



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 10:41 AM UTC

PDB ID : 4V5R / pdb_00004v5r
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)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

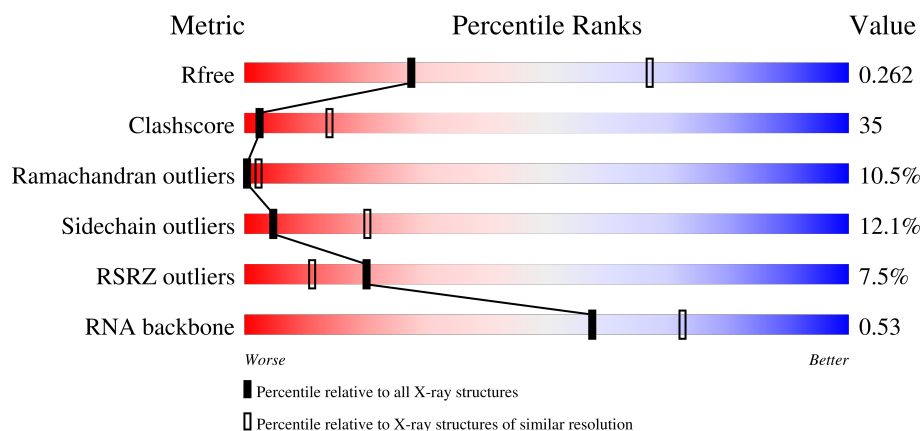
1 Overall quality at a glance ⓘ

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	2% 38% 48% 11% ..
1	CA	1522	4% 41% 45% 11% ..
2	AB	256	5% 26% 52% 13% . 9%
2	CB	256	8% 28% 49% 13% . 9%

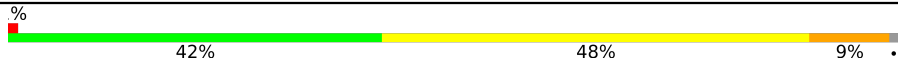
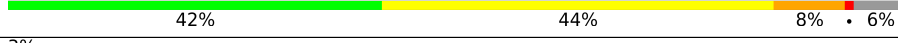
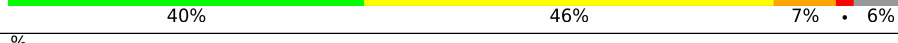
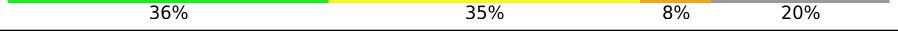
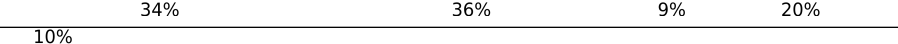
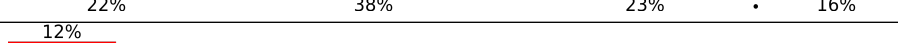
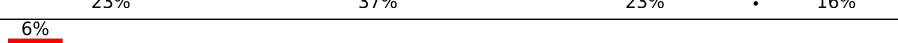
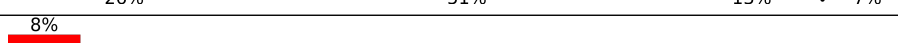
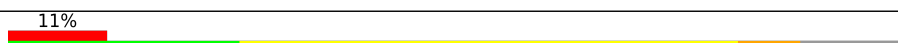
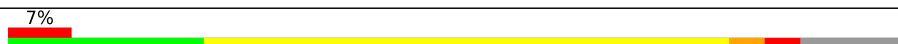
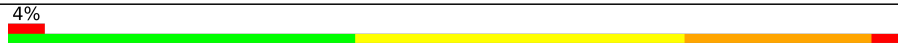
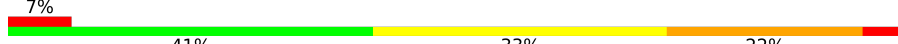
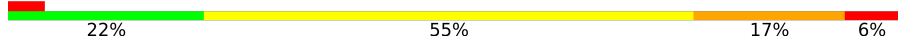
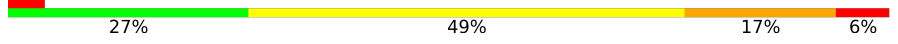
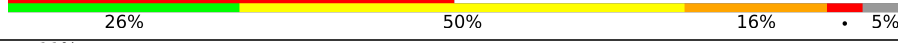
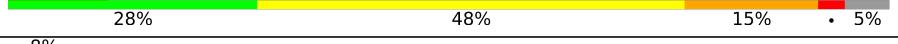
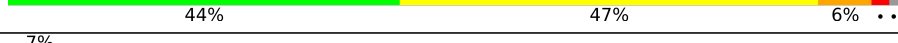
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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	131	
12	CL	131	
13	AM	126	
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	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	AW	76	
22	CV	76	
22	CW	76	
23	AX	27	
23	CX	27	
24	AY	77	
24	CY	77	
25	AZ	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	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229	
39	BD	276	

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Mol	Chain	Length	Quality of chain
39	DD	276	
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
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	-

2 Entry composition

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	C	N	O	P	0	0	0
			32451	14445	6010	10487	1509			
1	CA	1510	Total	C	N	O	P	0	0	0
			32451	14445	6010	10487	1509			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	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	0	0	0
			459	288	90	76	5			

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

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

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

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

- 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	0	0	0
			507	326	101	78	2			
34	D8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			
36	DA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
40	DE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

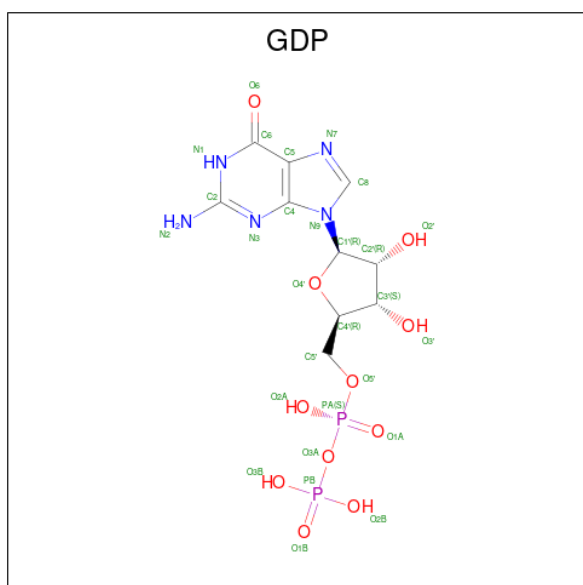
- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

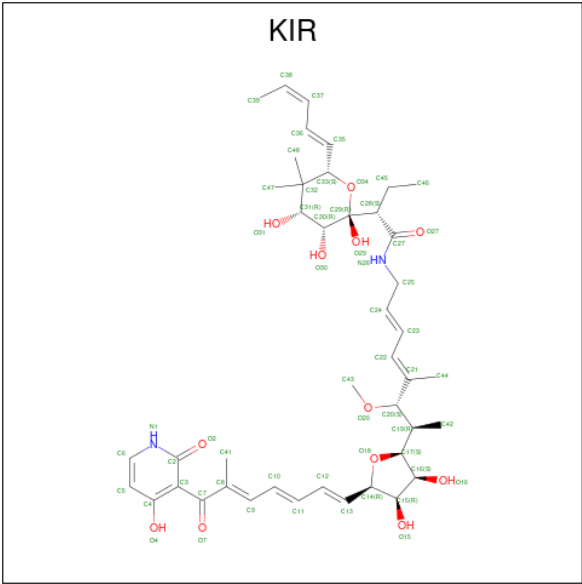
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B4	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 61 is KIRROMYCIN (CCD ID: KIR) (formula: C₄₃H₆₀N₂O₁₂).

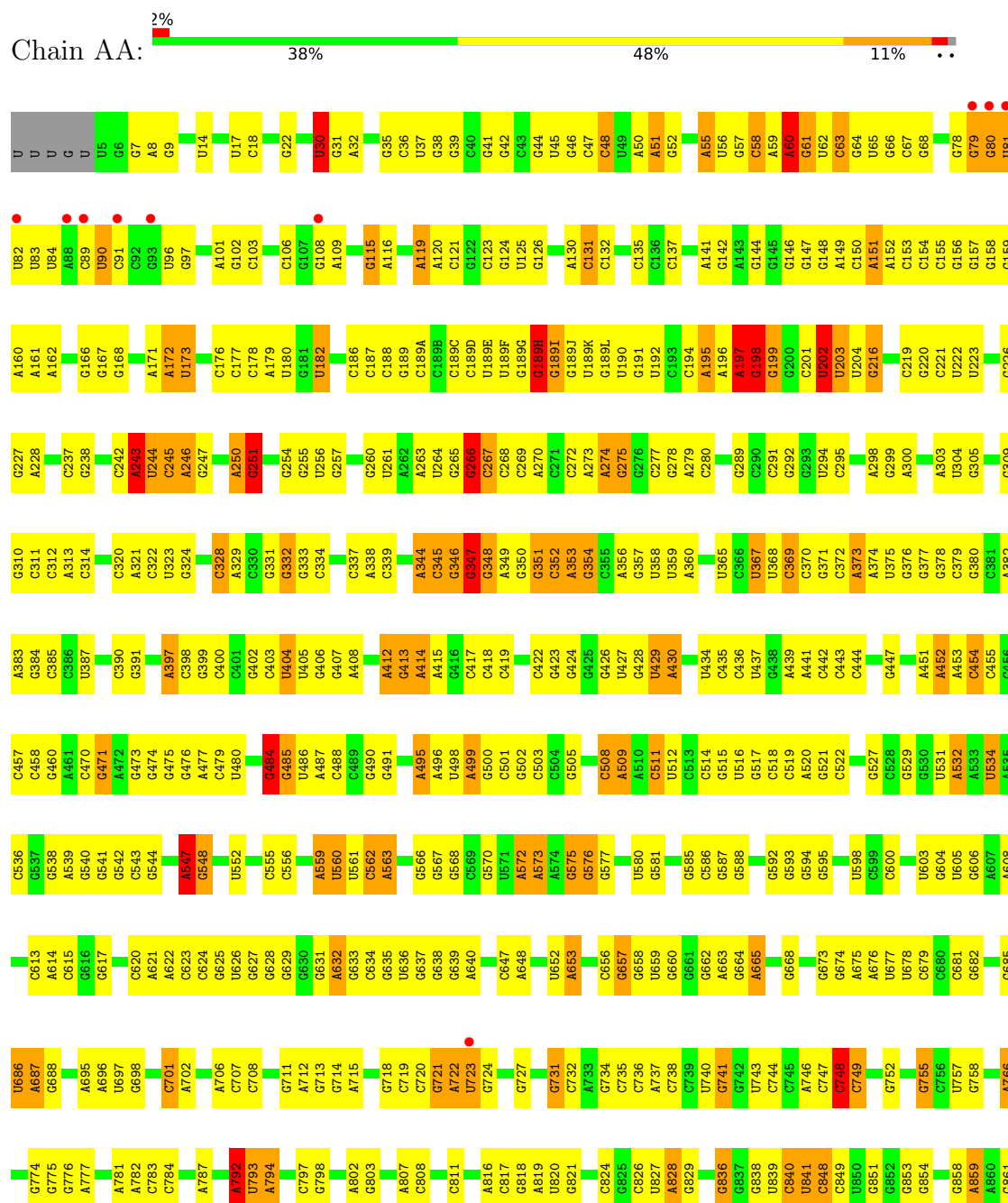


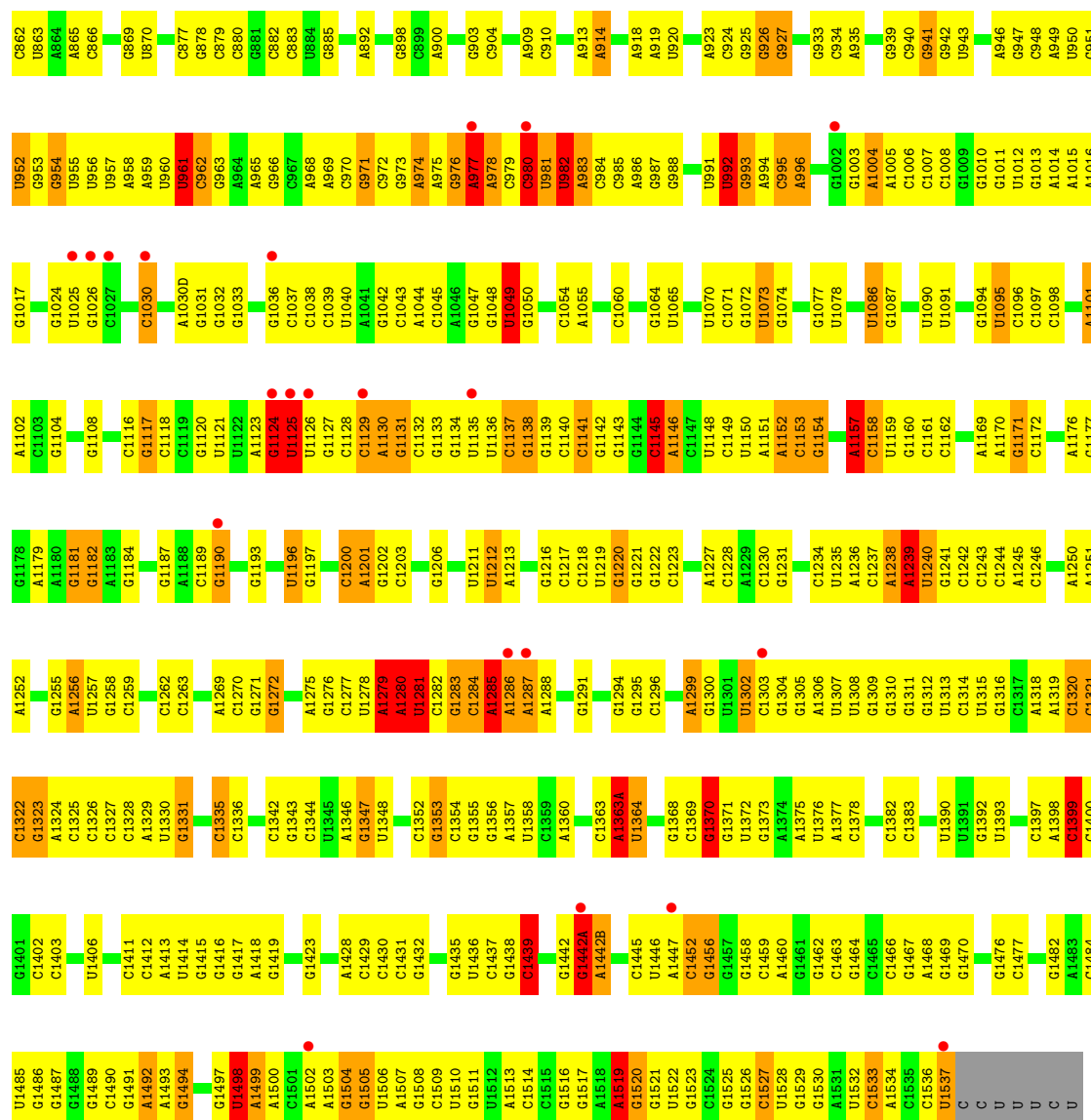
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AZ	1	Total	C	N	O		0	0
			57	43	2	12			
61	CZ	1	Total	C	N	O		0	0
			57	43	2	12			

3 Residue-property plots

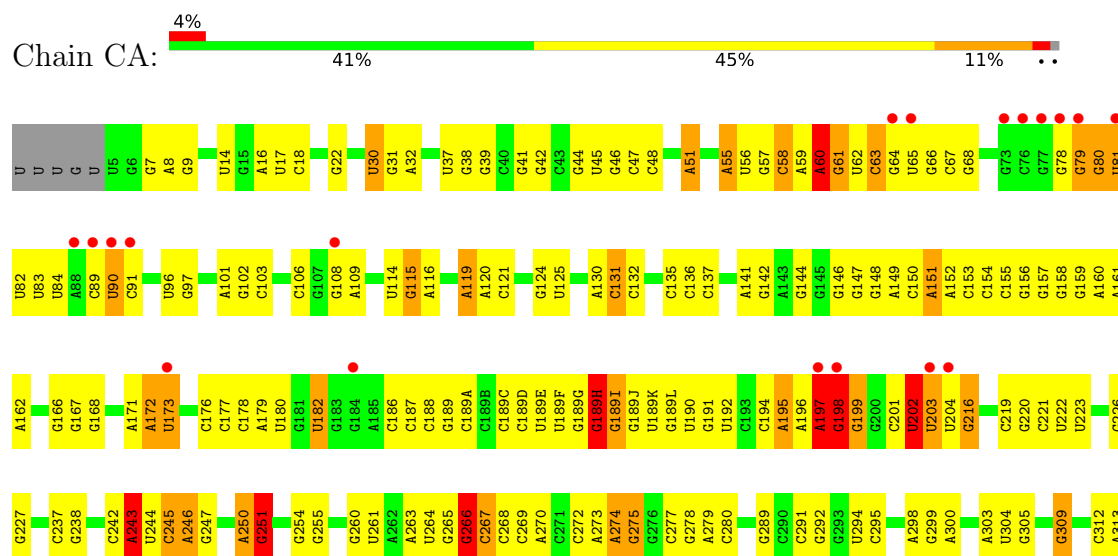
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

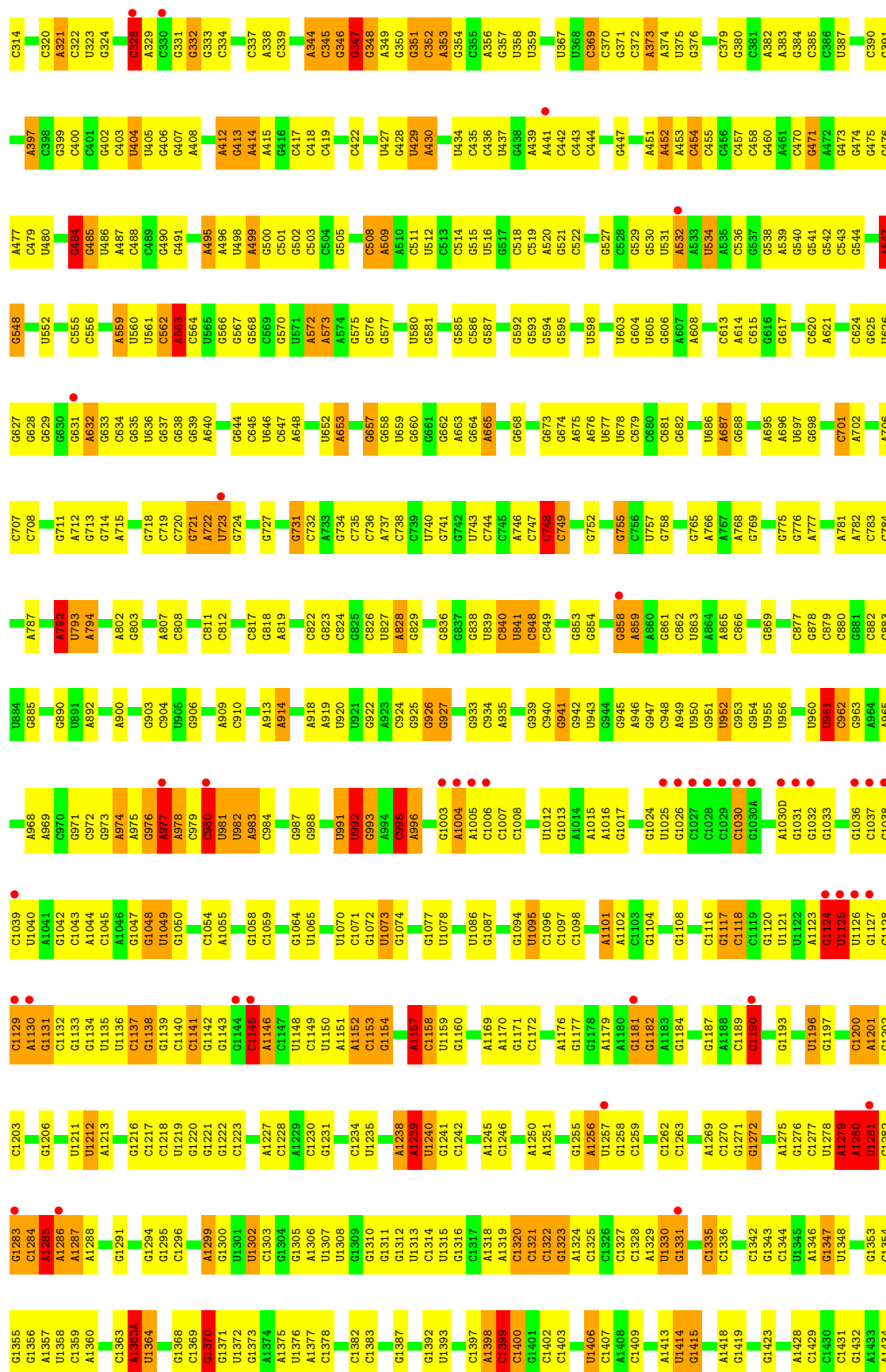
• Molecule 1: 16S rRNA

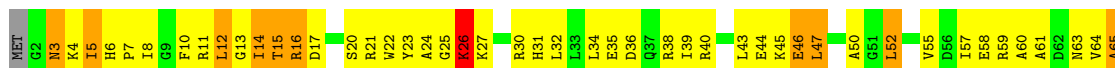


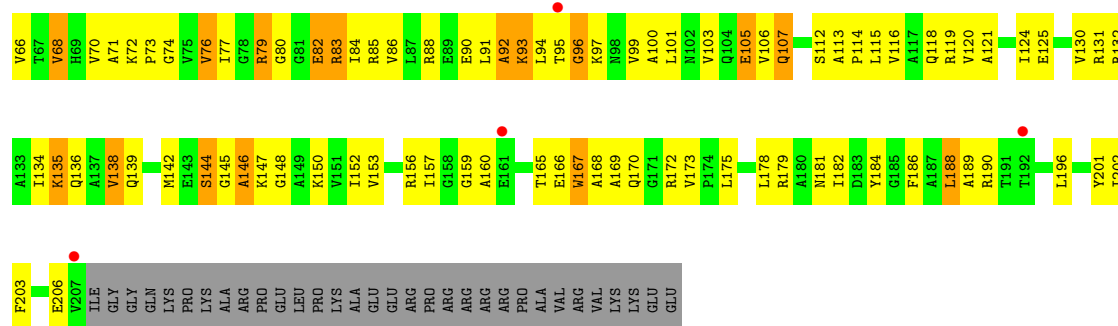


• Molecule 1: 16S rRNA

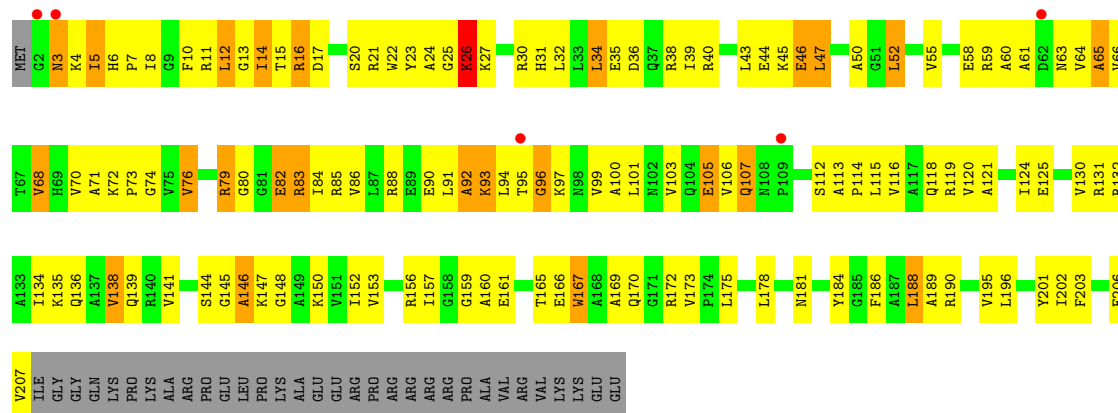




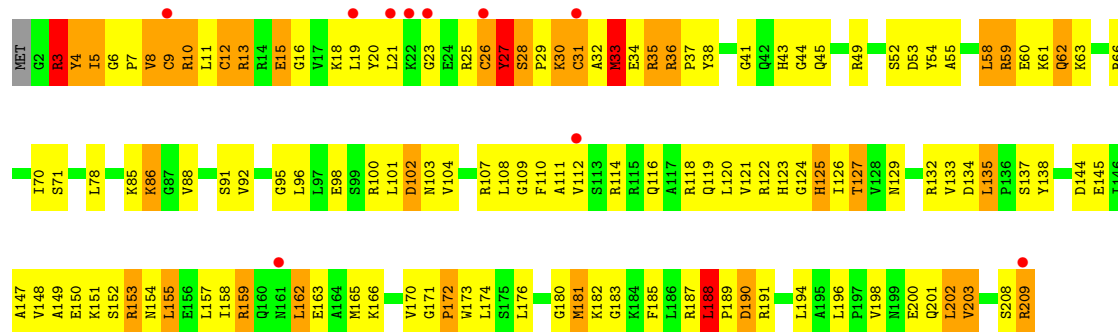




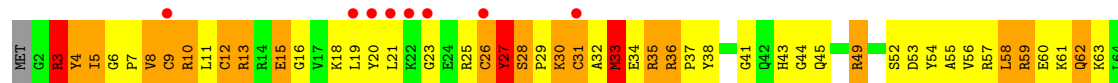
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

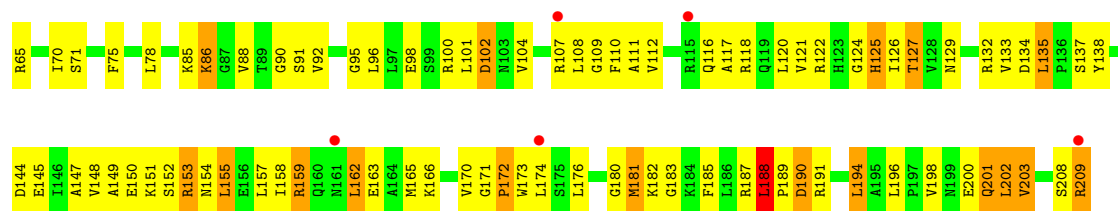


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

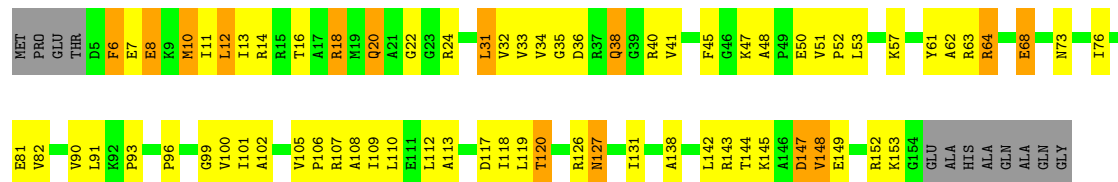


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

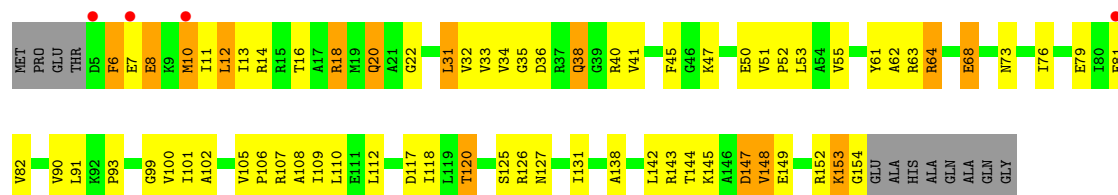




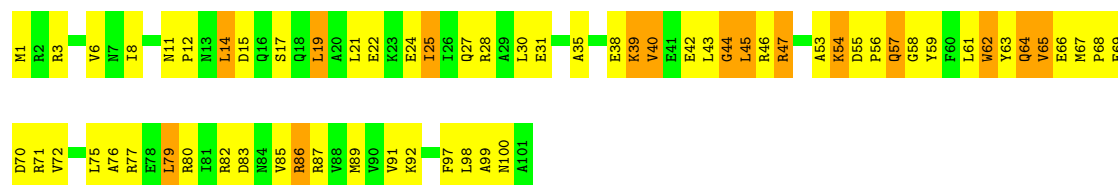
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



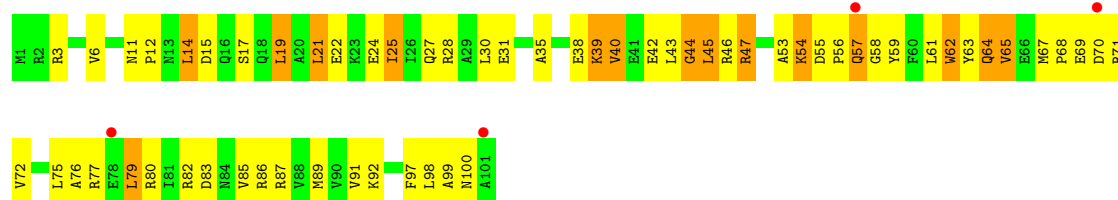
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

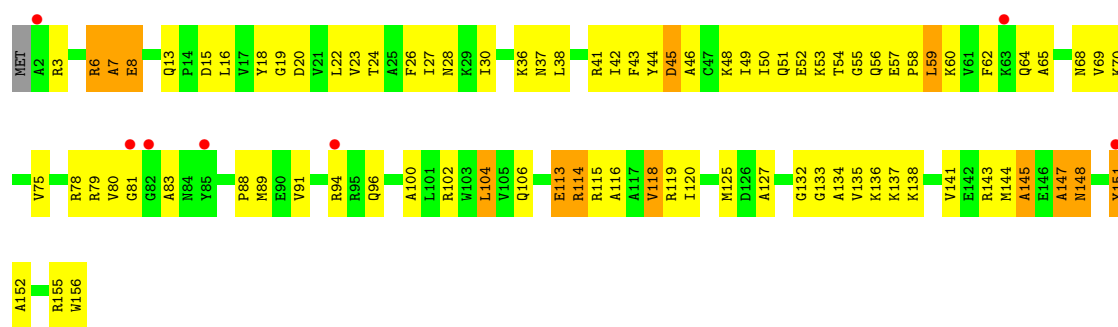


• Molecule 6: 30S RIBOSOMAL PROTEIN S6



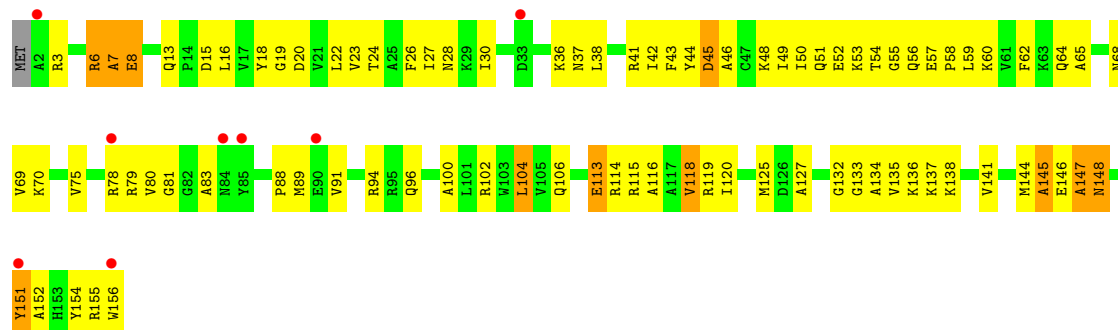
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG: 



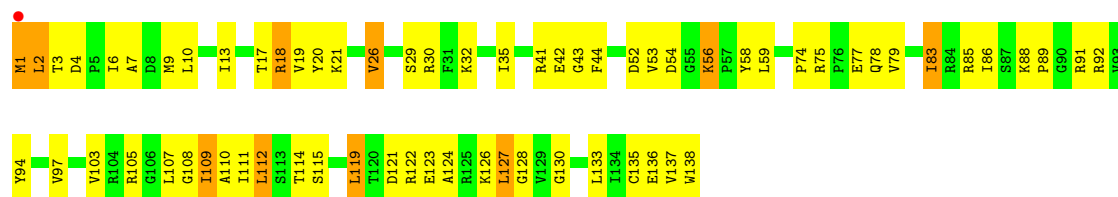
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG: 



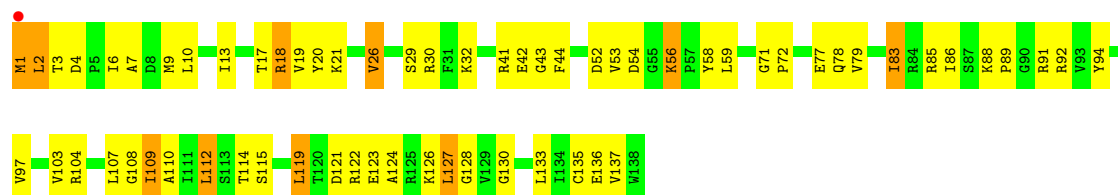
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH: 



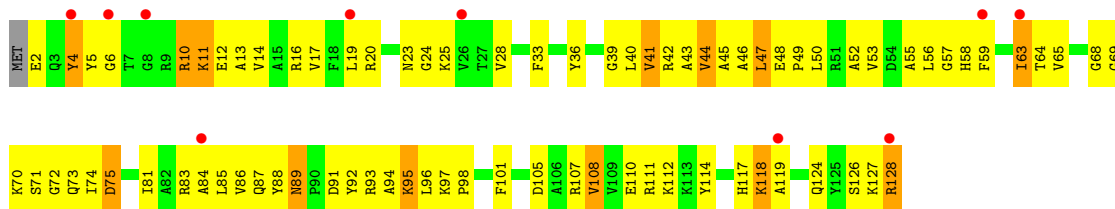
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH: 

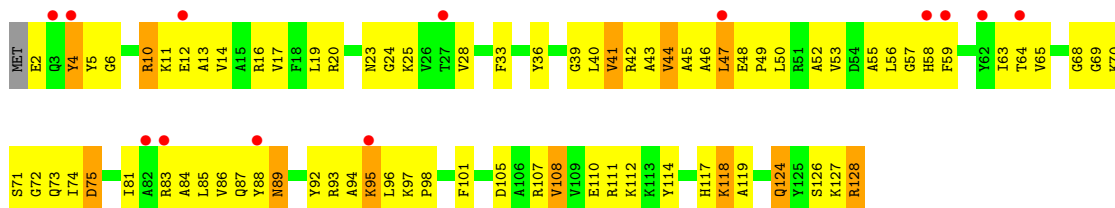


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

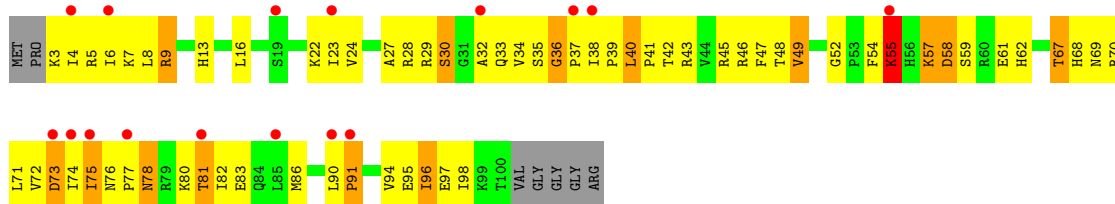
Chain AI: 



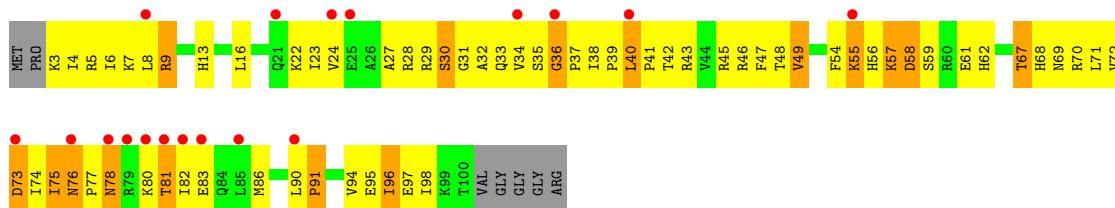
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



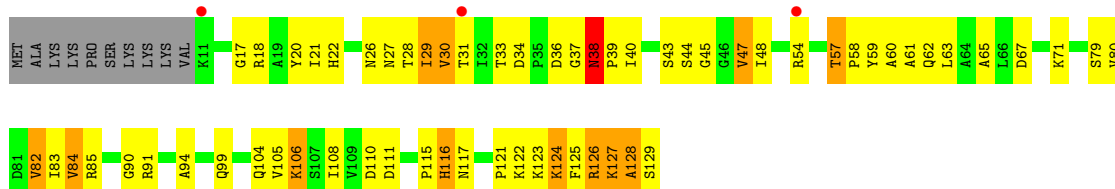
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



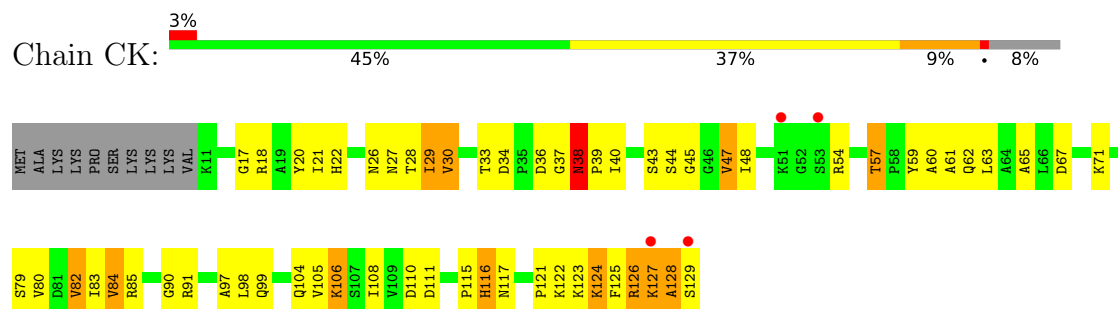
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



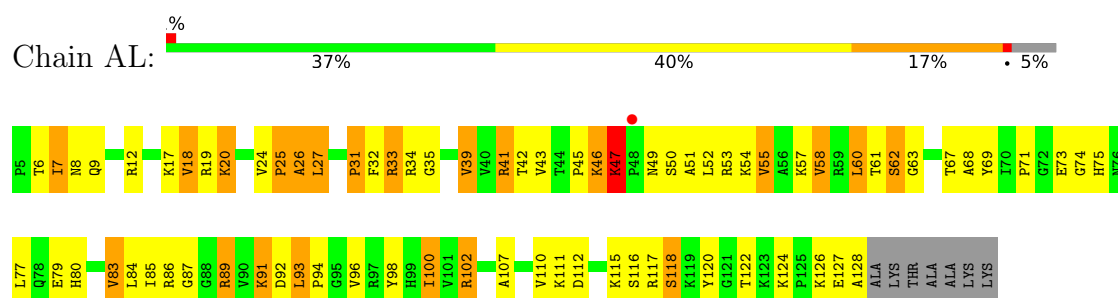
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



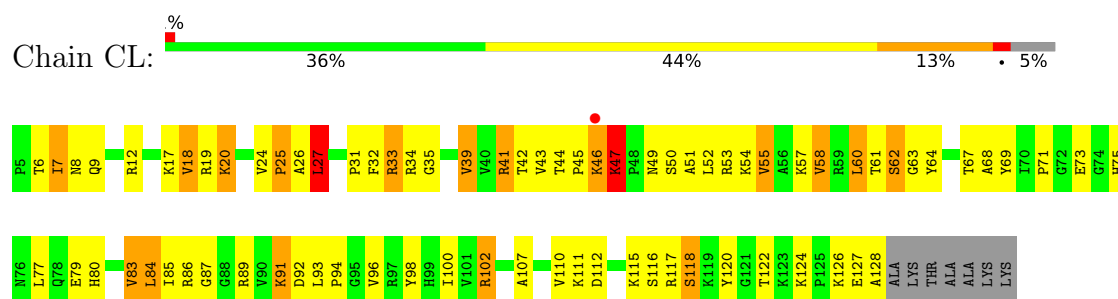
● Molecule 11: 30S RIBOSOMAL PROTEIN S11



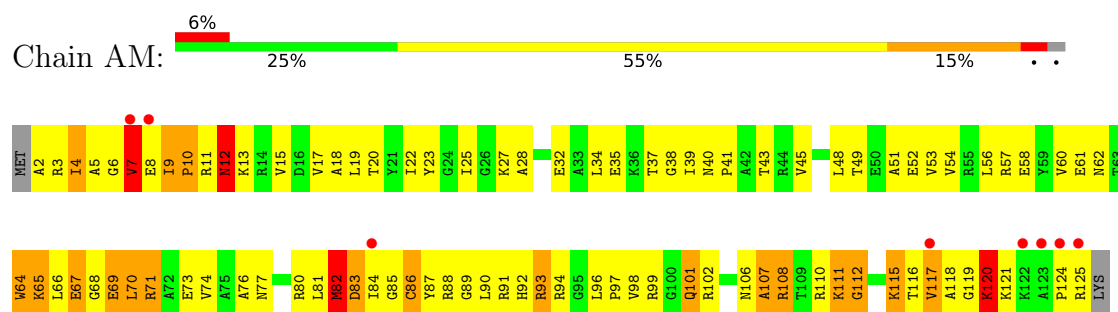
● Molecule 12: 30S RIBOSOMAL PROTEIN S12



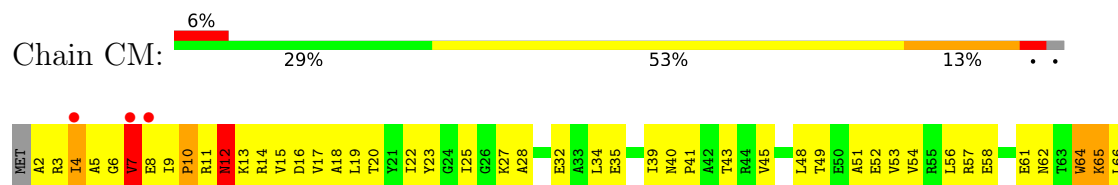
● Molecule 12: 30S RIBOSOMAL PROTEIN S12

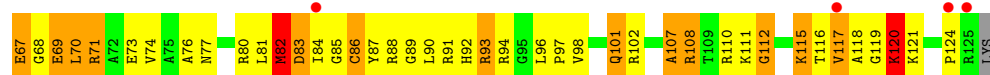


● Molecule 13: 30S RIBOSOMAL PROTEIN S13

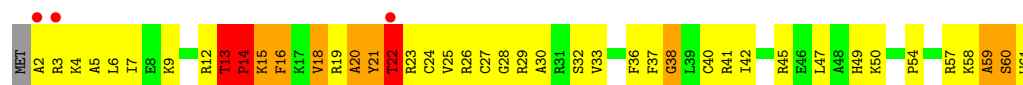


● Molecule 13: 30S RIBOSOMAL PROTEIN S13

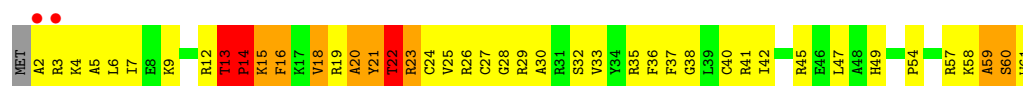




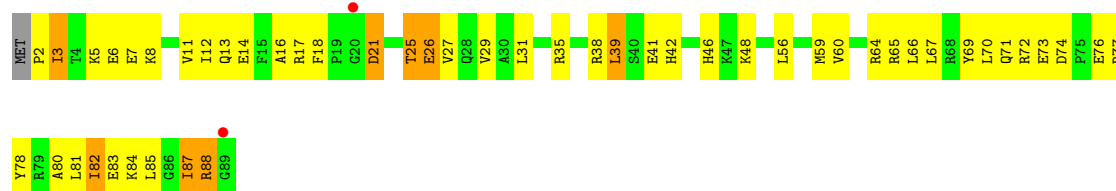
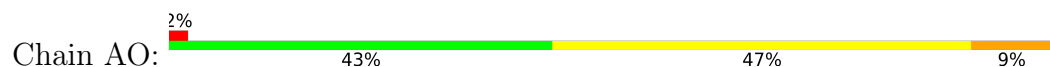
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



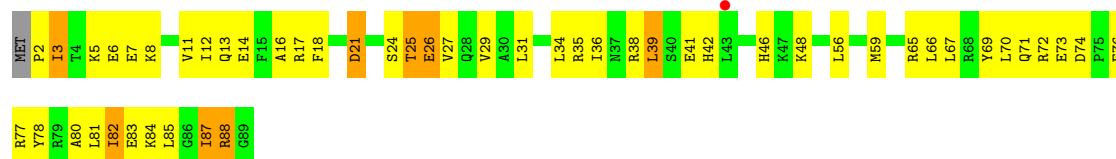
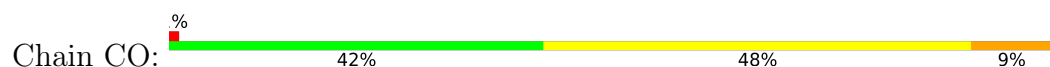
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



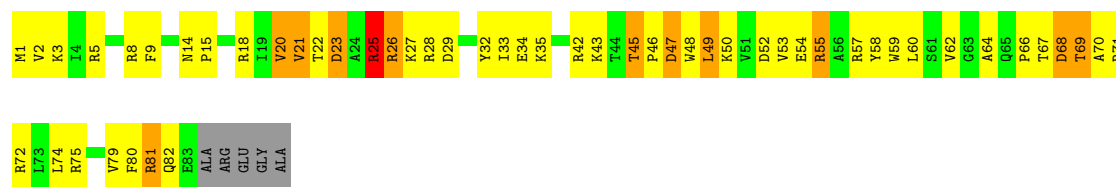
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



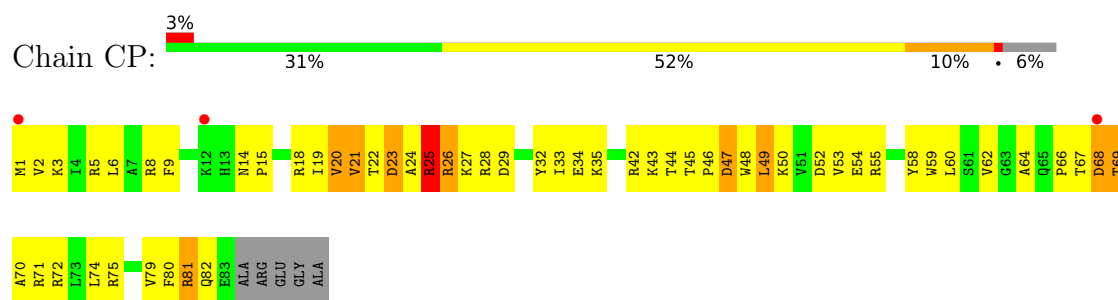
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



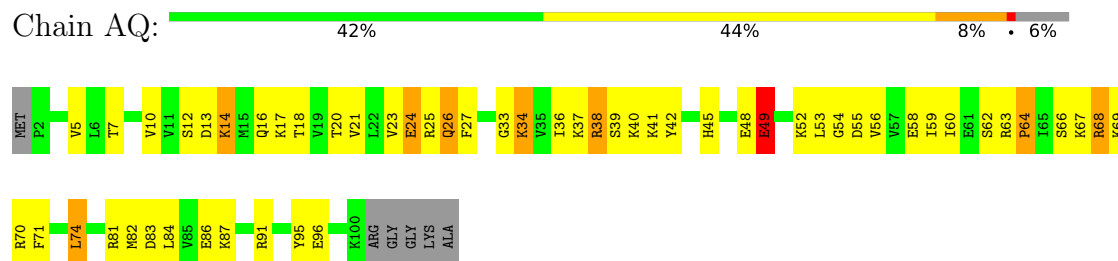
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



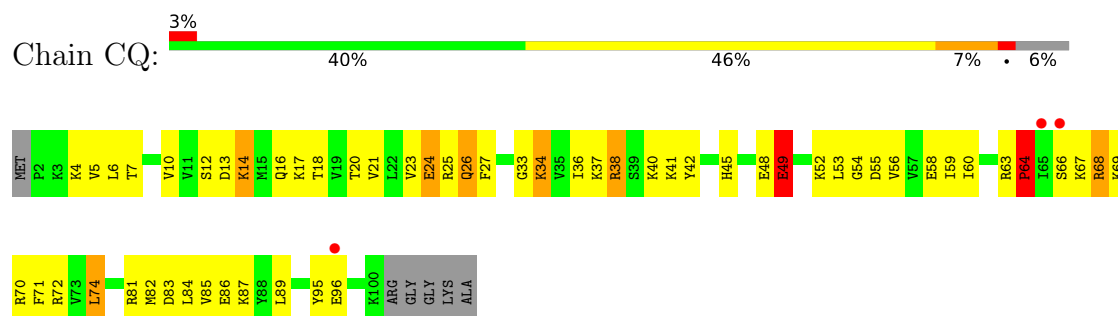
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



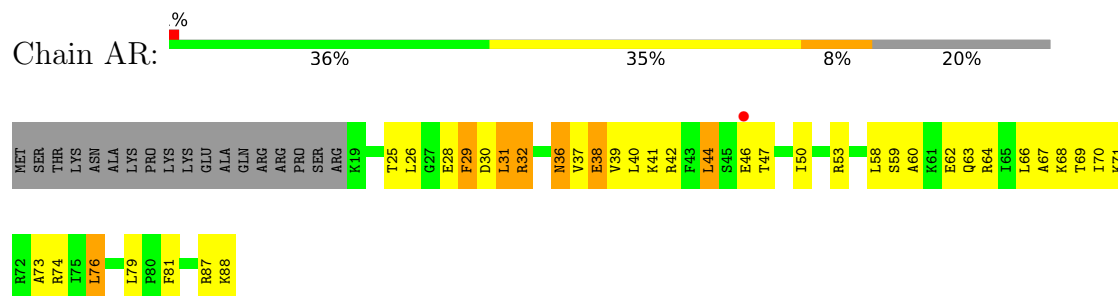
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



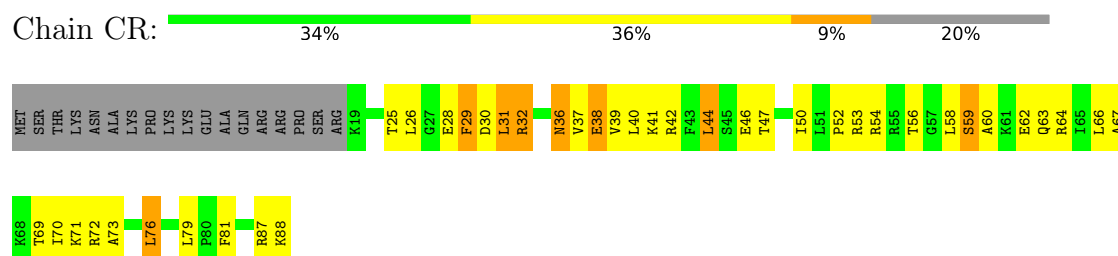
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



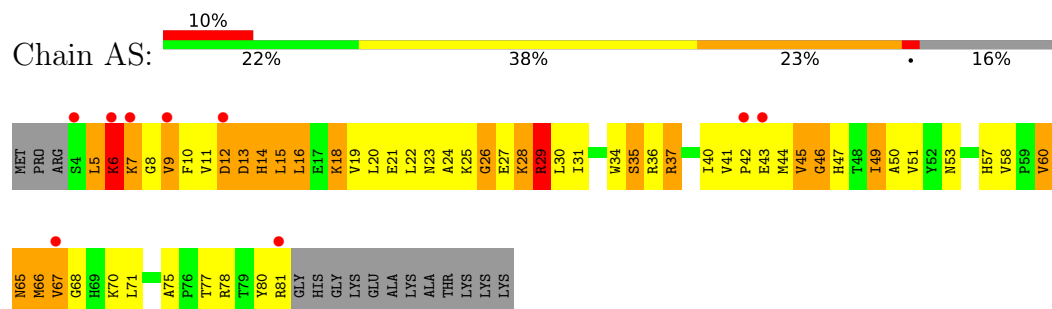
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



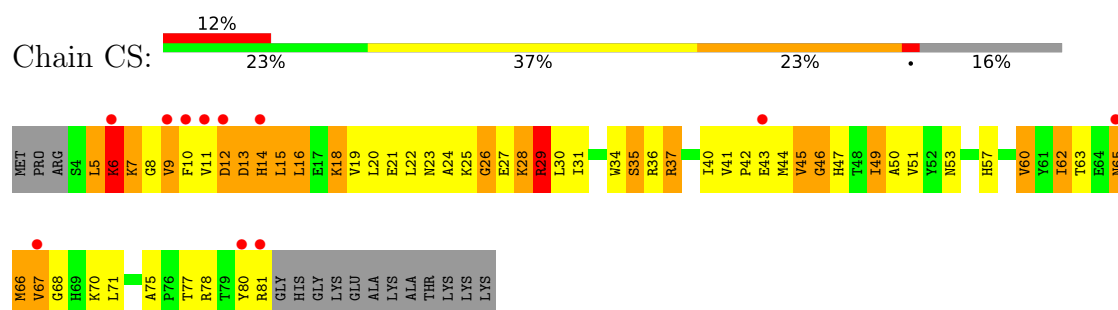
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



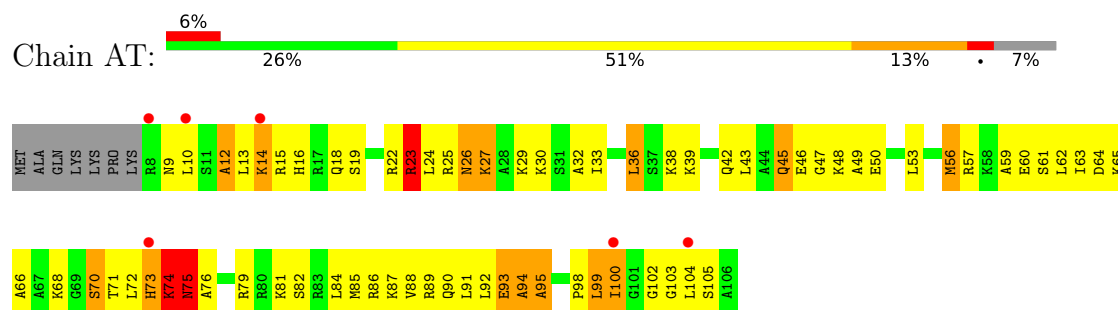
● Molecule 19: 30S RIBOSOMAL PROTEIN S19



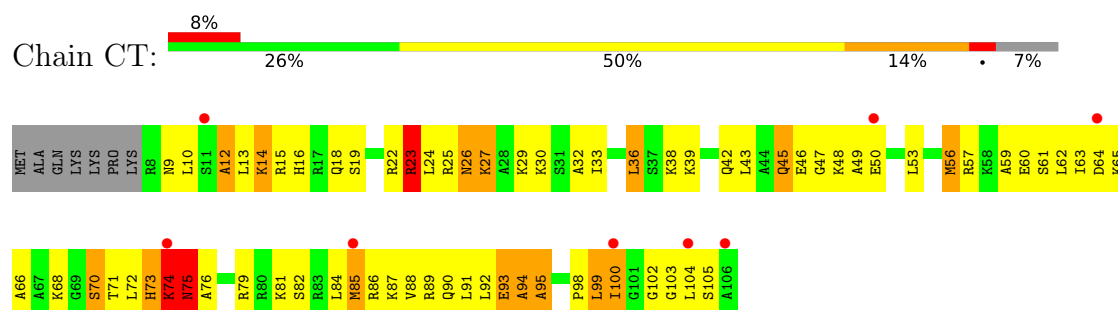
● Molecule 19: 30S RIBOSOMAL PROTEIN S19



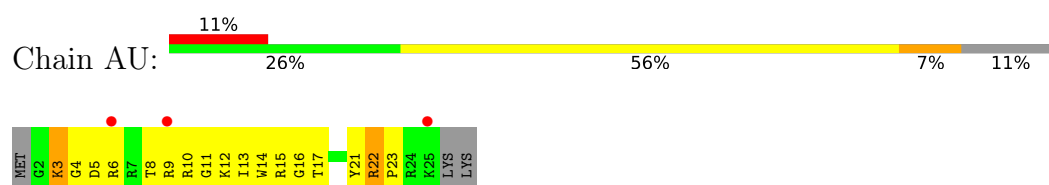
● Molecule 20: 30S RIBOSOMAL PROTEIN S20



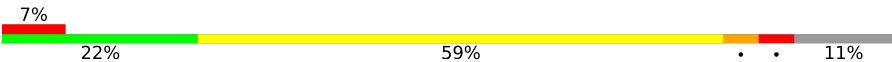
● Molecule 20: 30S RIBOSOMAL PROTEIN S20

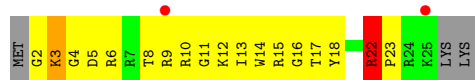


● Molecule 21: 30S RIBOSOMAL PROTEIN THX



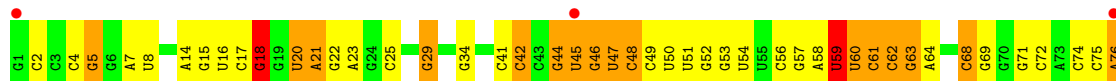
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU: 

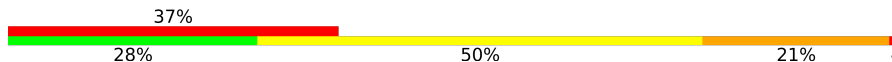


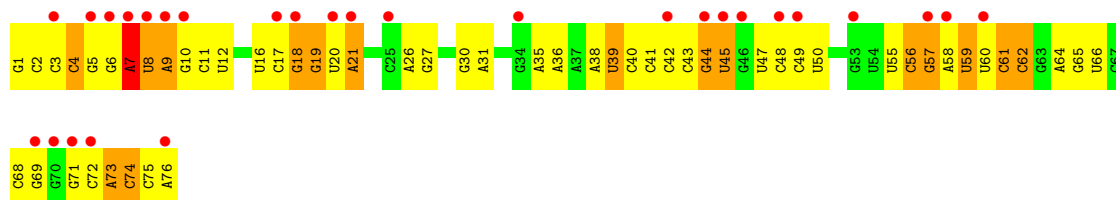
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AV: 



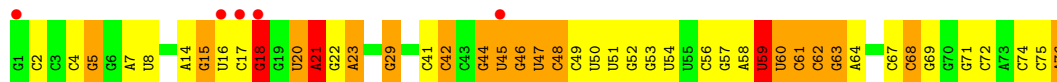
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AW: 



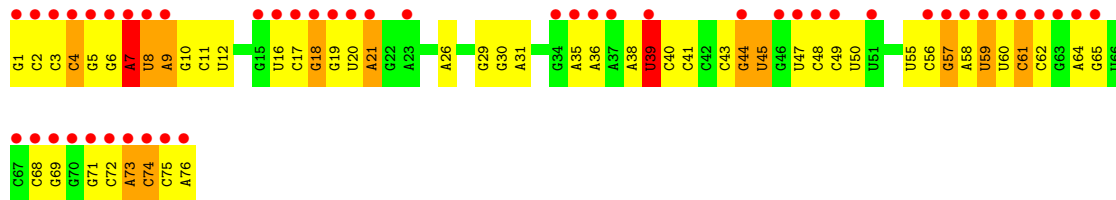
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain CV: 

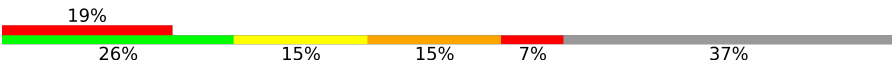


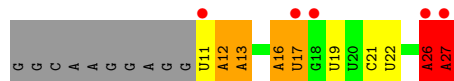
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain CW: 



- Molecule 23: MRNA

Chain AX: 



Chain CX:

Category	Percentage
G	15%
U11	19%
A12	30%
A13	7%
A16	7%
U17	37%
G18	
C21	
U22	
G23	
G24	
A25	
A26	
A27	

Chain AY:

Category	Value
A1	4%
A2	22%
A3	55%
A4	17%
A5	6%

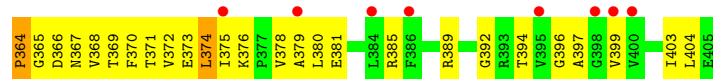
Chain CY:

Category	Percentage
A1	4%
A2	27%
A3	49%
A4	17%
A5	6%

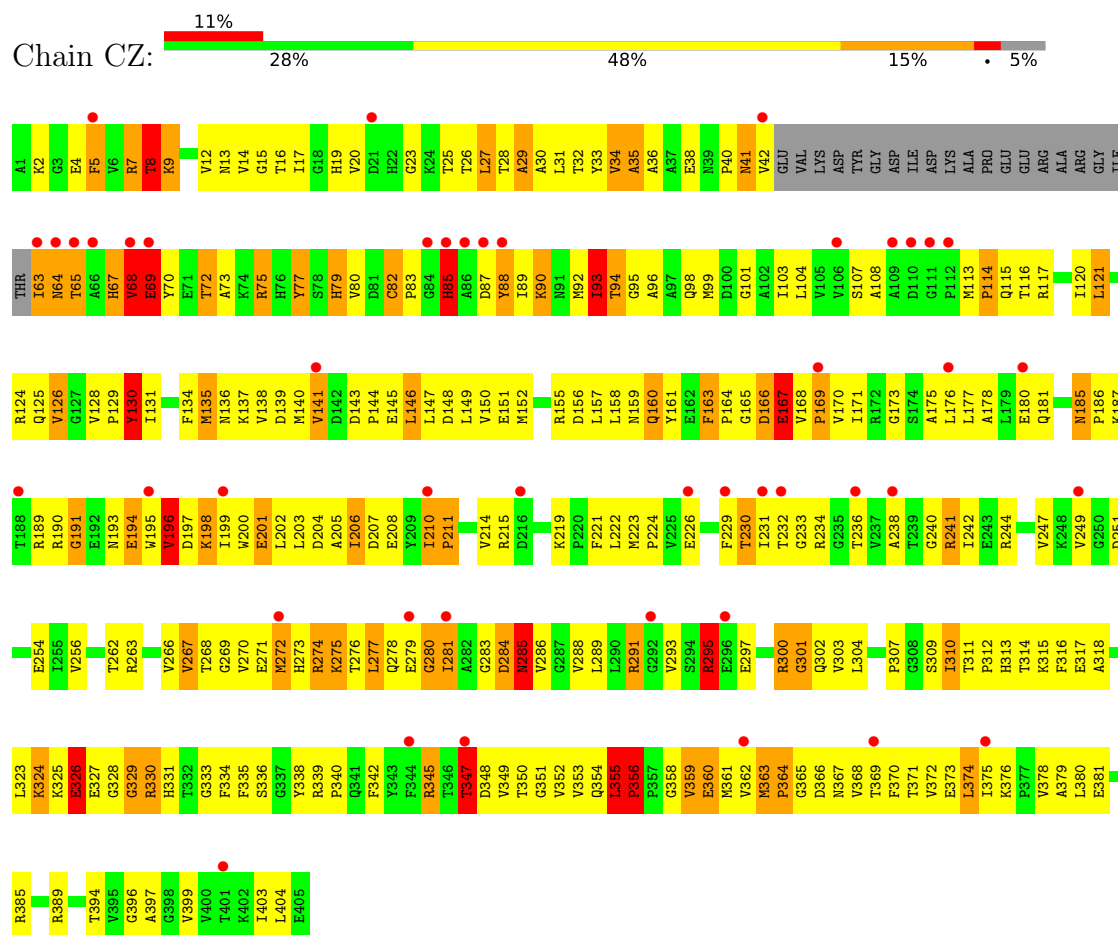
Chain AZ:

The visualization displays a chain of amino acids (AZ) and their corresponding chemical structures. The chain is represented by a horizontal bar at the top, divided into segments of different colors (red, orange, yellow, green, blue) representing different chemical classes. Below the bar, the amino acids are listed in a grid, with their chemical structures shown to the left and their names to the right. The grid is organized into rows and columns, with the amino acids grouped by their chemical class. The chain starts with LLE and ends with GLU.

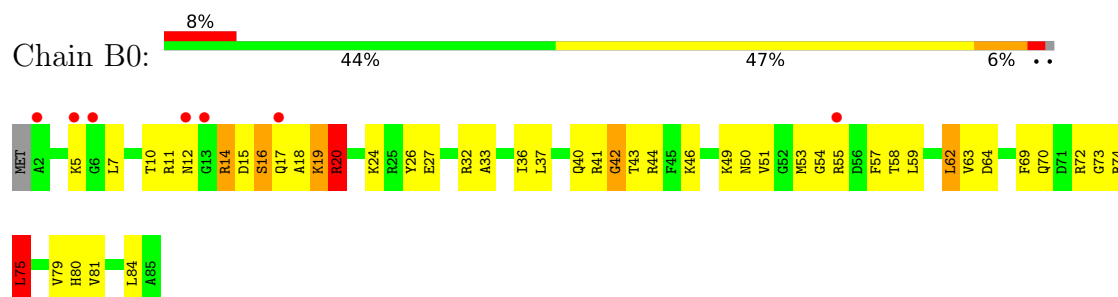
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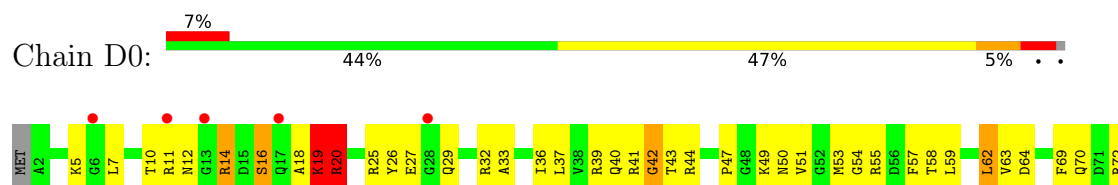
• Molecule 25: ELONGATION FACTOR TU

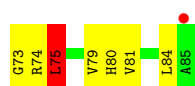


• Molecule 26: 50S RIBOSOMAL PROTEIN L27

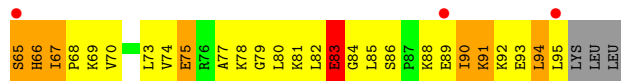
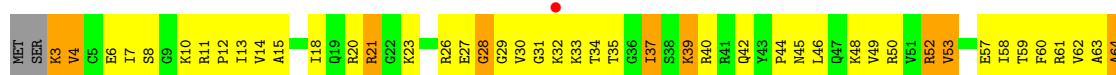


• Molecule 26: 50S RIBOSOMAL PROTEIN L27

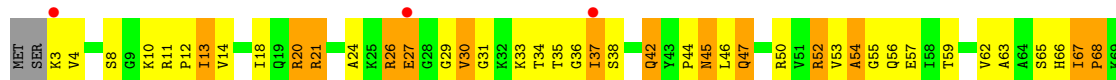




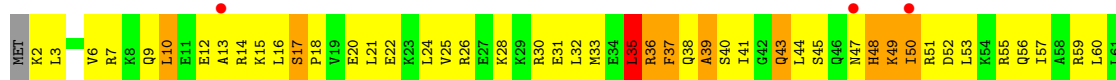
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



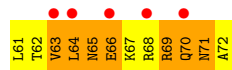
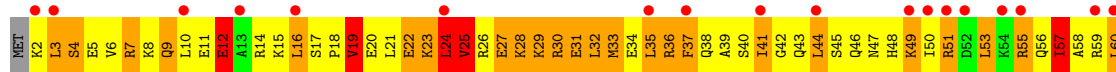
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



• Molecule 28: 50S RIBOSOMAL PROTEIN L29



• Molecule 28: 50S RIBOSOMAL PROTEIN L29

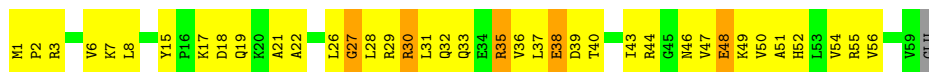


• Molecule 29: 50S RIBOSOMAL PROTEIN L30

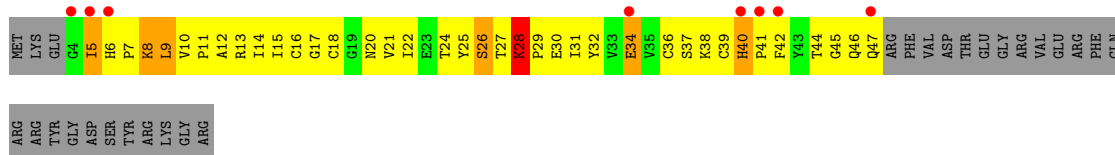




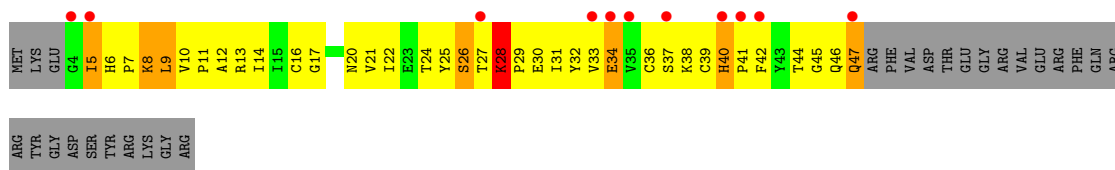
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



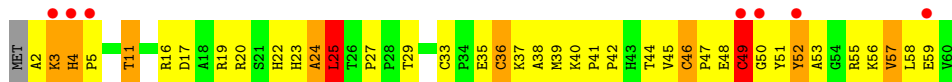
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



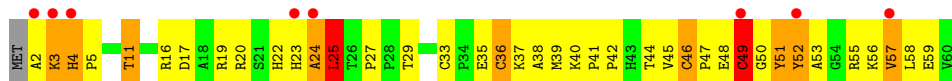
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



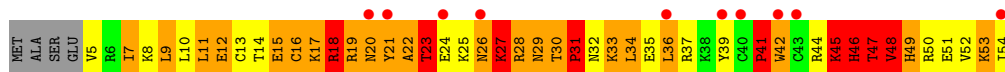
• Molecule 31: 50S RIBOSOMAL PROTEIN L32



• Molecule 31: 50S RIBOSOMAL PROTEIN L32

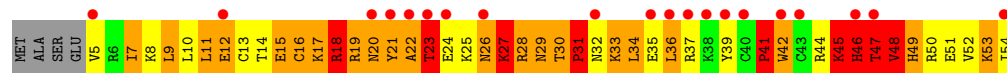


• Molecule 32: 50S RIBOSOMAL PROTEIN L33



- Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain D6: 



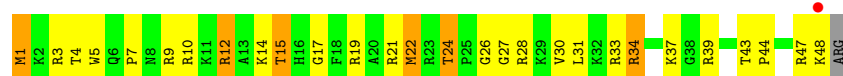
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain B7: 



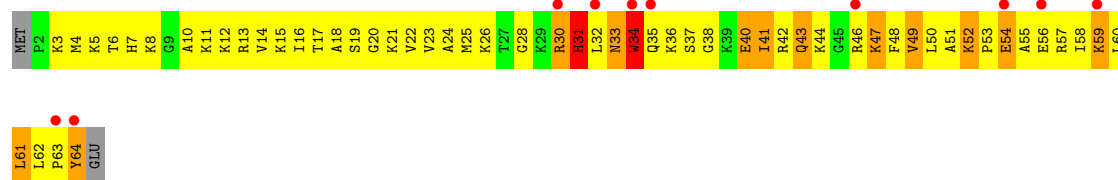
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain D7: 

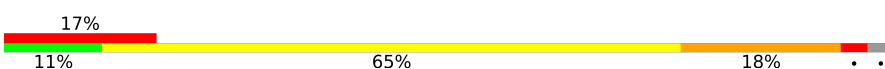


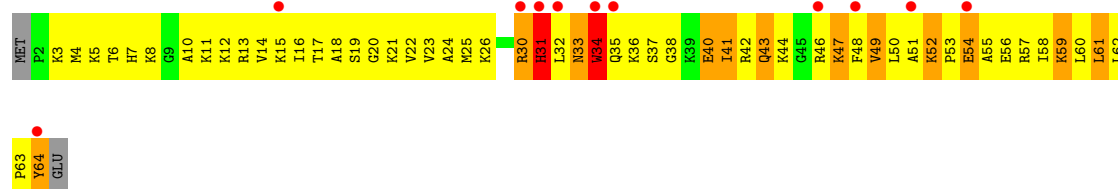
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain B8: 



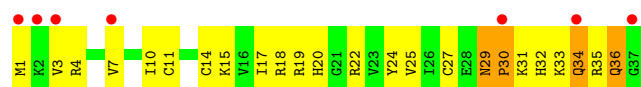
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain D8: 

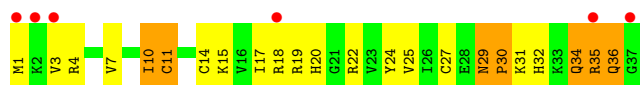
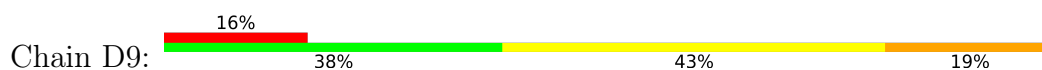


- Molecule 35: 50S RIBOSOMAL PROTEIN L36

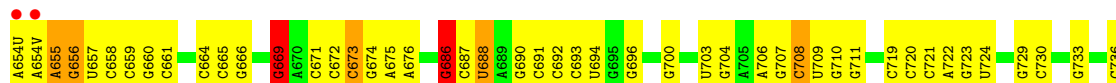
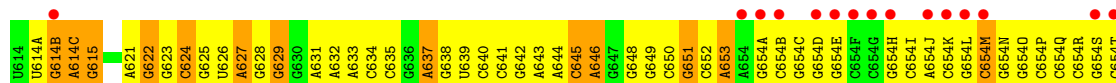
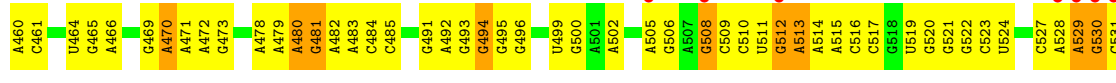
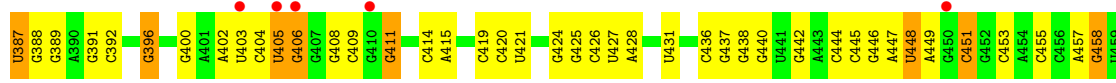
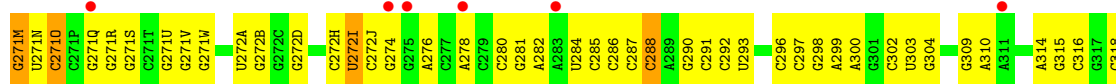
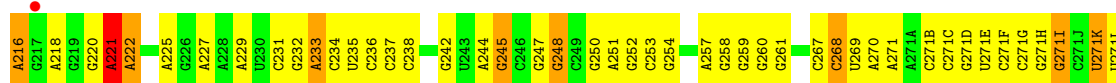
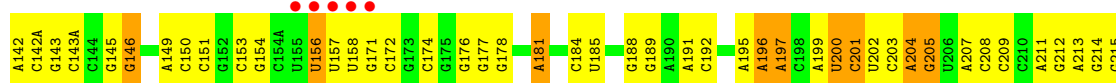
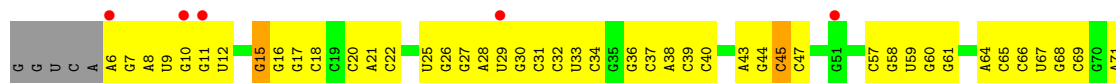
Chain B9: 

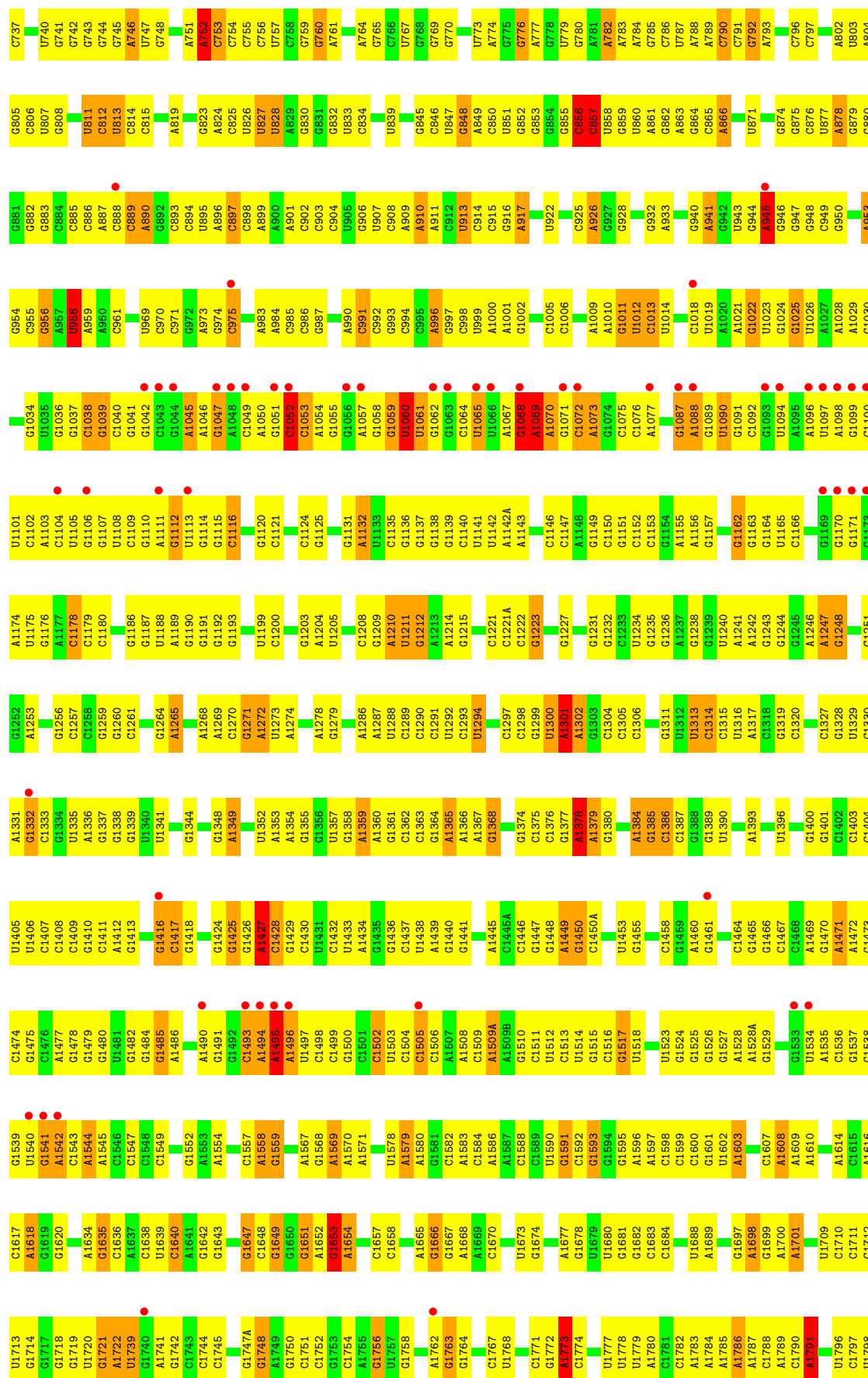


- Molecule 35: 50S RIBOSOMAL PROTEIN L36

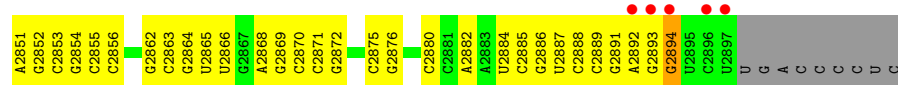


● Molecule 36: 23S RIBOSOMAL RNA

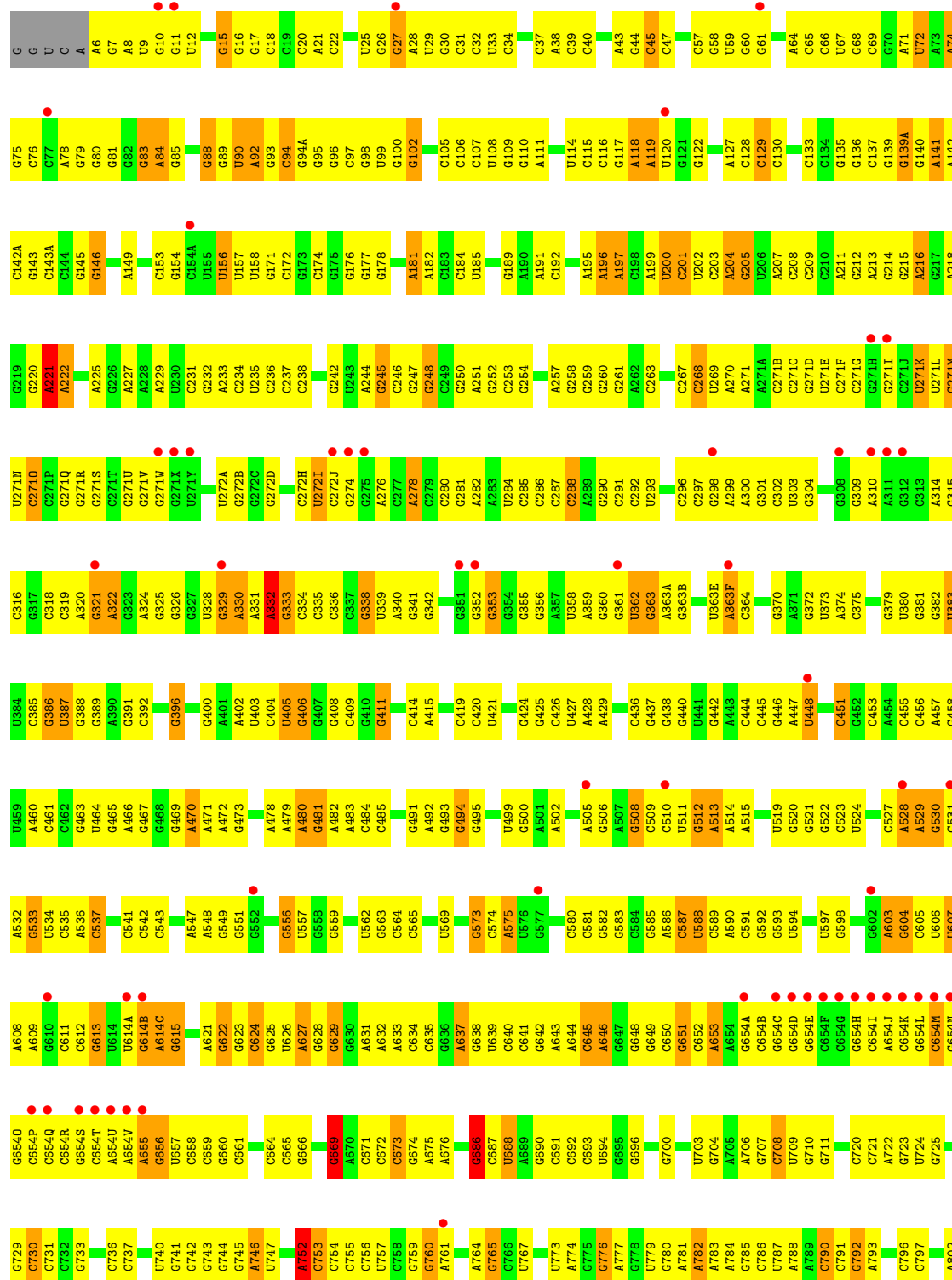






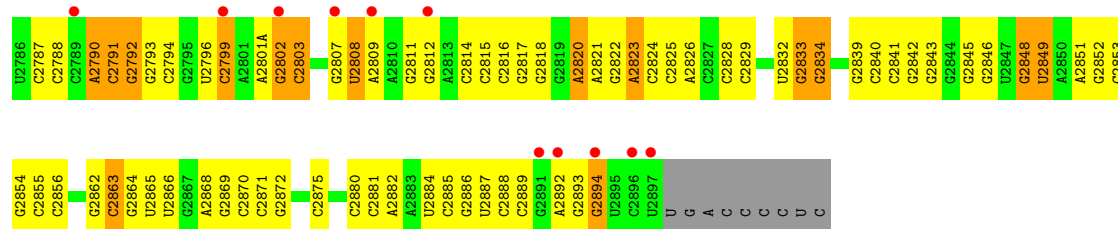


• Molecule 36: 23S RIBOSOMAL RNA

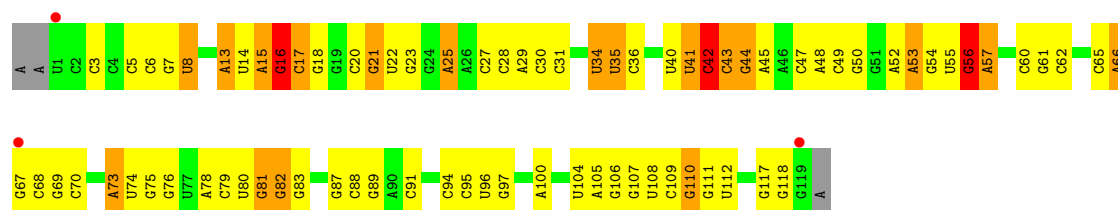




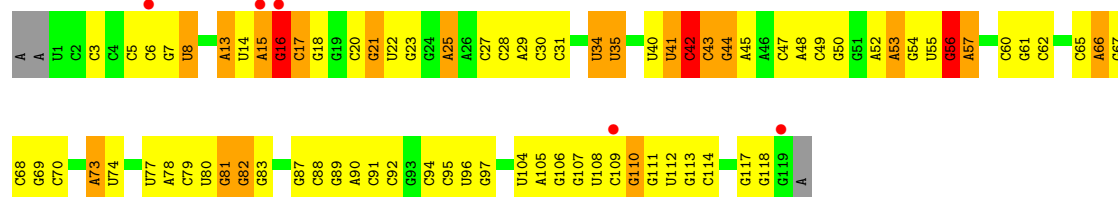
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G2714	A2632	C2558	G2484	G2416	C2343	G2184	U2122	G2045	C1961	C1881	A1801
			G2485	G2417	U2344	C2185	G2124	G2046	C1962	A1802	
U2720	U2635	U2562	G2486	A2418	G2345	G2187	G2125		U1963	A1803	C1804
A2721	U2636	A2563		U2419	A2346	G2188	A2126		C1967	U1805	C1804
G2722	A2639	A2564	U2491	G2420	C2347	G2189	G2127		G1968	A1885	C1806
C2723	G2640	A2565	U2492	C2421	U2348	G2190	G2128		G1969	G1886	G1807
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G2736	C2651	G2576	U2503	A2431	G2358	G2198	G2136		A1986	G1817	
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	A2665		A2518	G2445	G2374	G2221	G2149		U1999	U1915	
A2750	G2668	A2589	U2522	G2446	G2375	G2223	U2150		A2001	A1916	
G2751	G2689	C2591	G2523	G2447	A2376	G2224	G2151		C2006	G1917	
C2752	G2690	G2592	G2524	U2448	A2377	A2225	G2152		C2007	C1837	
A2753			G2525		A2378		G2153		C2008	C1838	
U2754		G2595	G2526	G2454	G2382	G2228	G2154		C2009	G1839	
G2755	G2672		G2527	G2455	G2383	G2229	G2155		G2010	U1841	
G2756	G2673	A2602	G2528	C2456	G2384	G2230	G2156		G2011	G1842	
A2757	A2674	U2603	U2528	U2457	G2385	G2231	A2157		G2012	C1843	
U2758	A2675	U2604	G2529	G2458	C2386		G2158		A2013	G1844	
		G2605		A2459	U2387	G2238	G2159		U2022	A1847	
G2759	C2678	C2606	A2533	U2460	A2388	G2239	G2160		G2023	A1848	
U2761	G2680	A2534	A2534	C2461	U2389	C2240	C2161		G2024	U1851	
G2762	C2681			U2462	G2390	A2241	G2162		C2025	A1854	
G2763	U2682	U2609	U2537	G2463	G2391	G2242	C2163		C2026	G1855	
A2765		U2610	C2538	C2464	A2392		G2166		C2027	G1856	
G2766		U2611	C2539	C2465	G2393	U2245	U2167		C2028	G1857	
		U2612	A2540	C2466	C2394	G2246	G2168		G2029	U1940	
C2771		A2614	A2541	C2467	C2395	U2247	A2169		A2030		
C2772		U2615	G2542	G2468	G2396	U2248	G2170		A2031	U1946	
C2773		G2616	G2543	A2469	G2397	G2250	A2171		G2032	C1947	
		C2617	G2544	G2470			U2172		A2033	G1948	
		G2618	U2545	C2471	G2400	U2257	A2173		U2034	G1949	
G2777	C2695	C2619	U2546	G2472	U2401	C2258	C2174		G2035		
A2778	U2696	G2620	U2547	U2473	C2402		G2175		C2036	A1952	
U2779	G2697		G2548	C2474	G2403	U2262	C2176		C2037	A1953	
G2780		G2624		C2475	C2404	C2263	A2177		C2038	G1866	
A2781	U2702	C2625	C2551	A2476	G2405	C2264	C2178		C2039	A1876	
G2782	C2703	C2626	U2552	C2477	U2406	U2265	C2179		C2040	U1877	
G2783		G2627	G2553	A2478	A2335	A2266	U2180				
		C2628	U2554	A2336	A2336	A2267	G2181				
G2785		A2629	U2555	G2481	U2408						



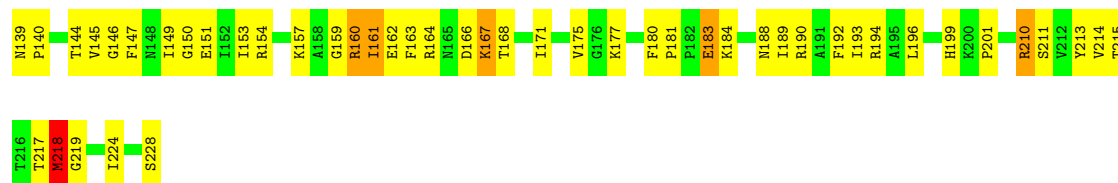
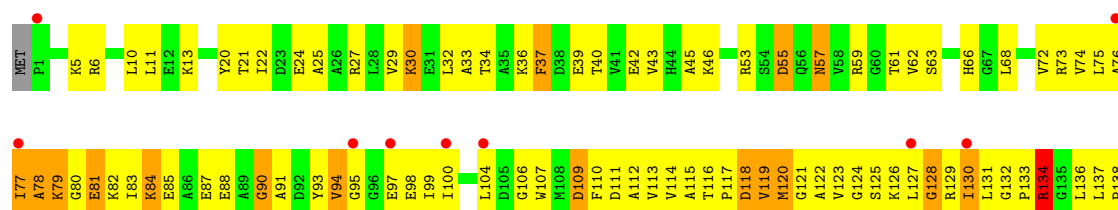
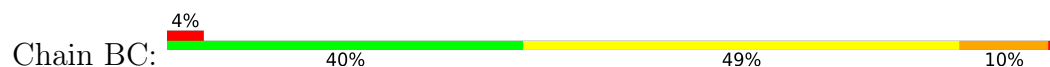
• Molecule 37: 5S RIBOSOMAL RNA



• Molecule 37: 5S RIBOSOMAL RNA

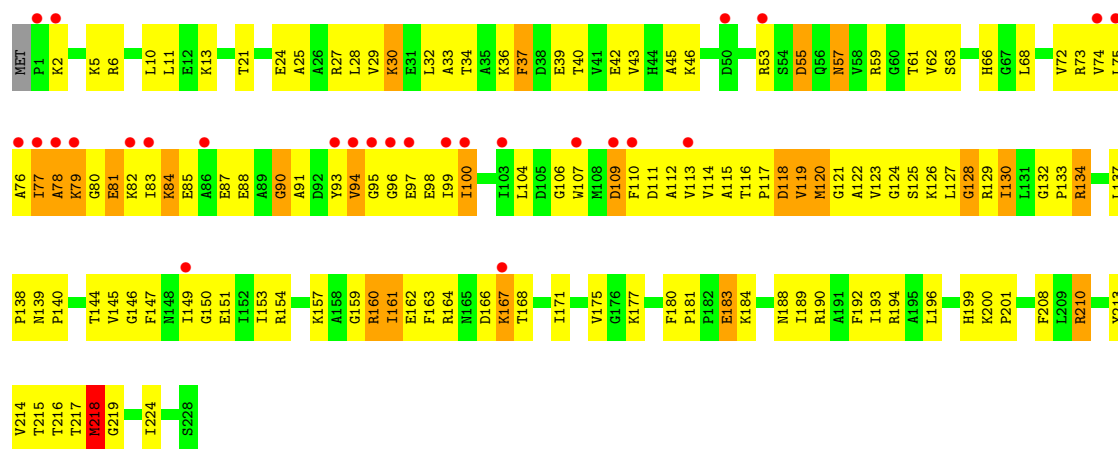


• Molecule 38: 50S RIBOSOMAL PROTEIN L1

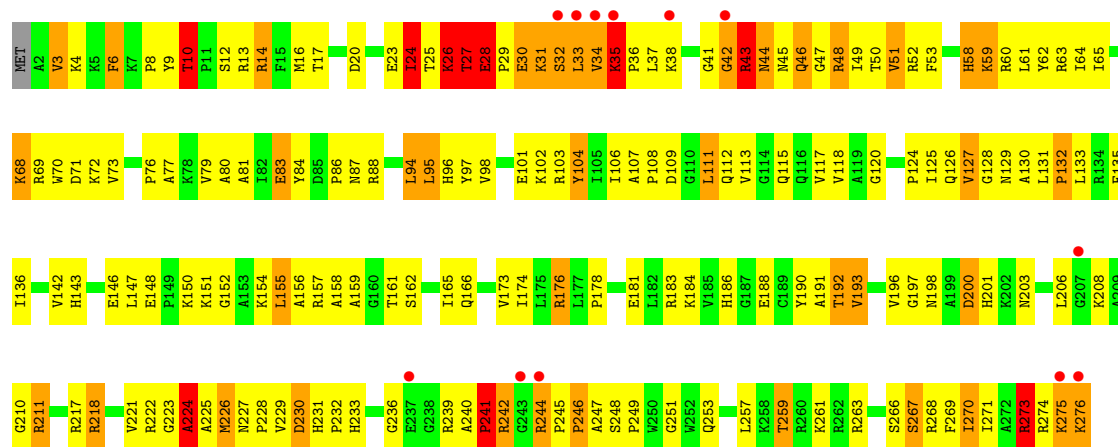


• Molecule 38: 50S RIBOSOMAL PROTEIN L1

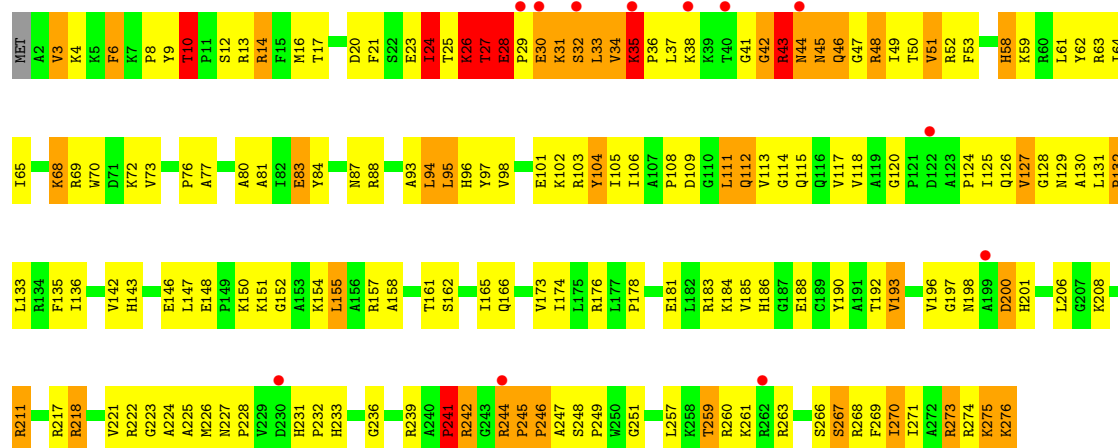




• Molecule 39: 50S RIBOSOMAL PROTEIN L2

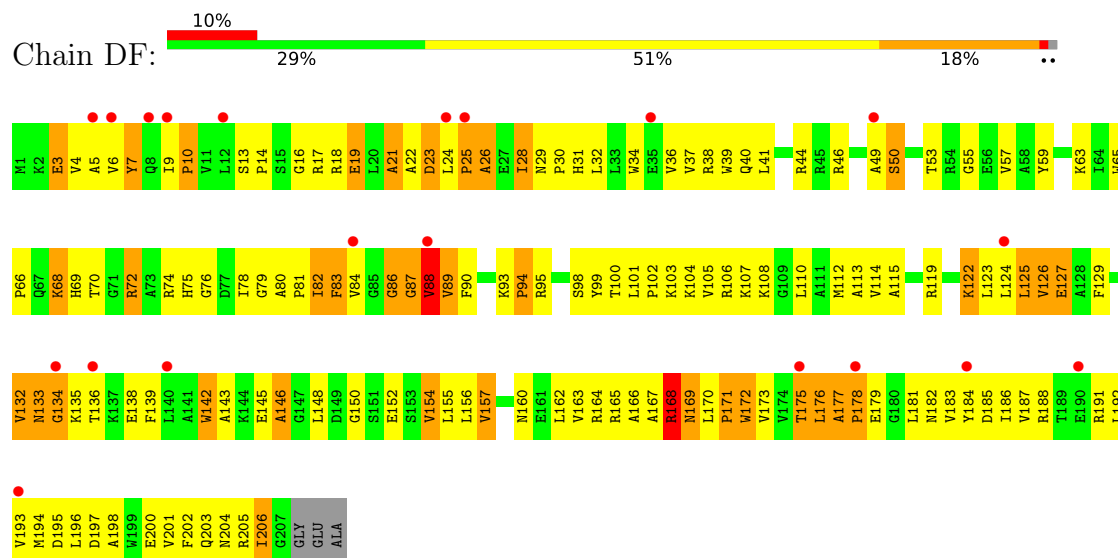


• Molecule 39: 50S RIBOSOMAL PROTEIN L2

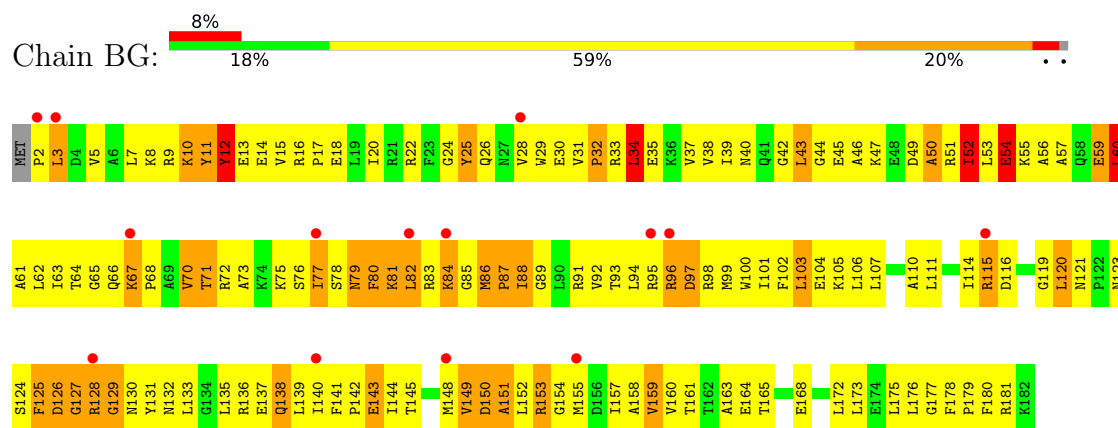


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

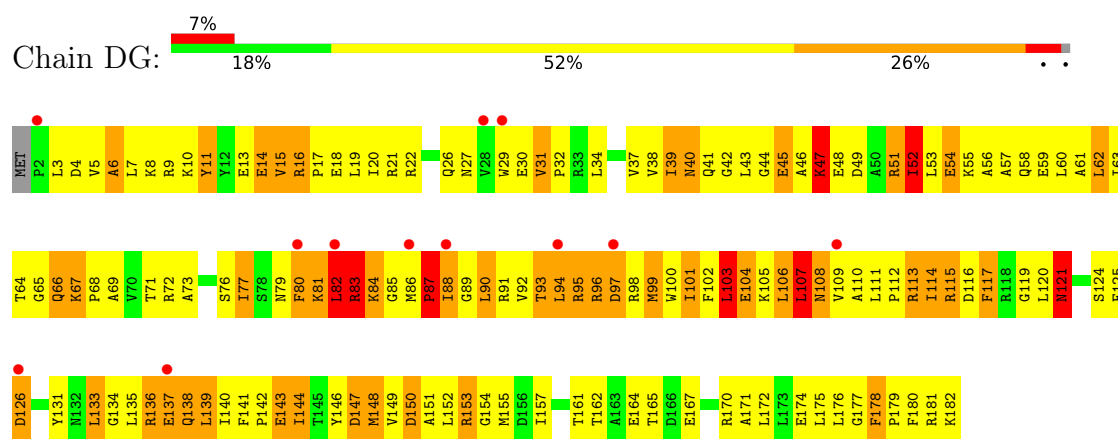
• Molecule 41: 50S RIBOSOMAL PROTEIN L4



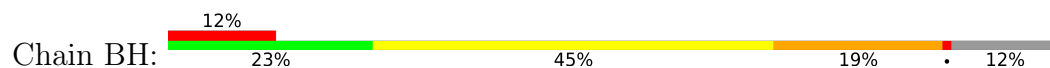
• Molecule 42: 50S RIBOSOMAL PROTEIN L5



• Molecule 42: 50S RIBOSOMAL PROTEIN L5



• Molecule 43: 50S RIBOSOMAL PROTEIN L6



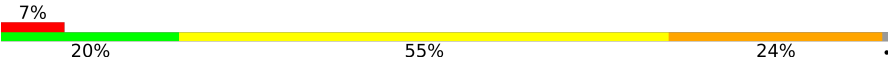


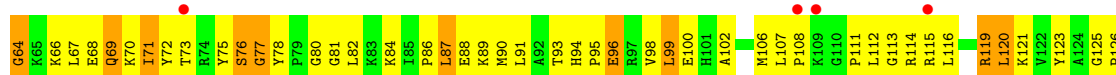
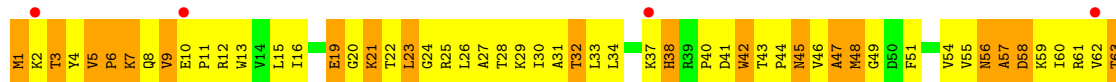
- Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain DK:  83% 12% 5%

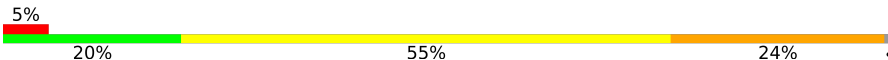


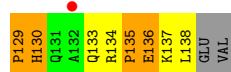
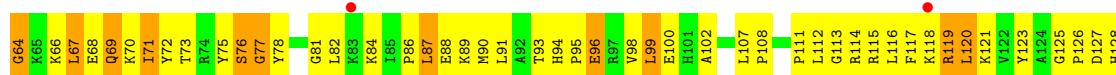
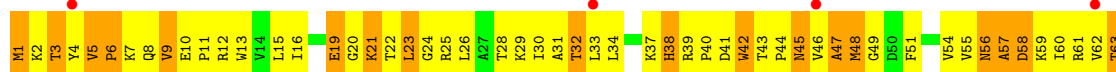
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:  7% 20% 55% 24%

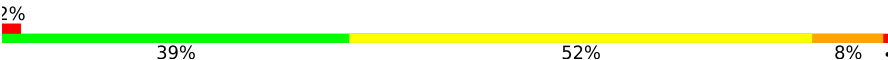


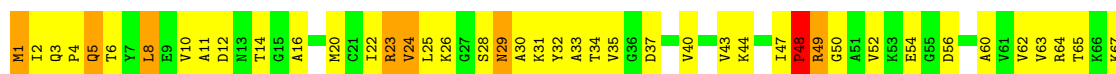
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN:  5% 20% 55% 24%



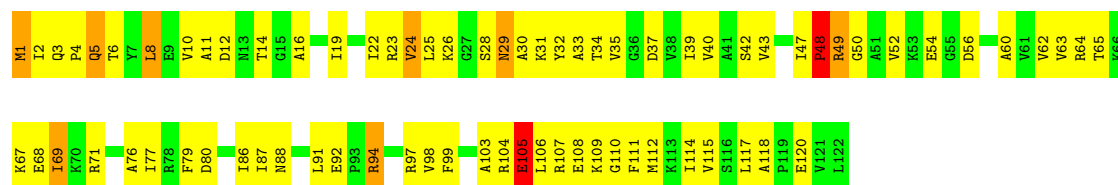
- Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:  2% 39% 52% 8%

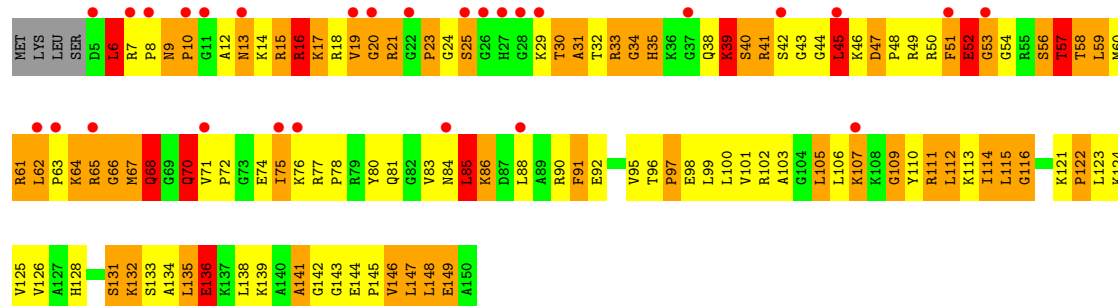
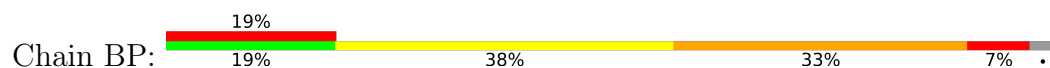


- Molecule 47: 50S RIBOSOMAL PROTEIN L14

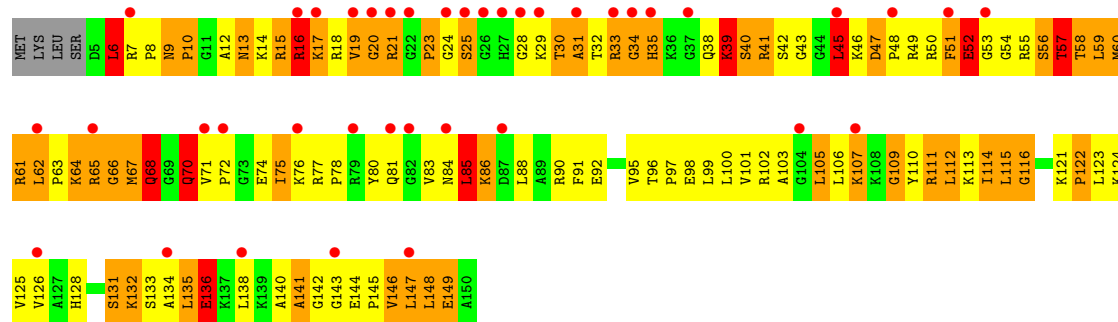
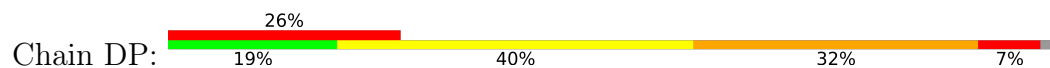
Chain DO:  39% 53% 7%



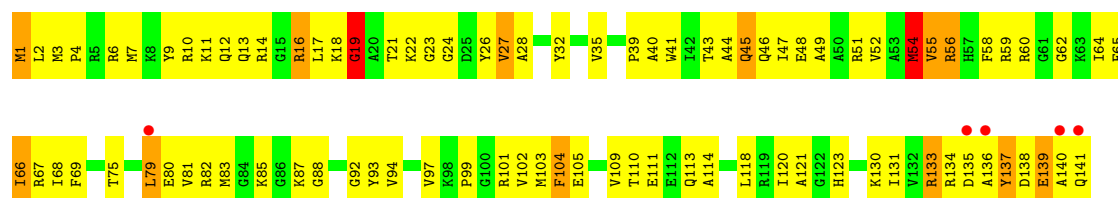
• Molecule 48: 50S RIBOSOMAL PROTEIN L15



• Molecule 48: 50S RIBOSOMAL PROTEIN L15

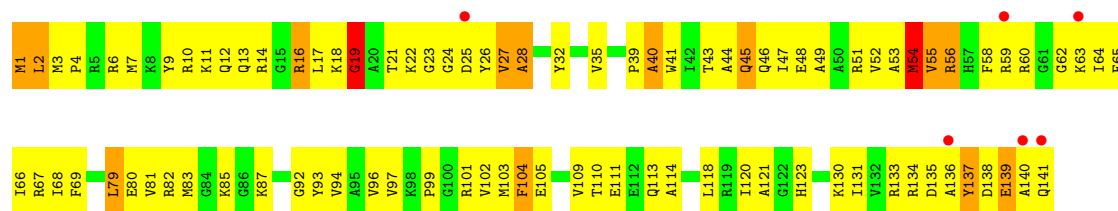


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

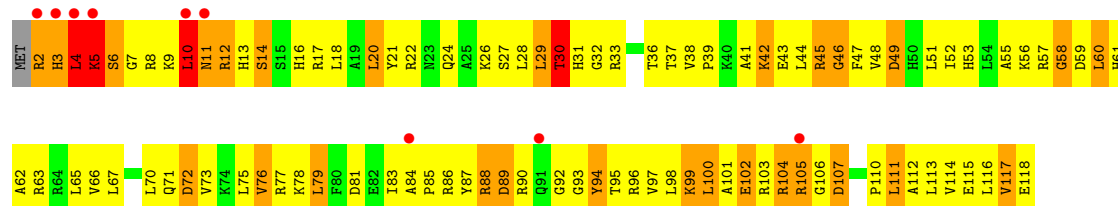
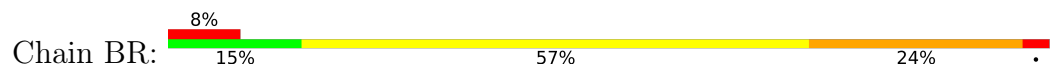


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

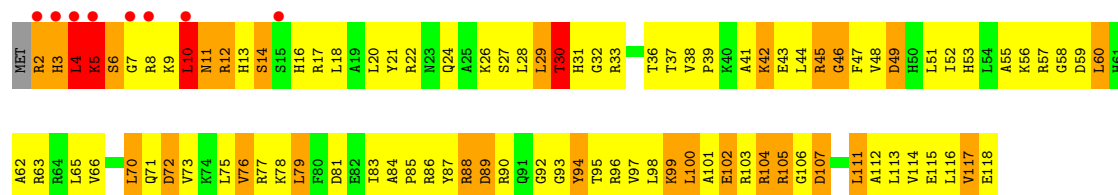
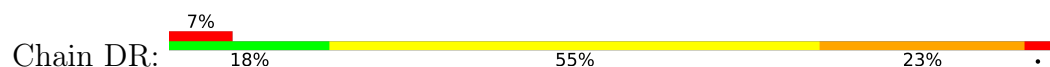




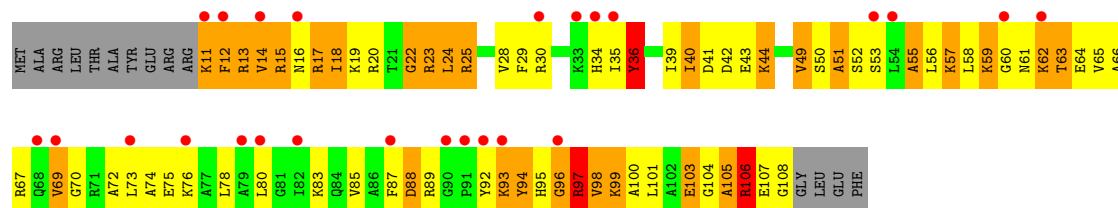
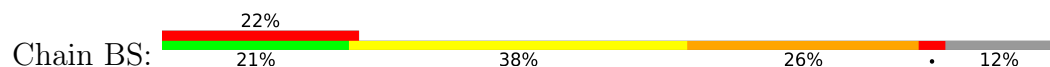
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



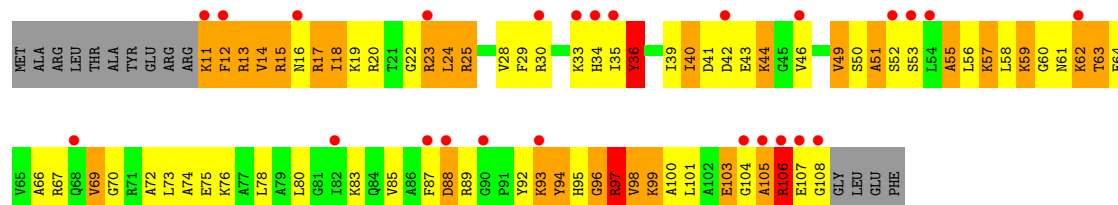
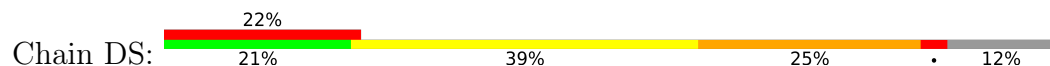
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



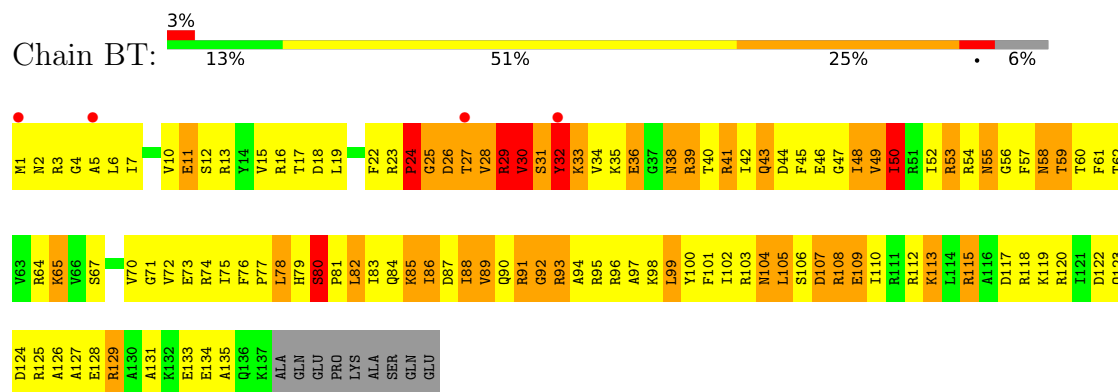
• Molecule 51: 50S RIBOSOMAL PROTEIN L18



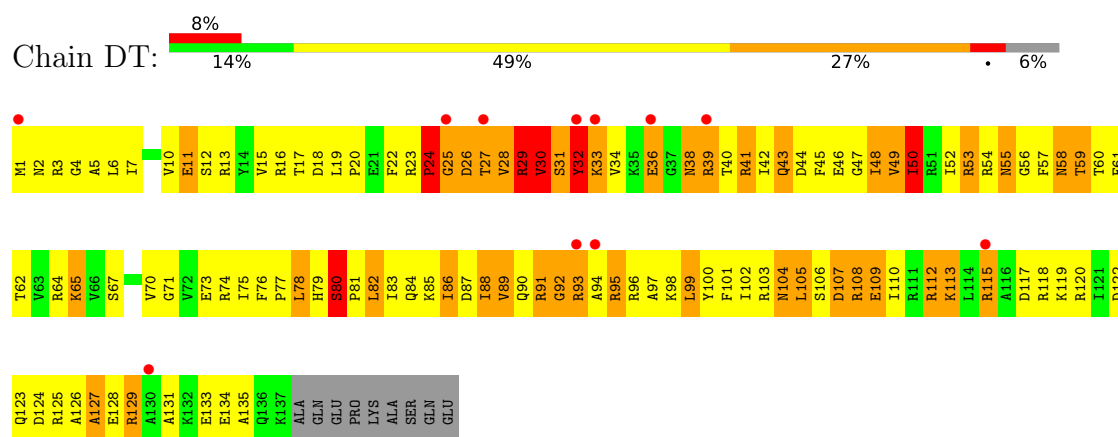
• Molecule 51: 50S RIBOSOMAL PROTEIN L18



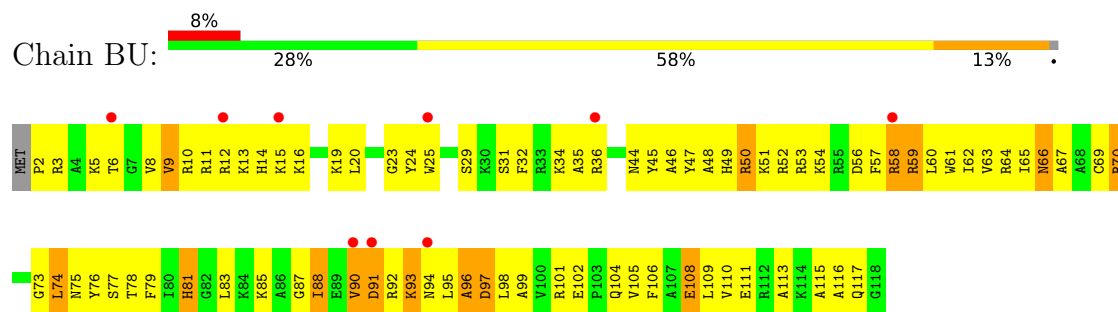
- Molecule 52: 50S RIBOSOMAL PROTEIN L19



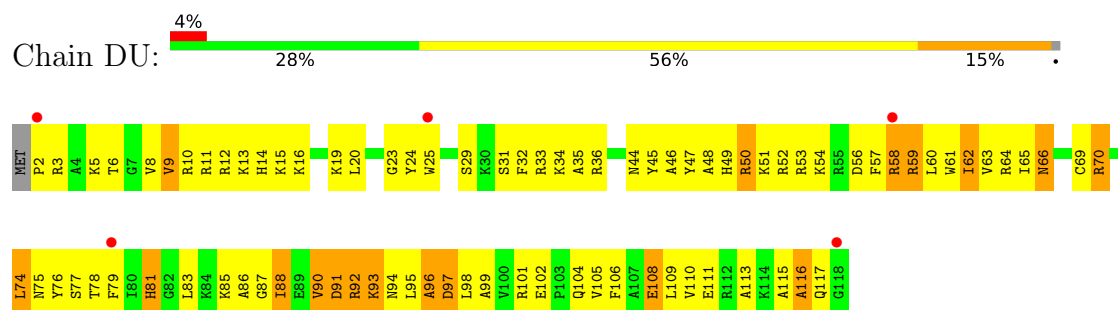
- Molecule 52: 50S RIBOSOMAL PROTEIN L19



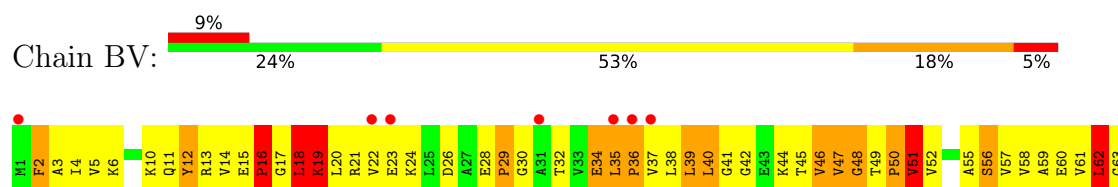
- Molecule 53: 50S RIBOSOMAL PROTEIN L20



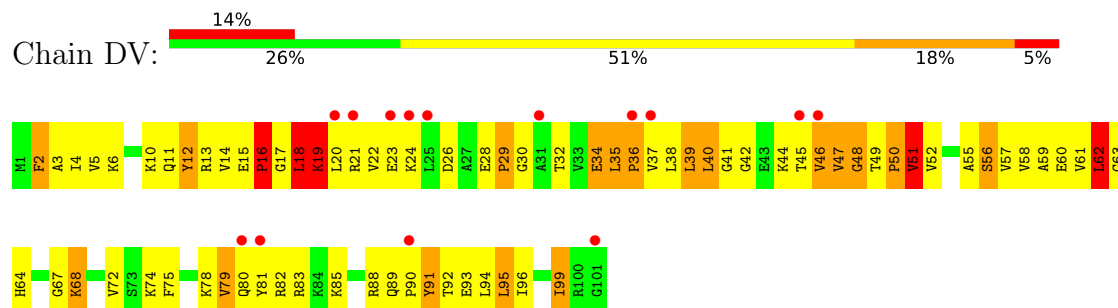
- Molecule 53: 50S RIBOSOMAL PROTEIN L20



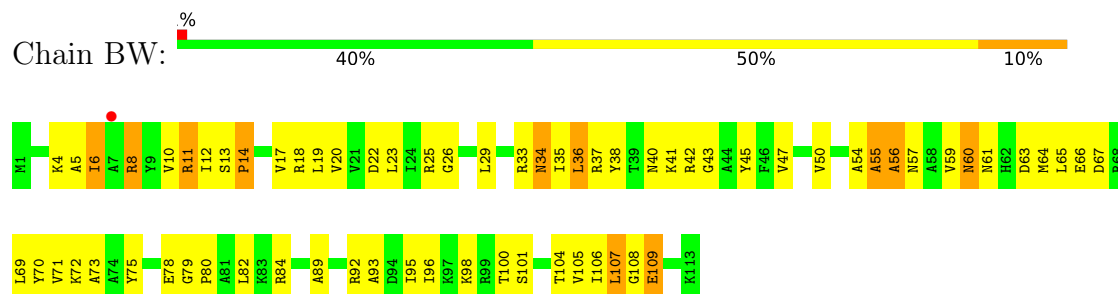
- Molecule 54: 50S RIBOSOMAL PROTEIN L21



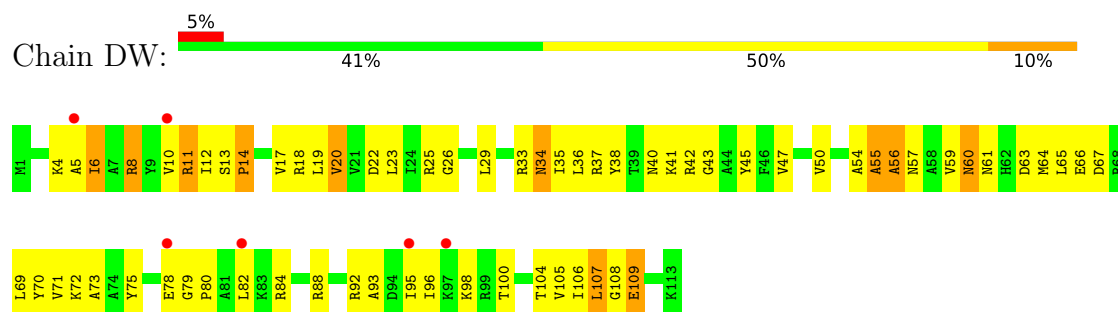
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



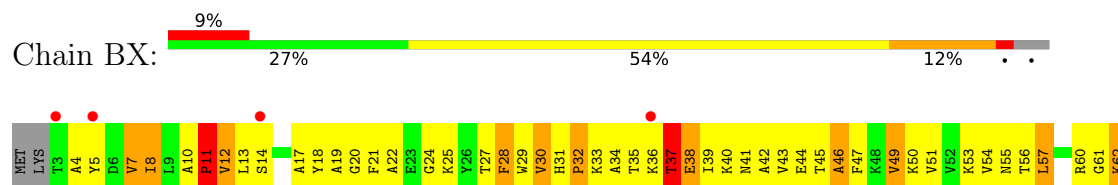
• Molecule 55: 50S RIBOSOMAL PROTEIN L22

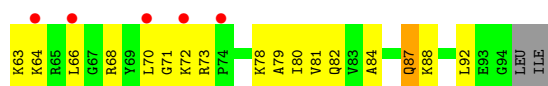


• Molecule 55: 50S RIBOSOMAL PROTEIN L22

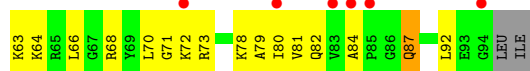


• Molecule 56: 50S RIBOSOMAL PROTEIN L23

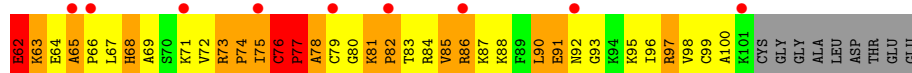
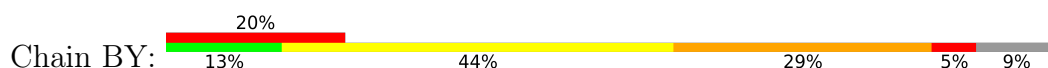




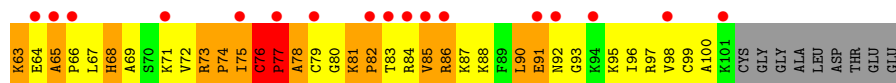
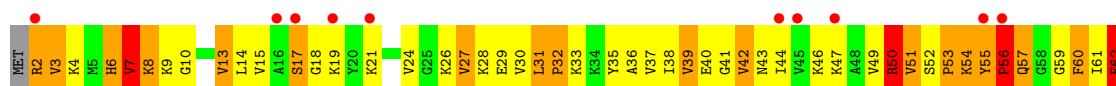
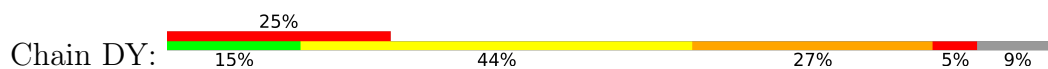
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



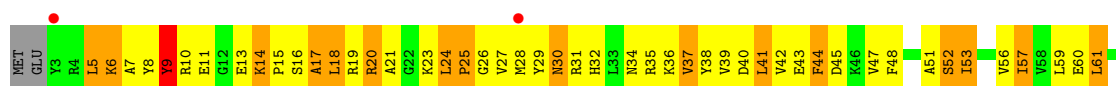
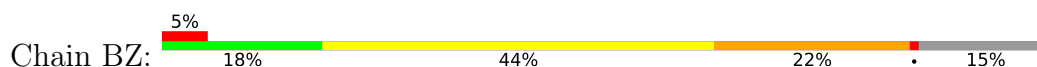
• Molecule 57: 50S RIBOSOMAL PROTEIN L24



• Molecule 57: 50S RIBOSOMAL PROTEIN L24

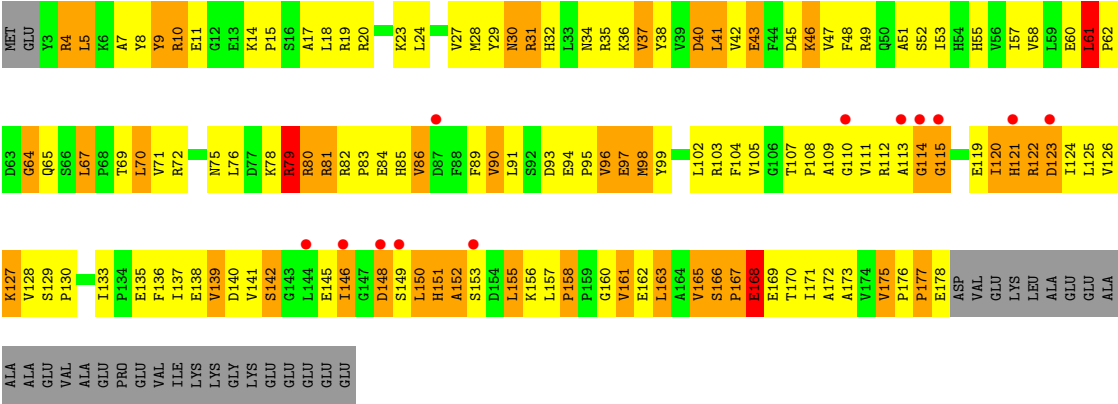
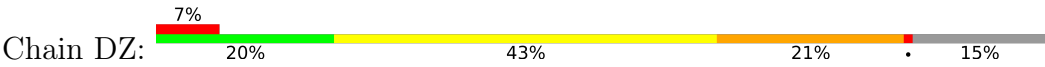


• Molecule 58: 50S RIBOSOMAL PROTEIN L25



ALA
GLU
PRO
GLU
VAL
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU

● Molecule 58: 50S RIBOSOMAL PROTEIN L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	290.20Å 269.20Å 404.00Å 90.00° 91.54° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.10) 99.8 (50.00-3.10)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.237 , 0.264 0.236 , 0.262	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)	0.28 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.48	2/36325 (0.0%)	0.72	59/56695 (0.1%)
1	CA	0.50	3/36325 (0.0%)	0.73	67/56695 (0.1%)
2	AB	0.56	0/1935	1.06	8/2609 (0.3%)
2	CB	0.61	0/1935	1.05	11/2609 (0.4%)
3	AC	0.61	0/1636	1.05	3/2205 (0.1%)
3	CC	0.76	0/1636	1.04	4/2205 (0.2%)
4	AD	0.50	0/1733	1.00	12/2318 (0.5%)
4	CD	0.51	0/1733	1.00	12/2318 (0.5%)
5	AE	0.64	0/1162	1.10	5/1564 (0.3%)
5	CE	0.75	0/1162	1.09	4/1564 (0.3%)
6	AF	0.51	0/856	0.98	3/1154 (0.3%)
6	CF	0.55	0/856	0.98	3/1154 (0.3%)
7	AG	0.52	0/1276	1.03	8/1709 (0.5%)
7	CG	0.61	0/1276	1.06	9/1709 (0.5%)
8	AH	0.58	0/1136	1.09	1/1527 (0.1%)
8	CH	0.63	0/1136	1.11	1/1527 (0.1%)
9	AI	0.49	0/1029	0.97	3/1379 (0.2%)
9	CI	0.56	0/1029	0.96	3/1379 (0.2%)
10	AJ	0.53	0/807	1.12	6/1085 (0.6%)
10	CJ	0.63	0/807	1.15	8/1085 (0.7%)
11	AK	0.56	0/900	1.09	5/1213 (0.4%)
11	CK	0.68	0/900	1.10	5/1213 (0.4%)
12	AL	0.58	0/986	1.11	8/1320 (0.6%)
12	CL	0.63	0/986	1.14	5/1320 (0.4%)
13	AM	0.55	0/998	1.11	7/1336 (0.5%)
13	CM	0.61	0/998	1.11	6/1336 (0.4%)
14	AN	0.66	0/501	1.18	5/664 (0.8%)
14	CN	0.69	0/501	1.17	3/664 (0.5%)
15	AO	0.59	0/745	0.98	1/992 (0.1%)
15	CO	0.62	0/745	0.99	2/992 (0.2%)
16	AP	0.54	0/716	1.01	4/963 (0.4%)
16	CP	0.55	0/716	1.01	3/963 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.56	0/836	1.02	4/1117 (0.4%)
17	CQ	0.58	0/836	1.01	2/1117 (0.2%)
18	AR	0.56	0/579	0.97	2/768 (0.3%)
18	CR	0.56	0/579	0.97	3/768 (0.4%)
19	AS	0.53	0/642	0.98	2/865 (0.2%)
19	CS	0.58	0/642	0.99	2/865 (0.2%)
20	AT	0.49	0/765	1.09	6/1007 (0.6%)
20	CT	0.52	0/765	1.10	6/1007 (0.6%)
21	AU	0.53	0/212	0.91	0/277
21	CU	0.56	0/212	0.90	2/277 (0.7%)
22	AV	0.52	0/1809	0.82	1/2819 (0.0%)
22	AW	0.52	0/1809	0.69	1/2819 (0.0%)
22	CV	0.54	0/1809	0.83	4/2819 (0.1%)
22	CW	0.52	0/1809	0.69	2/2819 (0.1%)
23	AX	0.60	0/406	0.93	2/631 (0.3%)
23	CX	0.67	0/406	0.96	3/631 (0.5%)
24	AY	0.45	1/1619 (0.1%)	0.61	0/2516
24	CY	0.45	0/1619	0.61	0/2516
25	AZ	0.89	4/3042 (0.1%)	1.06	26/4129 (0.6%)
25	CZ	0.87	4/3042 (0.1%)	1.05	24/4129 (0.6%)
26	B0	0.48	0/671	0.98	0/892
26	D0	0.50	0/671	0.99	2/892 (0.2%)
27	B1	0.56	0/738	1.10	3/981 (0.3%)
27	D1	0.61	0/738	1.21	8/981 (0.8%)
28	B2	0.40	0/600	1.04	6/793 (0.8%)
28	D2	0.52	0/600	1.36	16/793 (2.0%)
29	B3	0.44	0/472	0.91	0/634
29	D3	0.49	0/472	0.91	0/634
30	B4	0.53	0/349	0.94	0/474
30	D4	0.54	0/349	0.97	0/474
31	B5	0.56	0/473	0.96	2/639 (0.3%)
31	D5	0.53	0/473	0.95	3/639 (0.5%)
32	B6	0.74	0/440	1.29	6/586 (1.0%)
32	D6	0.78	0/440	1.33	6/586 (1.0%)
33	B7	0.53	0/426	1.08	2/561 (0.4%)
33	D7	0.54	0/426	1.13	2/561 (0.4%)
34	B8	0.62	0/515	1.08	1/679 (0.1%)
34	D8	0.67	0/515	1.08	1/679 (0.1%)
35	B9	0.66	0/310	1.05	0/407
35	D9	0.63	0/310	1.07	0/407
36	BA	0.46	1/69976 (0.0%)	0.68	68/109244 (0.1%)
36	DA	0.46	1/69976 (0.0%)	0.68	71/109244 (0.1%)
37	BB	0.45	0/2853	0.71	3/4451 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DB	0.43	0/2853	0.70	3/4451 (0.1%)
38	BC	0.52	4/1774 (0.2%)	0.93	6/2391 (0.3%)
38	DC	0.56	2/1774 (0.1%)	0.93	7/2391 (0.3%)
39	BD	0.63	0/2195	1.19	17/2955 (0.6%)
39	DD	0.68	0/2195	1.20	19/2955 (0.6%)
40	BE	0.53	0/1596	1.13	15/2153 (0.7%)
40	DE	0.54	0/1596	1.14	12/2153 (0.6%)
41	BF	0.45	0/1658	1.00	9/2244 (0.4%)
41	DF	0.45	0/1658	1.00	8/2244 (0.4%)
42	BG	0.47	0/1499	1.06	11/2016 (0.5%)
42	DG	0.57	0/1499	1.20	22/2016 (1.1%)
43	BH	0.47	0/1245	1.07	8/1682 (0.5%)
43	DH	0.48	0/1245	1.08	9/1682 (0.5%)
46	BN	0.47	0/1131	1.02	3/1525 (0.2%)
46	DN	0.49	0/1131	1.03	4/1525 (0.3%)
47	BO	0.59	0/943	1.07	2/1269 (0.2%)
47	DO	0.62	0/943	1.07	3/1269 (0.2%)
48	BP	0.52	0/1131	1.28	16/1504 (1.1%)
48	DP	0.56	0/1131	1.30	16/1504 (1.1%)
49	BQ	0.60	0/1143	1.04	3/1527 (0.2%)
49	DQ	0.65	0/1143	1.04	4/1527 (0.3%)
50	BR	0.51	0/974	1.01	5/1302 (0.4%)
50	DR	0.52	0/974	1.02	5/1302 (0.4%)
51	BS	0.49	0/778	1.05	5/1036 (0.5%)
51	DS	0.50	0/778	1.05	5/1036 (0.5%)
52	BT	0.55	0/1155	1.18	16/1542 (1.0%)
52	DT	0.56	0/1155	1.18	16/1542 (1.0%)
53	BU	0.47	0/975	1.11	9/1297 (0.7%)
53	DU	0.49	0/975	1.12	9/1297 (0.7%)
54	BV	0.46	0/790	0.94	2/1057 (0.2%)
54	DV	0.46	0/790	0.95	2/1057 (0.2%)
55	BW	0.47	0/907	0.96	3/1216 (0.2%)
55	DW	0.49	0/907	0.96	3/1216 (0.2%)
56	BX	0.47	0/739	1.06	6/993 (0.6%)
56	DX	0.49	0/739	1.05	5/993 (0.5%)
57	BY	0.50	0/788	1.09	7/1051 (0.7%)
57	DY	0.50	0/788	1.08	7/1051 (0.7%)
58	BZ	0.52	0/1435	1.10	9/1949 (0.5%)
58	DZ	0.56	0/1435	1.19	17/1949 (0.9%)
All	All	0.51	22/330278 (0.0%)	0.82	904/493462 (0.2%)

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 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	CZ	68	VAL	C-O	-33.22	0.84	1.24
25	AZ	68	VAL	C-O	-32.45	0.85	1.24
25	AZ	68	VAL	CA-CB	-9.72	1.41	1.54
25	CZ	68	VAL	CA-CB	-9.49	1.41	1.54
1	CA	1125	U	O5'-C5'	7.57	1.53	1.42

The worst 5 of 904 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1498	U	C2'-C3'-O3'	16.45	134.18	109.50
1	AA	1498	U	C2'-C3'-O3'	16.09	133.63	109.50
1	CA	1363(A)	A	C2'-C3'-O3'	15.77	133.16	109.50
1	AA	1363(A)	A	C2'-C3'-O3'	15.01	132.02	109.50
1	CA	508	C	C2'-C3'-O3'	14.86	131.78	109.50

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 [i](#)

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	856	0
2	AB	1900	0	1951	204	2
2	CB	1900	0	1951	195	2
3	AC	1612	0	1677	148	0
3	CC	1612	0	1677	147	0
4	AD	1703	0	1765	179	0
4	CD	1703	0	1765	169	0
5	AE	1146	0	1207	75	0
5	CE	1146	0	1207	72	0
6	AF	843	0	857	66	0
6	CF	843	0	857	61	0
7	AG	1257	0	1296	75	0
7	CG	1257	0	1296	69	0
8	AH	1116	0	1177	62	0
8	CH	1116	0	1177	55	0
9	AI	1010	0	1037	113	0
9	CI	1010	0	1037	112	0
10	AJ	794	0	840	119	0
10	CJ	794	0	840	117	0
11	AK	885	0	904	64	0
11	CK	885	0	904	65	0
12	AL	970	0	1057	100	0
12	CL	970	0	1057	97	0
13	AM	987	0	1059	119	0
13	CM	987	0	1059	122	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	48	0
15	CO	734	0	771	47	0
16	AP	700	0	720	84	0
16	CP	700	0	720	88	0
17	AQ	823	0	891	65	0
17	CQ	823	0	891	67	0
18	AR	574	0	644	49	0
18	CR	574	0	644	52	0
19	AS	629	0	652	81	0
19	CS	629	0	652	82	0
20	AT	763	0	861	102	0
20	CT	763	0	861	102	0
21	AU	208	0	221	26	0
21	CU	208	0	221	28	0
22	AV	1619	0	822	58	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	14	0
23	CX	362	0	184	14	0
24	AY	1645	0	853	133	0
24	CY	1645	0	853	89	0
25	AZ	2984	0	2997	494	0
25	CZ	2984	0	2997	400	0
26	B0	662	0	688	69	0
26	D0	662	0	688	67	0
27	B1	731	0	808	86	0
27	D1	731	0	808	83	0
28	B2	598	0	653	90	0
28	D2	598	0	653	227	0
29	B3	467	0	523	36	0
29	D3	467	0	523	37	0
30	B4	340	0	337	53	0
30	D4	340	0	336	58	0
31	B5	459	0	480	83	0
31	D5	459	0	480	75	0
32	B6	433	0	461	126	0
32	D6	433	0	461	126	0
33	B7	418	0	467	40	0
33	D7	418	0	467	39	0
34	B8	507	0	576	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D8	507	0	576	130	0
35	B9	307	0	337	35	0
35	D9	307	0	335	32	0
36	BA	62477	0	31497	2074	0
36	DA	62477	0	31497	2077	0
37	BB	2551	0	1295	92	0
37	DB	2551	0	1295	100	0
38	BC	1742	0	1800	172	2
38	DC	1742	0	1800	162	2
39	BD	2145	0	2234	264	0
39	DD	2145	0	2234	246	0
40	BE	1563	0	1629	248	0
40	DE	1563	0	1629	249	0
41	BF	1623	0	1677	225	0
41	DF	1623	0	1677	223	0
42	BG	1474	0	1535	249	0
42	DG	1474	0	1535	279	0
43	BH	1222	0	1282	168	0
43	DH	1222	0	1282	162	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	167	0
46	DN	1104	0	1180	167	0
47	BO	933	0	996	94	0
47	DO	933	0	996	92	0
48	BP	1114	0	1187	279	0
48	DP	1114	0	1187	276	0
49	BQ	1122	0	1179	128	0
49	DQ	1122	0	1179	139	0
50	BR	960	0	1021	157	0
50	DR	960	0	1021	157	0
51	BS	770	0	832	141	0
51	DS	770	0	832	142	0
52	BT	1141	0	1202	213	0
52	DT	1141	0	1202	217	0
53	BU	958	0	1015	137	0
53	DU	958	0	1015	138	0
54	BV	779	0	852	139	0
54	DV	779	0	852	143	0
55	BW	896	0	953	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	DW	896	0	953	87	0
56	BX	725	0	778	104	0
56	DX	725	0	778	99	0
57	BY	775	0	870	179	0
57	DY	775	0	870	174	0
58	BZ	1403	0	1432	219	0
58	DZ	1403	0	1432	196	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	17856	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 35.

The worst 5 of 17856 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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	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	6
3	CC	204/239 (85%)	171 (84%)	21 (10%)	12 (6%)	1	8
4	AD	206/209 (99%)	149 (72%)	39 (19%)	18 (9%)	0	4
4	CD	206/209 (99%)	149 (72%)	38 (18%)	19 (9%)	0	3
5	AE	148/162 (91%)	136 (92%)	10 (7%)	2 (1%)	9	34
5	CE	148/162 (91%)	136 (92%)	9 (6%)	3 (2%)	6	25
6	AF	99/101 (98%)	72 (73%)	18 (18%)	9 (9%)	0	3
6	CF	99/101 (98%)	73 (74%)	17 (17%)	9 (9%)	0	3
7	AG	153/156 (98%)	127 (83%)	22 (14%)	4 (3%)	4	21
7	CG	153/156 (98%)	129 (84%)	21 (14%)	3 (2%)	6	25
8	AH	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8	32
8	CH	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8	32
9	AI	125/128 (98%)	83 (66%)	34 (27%)	8 (6%)	1	6
9	CI	125/128 (98%)	83 (66%)	35 (28%)	7 (6%)	1	8
10	AJ	96/105 (91%)	69 (72%)	21 (22%)	6 (6%)	1	6
10	CJ	96/105 (91%)	71 (74%)	19 (20%)	6 (6%)	1	6
11	AK	117/129 (91%)	98 (84%)	18 (15%)	1 (1%)	14	44
11	CK	117/129 (91%)	99 (85%)	17 (14%)	1 (1%)	14	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AL	122/131 (93%)	104 (85%)	10 (8%)	8 (7%)	1	6
12	CL	122/131 (93%)	104 (85%)	10 (8%)	8 (7%)	1	6
13	AM	122/126 (97%)	85 (70%)	27 (22%)	10 (8%)	0	4
13	CM	122/126 (97%)	85 (70%)	28 (23%)	9 (7%)	1	5
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%)	5	23
15	CO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	5	23
16	AP	81/88 (92%)	58 (72%)	17 (21%)	6 (7%)	1	5
16	CP	81/88 (92%)	59 (73%)	16 (20%)	6 (7%)	1	5
17	AQ	97/105 (92%)	85 (88%)	7 (7%)	5 (5%)	1	10
17	CQ	97/105 (92%)	85 (88%)	7 (7%)	5 (5%)	1	10
18	AR	68/88 (77%)	55 (81%)	11 (16%)	2 (3%)	3	19
18	CR	68/88 (77%)	56 (82%)	10 (15%)	2 (3%)	3	19
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%)	0	4
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	12
21	CU	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	2	12
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%)	1	11
26	D0	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	1	11
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%)	0	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%)	0	3
29	D3	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	0	3
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%)	0	4
35	D9	35/37 (95%)	25 (71%)	7 (20%)	3 (9%)	0	4
38	BC	226/229 (99%)	170 (75%)	40 (18%)	16 (7%)	1	5
38	DC	226/229 (99%)	170 (75%)	40 (18%)	16 (7%)	1	5
39	BD	273/276 (99%)	214 (78%)	33 (12%)	26 (10%)	0	3
39	DD	273/276 (99%)	214 (78%)	34 (12%)	25 (9%)	0	3
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	0
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%)	2	13
47	DO	120/122 (98%)	100 (83%)	15 (12%)	5 (4%)	2	13
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	12
49	DQ	139/141 (99%)	108 (78%)	25 (18%)	6 (4%)	2	12

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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	12
53	DU	115/118 (98%)	82 (71%)	28 (24%)	5 (4%)	2	12
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%)	1	9
55	DW	111/113 (98%)	84 (76%)	21 (19%)	6 (5%)	1	9
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	2

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%)	181 (90%)	21 (10%)	7	27
3	AC	160/188 (85%)	138 (86%)	22 (14%)	3	15
3	CC	160/188 (85%)	138 (86%)	22 (14%)	3	15
4	AD	180/181 (99%)	163 (91%)	17 (9%)	8	31
4	CD	180/181 (99%)	162 (90%)	18 (10%)	7	29
5	AE	115/123 (94%)	103 (90%)	12 (10%)	7	27
5	CE	115/123 (94%)	102 (89%)	13 (11%)	5	23
6	AF	90/90 (100%)	79 (88%)	11 (12%)	5	20
6	CF	90/90 (100%)	79 (88%)	11 (12%)	5	20
7	AG	126/127 (99%)	116 (92%)	10 (8%)	11	37
7	CG	126/127 (99%)	115 (91%)	11 (9%)	9	34
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%)	91 (93%)	7 (7%)	13	41
9	CI	98/99 (99%)	91 (93%)	7 (7%)	13	41
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	5	23
10	CJ	88/92 (96%)	78 (89%)	10 (11%)	5	23
11	AK	90/99 (91%)	78 (87%)	12 (13%)	4	17
11	CK	90/99 (91%)	79 (88%)	11 (12%)	5	20
12	AL	104/108 (96%)	90 (86%)	14 (14%)	4	16
12	CL	104/108 (96%)	89 (86%)	15 (14%)	3	14
13	AM	99/101 (98%)	85 (86%)	14 (14%)	3	15
13	CM	99/101 (98%)	86 (87%)	13 (13%)	4	17
14	AN	49/50 (98%)	44 (90%)	5 (10%)	7	28
14	CN	49/50 (98%)	44 (90%)	5 (10%)	7	28
15	AO	79/80 (99%)	69 (87%)	10 (13%)	4	18
15	CO	79/80 (99%)	69 (87%)	10 (13%)	4	18
16	AP	72/74 (97%)	65 (90%)	7 (10%)	8	30
16	CP	72/74 (97%)	66 (92%)	6 (8%)	10	35
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	13	40
18	AR	61/77 (79%)	53 (87%)	8 (13%)	4	17
18	CR	61/77 (79%)	52 (85%)	9 (15%)	3	13
19	AS	69/80 (86%)	55 (80%)	14 (20%)	1	5
19	CS	69/80 (86%)	55 (80%)	14 (20%)	1	5
20	AT	76/82 (93%)	68 (90%)	8 (10%)	6	26
20	CT	76/82 (93%)	68 (90%)	8 (10%)	6	26
21	AU	19/22 (86%)	18 (95%)	1 (5%)	20	51
21	CU	19/22 (86%)	18 (95%)	1 (5%)	20	51
25	AZ	322/338 (95%)	277 (86%)	45 (14%)	3	15
25	CZ	322/338 (95%)	276 (86%)	46 (14%)	3	14
26	B0	66/67 (98%)	58 (88%)	8 (12%)	5	20
26	D0	66/67 (98%)	58 (88%)	8 (12%)	5	20
27	B1	78/83 (94%)	67 (86%)	11 (14%)	3	15
27	D1	78/83 (94%)	67 (86%)	11 (14%)	3	15
28	B2	66/67 (98%)	61 (92%)	5 (8%)	12	39
28	D2	66/67 (98%)	55 (83%)	11 (17%)	2	10
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%)	34 (87%)	5 (13%)	4	18
30	D4	39/63 (62%)	34 (87%)	5 (13%)	4	18
31	B5	51/52 (98%)	46 (90%)	5 (10%)	7	29
31	D5	51/52 (98%)	46 (90%)	5 (10%)	7	29
32	B6	49/52 (94%)	32 (65%)	17 (35%)	0	0
32	D6	49/52 (94%)	32 (65%)	17 (35%)	0	0
33	B7	41/42 (98%)	36 (88%)	5 (12%)	5	20
33	D7	41/42 (98%)	36 (88%)	5 (12%)	5	20
34	B8	53/55 (96%)	42 (79%)	11 (21%)	1	5
34	D8	53/55 (96%)	42 (79%)	11 (21%)	1	5
35	B9	34/34 (100%)	31 (91%)	3 (9%)	9	33
35	D9	34/34 (100%)	30 (88%)	4 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BC	180/181 (99%)	170 (94%)	10 (6%)	19	49
38	DC	180/181 (99%)	170 (94%)	10 (6%)	19	49
39	BD	217/218 (100%)	185 (85%)	32 (15%)	3	14
39	DD	217/218 (100%)	187 (86%)	30 (14%)	3	15
40	BE	165/166 (99%)	142 (86%)	23 (14%)	3	15
40	DE	165/166 (99%)	143 (87%)	22 (13%)	4	17
41	BF	165/166 (99%)	153 (93%)	12 (7%)	13	40
41	DF	165/166 (99%)	153 (93%)	12 (7%)	13	40
42	BG	155/156 (99%)	137 (88%)	18 (12%)	5	22
42	DG	155/156 (99%)	127 (82%)	28 (18%)	2	8
43	BH	132/148 (89%)	119 (90%)	13 (10%)	7	29
43	DH	132/148 (89%)	120 (91%)	12 (9%)	9	32
46	BN	117/119 (98%)	102 (87%)	15 (13%)	4	18
46	DN	117/119 (98%)	102 (87%)	15 (13%)	4	18
47	BO	100/100 (100%)	93 (93%)	7 (7%)	14	41
47	DO	100/100 (100%)	92 (92%)	8 (8%)	11	37
48	BP	112/116 (97%)	90 (80%)	22 (20%)	1	6
48	DP	112/116 (97%)	91 (81%)	21 (19%)	1	7
49	BQ	111/111 (100%)	101 (91%)	10 (9%)	9	33
49	DQ	111/111 (100%)	102 (92%)	9 (8%)	11	36
50	BR	100/101 (99%)	85 (85%)	15 (15%)	3	13
50	DR	100/101 (99%)	84 (84%)	16 (16%)	2	12
51	BS	77/88 (88%)	67 (87%)	10 (13%)	4	18
51	DS	77/88 (88%)	67 (87%)	10 (13%)	4	18
52	BT	120/127 (94%)	101 (84%)	19 (16%)	2	12
52	DT	120/127 (94%)	101 (84%)	19 (16%)	2	12
53	BU	92/94 (98%)	87 (95%)	5 (5%)	20	50
53	DU	92/94 (98%)	86 (94%)	6 (6%)	15	44
54	BV	82/82 (100%)	67 (82%)	15 (18%)	2	8
54	DV	82/82 (100%)	67 (82%)	15 (18%)	2	8
55	BW	91/92 (99%)	84 (92%)	7 (8%)	12	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	DW	91/92 (99%)	84 (92%)	7 (8%)	12	38
56	BX	74/78 (95%)	67 (90%)	7 (10%)	8	30
56	DX	74/78 (95%)	68 (92%)	6 (8%)	11	36
57	BY	84/91 (92%)	73 (87%)	11 (13%)	4	17
57	DY	84/91 (92%)	73 (87%)	11 (13%)	4	17
58	BZ	155/179 (87%)	128 (83%)	27 (17%)	2	9
58	DZ	155/179 (87%)	131 (84%)	24 (16%)	2	12
All	All	10338/10854 (95%)	9084 (88%)	1254 (12%)	5	20

5 of 1254 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	D4	5	ILE
50	DR	70	LEU
33	D7	1	MET
29	D3	48	GLU
41	DF	88	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 355 such sidechains are listed below:

Mol	Chain	Res	Type
14	CN	49	HIS
39	DD	116	GLN
17	CQ	26	GLN
25	CZ	285	ASN
40	DE	180	ASN

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%)	225 (14%)	46 (3%)
22	AV	75/76 (98%)	22 (29%)	1 (1%)
22	AW	75/76 (98%)	22 (29%)	2 (2%)
22	CV	75/76 (98%)	23 (30%)	1 (1%)
22	CW	75/76 (98%)	22 (29%)	3 (4%)
23	AX	16/27 (59%)	7 (43%)	1 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	CX	16/27 (59%)	5 (31%)	1 (6%)
24	AY	75/77 (97%)	25 (33%)	3 (4%)
24	CY	75/77 (97%)	25 (33%)	3 (4%)
36	BA	2900/2915 (99%)	498 (17%)	45 (1%)
36	DA	2900/2915 (99%)	496 (17%)	45 (1%)
37	BB	118/122 (96%)	22 (18%)	3 (2%)
37	DB	118/122 (96%)	22 (18%)	3 (2%)
All	All	9536/9630 (99%)	1641 (17%)	200 (2%)

5 of 1641 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 [i](#)

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	5MU	AY	54	24	19,22,23	0.33	0	27,32,35	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PSU	CY	55	24	18,21,22	0.89	1 (5%)	21,30,33	1.93	5 (23%)
24	H2U	AY	20	24	18,21,22	0.74	0	19,30,33	1.67	4 (21%)
24	H2U	CY	16	24	18,21,22	1.02	1 (5%)	19,30,33	1.64	3 (15%)
24	H2U	AY	16	24	18,21,22	1.03	1 (5%)	19,30,33	1.66	3 (15%)
24	5MU	CY	54	24	19,22,23	0.36	0	27,32,35	0.46	0
24	MIA	CY	37	24	28,31,32	0.84	2 (7%)	38,44,47	1.05	1 (2%)
24	H2U	CY	20	24	18,21,22	0.74	0	19,30,33	1.69	4 (21%)
24	H2U	AY	17	24	18,21,22	1.01	0	19,30,33	1.72	4 (21%)
24	OMC	AY	32	24	19,22,23	0.39	0	25,31,34	0.68	1 (4%)
24	H2U	CY	17	24	18,21,22	1.00	1 (5%)	19,30,33	1.72	4 (21%)
24	OMC	CY	32	24	19,22,23	0.33	0	25,31,34	0.67	1 (4%)
24	4SU	AY	8	24	18,21,22	0.53	0	25,30,33	0.83	2 (8%)
24	7MG	CY	46	24	23,26,27	2.66	3 (13%)	27,39,42	1.73	3 (11%)
24	PSU	AY	55	24	18,21,22	0.91	2 (11%)	21,30,33	1.88	5 (23%)
24	MIA	AY	37	24	28,31,32	0.72	1 (3%)	38,44,47	1.02	1 (2%)
24	7MG	AY	46	24	23,26,27	2.62	3 (13%)	27,39,42	1.74	3 (11%)
24	4SU	CY	8	24	18,21,22	0.49	0	25,30,33	0.87	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
24	H2U	AY	20	24	-	0/7/38/39	0/2/2/2
24	H2U	CY	16	24	-	0/7/38/39	0/2/2/2
24	H2U	AY	16	24	-	0/7/38/39	0/2/2/2
24	5MU	CY	54	24	-	0/7/25/26	0/2/2/2
24	MIA	CY	37	24	-	2/15/33/34	0/3/3/3
24	H2U	CY	20	24	-	0/7/38/39	0/2/2/2
24	H2U	AY	17	24	-	3/7/38/39	0/2/2/2
24	OMC	AY	32	24	-	0/9/27/28	0/2/2/2
24	H2U	CY	17	24	-	3/7/38/39	0/2/2/2
24	OMC	CY	32	24	-	0/9/27/28	0/2/2/2
24	4SU	AY	8	24	-	0/7/25/26	0/2/2/2
24	7MG	CY	46	24	-	1/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSU	AY	55	24	-	2/7/25/26	0/2/2/2
24	MIA	AY	37	24	-	2/15/33/34	0/3/3/3
24	7MG	AY	46	24	-	1/7/37/38	0/3/3/3
24	4SU	CY	8	24	-	0/7/25/26	0/2/2/2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	46	7MG	C8-N9	-11.95	1.38	1.45
24	AY	46	7MG	C8-N9	-11.85	1.38	1.45
24	CY	46	7MG	C5-N7	3.09	1.39	1.35
24	AY	46	7MG	C5-N7	3.06	1.39	1.35
24	CY	37	MIA	C2-S10	2.79	1.78	1.75

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	46	7MG	N9-C8-N7	6.90	113.14	103.37
24	CY	46	7MG	N9-C8-N7	6.87	113.09	103.37
24	CY	37	MIA	C11-S10-C2	5.43	106.32	102.25
24	AY	37	MIA	C11-S10-C2	5.17	106.13	102.25
24	CY	55	PSU	N1-C2-N3	4.89	120.33	115.17

There are no chirality outliers.

5 of 16 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.

11 monomers are involved in 18 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CY	37	MIA	1	0
24	CY	20	H2U	1	0
24	AY	17	H2U	3	0
24	CY	17	H2U	4	0
24	AY	8	4SU	1	0
24	CY	46	7MG	3	0
24	AY	46	7MG	3	0
24	CY	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
61	KIR	CZ	502	-	56,59,59	3.63	22 (39%)	60,84,84	1.63	11 (18%)
60	GDP	CZ	501	-	29,30,30	1.06	2 (6%)	45,47,47	1.80	6 (13%)
60	GDP	AZ	501	-	29,30,30	0.97	1 (3%)	45,47,47	1.49	6 (13%)
61	KIR	AZ	502	-	56,59,59	3.66	23 (41%)	60,84,84	1.62	11 (18%)

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
61	KIR	CZ	502	-	-	8/54/98/98	0/3/3/3
60	GDP	CZ	501	-	-	0/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	GDP	AZ	501	-	-	2/16/32/32	0/3/3/3
61	KIR	AZ	502	-	-	8/54/98/98	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CZ	502	KIR	O18-C17	-14.79	1.22	1.44
61	AZ	502	KIR	O18-C17	-14.51	1.23	1.44
61	AZ	502	KIR	O30-C30	-12.80	1.17	1.42
61	CZ	502	KIR	O30-C30	-12.45	1.18	1.42
61	CZ	502	KIR	O34-C33	-9.29	1.29	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CZ	501	GDP	C5-C4-N3	-6.25	118.45	128.39
60	CZ	501	GDP	C2-N3-C4	5.61	121.96	112.30
61	AZ	502	KIR	O29-C29-O34	-5.14	101.68	110.15
61	CZ	502	KIR	O29-C29-O34	-5.07	101.79	110.15
61	CZ	502	KIR	C48-C32-C47	-4.60	101.43	107.70

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	C4-C3-C7-C8
61	AZ	502	KIR	O18-C17-C19-C42
61	CZ	502	KIR	C4-C3-C7-C8
61	CZ	502	KIR	O18-C17-C19-C42

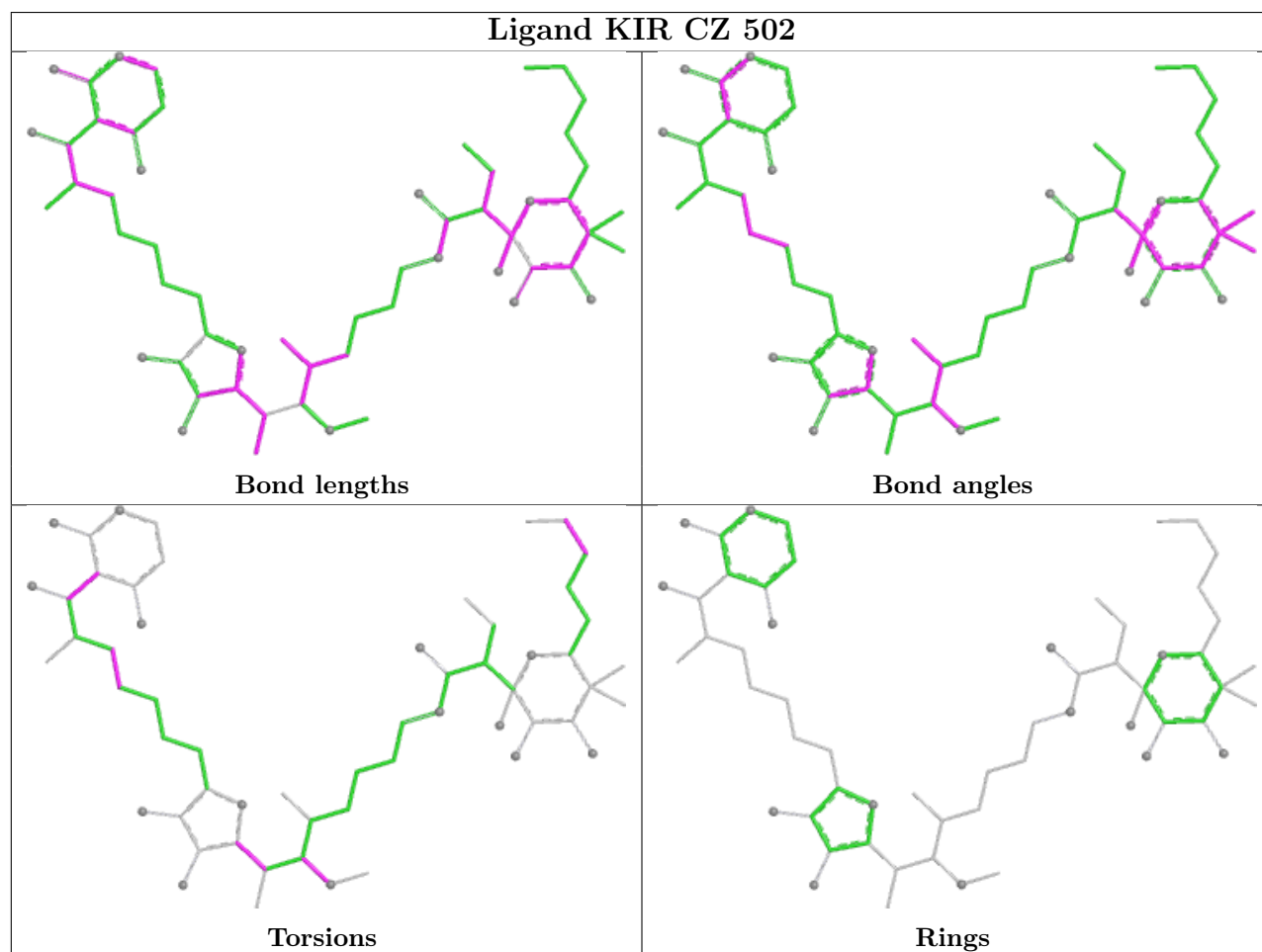
There are no ring outliers.

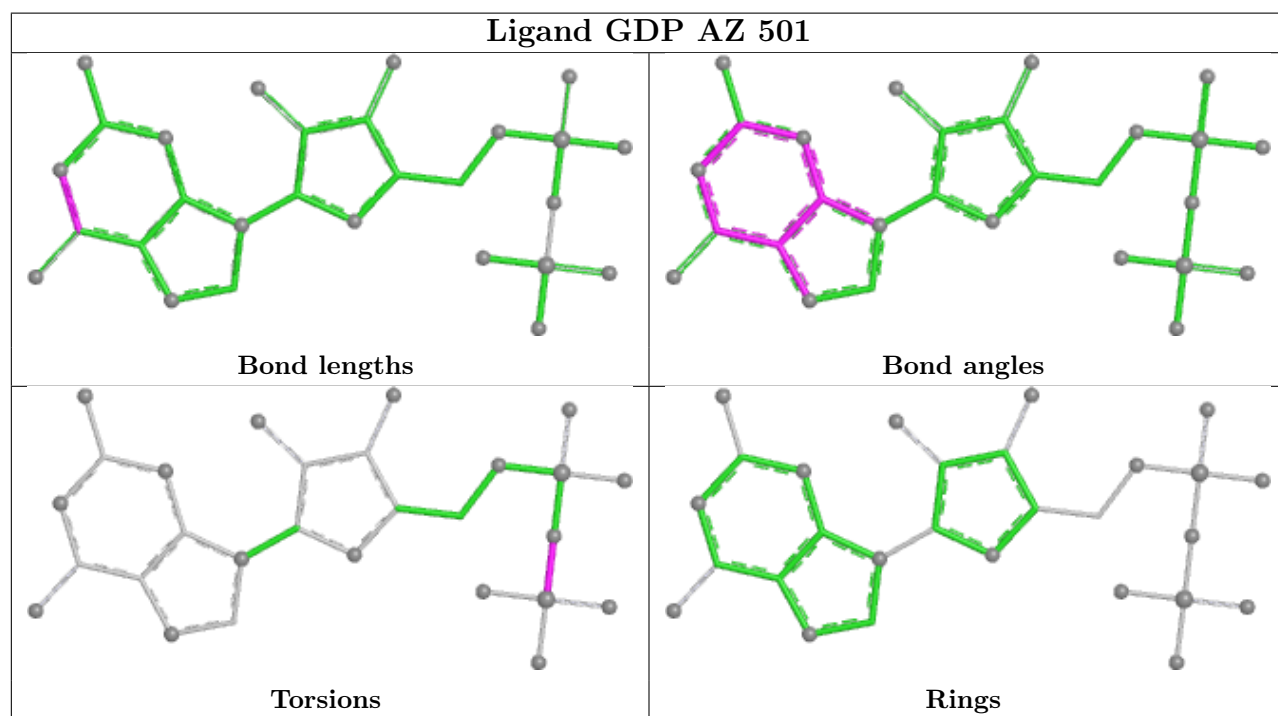
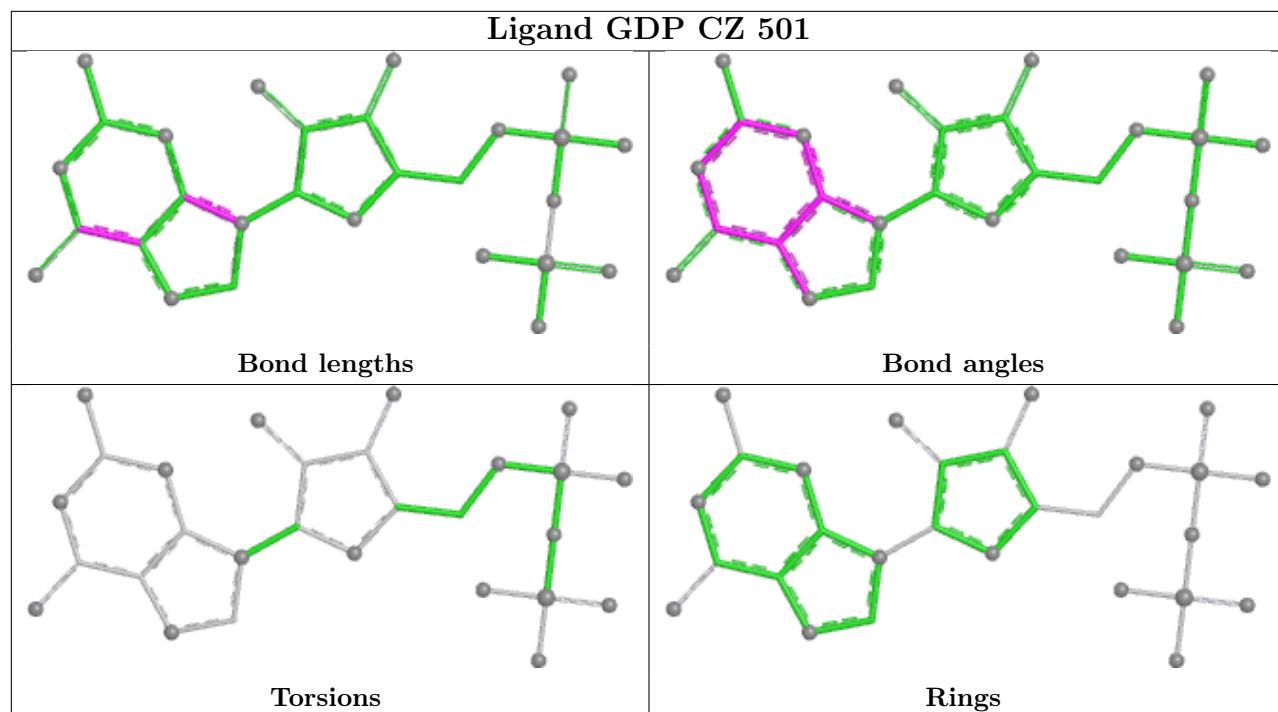
4 monomers are involved in 45 short contacts:

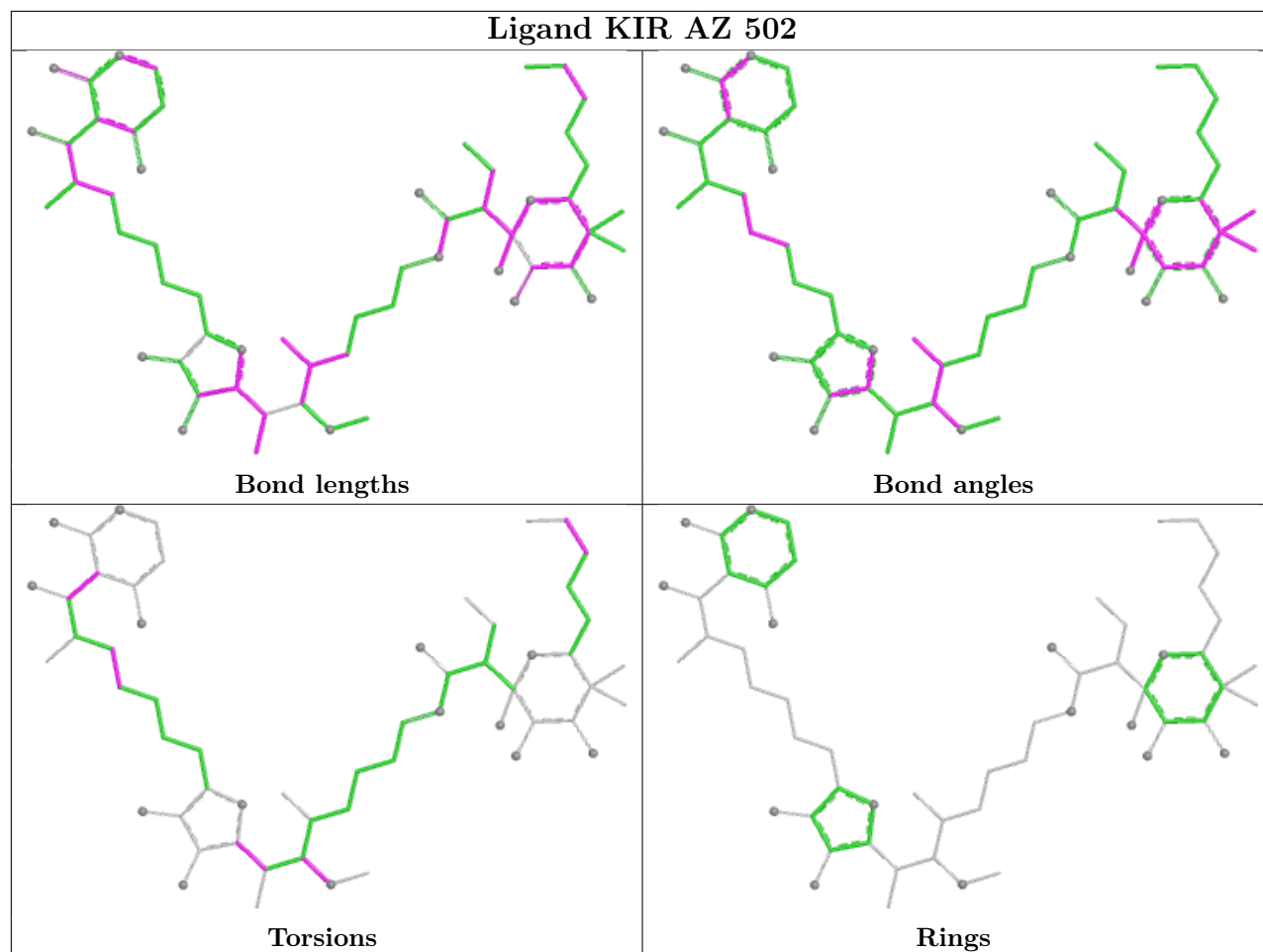
Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	CZ	502	KIR	9	0
60	CZ	501	GDP	8	0
60	AZ	501	GDP	15	0
61	AZ	502	KIR	13	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1510/1522 (99%)	0.07	31 (2%) 63 42	44, 78, 160, 200	0
1	CA	1510/1522 (99%)	0.21	68 (4%) 38 20	37, 73, 161, 200	0
2	AB	234/256 (91%)	0.46	13 (5%) 30 16	58, 88, 152, 164	0
2	CB	234/256 (91%)	0.52	20 (8%) 16 9	54, 86, 151, 164	0
3	AC	206/239 (86%)	0.21	4 (1%) 66 45	52, 75, 101, 110	0
3	CC	206/239 (86%)	0.33	5 (2%) 59 38	46, 70, 100, 109	0
4	AD	208/209 (99%)	0.53	10 (4%) 35 19	71, 97, 124, 132	0
4	CD	208/209 (99%)	0.67	13 (6%) 26 14	67, 96, 123, 131	0
5	AE	150/162 (92%)	-0.10	0 100 100	53, 65, 89, 110	0
5	CE	150/162 (92%)	-0.08	4 (2%) 56 35	49, 63, 88, 109	0
6	AF	101/101 (100%)	0.29	0 100 100	71, 99, 115, 122	0
6	CF	101/101 (100%)	0.56	4 (3%) 42 23	68, 97, 114, 121	0
7	AG	155/156 (99%)	0.43	7 (4%) 38 20	66, 89, 113, 130	0
7	CG	155/156 (99%)	0.54	8 (5%) 33 17	59, 86, 112, 129	0
8	AH	138/138 (100%)	0.03	1 (0%) 84 68	54, 70, 87, 95	0
8	CH	138/138 (100%)	0.07	1 (0%) 84 68	52, 67, 87, 94	0
9	AI	127/128 (99%)	0.76	10 (7%) 18 10	62, 96, 128, 139	0
9	CI	127/128 (99%)	0.98	13 (10%) 12 6	54, 93, 127, 139	0
10	AJ	98/105 (93%)	1.13	16 (16%) 4 2	59, 99, 141, 145	0
10	CJ	98/105 (93%)	1.18	18 (18%) 3 1	54, 95, 140, 144	0
11	AK	119/129 (92%)	0.18	3 (2%) 58 37	55, 73, 107, 134	0
11	CK	119/129 (92%)	0.29	4 (3%) 48 28	51, 68, 108, 133	0
12	AL	124/131 (94%)	0.07	1 (0%) 82 65	55, 70, 94, 132	0
12	CL	124/131 (94%)	0.06	1 (0%) 82 65	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%)	0.59	8 (6%)	25	13	71, 97, 124, 152	0
13	CM	124/126 (98%)	0.75	7 (5%)	30	16	67, 95, 123, 152	0
14	AN	60/61 (98%)	0.49	3 (5%)	34	18	57, 72, 93, 96	0
14	CN	60/61 (98%)	0.54	2 (3%)	49	29	49, 66, 91, 96	0
15	AO	88/89 (98%)	0.19	2 (2%)	61	39	57, 75, 99, 105	0
15	CO	88/89 (98%)	0.28	1 (1%)	78	59	56, 74, 98, 104	0
16	AP	83/88 (94%)	0.35	0	100	100	74, 91, 109, 135	0
16	CP	83/88 (94%)	0.62	3 (3%)	46	26	72, 89, 108, 136	0
17	AQ	99/105 (94%)	0.20	0	100	100	60, 79, 95, 108	0
17	CQ	99/105 (94%)	0.22	3 (3%)	52	31	57, 78, 93, 107	0
18	AR	70/88 (79%)	0.18	1 (1%)	73	53	58, 82, 106, 119	0
18	CR	70/88 (79%)	0.08	0	100	100	56, 79, 105, 118	0
19	AS	78/93 (83%)	0.86	9 (11%)	9	5	75, 99, 137, 139	0
19	CS	78/93 (83%)	0.99	11 (14%)	6	3	71, 99, 136, 139	0
20	AT	99/106 (93%)	0.56	6 (6%)	27	15	75, 97, 131, 135	0
20	CT	99/106 (93%)	0.68	8 (8%)	18	10	71, 96, 132, 135	0
21	AU	24/27 (88%)	0.94	3 (12%)	8	5	66, 84, 103, 114	0
21	CU	24/27 (88%)	0.90	2 (8%)	17	9	64, 78, 99, 115	0
22	AV	76/76 (100%)	0.44	3 (3%)	43	24	56, 91, 128, 148	0
22	AW	76/76 (100%)	1.95	28 (36%)	1	0	103, 172, 200, 200	0
22	CV	76/76 (100%)	0.57	5 (6%)	24	13	50, 89, 128, 147	0
22	CW	76/76 (100%)	2.43	48 (63%)	0	0	100, 172, 200, 200	0
23	AX	17/27 (62%)	1.01	5 (29%)	1	1	50, 97, 156, 157	0
23	CX	17/27 (62%)	0.88	4 (23%)	2	1	45, 95, 156, 157	0
24	AY	68/77 (88%)	0.53	3 (4%)	39	21	61, 140, 171, 190	0
24	CY	68/77 (88%)	0.45	3 (4%)	39	21	57, 140, 170, 190	0
25	AZ	385/405 (95%)	2.30	202 (52%)	0	0	116, 142, 165, 183	0
25	CZ	385/405 (95%)	0.99	46 (11%)	9	5	113, 141, 165, 183	0
26	B0	84/85 (98%)	0.72	7 (8%)	17	9	77, 91, 118, 131	0
26	D0	84/85 (98%)	0.60	6 (7%)	22	12	76, 90, 119, 131	0
27	B1	93/98 (94%)	0.48	4 (4%)	40	22	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%)	0.48	6 (6%) 25 13	56, 76, 130, 142	0
28	B2	71/72 (98%)	0.38	3 (4%) 40 22	110, 133, 148, 157	0
28	D2	71/72 (98%)	1.65	23 (32%) 1 0	134, 154, 174, 175	0
29	B3	59/60 (98%)	0.61	3 (5%) 33 18	80, 99, 120, 142	0
29	D3	59/60 (98%)	0.53	0 100 100	80, 97, 120, 142	0
30	B4	44/71 (61%)	0.89	8 (18%) 3 1	124, 149, 160, 163	0
30	D4	44/71 (61%)	1.65	11 (25%) 2 1	123, 147, 158, 163	0
31	B5	59/60 (98%)	1.02	7 (11%) 9 5	73, 105, 158, 176	0
31	D5	59/60 (98%)	1.00	8 (13%) 7 4	72, 104, 158, 176	0
32	B6	50/54 (92%)	1.19	10 (20%) 3 1	74, 106, 116, 125	0
32	D6	50/54 (92%)	2.00	20 (40%) 1 0	73, 104, 115, 123	0
33	B7	48/49 (97%)	0.56	1 (2%) 63 42	70, 79, 119, 139	0
33	D7	48/49 (97%)	0.60	1 (2%) 63 42	68, 78, 119, 140	0
34	B8	63/65 (96%)	1.05	10 (15%) 5 2	80, 90, 104, 131	0
34	D8	63/65 (96%)	1.06	11 (17%) 4 2	78, 88, 104, 131	0
35	B9	37/37 (100%)	1.15	7 (18%) 3 1	76, 90, 104, 108	0
35	D9	37/37 (100%)	0.97	6 (16%) 4 2	76, 90, 104, 107	0
36	BA	2901/2915 (99%)	0.43	142 (4%) 35 18	49, 95, 190, 200	0
36	DA	2901/2915 (99%)	0.53	144 (4%) 34 18	46, 93, 190, 200	0
37	BB	119/122 (97%)	0.50	3 (2%) 58 37	78, 108, 134, 157	0
37	DB	119/122 (97%)	0.66	5 (4%) 40 22	75, 107, 133, 157	0
38	BC	228/229 (99%)	0.51	9 (3%) 43 24	69, 99, 177, 186	0
38	DC	228/229 (99%)	0.76	27 (11%) 9 5	67, 97, 177, 187	0
39	BD	275/276 (99%)	0.19	12 (4%) 39 21	50, 68, 98, 123	0
39	DD	275/276 (99%)	0.25	12 (4%) 39 21	47, 66, 97, 123	0
40	BE	204/206 (99%)	0.79	21 (10%) 12 6	64, 93, 141, 152	0
40	DE	204/206 (99%)	0.78	17 (8%) 17 9	64, 93, 141, 152	0
41	BF	207/210 (98%)	0.83	20 (9%) 13 7	73, 128, 176, 184	0
41	DF	207/210 (98%)	0.92	20 (9%) 13 7	70, 127, 176, 184	0
42	BG	181/182 (99%)	0.70	14 (7%) 19 10	97, 125, 147, 157	0
42	DG	181/182 (99%)	0.59	12 (6%) 24 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%)	0.97	21 (13%) 7 4	106, 142, 163, 165	0
43	DH	159/180 (88%)	1.01	22 (13%) 6 4	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%)	0.62	10 (7%) 21 11	78, 104, 145, 148	0
46	DN	138/140 (98%)	0.74	7 (5%) 33 18	77, 104, 144, 147	0
47	BO	122/122 (100%)	0.05	3 (2%) 58 37	58, 76, 90, 97	0
47	DO	122/122 (100%)	0.17	0 100 100	57, 76, 89, 97	0
48	BP	146/150 (97%)	1.19	28 (19%) 3 1	73, 121, 146, 162	0
48	DP	146/150 (97%)	1.65	39 (26%) 1 1	72, 120, 145, 162	0
49	BQ	141/141 (100%)	0.44	5 (3%) 47 27	61, 78, 107, 138	0
49	DQ	141/141 (100%)	0.46	6 (4%) 40 22	60, 77, 107, 139	0
50	BR	117/118 (99%)	0.67	9 (7%) 19 10	76, 98, 114, 129	0
50	DR	117/118 (99%)	0.68	8 (6%) 23 12	75, 98, 115, 129	0
51	BS	98/112 (87%)	1.35	25 (25%) 1 1	89, 112, 137, 141	0
51	DS	98/112 (87%)	1.44	25 (25%) 1 1	88, 111, 136, 140	0
52	BT	137/146 (93%)	0.58	4 (2%) 53 32	74, 97, 155, 179	0
52	DT	137/146 (93%)	0.69	11 (8%) 18 10	73, 97, 154, 179	0
53	BU	117/118 (99%)	0.71	9 (7%) 19 10	81, 98, 125, 142	0
53	DU	117/118 (99%)	0.70	5 (4%) 40 22	78, 97, 125, 142	0
54	BV	101/101 (100%)	0.97	9 (8%) 15 8	79, 130, 146, 150	0
54	DV	101/101 (100%)	1.11	14 (13%) 6 4	79, 129, 146, 150	0
55	BW	113/113 (100%)	0.43	1 (0%) 81 63	85, 100, 133, 165	0
55	DW	113/113 (100%)	0.68	6 (5%) 32 17	82, 100, 133, 165	0
56	BX	92/96 (95%)	0.87	9 (9%) 13 7	83, 109, 125, 134	0
56	DX	92/96 (95%)	1.06	13 (14%) 6 3	83, 108, 124, 134	0
57	BY	100/110 (90%)	1.45	22 (22%) 2 1	127, 146, 179, 187	0
57	DY	100/110 (90%)	1.46	27 (27%) 1 1	126, 146, 179, 187	0
58	BZ	176/206 (85%)	0.63	10 (5%) 29 16	75, 103, 135, 144	0
58	DZ	176/206 (85%)	0.61	14 (7%) 18 10	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%)	0.57	1643 (7%) 20 11	37, 93, 162, 200	0

The worst 5 of 1643 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	BQ	141	GLN	11.8
49	DQ	141	GLN	9.5
14	CN	2	ALA	9.3
25	CZ	63	ILE	8.7
25	AZ	203	LEU	8.6

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	AY	17	20/21	0.42	0.16	194,195,195,195	0
24	H2U	CY	17	20/21	0.42	0.19	194,195,195,195	0
24	H2U	CY	16	20/21	0.47	0.21	181,191,191,193	0
24	H2U	AY	16	20/21	0.49	0.16	181,191,192,193	0
24	H2U	AY	20	20/21	0.49	0.14	186,186,188,188	0
24	7MG	AY	46	24/25	0.60	0.17	166,169,171,171	0
24	H2U	CY	20	20/21	0.62	0.16	185,186,187,187	0
24	7MG	CY	46	24/25	0.68	0.15	166,168,170,170	0
24	PSU	AY	55	20/21	0.69	0.11	157,166,168,168	0
24	PSU	CY	55	20/21	0.73	0.11	158,166,168,168	0
24	4SU	AY	8	20/21	0.77	0.17	140,143,144,144	0
24	5MU	CY	54	21/22	0.82	0.10	142,153,154,156	0
24	5MU	AY	54	21/22	0.84	0.10	143,153,153,156	0
24	OMC	CY	32	21/22	0.88	0.12	96,103,108,109	0
24	OMC	AY	32	21/22	0.88	0.14	98,106,112,113	0
24	MIA	CY	37	29/30	0.89	0.16	60,80,107,108	0
24	MIA	AY	37	29/30	0.90	0.15	63,84,108,108	0
24	4SU	CY	8	20/21	0.90	0.16	140,141,142,142	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.76	0.23	139,147,150,150	0
61	KIR	CZ	502	57/57	0.81	0.18	139,145,150,151	0
60	GDP	AZ	501	28/28	0.83	0.14	151,157,158,158	0
59	ZN	B4	101	1/1	0.88	0.09	200,200,200,200	0
60	GDP	CZ	501	28/28	0.89	0.12	141,145,153,153	0
59	ZN	B9	101	1/1	0.94	0.08	200,200,200,200	0
59	ZN	AD	301	1/1	0.97	0.19	99,99,99,99	0
59	ZN	D4	101	1/1	0.99	0.03	129,129,129,129	0
59	ZN	D9	101	1/1	0.99	0.02	133,133,133,133	0
59	ZN	CD	301	1/1	0.99	0.18	85,85,85,85	0
59	ZN	AN	101	1/1	1.00	0.01	84,84,84,84	0
59	ZN	CN	101	1/1	1.00	0.01	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.