wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 09:20 am GMT

PDB ID	:	4V5R
Title	:	The crystal structure of EF-Tu and Trp-tRNA-Trp bound to a 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:

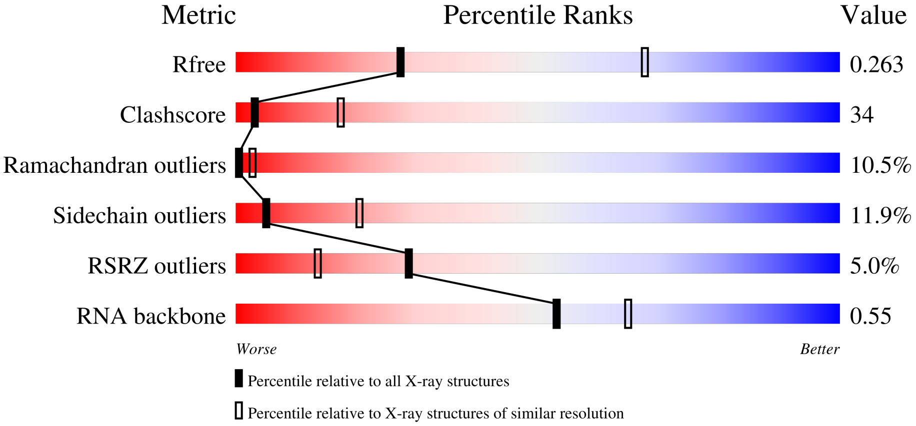
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance ⓘ

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

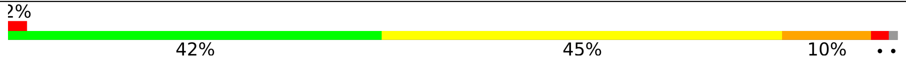
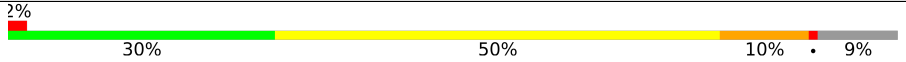
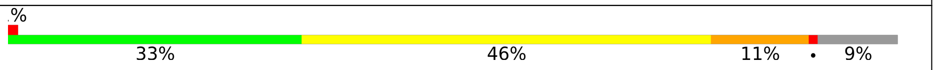
The reported resolution of this entry is 3.10 Å.

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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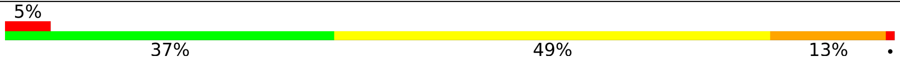
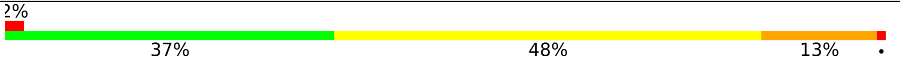
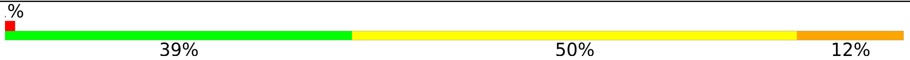
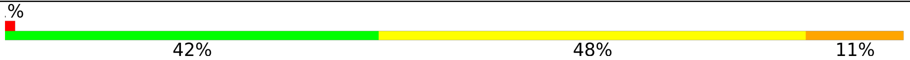
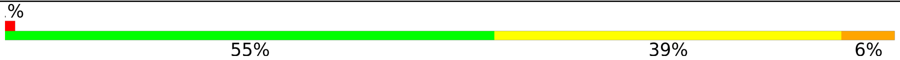
Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
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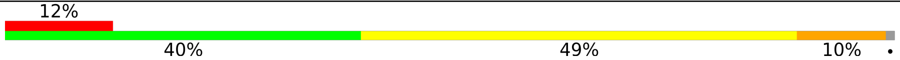
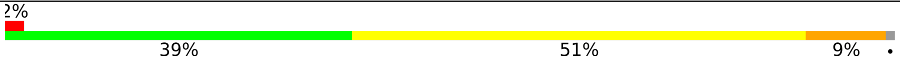
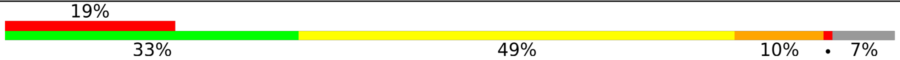
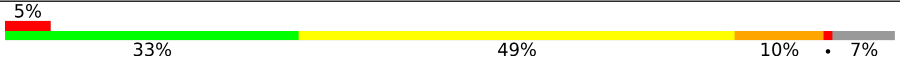
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
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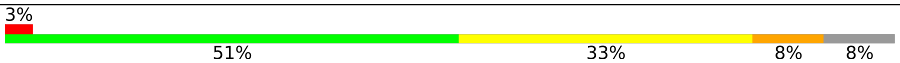
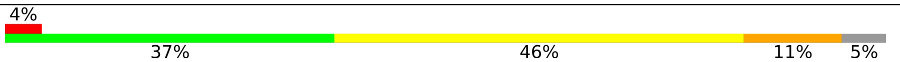
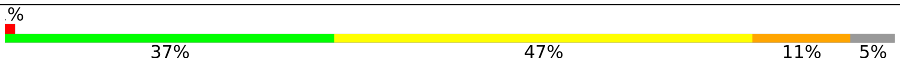
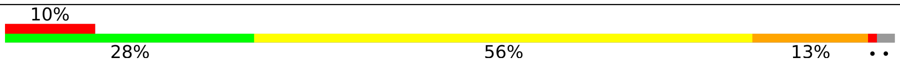
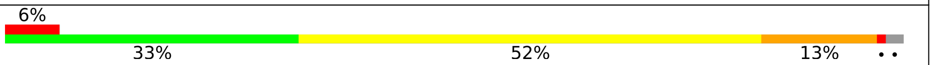
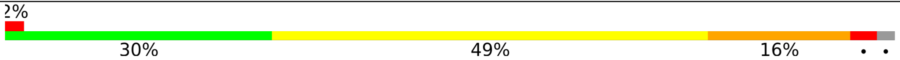
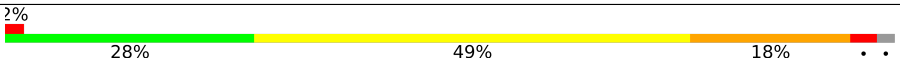
11	CK	129	
12	AL	131	
12	CL	131	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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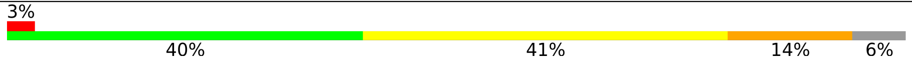
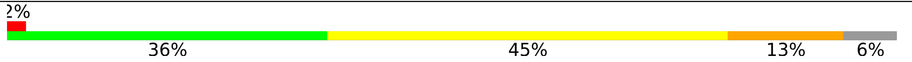
Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
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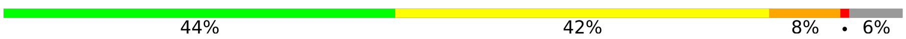
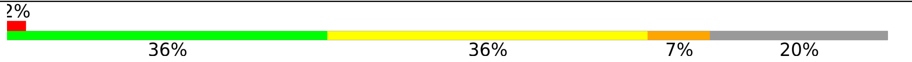
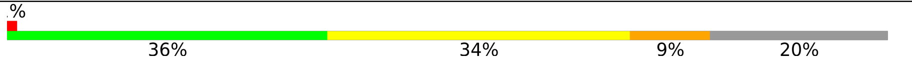
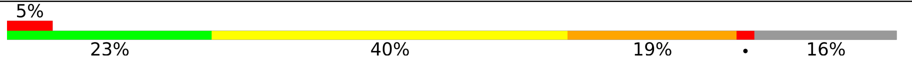
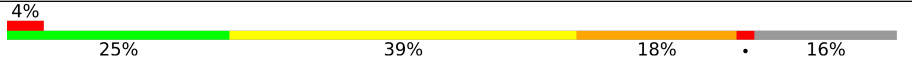
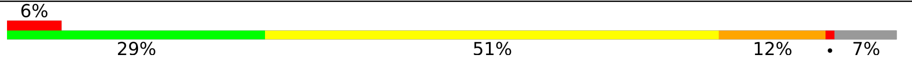
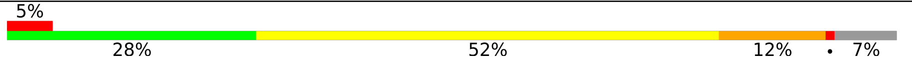
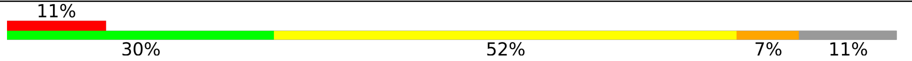
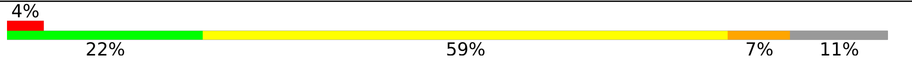
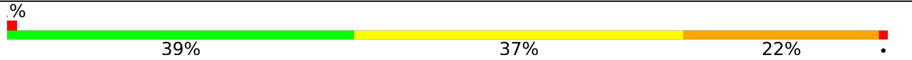
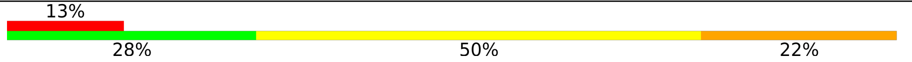
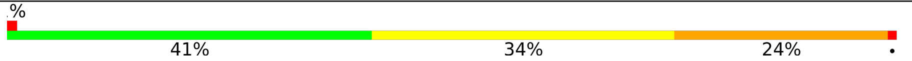
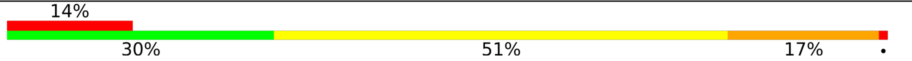
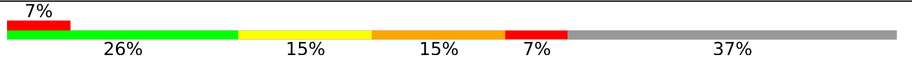
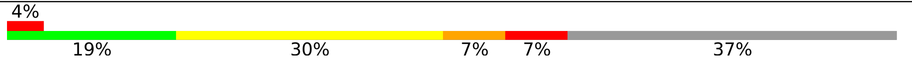
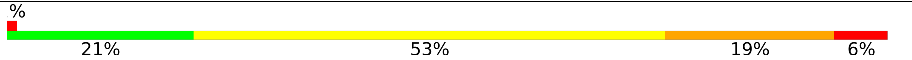
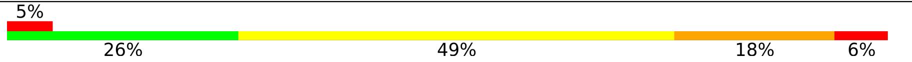
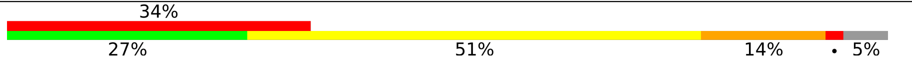
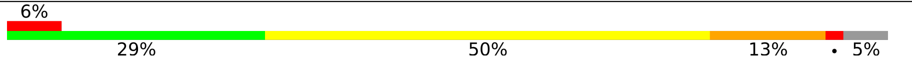
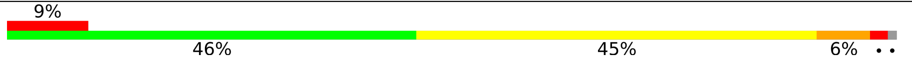
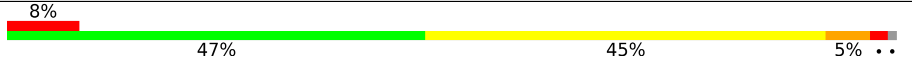
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	AW	76	
22	CV	76	
22	CW	76	
23	AX	27	
23	CX	27	
24	AY	77	
24	CY	77	
25	AZ	405	
25	CZ	405	
26	B0	85	
26	D0	85	

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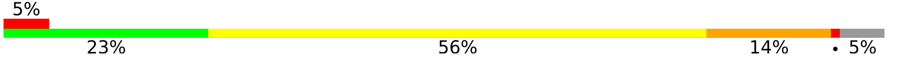
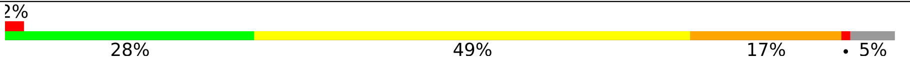
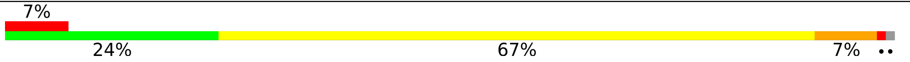
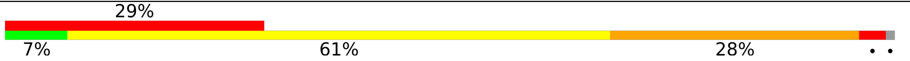
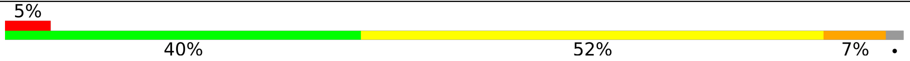
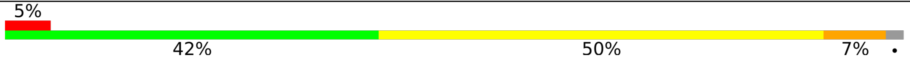
Mol	Chain	Length	Quality of chain
27	B1	98	
27	D1	98	
28	B2	72	
28	D2	72	
29	B3	60	
29	D3	60	
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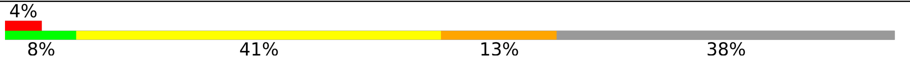
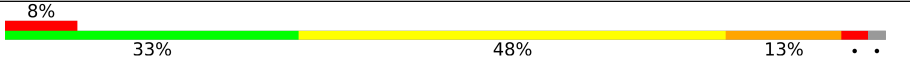
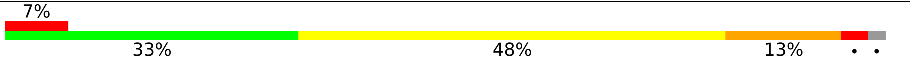
30	D4	71	
31	B5	60	
31	D5	60	
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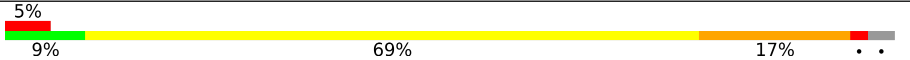
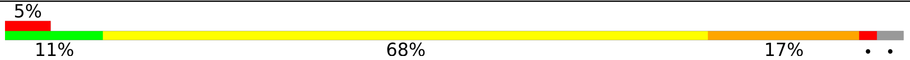
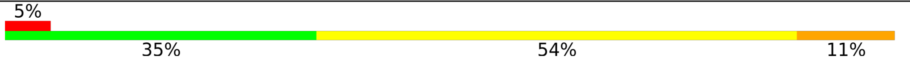
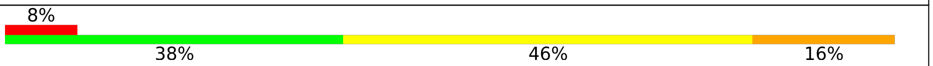
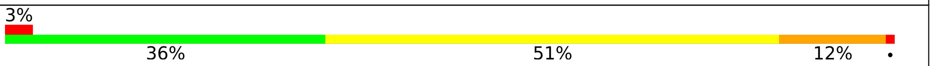
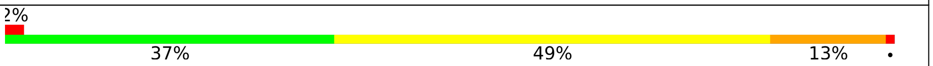
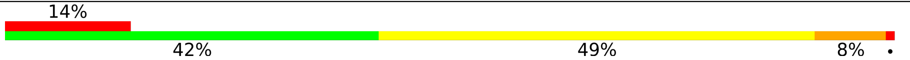
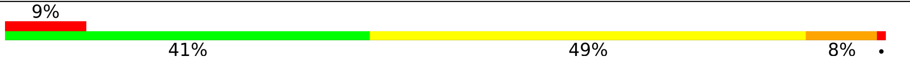
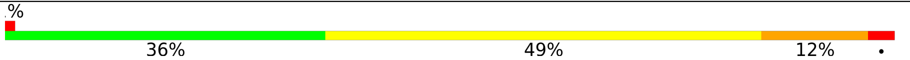
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229	
39	BD	276	

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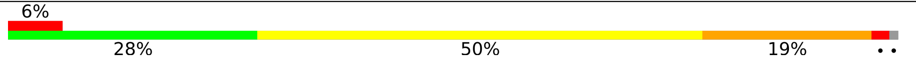
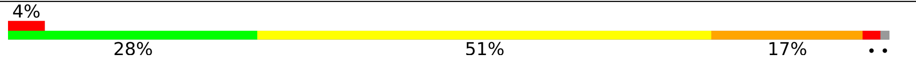
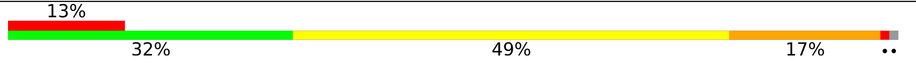
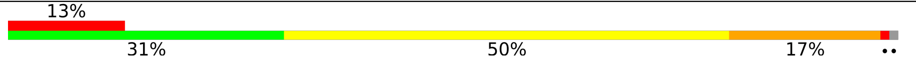
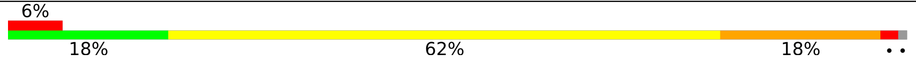
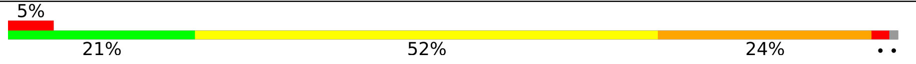
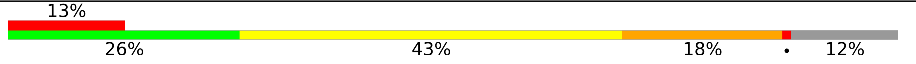
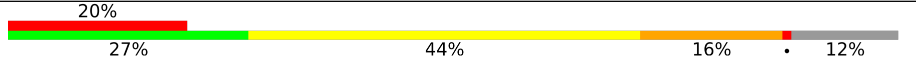
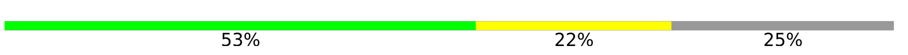
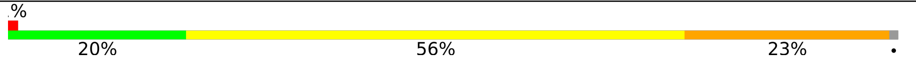
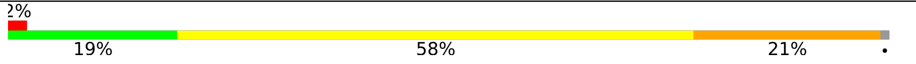
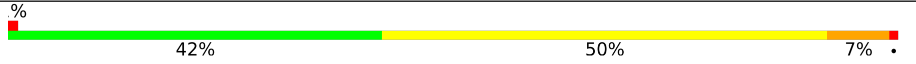
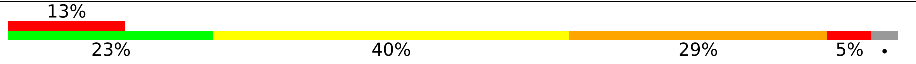
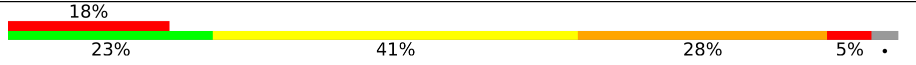
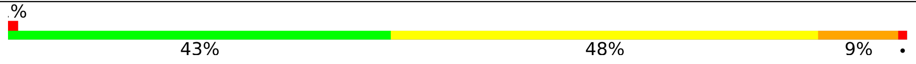
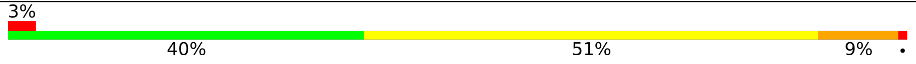
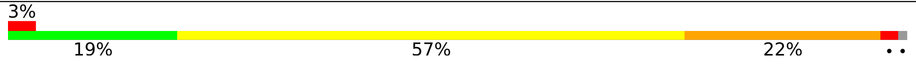
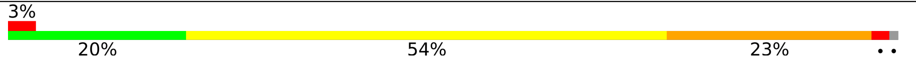
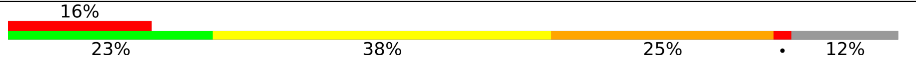
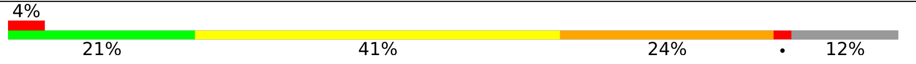
Mol	Chain	Length	Quality of chain
39	DD	276	
40	BE	206	
40	DE	206	
41	BF	210	
41	DF	210	
42	BG	182	
42	DG	182	
43	BH	180	
43	DH	180	
44	BJ	173	
44	DJ	173	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	

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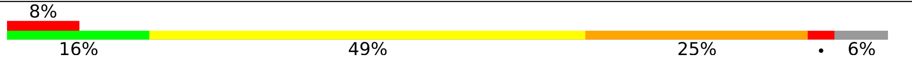
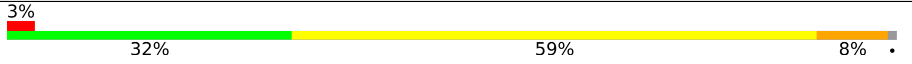
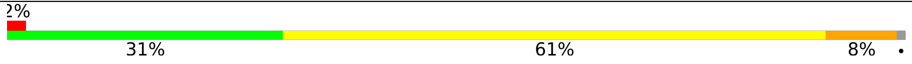
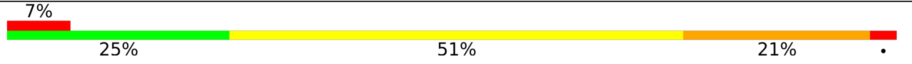
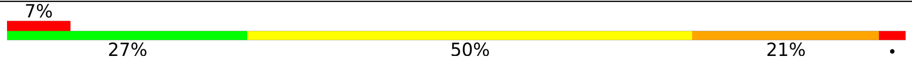
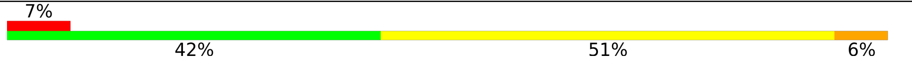
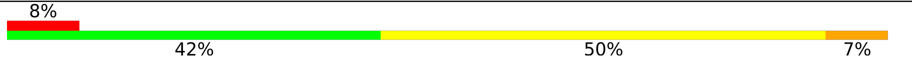
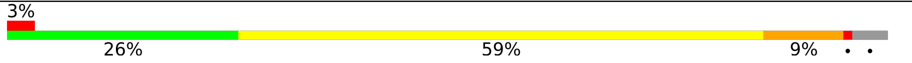
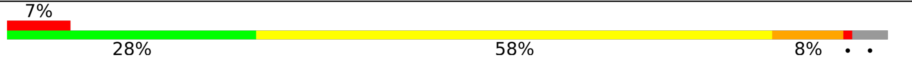
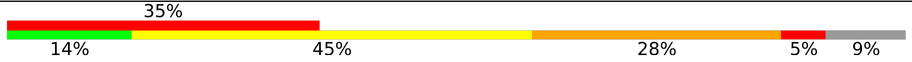
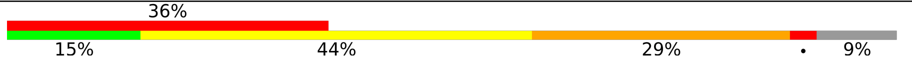
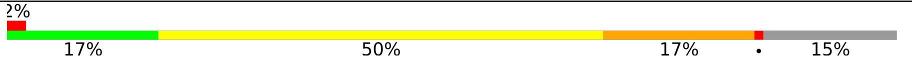
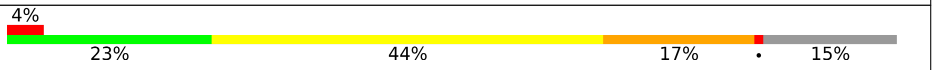
Mol	Chain	Length	Quality of chain
52	BT	146	
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	

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	AD	301	-	-	X	-
59	ZN	AN	101	-	-	X	-
59	ZN	CD	301	-	-	X	-
59	ZN	CN	101	-	-	X	-
60	GDP	AZ	501	-	-	X	-
61	KIR	AZ	502	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 307330 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	1510	Total 32451	C 14445	N 6010	O 10487	P 1509	0	0	0
1	CA	1510	Total 32451	C 14445	N 6010	O 10487	P 1509	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
5	AE	150	Total 1146	C 724	N 217	O 201	S 4	0	0	0
5	CE	150	Total 1146	C 724	N 217	O 201	S 4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	AP	83	700	443	139	117	1	0	0	0
16	CP	83	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
			Total	C	N	O	S			
17	AQ	99	823	528	151	142	2	0	0	0
17	CQ	99	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
			Total	C	N	O			
18	AR	70	574	367	112	95	0	0	0
18	CR	70	574	367	112	95	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AS	78	629	403	114	110	2	0	0	0
19	CS	78	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
			Total	C	N	O	S			
20	AT	99	763	470	162	129	2	0	0	0
20	CT	99	763	470	162	129	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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
			362	164	68	114	16			
23	CX	17	Total	C	N	O	P	0	0	0
			362	164	68	114	16			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AY	77	Total	C	N	O	P	S	0	0	0
			1645	742	289	536	76	2			
24	CY	77	Total	C	N	O	P	S	0	0	0
			1645	742	289	536	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	C	N	O	S	0	0	0
			662	410	140	111	1			
26	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

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

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

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

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

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

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

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

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

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

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

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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
			Total	C	N	O	S			
42	BG	181	1474	942	268	260	4	0	0	0
42	DG	181	1474	942	268	260	4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	BU	117	958	604	202	151	1	0	0	0
53	DU	117	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
			Total	C	N	O	S			
54	BV	101	779	501	142	135	1	0	0	0
54	DV	101	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
			Total	C	N	O	S			
55	BW	113	896	563	176	155	2	0	0	0
55	DW	113	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
			Total	C	N	O			
56	BX	92	725	471	131	123	0	0	0
56	DX	92	725	471	131	123	0	0	0

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

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

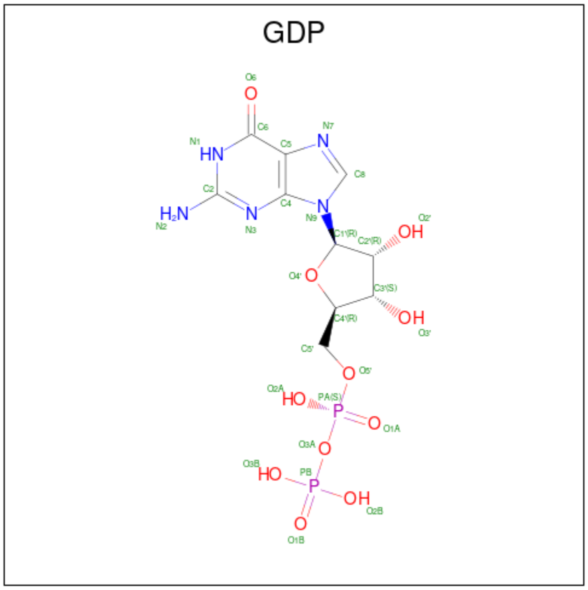
- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

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

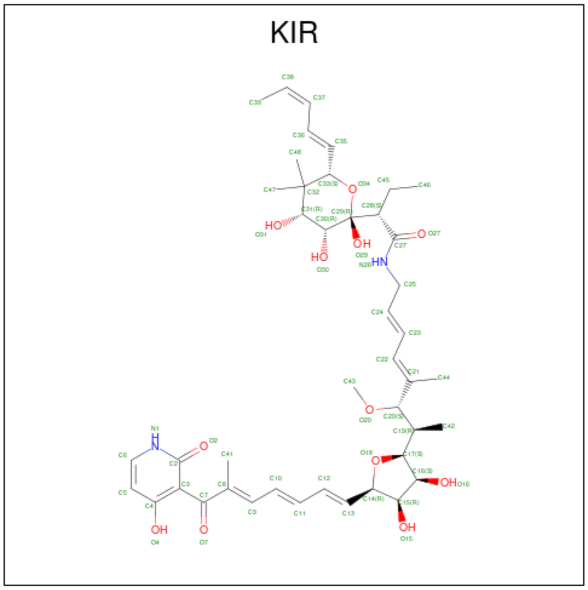
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	1	Total 1	Zn 1	0	0
59	AN	1	Total 1	Zn 1	0	0
59	B4	1	Total 1	Zn 1	0	0
59	B9	1	Total 1	Zn 1	0	0
59	CD	1	Total 1	Zn 1	0	0
59	CN	1	Total 1	Zn 1	0	0
59	D4	1	Total 1	Zn 1	0	0
59	D9	1	Total 1	Zn 1	0	0

- 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 28	C 10	N 5	O 11	P 2	0	0
60	CZ	1	Total 28	C 10	N 5	O 11	P 2	0	0

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



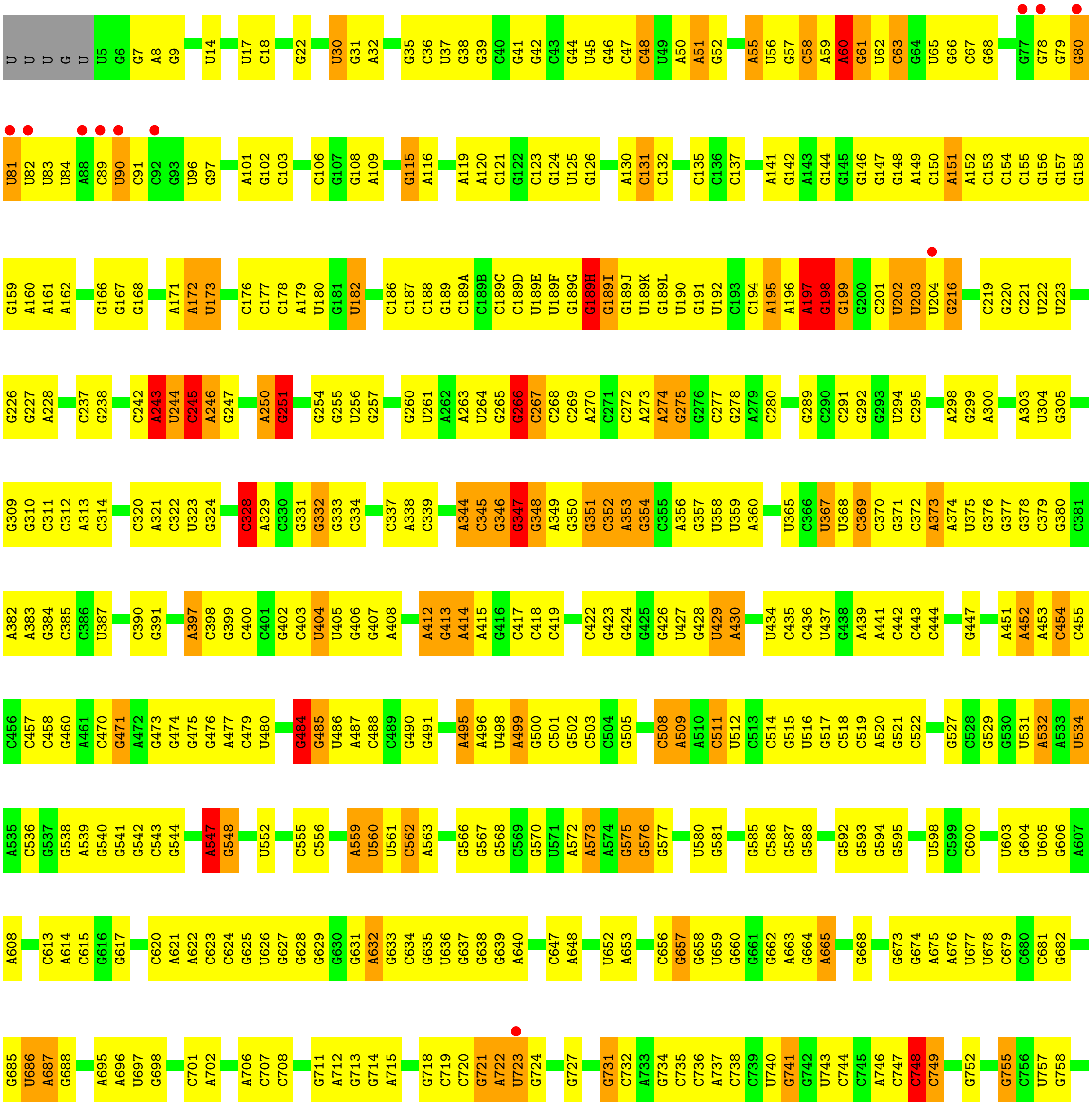
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
61	AZ	1	Total 57	C 43	N 2	O 12	0	0
61	CZ	1	Total 57	C 43	N 2	O 12	0	0

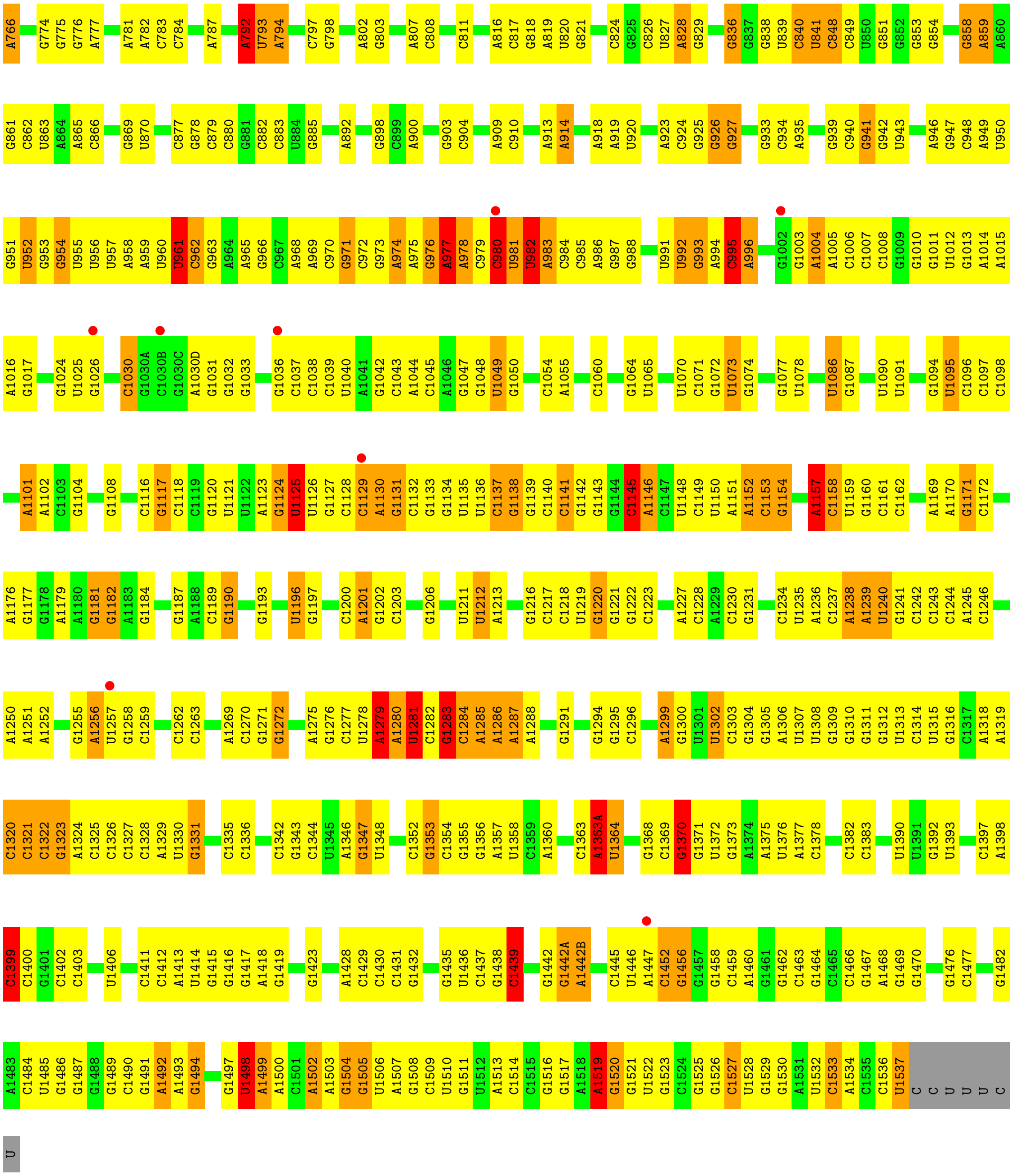
3 Residue-property plots

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

- Molecule 1: 16S RRNA

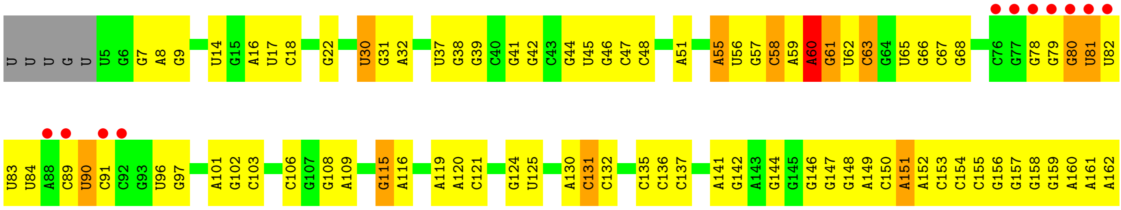
Chain AA:

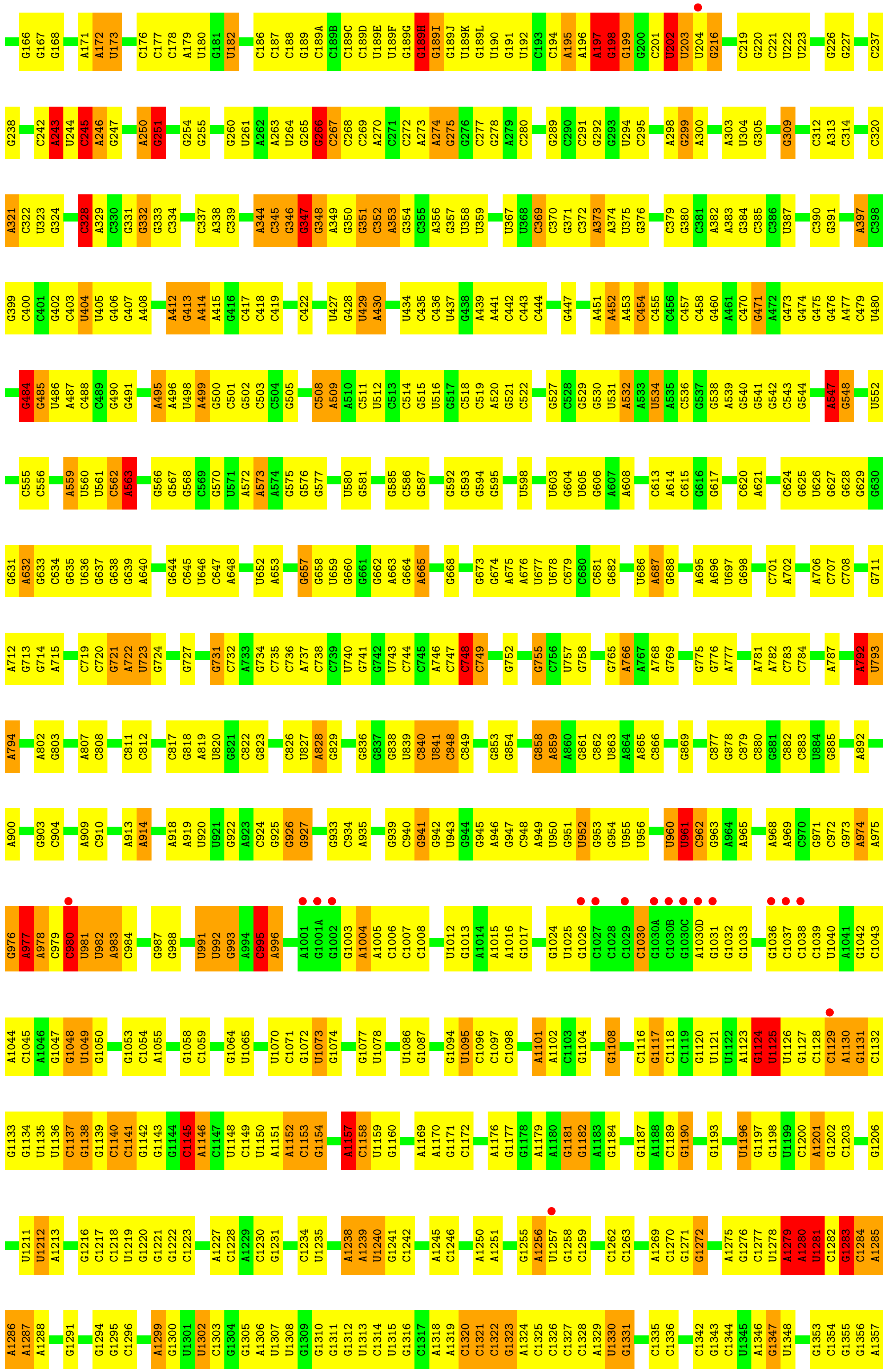




- Molecule 1: 16S RRNA

Chain CA:

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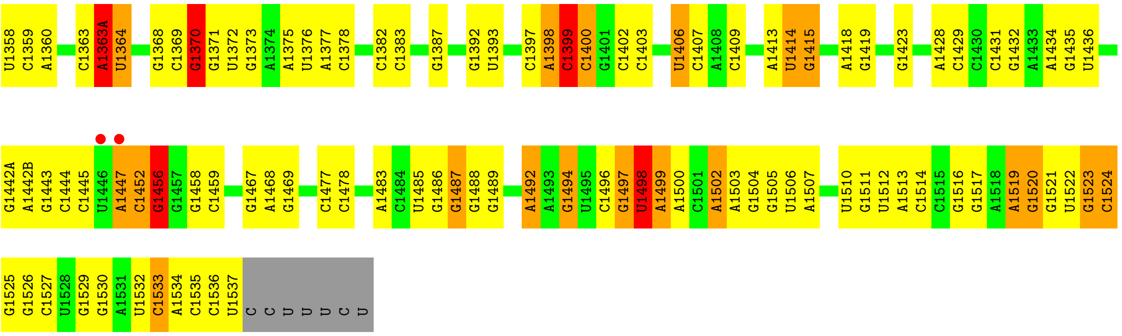
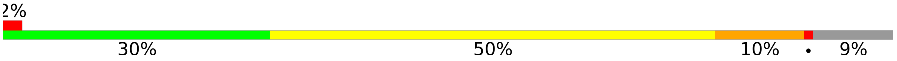
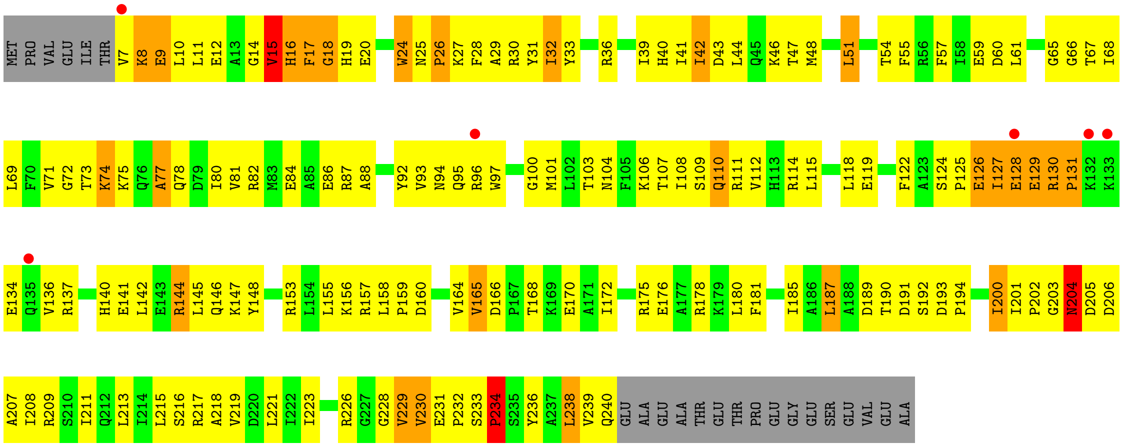


- Molecule 2: 30S RIBOSOMAL PROTEIN S2

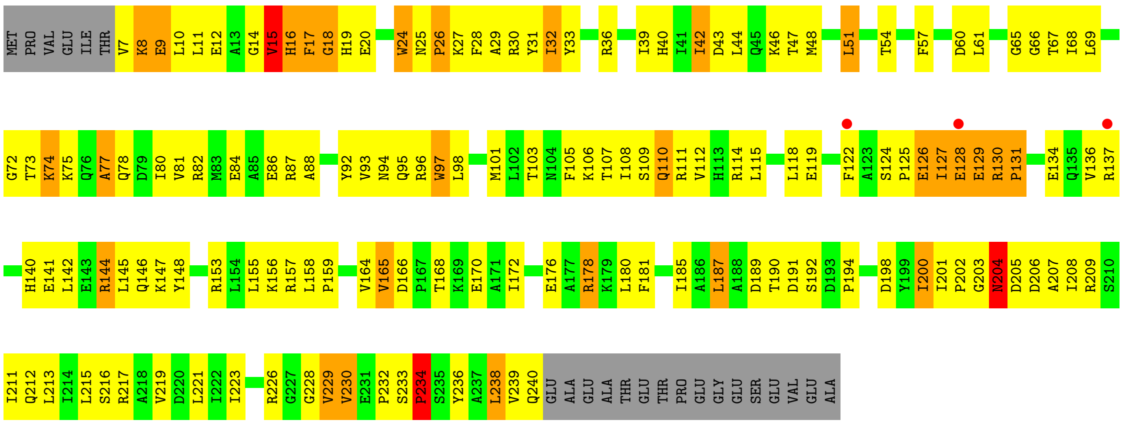
Chain AB:





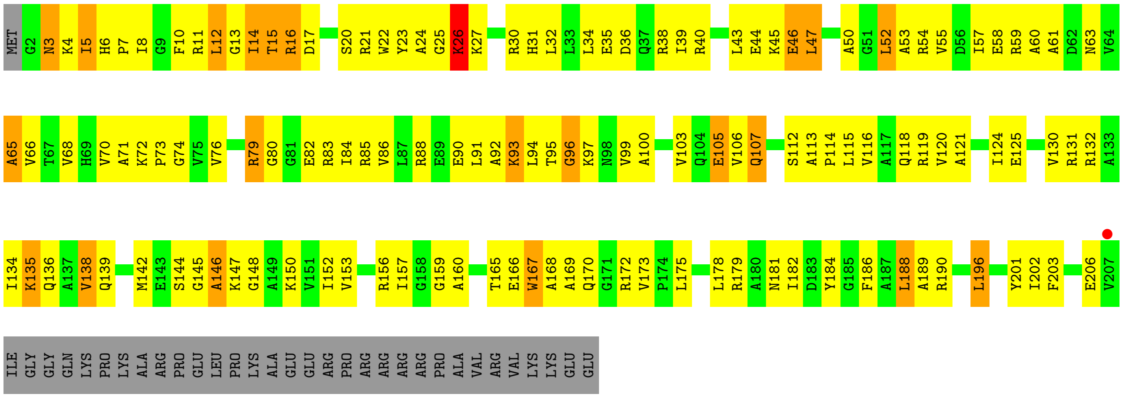
- Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain CB:



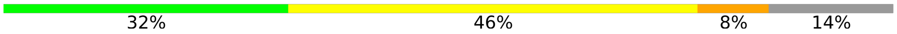
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

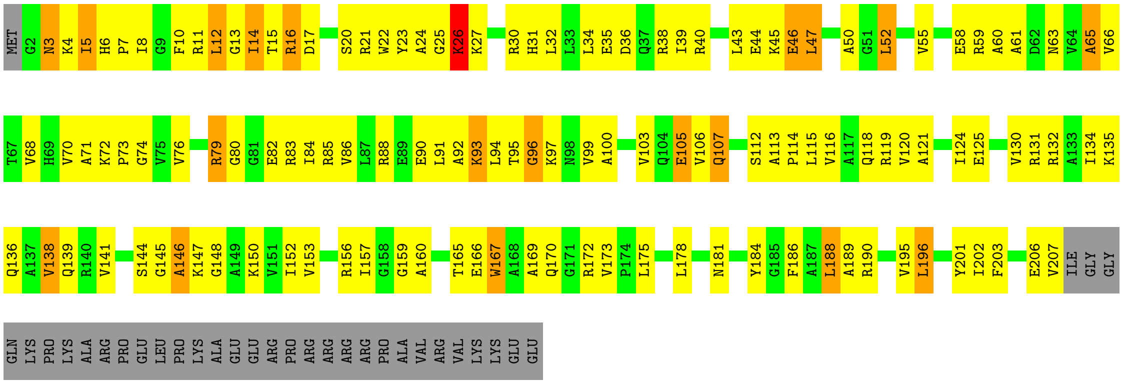
Chain AC:



- Molecule 3: 30S RIBOSOMAL PROTEIN S3

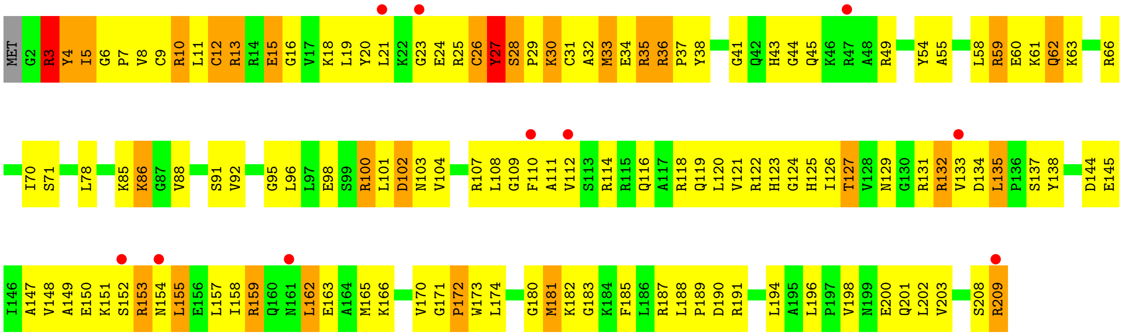
Chain CC:





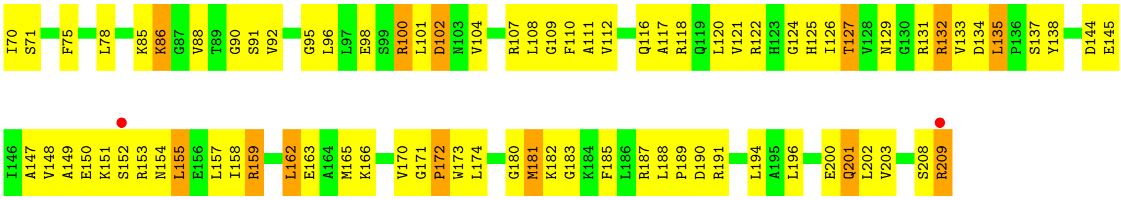
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



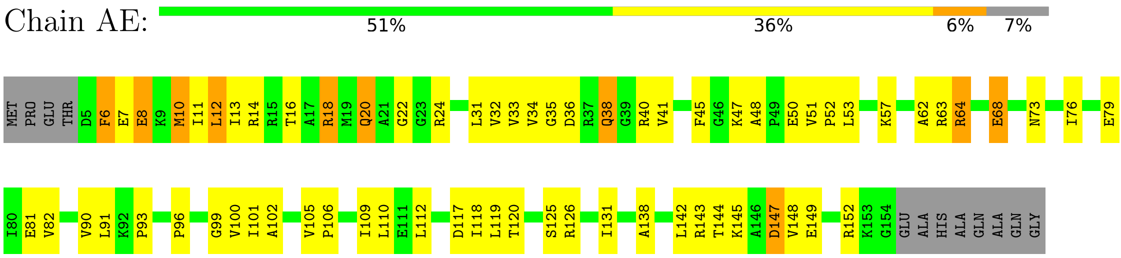
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD:



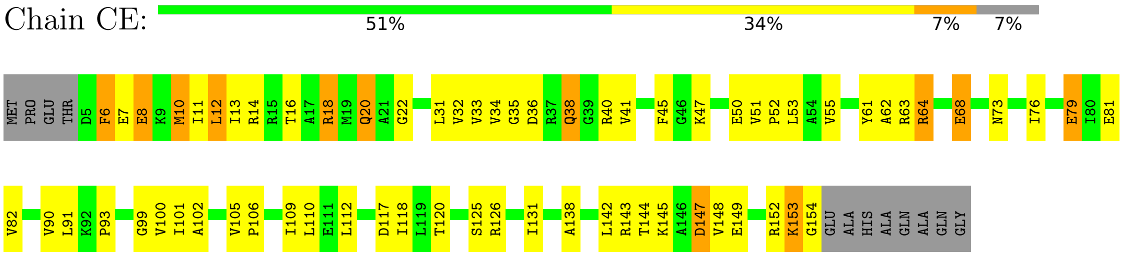
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:



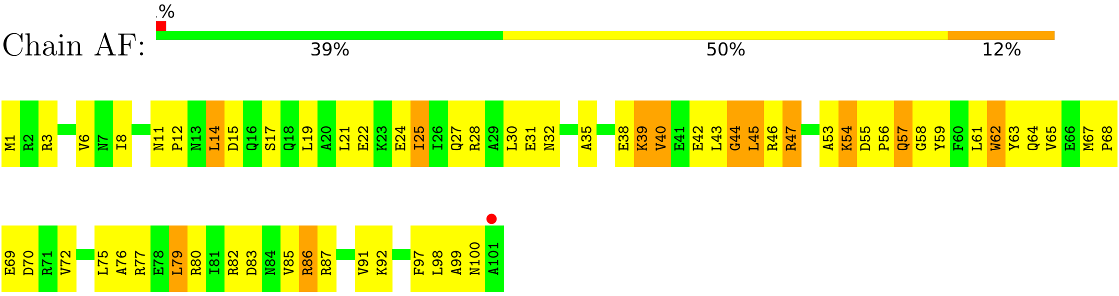
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:



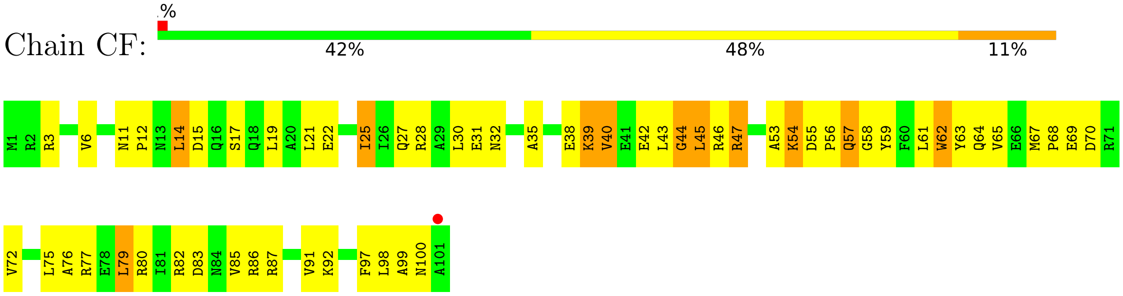
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



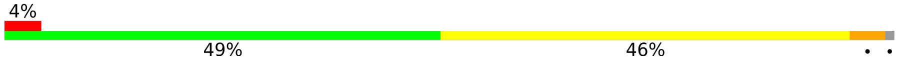
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

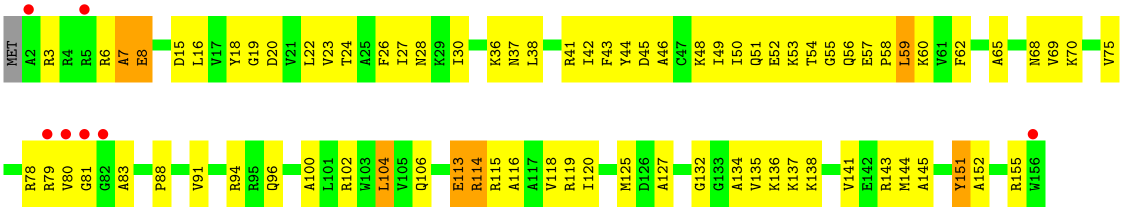
Chain CF:



- Molecule 7: 30S RIBOSOMAL PROTEIN S7

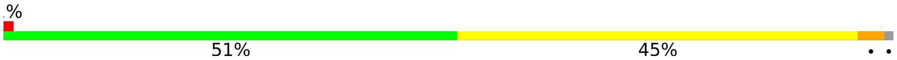
Chain AG:

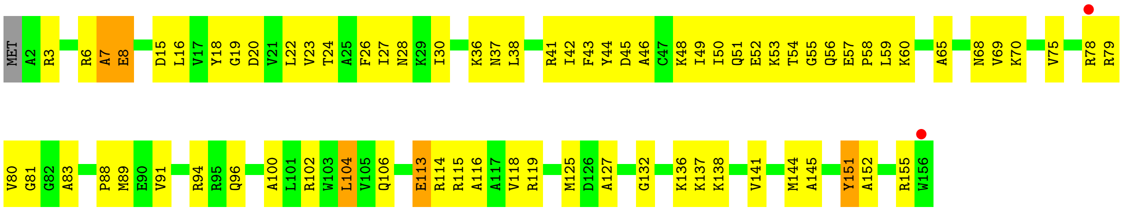




- Molecule 7: 30S RIBOSOMAL PROTEIN S7

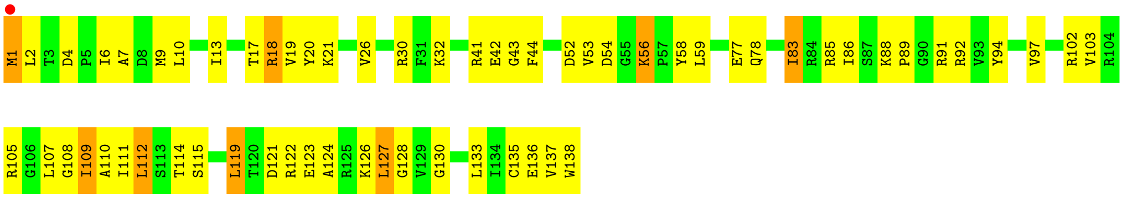
Chain CG:





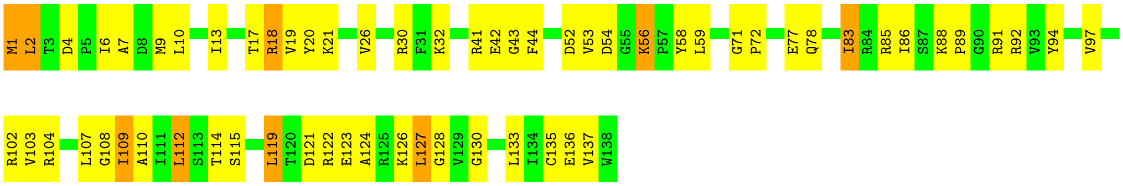
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



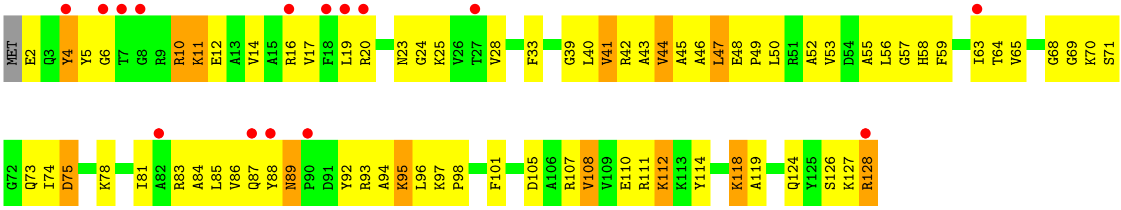
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:

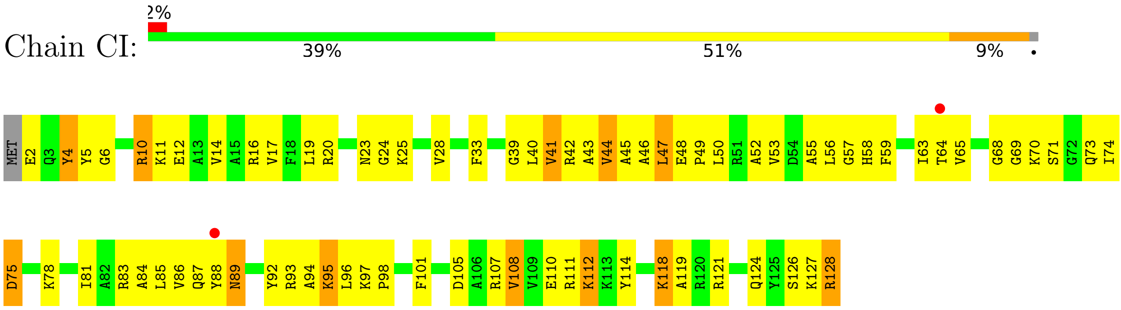


- Molecule 9: 30S RIBOSOMAL PROTEIN S9

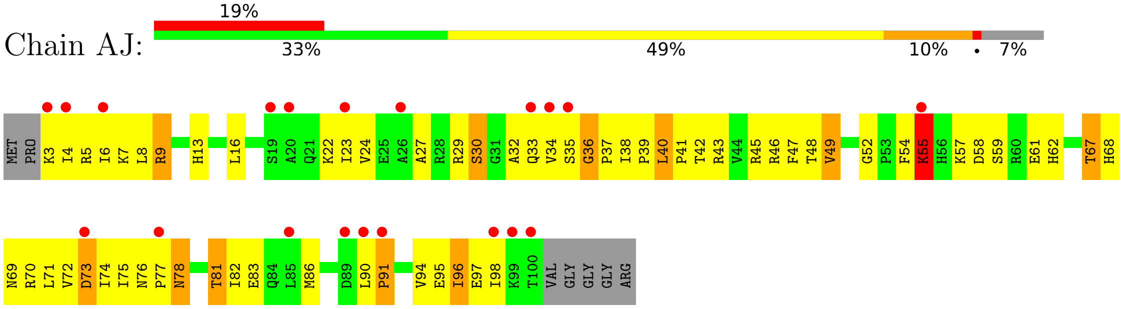
Chain AI:



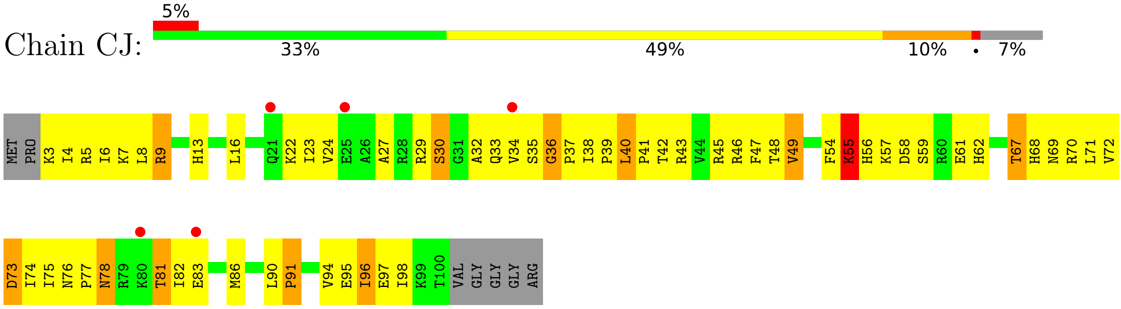
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



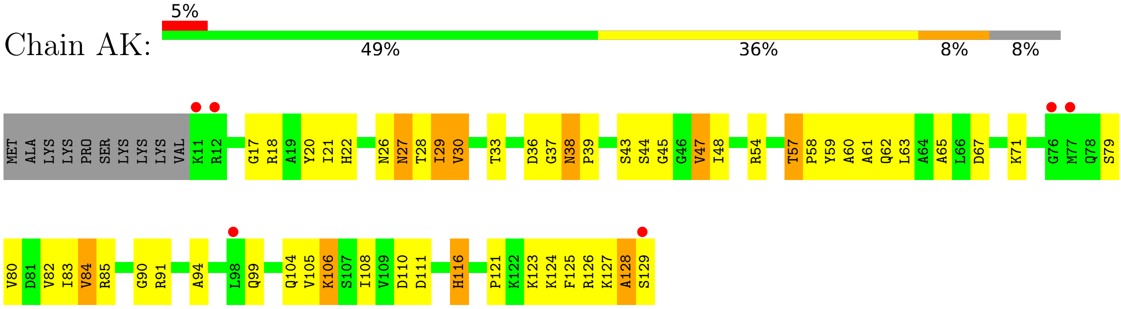
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



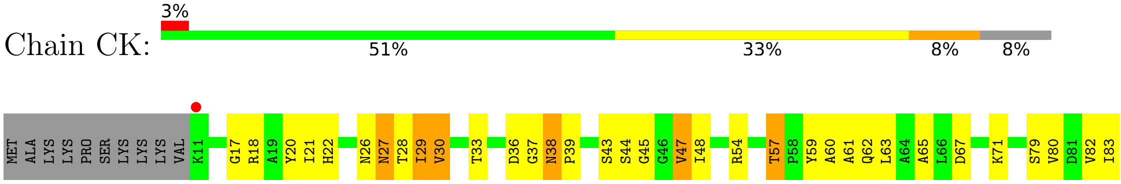
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



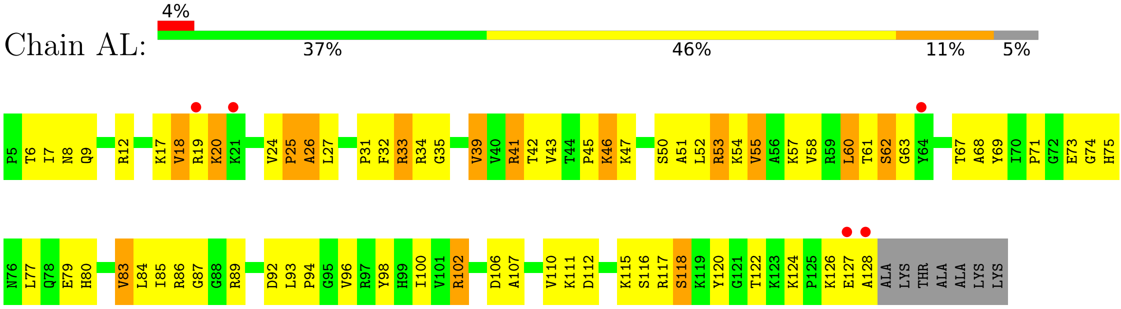
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



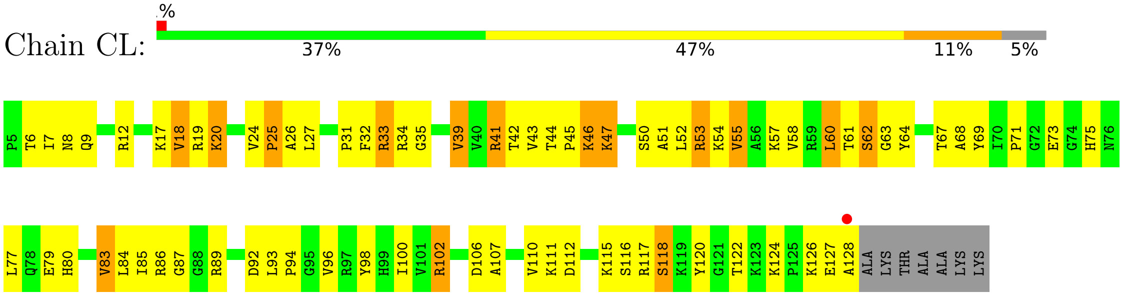
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



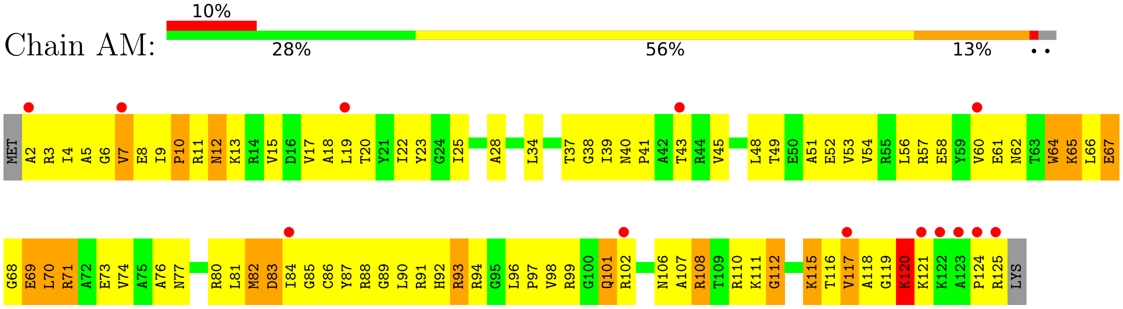
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



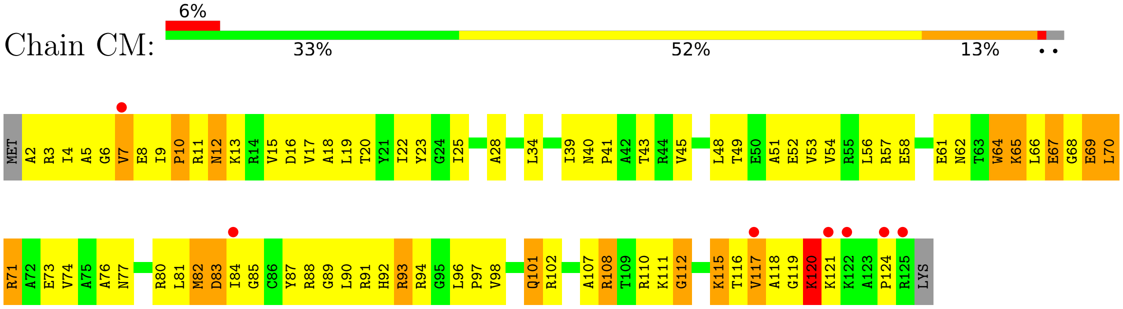
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



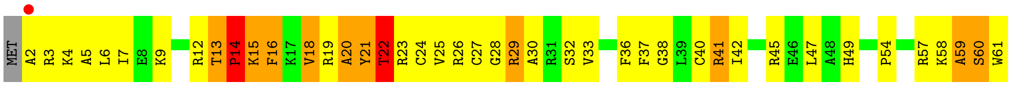
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

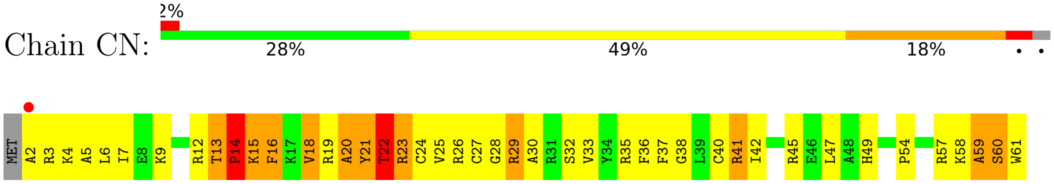


- Molecule 14: 30S RIBOSOMAL PROTEIN S14



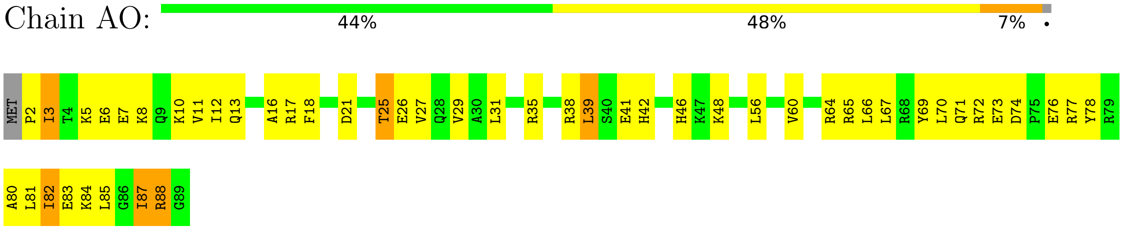
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CN:



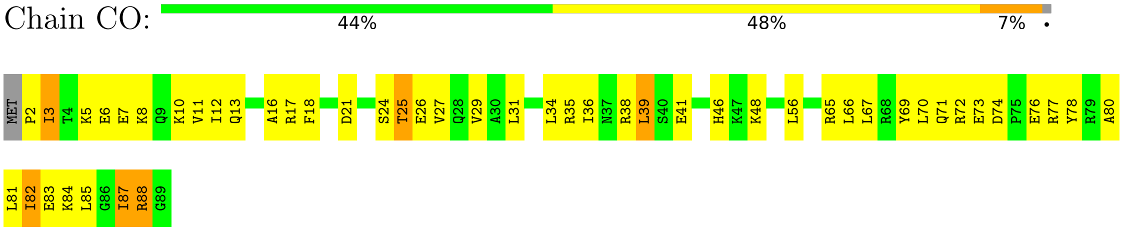
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



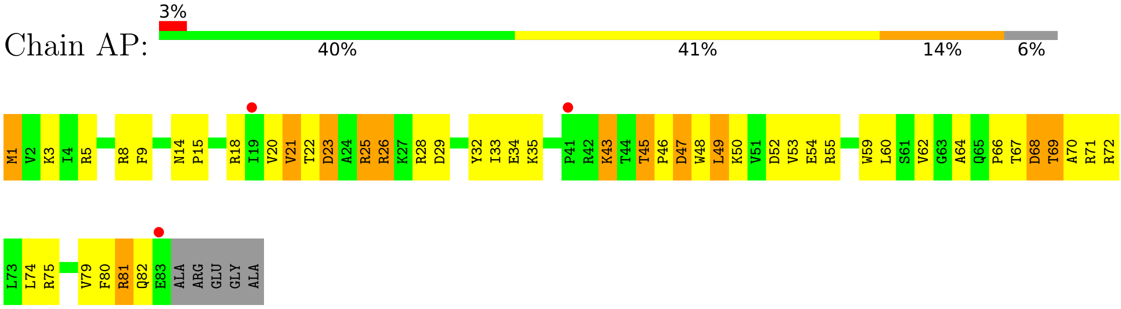
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



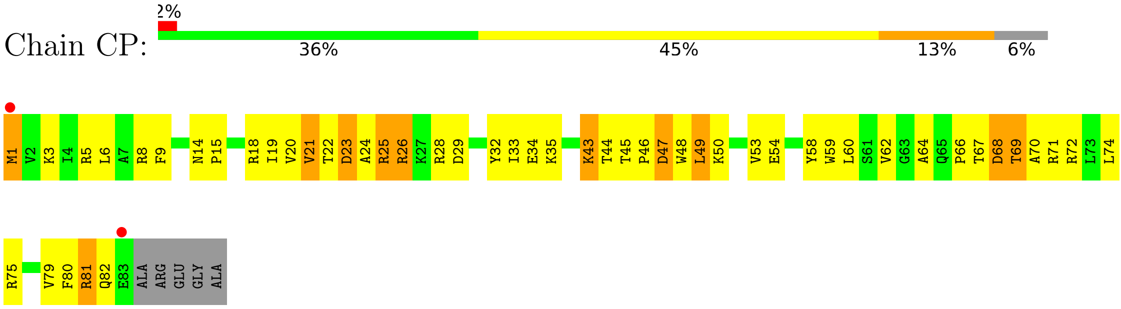
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:

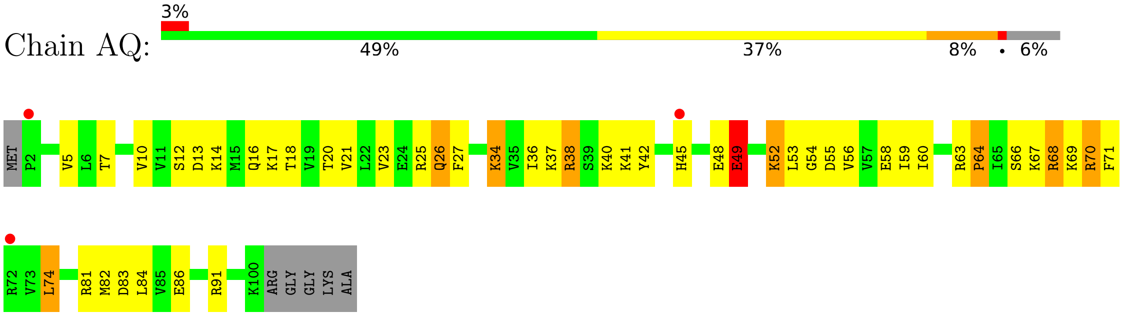


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

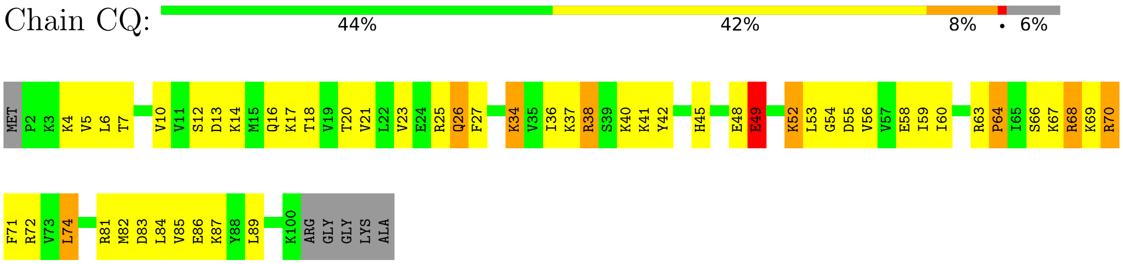
Chain CP:



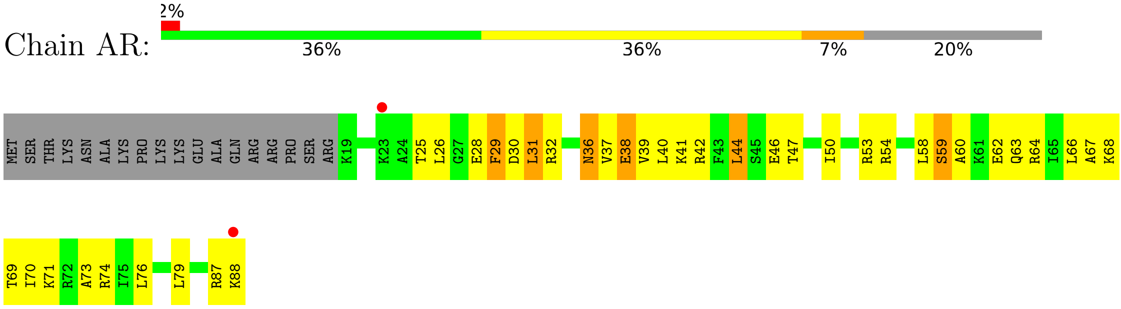
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



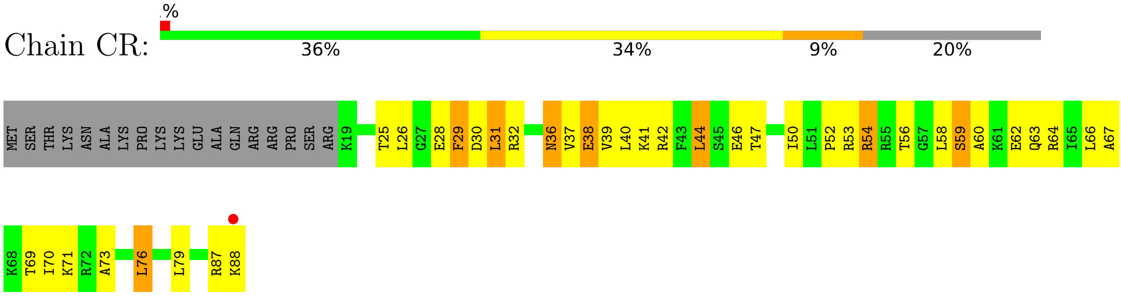
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



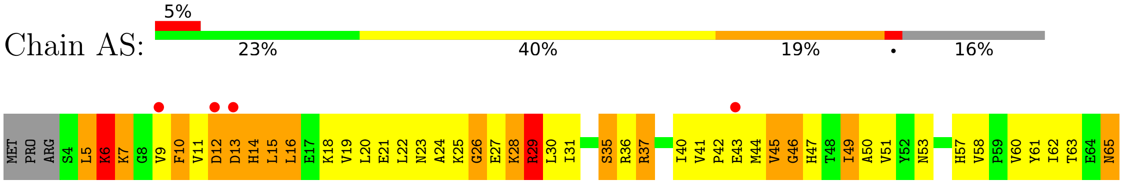
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

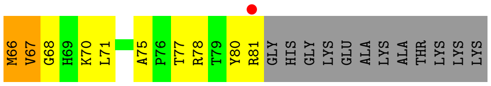


- Molecule 18: 30S RIBOSOMAL PROTEIN S18



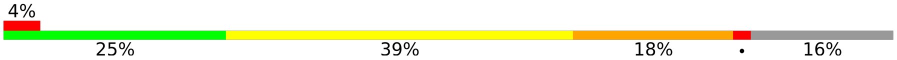
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

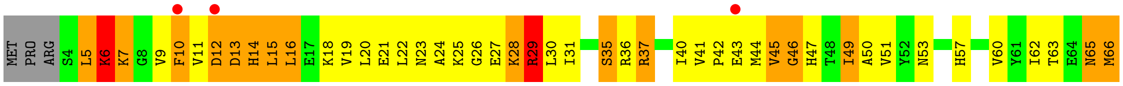


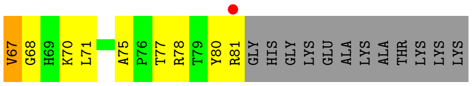


- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:

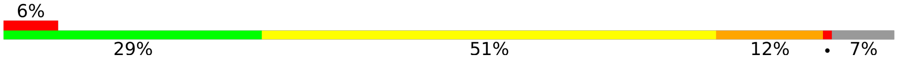


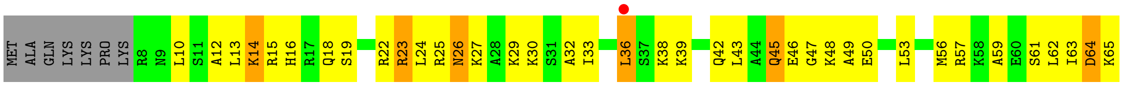


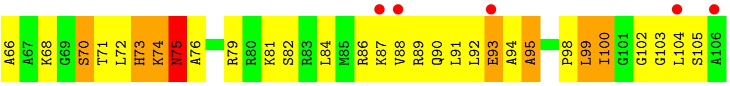


- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:

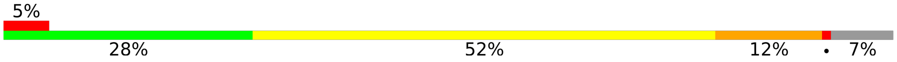


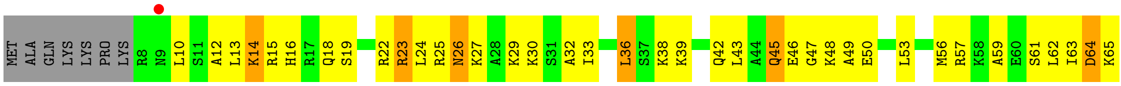


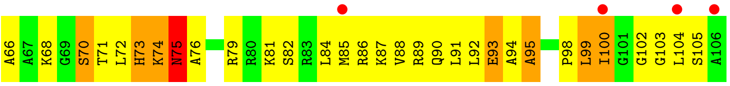


- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CT:

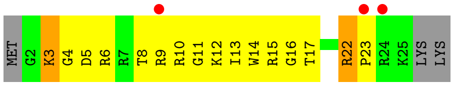






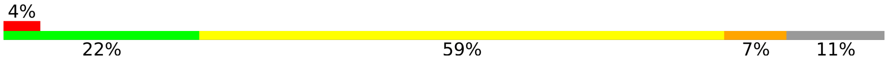
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

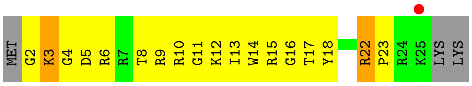
Chain AU:



- Molecule 21: 30S RIBOSOMAL PROTEIN THX

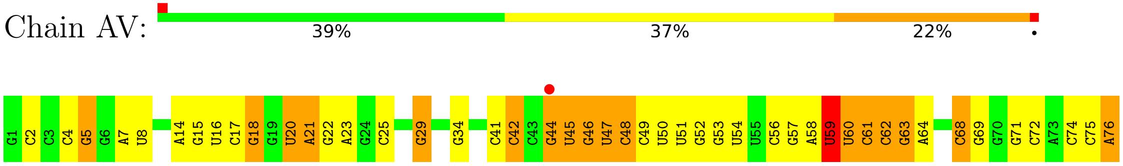
Chain CU:





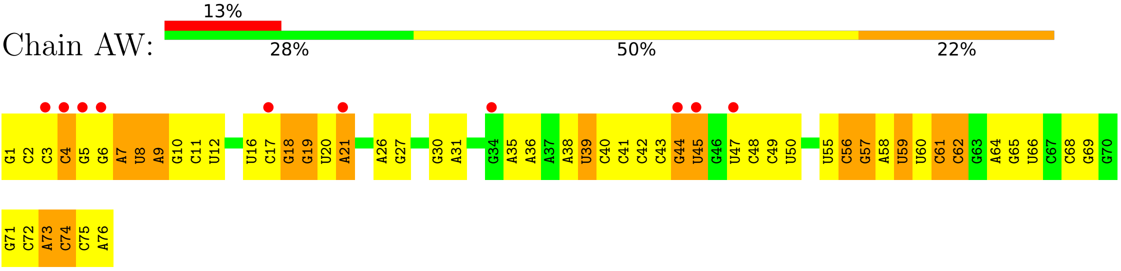
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AV:



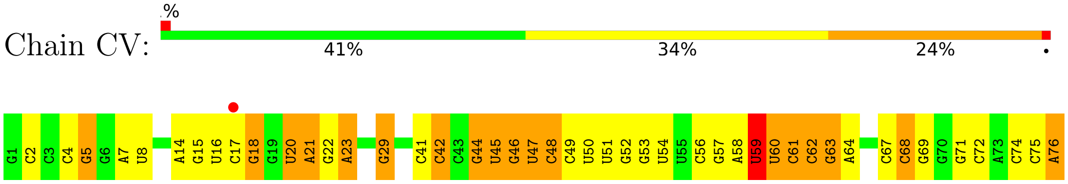
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AW:



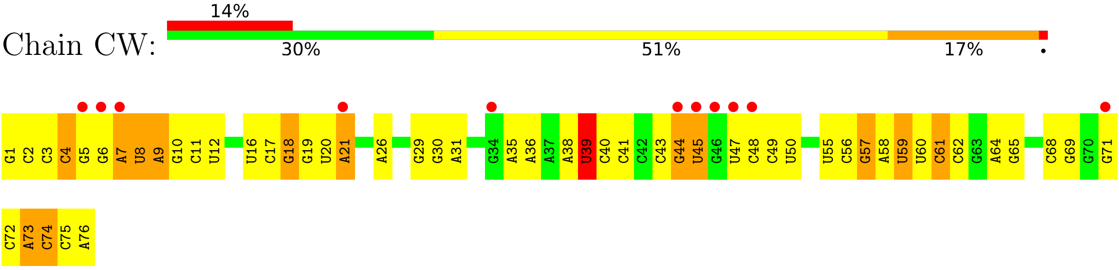
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain CV:



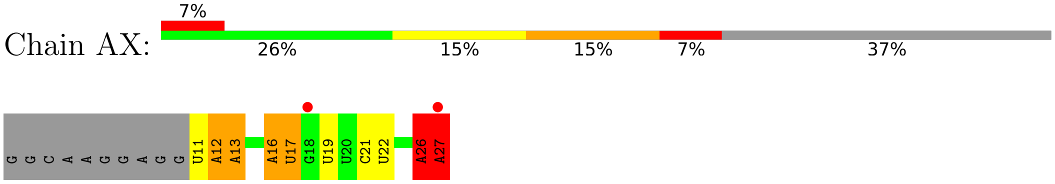
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain CW:



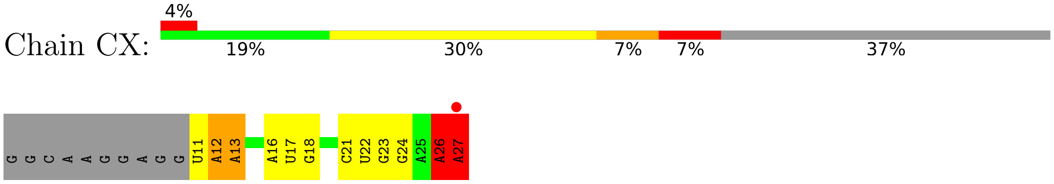
- Molecule 23: MRNA

Chain AX:

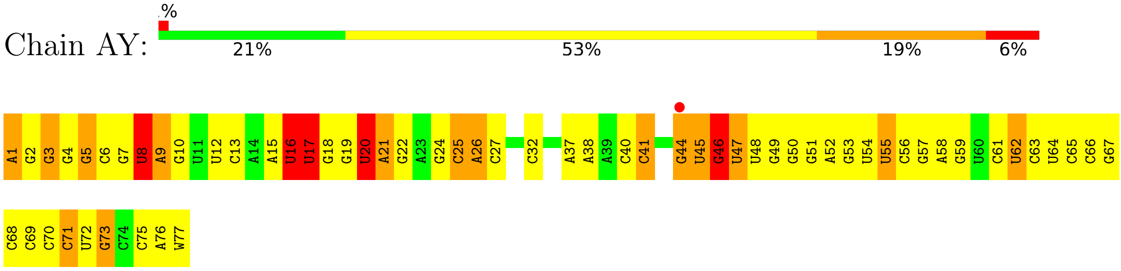


- Molecule 23: MRNA

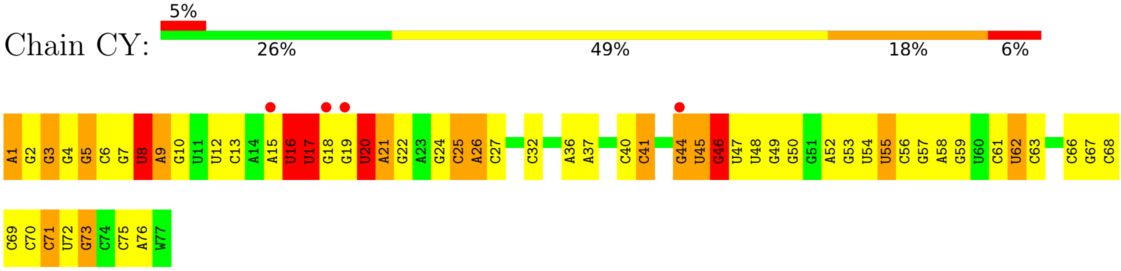
Chain CX:



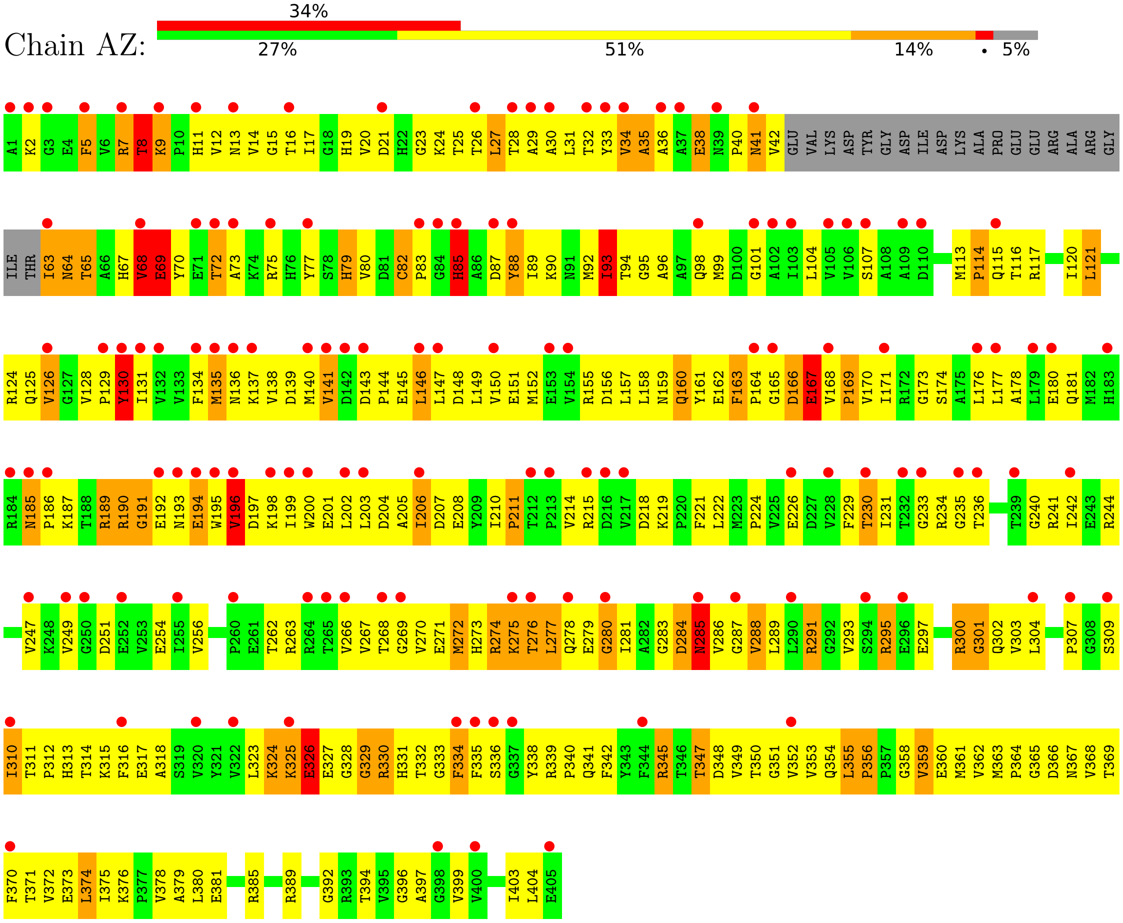
- Molecule 24: A-SITE TRNA TRP-TRNA TRP



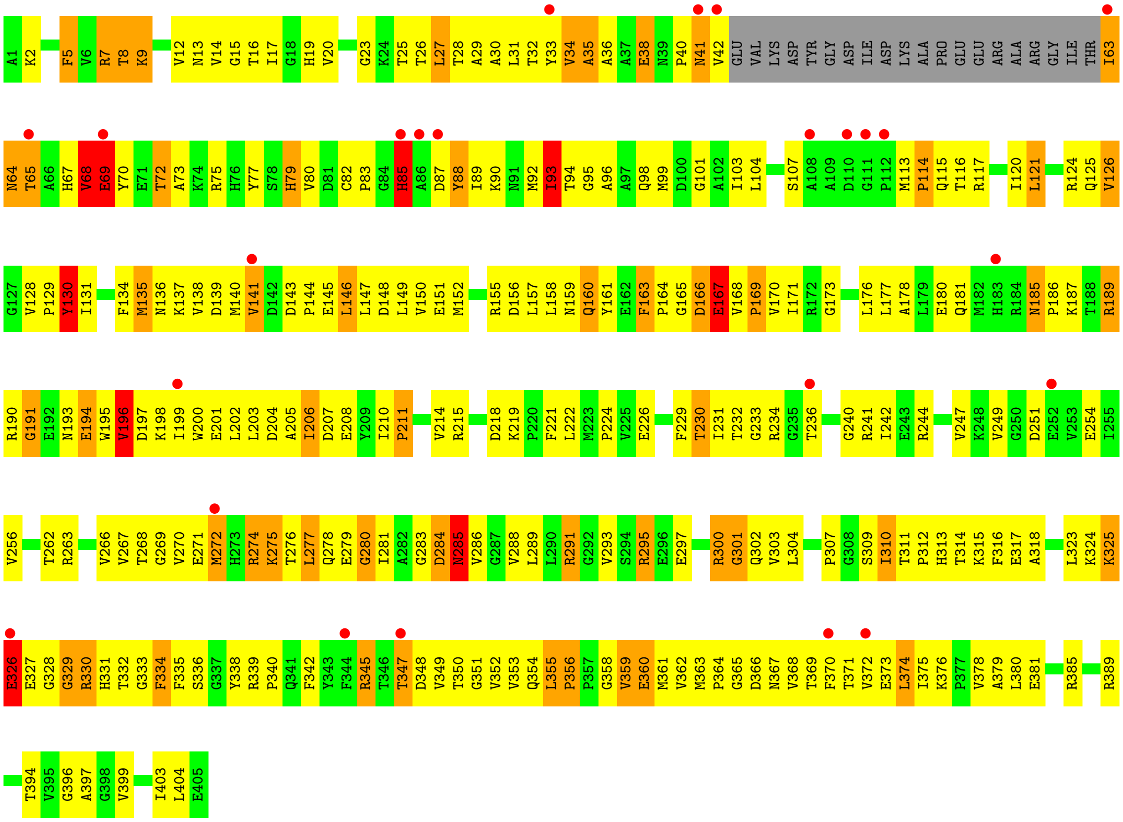
- Molecule 24: A-SITE TRNA TRP-TRNA TRP



- Molecule 25: ELONGATION FACTOR TU

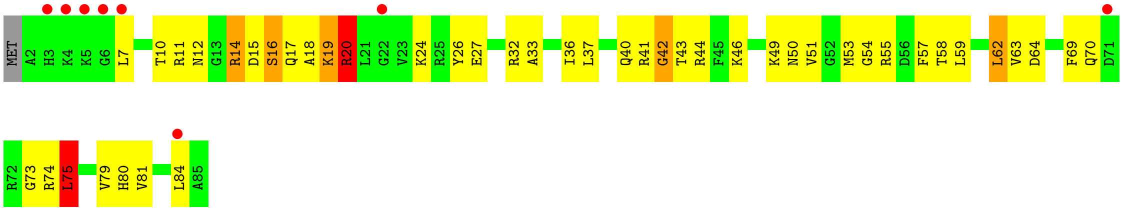


- Molecule 25: ELONGATION FACTOR TU



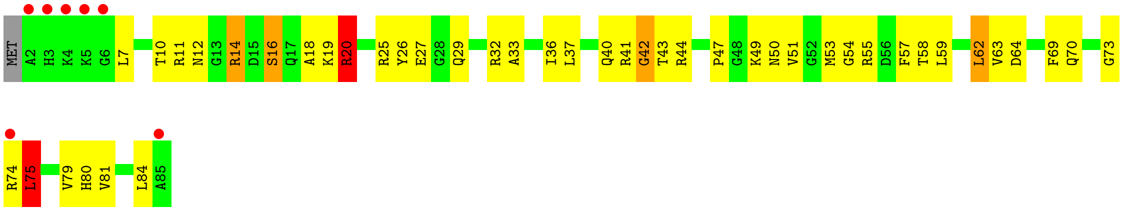
- Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain B0:



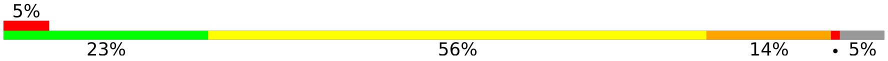
- Molecule 26: 50S RIBOSOMAL PROTEIN L27

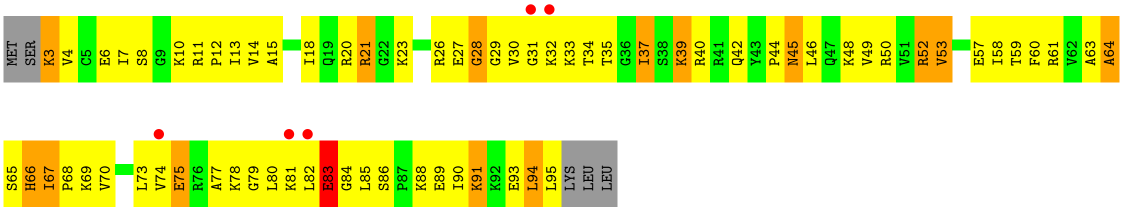
Chain D0:



- Molecule 27: 50S RIBOSOMAL PROTEIN L28

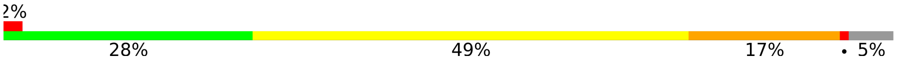
Chain B1:

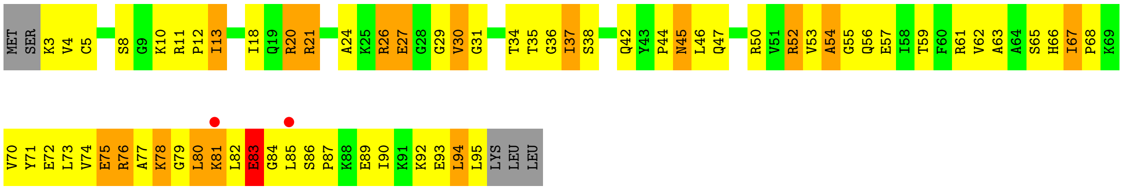




- Molecule 27: 50S RIBOSOMAL PROTEIN L28

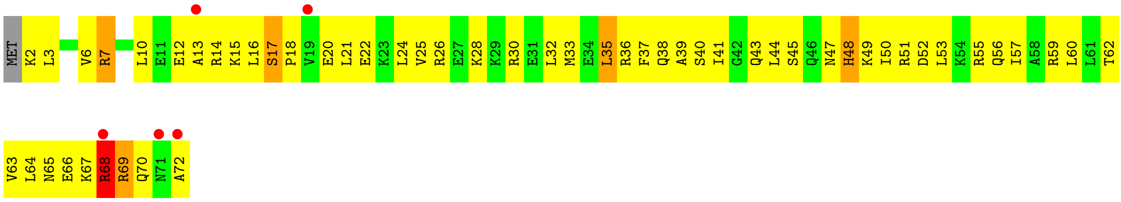
Chain D1:





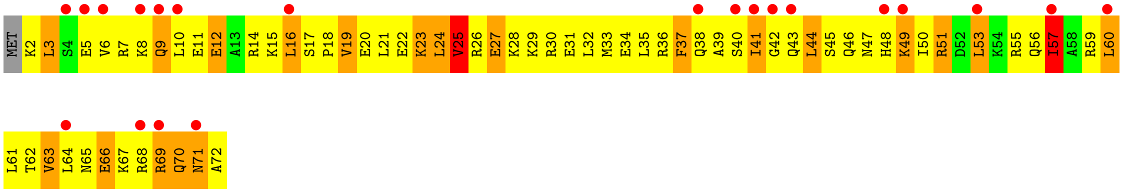
- Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain B2:



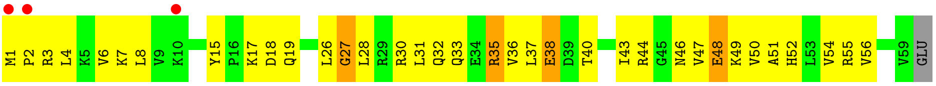
- Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain D2:



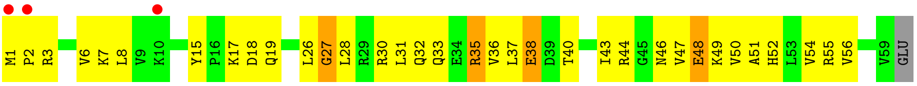
- Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain B3:

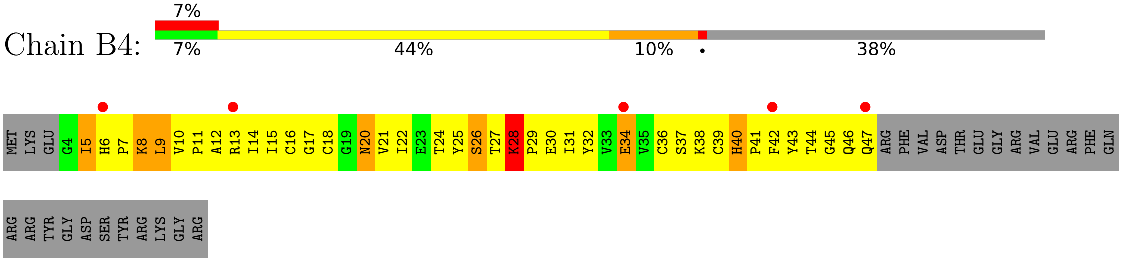


- Molecule 29: 50S RIBOSOMAL PROTEIN L30

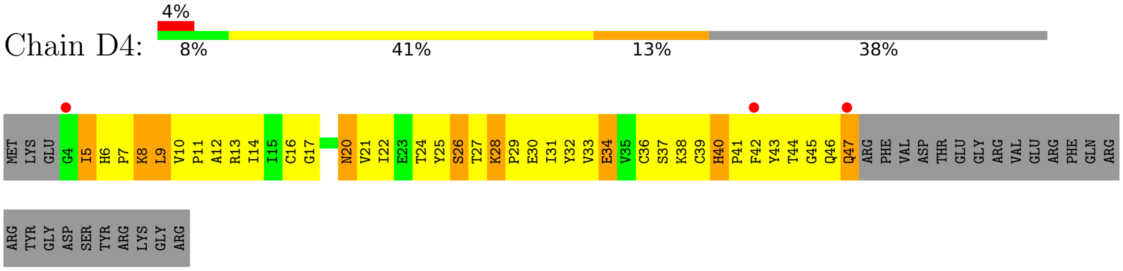
Chain D3:



- Molecule 30: 50S RIBOSOMAL PROTEIN L31



- Molecule 30: 50S RIBOSOMAL PROTEIN L31



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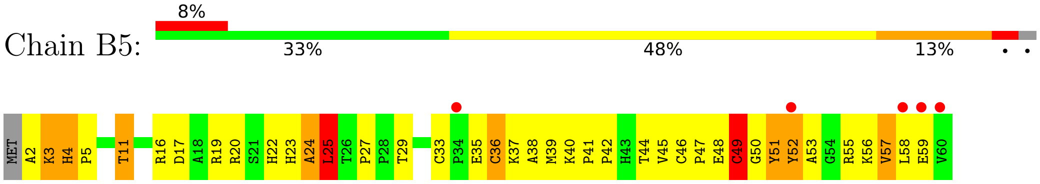

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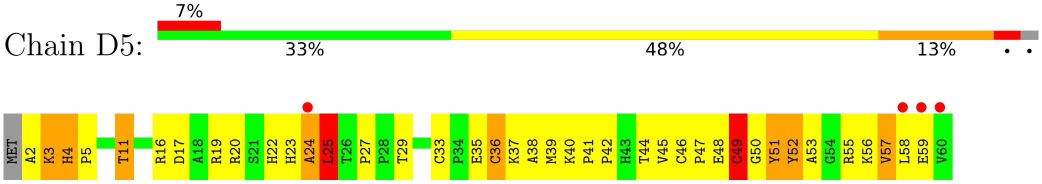

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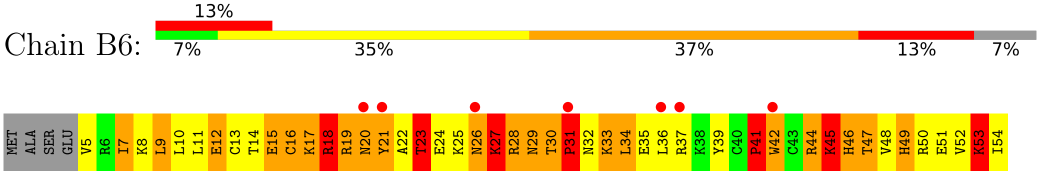

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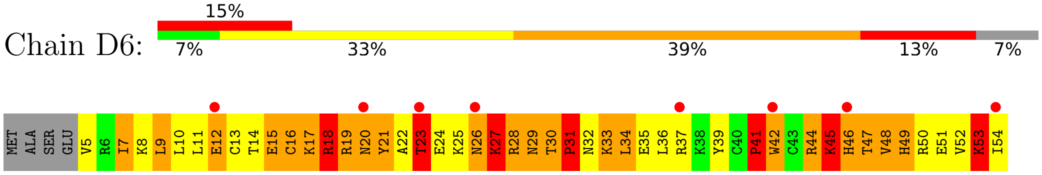

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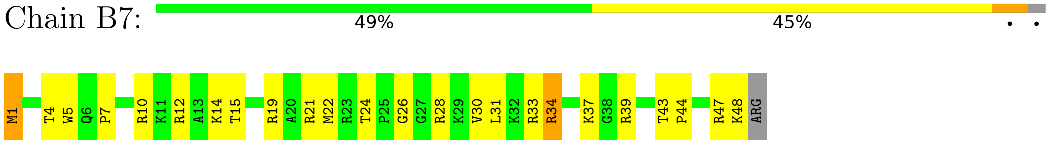

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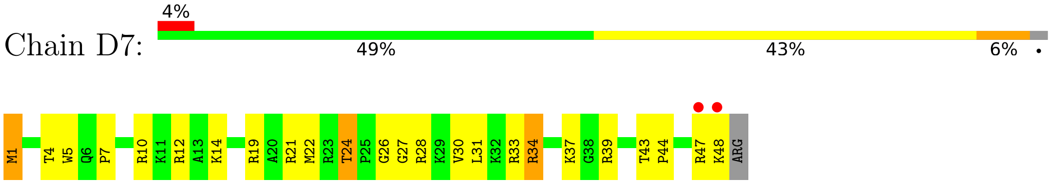

- Molecule 34: 50S RIBOSOMAL PROTEIN L35

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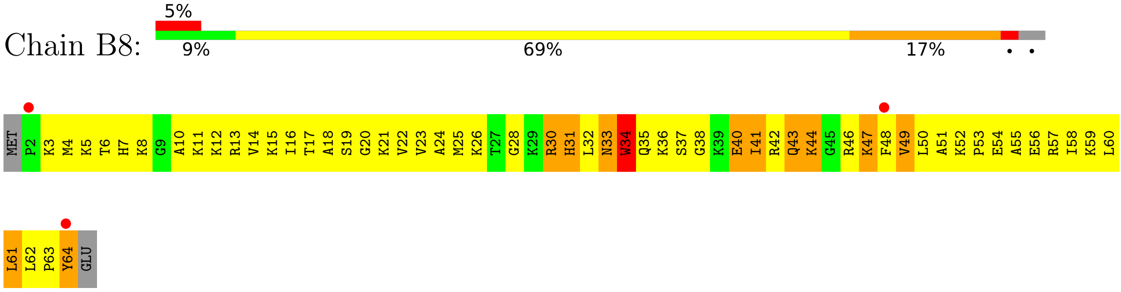

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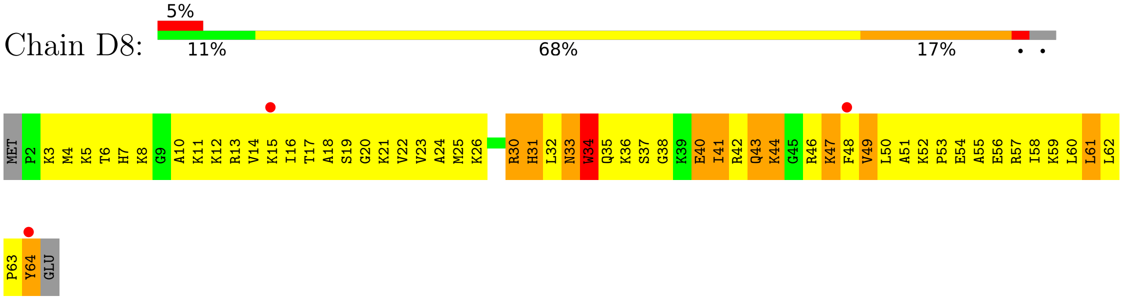

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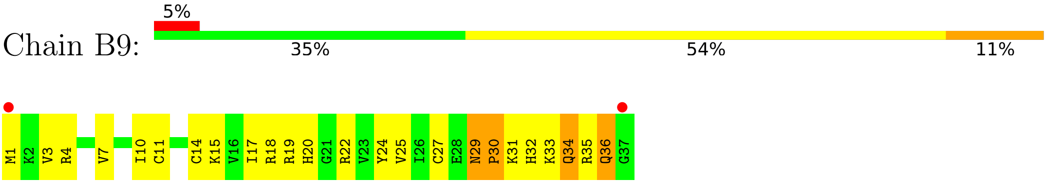

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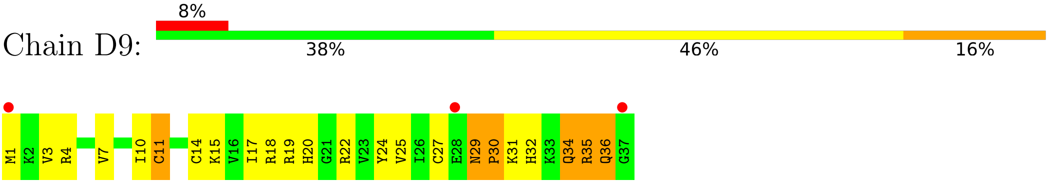
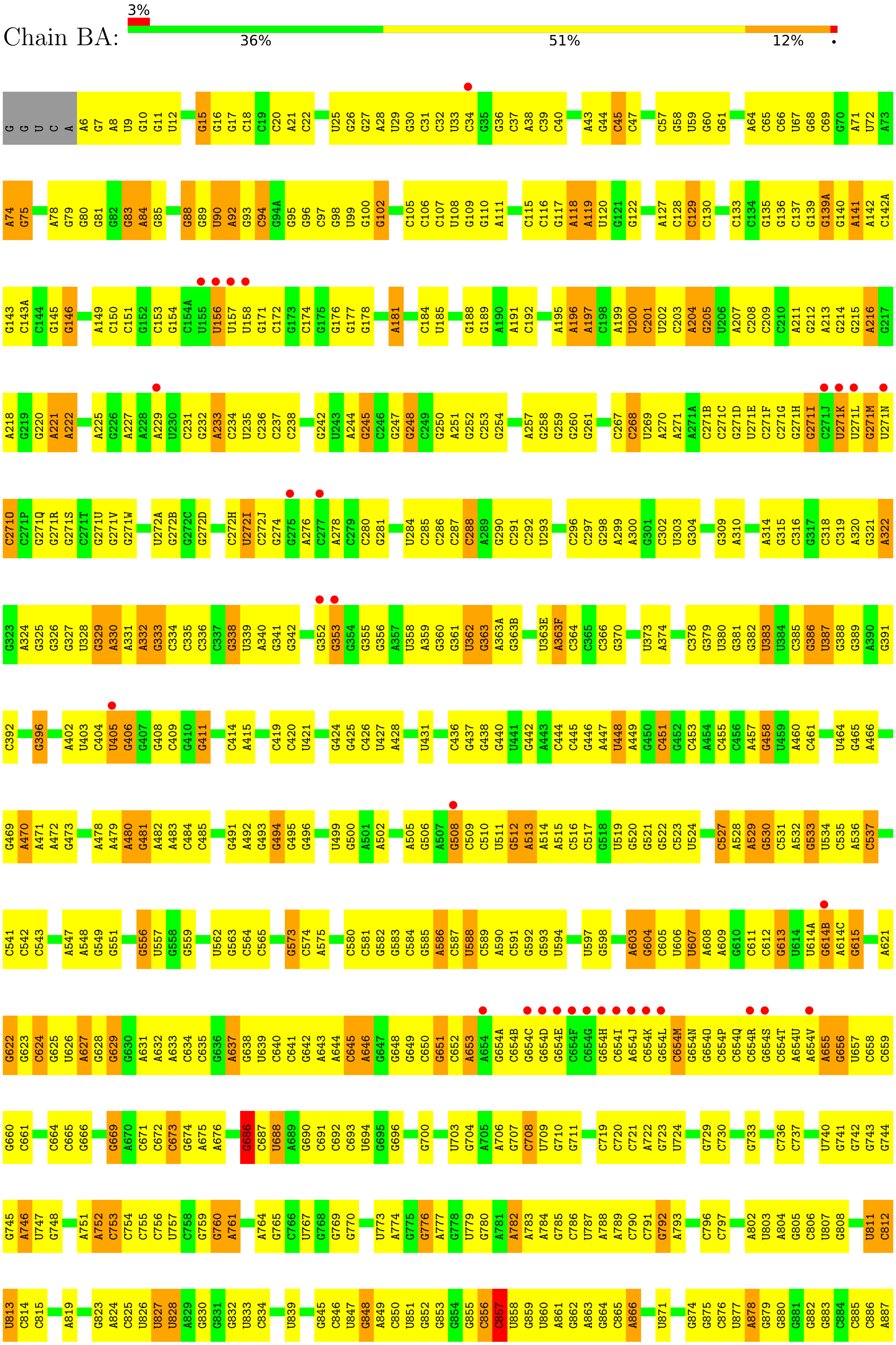


- Molecule 36: 23S RIBOSOMAL RNA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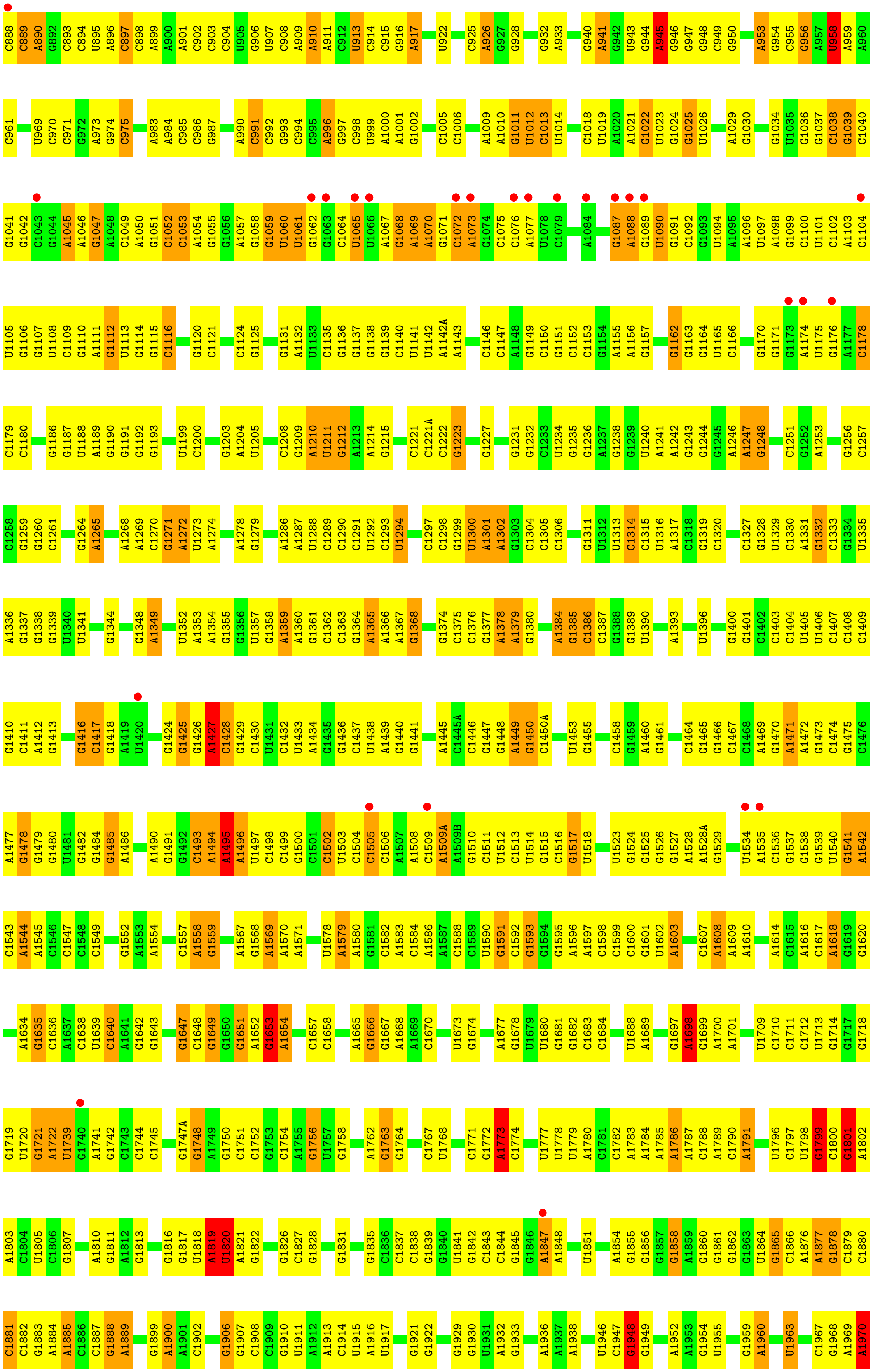
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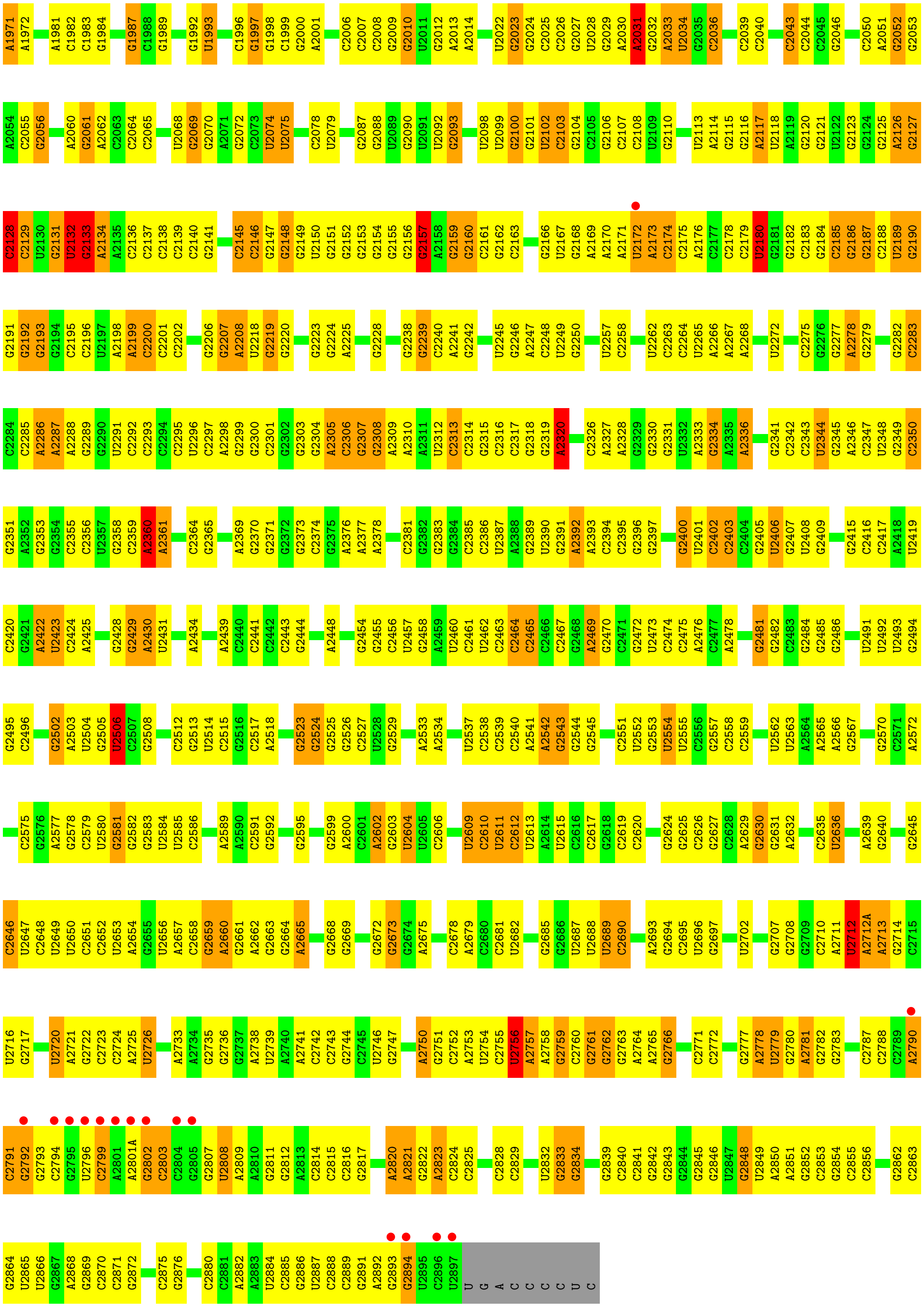

- Molecule 36: 23S RIBOSOMAL RNA

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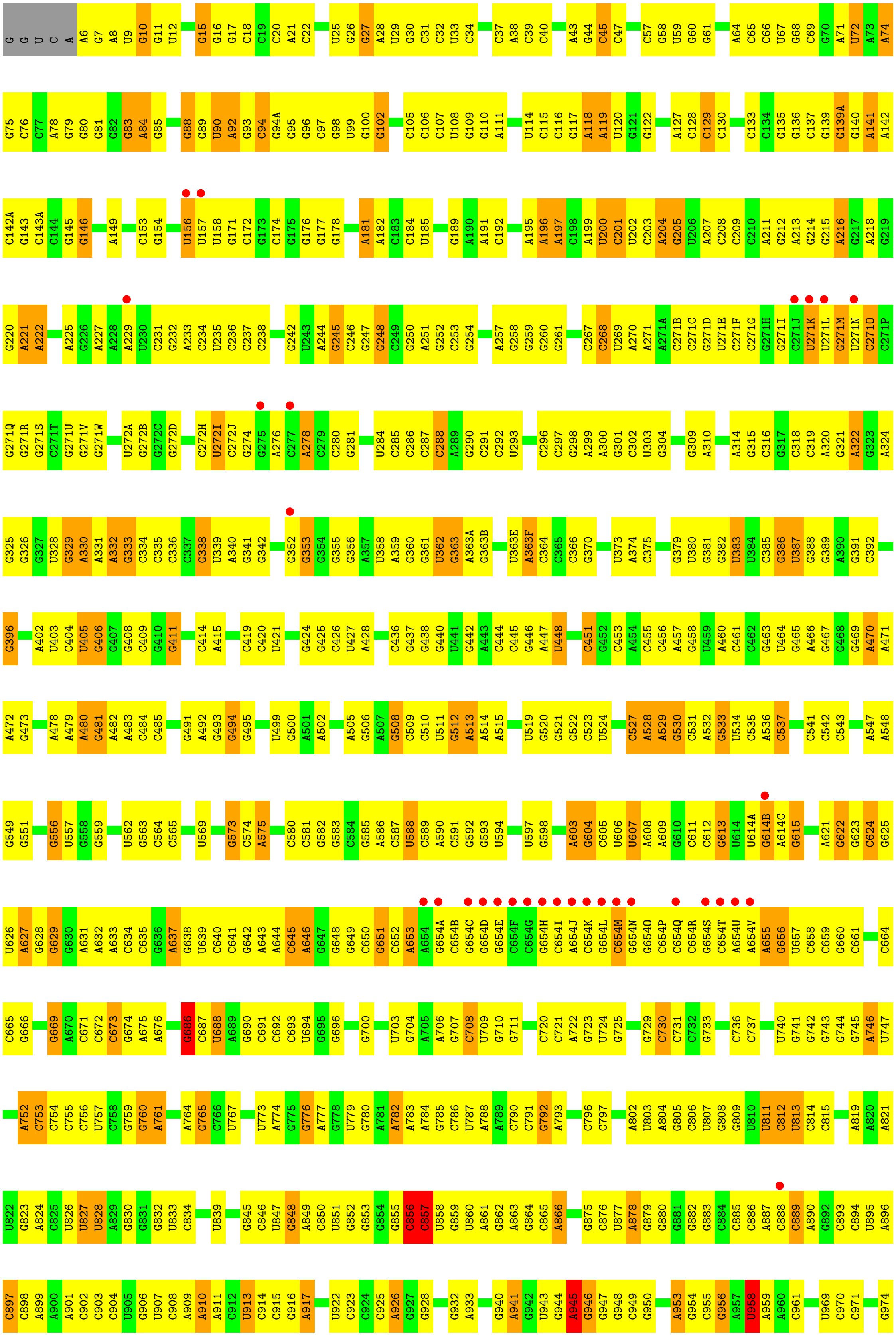
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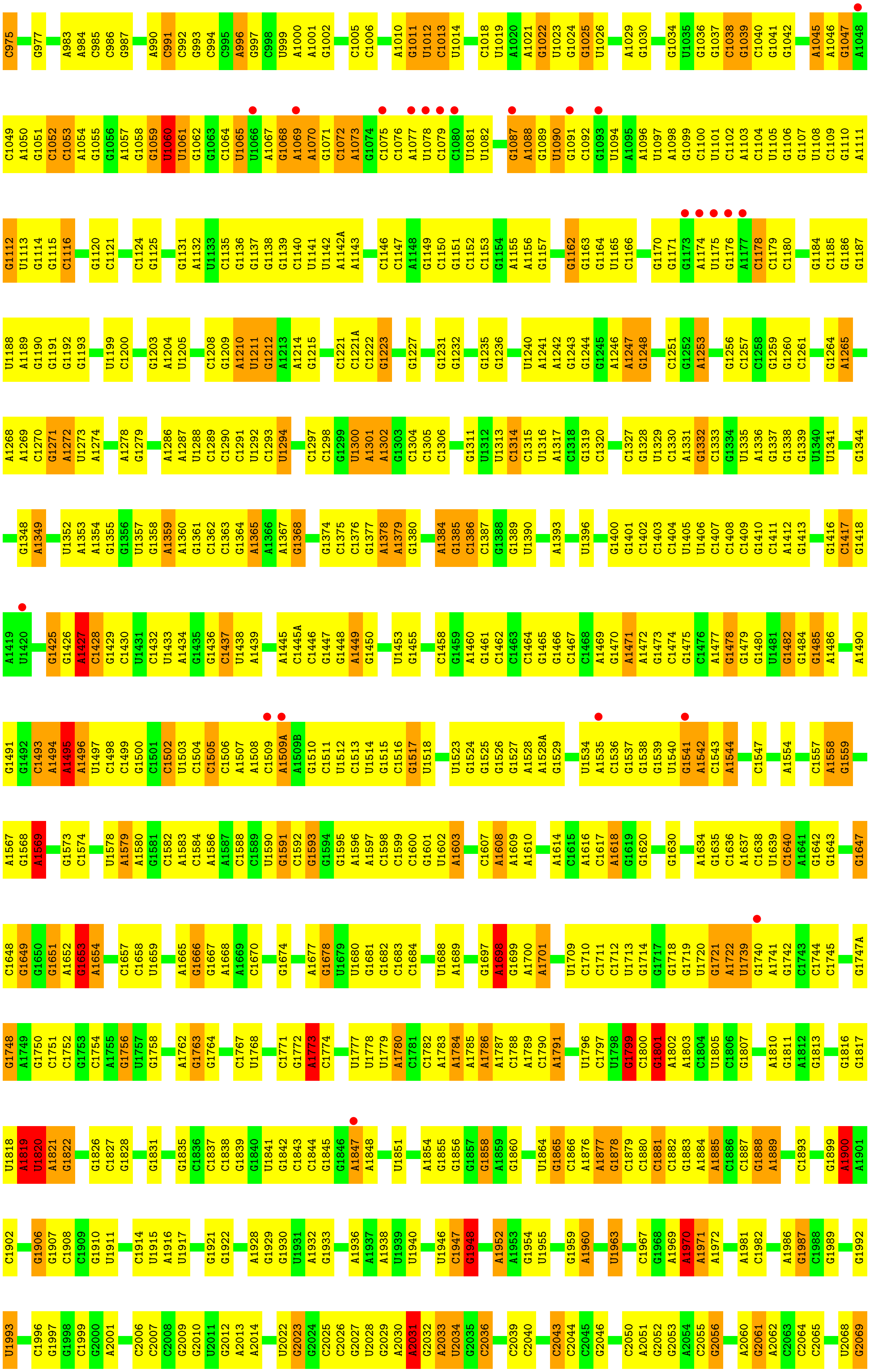
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G1748 A1749 G1750 C1751 C1752 G1753 C1754 A1755 G1756 U1757 G1758 A1762 G1763 G1764 C1767 U1768 C1771 G1772 A1773 C1774 U1777 G1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 U1805 C1806 G1807 A1810 G1811 A1812 G1813 G1816 G1817
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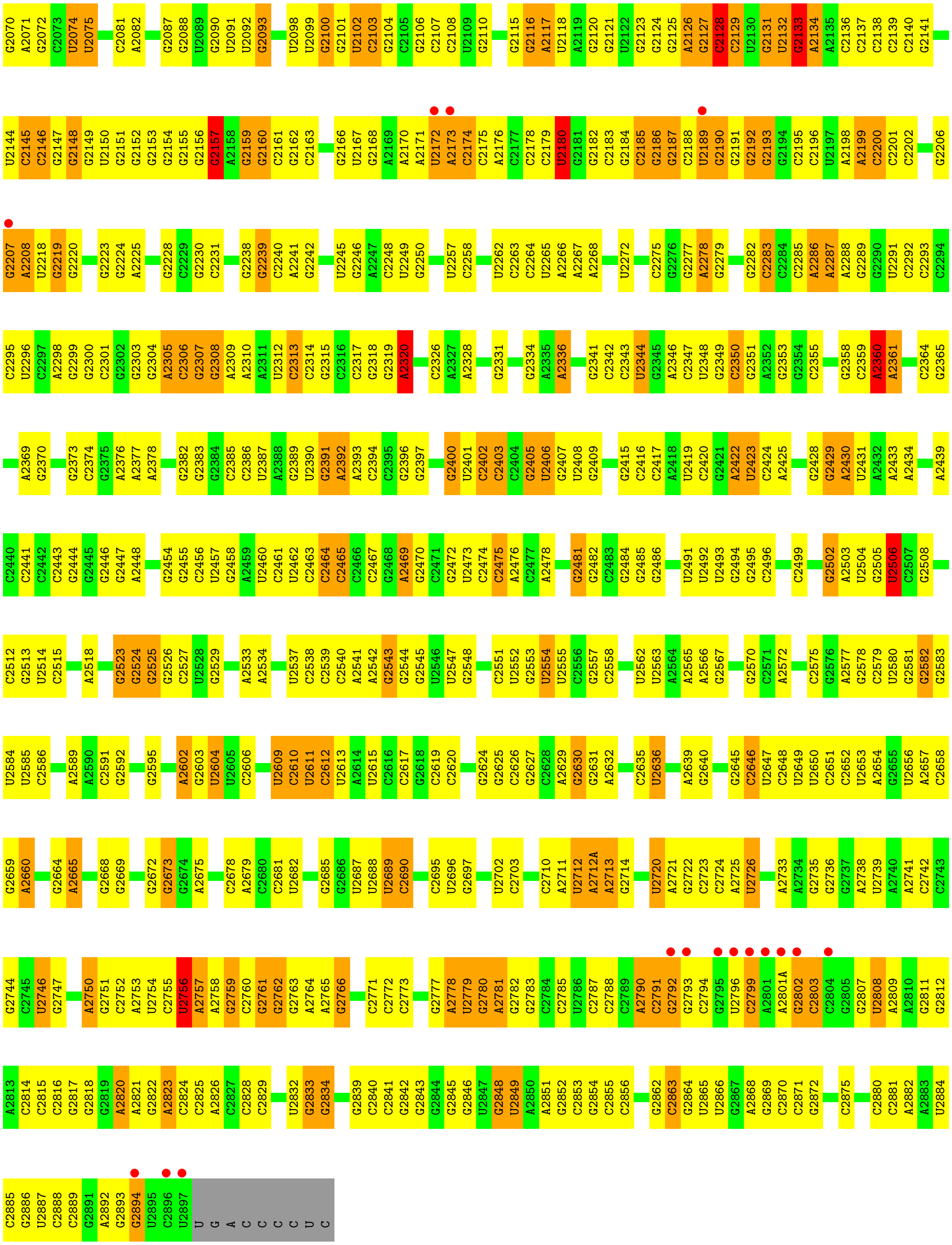
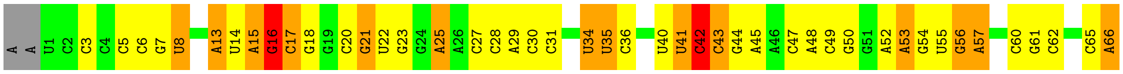
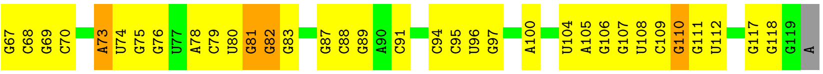


- Molecule 37: 5S RIBOSOMAL RNA

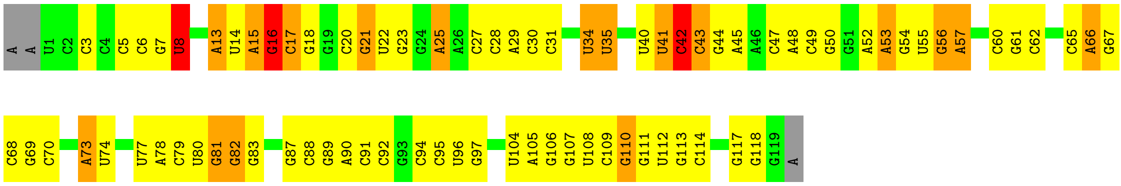
Chain BB:





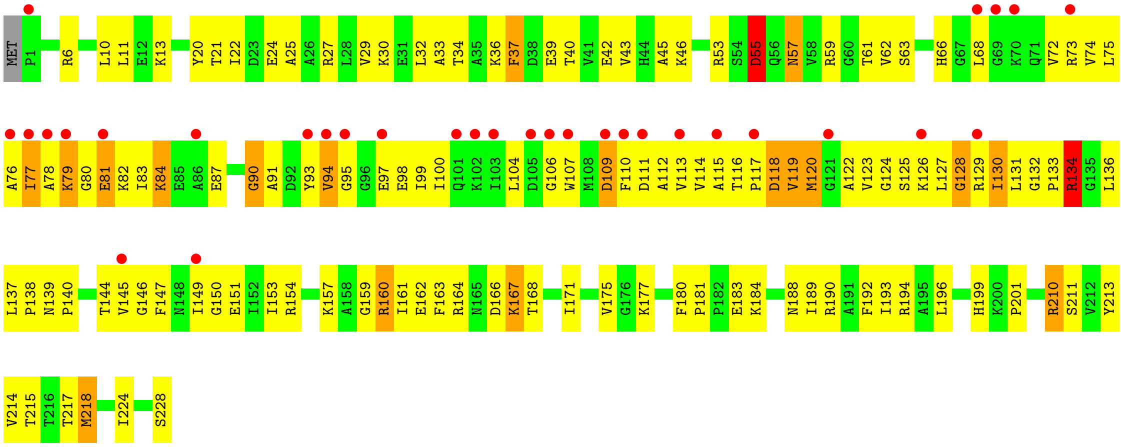
- Molecule 37: 5S RIBOSOMAL RNA

Chain DB:



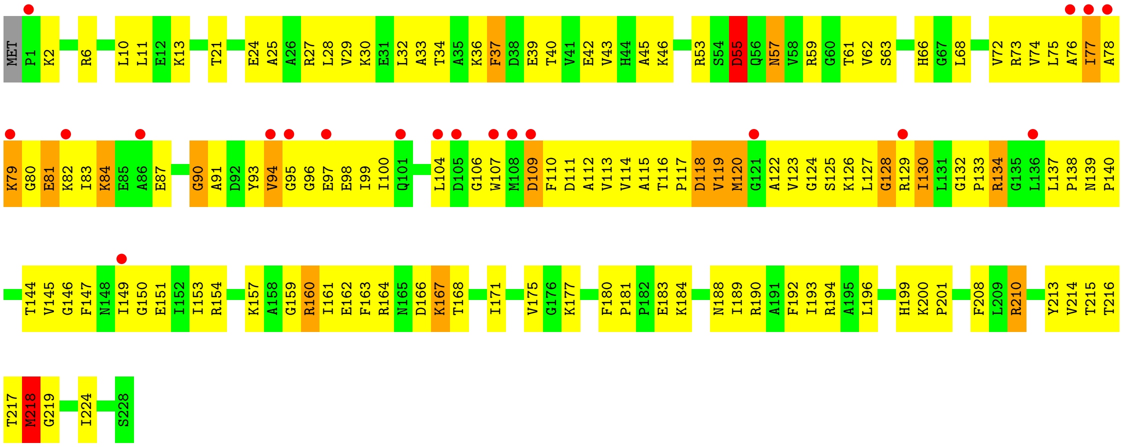
- Molecule 38: 50S RIBOSOMAL PROTEIN L1

Chain BC:



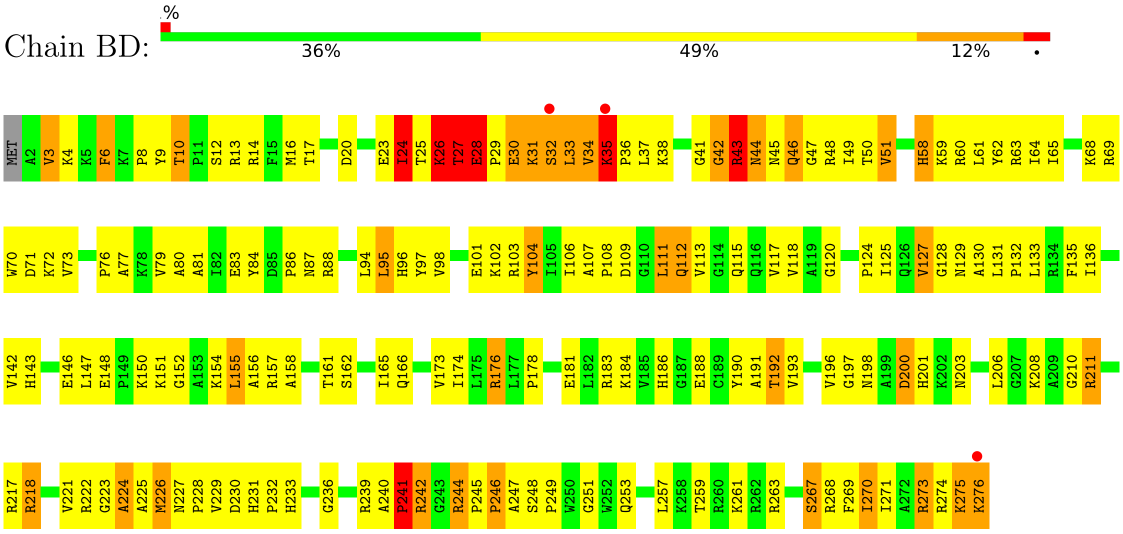
- Molecule 38: 50S RIBOSOMAL PROTEIN L1

Chain DC:



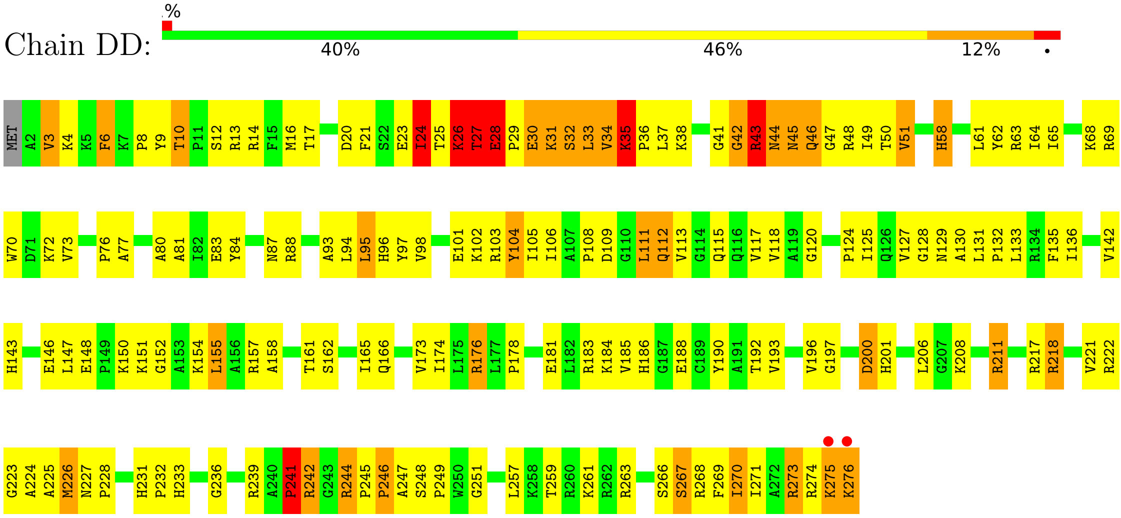
- Molecule 39: 50S RIBOSOMAL PROTEIN L2

Chain BD:



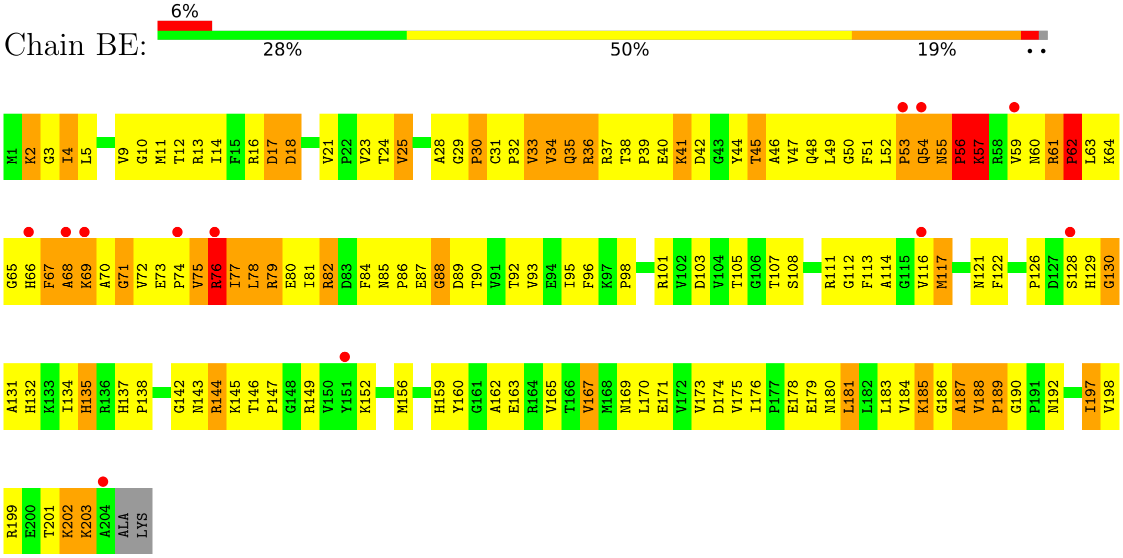
- Molecule 39: 50S RIBOSOMAL PROTEIN L2

Chain DD:



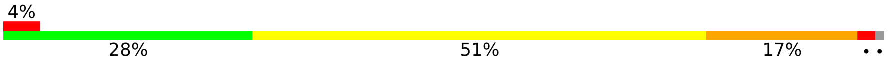
- Molecule 40: 50S RIBOSOMAL PROTEIN L3

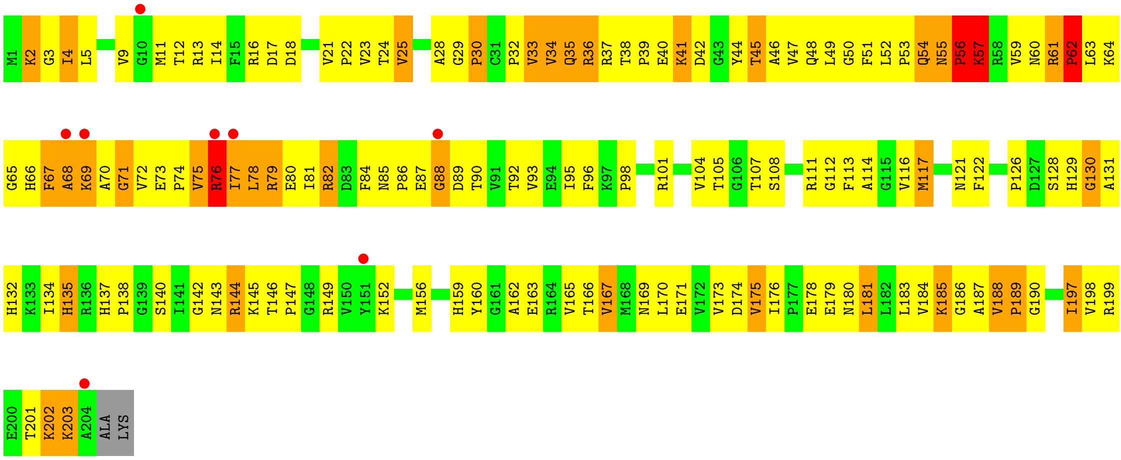
Chain BE:



- Molecule 40: 50S RIBOSOMAL PROTEIN L3

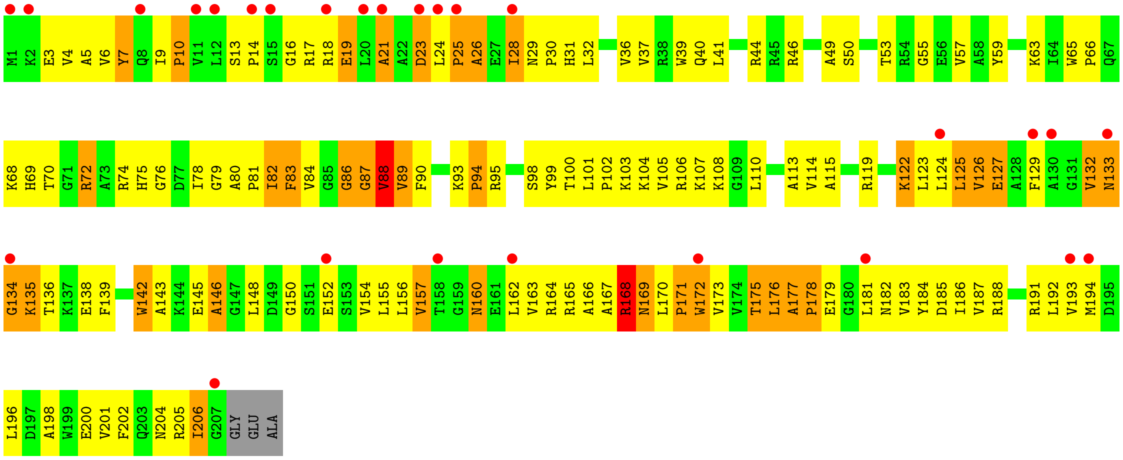
Chain DE:





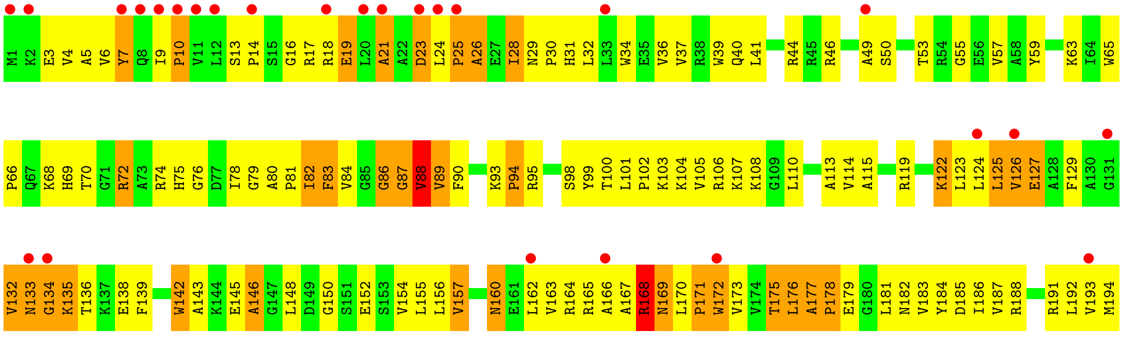
- Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain BF:



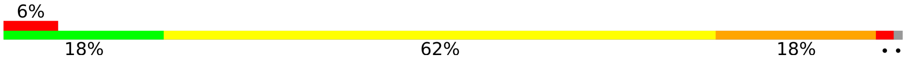
- Molecule 41: 50S RIBOSOMAL PROTEIN L4

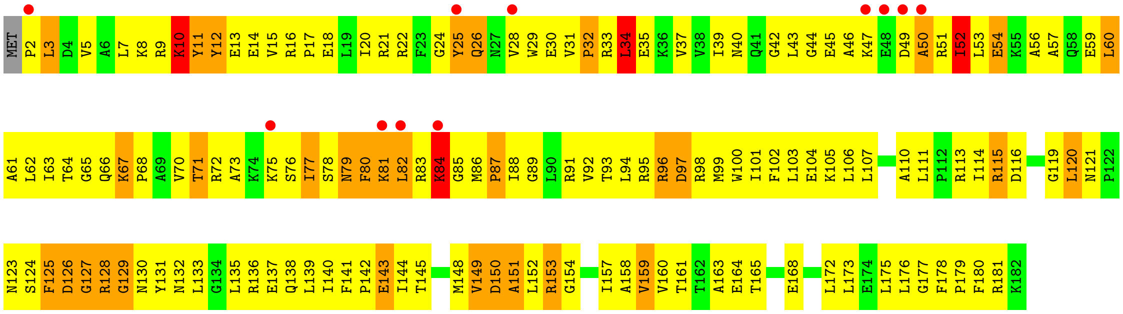
Chain DF:



- Molecule 42: 50S RIBOSOMAL PROTEIN L5

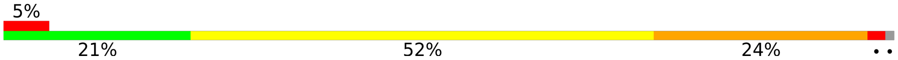
Chain BG:

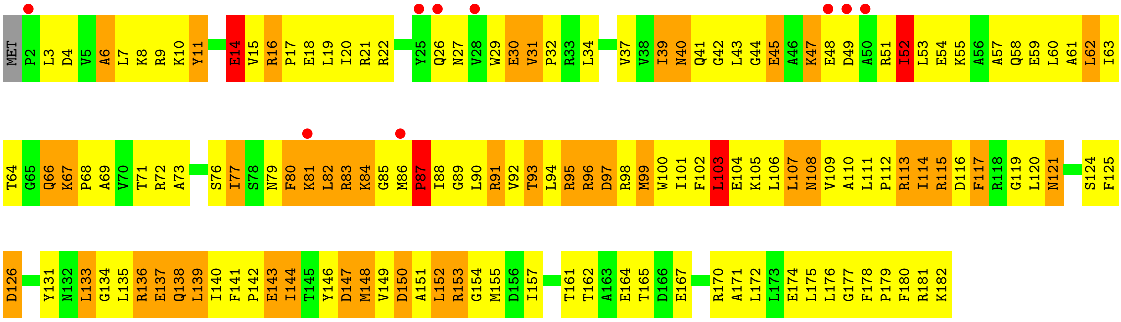




- Molecule 42: 50S RIBOSOMAL PROTEIN L5

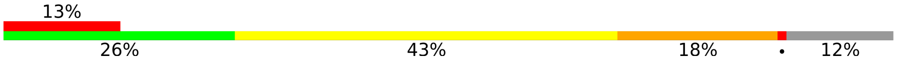
Chain DG:

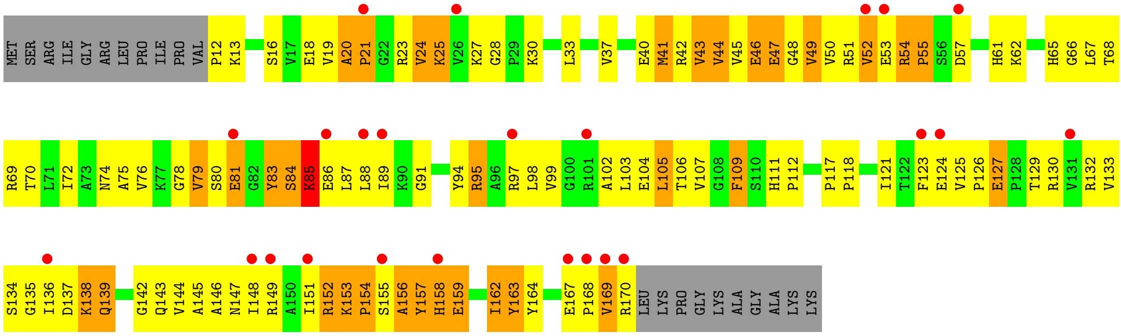




- Molecule 43: 50S RIBOSOMAL PROTEIN L6

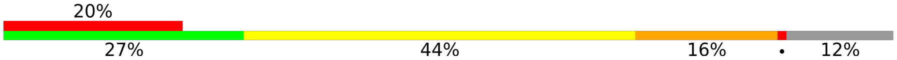
Chain BH:

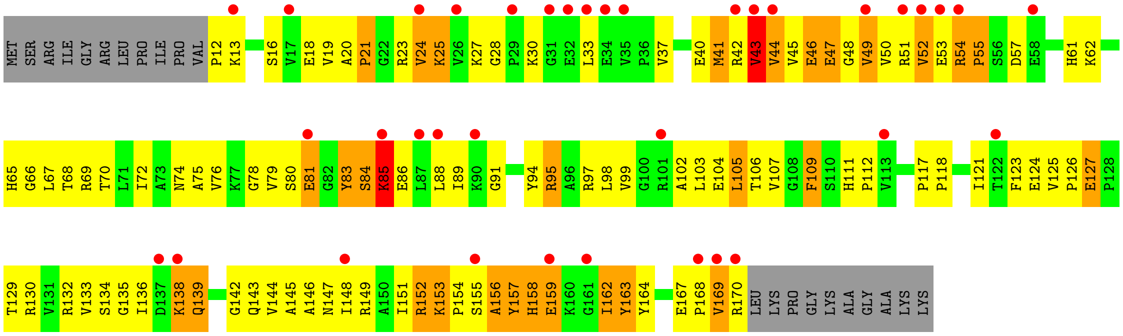




- Molecule 43: 50S RIBOSOMAL PROTEIN L6

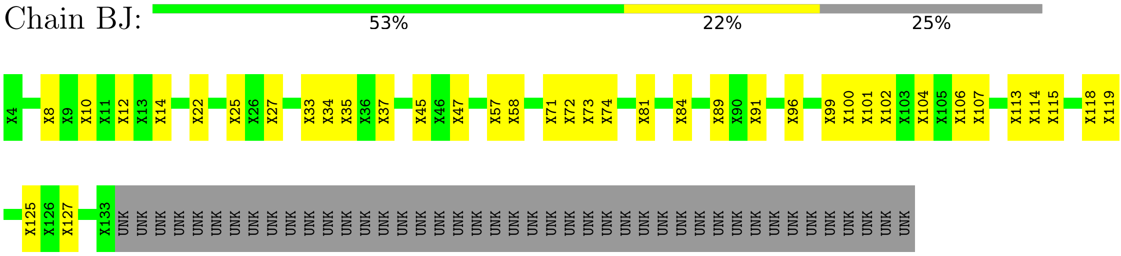
Chain DH:





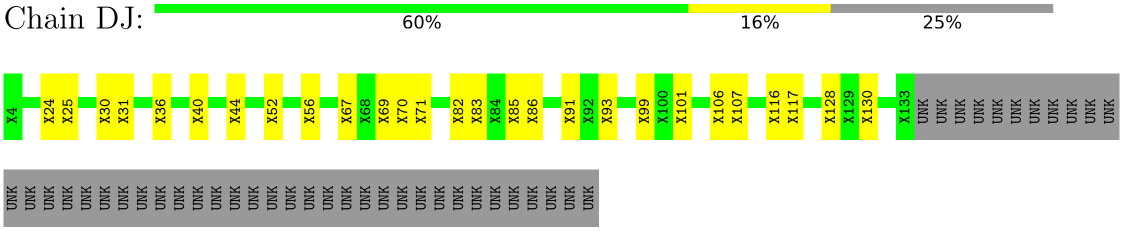
- Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



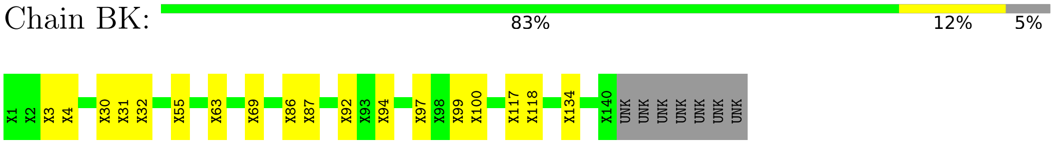
- Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain DJ:



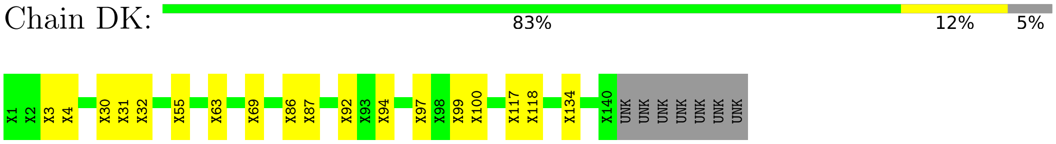
- Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK:



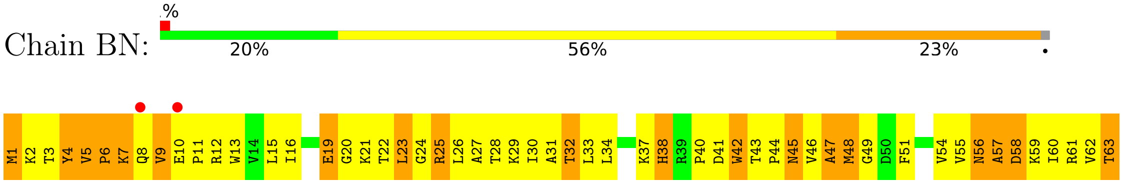
- Molecule 45: 50S RIBOSOMAL PROTEIN L11

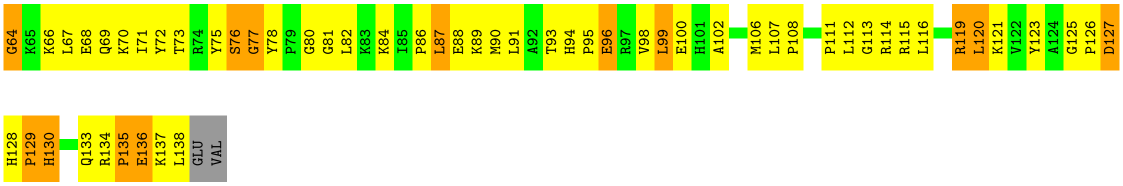
Chain DK:



- Molecule 46: 50S RIBOSOMAL PROTEIN L13

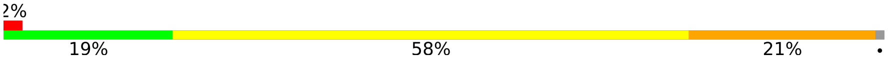
Chain BN:

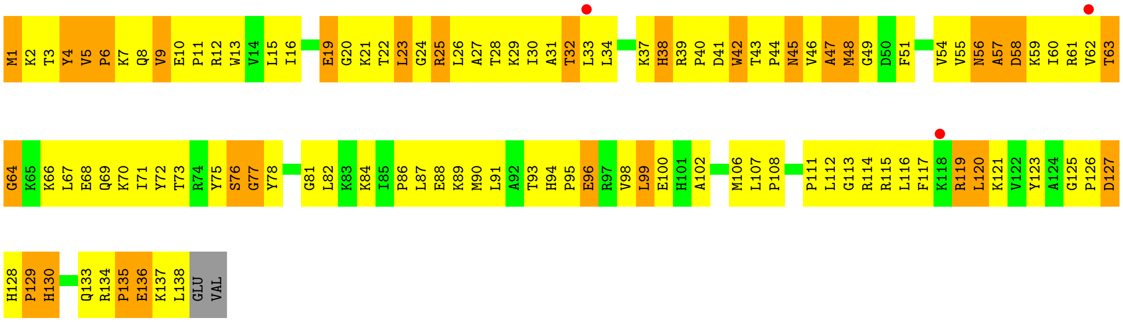




- Molecule 46: 50S RIBOSOMAL PROTEIN L13

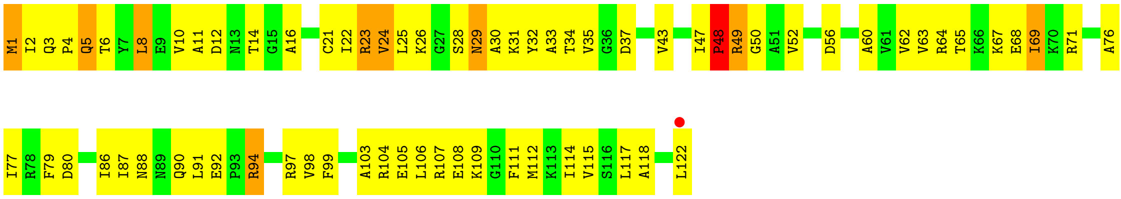
Chain DN:





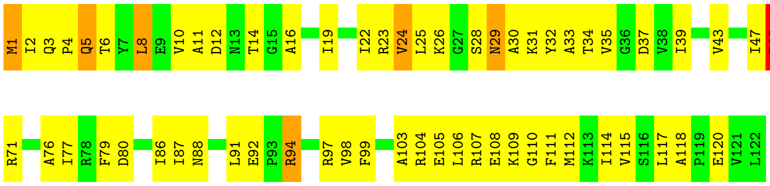
- Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:



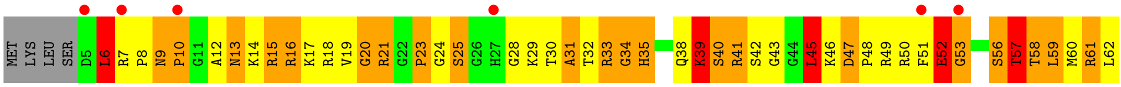
- Molecule 47: 50S RIBOSOMAL PROTEIN L14

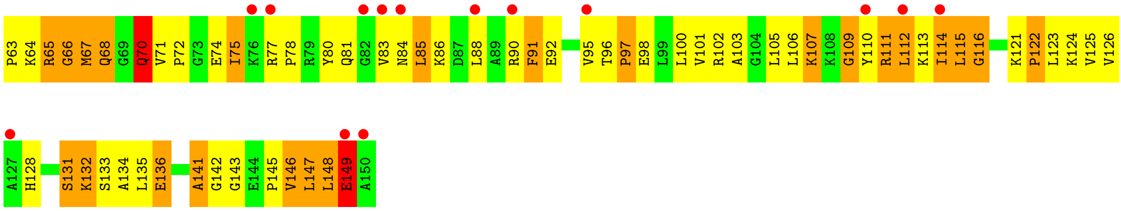
Chain DO:



- Molecule 48: 50S RIBOSOMAL PROTEIN L15

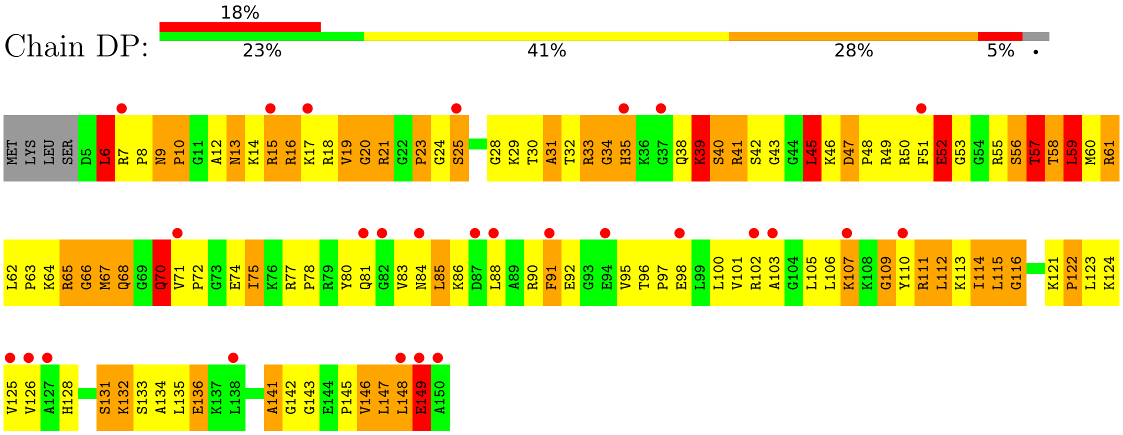
Chain BP:





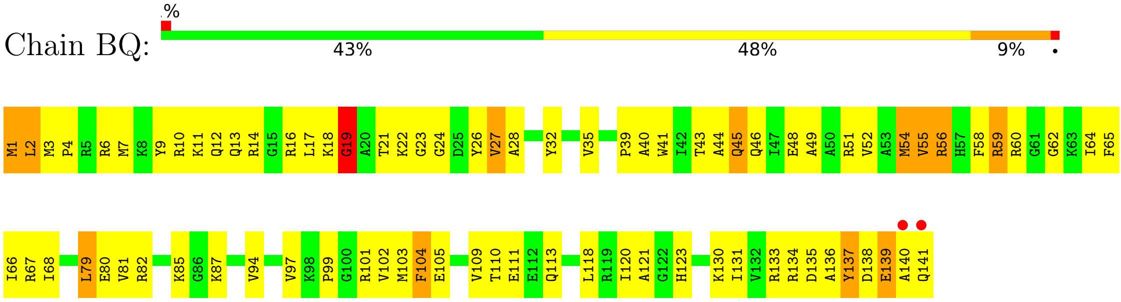
- Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP:



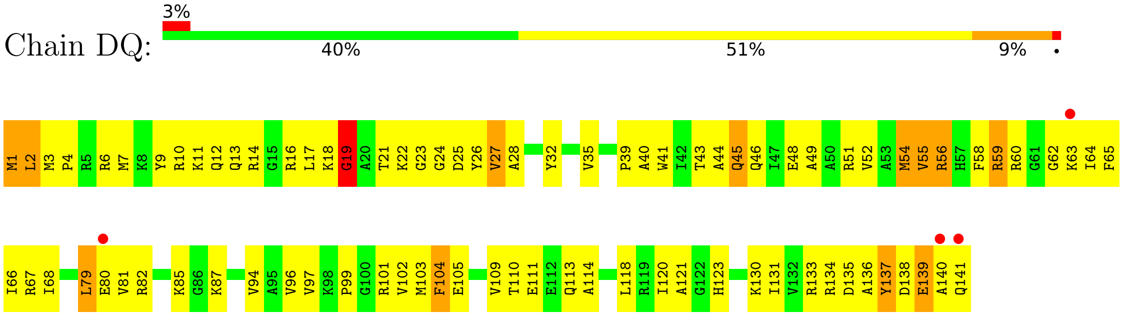
- Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



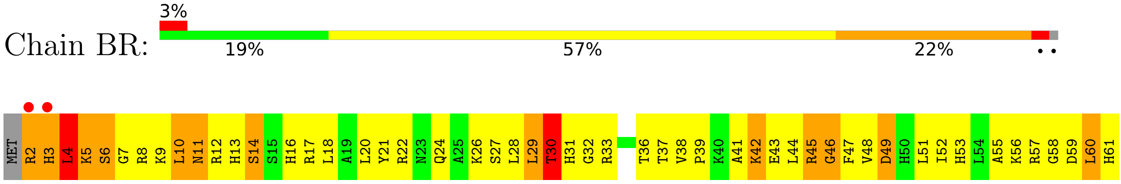
- Molecule 49: 50S RIBOSOMAL PROTEIN L16

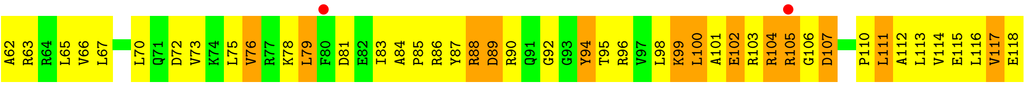
Chain DQ:



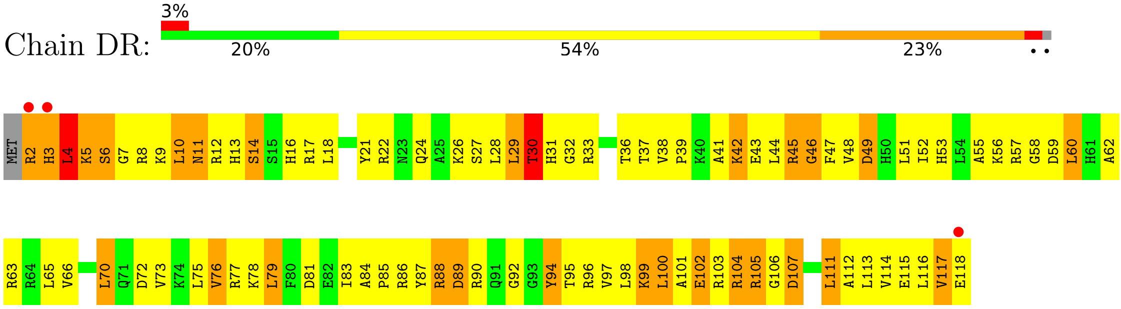
- Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain BR:

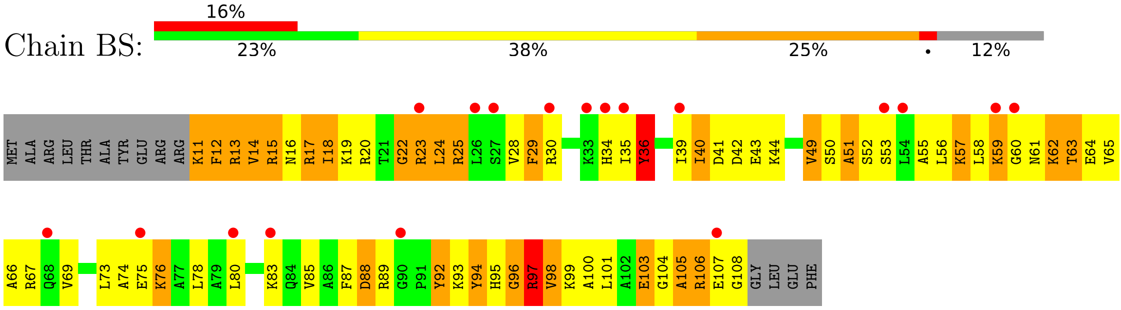




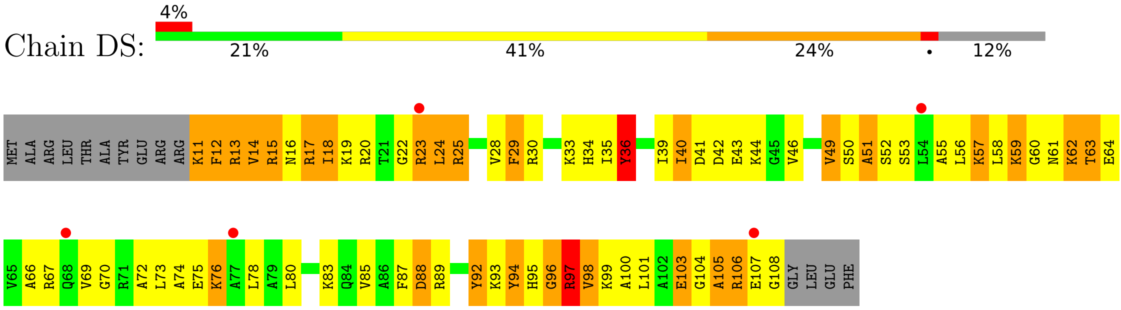
- Molecule 50: 50S RIBOSOMAL PROTEIN L17



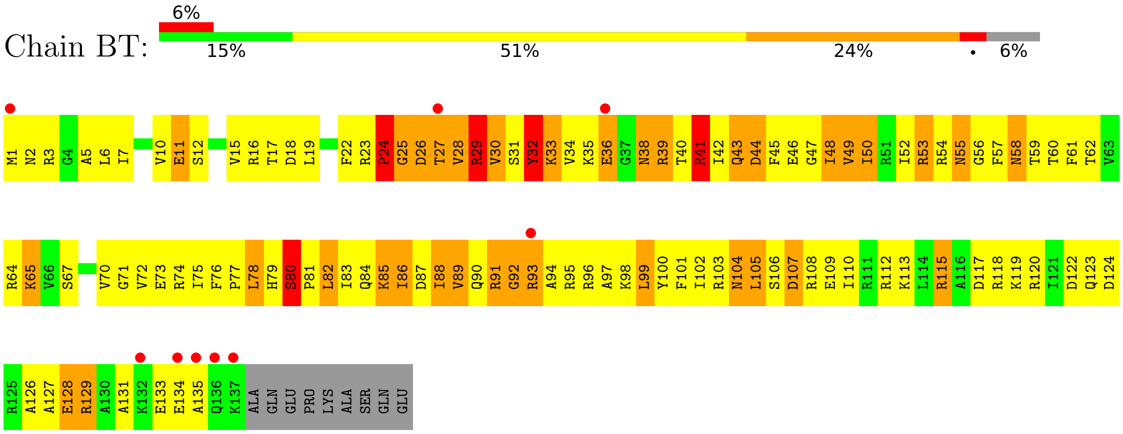
- Molecule 51: 50S RIBOSOMAL PROTEIN L18



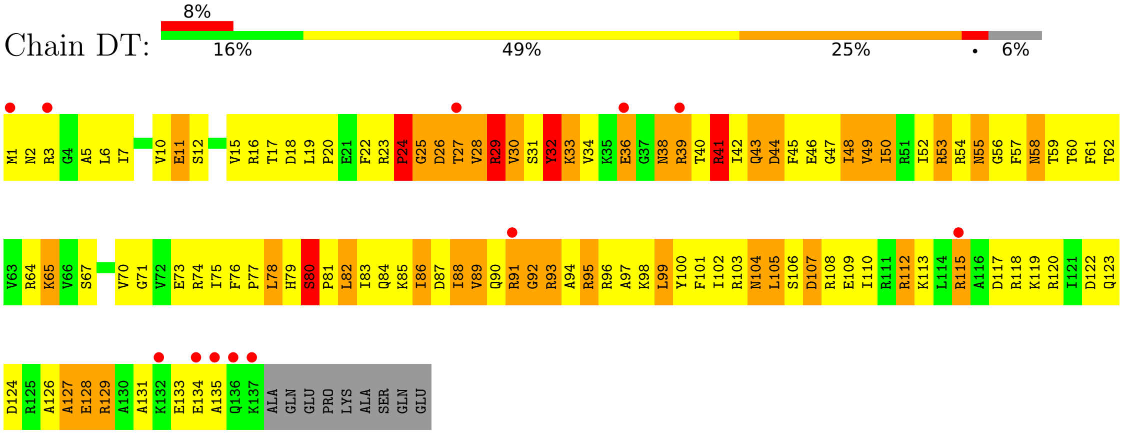
- Molecule 51: 50S RIBOSOMAL PROTEIN L18



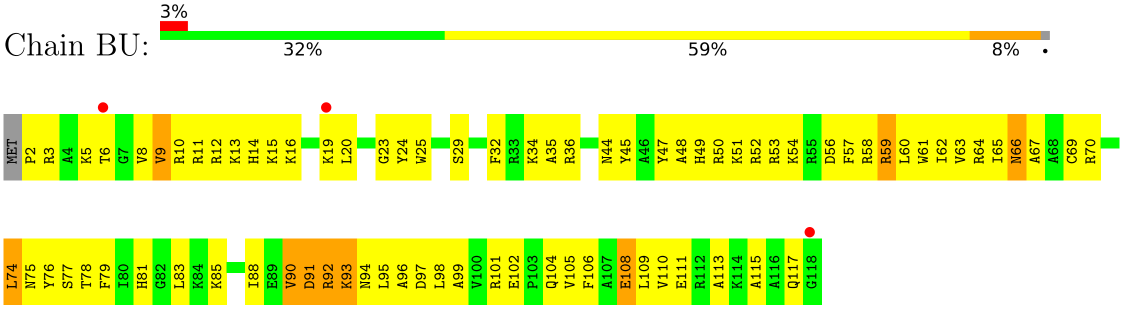
- Molecule 52: 50S RIBOSOMAL PROTEIN L19



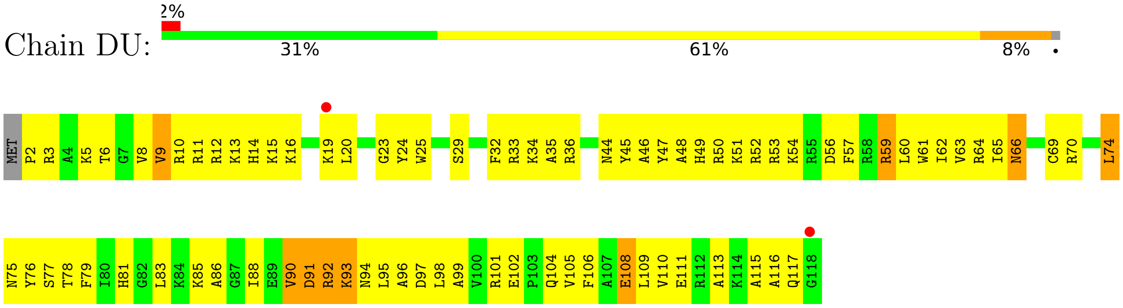
- Molecule 52: 50S RIBOSOMAL PROTEIN L19



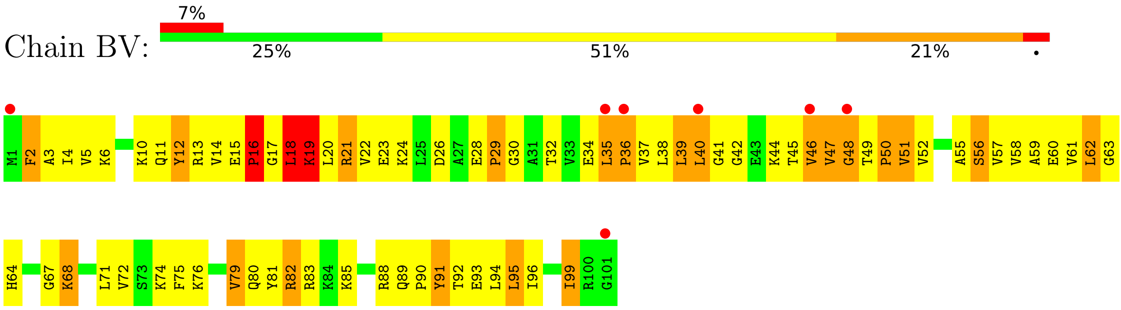
- Molecule 53: 50S RIBOSOMAL PROTEIN L20



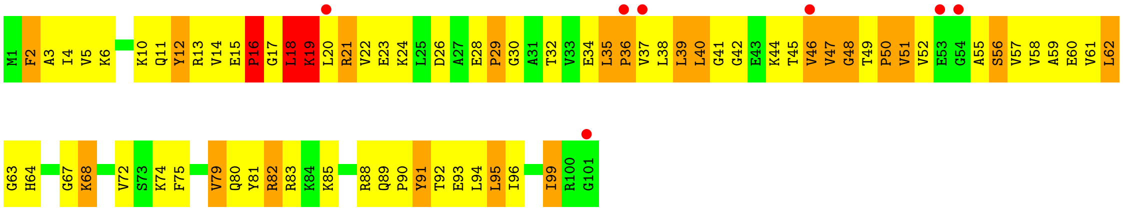
- Molecule 53: 50S RIBOSOMAL PROTEIN L20



- Molecule 54: 50S RIBOSOMAL PROTEIN L21

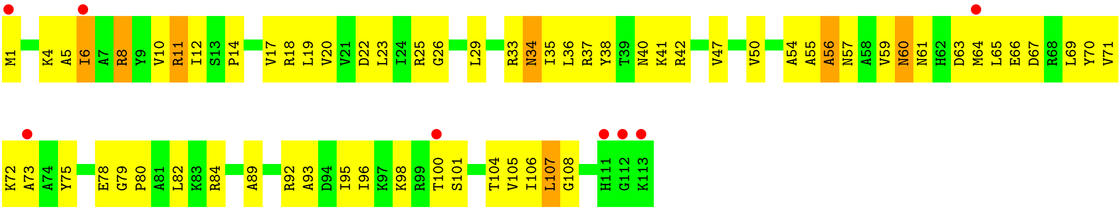


- Molecule 54: 50S RIBOSOMAL PROTEIN L21



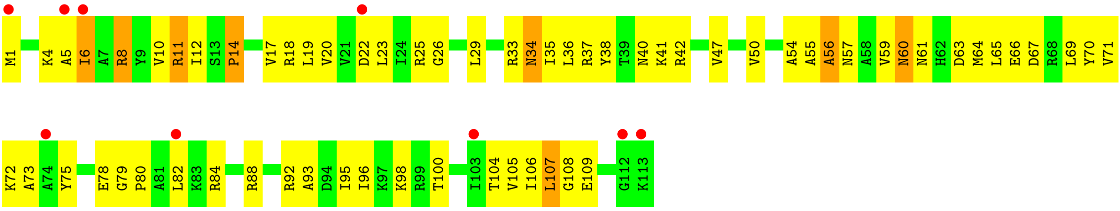
- Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain BW:



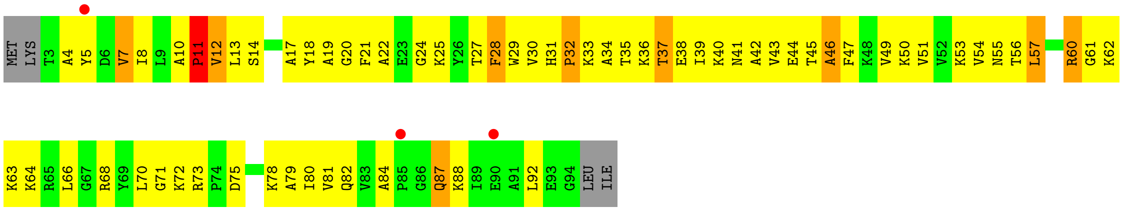
- Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain DW:



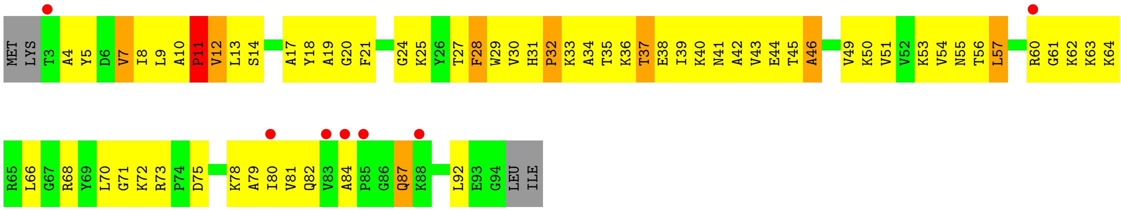
- Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



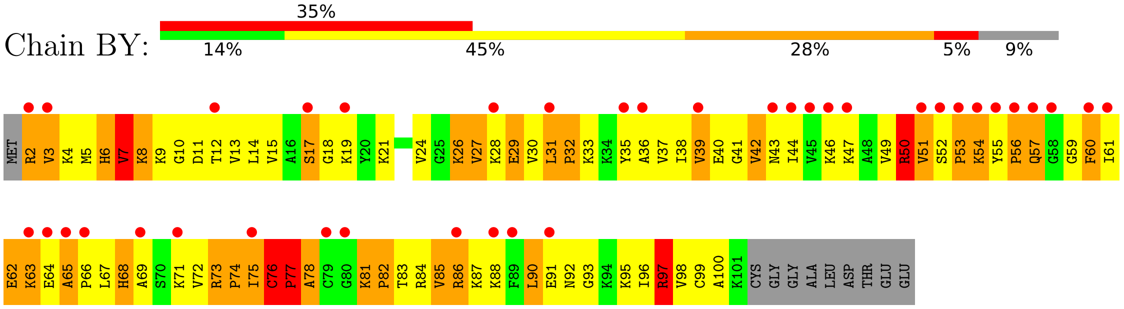
- Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain DX:



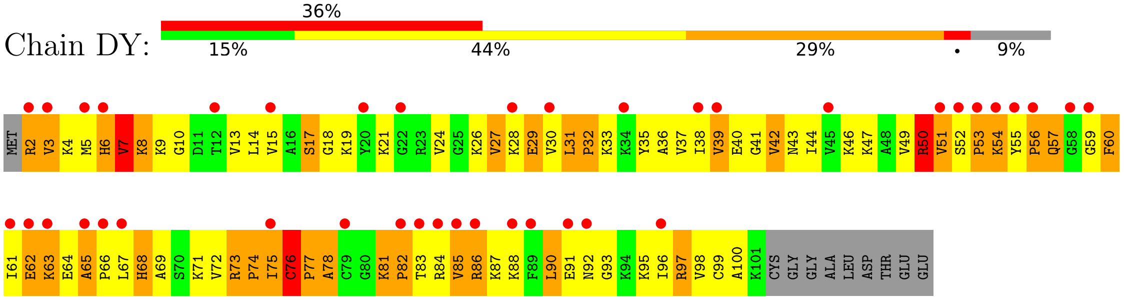
- Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY:



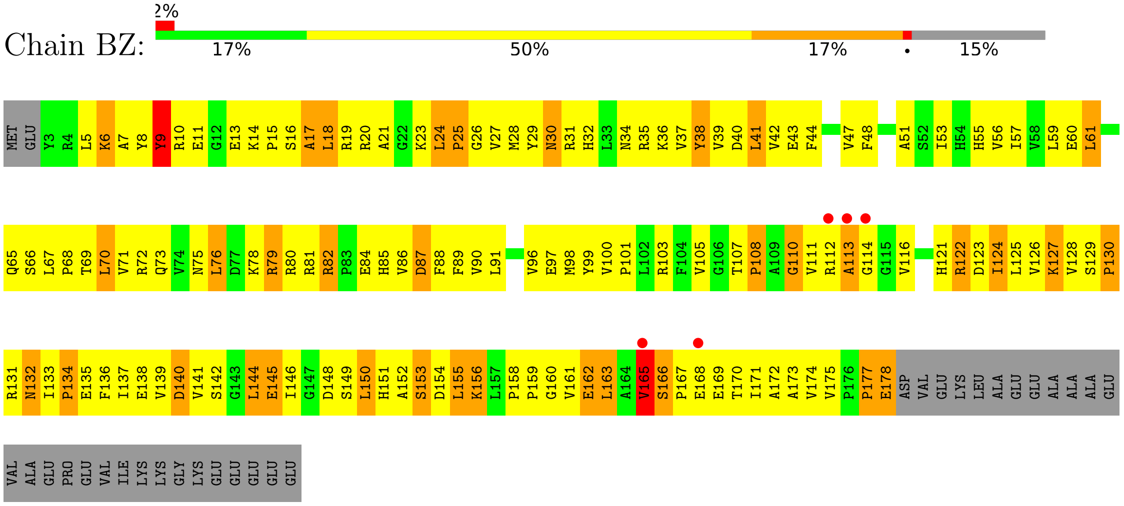
- Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain DY:



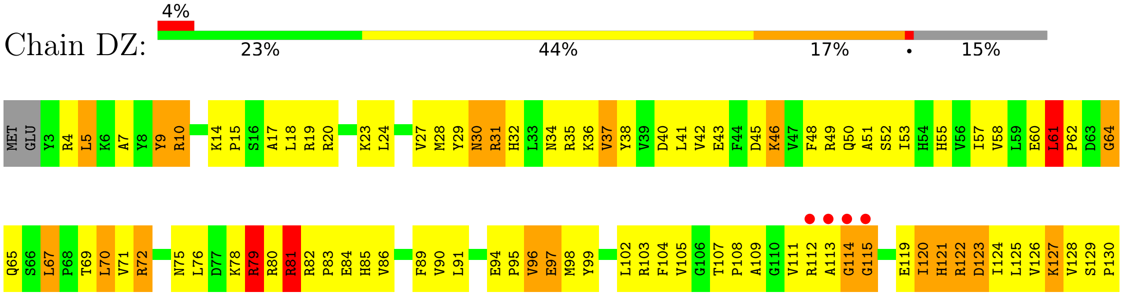
- Molecule 58: 50S RIBOSOMAL PROTEIN L25

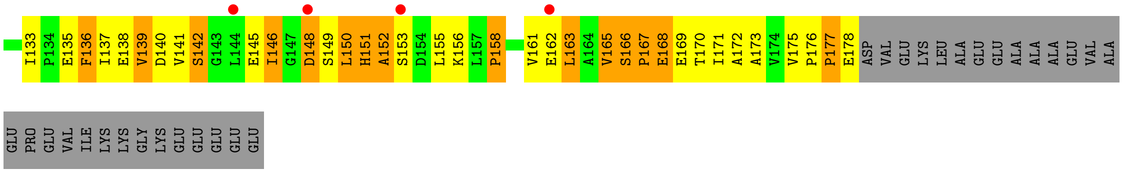
Chain BZ:



- Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain DZ:




I133
P134
E135
F136
I137
E138
V139
D140
V141
S142
G143
L144
E145
I146
G147
D148
S149
L150
H151
A152
S153
D154
L155
K156
L157
P158
V161
E162
L163
A164
V165
S166
P167
E168
E169
T170
I171
A172
A173
V174
V175
P176
P177
E178
ASP
VAL
GLU
LYS
LEU
ALA
GLU
GLU
ALA
ALA
ALA
GLU
VAL
ALA
GLU
PRO
GLU
VAL
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU
GLU

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	290.20Å 269.20Å 404.00Å 90.00° 91.54° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.10) 92.4 (49.51-2.90)	Depositor EDS
R$_{merge}$	0.02	Depositor
R$_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R$_{free}$	0.237 , 0.264 0.236 , 0.263	Depositor DCC
R$_{free}$ test set	62894 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	79.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 67.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F$_o$,F$_c$ correlation	0.93	EDS
Total number of atoms	307330	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5MU, 7MG, KIR, MIA, OMC, 4SU, GDP, H2U, PSU

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	0.57	6/36325 (0.0%)	0.75	35/56695 (0.1%)
1	CA	0.64	11/36325 (0.0%)	0.76	45/56695 (0.1%)
2	AB	0.49	0/1935	0.69	0/2609
2	CB	0.49	0/1935	0.69	0/2609
3	AC	0.53	0/1636	0.72	1/2205 (0.0%)
3	CC	0.58	0/1636	0.73	1/2205 (0.0%)
4	AD	0.45	0/1733	0.69	1/2318 (0.0%)
4	CD	0.43	0/1733	0.68	1/2318 (0.0%)
5	AE	0.56	0/1162	0.75	0/1564
5	CE	0.59	0/1162	0.76	0/1564
6	AF	0.43	0/856	0.68	0/1154
6	CF	0.42	0/856	0.67	0/1154
7	AG	0.45	0/1276	0.64	0/1709
7	CG	0.47	0/1276	0.64	0/1709
8	AH	0.48	0/1136	0.73	0/1527
8	CH	0.49	0/1136	0.75	0/1527
9	AI	0.45	0/1029	0.68	0/1379
9	CI	0.46	0/1029	0.68	0/1379
10	AJ	0.44	0/807	0.73	0/1085
10	CJ	0.47	0/807	0.74	0/1085
11	AK	0.49	0/900	0.72	0/1213
11	CK	0.52	0/900	0.72	0/1213
12	AL	0.49	0/986	0.77	0/1320
12	CL	0.51	0/986	0.78	0/1320
13	AM	0.45	0/998	0.73	0/1336
13	CM	0.46	0/998	0.73	0/1336
14	AN	0.62	0/501	0.81	0/664
14	CN	0.56	0/501	0.80	0/664
15	AO	0.47	0/745	0.67	0/992
15	CO	0.47	0/745	0.67	0/992
16	AP	0.43	0/716	0.70	0/963
16	CP	0.43	0/716	0.70	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.50	0/836	0.70	0/1117
17	CQ	0.50	0/836	0.70	0/1117
18	AR	0.50	0/579	0.66	0/768
18	CR	0.47	0/579	0.65	0/768
19	AS	0.47	0/642	0.71	0/865
19	CS	0.49	0/642	0.72	0/865
20	AT	0.40	0/765	0.66	0/1007
20	CT	0.42	0/765	0.67	0/1007
21	AU	0.51	0/212	0.65	0/277
21	CU	0.47	0/212	0.64	0/277
22	AV	0.66	0/1809	0.83	1/2819 (0.0%)
22	AW	0.55	0/1809	0.75	0/2819
22	CV	0.72	0/1809	0.82	1/2819 (0.0%)
22	CW	0.57	1/1809 (0.1%)	0.76	0/2819
23	AX	0.69	0/406	0.87	2/631 (0.3%)
23	CX	0.80	0/406	0.90	3/631 (0.5%)
24	AY	0.49	1/1619 (0.1%)	0.70	0/2516
24	CY	0.50	1/1619 (0.1%)	0.70	0/2516
25	AZ	0.67	3/3042 (0.1%)	0.76	7/4129 (0.2%)
25	CZ	0.65	4/3042 (0.1%)	0.76	6/4129 (0.1%)
26	B0	0.45	0/671	0.70	0/892
26	D0	0.44	0/671	0.70	0/892
27	B1	0.43	0/738	0.72	0/981
27	D1	0.51	0/738	0.83	0/981
28	B2	0.35	0/600	0.63	0/793
28	D2	0.40	0/600	0.82	0/793
29	B3	0.35	0/472	0.60	0/634
29	D3	0.36	0/472	0.61	0/634
30	B4	0.41	0/349	0.64	0/474
30	D4	0.42	0/349	0.65	0/474
31	B5	0.40	0/473	0.64	0/639
31	D5	0.39	0/473	0.63	0/639
32	B6	0.62	0/440	0.95	0/586
32	D6	0.67	0/440	0.97	0/586
33	B7	0.45	0/426	0.71	0/561
33	D7	0.43	0/426	0.72	0/561
34	B8	0.55	0/515	0.77	0/679
34	D8	0.58	0/515	0.77	0/679
35	B9	0.53	0/310	0.70	0/407
35	D9	0.50	0/310	0.69	0/407
36	BA	0.52	5/69976 (0.0%)	0.72	27/109244 (0.0%)
36	DA	0.53	5/69976 (0.0%)	0.72	35/109244 (0.0%)
37	BB	0.49	0/2853	0.74	0/4451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	DB	0.44	0/2853	0.74	1/4451 (0.0%)
38	BC	0.42	1/1774 (0.1%)	0.74	3/2391 (0.1%)
38	DC	0.43	2/1774 (0.1%)	0.75	3/2391 (0.1%)
39	BD	0.52	0/2195	0.88	4/2955 (0.1%)
39	DD	0.54	0/2195	0.90	4/2955 (0.1%)
40	BE	0.43	0/1596	0.71	0/2153
40	DE	0.44	0/1596	0.71	0/2153
41	BF	0.38	0/1658	0.74	3/2244 (0.1%)
41	DF	0.36	0/1658	0.74	3/2244 (0.1%)
42	BG	0.39	0/1499	0.70	1/2016 (0.0%)
42	DG	0.47	0/1499	0.80	0/2016
43	BH	0.35	0/1245	0.67	0/1682
43	DH	0.35	0/1245	0.67	0/1682
46	BN	0.39	0/1131	0.71	1/1525 (0.1%)
46	DN	0.39	0/1131	0.71	1/1525 (0.1%)
47	BO	0.52	1/943 (0.1%)	0.71	0/1269
47	DO	0.51	0/943	0.72	0/1269
48	BP	0.43	0/1131	0.89	3/1504 (0.2%)
48	DP	0.44	0/1131	0.90	4/1504 (0.3%)
49	BQ	0.51	0/1143	0.72	1/1527 (0.1%)
49	DQ	0.54	0/1143	0.72	1/1527 (0.1%)
50	BR	0.38	0/974	0.72	1/1302 (0.1%)
50	DR	0.39	0/974	0.72	1/1302 (0.1%)
51	BS	0.43	0/778	0.75	0/1036
51	DS	0.41	0/778	0.75	0/1036
52	BT	0.44	0/1155	0.76	2/1542 (0.1%)
52	DT	0.45	0/1155	0.77	2/1542 (0.1%)
53	BU	0.44	0/975	0.67	0/1297
53	DU	0.42	0/975	0.67	0/1297
54	BV	0.38	0/790	0.67	0/1057
54	DV	0.36	0/790	0.67	0/1057
55	BW	0.38	0/907	0.64	0/1216
55	DW	0.37	0/907	0.65	0/1216
56	BX	0.43	0/739	0.91	3/993 (0.3%)
56	DX	0.42	0/739	0.89	3/993 (0.3%)
57	BY	0.37	0/788	0.68	1/1051 (0.1%)
57	DY	0.37	0/788	0.68	1/1051 (0.1%)
58	BZ	0.46	0/1435	0.74	0/1949
58	DZ	0.49	0/1435	0.79	3/1949 (0.2%)
All	All	0.53	41/330278 (0.0%)	0.73	216/493462 (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	4	59
1	CA	4	49
22	AV	0	3
22	CV	0	2
23	AX	0	2
23	CX	0	1
36	BA	2	63
36	DA	2	72
37	BB	0	2
37	DB	0	2
49	BQ	0	1
49	DQ	0	1
All	All	12	257

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	CZ	68	VAL	C-O	-20.43	0.84	1.23
25	AZ	68	VAL	C-O	-19.95	0.85	1.23
36	DA	761	A	C5-C6	-10.79	1.31	1.41
36	BA	761	A	C5-C6	-10.15	1.31	1.41
1	CA	858	G	C5-C6	-10.08	1.32	1.42

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	DC	134	ARG	NE-CZ-NH2	-14.36	113.12	120.30
39	DD	43	ARG	NE-CZ-NH1	14.15	127.37	120.30
41	BF	168	ARG	NE-CZ-NH2	-13.66	113.47	120.30
38	DC	134	ARG	NE-CZ-NH1	13.54	127.07	120.30
38	BC	134	ARG	NE-CZ-NH2	-13.34	113.63	120.30

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	508	C	C3’
1	AA	1363(A)	A	C3’
1	AA	1399	C	C3’
1	AA	1498	U	C3’
36	BA	1819	A	C3’

5 of 257 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	14	U	Sidechain
1	AA	189(G)	G	Sidechain
1	AA	30	U	Sidechain
1	AA	37	U	Sidechain
1	AA	60	A	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	32451	0	16382	929	0
1	CA	32451	0	16382	850	0
2	AB	1900	0	1951	185	2
2	CB	1900	0	1951	176	2
3	AC	1612	0	1677	145	0
3	CC	1612	0	1677	141	0
4	AD	1703	0	1765	170	0
4	CD	1703	0	1765	157	0
5	AE	1146	0	1207	69	0
5	CE	1146	0	1207	69	0
6	AF	843	0	857	64	0
6	CF	843	0	857	59	0
7	AG	1257	0	1296	70	0
7	CG	1257	0	1296	63	0
8	AH	1116	0	1177	55	0
8	CH	1116	0	1177	49	0
9	AI	1010	0	1037	109	0
9	CI	1010	0	1037	109	0
10	AJ	794	0	840	116	0
10	CJ	794	0	840	116	0
11	AK	885	0	904	58	0
11	CK	885	0	904	57	0
12	AL	970	0	1057	99	0
12	CL	970	0	1057	97	0
13	AM	987	0	1059	116	0
13	CM	987	0	1059	116	0
14	AN	492	0	530	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	530	63	0
15	AO	734	0	771	44	0
15	CO	734	0	771	43	0
16	AP	700	0	720	75	0
16	CP	700	0	720	80	0
17	AQ	823	0	891	60	0
17	CQ	823	0	891	62	0
18	AR	574	0	644	46	0
18	CR	574	0	644	50	0
19	AS	629	0	652	76	0
19	CS	629	0	652	73	0
20	AT	763	0	861	97	0
20	CT	763	0	861	99	0
21	AU	208	0	221	25	0
21	CU	208	0	221	29	0
22	AV	1619	0	822	59	0
22	AW	1619	0	822	79	0
22	CV	1619	0	822	58	0
22	CW	1619	0	822	73	0
23	AX	362	0	184	15	0
23	CX	362	0	184	14	0
24	AY	1645	0	853	132	0
24	CY	1645	0	853	89	0
25	AZ	2984	0	2997	475	0
25	CZ	2984	0	2997	384	0
26	B0	662	0	688	66	0
26	D0	662	0	688	65	0
27	B1	731	0	808	84	0
27	D1	731	0	808	80	0
28	B2	598	0	653	87	0
28	D2	598	0	653	215	0
29	B3	467	0	523	35	0
29	D3	467	0	523	35	0
30	B4	340	0	337	53	0
30	D4	340	0	336	58	0
31	B5	459	0	480	84	0
31	D5	459	0	480	76	0
32	B6	433	0	461	123	0
32	D6	433	0	461	121	0
33	B7	418	0	467	38	0
33	D7	418	0	467	37	0
34	B8	507	0	576	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D8	507	0	576	128	0
35	B9	307	0	337	33	0
35	D9	307	0	335	31	0
36	BA	62477	0	31497	2071	0
36	DA	62477	0	31497	2074	0
37	BB	2551	0	1295	93	0
37	DB	2551	0	1295	101	0
38	BC	1742	0	1800	162	2
38	DC	1742	0	1800	153	2
39	BD	2145	0	2234	254	0
39	DD	2145	0	2234	240	0
40	BE	1563	0	1629	237	0
40	DE	1563	0	1629	235	0
41	BF	1623	0	1677	214	0
41	DF	1623	0	1677	216	0
42	BG	1474	0	1535	236	0
42	DG	1474	0	1535	269	0
43	BH	1222	0	1282	159	0
43	DH	1222	0	1282	155	0
44	BJ	651	0	156	23	0
44	DJ	651	0	166	16	0
45	BK	700	0	167	9	0
45	DK	700	0	167	9	0
46	BN	1104	0	1180	160	0
46	DN	1104	0	1180	157	0
47	BO	933	0	996	86	0
47	DO	933	0	996	88	0
48	BP	1114	0	1187	267	0
48	DP	1114	0	1187	264	0
49	BQ	1122	0	1179	119	0
49	DQ	1122	0	1179	128	0
50	BR	960	0	1021	151	0
50	DR	960	0	1021	150	0
51	BS	770	0	832	135	0
51	DS	770	0	832	138	0
52	BT	1141	0	1202	207	0
52	DT	1141	0	1202	207	0
53	BU	958	0	1015	129	0
53	DU	958	0	1015	132	0
54	BV	779	0	852	139	0
54	DV	779	0	852	141	0
55	BW	896	0	953	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	DW	896	0	953	84	0
56	BX	725	0	778	100	0
56	DX	725	0	778	92	0
57	BY	775	0	870	177	0
57	DY	775	0	870	169	0
58	BZ	1403	0	1432	211	0
58	DZ	1403	0	1432	189	0
59	AD	1	0	0	3	0
59	AN	1	0	0	2	0
59	B4	1	0	0	1	0
59	B9	1	0	0	1	0
59	CD	1	0	0	2	0
59	CN	1	0	0	2	0
59	D4	1	0	0	0	0
59	D9	1	0	0	0	0
60	AZ	28	0	12	15	0
60	CZ	28	0	12	8	0
61	AZ	57	0	58	13	0
61	CZ	57	0	58	9	0
All	All	307330	0	208699	17314	4

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 34.

The worst 5 of 17314 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AZ:355:LEU:CD2	25:AZ:370:PHE:HB3	1.63	1.28
25:CZ:355:LEU:CD2	25:CZ:370:PHE:HB3	1.63	1.24
39:DD:35:LYS:HG3	39:DD:104:TYR:CE2	1.73	1.23
25:AZ:2:LYS:O	25:AZ:275:LYS:HE3	1.42	1.20
25:CZ:355:LEU:HD23	25:CZ:370:PHE:CB	1.73	1.19

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:65:GLY:O	38:DC:27:ARG:NH2[2_445]	1.97	0.23
2:AB:65:GLY:O	38:BC:27:ARG:NH2[2_646]	2.02	0.18
2:CB:66:GLY:CA	38:DC:27:ARG:NH2[2_445]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:66:GLY:CA	38:BC:27:ARG:NH2[2_646]	2.18	0.02

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%)	161 (69%)	48 (21%)	23 (10%)	0	3
2	CB	232/256 (91%)	164 (71%)	45 (19%)	23 (10%)	0	3
3	AC	204/239 (85%)	169 (83%)	22 (11%)	13 (6%)	1	8
3	CC	204/239 (85%)	171 (84%)	21 (10%)	12 (6%)	1	10
4	AD	206/209 (99%)	149 (72%)	39 (19%)	18 (9%)	1	4
4	CD	206/209 (99%)	149 (72%)	38 (18%)	19 (9%)	1	4
5	AE	148/162 (91%)	136 (92%)	10 (7%)	2 (1%)	11	40
5	CE	148/162 (91%)	136 (92%)	9 (6%)	3 (2%)	7	31
6	AF	99/101 (98%)	72 (73%)	18 (18%)	9 (9%)	1	4
6	CF	99/101 (98%)	73 (74%)	17 (17%)	9 (9%)	1	4
7	AG	153/156 (98%)	127 (83%)	22 (14%)	4 (3%)	5	26
7	CG	153/156 (98%)	129 (84%)	21 (14%)	3 (2%)	7	31
8	AH	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	10	39
8	CH	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	10	39
9	AI	125/128 (98%)	83 (66%)	34 (27%)	8 (6%)	1	8
9	CI	125/128 (98%)	83 (66%)	35 (28%)	7 (6%)	2	11
10	AJ	96/105 (91%)	69 (72%)	21 (22%)	6 (6%)	1	8
10	CJ	96/105 (91%)	71 (74%)	19 (20%)	6 (6%)	1	8
11	AK	117/129 (91%)	98 (84%)	18 (15%)	1 (1%)	17	52
11	CK	117/129 (91%)	99 (85%)	17 (14%)	1 (1%)	17	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AL	122/131 (93%)	104 (85%)	10 (8%)	8 (7%)	1	7
12	CL	122/131 (93%)	104 (85%)	10 (8%)	8 (7%)	1	7
13	AM	122/126 (97%)	85 (70%)	27 (22%)	10 (8%)	1	5
13	CM	122/126 (97%)	85 (70%)	28 (23%)	9 (7%)	1	6
14	AN	58/61 (95%)	42 (72%)	9 (16%)	7 (12%)	0	1
14	CN	58/61 (95%)	43 (74%)	7 (12%)	8 (14%)	0	1
15	AO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	6	28
15	CO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	6	28
16	AP	81/88 (92%)	58 (72%)	17 (21%)	6 (7%)	1	6
16	CP	81/88 (92%)	59 (73%)	16 (20%)	6 (7%)	1	6
17	AQ	97/105 (92%)	85 (88%)	7 (7%)	5 (5%)	2	12
17	CQ	97/105 (92%)	85 (88%)	7 (7%)	5 (5%)	2	12
18	AR	68/88 (77%)	55 (81%)	11 (16%)	2 (3%)	4	24
18	CR	68/88 (77%)	56 (82%)	10 (15%)	2 (3%)	4	24
19	AS	76/93 (82%)	48 (63%)	15 (20%)	13 (17%)	0	0
19	CS	76/93 (82%)	47 (62%)	16 (21%)	13 (17%)	0	0
20	AT	97/106 (92%)	67 (69%)	22 (23%)	8 (8%)	1	5
20	CT	97/106 (92%)	67 (69%)	21 (22%)	9 (9%)	0	3
21	AU	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	2	15
21	CU	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	2	15
25	AZ	381/405 (94%)	263 (69%)	80 (21%)	38 (10%)	0	3
25	CZ	381/405 (94%)	266 (70%)	77 (20%)	38 (10%)	0	3
26	B0	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	2	14
26	D0	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	2	14
27	B1	91/98 (93%)	68 (75%)	13 (14%)	10 (11%)	0	2
27	D1	91/98 (93%)	63 (69%)	10 (11%)	18 (20%)	0	0
28	B2	69/72 (96%)	46 (67%)	17 (25%)	6 (9%)	1	4
28	D2	69/72 (96%)	37 (54%)	16 (23%)	16 (23%)	0	0
29	B3	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	1	4
29	D3	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	1	4
30	B4	42/71 (59%)	24 (57%)	11 (26%)	7 (17%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	D4	42/71 (59%)	24 (57%)	11 (26%)	7 (17%)	0	0
31	B5	57/60 (95%)	41 (72%)	7 (12%)	9 (16%)	0	0
31	D5	57/60 (95%)	40 (70%)	8 (14%)	9 (16%)	0	0
32	B6	48/54 (89%)	23 (48%)	8 (17%)	17 (35%)	0	0
32	D6	48/54 (89%)	23 (48%)	8 (17%)	17 (35%)	0	0
33	B7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
33	D7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
34	B8	61/65 (94%)	43 (70%)	12 (20%)	6 (10%)	0	3
34	D8	61/65 (94%)	45 (74%)	10 (16%)	6 (10%)	0	3
35	B9	35/37 (95%)	25 (71%)	7 (20%)	3 (9%)	1	4
35	D9	35/37 (95%)	25 (71%)	7 (20%)	3 (9%)	1	4
38	BC	226/229 (99%)	170 (75%)	40 (18%)	16 (7%)	1	6
38	DC	226/229 (99%)	170 (75%)	40 (18%)	16 (7%)	1	6
39	BD	273/276 (99%)	214 (78%)	33 (12%)	26 (10%)	0	3
39	DD	273/276 (99%)	214 (78%)	34 (12%)	25 (9%)	1	4
40	BE	202/206 (98%)	125 (62%)	46 (23%)	31 (15%)	0	0
40	DE	202/206 (98%)	125 (62%)	47 (23%)	30 (15%)	0	0
41	BF	205/210 (98%)	153 (75%)	23 (11%)	29 (14%)	0	1
41	DF	205/210 (98%)	153 (75%)	23 (11%)	29 (14%)	0	1
42	BG	179/182 (98%)	103 (58%)	45 (25%)	31 (17%)	0	0
42	DG	179/182 (98%)	111 (62%)	40 (22%)	28 (16%)	0	0
43	BH	157/180 (87%)	105 (67%)	28 (18%)	24 (15%)	0	0
43	DH	157/180 (87%)	105 (67%)	29 (18%)	23 (15%)	0	1
46	BN	136/140 (97%)	85 (62%)	32 (24%)	19 (14%)	0	1
46	DN	136/140 (97%)	86 (63%)	32 (24%)	18 (13%)	0	1
47	BO	120/122 (98%)	100 (83%)	15 (12%)	5 (4%)	3	16
47	DO	120/122 (98%)	100 (83%)	15 (12%)	5 (4%)	3	16
48	BP	144/150 (96%)	72 (50%)	31 (22%)	41 (28%)	0	0
48	DP	144/150 (96%)	71 (49%)	33 (23%)	40 (28%)	0	0
49	BQ	139/141 (99%)	108 (78%)	25 (18%)	6 (4%)	2	16
49	DQ	139/141 (99%)	108 (78%)	25 (18%)	6 (4%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	BR	115/118 (98%)	81 (70%)	15 (13%)	19 (16%)	0	0
50	DR	115/118 (98%)	82 (71%)	14 (12%)	19 (16%)	0	0
51	BS	96/112 (86%)	44 (46%)	31 (32%)	21 (22%)	0	0
51	DS	96/112 (86%)	44 (46%)	32 (33%)	20 (21%)	0	0
52	BT	135/146 (92%)	85 (63%)	24 (18%)	26 (19%)	0	0
52	DT	135/146 (92%)	85 (63%)	24 (18%)	26 (19%)	0	0
53	BU	115/118 (98%)	82 (71%)	28 (24%)	5 (4%)	2	16
53	DU	115/118 (98%)	82 (71%)	28 (24%)	5 (4%)	2	16
54	BV	99/101 (98%)	67 (68%)	19 (19%)	13 (13%)	0	1
54	DV	99/101 (98%)	67 (68%)	19 (19%)	13 (13%)	0	1
55	BW	111/113 (98%)	82 (74%)	23 (21%)	6 (5%)	2	12
55	DW	111/113 (98%)	84 (76%)	21 (19%)	6 (5%)	2	12
56	BX	90/96 (94%)	63 (70%)	16 (18%)	11 (12%)	0	1
56	DX	90/96 (94%)	64 (71%)	15 (17%)	11 (12%)	0	1
57	BY	98/110 (89%)	32 (33%)	36 (37%)	30 (31%)	0	0
57	DY	98/110 (89%)	32 (33%)	37 (38%)	29 (30%)	0	0
58	BZ	174/206 (84%)	111 (64%)	36 (21%)	27 (16%)	0	0
58	DZ	174/206 (84%)	119 (68%)	31 (18%)	24 (14%)	0	1
All	All	12256/13098 (94%)	8805 (72%)	2168 (18%)	1283 (10%)	0	3

5 of 1283 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	18	GLY
2	AB	130	ARG
2	AB	234	PRO
3	AC	12	LEU

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%)	181 (90%)	21 (10%)	7	27
2	CB	202/220 (92%)	180 (89%)	22 (11%)	6	25
3	AC	160/188 (85%)	141 (88%)	19 (12%)	5	20
3	CC	160/188 (85%)	142 (89%)	18 (11%)	6	23
4	AD	180/181 (99%)	162 (90%)	18 (10%)	7	28
4	CD	180/181 (99%)	162 (90%)	18 (10%)	7	28
5	AE	115/123 (94%)	102 (89%)	13 (11%)	6	23
5	CE	115/123 (94%)	102 (89%)	13 (11%)	6	23
6	AF	90/90 (100%)	80 (89%)	10 (11%)	6	24
6	CF	90/90 (100%)	80 (89%)	10 (11%)	6	24
7	AG	126/127 (99%)	118 (94%)	8 (6%)	18	48
7	CG	126/127 (99%)	118 (94%)	8 (6%)	18	48
8	AH	119/119 (100%)	107 (90%)	12 (10%)	7	28
8	CH	119/119 (100%)	107 (90%)	12 (10%)	7	28
9	AI	98/99 (99%)	90 (92%)	8 (8%)	11	38
9	CI	98/99 (99%)	89 (91%)	9 (9%)	9	33
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	4	18
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	4	18
11	AK	90/99 (91%)	80 (89%)	10 (11%)	6	24
11	CK	90/99 (91%)	80 (89%)	10 (11%)	6	24
12	AL	104/108 (96%)	92 (88%)	12 (12%)	5	22
12	CL	104/108 (96%)	92 (88%)	12 (12%)	5	22
13	AM	99/101 (98%)	88 (89%)	11 (11%)	6	24
13	CM	99/101 (98%)	88 (89%)	11 (11%)	6	24
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3	14
14	CN	49/50 (98%)	42 (86%)	7 (14%)	3	14
15	AO	79/80 (99%)	70 (89%)	9 (11%)	5	23
15	CO	79/80 (99%)	70 (89%)	9 (11%)	5	23
16	AP	72/74 (97%)	64 (89%)	8 (11%)	6	24
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	30
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	17	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	17	48
18	AR	61/77 (79%)	51 (84%)	10 (16%)	2	10
18	CR	61/77 (79%)	51 (84%)	10 (16%)	2	10
19	AS	69/80 (86%)	56 (81%)	13 (19%)	1	6
19	CS	69/80 (86%)	56 (81%)	13 (19%)	1	6
20	AT	76/82 (93%)	68 (90%)	8 (10%)	7	26
20	CT	76/82 (93%)	68 (90%)	8 (10%)	7	26
21	AU	19/22 (86%)	18 (95%)	1 (5%)	22	54
21	CU	19/22 (86%)	18 (95%)	1 (5%)	22	54
25	AZ	322/338 (95%)	279 (87%)	43 (13%)	4	16
25	CZ	322/338 (95%)	281 (87%)	41 (13%)	4	18
26	B0	66/67 (98%)	59 (89%)	7 (11%)	6	26
26	D0	66/67 (98%)	59 (89%)	7 (11%)	6	26
27	B1	78/83 (94%)	67 (86%)	11 (14%)	3	15
27	D1	78/83 (94%)	68 (87%)	10 (13%)	4	18
28	B2	66/67 (98%)	64 (97%)	2 (3%)	41	71
28	D2	66/67 (98%)	57 (86%)	9 (14%)	3	16
29	B3	51/52 (98%)	45 (88%)	6 (12%)	5	21
29	D3	51/52 (98%)	45 (88%)	6 (12%)	5	21
30	B4	39/63 (62%)	32 (82%)	7 (18%)	2	8
30	D4	39/63 (62%)	33 (85%)	6 (15%)	2	11
31	B5	51/52 (98%)	45 (88%)	6 (12%)	5	21
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%)	31 (63%)	18 (37%)	0	0
33	B7	41/42 (98%)	38 (93%)	3 (7%)	14	43
33	D7	41/42 (98%)	38 (93%)	3 (7%)	14	43
34	B8	53/55 (96%)	44 (83%)	9 (17%)	2	9
34	D8	53/55 (96%)	44 (83%)	9 (17%)	2	9
35	B9	34/34 (100%)	31 (91%)	3 (9%)	10	36
35	D9	34/34 (100%)	31 (91%)	3 (9%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BC	180/181 (99%)	172 (96%)	8 (4%)	28	61
38	DC	180/181 (99%)	172 (96%)	8 (4%)	28	61
39	BD	217/218 (100%)	186 (86%)	31 (14%)	3	14
39	DD	217/218 (100%)	187 (86%)	30 (14%)	3	16
40	BE	165/166 (99%)	145 (88%)	20 (12%)	5	20
40	DE	165/166 (99%)	143 (87%)	22 (13%)	4	16
41	BF	165/166 (99%)	152 (92%)	13 (8%)	12	40
41	DF	165/166 (99%)	152 (92%)	13 (8%)	12	40
42	BG	155/156 (99%)	135 (87%)	20 (13%)	4	18
42	DG	155/156 (99%)	124 (80%)	31 (20%)	1	5
43	BH	132/148 (89%)	118 (89%)	14 (11%)	6	26
43	DH	132/148 (89%)	118 (89%)	14 (11%)	6	26
46	BN	117/119 (98%)	101 (86%)	16 (14%)	3	16
46	DN	117/119 (98%)	101 (86%)	16 (14%)	3	16
47	BO	100/100 (100%)	93 (93%)	7 (7%)	15	45
47	DO	100/100 (100%)	93 (93%)	7 (7%)	15	45
48	BP	112/116 (97%)	93 (83%)	19 (17%)	2	9
48	DP	112/116 (97%)	93 (83%)	19 (17%)	2	9
49	BQ	111/111 (100%)	101 (91%)	10 (9%)	9	34
49	DQ	111/111 (100%)	101 (91%)	10 (9%)	9	34
50	BR	100/101 (99%)	87 (87%)	13 (13%)	4	18
50	DR	100/101 (99%)	85 (85%)	15 (15%)	3	12
51	BS	77/88 (88%)	65 (84%)	12 (16%)	2	11
51	DS	77/88 (88%)	65 (84%)	12 (16%)	2	11
52	BT	120/127 (94%)	97 (81%)	23 (19%)	1	6
52	DT	120/127 (94%)	97 (81%)	23 (19%)	1	6
53	BU	92/94 (98%)	86 (94%)	6 (6%)	17	47
53	DU	92/94 (98%)	86 (94%)	6 (6%)	17	47
54	BV	82/82 (100%)	67 (82%)	15 (18%)	1	7
54	DV	82/82 (100%)	67 (82%)	15 (18%)	1	7
55	BW	91/92 (99%)	87 (96%)	4 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	DW	91/92 (99%)	86 (94%)	5 (6%)	21	53
56	BX	74/78 (95%)	67 (90%)	7 (10%)	8	31
56	DX	74/78 (95%)	68 (92%)	6 (8%)	11	39
57	BY	84/91 (92%)	71 (84%)	13 (16%)	2	11
57	DY	84/91 (92%)	72 (86%)	12 (14%)	3	14
58	BZ	155/179 (87%)	130 (84%)	25 (16%)	2	10
58	DZ	155/179 (87%)	131 (84%)	24 (16%)	2	11
All	All	10338/10854 (95%)	9112 (88%)	1226 (12%)	5	20

5 of 1226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	D8	30	ARG
52	DT	50	ILE
39	DD	44	ASN
33	D7	34	ARG
42	DG	153	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 325 such sidechains are listed below:

Mol	Chain	Res	Type
25	CZ	98	GLN
43	DH	74	ASN
25	CZ	367	ASN
39	DD	116	GLN
49	DQ	141	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1509/1522 (99%)	227 (15%)	43 (2%)
1	CA	1509/1522 (99%)	222 (14%)	46 (3%)
22	AV	75/76 (98%)	22 (29%)	1 (1%)
22	AW	75/76 (98%)	21 (28%)	2 (2%)
22	CV	75/76 (98%)	23 (30%)	1 (1%)
22	CW	75/76 (98%)	21 (28%)	3 (4%)
23	AX	16/27 (59%)	6 (37%)	1 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	CX	16/27 (59%)	5 (31%)	1 (6%)
24	AY	74/77 (96%)	25 (33%)	3 (4%)
24	CY	74/77 (96%)	25 (33%)	3 (4%)
36	BA	2900/2915 (99%)	494 (17%)	45 (1%)
36	DA	2900/2915 (99%)	492 (16%)	45 (1%)
37	BB	118/122 (96%)	22 (18%)	3 (2%)
37	DB	118/122 (96%)	22 (18%)	3 (2%)
All	All	9534/9630 (99%)	1627 (17%)	200 (2%)

5 of 1627 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 200 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	495	A
1	CA	1529	G
37	DB	66	A
1	CA	560	U
1	CA	1049	U

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	AY	20	24	18,21,22	0.73	0	21,30,33	1.91	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	5MU	CY	54	24	19,22,23	0.42	0	28,32,35	0.44	0
24	MIA	AY	37	24	24,31,32	0.97	2 (8%)	26,44,47	1.69	4 (15%)
24	7MG	AY	46	24	22,26,27	3.08	2 (9%)	29,39,42	1.60	2 (6%)
24	H2U	CY	17	24	18,21,22	0.97	0	21,30,33	1.90	5 (23%)
24	7MG	CY	46	24	22,26,27	3.12	2 (9%)	29,39,42	1.59	2 (6%)
24	OMC	AY	32	24	19,22,23	0.39	0	26,31,34	0.66	1 (3%)
24	OMC	CY	32	24	19,22,23	0.32	0	26,31,34	0.66	1 (3%)
24	4SU	CY	8	24	18,21,22	0.51	0	26,30,33	0.86	2 (7%)
24	H2U	CY	16	24	18,21,22	0.98	1 (5%)	21,30,33	1.79	4 (19%)
24	4SU	AY	8	24	18,21,22	0.55	0	26,30,33	0.82	2 (7%)
24	H2U	CY	20	24	18,21,22	0.73	0	21,30,33	1.92	5 (23%)
24	5MU	AY	54	24	19,22,23	0.38	0	28,32,35	0.43	0
24	PSU	CY	55	24	18,21,22	0.86	1 (5%)	22,30,33	1.80	5 (22%)
24	H2U	AY	17	24	18,21,22	0.98	0	21,30,33	1.90	5 (23%)
24	MIA	CY	37	24	24,31,32	1.08	3 (12%)	26,44,47	1.70	4 (15%)
24	H2U	AY	16	24	18,21,22	0.99	1 (5%)	21,30,33	1.82	4 (19%)
24	PSU	AY	55	24	18,21,22	0.89	2 (11%)	22,30,33	1.76	5 (22%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	H2U	AY	17	24	-	3/7/38/39	0/2/2/2
24	MIA	CY	37	24	-	2/11/33/34	0/3/3/3
24	H2U	AY	16	24	-	0/7/38/39	0/2/2/2
24	PSU	AY	55	24	-	2/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	46	7MG	C8-N9	-14.07	1.38	1.46
24	AY	46	7MG	C8-N9	-13.95	1.38	1.46
24	CY	46	7MG	C5-N7	3.40	1.39	1.35
24	AY	46	7MG	C5-N7	3.37	1.39	1.35
24	CY	37	MIA	C2-S10	2.71	1.78	1.75

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AY	46	7MG	N9-C8-N7	6.83	113.14	103.38
24	CY	46	7MG	N9-C8-N7	6.79	113.09	103.38
24	CY	37	MIA	C11-S10-C2	5.43	106.32	102.27
24	AY	20	H2U	C4-N3-C2	-5.23	121.45	125.79
24	CY	20	H2U	C4-N3-C2	-5.22	121.46	125.79

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	17	H2U	C4'-C5'-O5'-P
24	AY	37	MIA	C5-C6-N6-C12
24	CY	17	H2U	C4'-C5'-O5'-P
24	CY	37	MIA	C5-C6-N6-C12
24	AY	17	H2U	O4'-C4'-C5'-O5'

There are no ring outliers.

14 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	20	H2U	1	0
24	CY	54	5MU	1	0
24	AY	46	7MG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CY	17	H2U	4	0
24	CY	46	7MG	3	0
24	CY	8	4SU	1	0
24	CY	16	H2U	4	0
24	AY	8	4SU	1	0
24	CY	20	H2U	1	0
24	AY	54	5MU	1	0
24	CY	55	PSU	1	0
24	AY	17	H2U	3	0
24	AY	16	H2U	3	0
24	AY	55	PSU	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	CZ	501	-	24,30,30	1.57	3 (12%)	30,47,47	1.47	3 (10%)
61	KIR	CZ	502	-	56,59,59	3.39	22 (39%)	62,84,84	1.66	13 (20%)
61	KIR	AZ	502	-	56,59,59	3.42	22 (39%)	62,84,84	1.63	13 (20%)
60	GDP	AZ	501	-	24,30,30	1.65	5 (20%)	30,47,47	1.52	5 (16%)

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	CZ	501	-	-	0/12/32/32	0/3/3/3
61	KIR	CZ	502	-	-	8/54/98/98	0/3/3/3
61	KIR	AZ	502	-	-	8/54/98/98	0/3/3/3
60	GDP	AZ	501	-	-	2/12/32/32	0/3/3/3

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CZ	502	KIR	O18-C17	-14.49	1.22	1.44
61	AZ	502	KIR	O18-C17	-14.21	1.23	1.44
61	AZ	502	KIR	O30-C30	-12.64	1.17	1.42
61	CZ	502	KIR	O30-C30	-12.30	1.18	1.42
60	CZ	501	GDP	C5-C6	-5.70	1.35	1.47

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	AZ	502	KIR	O29-C29-O34	-5.09	101.68	110.21
61	CZ	502	KIR	O29-C29-O34	-5.02	101.79	110.21
61	CZ	502	KIR	C48-C32-C47	-4.41	101.43	107.72
60	CZ	501	GDP	PA-O3A-PB	-4.30	118.08	132.83
60	AZ	501	GDP	C2-N1-C6	-4.23	117.32	125.10

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	AZ	501	GDP	PA-O3A-PB-O2B
61	AZ	502	KIR	O18-C17-C19-C42
61	CZ	502	KIR	O18-C17-C19-C42
61	AZ	502	KIR	C11-C10-C9-C8
61	CZ	502	KIR	C11-C10-C9-C8

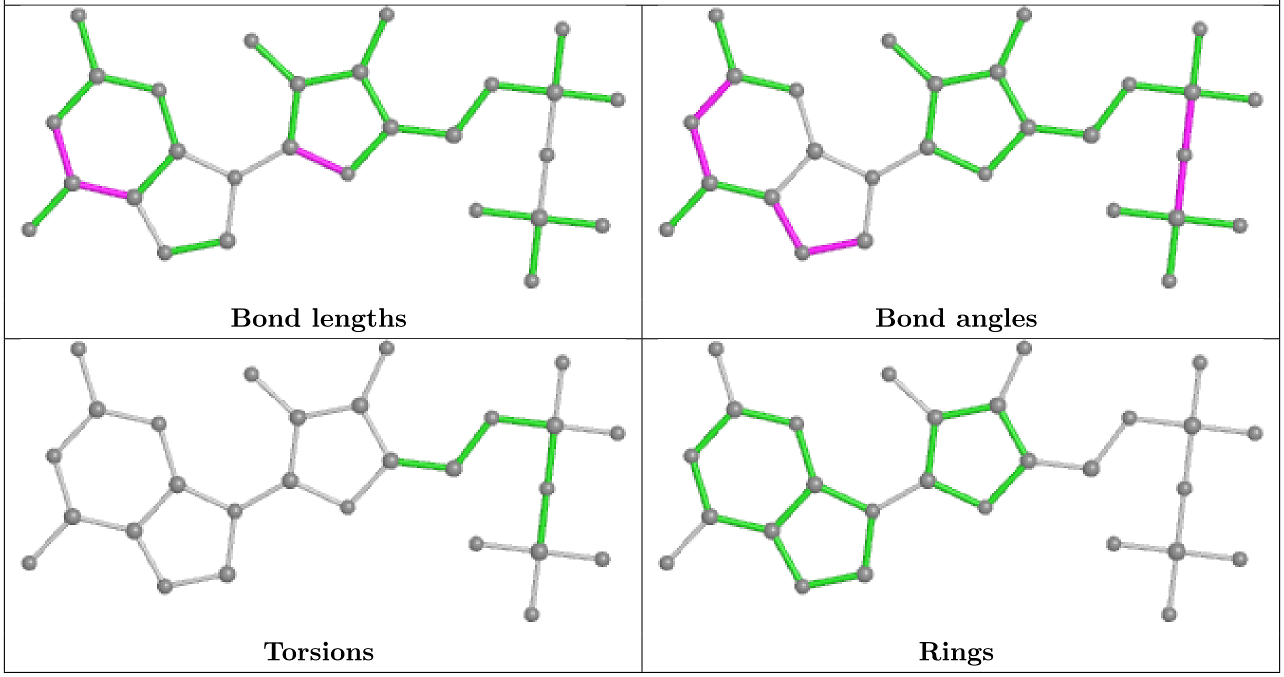
There are no ring outliers.

4 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	CZ	501	GDP	8	0
61	CZ	502	KIR	9	0
61	AZ	502	KIR	13	0
60	AZ	501	GDP	15	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 CZ 501



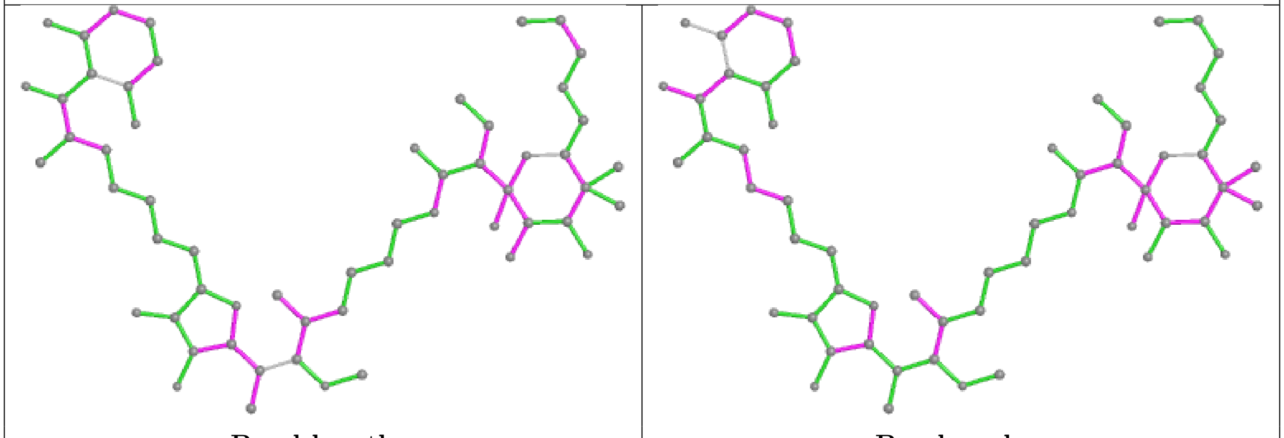
Bond lengths

Bond angles

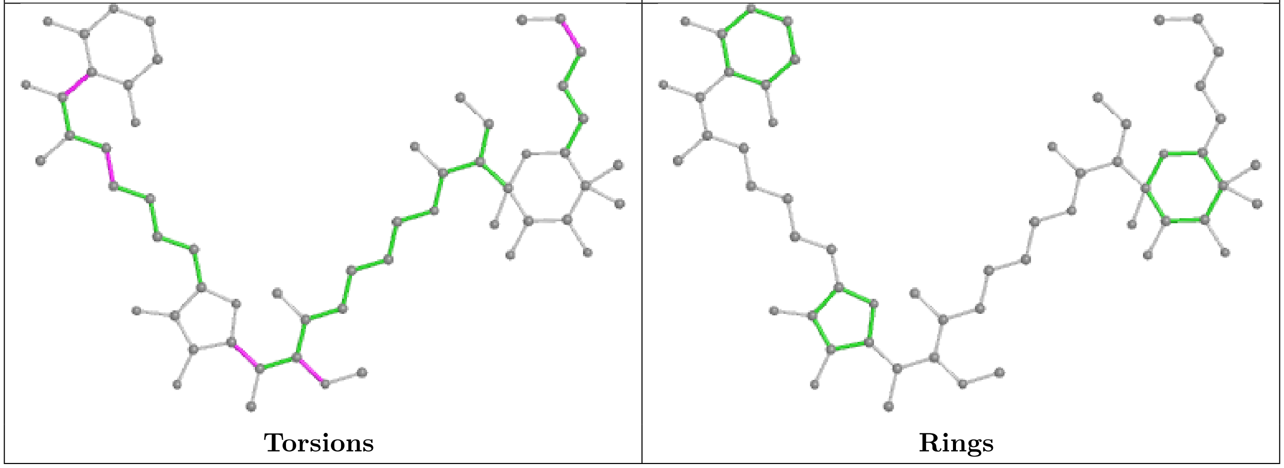
Torsions

Rings

Ligand KIR CZ 502

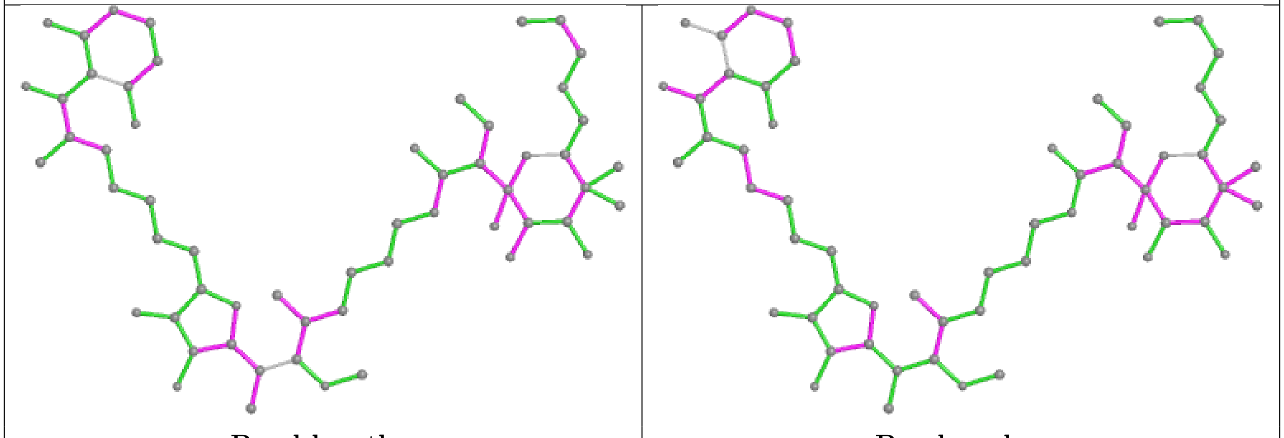


Bond lengths **Bond angles**



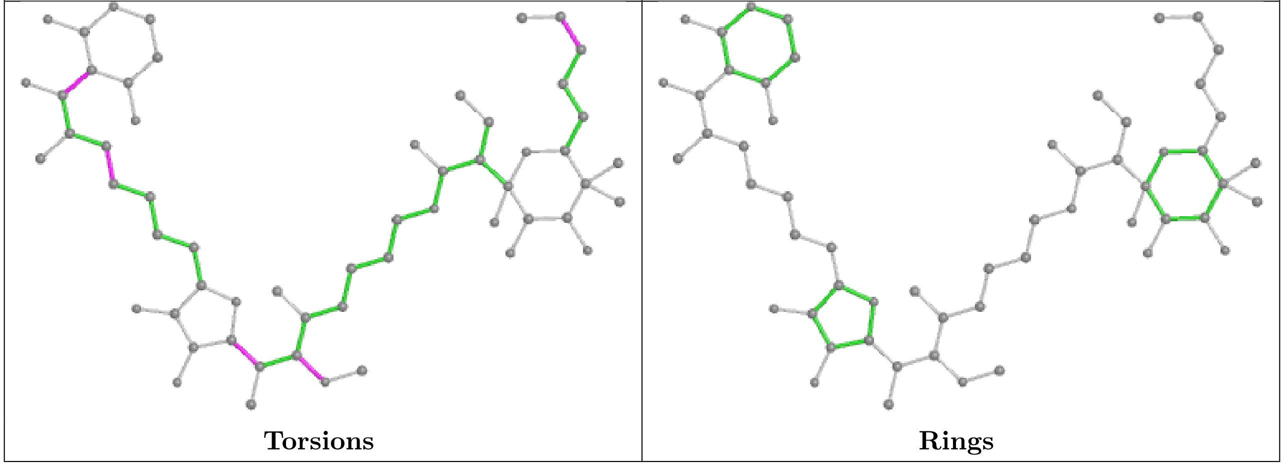
Torsions **Rings**

Ligand KIR AZ 502



Bond lengths

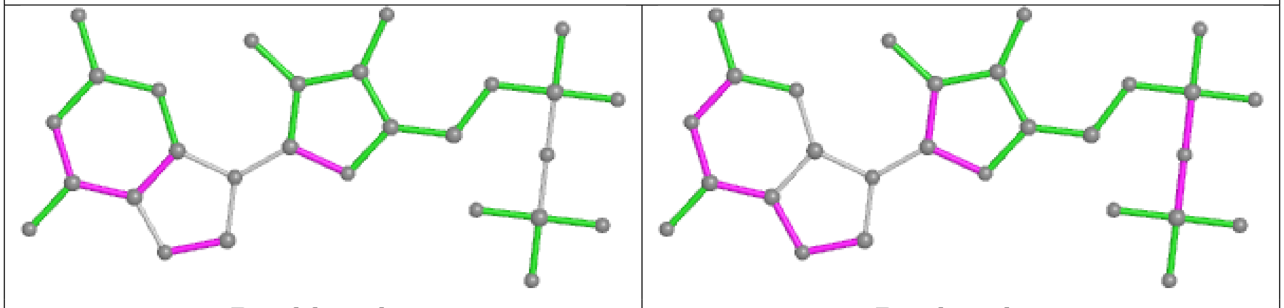
Bond angles



Torsions

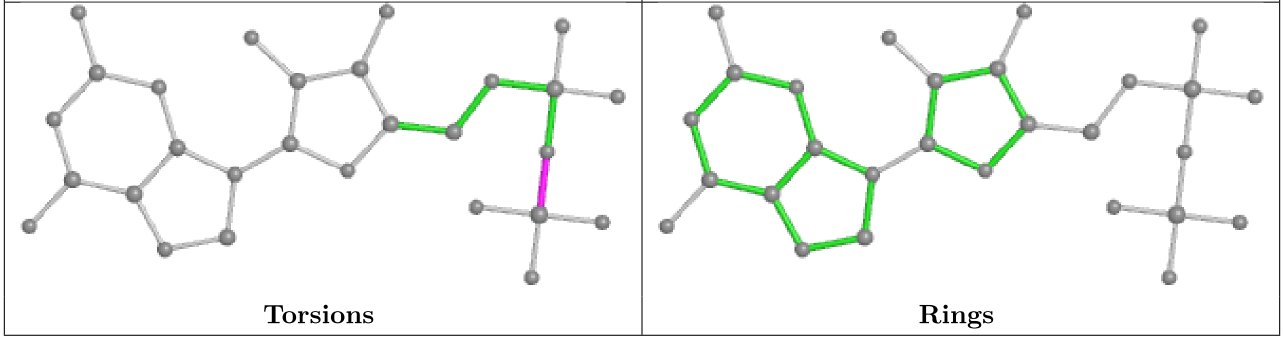
Rings

Ligand GDP AZ 501



Bond lengths

Bond angles



Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95^{th} 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	1510/1522 (99%)	-0.29	19 (1%) 77 59	44, 78, 160, 200	0
1	CA	1510/1522 (99%)	-0.07	31 (2%) 63 43	37, 73, 161, 200	0
2	AB	234/256 (91%)	-0.10	6 (2%) 56 33	58, 88, 152, 164	0
2	CB	234/256 (91%)	-0.19	3 (1%) 77 59	54, 86, 151, 164	0
3	AC	206/239 (86%)	-0.30	1 (0%) 91 81	52, 75, 101, 110	0
3	CC	206/239 (86%)	-0.30	0 100 100	46, 70, 100, 109	0
4	AD	208/209 (99%)	0.11	10 (4%) 30 14	71, 97, 124, 132	0
4	CD	208/209 (99%)	0.05	4 (1%) 66 46	67, 96, 123, 131	0
5	AE	150/162 (92%)	-0.35	0 100 100	53, 65, 89, 110	0
5	CE	150/162 (92%)	-0.35	0 100 100	49, 63, 88, 109	0
6	AF	101/101 (100%)	0.04	1 (0%) 82 67	71, 99, 115, 122	0
6	CF	101/101 (100%)	-0.15	1 (0%) 82 67	68, 97, 114, 121	0
7	AG	155/156 (99%)	0.18	7 (4%) 33 16	66, 89, 113, 130	0
7	CG	155/156 (99%)	-0.11	2 (1%) 77 59	59, 86, 112, 129	0
8	AH	138/138 (100%)	-0.28	1 (0%) 87 75	54, 70, 87, 95	0
8	CH	138/138 (100%)	-0.30	0 100 100	52, 67, 87, 94	0
9	AI	127/128 (99%)	0.64	15 (11%) 4 2	62, 96, 128, 139	0
9	CI	127/128 (99%)	0.23	2 (1%) 72 51	54, 93, 127, 139	0
10	AJ	98/105 (93%)	0.81	20 (20%) 1 0	59, 99, 141, 145	0
10	CJ	98/105 (93%)	0.35	5 (5%) 28 13	54, 95, 140, 144	0
11	AK	119/129 (92%)	0.04	6 (5%) 28 13	55, 73, 107, 134	0
11	CK	119/129 (92%)	-0.04	4 (3%) 45 24	51, 68, 108, 133	0
12	AL	124/131 (94%)	0.02	5 (4%) 38 19	55, 70, 94, 132	0
12	CL	124/131 (94%)	-0.12	1 (0%) 86 72	51, 68, 93, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	124/126 (98%)	0.34	13 (10%) 6 2	71, 97, 124, 152	0
13	CM	124/126 (98%)	0.13	7 (5%) 24 11	67, 95, 123, 152	0
14	AN	60/61 (98%)	-0.17	1 (1%) 70 49	57, 72, 93, 96	0
14	CN	60/61 (98%)	-0.02	1 (1%) 70 49	49, 66, 91, 96	0
15	AO	88/89 (98%)	-0.08	0 100 100	57, 75, 99, 105	0
15	CO	88/89 (98%)	-0.05	0 100 100	56, 74, 98, 104	0
16	AP	83/88 (94%)	0.40	3 (3%) 42 22	74, 91, 109, 135	0
16	CP	83/88 (94%)	0.38	2 (2%) 59 37	72, 89, 108, 136	0
17	AQ	99/105 (94%)	-0.00	3 (3%) 50 27	60, 79, 95, 108	0
17	CQ	99/105 (94%)	-0.06	0 100 100	57, 78, 93, 107	0
18	AR	70/88 (79%)	-0.05	2 (2%) 51 28	58, 82, 106, 119	0
18	CR	70/88 (79%)	-0.30	1 (1%) 75 56	56, 79, 105, 118	0
19	AS	78/93 (83%)	0.43	5 (6%) 19 8	75, 99, 137, 139	0
19	CS	78/93 (83%)	0.45	4 (5%) 28 13	71, 99, 136, 139	0
20	AT	99/106 (93%)	0.44	6 (6%) 21 9	75, 97, 131, 135	0
20	CT	99/106 (93%)	0.43	5 (5%) 28 13	71, 96, 132, 135	0
21	AU	24/27 (88%)	0.77	3 (12%) 3 1	66, 84, 103, 114	0
21	CU	24/27 (88%)	0.37	1 (4%) 36 18	64, 78, 99, 115	0
22	AV	76/76 (100%)	-0.29	1 (1%) 77 59	56, 91, 128, 148	0
22	AW	76/76 (100%)	0.78	10 (13%) 3 1	103, 172, 200, 200	0
22	CV	76/76 (100%)	-0.22	1 (1%) 77 59	50, 89, 128, 147	0
22	CW	76/76 (100%)	0.70	11 (14%) 2 1	100, 172, 200, 200	0
23	AX	17/27 (62%)	0.58	2 (11%) 4 2	50, 97, 156, 157	0
23	CX	17/27 (62%)	0.53	1 (5%) 22 10	45, 95, 156, 157	0
24	AY	68/77 (88%)	0.04	1 (1%) 73 54	61, 140, 171, 190	0
24	CY	68/77 (88%)	-0.01	4 (5%) 22 10	57, 140, 170, 190	0
25	AZ	385/405 (95%)	1.76	136 (35%) 0 0	116, 142, 165, 183	0
25	CZ	385/405 (95%)	0.44	24 (6%) 20 9	113, 141, 165, 183	0
26	B0	84/85 (98%)	0.62	8 (9%) 8 2	77, 91, 118, 131	0
26	D0	84/85 (98%)	0.55	7 (8%) 11 4	76, 90, 119, 131	0
27	B1	93/98 (94%)	0.43	5 (5%) 25 12	74, 95, 134, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
27	D1	93/98 (94%)	0.24	2 (2%) 62 41	56, 76, 130, 142	0
28	B2	71/72 (98%)	0.45	5 (7%) 16 7	110, 133, 148, 157	0
28	D2	71/72 (98%)	1.39	21 (29%) 0 0	134, 154, 174, 175	0
29	B3	59/60 (98%)	0.66	3 (5%) 28 13	80, 99, 120, 142	0
29	D3	59/60 (98%)	0.54	3 (5%) 28 13	80, 97, 120, 142	0
30	B4	44/71 (61%)	0.21	5 (11%) 5 2	124, 149, 160, 163	0
30	D4	44/71 (61%)	0.38	3 (6%) 17 7	123, 147, 158, 163	0
31	B5	59/60 (98%)	0.31	5 (8%) 10 4	73, 105, 158, 176	0
31	D5	59/60 (98%)	0.14	4 (6%) 17 7	72, 104, 158, 176	0
32	B6	50/54 (92%)	0.81	7 (14%) 2 1	74, 106, 116, 125	0
32	D6	50/54 (92%)	0.85	8 (16%) 1 1	73, 104, 115, 123	0
33	B7	48/49 (97%)	0.43	0 100 100	70, 79, 119, 139	0
33	D7	48/49 (97%)	0.58	2 (4%) 36 18	68, 78, 119, 140	0
34	B8	63/65 (96%)	0.49	3 (4%) 30 14	80, 90, 104, 131	0
34	D8	63/65 (96%)	0.41	3 (4%) 30 14	78, 88, 104, 131	0
35	B9	37/37 (100%)	0.63	2 (5%) 25 12	76, 90, 104, 108	0
35	D9	37/37 (100%)	0.29	3 (8%) 12 5	76, 90, 104, 107	0
36	BA	2901/2915 (99%)	-0.10	73 (2%) 57 34	49, 95, 190, 200	0
36	DA	2901/2915 (99%)	-0.02	70 (2%) 59 37	46, 93, 190, 200	0
37	BB	119/122 (97%)	-0.46	0 100 100	78, 108, 134, 157	0
37	DB	119/122 (97%)	-0.37	0 100 100	75, 107, 133, 157	0
38	BC	228/229 (99%)	0.71	32 (14%) 2 1	69, 99, 177, 187	0
38	DC	228/229 (99%)	0.33	20 (8%) 10 4	67, 97, 177, 187	0
39	BD	275/276 (99%)	-0.15	3 (1%) 80 64	50, 68, 98, 123	0
39	DD	275/276 (99%)	-0.16	2 (0%) 87 75	47, 66, 97, 123	0
40	BE	204/206 (99%)	0.28	12 (5%) 22 10	64, 93, 141, 152	0
40	DE	204/206 (99%)	0.25	8 (3%) 39 20	64, 93, 141, 152	0
41	BF	207/210 (98%)	0.76	27 (13%) 3 1	73, 128, 176, 184	0
41	DF	207/210 (98%)	0.68	27 (13%) 3 1	70, 127, 176, 184	0
42	BG	181/182 (99%)	0.25	11 (6%) 21 9	97, 125, 147, 157	0
42	DG	181/182 (99%)	0.08	9 (4%) 28 13	75, 96, 125, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	BH	159/180 (88%)	0.79	24 (15%) 2 1	106, 142, 163, 165	0
43	DH	159/180 (88%)	1.16	36 (22%) 0 0	106, 142, 163, 165	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	138/140 (98%)	0.20	2 (1%) 75 56	78, 104, 145, 148	0
46	DN	138/140 (98%)	0.17	3 (2%) 62 41	77, 104, 144, 147	0
47	BO	122/122 (100%)	-0.16	1 (0%) 86 72	58, 76, 90, 97	0
47	DO	122/122 (100%)	-0.06	0 100 100	57, 76, 89, 97	0
48	BP	146/150 (97%)	0.95	20 (13%) 3 1	73, 121, 146, 162	0
48	DP	146/150 (97%)	0.96	27 (18%) 1 0	72, 120, 145, 162	0
49	BQ	141/141 (100%)	0.02	2 (1%) 75 56	61, 78, 107, 138	0
49	DQ	141/141 (100%)	0.05	4 (2%) 53 30	60, 77, 107, 139	0
50	BR	117/118 (99%)	0.32	4 (3%) 45 24	76, 98, 114, 129	0
50	DR	117/118 (99%)	0.31	3 (2%) 56 33	75, 98, 115, 129	0
51	BS	98/112 (87%)	0.87	18 (18%) 1 0	89, 112, 137, 141	0
51	DS	98/112 (87%)	0.46	5 (5%) 28 13	88, 111, 136, 140	0
52	BT	137/146 (93%)	0.13	9 (6%) 18 7	74, 97, 155, 179	0
52	DT	137/146 (93%)	0.23	12 (8%) 10 4	73, 97, 154, 179	0
53	BU	117/118 (99%)	0.14	3 (2%) 56 33	81, 98, 125, 142	0
53	DU	117/118 (99%)	0.13	2 (1%) 70 49	78, 97, 125, 142	0
54	BV	101/101 (100%)	0.56	7 (6%) 16 7	79, 130, 146, 150	0
54	DV	101/101 (100%)	0.50	7 (6%) 16 7	79, 129, 146, 150	0
55	BW	113/113 (100%)	0.47	8 (7%) 16 6	85, 100, 133, 165	0
55	DW	113/113 (100%)	0.39	9 (7%) 12 5	82, 100, 133, 165	0
56	BX	92/96 (95%)	0.49	3 (3%) 46 24	83, 109, 125, 134	0
56	DX	92/96 (95%)	0.40	7 (7%) 13 5	83, 108, 124, 134	0
57	BY	100/110 (90%)	1.80	38 (38%) 0 0	127, 146, 179, 187	0
57	DY	100/110 (90%)	1.76	40 (40%) 0 0	126, 146, 179, 187	0
58	BZ	176/206 (85%)	0.09	5 (2%) 53 30	75, 103, 135, 144	0
58	DZ	176/206 (85%)	0.05	8 (4%) 33 16	64, 94, 140, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	21994/23368 (94%)	0.13	1092 (4%)	28	13	37, 93, 162, 200	0

The worst 5 of 1092 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	DQ	141	GLN	14.3
49	BQ	141	GLN	12.8
38	BC	1	PRO	11.6
43	DH	170	ARG	11.5
53	DU	118	GLY	11.2

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	0.56	0.69	181,191,191,193	0
24	H2U	AY	16	20/21	0.58	0.66	181,191,192,193	0
24	7MG	AY	46	24/25	0.65	0.39	166,169,171,171	0
24	H2U	AY	20	20/21	0.74	0.35	186,186,188,188	0
24	4SU	AY	8	20/21	0.76	0.30	140,143,144,144	0
24	H2U	CY	20	20/21	0.79	0.38	185,186,187,187	0
24	PSU	CY	55	20/21	0.79	0.18	158,166,168,168	0
24	H2U	CY	17	20/21	0.80	0.58	194,195,195,195	0
24	PSU	AY	55	20/21	0.80	0.19	157,166,168,168	0
24	H2U	AY	17	20/21	0.80	0.54	194,195,195,195	0
24	7MG	CY	46	24/25	0.84	0.23	166,168,170,170	0
24	4SU	CY	8	20/21	0.85	0.24	140,141,142,142	0
24	5MU	CY	54	21/22	0.89	0.15	142,153,154,156	0
24	OMC	CY	32	21/22	0.90	0.17	96,103,108,109	0
24	5MU	AY	54	21/22	0.92	0.20	143,153,153,156	0
24	OMC	AY	32	21/22	0.92	0.29	98,106,112,113	0
24	MIA	CY	37	29/30	0.93	0.28	60,80,107,108	0
24	MIA	AY	37	29/30	0.94	0.26	63,84,108,108	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, 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
61	KIR	AZ	502	57/57	0.74	0.57	139,147,150,150	0
60	GDP	CZ	501	28/28	0.81	0.25	141,145,153,153	0
60	GDP	AZ	501	28/28	0.84	0.23	151,157,158,158	0
61	KIR	CZ	502	57/57	0.84	0.34	139,145,150,151	0
59	ZN	B4	101	1/1	0.88	0.08	200,200,200,200	0
59	ZN	B9	101	1/1	0.94	0.14	200,200,200,200	0
59	ZN	D9	101	1/1	0.97	0.11	133,133,133,133	0
59	ZN	AN	101	1/1	0.99	0.16	84,84,84,84	0
59	ZN	CD	301	1/1	0.99	0.31	85,85,85,85	0
59	ZN	D4	101	1/1	0.99	0.14	129,129,129,129	0
59	ZN	AD	301	1/1	0.99	0.29	99,99,99,99	0
59	ZN	CN	101	1/1	1.00	0.17	63,63,63,63	0

6.5 Other polymers ⓘ

There are no such residues in this entry.