



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 30, 2026 – 01:36 PM EDT

PDB ID : 4V5P / pdb_00004v5p
Title : The crystal structure of EF-Tu and A9C-tRNA-Trp bound to a near- cognate codon on the 70S ribosome
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.
Deposited on : 2010-12-07
Resolution : 3.10 Å(reported)

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

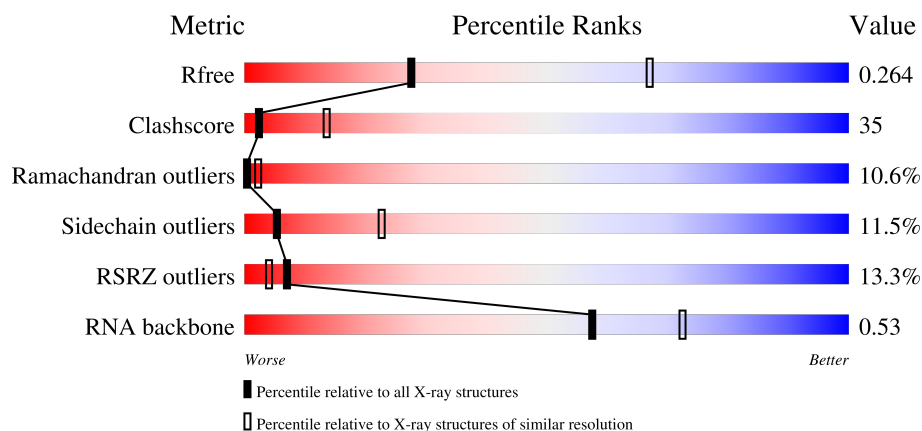
1 Overall quality at a glance

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	11% 36% 49% 12% • •
1	CA	1522	6% 34% 51% 11% • •
2	AB	256	15% 27% 49% 14% • 9%
2	CB	256	9% 24% 52% 14% • 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	135	
12	CL	135	
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
24	PSU	AY	55	X	-	-	-
24	PSU	CY	55	X	-	-	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 307322 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			

There are 8 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	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			

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

- Molecule 24 is a RNA chain called A-SITE TRNA A9C TRP-TRNA TRP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AY	77	Total	C	N	O	P	S	0	0	0
			1643	741	287	537	76	2			
24	CY	77	Total	C	N	O	P	S	0	0	0
			1643	741	287	537	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
			2983	1886	522	563	12				
25	CZ	385	Total	C	N	O	S		0	0	0
			2983	1886	522	563	12				

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	6	ILE	VAL	conflict	UNP Q5SHN6
AZ	264	LYS	ARG	conflict	UNP Q5SHN6
CZ	6	ILE	VAL	conflict	UNP Q5SHN6
CZ	264	LYS	ARG	conflict	UNP Q5SHN6

- 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				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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				

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

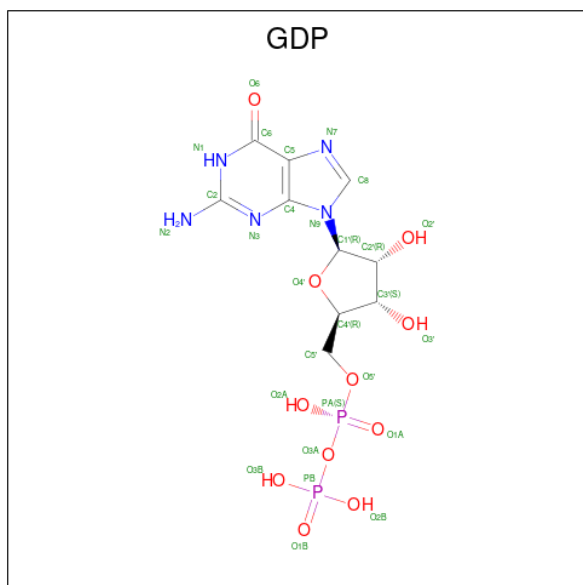
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B4	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		

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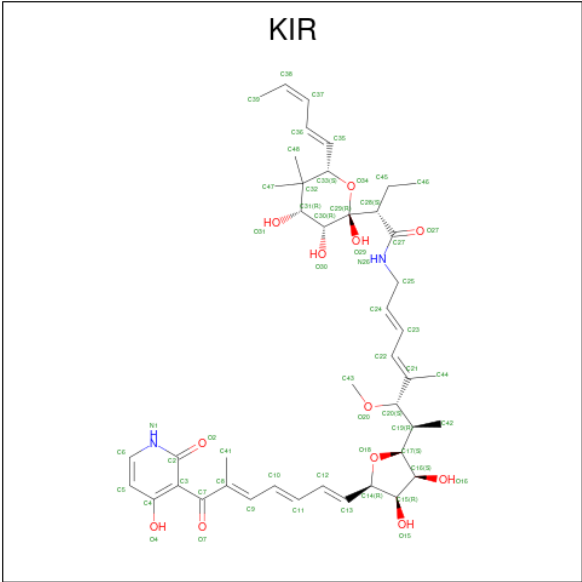
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CN	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		

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

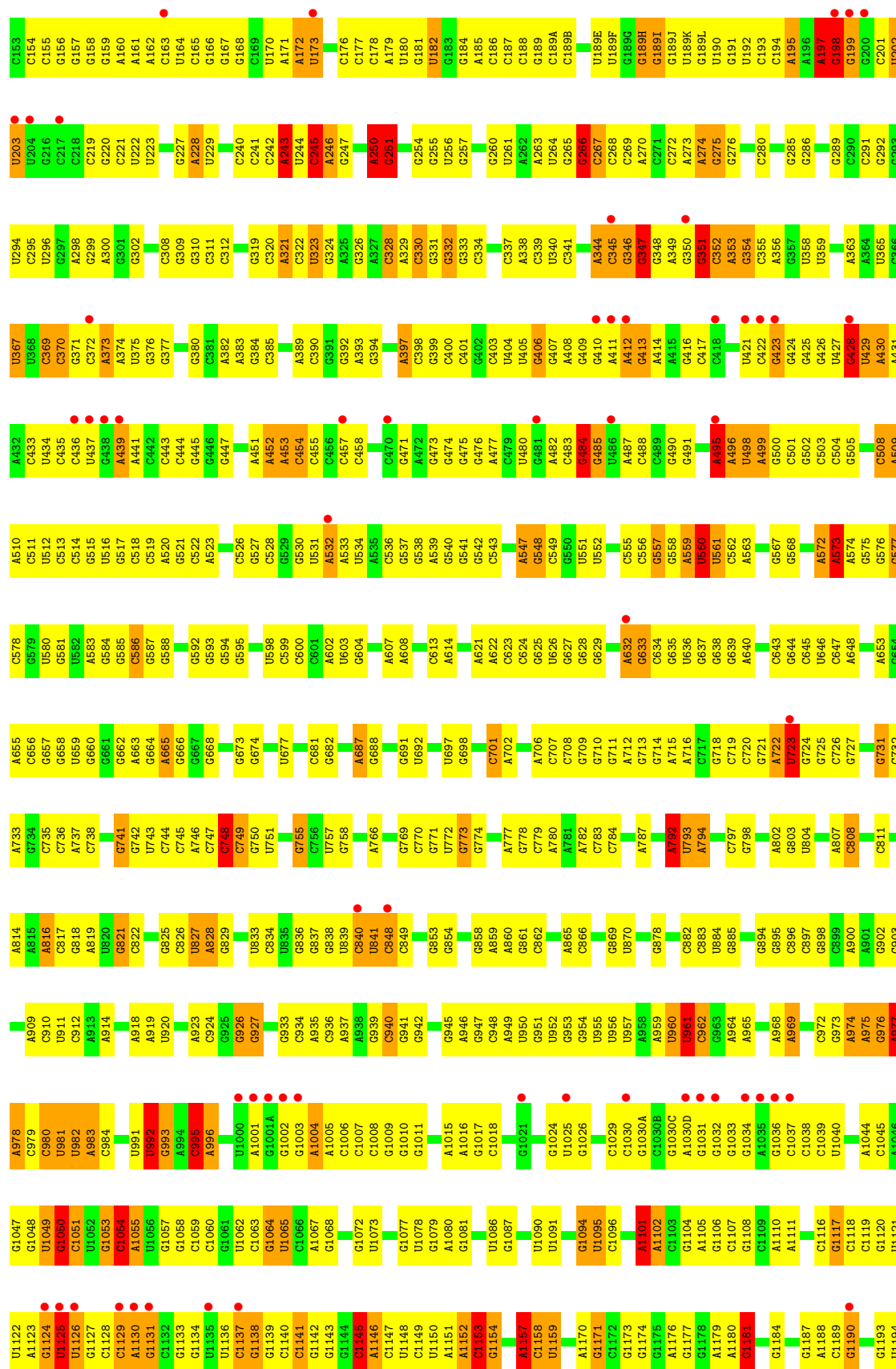


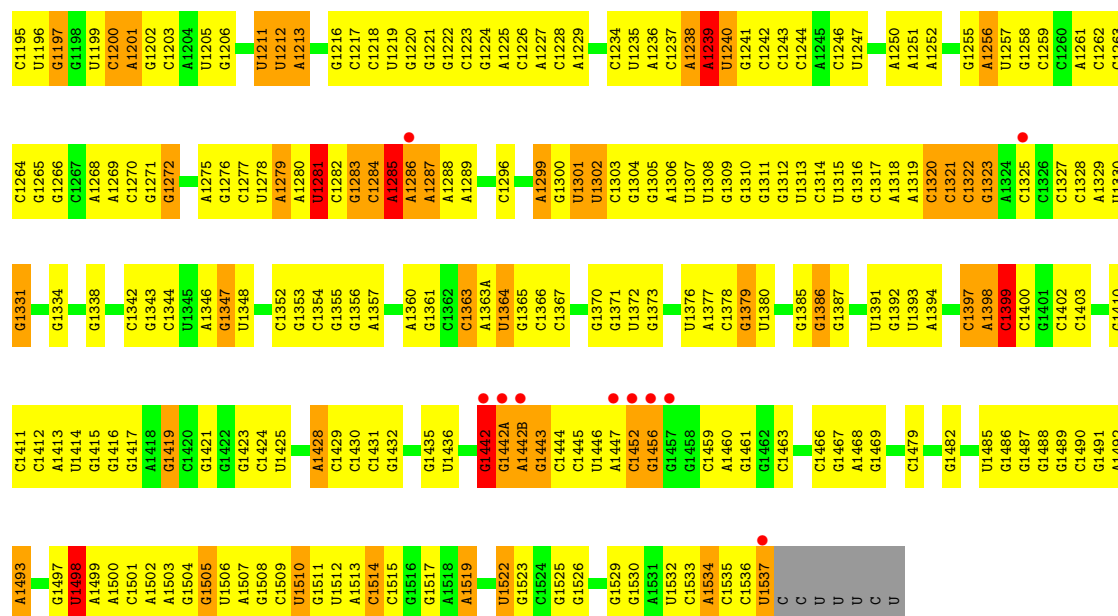
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
60	AZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
60	CZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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

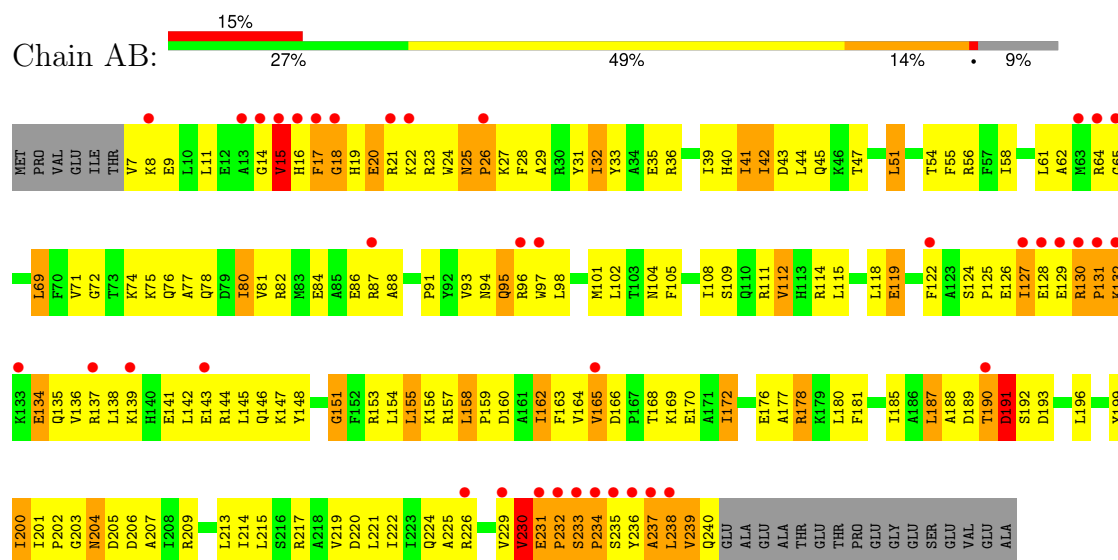


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
61	AZ	1	Total	C	N	O	0	0
			57	43	2	12		
61	CZ	1	Total	C	N	O	0	0
			57	43	2	12		

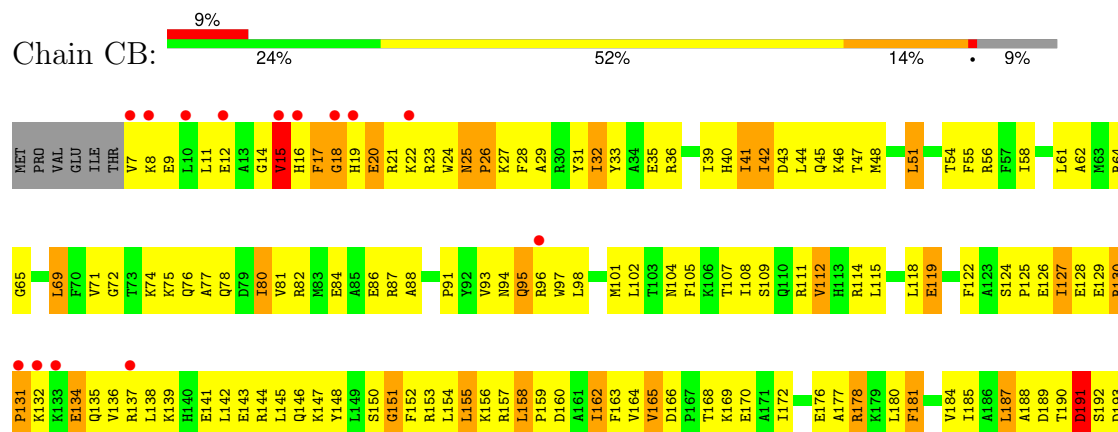


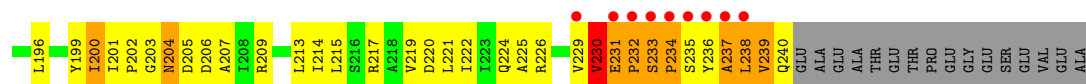


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

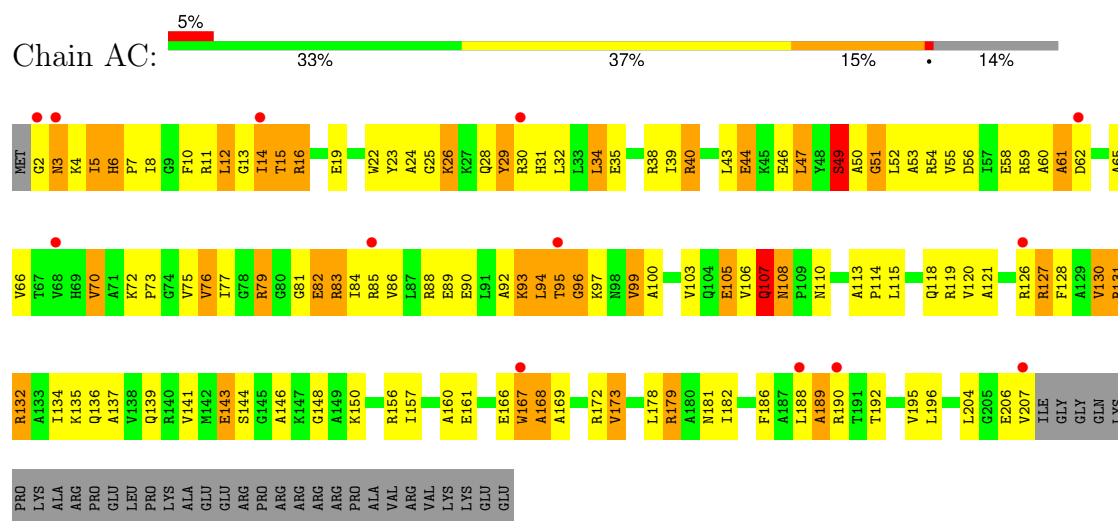


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

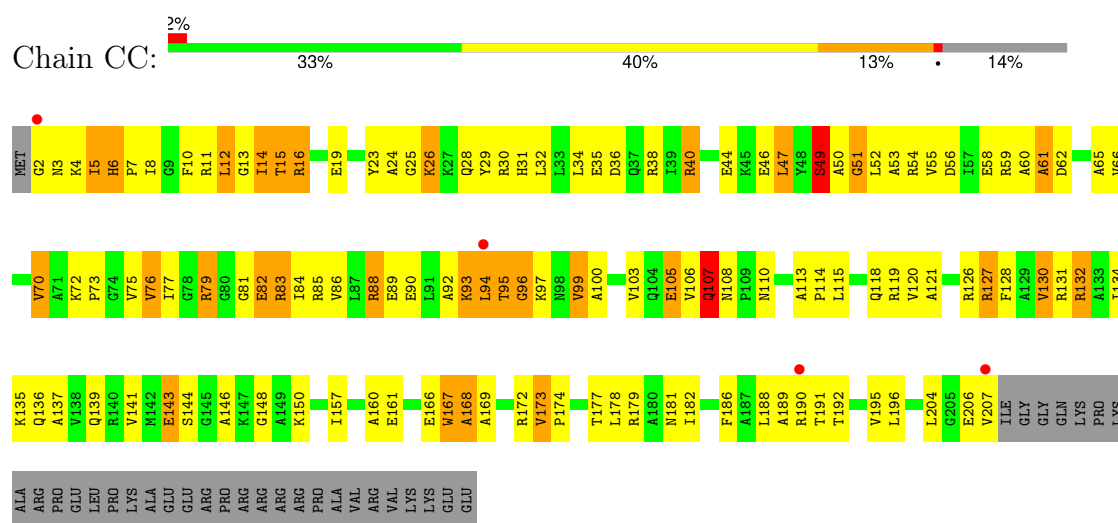




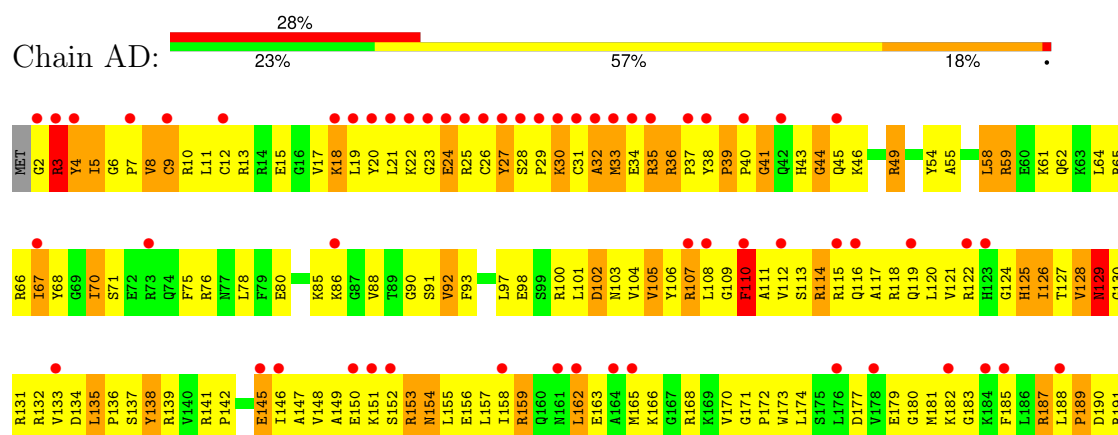
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



• Molecule 3: 30S RIBOSOMAL PROTEIN S3

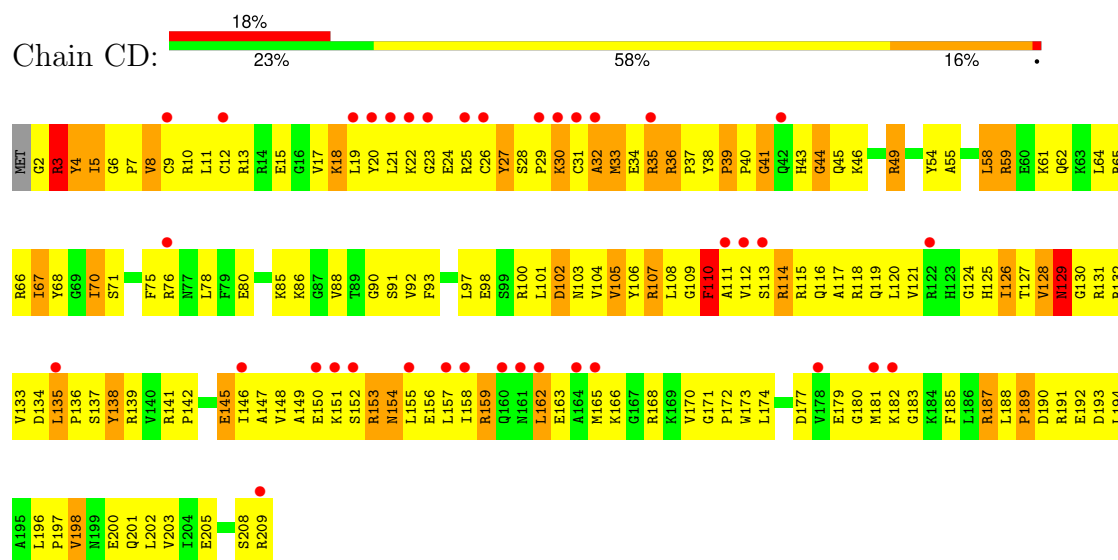


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

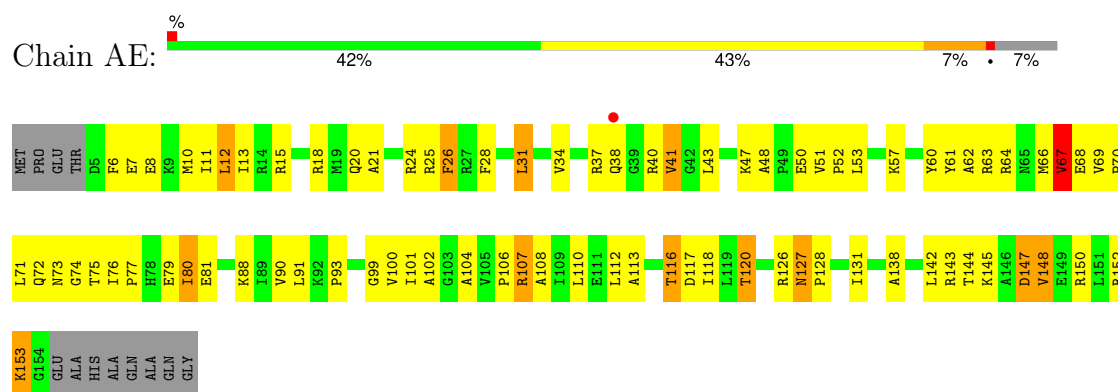




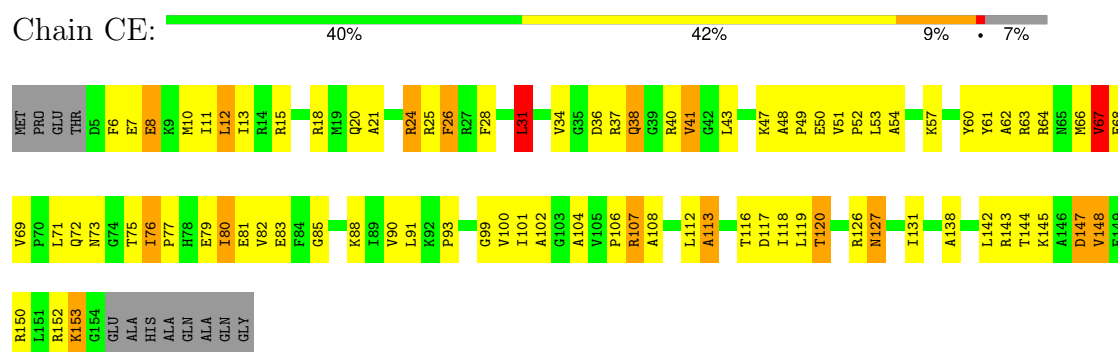
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



• Molecule 5: 30S RIBOSOMAL PROTEIN S5



• Molecule 5: 30S RIBOSOMAL PROTEIN S5



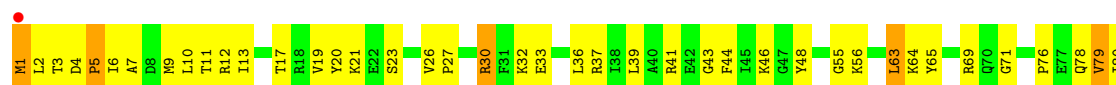
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



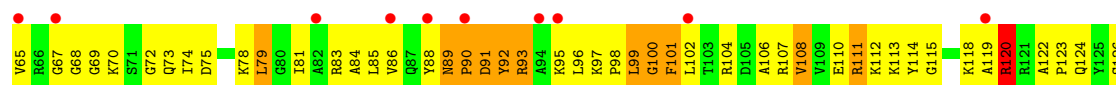
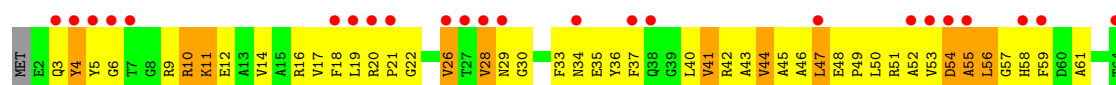




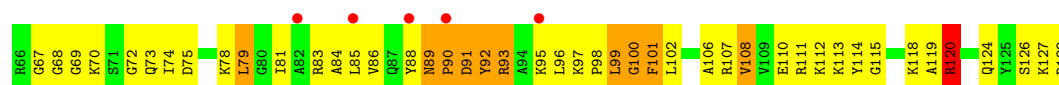
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



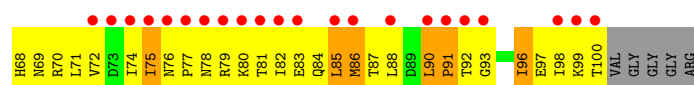
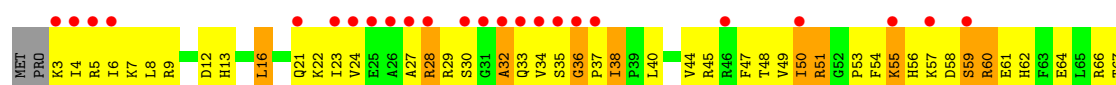
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



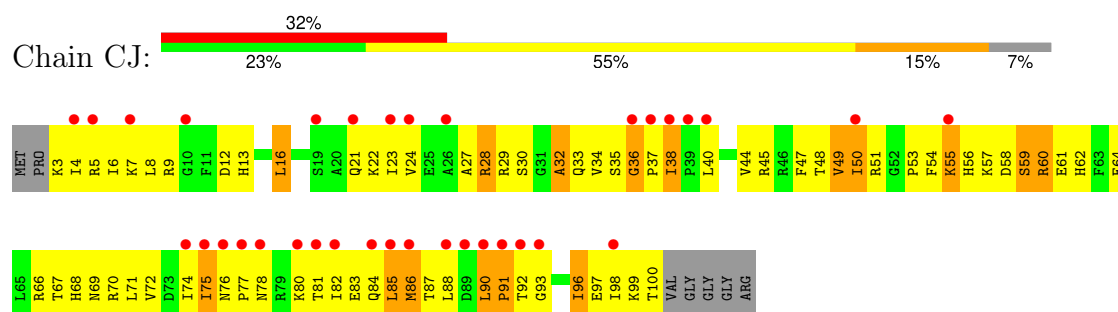
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



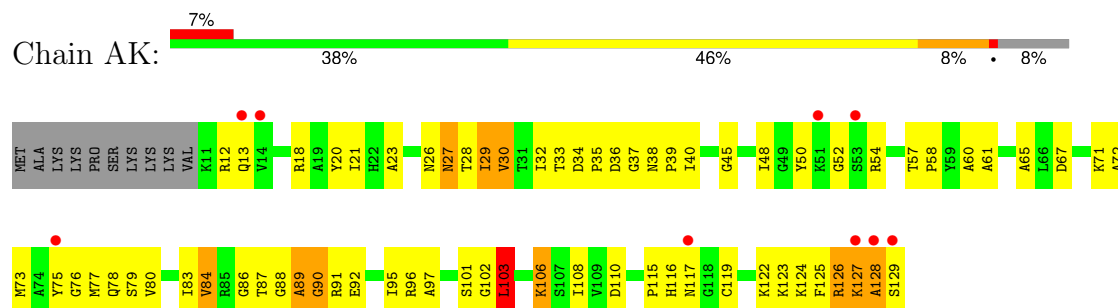
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



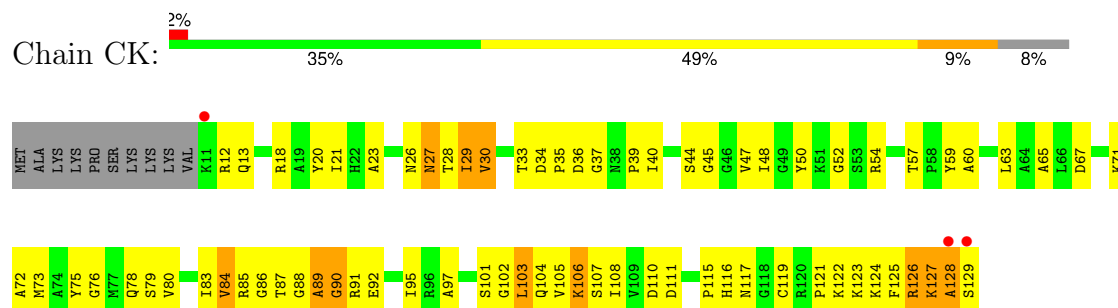
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



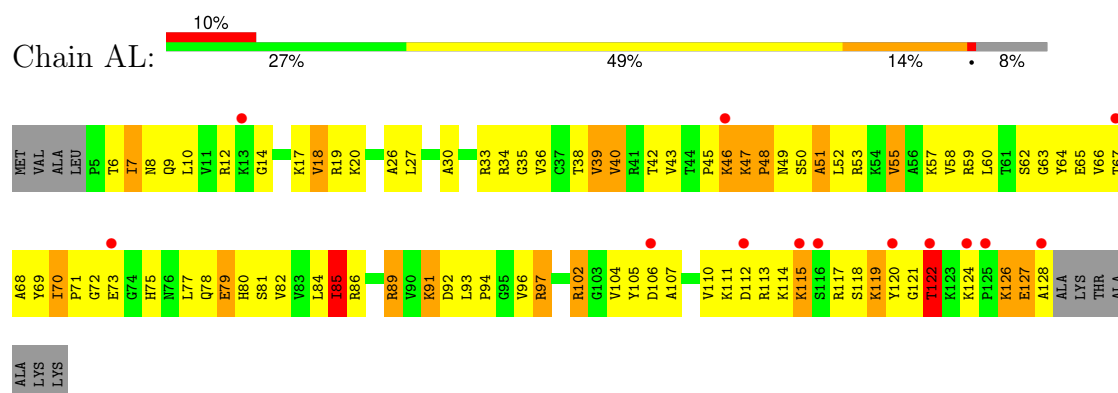
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



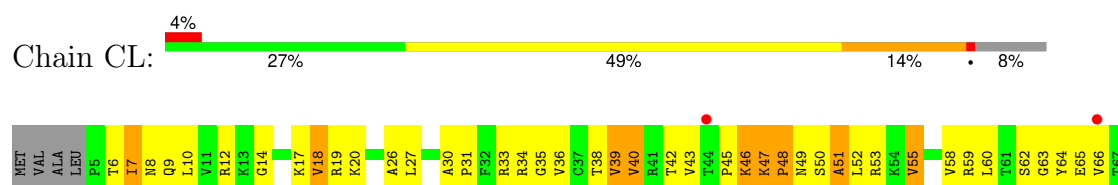
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



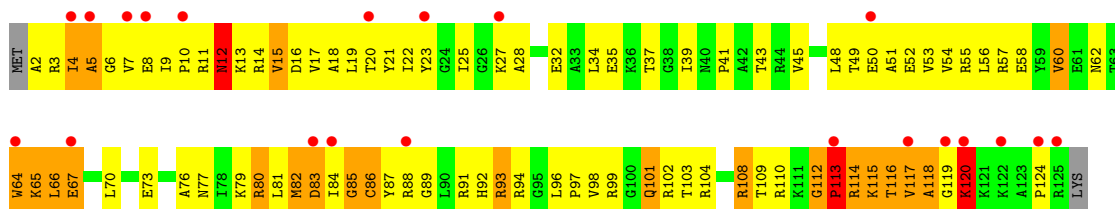
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



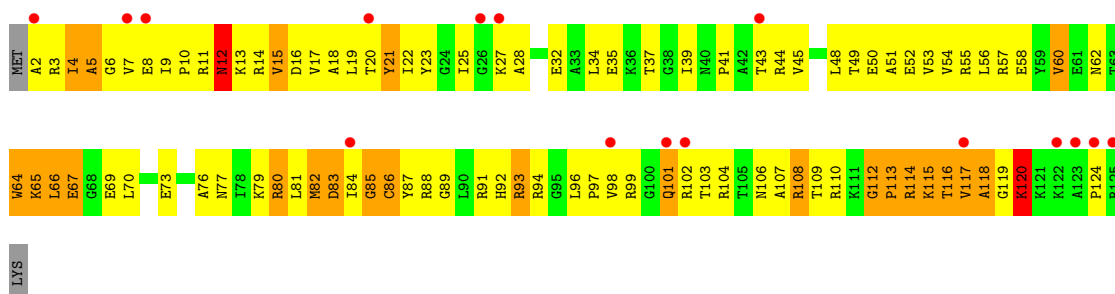
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



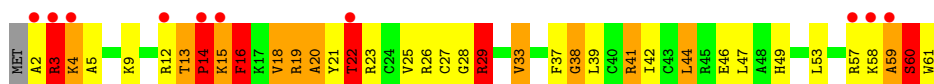
● Molecule 13: 30S RIBOSOMAL PROTEIN S13



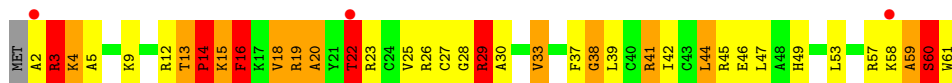
● Molecule 13: 30S RIBOSOMAL PROTEIN S13



- Molecule 14: 30S RIBOSOMAL PROTEIN S14

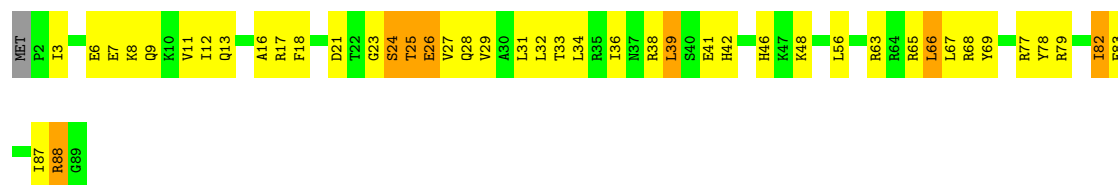


- Molecule 14: 30S RIBOSOMAL PROTEIN S14



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

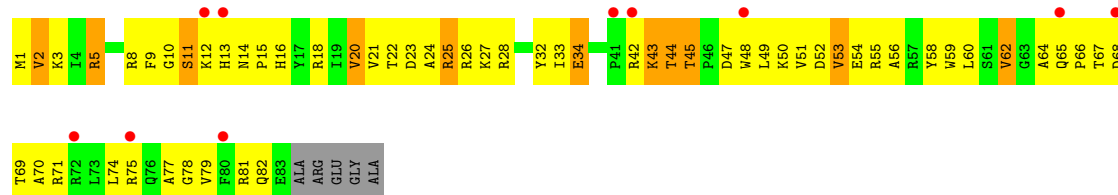




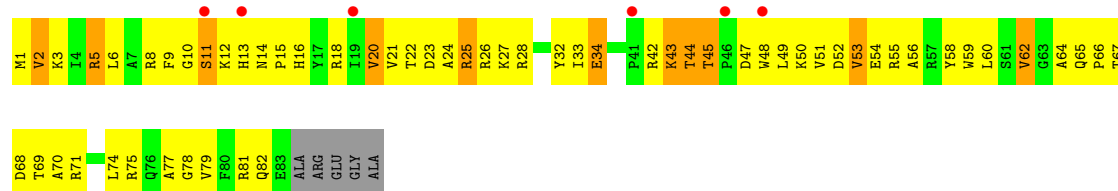
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



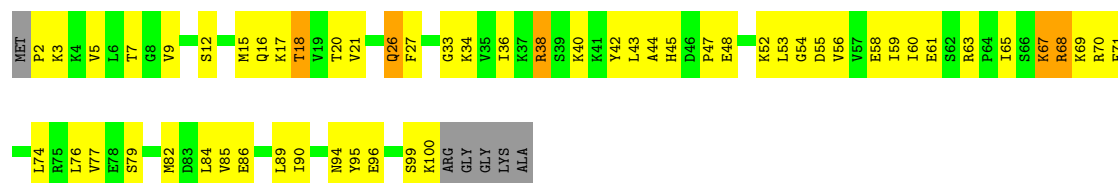
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



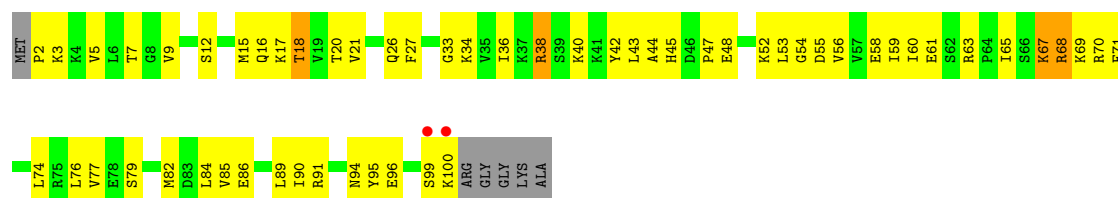
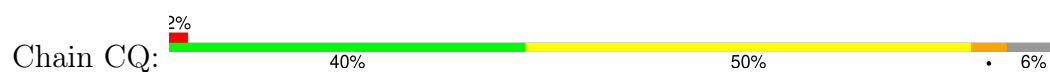
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



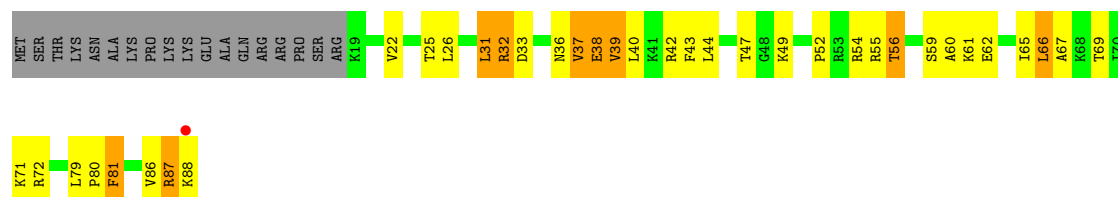
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



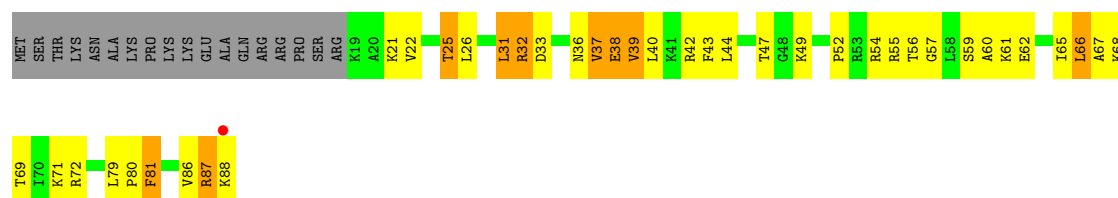
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



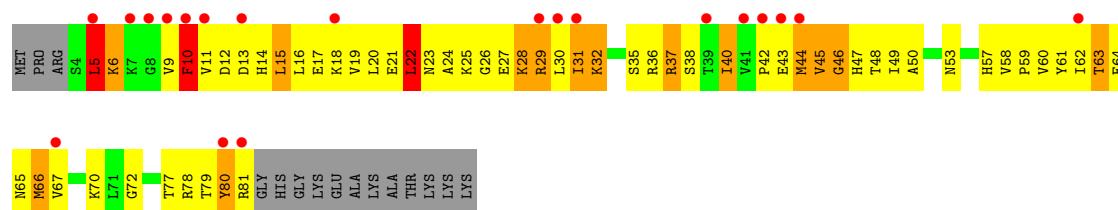
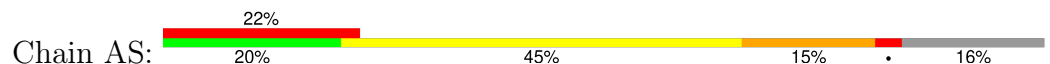
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



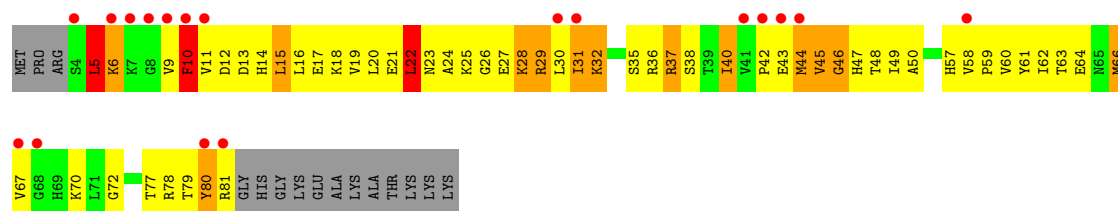
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



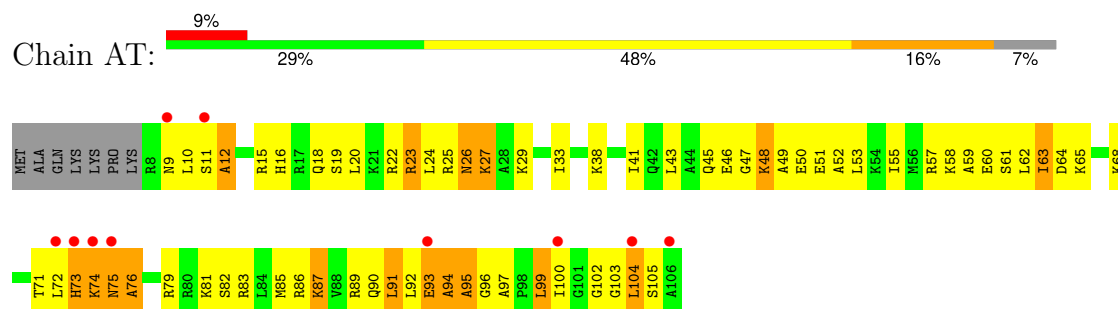
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



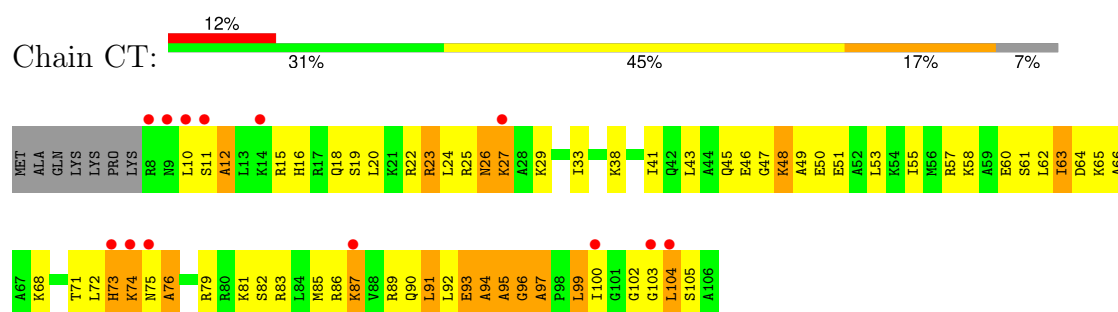
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



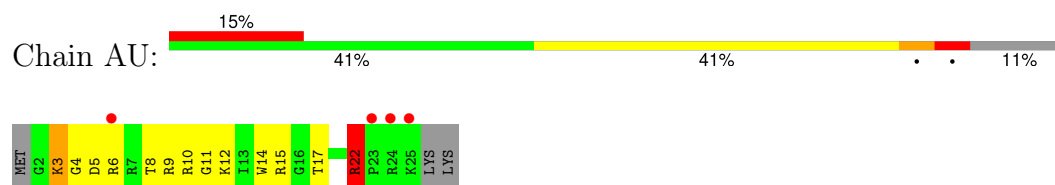
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



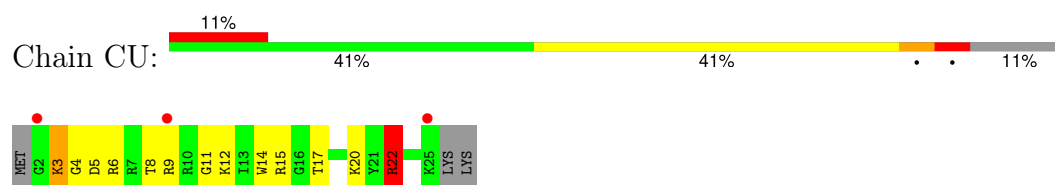
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



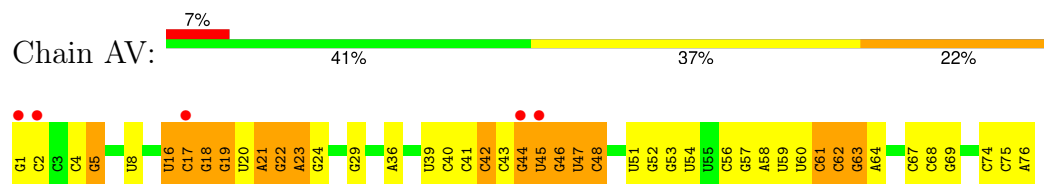
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



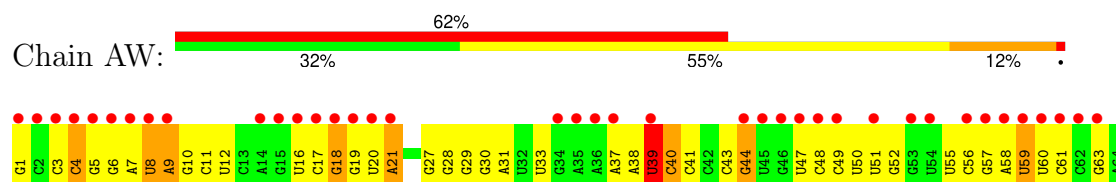
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

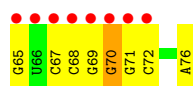


- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



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

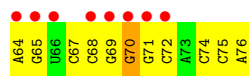
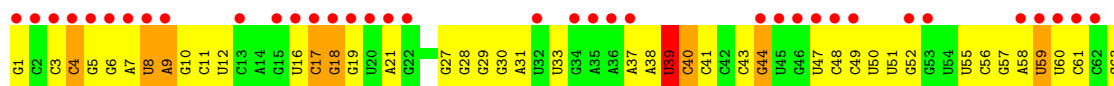




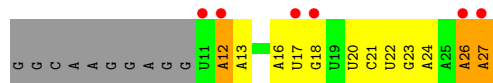
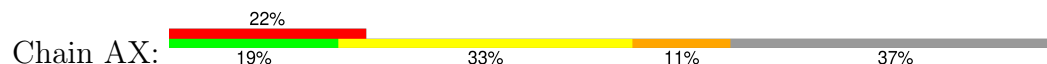
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



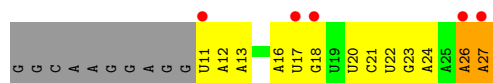
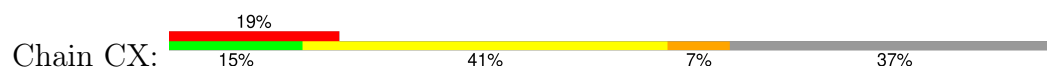
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



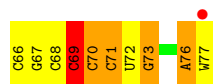
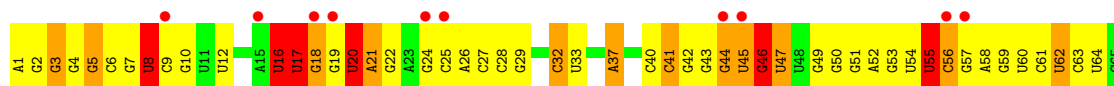
- Molecule 23: MRNA



- Molecule 23: MRNA



- Molecule 24: A-SITE TRNA A9C TRP-TRNA TRP

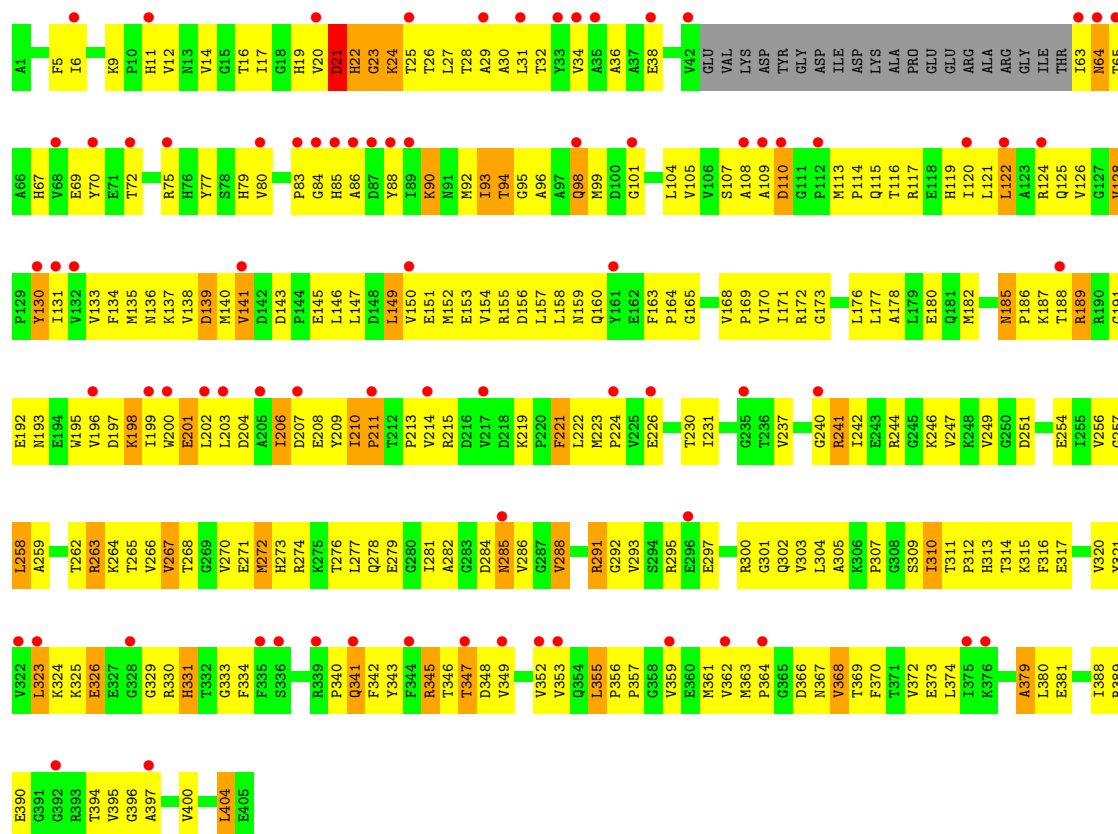


- Molecule 24: A-SITE TRNA A9C TRP-TRNA TRP

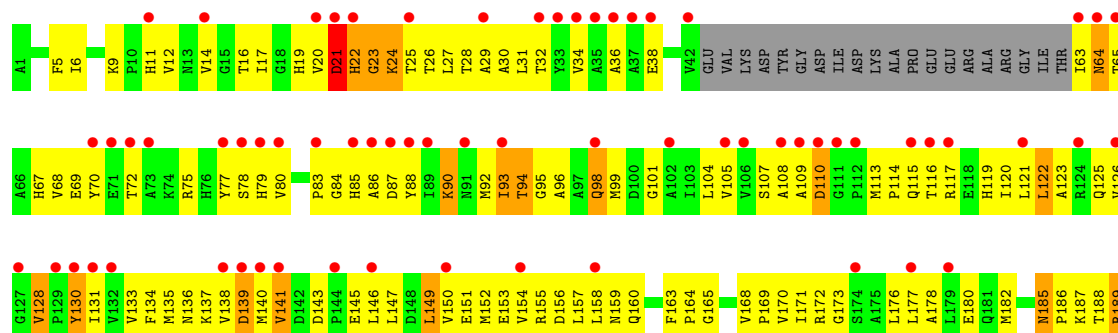


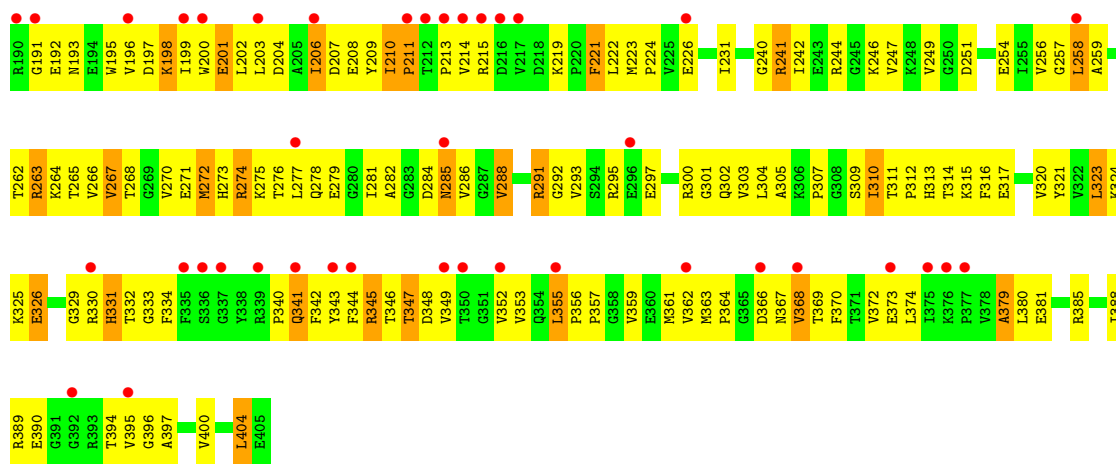


● Molecule 25: ELONGATION FACTOR TU

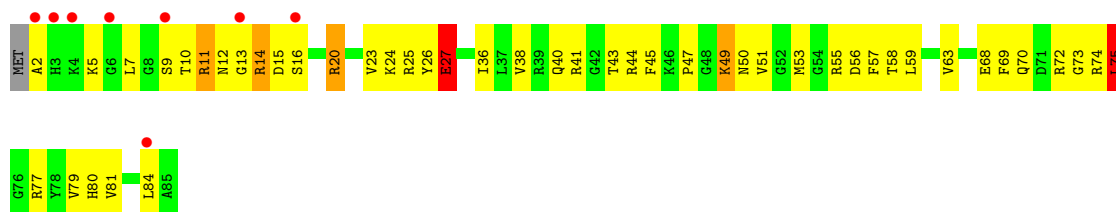
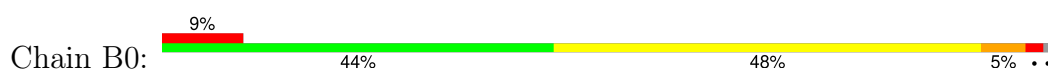


● Molecule 25: ELONGATION FACTOR TU

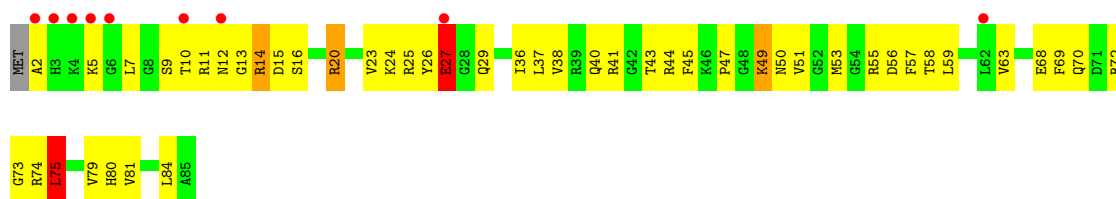
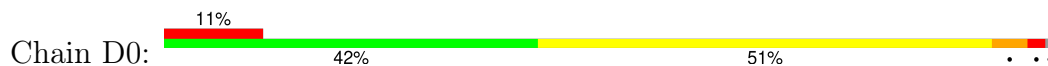




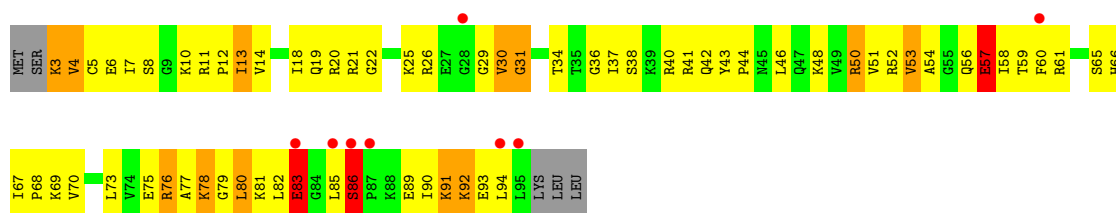
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



• Molecule 26: 50S RIBOSOMAL PROTEIN L27

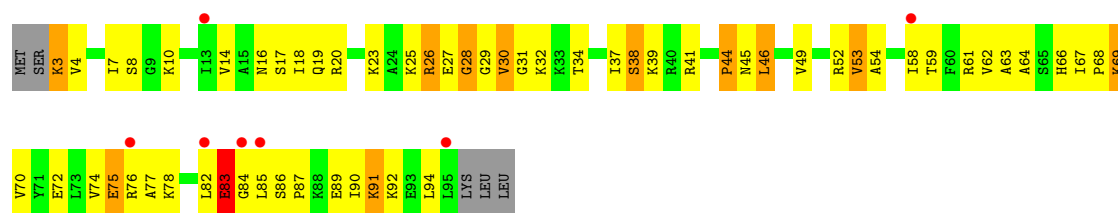


• Molecule 27: 50S RIBOSOMAL PROTEIN L28

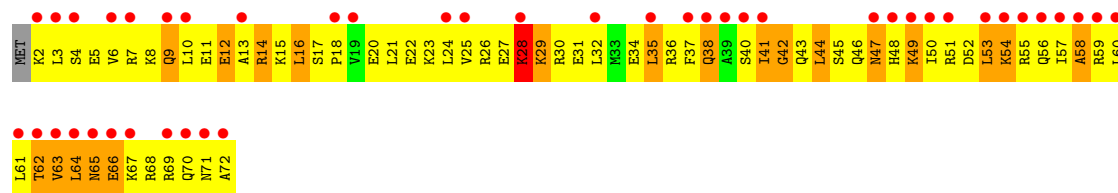
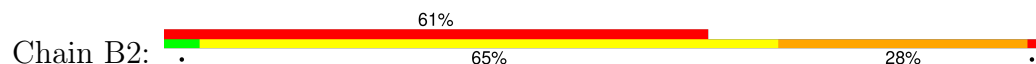


• Molecule 27: 50S RIBOSOMAL PROTEIN L28

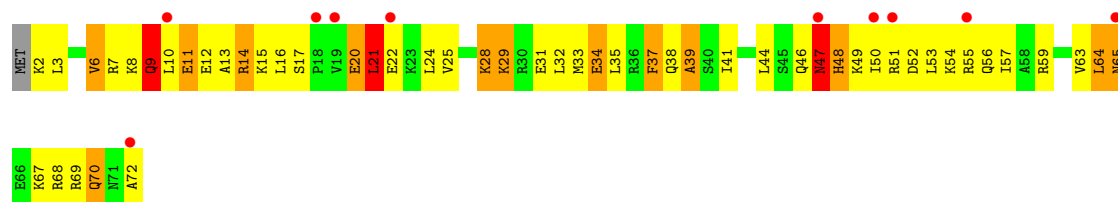




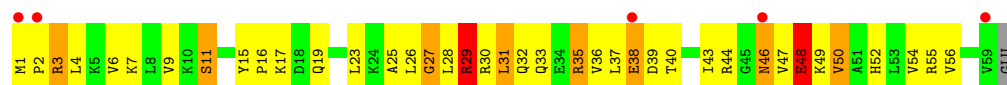
● Molecule 28: 50S RIBOSOMAL PROTEIN L29



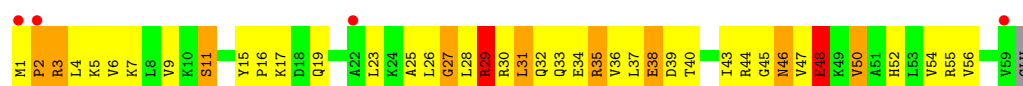
● Molecule 28: 50S RIBOSOMAL PROTEIN L29



● Molecule 29: 50S RIBOSOMAL PROTEIN L30



● Molecule 29: 50S RIBOSOMAL PROTEIN L30



● Molecule 30: 50S RIBOSOMAL PROTEIN L31



ARG
ARG
TYR
GLY
ASP
SER
TYR
ARG
LYS
GLY
ARG

• Molecule 30: 50S RIBOSOMAL PROTEIN L31



MET LYS GLU G4 I5 H6 P7 K8 L9 V10 P11 A12 R13 R14 I14 I15 C18 G19 N20 V21 T22 E23 T24 Y25 S26 T27 K28 P29 E30 E31 Y32 Y33 E34 V35 C36 C37 K38 C39 H40 P41 F42 V43 T44 G45 Q46 Q47 ARG PHE VAL ASP THR GLY ARG VAL GLU ARG PHE GLN ARG

ARG
TYR
GLY
ASP
SER
TYR
ARG
LYS
GLY
ARG

• Molecule 31: 50S RIBOSOMAL PROTEIN L32



MET A2 K3 H4 P5 V6 P7 T11 R15 R16 D17 R20 H23 A24 L25 T29 L30 V31 P32 C33 P34 E35 C36 K37 A38 M39 K40 P41 P42 H43 T44 V45 C46 P47 E48 C49 G50 Y51 Y52 A53 G54 R55 K56 V57 L58 E59 V60

• Molecule 31: 50S RIBOSOMAL PROTEIN L32



MET A2 K3 H4 P5 V6 P7 T11 R15 R16 D17 A18 R19 R20 H23 A24 L25 T29 L30 V31 P32 C33 P34 E35 C36 K37 A38 M39 K40 P41 P42 H43 T44 V45 C46 P47 E48 C49 G50 Y51 Y52 A53 G54 R55 K56 V57 L58 E59 V60

• Molecule 32: 50S RIBOSOMAL PROTEIN L33



MET ALA SER GLU V5 R6 R7 K8 L9 L10 L11 E12 C13 T14 E15 C16 C17 K18 R19 N20 N21 A22 T23 E24 K25 N26 K27 R28 N29 T30 T31 N32 K33 L34 E35 L36 R37 K38 Y39 C40 P41 V42 C43 R44 R45 H46 V48 H49 R50 E51 V52 K53 I54

• Molecule 32: 50S RIBOSOMAL PROTEIN L33



MET ALA SER GLU V5 R6 R7 K8 L9 L10 L11 E12 C13 T14 E15 C16 C17 K18 R19 N20 N21 A22 T23 E24 K25 N26 K27 R28 N29 T30 T31 N32 K33 L34 E35 L36 R37 K38 Y39 C40 P41 V42 C43 R44 R45 H46 V48 H49 R50 E51 V52 K53 I54

• Molecule 33: 50S RIBOSOMAL PROTEIN L34

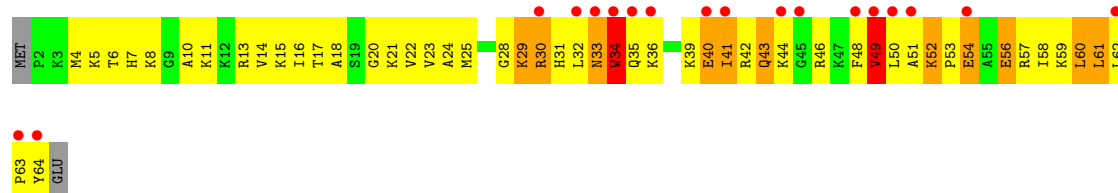


M1 T4 W5 Q6 R9 R10 R11 R12 G17 F18 R19 A20 R21 T24 G27 R28 L31 K32 R33 R34 R35 Q36 K37 G38 R39 R40 V40 R41 L42 T43 P44 A45 V46 R47 R48 ARG

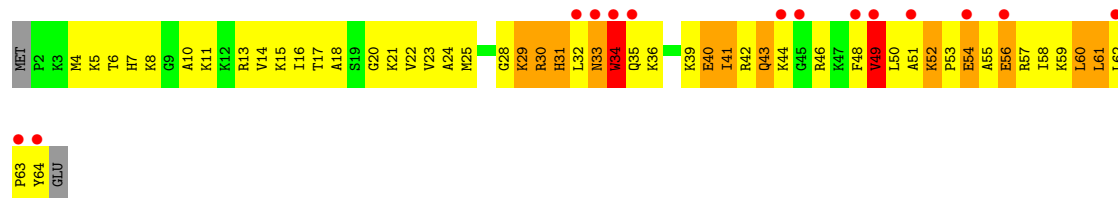
• Molecule 33: 50S RIBOSOMAL PROTEIN L34



• Molecule 34: 50S RIBOSOMAL PROTEIN L35



• Molecule 34: 50S RIBOSOMAL PROTEIN L35



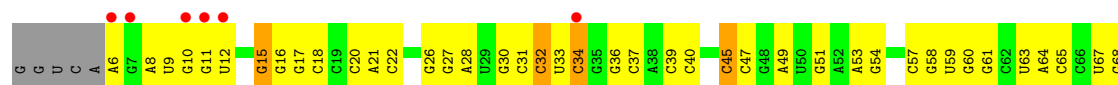
• Molecule 35: 50S RIBOSOMAL PROTEIN L36



• Molecule 35: 50S RIBOSOMAL PROTEIN L36



• Molecule 36: 23S RIBOSOMAL RNA

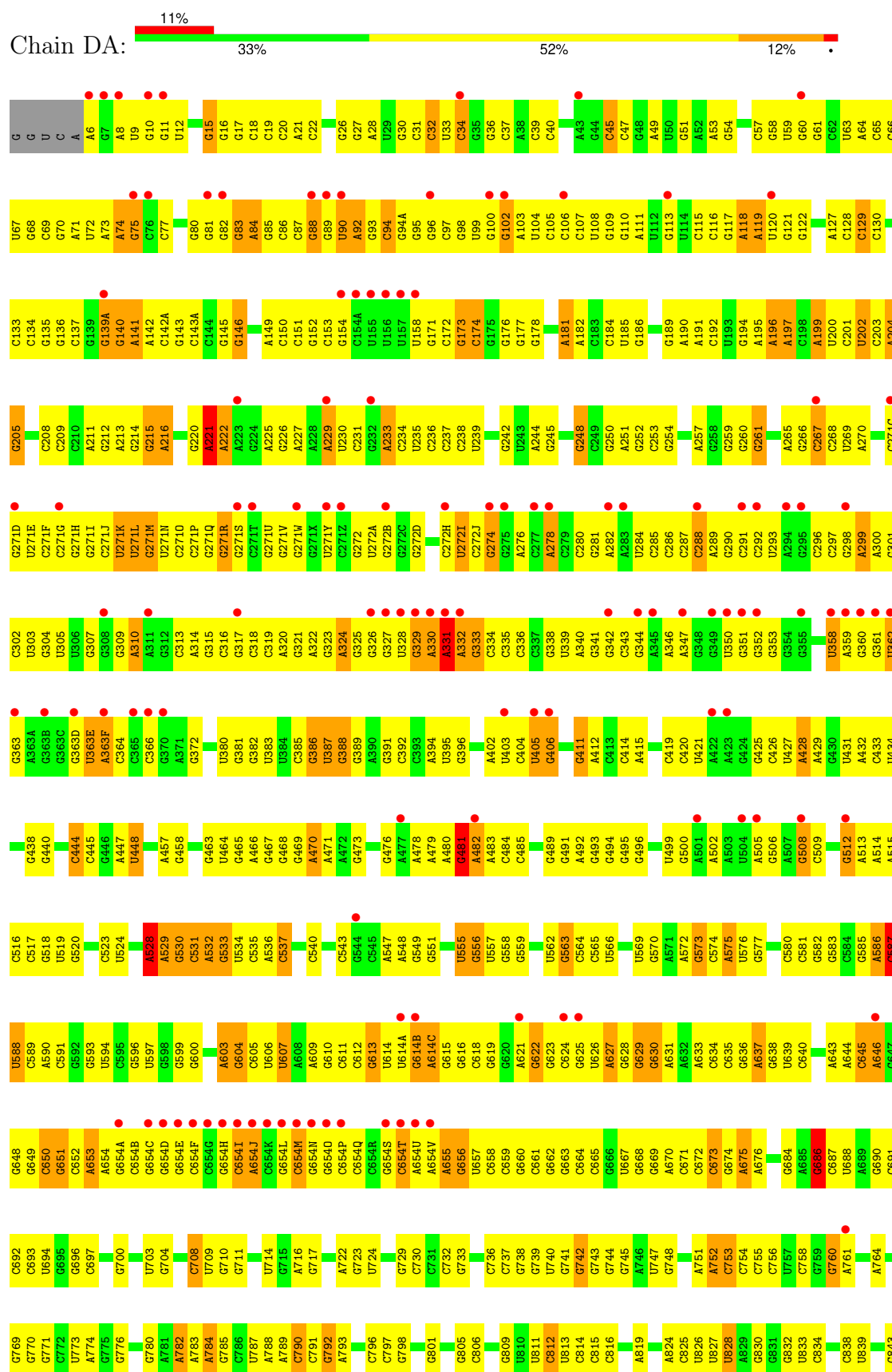




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A1859	U1777	C1684	A1608	A1535	G1472	C1403	U1329	G1257	G1184	G1055	G1055	A988
G1860	U1778	C1685	A1609	C1536	G1473	C1404	U1330	G1258	C1115	C1116	G1056	G989
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G1863	A1689	A1689	C1611	G1539	G1476	C1407	C1332	G1261	C1121	C1121	U1059	C992
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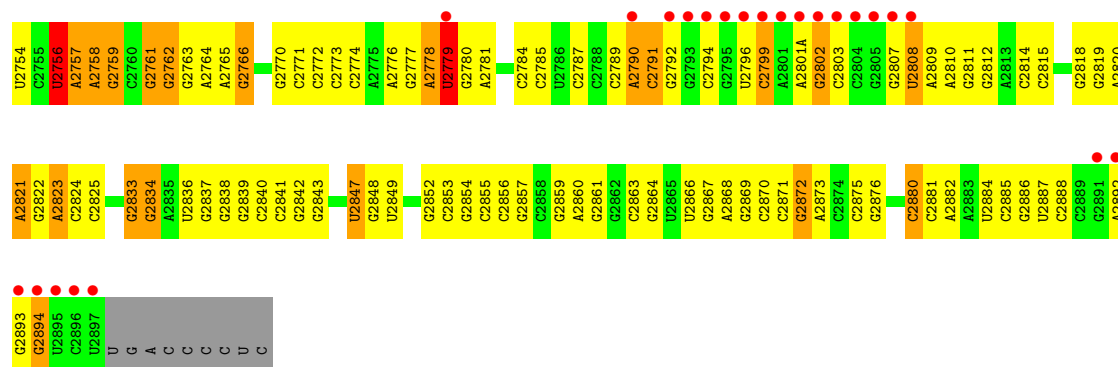
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	C2771	G2627	C2539	U2467	A2392	G2318	G2162	U2098	A2019	
	C2772	C2628	U2542	G2468	A2393	C2163	G2163	U2099	A2020	
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• Molecule 36: 23S RIBOSOMAL RNA

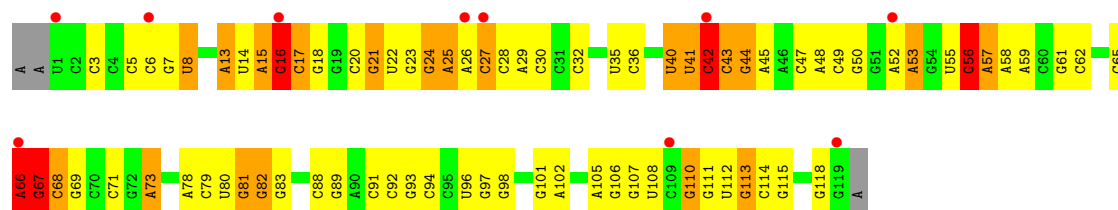




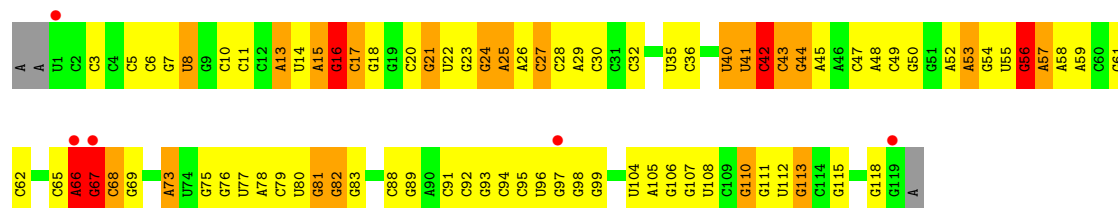
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A1796	C1880	G2037	G2112	C2174	U2248	A2322	A2393	C2466	U2537	G2617	U2696
C1797	C1881	G2038	U2113	C2175	U2249	A2323	G2396	U2467	C2538	G2618	G2697
U1908	G1882	C2039	A2114	A2176	U2250	G2324	G2397	U2468	C2539	C2626	U2698
G1798	C1883	U2041	G2115	C2177	U2251	G2325	U2398	A2469	A2542	G2627	C2699
G1799	A1884	U2042	G2116	C2178	C2252	G2326	C2402	G2470	G2543	C2628	C2700
C1800	A1885	C2043	A2117	C2179	U2253	A2327	C2403	G2471	G2544	A2629	C2701
G1801	G1886	G2052	U2118	U2180	C2261	A2328	C2404	G2472	G2545	G2630	U2702
G1807	C1887	G2053	A2119	G2181	U2262	G2329	G2405	U2473	U2546	C2631	C2703
U1808	A1888	G2054	G2120	G2182	C2263	A2330	U2406	C2474	C2552	A2632	C2704
A1810	A1889	C2055	U2121	C2183	U2264	A2331	G2407	A2475	G2553	U2636	C2710
G1811	G1899	G2056	G2122	G2184	A2265	G2332	U2408	C2476	U2554	U2637	U2711
G1812	A1900	A2060	G2123	C2185	A2266	G2333	G2409	C2477	U2555	A2639	U2712
G1813	A1901	G2061	G2124	G2186	A2267	A2334	U2410	A2478	C2556	G2640	A2712A
G1816	C1902	U2062	A2126	C2187	A2268	A2335	G2411	C2479	C2557	U2641	A2713
G1817	G1903	C2063	G2127	U2189	U2269	G2337	U2398	C2481	C2558	G2642	C2714
U1818	G1906	C2064	C2128	G2190	A2274	U2340	G2413	G2482	U2559	G2643	U2715
A1819	G1907	C2065	G2131	G2191	C2275	G2341	G2414	G2485	U2562	G2644	U2716
U1820	C1908	C2066	G2132	C2192	G2276	G2342	G2415	G2486	U2563	G2645	G2717
A1821	C1909	U2068	G2133	G2193	U2277	C2343	C2416	U2487	A2564	C2646	U2718
C1826	G1910	G2069	A2134	G2194	A2278	G2344	G2417	A2488	A2565	U2647	G2719
G1827	U1911	C2070	C2135	C2195	C2282	U2345	U2418	G2489	A2566	U2648	U2720
G1828	A1912	U2071	G2136	C2196	G2283	G2346	G2419	C2490	G2567	U2649	A2721
G1831	C1913	U2072	C2137	U2197	C2284	A2352	G2421	U2491	C2568	U2650	G2722
U1833	A1914	G2073	G2138	A2199	C2285	A2353	U2422	U2492	G2569	C2651	C2723
U1836	C1915	U2074	C2139	A2200	A2286	C2355	A2423	U2493	C2570	U2652	C2724
C1837	U1916	U2075	C2140	C2201	A2287	G2356	C2424	C2494	C2571	A2654	U2725
C1925	U1917	C2078	G2143	C2202	G2288	G2357	A2425	C2499	C2572	U2655	U2726
U1841	U1926	U2086	U2144	G2206	G2289	A2358	G2428	G2502	C2573	U2656	G2732
G1842	G1929	G2087	U2145	G2207	U2291	A2359	G2429	A2503	A2577	A2657	G2733
G1843	U2011	G2088	C2146	A2208	C2292	A2360	U2430	U2504	G2578	C2658	A2734
C1844	U1931	U2089	G2147	A2218	C2293	A2361	U2431	G2505	G2579	C2659	G2735
C1847	A1932	U2091	G2151	G2219	C2294	A2362	A2432	U2506	U2580	A2660	G2736
C1851	G1933	G2093	G2152	G2221	G2295	A2363	U2433	C2507	C2581	G2661	U2740
U1851	A1936	G2094	G2153	A2226	U2296	A2364	A2434	G2508	G2582	C2662	A2741
C1852	A1937	U2095	G2154	A2227	C2297	A2365	U2438	U2511	U2585	A2665	C2742
A1854	A1938	C2097	G2155	G2228	C2298	A2366	A2439	C2512	C2586	C2666	C2743
			G2156	G2229	G2299	A2367	G2440	G2513	A2589	C2667	C2744
			G2157	G2230	G2300	A2368	C2441	U2514	C2590	G2668	U2746
			G2159	G2231	G2301	A2369	C2442	C2515	C2591	G2669	G2747
				G2232	A2305	A2370	C2443	U2518	G2592	C2670	A2750
				G2233	C2306	A2371	G2444	U2519	C2593	G2671	G2751
				G2234	G2307	A2372	G2445	C2520	G2595	C2672	C2752
				G2235	G2308	A2373				C2673	A2753



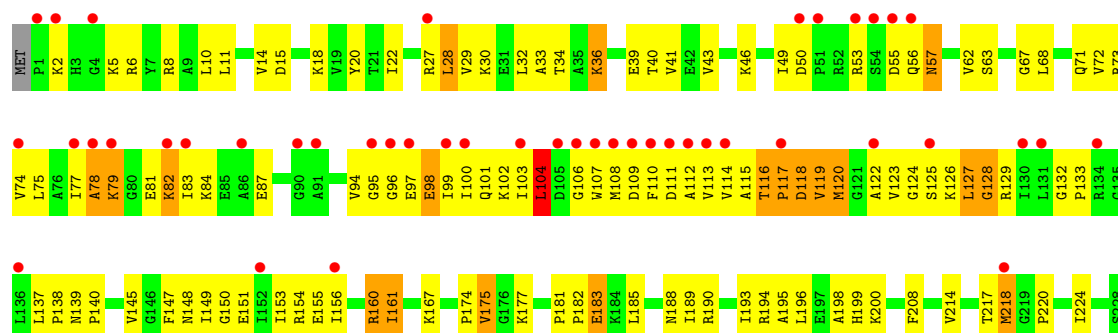
• Molecule 37: 5S RIBOSOMAL RNA



• Molecule 37: 5S RIBOSOMAL RNA

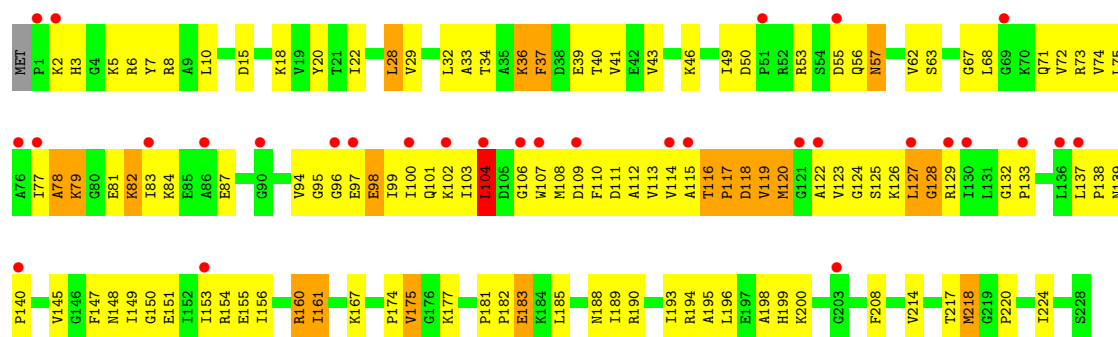


• Molecule 38: 50S RIBOSOMAL PROTEIN L1

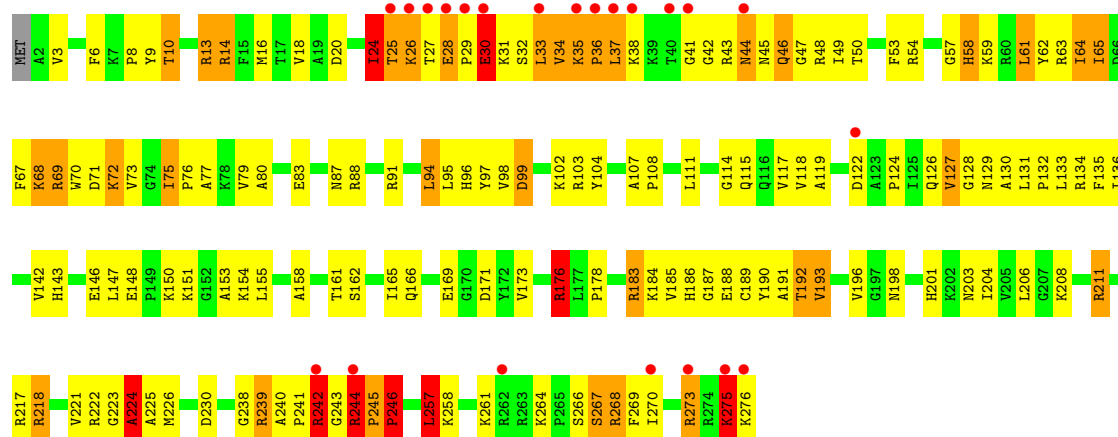
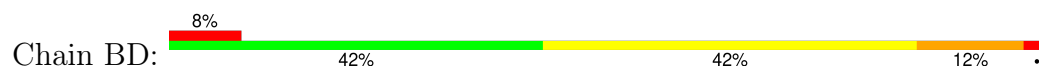


• Molecule 38: 50S RIBOSOMAL PROTEIN L1

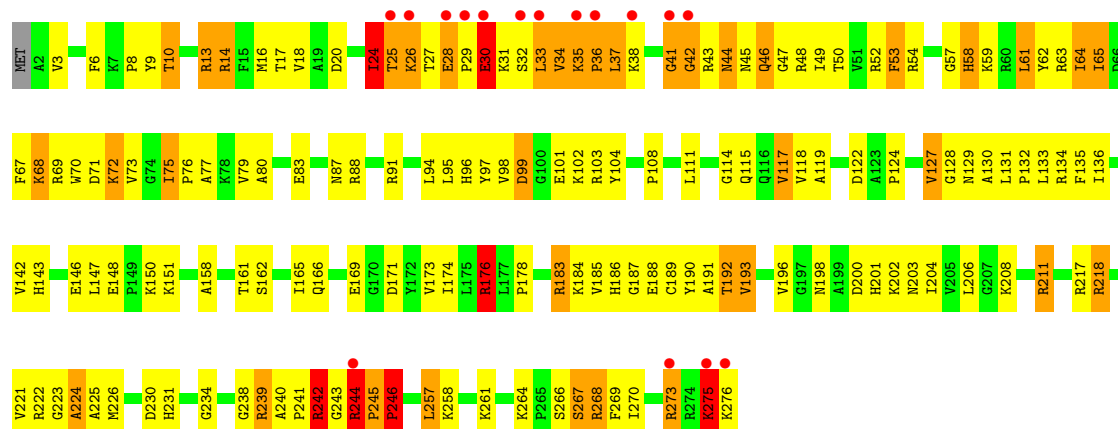




• Molecule 39: 50S RIBOSOMAL PROTEIN L2

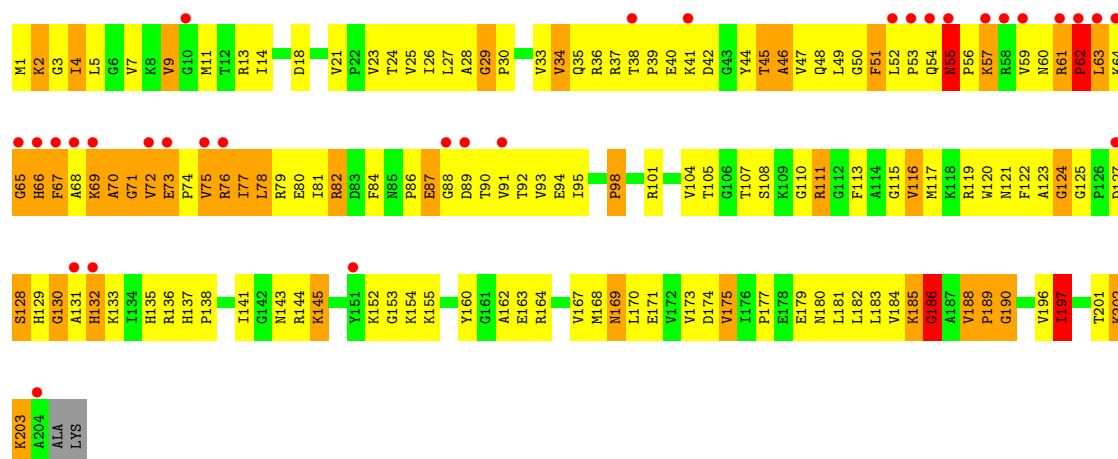


• Molecule 39: 50S RIBOSOMAL PROTEIN L2

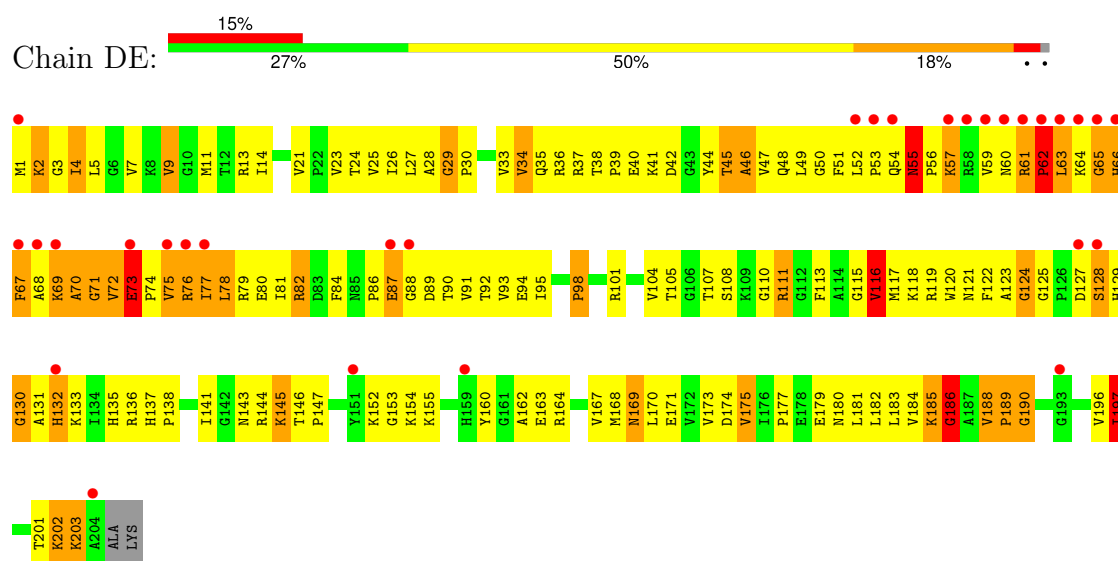


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

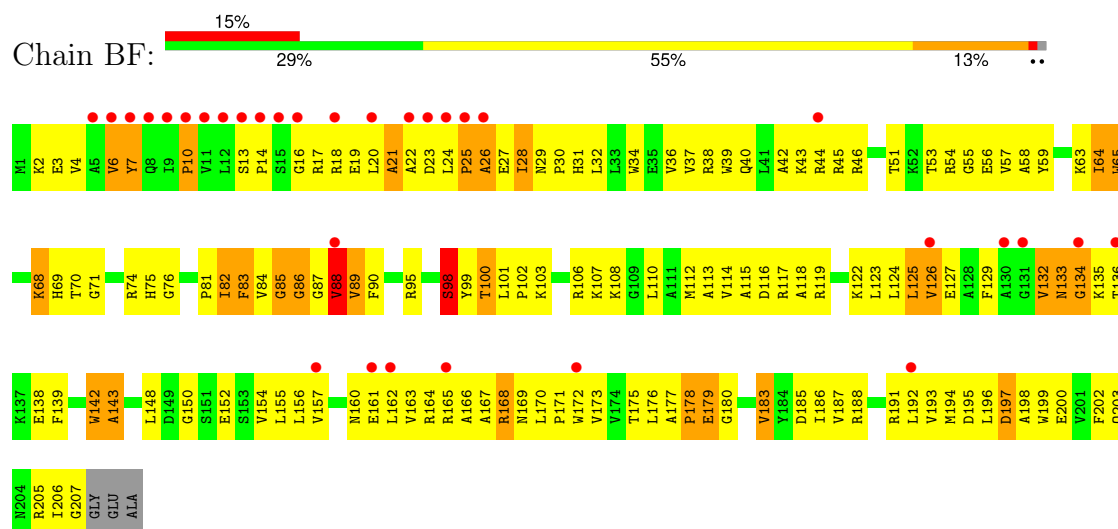




• Molecule 40: 50S RIBOSOMAL PROTEIN L3

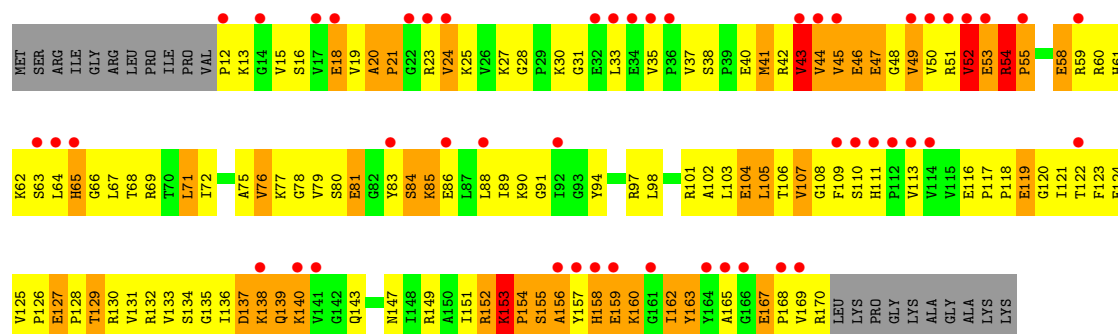


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

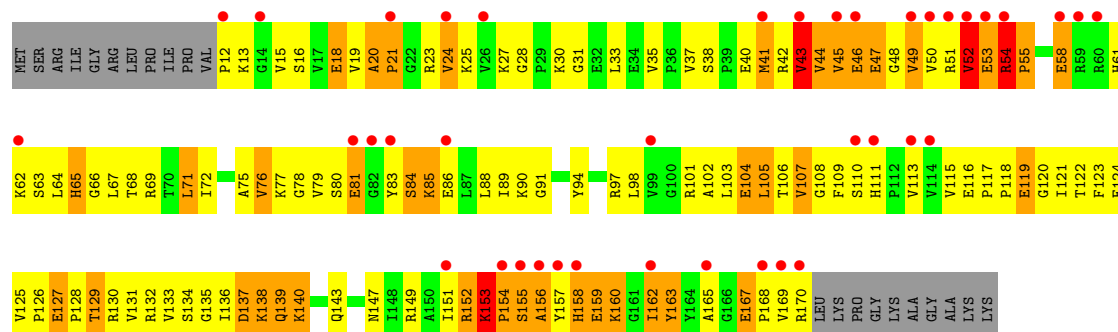
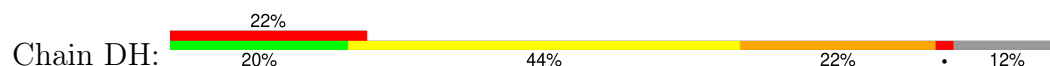


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

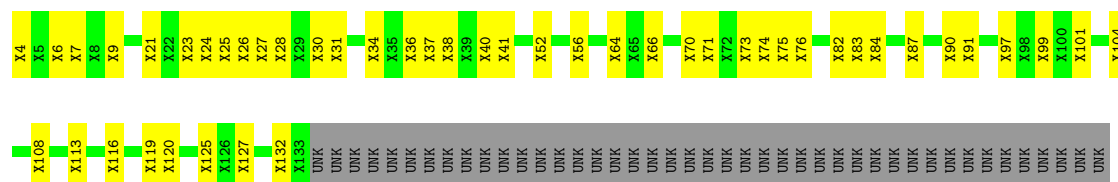
Chain BH: 27% 19% 45% 22% 12%



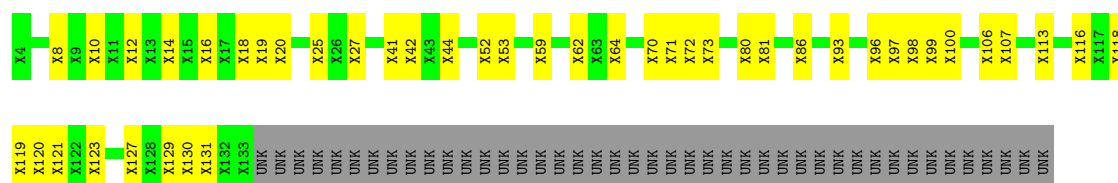
• Molecule 43: 50S RIBOSOMAL PROTEIN L6



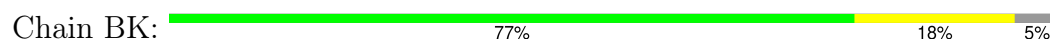
• Molecule 44: 50S RIBOSOMAL PROTEIN L10



• Molecule 44: 50S RIBOSOMAL PROTEIN L10



• Molecule 45: 50S RIBOSOMAL PROTEIN L11





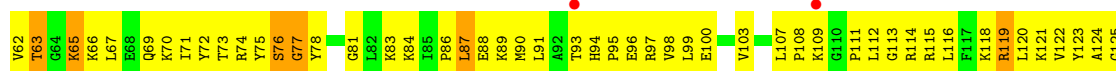
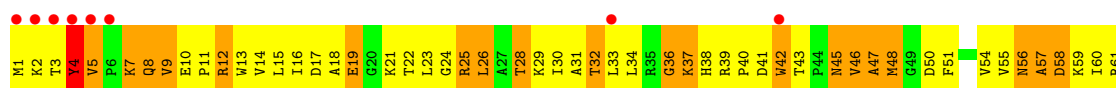
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain DK: 79% 16% 5%



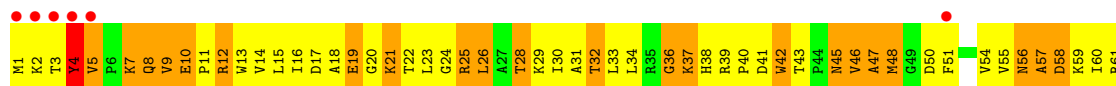
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN: 9% 17% 59% 22% ..



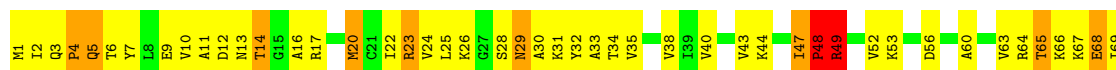
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN: 8% 16% 59% 23% ..

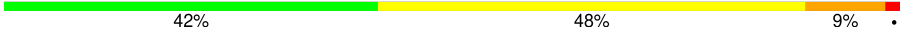


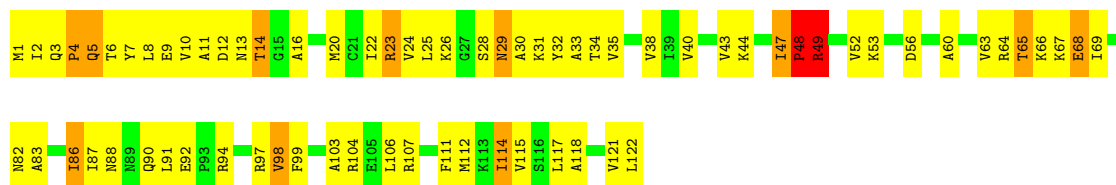
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO: 43% 47% 9% .



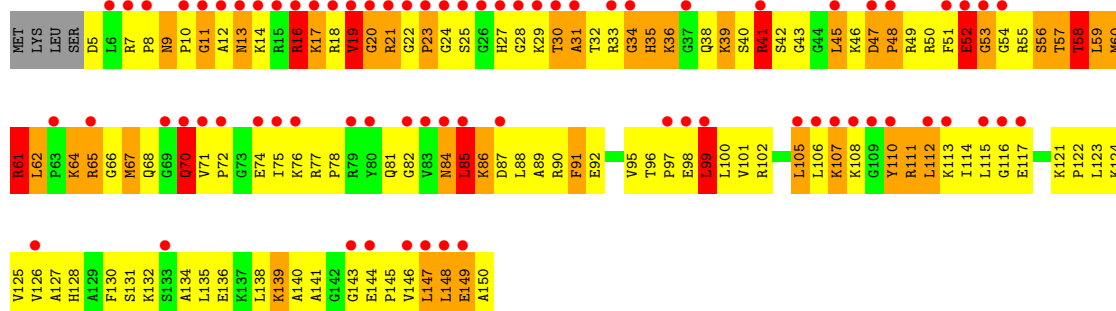
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO: 

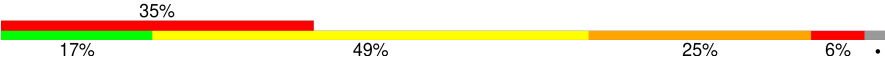


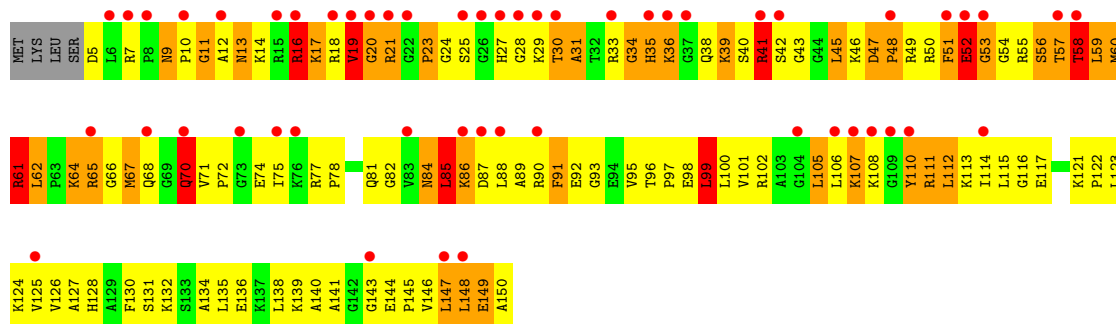
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP: 



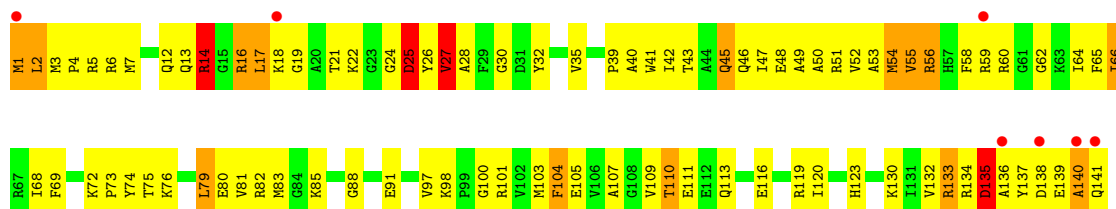
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP: 



• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ: 

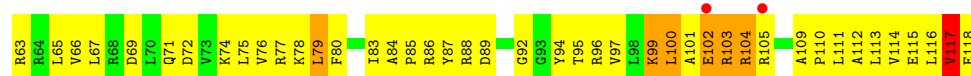


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

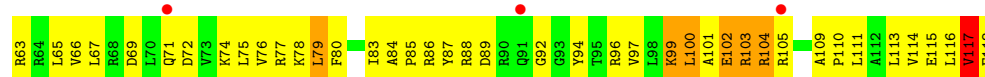
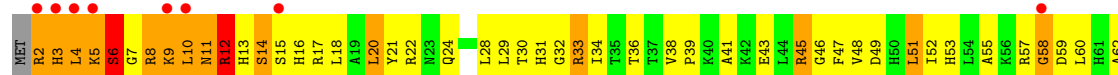
Chain DQ: 



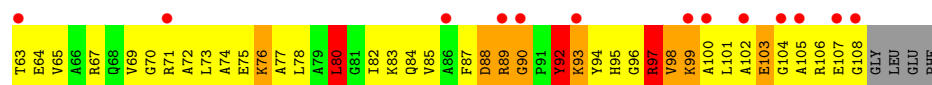
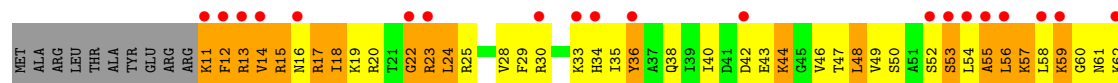
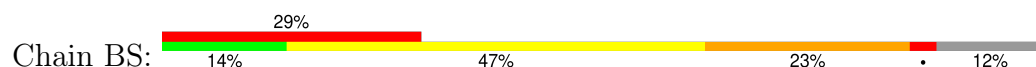
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



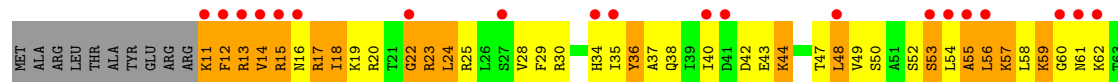
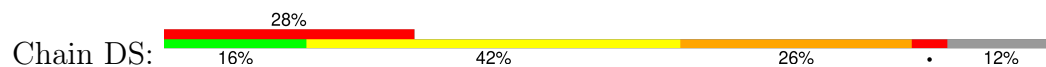
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



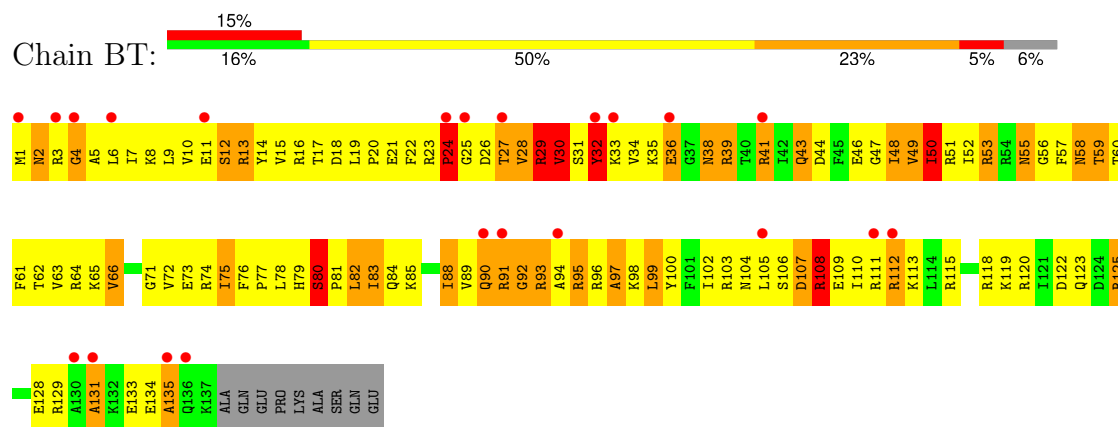
• Molecule 51: 50S RIBOSOMAL PROTEIN L18



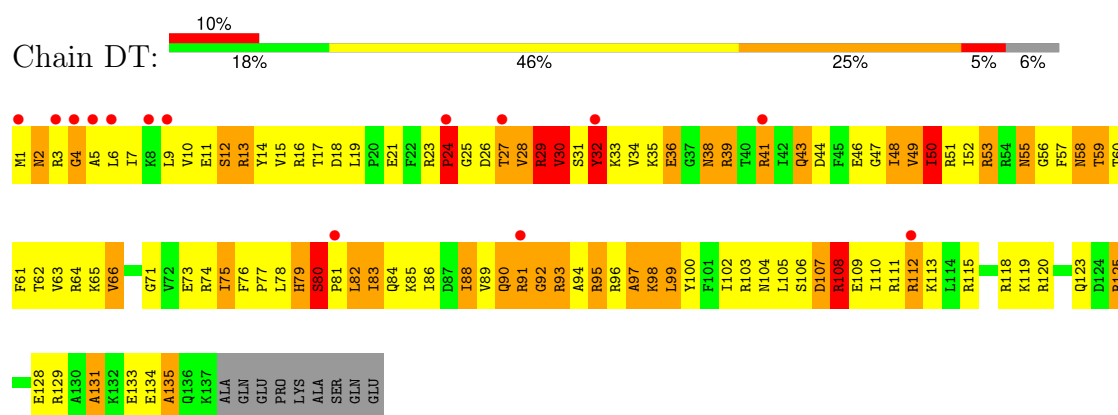
• Molecule 51: 50S RIBOSOMAL PROTEIN L18



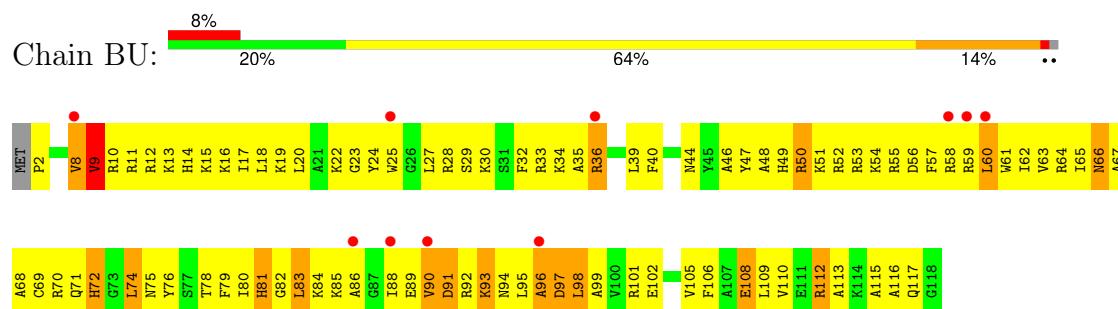
- Molecule 52: 50S RIBOSOMAL PROTEIN L19



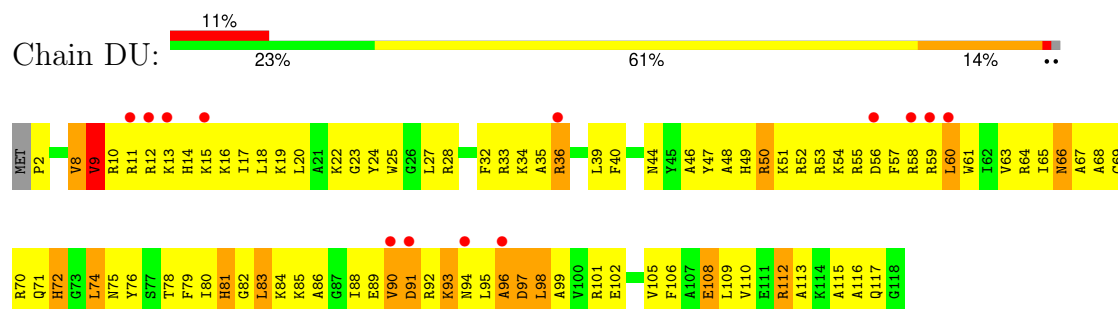
- Molecule 52: 50S RIBOSOMAL PROTEIN L19



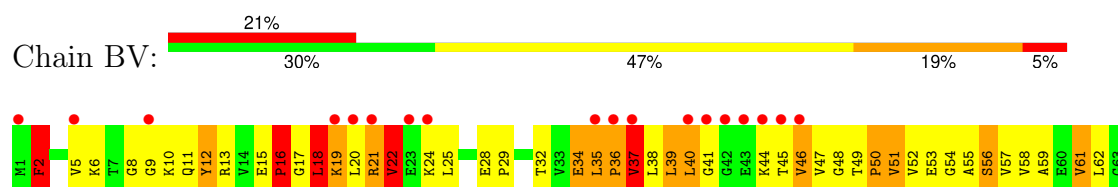
- Molecule 53: 50S RIBOSOMAL PROTEIN L20



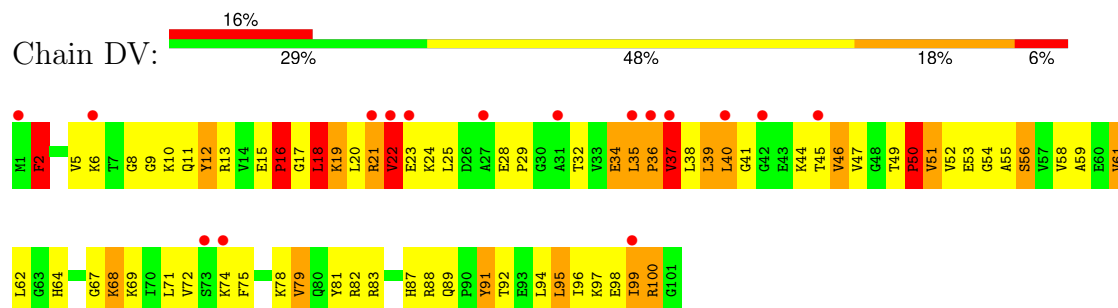
- Molecule 53: 50S RIBOSOMAL PROTEIN L20



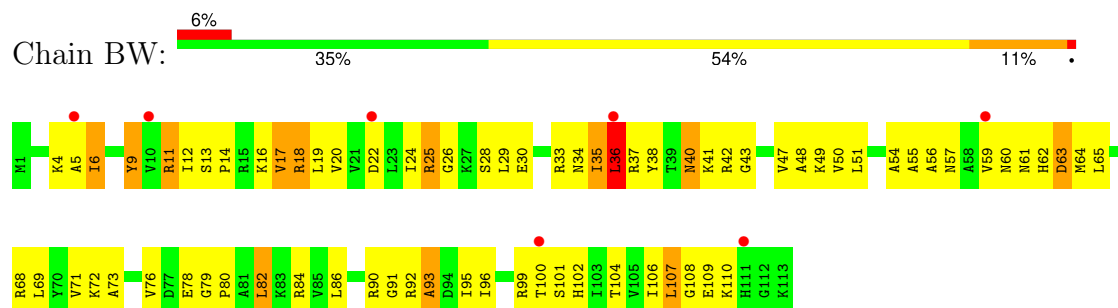
- Molecule 54: 50S RIBOSOMAL PROTEIN L21



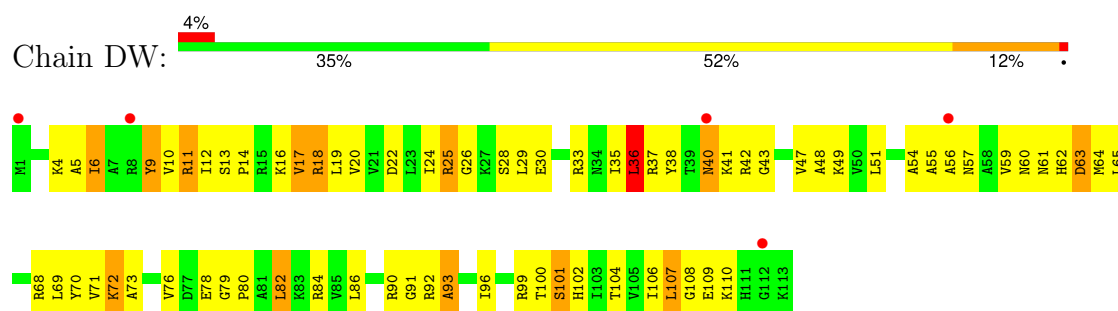
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



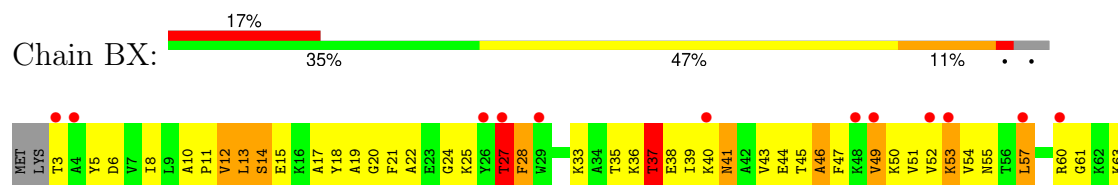
• Molecule 55: 50S RIBOSOMAL PROTEIN L22

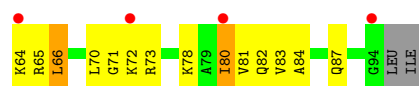


• Molecule 55: 50S RIBOSOMAL PROTEIN L22

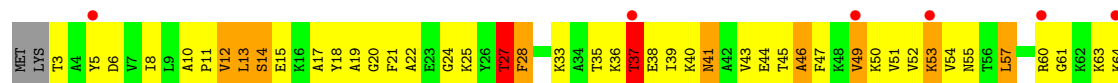


• Molecule 56: 50S RIBOSOMAL PROTEIN L23

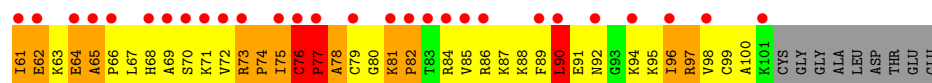
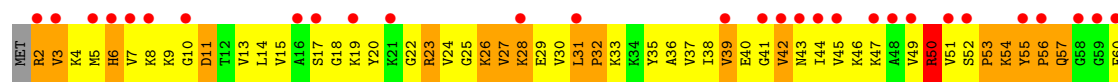




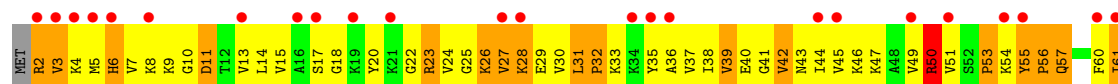
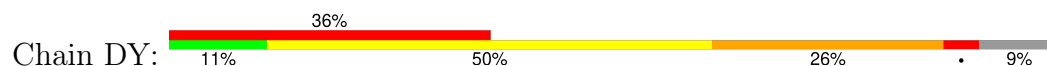
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



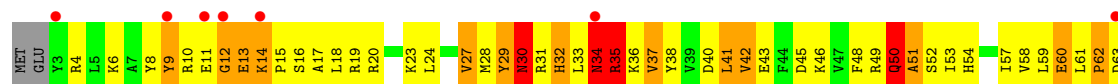
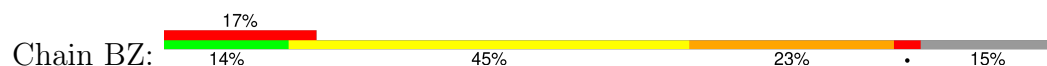
• Molecule 57: 50S RIBOSOMAL PROTEIN L24



• Molecule 57: 50S RIBOSOMAL PROTEIN L24

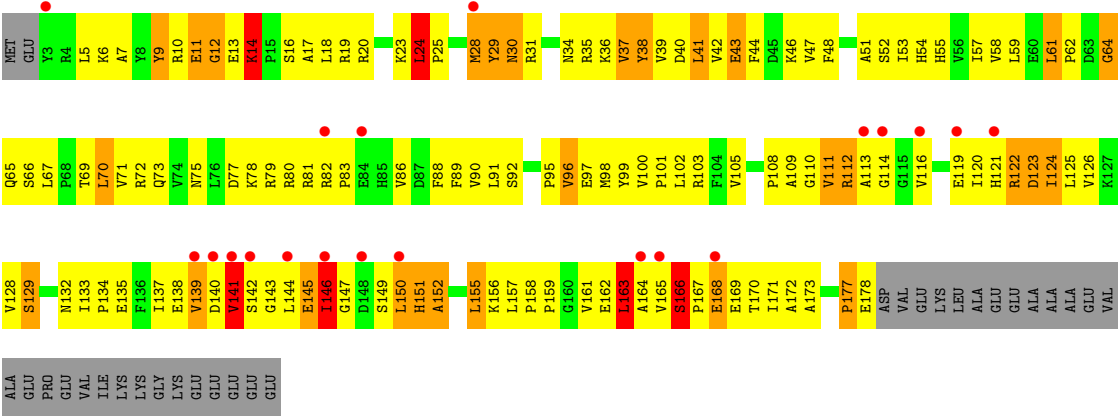
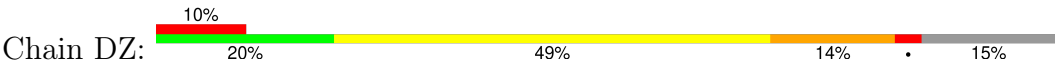


• Molecule 58: 50S RIBOSOMAL PROTEIN L25



ALA
GLU
VAL
ALA
GLU
PRO
GLU
VAL
TLE
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	289.90Å 268.50Å 403.60Å 90.00° 91.62° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-3.10) 97.9 (50.00-3.10)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.243 , 0.267 0.240 , 0.264	Depositor DCC
R_{free} test set	59600 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	307322	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% 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: PSU, KIR, OMC, H2U, 7MG, MIA, GDP, 4SU, ZN, 5MU

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	0.46	1/36325 (0.0%)	0.72	64/56695 (0.1%)
1	CA	0.45	1/36325 (0.0%)	0.71	61/56695 (0.1%)
2	AB	0.58	0/1935	1.07	14/2609 (0.5%)
2	CB	0.51	0/1935	1.07	15/2609 (0.6%)
3	AC	0.66	0/1636	1.06	11/2205 (0.5%)
3	CC	0.52	0/1636	1.07	8/2205 (0.4%)
4	AD	0.45	0/1733	0.97	6/2318 (0.3%)
4	CD	0.44	0/1733	0.97	5/2318 (0.2%)
5	AE	0.71	0/1162	1.14	7/1564 (0.4%)
5	CE	0.63	0/1162	1.14	10/1564 (0.6%)
6	AF	0.50	0/856	0.98	2/1154 (0.2%)
6	CF	0.45	0/856	0.98	2/1154 (0.2%)
7	AG	0.57	0/1276	0.96	5/1709 (0.3%)
7	CG	0.48	0/1276	0.96	5/1709 (0.3%)
8	AH	0.62	0/1136	1.06	6/1527 (0.4%)
8	CH	0.56	0/1136	1.06	5/1527 (0.3%)
9	AI	0.54	0/1029	1.00	6/1379 (0.4%)
9	CI	0.47	0/1029	0.98	5/1379 (0.4%)
10	AJ	0.56	0/807	1.02	3/1085 (0.3%)
10	CJ	0.47	0/807	1.00	2/1085 (0.2%)
11	AK	0.64	0/900	1.08	8/1213 (0.7%)
11	CK	0.54	0/900	1.09	5/1213 (0.4%)
12	AL	0.51	0/986	1.04	6/1320 (0.5%)
12	CL	0.49	0/986	1.03	4/1320 (0.3%)
13	AM	0.55	0/998	1.09	8/1336 (0.6%)
13	CM	0.47	0/998	1.10	8/1336 (0.6%)
14	AN	0.59	0/501	1.18	4/664 (0.6%)
14	CN	0.52	0/501	1.17	5/664 (0.8%)
15	AO	0.57	0/745	0.94	2/992 (0.2%)
15	CO	0.54	0/745	0.91	1/992 (0.1%)
16	AP	0.48	0/716	0.94	3/963 (0.3%)
16	CP	0.45	0/716	0.94	3/963 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.55	0/836	1.02	1/1117 (0.1%)
17	CQ	0.49	0/836	1.01	1/1117 (0.1%)
18	AR	0.51	0/579	1.02	5/768 (0.7%)
18	CR	0.48	0/579	1.02	5/768 (0.7%)
19	AS	0.53	0/642	1.06	5/865 (0.6%)
19	CS	0.46	0/642	1.05	5/865 (0.6%)
20	AT	0.47	0/765	1.15	8/1007 (0.8%)
20	CT	0.43	0/765	1.13	6/1007 (0.6%)
21	AU	0.54	0/212	1.03	2/277 (0.7%)
21	CU	0.50	0/212	0.98	2/277 (0.7%)
22	AV	0.45	0/1809	0.70	1/2819 (0.0%)
22	AW	0.39	0/1809	0.67	2/2819 (0.1%)
22	CV	0.44	0/1809	0.69	1/2819 (0.0%)
22	CW	0.40	0/1809	0.67	2/2819 (0.1%)
23	AX	0.49	0/405	0.72	0/629
23	CX	0.47	0/405	0.72	0/629
24	AY	0.42	0/1616	0.59	2/2511 (0.1%)
24	CY	0.43	0/1616	0.59	2/2511 (0.1%)
25	AZ	0.40	0/3041	0.89	6/4127 (0.1%)
25	CZ	0.41	0/3041	0.89	6/4127 (0.1%)
26	B0	0.47	0/671	1.02	3/892 (0.3%)
26	D0	0.45	0/671	1.01	2/892 (0.2%)
27	B1	0.55	0/738	1.11	3/981 (0.3%)
27	D1	0.48	0/738	0.98	3/981 (0.3%)
28	B2	0.43	0/600	1.09	6/793 (0.8%)
28	D2	0.41	0/600	1.07	5/793 (0.6%)
29	B3	0.50	0/472	0.98	3/634 (0.5%)
29	D3	0.43	0/472	0.97	3/634 (0.5%)
30	B4	0.48	0/349	0.93	1/474 (0.2%)
30	D4	0.46	0/349	0.92	1/474 (0.2%)
31	B5	0.53	0/473	1.06	2/639 (0.3%)
31	D5	0.53	0/473	1.06	1/639 (0.2%)
32	B6	0.64	0/440	1.16	5/586 (0.9%)
32	D6	0.60	0/440	1.14	4/586 (0.7%)
33	B7	0.57	0/426	1.10	5/561 (0.9%)
33	D7	0.51	0/426	1.08	5/561 (0.9%)
34	B8	0.62	0/515	1.21	5/679 (0.7%)
34	D8	0.56	0/515	1.19	5/679 (0.7%)
35	B9	0.53	0/310	0.96	0/407
35	D9	0.52	0/310	0.96	0/407
36	BA	0.44	1/69976 (0.0%)	0.68	60/109244 (0.1%)
36	DA	0.44	1/69976 (0.0%)	0.68	61/109244 (0.1%)
37	BB	0.41	0/2853	0.69	2/4451 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DB	0.42	0/2853	0.70	3/4451 (0.1%)
38	BC	0.53	3/1774 (0.2%)	0.94	5/2391 (0.2%)
38	DC	0.49	4/1774 (0.2%)	0.93	4/2391 (0.2%)
39	BD	0.66	0/2195	1.17	20/2955 (0.7%)
39	DD	0.61	0/2195	1.17	20/2955 (0.7%)
40	BE	0.54	0/1596	1.18	12/2153 (0.6%)
40	DE	0.53	0/1596	1.18	13/2153 (0.6%)
41	BF	0.46	0/1658	1.00	10/2244 (0.4%)
41	DF	0.44	0/1658	1.00	9/2244 (0.4%)
42	BG	0.51	0/1499	1.18	12/2016 (0.6%)
42	DG	0.45	0/1499	1.06	10/2016 (0.5%)
43	BH	0.44	0/1245	1.03	8/1682 (0.5%)
43	DH	0.43	0/1245	1.03	8/1682 (0.5%)
46	BN	0.46	0/1131	0.97	1/1525 (0.1%)
46	DN	0.43	0/1131	0.96	1/1525 (0.1%)
47	BO	0.57	0/943	1.02	1/1269 (0.1%)
47	DO	0.55	0/943	1.01	1/1269 (0.1%)
48	BP	0.55	0/1131	1.28	15/1504 (1.0%)
48	DP	0.52	0/1131	1.28	16/1504 (1.1%)
49	BQ	0.60	0/1143	1.07	6/1527 (0.4%)
49	DQ	0.56	0/1143	1.06	8/1527 (0.5%)
50	BR	0.50	0/974	0.96	2/1302 (0.2%)
50	DR	0.49	0/974	0.95	2/1302 (0.2%)
51	BS	0.46	0/778	1.11	4/1036 (0.4%)
51	DS	0.43	0/778	1.10	6/1036 (0.6%)
52	BT	0.55	0/1155	1.14	16/1542 (1.0%)
52	DT	0.53	0/1155	1.14	17/1542 (1.1%)
53	BU	0.49	0/975	1.11	10/1297 (0.8%)
53	DU	0.46	0/975	1.10	10/1297 (0.8%)
54	BV	0.47	0/790	0.92	2/1057 (0.2%)
54	DV	0.47	0/790	0.92	2/1057 (0.2%)
55	BW	0.47	0/907	0.96	1/1216 (0.1%)
55	DW	0.45	0/907	0.95	1/1216 (0.1%)
56	BX	0.45	0/739	1.01	5/993 (0.5%)
56	DX	0.44	0/739	1.01	5/993 (0.5%)
57	BY	0.47	0/788	1.11	5/1051 (0.5%)
57	DY	0.46	0/788	1.10	5/1051 (0.5%)
58	BZ	0.56	0/1435	1.15	9/1949 (0.5%)
58	DZ	0.49	0/1435	1.16	14/1949 (0.7%)
All	All	0.46	11/330268 (0.0%)	0.81	845/493444 (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	5	49
1	CA	4	49
22	AW	1	1
22	CW	1	1
24	AY	2	0
24	CY	2	0
36	BA	2	66
36	DA	2	67
37	BB	0	6
37	DB	0	6
All	All	19	245

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	BC	218	MET	SD-CE	7.06	1.97	1.79
38	DC	218	MET	CG-SD	6.65	1.97	1.80
36	BA	2173	A	O5'-C5'	6.38	1.52	1.42
38	DC	218	MET	SD-CE	6.37	1.95	1.79
36	DA	2173	A	O5'-C5'	6.15	1.52	1.42

The worst 5 of 845 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1498	U	C2'-C3'-O3'	15.95	133.42	109.50
1	AA	1498	U	C2'-C3'-O3'	15.66	132.99	109.50
1	AA	508	C	C2'-C3'-O3'	14.29	130.93	109.50
36	DA	1820	U	C2'-C3'-O3'	14.02	130.53	109.50
1	CA	508	C	C2'-C3'-O3'	14.01	130.51	109.50

5 of 19 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	508	C	C3'
1	AA	1239	A	C3'
1	AA	1498	U	C3'
1	AA	1504	G	C3'
1	AA	1531	A	C3'

5 of 245 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	108	G	Sidechain
1	AA	14	U	Sidechain
1	AA	189(G)	G	Sidechain
1	AA	189(H)	G	Sidechain
1	AA	21	G	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32451	0	16382	1017	0
1	CA	32451	0	16382	1043	0
2	AB	1900	0	1951	215	0
2	CB	1900	0	1951	215	0
3	AC	1612	0	1677	155	0
3	CC	1612	0	1677	165	0
4	AD	1703	0	1764	233	0
4	CD	1703	0	1763	237	0
5	AE	1146	0	1207	80	0
5	CE	1146	0	1207	91	0
6	AF	843	0	857	85	0
6	CF	843	0	857	84	0
7	AG	1257	0	1296	95	0
7	CG	1257	0	1296	93	0
8	AH	1116	0	1177	55	0
8	CH	1116	0	1177	59	0
9	AI	1010	0	1037	145	0
9	CI	1010	0	1037	145	0
10	AJ	794	0	840	117	0
10	CJ	794	0	840	120	0
11	AK	885	0	904	64	0
11	CK	885	0	904	67	0
12	AL	970	0	1057	111	0
12	CL	970	0	1057	115	0
13	AM	987	0	1059	144	0
13	CM	987	0	1059	146	0
14	AN	492	0	529	58	0
14	CN	492	0	529	60	0
15	AO	734	0	771	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	734	0	771	46	0
16	AP	700	0	720	79	0
16	CP	700	0	720	79	0
17	AQ	823	0	891	56	0
17	CQ	823	0	891	60	0
18	AR	574	0	644	35	0
18	CR	574	0	644	39	0
19	AS	629	0	652	81	0
19	CS	629	0	652	82	0
20	AT	763	0	861	83	0
20	CT	763	0	861	83	0
21	AU	208	0	221	13	0
21	CU	208	0	221	13	0
22	AV	1619	0	822	59	0
22	AW	1619	0	822	65	0
22	CV	1619	0	822	62	0
22	CW	1619	0	822	69	0
23	AX	361	0	184	7	0
23	CX	361	0	184	11	0
24	AY	1643	0	853	75	0
24	CY	1643	0	853	75	0
25	AZ	2983	0	2999	294	0
25	CZ	2983	0	2999	299	0
26	B0	662	0	688	62	0
26	D0	662	0	688	64	0
27	B1	731	0	808	74	0
27	D1	731	0	808	72	0
28	B2	598	0	653	165	0
28	D2	598	0	653	73	0
29	B3	467	0	523	51	0
29	D3	467	0	523	51	0
30	B4	340	0	336	51	0
30	D4	340	0	336	55	0
31	B5	459	0	480	66	0
31	D5	459	0	480	68	0
32	B6	433	0	461	136	0
32	D6	433	0	461	136	0
33	B7	418	0	467	29	0
33	D7	418	0	467	27	0
34	B8	507	0	576	125	0
34	D8	507	0	576	123	0
35	B9	307	0	336	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	D9	307	0	335	42	0
36	BA	62477	0	31497	2136	0
36	DA	62477	0	31497	2207	0
37	BB	2551	0	1295	84	0
37	DB	2551	0	1295	94	0
38	BC	1742	0	1800	150	0
38	DC	1742	0	1800	140	0
39	BD	2145	0	2234	234	0
39	DD	2145	0	2234	242	0
40	BE	1563	0	1629	229	0
40	DE	1563	0	1629	230	0
41	BF	1623	0	1677	201	0
41	DF	1623	0	1677	207	0
42	BG	1474	0	1535	257	0
42	DG	1474	0	1535	246	0
43	BH	1222	0	1282	185	0
43	DH	1222	0	1282	191	0
44	BJ	651	0	164	27	0
44	DJ	651	0	164	31	0
45	BK	700	0	173	18	0
45	DK	700	0	173	15	0
46	BN	1104	0	1180	183	0
46	DN	1104	0	1180	179	0
47	BO	933	0	996	87	0
47	DO	933	0	996	87	0
48	BP	1114	0	1187	271	0
48	DP	1114	0	1187	272	0
49	BQ	1122	0	1179	121	0
49	DQ	1122	0	1179	113	0
50	BR	960	0	1021	138	0
50	DR	960	0	1021	133	0
51	BS	770	0	832	162	0
51	DS	770	0	832	160	0
52	BT	1141	0	1202	235	0
52	DT	1141	0	1202	227	0
53	BU	958	0	1015	141	0
53	DU	958	0	1015	141	0
54	BV	779	0	852	118	0
54	DV	779	0	852	121	0
55	BW	896	0	953	90	0
55	DW	896	0	953	89	0
56	BX	725	0	778	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DX	725	0	778	88	0
57	BY	775	0	870	176	0
57	DY	775	0	870	167	0
58	BZ	1403	0	1432	224	0
58	DZ	1403	0	1432	208	0
59	AD	1	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B9	1	0	0	0	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D9	1	0	0	0	0
60	AZ	28	0	12	2	0
60	CZ	28	0	12	6	0
61	AZ	57	0	58	3	0
61	CZ	57	0	59	2	0
All	All	307322	0	208715	18175	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

The worst 5 of 18175 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)
38:DC:123:VAL:CG2	38:DC:127:LEU:HD23	1.33	1.53
38:BC:123:VAL:CG2	38:BC:127:LEU:HD23	1.33	1.51
38:DC:123:VAL:HG23	38:DC:127:LEU:CD2	1.50	1.42
38:BC:123:VAL:HG23	38:BC:127:LEU:CD2	1.50	1.41
36:DA:1899:G:N2	36:DA:1902:C:H41	1.34	1.24

There are no symmetry-related clashes.

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%)	175 (75%)	39 (17%)	18 (8%)	1	4
2	CB	232/256 (91%)	173 (75%)	41 (18%)	18 (8%)	1	4
3	AC	204/239 (85%)	161 (79%)	23 (11%)	20 (10%)	0	3
3	CC	204/239 (85%)	159 (78%)	28 (14%)	17 (8%)	0	4
4	AD	206/209 (99%)	134 (65%)	46 (22%)	26 (13%)	0	1
4	CD	206/209 (99%)	133 (65%)	48 (23%)	25 (12%)	0	1
5	AE	148/162 (91%)	138 (93%)	5 (3%)	5 (3%)	3	16
5	CE	148/162 (91%)	138 (93%)	6 (4%)	4 (3%)	4	20
6	AF	99/101 (98%)	80 (81%)	12 (12%)	7 (7%)	1	5
6	CF	99/101 (98%)	81 (82%)	11 (11%)	7 (7%)	1	5
7	AG	153/156 (98%)	123 (80%)	22 (14%)	8 (5%)	1	10
7	CG	153/156 (98%)	123 (80%)	22 (14%)	8 (5%)	1	10
8	AH	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	18	49
8	CH	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	18	49
9	AI	125/128 (98%)	85 (68%)	23 (18%)	17 (14%)	0	1
9	CI	125/128 (98%)	84 (67%)	24 (19%)	17 (14%)	0	1
10	AJ	96/105 (91%)	75 (78%)	12 (12%)	9 (9%)	0	3
10	CJ	96/105 (91%)	75 (78%)	12 (12%)	9 (9%)	0	3
11	AK	117/129 (91%)	100 (86%)	10 (8%)	7 (6%)	1	7
11	CK	117/129 (91%)	101 (86%)	9 (8%)	7 (6%)	1	7
12	AL	122/135 (90%)	94 (77%)	15 (12%)	13 (11%)	0	2
12	CL	122/135 (90%)	91 (75%)	18 (15%)	13 (11%)	0	2
13	AM	122/126 (97%)	82 (67%)	26 (21%)	14 (12%)	0	1
13	CM	122/126 (97%)	84 (69%)	24 (20%)	14 (12%)	0	1
14	AN	58/61 (95%)	41 (71%)	6 (10%)	11 (19%)	0	0
14	CN	58/61 (95%)	40 (69%)	7 (12%)	11 (19%)	0	0
15	AO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	CO	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	37
16	AP	81/88 (92%)	52 (64%)	22 (27%)	7 (9%)	0	4
16	CP	81/88 (92%)	52 (64%)	22 (27%)	7 (9%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	5	25
17	CQ	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	5	25
18	AR	68/88 (77%)	56 (82%)	11 (16%)	1 (2%)	8	32
18	CR	68/88 (77%)	57 (84%)	10 (15%)	1 (2%)	8	32
19	AS	76/93 (82%)	50 (66%)	16 (21%)	10 (13%)	0	1
19	CS	76/93 (82%)	50 (66%)	16 (21%)	10 (13%)	0	1
20	AT	97/106 (92%)	64 (66%)	24 (25%)	9 (9%)	0	3
20	CT	97/106 (92%)	62 (64%)	26 (27%)	9 (9%)	0	3
21	AU	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	2	12
21	CU	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	2	12
25	AZ	381/405 (94%)	269 (71%)	82 (22%)	30 (8%)	1	4
25	CZ	381/405 (94%)	268 (70%)	83 (22%)	30 (8%)	1	4
26	B0	82/85 (96%)	69 (84%)	10 (12%)	3 (4%)	2	15
26	D0	82/85 (96%)	69 (84%)	10 (12%)	3 (4%)	2	15
27	B1	91/98 (93%)	70 (77%)	10 (11%)	11 (12%)	0	1
27	D1	91/98 (93%)	71 (78%)	14 (15%)	6 (7%)	1	6
28	B2	69/72 (96%)	40 (58%)	15 (22%)	14 (20%)	0	0
28	D2	69/72 (96%)	44 (64%)	18 (26%)	7 (10%)	0	3
29	B3	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	0	3
29	D3	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	0	3
30	B4	42/71 (59%)	20 (48%)	17 (40%)	5 (12%)	0	1
30	D4	42/71 (59%)	20 (48%)	17 (40%)	5 (12%)	0	1
31	B5	57/60 (95%)	39 (68%)	8 (14%)	10 (18%)	0	0
31	D5	57/60 (95%)	39 (68%)	8 (14%)	10 (18%)	0	0
32	B6	48/54 (89%)	24 (50%)	8 (17%)	16 (33%)	0	0
32	D6	48/54 (89%)	24 (50%)	8 (17%)	16 (33%)	0	0
33	B7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	5	24
33	D7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	5	24
34	B8	61/65 (94%)	34 (56%)	21 (34%)	6 (10%)	0	3
34	D8	61/65 (94%)	34 (56%)	21 (34%)	6 (10%)	0	3
35	B9	35/37 (95%)	25 (71%)	6 (17%)	4 (11%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	D9	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	0	4
38	BC	226/229 (99%)	170 (75%)	45 (20%)	11 (5%)	1	11
38	DC	226/229 (99%)	171 (76%)	43 (19%)	12 (5%)	1	10
39	BD	273/276 (99%)	219 (80%)	31 (11%)	23 (8%)	0	4
39	DD	273/276 (99%)	217 (80%)	31 (11%)	25 (9%)	0	3
40	BE	202/206 (98%)	134 (66%)	39 (19%)	29 (14%)	0	0
40	DE	202/206 (98%)	134 (66%)	39 (19%)	29 (14%)	0	0
41	BF	205/210 (98%)	148 (72%)	35 (17%)	22 (11%)	0	2
41	DF	205/210 (98%)	149 (73%)	34 (17%)	22 (11%)	0	2
42	BG	179/182 (98%)	118 (66%)	33 (18%)	28 (16%)	0	0
42	DG	179/182 (98%)	119 (66%)	31 (17%)	29 (16%)	0	0
43	BH	157/180 (87%)	93 (59%)	34 (22%)	30 (19%)	0	0
43	DH	157/180 (87%)	94 (60%)	33 (21%)	30 (19%)	0	0
46	BN	136/140 (97%)	93 (68%)	20 (15%)	23 (17%)	0	0
46	DN	136/140 (97%)	93 (68%)	20 (15%)	23 (17%)	0	0
47	BO	120/122 (98%)	106 (88%)	8 (7%)	6 (5%)	1	11
47	DO	120/122 (98%)	106 (88%)	8 (7%)	6 (5%)	1	11
48	BP	144/150 (96%)	78 (54%)	36 (25%)	30 (21%)	0	0
48	DP	144/150 (96%)	77 (54%)	37 (26%)	30 (21%)	0	0
49	BQ	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	2	16
49	DQ	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	2	16
50	BR	115/118 (98%)	83 (72%)	16 (14%)	16 (14%)	0	1
50	DR	115/118 (98%)	83 (72%)	17 (15%)	15 (13%)	0	1
51	BS	96/112 (86%)	50 (52%)	24 (25%)	22 (23%)	0	0
51	DS	96/112 (86%)	49 (51%)	23 (24%)	24 (25%)	0	0
52	BT	135/146 (92%)	82 (61%)	30 (22%)	23 (17%)	0	0
52	DT	135/146 (92%)	82 (61%)	30 (22%)	23 (17%)	0	0
53	BU	115/118 (98%)	83 (72%)	25 (22%)	7 (6%)	1	7
53	DU	115/118 (98%)	83 (72%)	25 (22%)	7 (6%)	1	7
54	BV	99/101 (98%)	61 (62%)	23 (23%)	15 (15%)	0	0
54	DV	99/101 (98%)	62 (63%)	22 (22%)	15 (15%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BW	111/113 (98%)	87 (78%)	12 (11%)	12 (11%)	0	2
55	DW	111/113 (98%)	85 (77%)	14 (13%)	12 (11%)	0	2
56	BX	90/96 (94%)	64 (71%)	20 (22%)	6 (7%)	1	6
56	DX	90/96 (94%)	65 (72%)	19 (21%)	6 (7%)	1	6
57	BY	98/110 (89%)	41 (42%)	31 (32%)	26 (26%)	0	0
57	DY	98/110 (89%)	43 (44%)	29 (30%)	26 (26%)	0	0
58	BZ	174/206 (84%)	109 (63%)	27 (16%)	38 (22%)	0	0
58	DZ	174/206 (84%)	109 (63%)	47 (27%)	18 (10%)	0	2
All	All	12256/13106 (94%)	8858 (72%)	2104 (17%)	1294 (11%)	0	2

5 of 1294 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	18	GLY
2	AB	190	THR
2	AB	191	ASP
2	AB	230	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	177 (88%)	25 (12%)	4	19
2	CB	202/220 (92%)	177 (88%)	25 (12%)	4	19
3	AC	160/188 (85%)	141 (88%)	19 (12%)	5	21
3	CC	160/188 (85%)	142 (89%)	18 (11%)	5	23
4	AD	180/181 (99%)	157 (87%)	23 (13%)	4	18
4	CD	180/181 (99%)	157 (87%)	23 (13%)	4	18
5	AE	115/123 (94%)	103 (90%)	12 (10%)	7	27
5	CE	115/123 (94%)	101 (88%)	14 (12%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AF	90/90 (100%)	81 (90%)	9 (10%)	7	29
6	CF	90/90 (100%)	80 (89%)	10 (11%)	6	24
7	AG	126/127 (99%)	115 (91%)	11 (9%)	9	34
7	CG	126/127 (99%)	116 (92%)	10 (8%)	11	37
8	AH	119/119 (100%)	109 (92%)	10 (8%)	10	35
8	CH	119/119 (100%)	109 (92%)	10 (8%)	10	35
9	AI	98/99 (99%)	89 (91%)	9 (9%)	8	31
9	CI	98/99 (99%)	89 (91%)	9 (9%)	8	31
10	AJ	88/92 (96%)	79 (90%)	9 (10%)	7	28
10	CJ	88/92 (96%)	79 (90%)	9 (10%)	7	28
11	AK	90/99 (91%)	82 (91%)	8 (9%)	9	33
11	CK	90/99 (91%)	82 (91%)	8 (9%)	9	33
12	AL	104/111 (94%)	95 (91%)	9 (9%)	9	34
12	CL	104/111 (94%)	96 (92%)	8 (8%)	12	38
13	AM	99/101 (98%)	87 (88%)	12 (12%)	5	20
13	CM	99/101 (98%)	87 (88%)	12 (12%)	5	20
14	AN	49/50 (98%)	39 (80%)	10 (20%)	1	5
14	CN	49/50 (98%)	39 (80%)	10 (20%)	1	5
15	AO	79/80 (99%)	70 (89%)	9 (11%)	5	23
15	CO	79/80 (99%)	70 (89%)	9 (11%)	5	23
16	AP	72/74 (97%)	65 (90%)	7 (10%)	8	30
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	30
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	20	51
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	20	51
18	AR	61/77 (79%)	54 (88%)	7 (12%)	5	23
18	CR	61/77 (79%)	54 (88%)	7 (12%)	5	23
19	AS	69/80 (86%)	57 (83%)	12 (17%)	2	9
19	CS	69/80 (86%)	57 (83%)	12 (17%)	2	9
20	AT	76/82 (93%)	71 (93%)	5 (7%)	15	43
20	CT	76/82 (93%)	71 (93%)	5 (7%)	15	43
21	AU	19/22 (86%)	18 (95%)	1 (5%)	20	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CU	19/22 (86%)	18 (95%)	1 (5%)	20	51
25	AZ	322/338 (95%)	300 (93%)	22 (7%)	14	42
25	CZ	322/338 (95%)	300 (93%)	22 (7%)	14	42
26	B0	66/67 (98%)	59 (89%)	7 (11%)	6	26
26	D0	66/67 (98%)	59 (89%)	7 (11%)	6	26
27	B1	78/83 (94%)	67 (86%)	11 (14%)	3	15
27	D1	78/83 (94%)	71 (91%)	7 (9%)	9	33
28	B2	66/67 (98%)	61 (92%)	5 (8%)	12	39
28	D2	66/67 (98%)	59 (89%)	7 (11%)	6	26
29	B3	51/52 (98%)	44 (86%)	7 (14%)	3	15
29	D3	51/52 (98%)	44 (86%)	7 (14%)	3	15
30	B4	39/63 (62%)	32 (82%)	7 (18%)	2	9
30	D4	39/63 (62%)	32 (82%)	7 (18%)	2	9
31	B5	51/52 (98%)	44 (86%)	7 (14%)	3	15
31	D5	51/52 (98%)	44 (86%)	7 (14%)	3	15
32	B6	49/52 (94%)	34 (69%)	15 (31%)	0	0
32	D6	49/52 (94%)	34 (69%)	15 (31%)	0	0
33	B7	41/42 (98%)	32 (78%)	9 (22%)	1	4
33	D7	41/42 (98%)	32 (78%)	9 (22%)	1	4
34	B8	53/55 (96%)	44 (83%)	9 (17%)	2	10
34	D8	53/55 (96%)	43 (81%)	10 (19%)	1	7
35	B9	34/34 (100%)	30 (88%)	4 (12%)	5	21
35	D9	34/34 (100%)	30 (88%)	4 (12%)	5	21
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%)	145 (88%)	20 (12%)	5	20
40	DE	165/166 (99%)	145 (88%)	20 (12%)	5	20
41	BF	165/166 (99%)	154 (93%)	11 (7%)	15	43
41	DF	165/166 (99%)	154 (93%)	11 (7%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BG	155/156 (99%)	130 (84%)	25 (16%)	2	11
42	DG	155/156 (99%)	136 (88%)	19 (12%)	4	20
43	BH	132/148 (89%)	118 (89%)	14 (11%)	6	26
43	DH	132/148 (89%)	118 (89%)	14 (11%)	6	26
46	BN	117/119 (98%)	105 (90%)	12 (10%)	7	27
46	DN	117/119 (98%)	103 (88%)	14 (12%)	5	21
47	BO	100/100 (100%)	90 (90%)	10 (10%)	7	29
47	DO	100/100 (100%)	90 (90%)	10 (10%)	7	29
48	BP	112/116 (97%)	94 (84%)	18 (16%)	2	11
48	DP	112/116 (97%)	95 (85%)	17 (15%)	3	13
49	BQ	111/111 (100%)	96 (86%)	15 (14%)	4	16
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	4	19
50	BR	100/101 (99%)	89 (89%)	11 (11%)	6	24
50	DR	100/101 (99%)	89 (89%)	11 (11%)	6	24
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%)	99 (82%)	21 (18%)	2	9
52	DT	120/127 (94%)	99 (82%)	21 (18%)	2	9
53	BU	92/94 (98%)	85 (92%)	7 (8%)	12	39
53	DU	92/94 (98%)	85 (92%)	7 (8%)	12	39
54	BV	82/82 (100%)	64 (78%)	18 (22%)	1	4
54	DV	82/82 (100%)	63 (77%)	19 (23%)	1	4
55	BW	91/92 (99%)	84 (92%)	7 (8%)	12	38
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%)	67 (90%)	7 (10%)	8	30
57	BY	84/91 (92%)	71 (84%)	13 (16%)	2	12
57	DY	84/91 (92%)	71 (84%)	13 (16%)	2	12
58	BZ	155/179 (87%)	127 (82%)	28 (18%)	2	8
58	DZ	155/179 (87%)	136 (88%)	19 (12%)	4	20
All	All	10338/10860 (95%)	9147 (88%)	1191 (12%)	5	23

5 of 1191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	DC	175	VAL
55	DW	11	ARG
39	DD	218	ARG
38	DC	161	ILE
47	DO	48	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 332 such sidechains are listed below:

Mol	Chain	Res	Type
25	CZ	125	GLN
46	DN	45	ASN
26	D0	40	GLN
39	DD	96	HIS
49	DQ	45	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1509/1522 (99%)	244 (16%)	49 (3%)
1	CA	1509/1522 (99%)	238 (15%)	47 (3%)
22	AV	75/76 (98%)	20 (26%)	2 (2%)
22	AW	75/76 (98%)	17 (22%)	0
22	CV	75/76 (98%)	19 (25%)	1 (1%)
22	CW	75/76 (98%)	17 (22%)	0
23	AX	16/27 (59%)	6 (37%)	0
23	CX	16/27 (59%)	6 (37%)	0
24	AY	75/77 (97%)	25 (33%)	5 (6%)
24	CY	75/77 (97%)	25 (33%)	5 (6%)
36	BA	2900/2915 (99%)	515 (17%)	46 (1%)
36	DA	2900/2915 (99%)	513 (17%)	46 (1%)
37	BB	118/122 (96%)	25 (21%)	2 (1%)
37	DB	118/122 (96%)	25 (21%)	2 (1%)
All	All	9536/9630 (99%)	1695 (17%)	205 (2%)

5 of 1695 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G

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

5 of 205 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	266	G
1	CA	1211	U
36	DA	2481	G
1	CA	351	G
1	CA	748	C

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	H2U	AY	20	24	18,21,22	0.90	0	19,30,33	1.70	3 (15%)
24	4SU	CY	8	24	18,21,22	0.54	0	25,30,33	0.83	2 (8%)
24	5MU	CY	54	24	19,22,23	0.28	0	27,32,35	0.41	0
24	4SU	AY	8	24	18,21,22	0.52	0	25,30,33	0.85	2 (8%)
24	H2U	CY	17	24	18,21,22	0.89	0	19,30,33	1.86	5 (26%)
24	H2U	AY	16	24	18,21,22	0.91	1 (5%)	19,30,33	1.57	3 (15%)
24	PSU	AY	55	24	18,21,22	1.03	1 (5%)	21,30,33	1.75	4 (19%)
24	H2U	CY	16	24	18,21,22	0.97	1 (5%)	19,30,33	1.57	3 (15%)
24	H2U	CY	20	24	18,21,22	0.88	0	19,30,33	1.68	3 (15%)
24	7MG	AY	46	24	23,26,27	2.48	3 (13%)	27,39,42	1.69	3 (11%)
24	OMC	AY	32	24	19,22,23	0.35	0	25,31,34	0.70	1 (4%)
24	MIA	AY	37	24	28,31,32	0.97	1 (3%)	38,44,47	1.02	1 (2%)
24	OMC	CY	32	24	19,22,23	0.34	0	25,31,34	0.70	1 (4%)
24	MIA	CY	37	24	28,31,32	0.79	1 (3%)	38,44,47	1.02	1 (2%)

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	1.02	2 (11%)	21,30,33	1.73	3 (14%)
24	H2U	AY	17	24	18,21,22	0.89	0	19,30,33	1.84	4 (21%)
24	5MU	AY	54	24	19,22,23	0.31	0	27,32,35	0.42	0
24	7MG	CY	46	24	23,26,27	2.48	3 (13%)	27,39,42	1.70	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	H2U	AY	20	24	-	0/7/38/39	0/2/2/2
24	4SU	CY	8	24	-	0/7/25/26	0/2/2/2
24	5MU	CY	54	24	-	0/7/25/26	0/2/2/2
24	4SU	AY	8	24	-	1/7/25/26	0/2/2/2
24	H2U	CY	17	24	-	3/7/38/39	0/2/2/2
24	PSU	AY	55	24	1/1/5/5	2/7/25/26	0/2/2/2
24	H2U	AY	16	24	-	0/7/38/39	0/2/2/2
24	H2U	CY	16	24	-	0/7/38/39	0/2/2/2
24	H2U	CY	20	24	-	0/7/38/39	0/2/2/2
24	7MG	AY	46	24	-	1/7/37/38	0/3/3/3
24	OMC	AY	32	24	-	0/9/27/28	0/2/2/2
24	MIA	AY	37	24	-	2/15/33/34	0/3/3/3
24	OMC	CY	32	24	-	0/9/27/28	0/2/2/2
24	MIA	CY	37	24	-	2/15/33/34	0/3/3/3
24	PSU	CY	55	24	1/1/5/5	2/7/25/26	0/2/2/2
24	H2U	AY	17	24	-	3/7/38/39	0/2/2/2
24	5MU	AY	54	24	-	0/7/25/26	0/2/2/2
24	7MG	CY	46	24	-	1/7/37/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	46	7MG	C8-N9	-11.14	1.38	1.45
24	AY	46	7MG	C8-N9	-11.13	1.38	1.45
24	AY	37	MIA	C2-S10	3.59	1.78	1.75
24	AY	46	7MG	C5-N7	3.09	1.39	1.35
24	CY	46	7MG	C5-N7	3.04	1.39	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CY	46	7MG	N9-C8-N7	6.70	112.85	103.37
24	AY	46	7MG	N9-C8-N7	6.67	112.81	103.37
24	CY	37	MIA	C11-S10-C2	5.58	106.44	102.25
24	AY	37	MIA	C11-S10-C2	5.50	106.38	102.25
24	AY	55	PSU	N1-C2-N3	4.98	120.43	115.17

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	AY	55	PSU	C3'
24	CY	55	PSU	C3'

5 of 17 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	AY	55	PSU	C2'-C1'-C5-C4
24	CY	17	H2U	C4'-C5'-O5'-P
24	CY	37	MIA	C5-C6-N6-C12

There are no ring outliers.

17 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	20	H2U	2	0
24	CY	8	4SU	1	0
24	CY	54	5MU	1	0
24	AY	8	4SU	1	0
24	CY	17	H2U	5	0
24	AY	16	H2U	3	0
24	AY	55	PSU	2	0
24	CY	16	H2U	3	0
24	CY	20	H2U	2	0
24	AY	46	7MG	4	0
24	AY	32	OMC	1	0
24	AY	37	MIA	1	0
24	CY	32	OMC	1	0
24	CY	55	PSU	1	0
24	AY	17	H2U	5	0
24	AY	54	5MU	1	0
24	CY	46	7MG	4	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	AZ	502	-	56,59,59	3.72	23 (41%)	60,84,84	1.68	11 (18%)
60	GDP	CZ	501	-	29,30,30	1.08	2 (6%)	45,47,47	1.83	12 (26%)
61	KIR	CZ	502	-	56,59,59	3.67	24 (42%)	60,84,84	1.68	10 (16%)
60	GDP	AZ	501	-	29,30,30	1.09	1 (3%)	45,47,47	1.71	10 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	KIR	AZ	502	-	-	7/54/98/98	0/3/3/3
60	GDP	CZ	501	-	-	0/16/32/32	0/3/3/3
61	KIR	CZ	502	-	-	5/54/98/98	0/3/3/3
60	GDP	AZ	501	-	-	0/16/32/32	0/3/3/3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	502	KIR	O18-C17	-15.14	1.22	1.44
61	CZ	502	KIR	O18-C17	-14.86	1.22	1.44
61	AZ	502	KIR	O30-C30	-12.72	1.17	1.42
61	CZ	502	KIR	O30-C30	-12.66	1.17	1.42
61	AZ	502	KIR	O34-C33	-9.35	1.29	1.44

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AZ	501	GDP	C2-N3-C4	5.69	122.10	112.30
60	CZ	501	GDP	C2-N3-C4	5.50	121.77	112.30
60	CZ	501	GDP	C5-C4-N3	-4.87	120.63	128.39
61	AZ	502	KIR	O29-C29-O34	-4.79	102.25	110.15
61	AZ	502	KIR	C48-C32-C47	-4.65	101.36	107.70

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

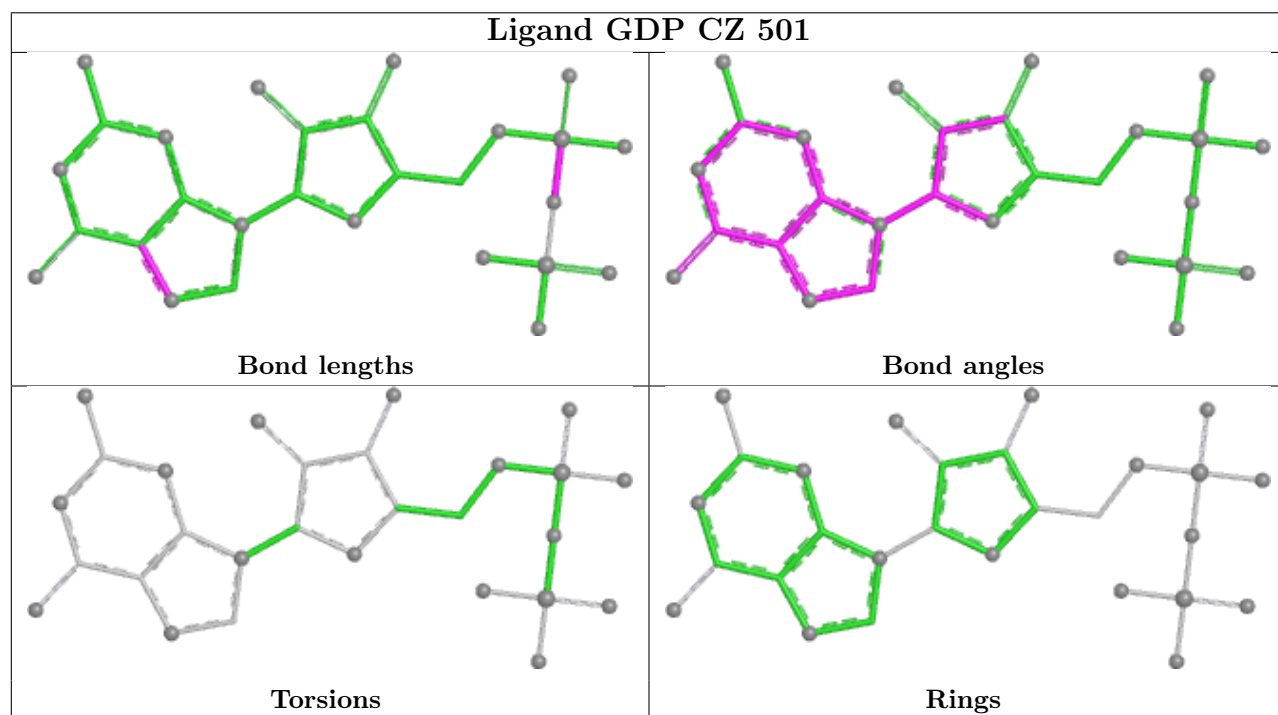
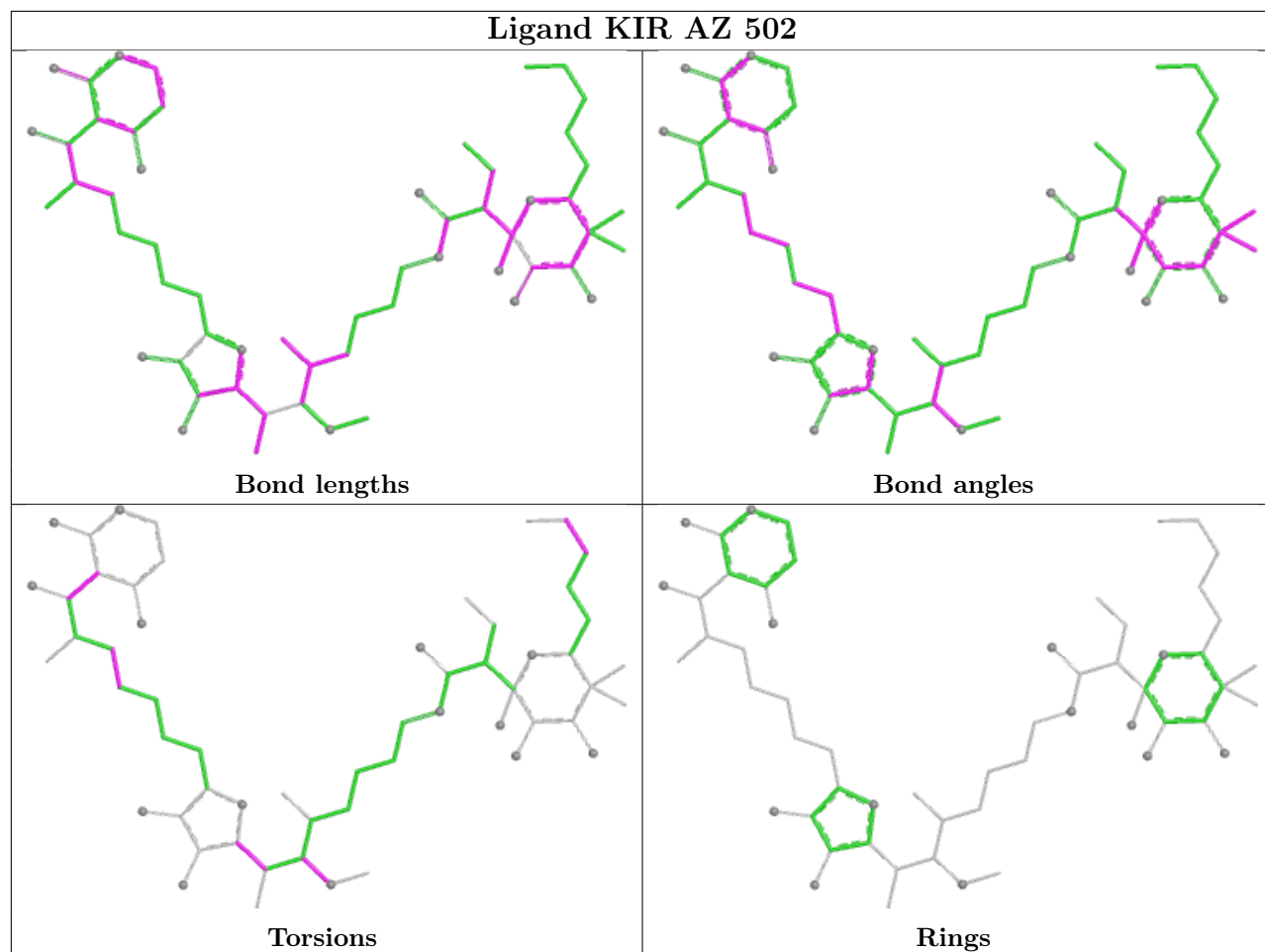
Mol	Chain	Res	Type	Atoms
61	AZ	502	KIR	C2-C3-C7-C8
61	AZ	502	KIR	C4-C3-C7-C8
61	AZ	502	KIR	C11-C10-C9-C8
61	CZ	502	KIR	C2-C3-C7-C8
61	CZ	502	KIR	C4-C3-C7-C8

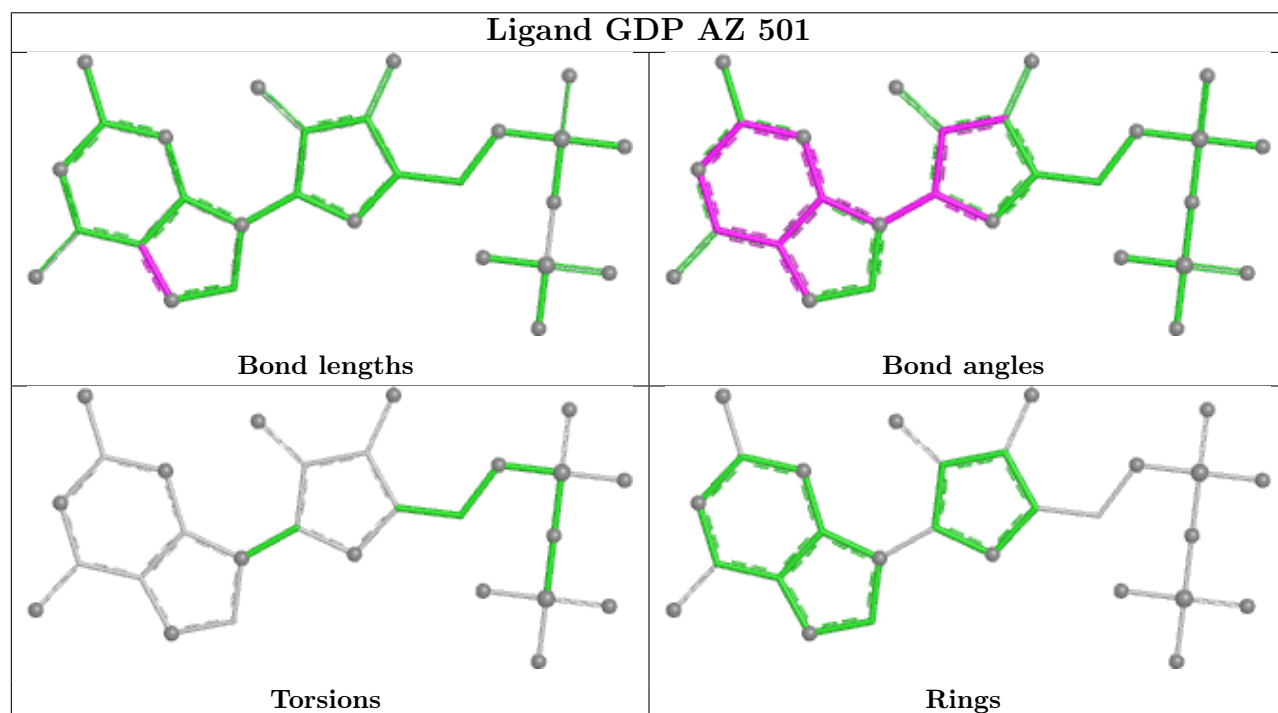
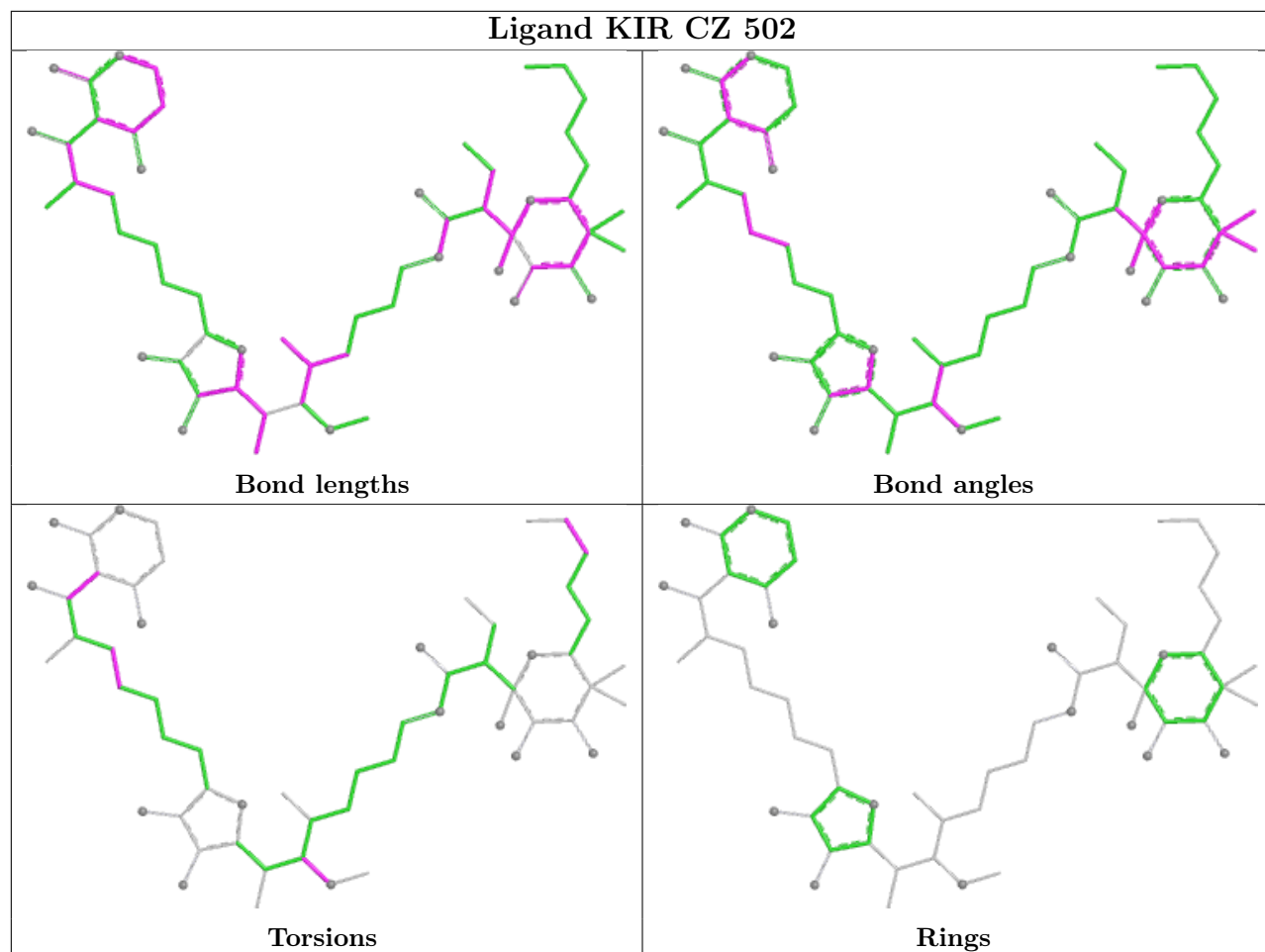
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AZ	502	KIR	3	0
60	CZ	501	GDP	6	0
61	CZ	502	KIR	2	0
60	AZ	501	GDP	2	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%)	0.51	161 (10%) 11 6	17, 54, 143, 200	0
1	CA	1510/1522 (99%)	0.37	84 (5%) 30 16	26, 58, 145, 200	0
2	AB	234/256 (91%)	0.86	39 (16%) 4 2	34, 64, 130, 141	0
2	CB	234/256 (91%)	0.72	23 (9%) 13 7	36, 65, 130, 142	0
3	AC	206/239 (86%)	0.45	13 (6%) 26 14	27, 48, 81, 86	0
3	CC	206/239 (86%)	0.27	4 (1%) 66 45	32, 52, 82, 88	0
4	AD	208/209 (99%)	1.59	59 (28%) 1 1	55, 89, 119, 122	0
4	CD	208/209 (99%)	1.18	37 (17%) 4 2	55, 90, 119, 122	0
5	AE	150/162 (92%)	-0.14	1 (0%) 84 68	23, 41, 62, 84	0
5	CE	150/162 (92%)	-0.08	0 100 100	30, 44, 64, 86	0
6	AF	101/101 (100%)	0.70	4 (3%) 42 23	48, 72, 88, 94	0
6	CF	101/101 (100%)	0.71	2 (1%) 65 44	52, 74, 90, 95	0
7	AG	155/156 (99%)	0.70	12 (7%) 19 10	40, 64, 100, 115	0
7	CG	155/156 (99%)	0.59	10 (6%) 25 13	45, 67, 101, 115	0
8	AH	138/138 (100%)	0.06	2 (1%) 73 53	30, 44, 61, 71	0
8	CH	138/138 (100%)	-0.04	1 (0%) 84 68	31, 47, 62, 72	0
9	AI	127/128 (99%)	1.47	35 (27%) 1 1	33, 73, 113, 120	0
9	CI	127/128 (99%)	1.06	14 (11%) 10 5	40, 77, 114, 120	0
10	AJ	98/105 (93%)	1.86	46 (46%) 0 0	41, 80, 133, 136	0
10	CJ	98/105 (93%)	1.61	34 (34%) 1 0	44, 84, 134, 137	0
11	AK	119/129 (92%)	0.44	9 (7%) 20 11	28, 49, 80, 104	0
11	CK	119/129 (92%)	0.28	3 (2%) 58 37	32, 53, 82, 104	0
12	AL	124/135 (91%)	0.87	13 (10%) 11 6	28, 66, 87, 125	0
12	CL	124/135 (91%)	0.75	6 (4%) 35 19	30, 67, 88, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	124/126 (98%)	1.15	21 (16%) 4 2	50, 73, 100, 137	0
13	CM	124/126 (98%)	0.96	16 (12%) 7 4	53, 76, 101, 137	0
14	AN	60/61 (98%)	0.85	10 (16%) 4 2	33, 48, 76, 79	0
14	CN	60/61 (98%)	0.70	3 (5%) 34 18	39, 53, 76, 80	0
15	AO	88/89 (98%)	0.20	0 100 100	36, 51, 73, 81	0
15	CO	88/89 (98%)	0.21	1 (1%) 78 59	37, 53, 73, 81	0
16	AP	83/88 (94%)	1.14	10 (12%) 9 5	62, 78, 99, 125	0
16	CP	83/88 (94%)	0.87	6 (7%) 21 11	62, 80, 100, 124	0
17	AQ	99/105 (94%)	0.28	0 100 100	33, 55, 72, 83	0
17	CQ	99/105 (94%)	0.22	2 (2%) 65 44	39, 56, 73, 83	0
18	AR	70/88 (79%)	0.31	1 (1%) 73 53	37, 55, 87, 99	0
18	CR	70/88 (79%)	0.33	1 (1%) 73 53	43, 59, 88, 99	0
19	AS	78/93 (83%)	1.58	20 (25%) 1 1	61, 81, 116, 125	0
19	CS	78/93 (83%)	1.26	18 (23%) 2 1	63, 83, 117, 125	0
20	AT	99/106 (93%)	1.01	10 (10%) 12 6	49, 77, 112, 115	0
20	CT	99/106 (93%)	0.89	13 (13%) 7 4	52, 78, 113, 115	0
21	AU	24/27 (88%)	1.16	4 (16%) 4 2	43, 55, 76, 93	0
21	CU	24/27 (88%)	1.13	3 (12%) 8 5	46, 59, 78, 92	0
22	AV	76/76 (100%)	0.33	5 (6%) 24 13	34, 64, 95, 113	0
22	AW	76/76 (100%)	2.76	47 (61%) 0 0	60, 165, 193, 200	0
22	CV	76/76 (100%)	0.29	3 (3%) 43 24	38, 66, 97, 114	0
22	CW	76/76 (100%)	2.29	44 (57%) 0 0	63, 166, 193, 200	0
23	AX	17/27 (62%)	1.58	6 (35%) 1 0	27, 87, 137, 139	0
23	CX	17/27 (62%)	1.47	5 (29%) 1 1	32, 88, 137, 140	0
24	AY	68/77 (88%)	1.38	11 (16%) 4 2	70, 145, 175, 178	0
24	CY	68/77 (88%)	1.49	18 (26%) 1 1	72, 146, 174, 178	0
25	AZ	385/405 (95%)	1.35	77 (20%) 3 1	84, 129, 155, 177	0
25	CZ	385/405 (95%)	1.55	106 (27%) 1 1	85, 129, 155, 177	0
26	B0	84/85 (98%)	0.84	8 (9%) 14 7	47, 64, 95, 108	0
26	D0	84/85 (98%)	0.95	9 (10%) 11 6	50, 66, 95, 108	0
27	B1	93/98 (94%)	0.58	8 (8%) 16 9	38, 55, 114, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9
27	D1	93/98 (94%)	0.77	7 (7%) 20 11	54, 71, 121, 129	0
28	B2	71/72 (98%)	2.80	44 (61%) 0 0	108, 136, 147, 149	0
28	D2	71/72 (98%)	1.20	10 (14%) 6 3	88, 107, 126, 142	0
29	B3	59/60 (98%)	0.81	5 (8%) 16 9	50, 71, 91, 116	0
29	D3	59/60 (98%)	0.72	4 (6%) 23 12	51, 72, 91, 116	0
30	B4	44/71 (61%)	3.59	39 (88%) 0 0	109, 148, 172, 176	0
30	D4	44/71 (61%)	2.30	23 (52%) 0 0	110, 148, 172, 176	0
31	B5	59/60 (98%)	1.24	13 (22%) 2 1	45, 71, 131, 148	0
31	D5	59/60 (98%)	1.30	11 (18%) 3 1	46, 73, 130, 148	0
32	B6	50/54 (92%)	2.65	25 (50%) 0 0	50, 80, 106, 112	0
32	D6	50/54 (92%)	1.80	17 (34%) 1 0	54, 82, 106, 114	0
33	B7	48/49 (97%)	0.73	3 (6%) 26 14	45, 53, 90, 110	0
33	D7	48/49 (97%)	0.59	2 (4%) 40 22	47, 54, 89, 110	0
34	B8	63/65 (96%)	1.53	18 (28%) 1 1	49, 63, 79, 101	0
34	D8	63/65 (96%)	1.25	14 (22%) 2 1	51, 65, 80, 101	0
35	B9	37/37 (100%)	1.46	11 (29%) 1 1	62, 75, 95, 98	0
35	D9	37/37 (100%)	1.64	11 (29%) 1 1	61, 77, 96, 98	0
36	BA	2901/2915 (99%)	0.67	310 (10%) 11 6	21, 65, 173, 200	0
36	DA	2901/2915 (99%)	0.71	323 (11%) 10 5	26, 67, 173, 200	0
37	BB	119/122 (97%)	0.89	10 (8%) 17 9	52, 81, 104, 123	0
37	DB	119/122 (97%)	0.82	5 (4%) 40 22	55, 82, 104, 123	0
38	BC	228/229 (99%)	1.13	45 (19%) 3 1	47, 78, 152, 166	0
38	DC	228/229 (99%)	1.01	31 (13%) 7 4	51, 80, 152, 167	0
39	BD	275/276 (99%)	0.27	22 (8%) 18 10	27, 44, 71, 96	0
39	DD	275/276 (99%)	0.21	16 (5%) 29 16	29, 46, 71, 96	0
40	BE	204/206 (99%)	1.02	31 (15%) 5 3	40, 65, 114, 124	0
40	DE	204/206 (99%)	0.90	30 (14%) 6 3	41, 65, 114, 124	0
41	BF	207/210 (98%)	1.12	32 (15%) 5 2	45, 96, 152, 159	0
41	DF	207/210 (98%)	1.22	39 (18%) 3 1	45, 97, 152, 159	0
42	BG	181/182 (99%)	0.83	24 (13%) 7 4	50, 73, 111, 132	0
42	DG	181/182 (99%)	1.15	33 (18%) 3 1	78, 100, 124, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BH	159/180 (88%)	1.66	49 (30%) 1 1	84, 119, 144, 150	0
43	DH	159/180 (88%)	1.52	39 (24%) 2 1	83, 119, 144, 151	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	138/140 (98%)	0.90	13 (9%) 14 8	51, 74, 118, 123	0
46	DN	138/140 (98%)	0.92	11 (7%) 18 10	51, 75, 118, 123	0
47	BO	122/122 (100%)	-0.01	0 100 100	35, 49, 62, 66	0
47	DO	122/122 (100%)	0.03	0 100 100	35, 50, 62, 65	0
48	BP	146/150 (97%)	2.17	74 (50%) 0 0	47, 92, 118, 139	0
48	DP	146/150 (97%)	1.81	52 (35%) 1 0	49, 95, 118, 138	0
49	BQ	141/141 (100%)	0.46	7 (4%) 34 18	35, 54, 75, 117	0
49	DQ	141/141 (100%)	0.59	7 (4%) 34 18	39, 54, 76, 117	0
50	BR	117/118 (99%)	0.83	8 (6%) 23 12	51, 70, 88, 93	0
50	DR	117/118 (99%)	0.82	11 (9%) 14 8	52, 71, 89, 93	0
51	BS	98/112 (87%)	1.87	33 (33%) 1 0	69, 89, 114, 118	0
51	DS	98/112 (87%)	1.59	31 (31%) 1 1	71, 90, 114, 117	0
52	BT	137/146 (93%)	1.08	22 (16%) 4 2	50, 71, 133, 164	0
52	DT	137/146 (93%)	0.98	14 (10%) 12 6	51, 72, 134, 164	0
53	BU	117/118 (99%)	0.85	10 (8%) 16 9	51, 68, 90, 112	0
53	DU	117/118 (99%)	0.96	13 (11%) 10 5	52, 69, 89, 112	0
54	BV	101/101 (100%)	1.47	21 (20%) 2 1	52, 98, 113, 116	0
54	DV	101/101 (100%)	1.36	16 (15%) 5 2	52, 98, 113, 116	0
55	BW	113/113 (100%)	0.71	7 (6%) 26 14	56, 71, 102, 133	0
55	DW	113/113 (100%)	0.73	5 (4%) 39 21	56, 72, 103, 134	0
56	BX	92/96 (95%)	1.44	16 (17%) 4 2	64, 83, 101, 111	0
56	DX	92/96 (95%)	1.26	15 (16%) 4 2	65, 84, 102, 112	0
57	BY	100/110 (90%)	2.43	57 (57%) 0 0	93, 114, 151, 160	0
57	DY	100/110 (90%)	2.03	40 (40%) 1 0	93, 114, 151, 160	0
58	BZ	176/206 (85%)	1.02	36 (20%) 2 1	44, 71, 117, 123	0
58	DZ	176/206 (85%)	0.99	20 (11%) 10 5	56, 78, 111, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	21994/23376 (94%)	0.83	2933 (13%) 7 4	17, 69, 146, 200	0

The worst 5 of 2933 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
48	BP	107	LYS	11.3
49	DQ	141	GLN	10.9
36	BA	2173	A	10.4
32	B6	42	TRP	9.6
28	B2	64	LEU	9.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	7MG	AY	46	24/25	0.26	0.19	170,172,175,176	0
24	7MG	CY	46	24/25	0.28	0.20	170,172,175,176	0
24	H2U	CY	16	20/21	0.32	0.18	170,173,173,174	0
24	H2U	CY	20	20/21	0.32	0.19	178,179,179,180	0
24	H2U	AY	20	20/21	0.32	0.19	178,179,179,179	0
24	H2U	AY	16	20/21	0.35	0.22	169,173,173,174	0
24	H2U	AY	17	20/21	0.41	0.20	170,174,175,176	0
24	H2U	CY	17	20/21	0.50	0.14	170,173,175,176	0
24	4SU	AY	8	20/21	0.56	0.17	145,147,149,149	0
24	PSU	CY	55	20/21	0.56	0.18	154,160,160,160	0
24	PSU	AY	55	20/21	0.58	0.17	154,159,160,161	0
24	4SU	CY	8	20/21	0.63	0.15	146,147,148,149	0
24	5MU	AY	54	21/22	0.65	0.14	145,149,150,153	0
24	5MU	CY	54	21/22	0.73	0.16	144,149,151,153	0
24	OMC	CY	32	21/22	0.78	0.19	107,112,121,122	0
24	MIA	AY	37	29/30	0.81	0.20	71,88,103,104	0
24	OMC	AY	32	21/22	0.81	0.15	107,112,120,121	0
24	MIA	CY	37	29/30	0.83	0.15	74,88,101,102	0

6.3 Carbohydrates [i](#)

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
60	GDP	AZ	501	28/28	0.80	0.12	130,136,140,141	0
60	GDP	CZ	501	28/28	0.80	0.12	129,136,140,140	0
61	KIR	CZ	502	57/57	0.82	0.18	118,120,121,123	0
61	KIR	AZ	502	57/57	0.85	0.20	117,119,121,122	0
59	ZN	D9	101	1/1	0.99	0.03	81,81,81,81	0
59	ZN	B4	101	1/1	0.99	0.07	90,90,90,90	0
59	ZN	B9	101	1/1	0.99	0.03	82,82,82,82	0
59	ZN	CD	301	1/1	0.99	0.16	72,72,72,72	0
59	ZN	D4	101	1/1	0.99	0.04	115,115,115,115	0
59	ZN	AN	101	1/1	1.00	0.02	34,34,34,34	0
59	ZN	AD	301	1/1	1.00	0.14	59,59,59,59	0
59	ZN	CN	101	1/1	1.00	0.02	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.