



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:59 am GMT

PDB ID : 4V5R  
Title : The crystal structure of EF-Tu and Trp-tRNA-Trp bound to a cognate codon on the 70S ribosome.  
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.  
Deposited on : 2010-12-07  
Resolution : 3.10 Å(reported)

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28972

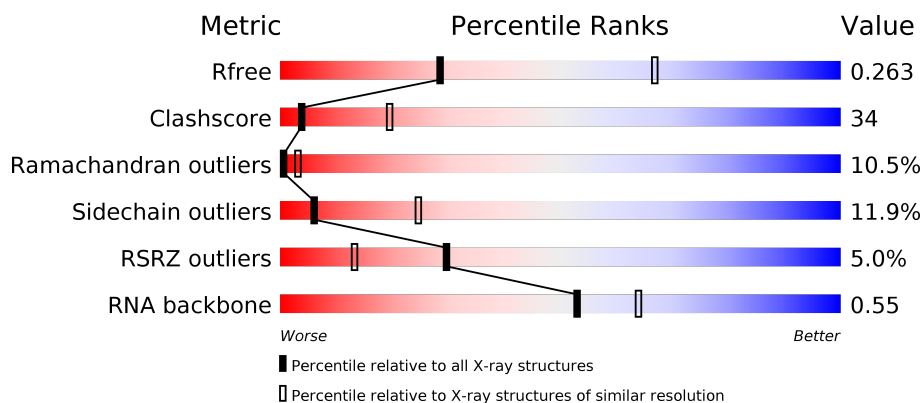
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)
RNA backbone	2435	1112 (3.50-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>0%</div> <div> <div></div> <div>38%</div> <div>49%</div> <div>11%</div> <div>..</div> </div> </div>
1	CA	1522	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>45%</div> <div>10%</div> <div>..</div> </div> </div>
2	AB	256	<div> <div>2%</div> <div> <div></div> <div>30%</div> <div>50%</div> <div>10%</div> <div>9%</div> </div> </div>
2	CB	256	<div> <div>0%</div> <div> <div></div> <div>33%</div> <div>46%</div> <div>11%</div> <div>9%</div> </div> </div>





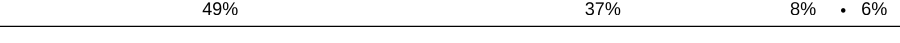
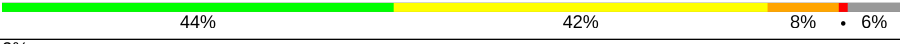
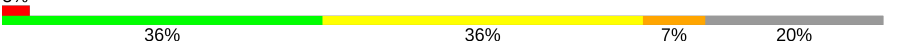

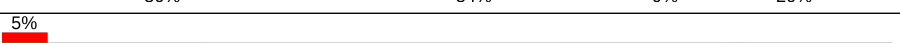
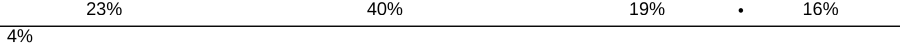
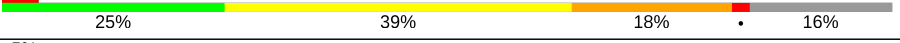
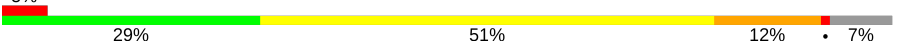

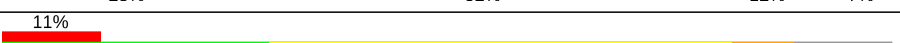
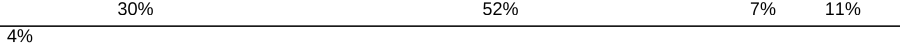
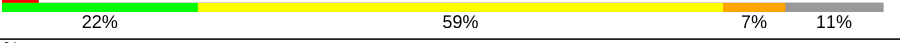

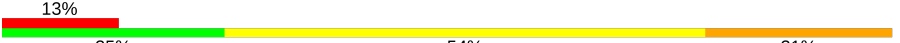
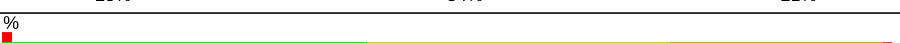


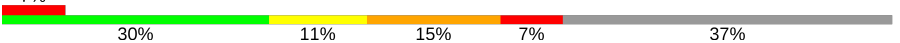

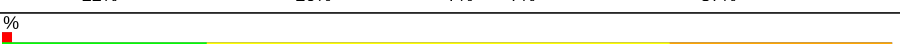
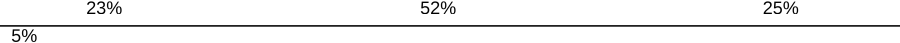
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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	131	
12	CL	131	
13	AM	126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

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

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	GDP	AZ	501	-	-	X	-
61	KIR	AZ	502	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 307330 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1510	Total	C	N	O	P	0	0	0
			32451	14445	6010	10487	1509			
1	CA	1510	Total	C	N	O	P	0	0	0
			32451	14445	6010	10487	1509			

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	24	Total	C	N	O	0	0	0
			208	128	50	30			
21	CU	24	Total	C	N	O	0	0	0
			208	128	50	30			

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

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

- Molecule 23 is a RNA chain called MRNA.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AY	77	Total	C	N	O	P	S	0	0	0
			1645	742	289	536	76	2			
24	CY	77	Total	C	N	O	P	S	0	0	0
			1645	742	289	536	76	2			

- Molecule 25 is a protein called ELONGATION FACTOR TU.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

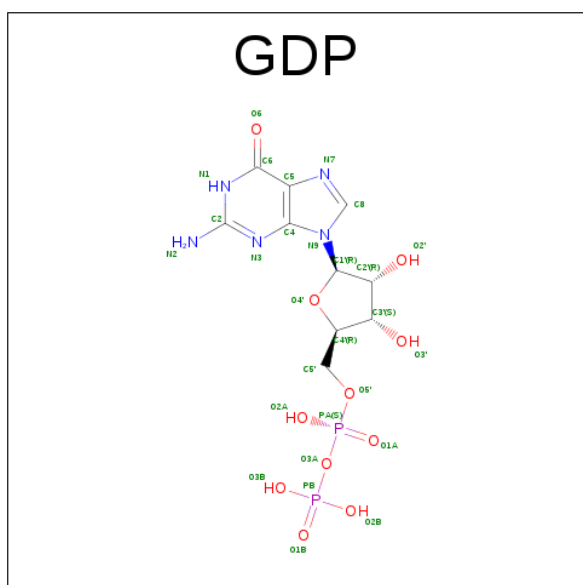
- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

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

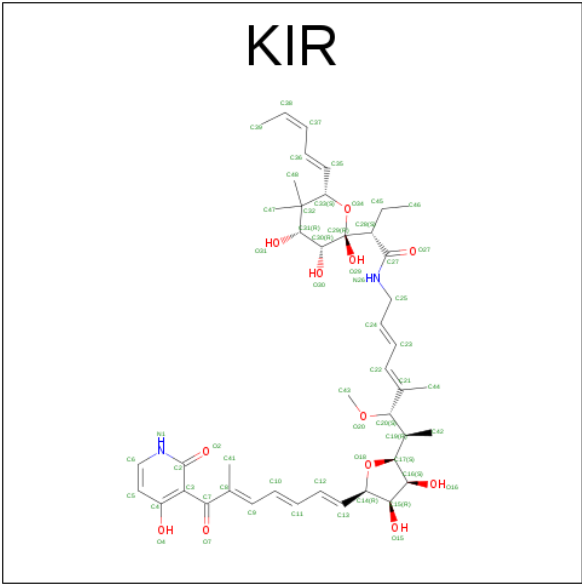
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

- Molecule 61 is KIRROMYCIN (three-letter code: KIR) (formula: C<sub>43</sub>H<sub>60</sub>N<sub>2</sub>O<sub>12</sub>).

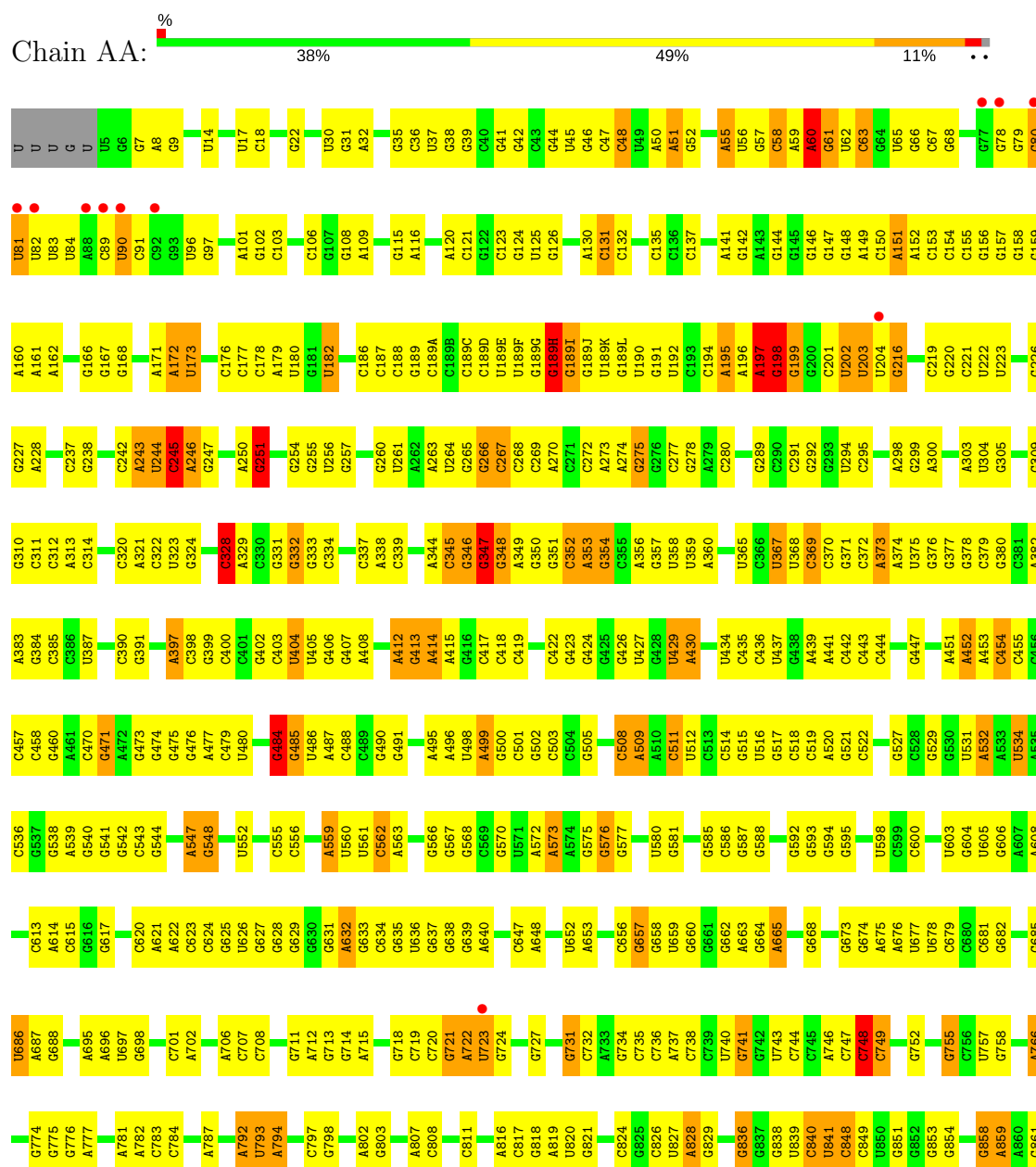


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AZ	1	Total	C	N	O		0	0
			57	43	2	12			
61	CZ	1	Total	C	N	O		0	0
			57	43	2	12			

### 3 Residue-property plots

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

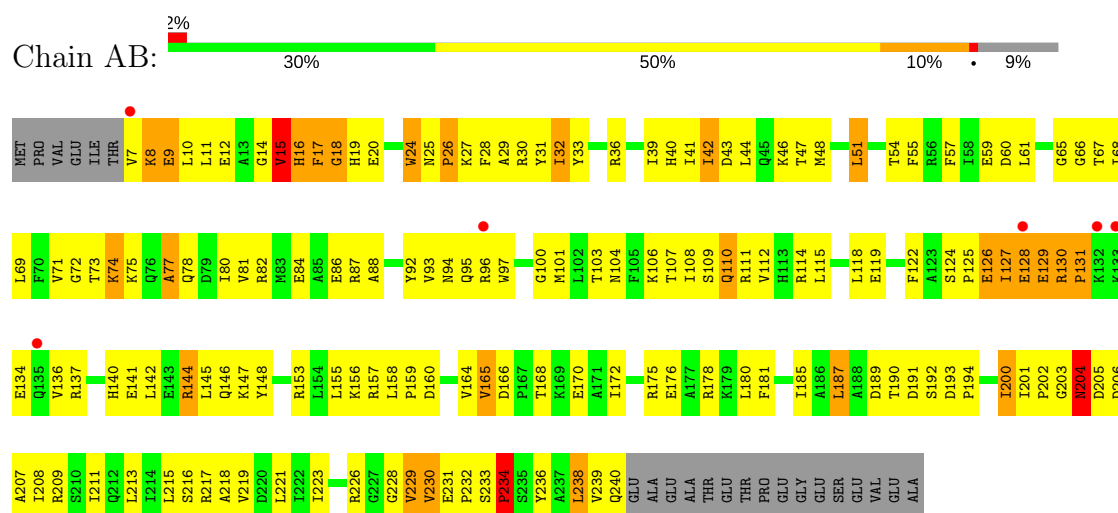
#### • Molecule 1: 16S rRNA



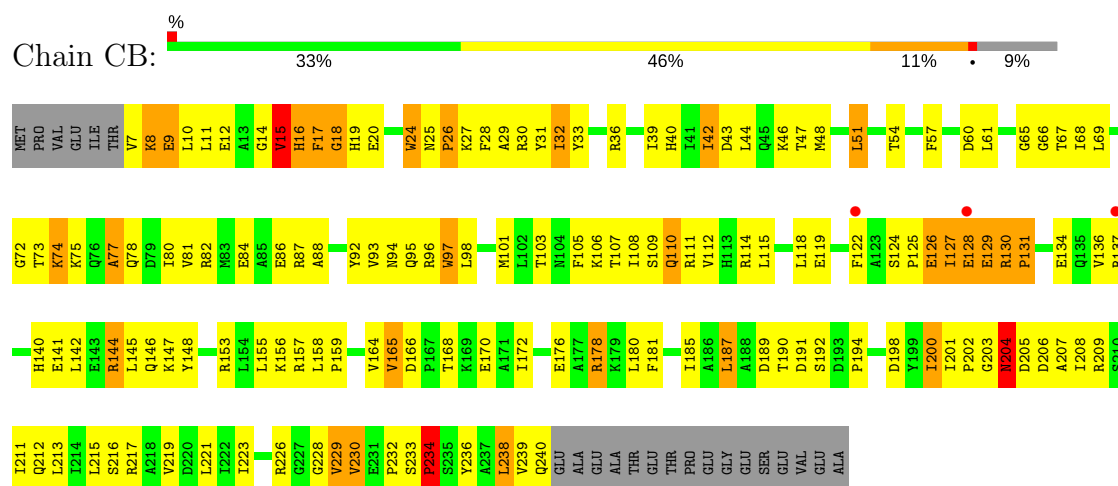


C1527	C1443	A1360	A1288	U1212	U1135	A1046	A978	G903	A802	G714	G633	C555	C484	C400
U1528	C1444	C1363	G1291	A1213	U1136	G1047	C979	C904	G803	A715	C634	C556	G485	C401
G1529	U1445	C1363	G1291	A1213	C1137	G1048	C980	A909	A807	C719	G635	A559	G486	C402
G1530	U1446	A1363A	G1291	A1213	U1049	U1049	U981	C910	C808	C720	U636	U561	A487	C403
U1531	G1294	U1364	G1295	C1217	G1139	G1050	A983	A913	C811	G721	G638	C562	C488	U404
U1532	C1452	U1364	C1296	U1219	C1141	G1054	C984	A914	C812	A722	G639	A563	G489	U405
C1533	G1456	C1368	A1299	G1221	G1142	C1054	G987	A918	C817	U723	A640	C566	G490	U406
A1534	G1457	C1369	G1370	G1222	G1143	C1055	G988	A919	C818	U724	G644	C567	G491	G407
C1535	U1458	G1371	U1300	G1223	G1144	C1058	U991	A918	C819	G727	G645	C568	A495	A408
U1537	C1459	U1372	U1301	C1223	G1145	C1059	U992	U920	A810	G731	U646	C569	A496	A412
C	G1467	G1373	U1302	A1227	C1147	C1064	U993	U921	U820	C732	C647	C570	U498	A414
C	G1468	A1374	G1303	C1228	U1148	U1065	G994	G922	G821	A733	A648	U571	A499	A415
U	G1469	A1375	G1305	A1229	C1149	U1066	A996	A923	G822	G734	U652	C572	C501	G416
U	C1477	U1376	A1306	C1230	U1150	U1071	C995	C924	G823	A735	C417	A573	G502	C417
U	C1478	C1378	U1307	G1231	A1151	C1072	A996	G925	G824	C736	A653	C574	C503	C418
C	A1483	C1382	U1308	U1234	A1152	U1073	A1001	G926	C826	A737	G657	C576	C504	C419
D	G1484	C1383	G1310	U1235	G1154	U1074	G1001A	G927	U827	C738	G658	C577	G505	C422
U1485	G1387	G1387	G1311	A1238	A1157	U1075	G1002	G933	A828	C739	U659	U580	C508	U427
G1486	U1392	G1387	G1312	A1239	C1158	G1077	G1003	C934	G829	U740	G660	C581	A509	G428
G1487	U1393	G1387	G1313	U1240	U1159	U1078	A1004	A935	G836	G741	G661	C582	C511	U429
G1488	U1393	G1387	G1314	G1241	G1160	U1086	A1005	G939	G837	U743	A663	C585	C512	A430
G1489	U1393	G1387	G1315	C1242	G1160	U1087	C1006	C940	U839	C744	G664	C586	U512	U430
A1492	C1397	C1387	G1316	U1242	A1169	G1087	C1007	G941	C840	C745	A665	C587	C513	U434
A1493	A1398	C1387	C1317	A1245	A1170	U1087	C1008	G942	U841	A746	C514	C588	C514	U435
A1494	C1399	C1387	G1318	C1246	A1171	U1094	U1012	G943	U842	C747	G668	C589	G515	C436
U1495	C1400	C1387	A1320	U1257	G1171	U1095	G1013	U943	C848	C748	G669	C590	U516	U437
U1496	G1401	C1387	C1321	G1258	C1172	C1096	A1014	G944	C849	C749	G673	C591	C517	U438
G1497	C1402	C1387	C1322	C1259	A1176	C1097	A1015	G945	G853	G752	G674	C592	C518	U439
U1498	C1403	C1387	G1323	U1261	G1177	C1098	G1017	U946	G854	G753	A675	C593	C519	A441
A1499	U1406	C1387	C1324	G1255	G1178	U1101	G1024	C948	G858	G755	U677	C594	A520	C442
A1500	C1407	C1387	C1325	A1256	A1179	A1102	U1025	G950	A859	C756	G678	C595	C522	C443
A1501	C1408	C1387	C1326	U1257	G1180	C1103	G1026	U952	A860	U757	C680	C596	G527	G447
A1503	C1409	C1387	C1327	G1258	G1181	C1104	G1027	G953	A861	G758	G679	C597	C528	A451
G1504	C1413	C1387	C1328	C1259	G1182	G1104	C1028	G954	C862	G765	C681	C606	G529	A452
U1506	U1414	C1387	U1330	C1262	A1183	G1108	C1029	U955	A864	A766	G682	A607	U531	A453
A1507	G1415	C1387	G1331	C1263	G1184	U1116	C1030	U956	A865	A767	U686	A608	U532	C455
U1510	A1418	C1387	C1335	A1269	G1187	C1116	G1030A	U960	C866	A768	A687	C613	U534	C456
G1511	G1419	C1387	C1336	C1270	C1188	G1117	C1030B	C962	G869	G776	G688	C615	U535	C457
U1512	G1423	C1387	G1342	G1271	G1189	C1118	G1030C	G963	C877	A775	A695	C616	C458	C460
C1514	G1423	C1387	C1344	G1272	G1190	G1119	G1031	G964	G878	A777	U696	G617	G538	G461
C1515	A1428	C1387	U1345	A1275	G1193	U1122	G1032	A965	C879	A781	C620	C621	A539	A461
G1516	C1429	C1387	U1346	G1276	U1196	G1123	G1033	A968	C880	A782	G701	G624	G540	C470
G1517	G1430	C1387	G1347	U1277	G1197	U1124	G1036	A969	G881	C783	A702	G625	G541	A471
A1518	C1431	C1387	U1348	A1278	U1199	U1125	C1037	C970	C882	C784	G626	U626	C542	A472
A1519	G1432	C1387	C1200	U1281	C1200	G1127	G1038	G971	C883	C784	G627	U627	C543	G473
G1520	A1433	C1387	A1281	U1281	C1201	C1128	C1039	G972	U884	A787	A706	G628	G544	G474
G1521	C1434	C1387	C1282	G1282	G1202	C1129	U1040	C973	G885	A787	C707	G629	G475	G475
U1522	G1435	C1387	G1283	G1283	C1203	A1130	U1041	G974	A892	A792	C708	G630	A547	A477
G1523	U1436	C1387	C1284	C1284	G1131	G1131	G1042	A975	A900	U793	G711	G631	G548	C479
C1524	G1442A	C1387	U1286	A1286	G1132	G1132	C1043	A976	A900	A794	A712	U552	U552	U480
G1525	A1442B	C1387	U1286	A1286	G1133	G1133	C1044	A977	A900	A794	G713	A632		
G1526		C1387	U1287	A1287	G1134	G1134	C1045							

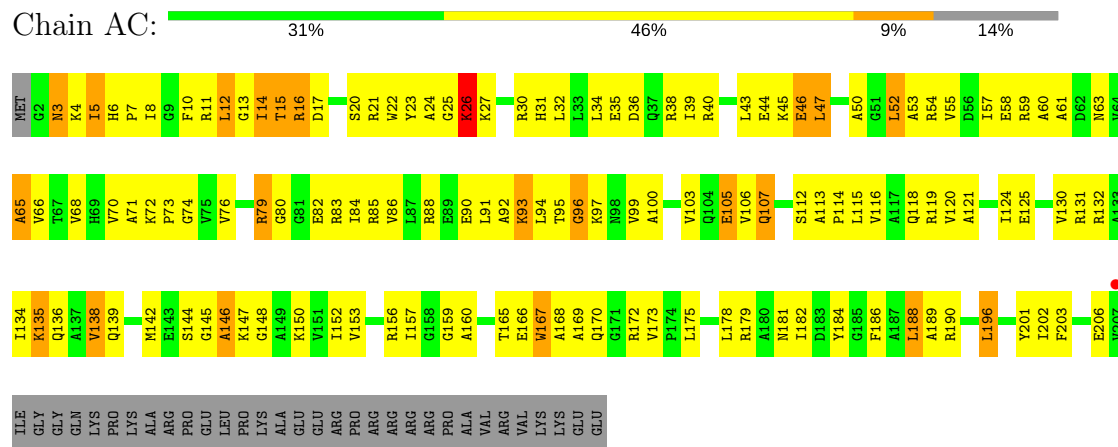
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



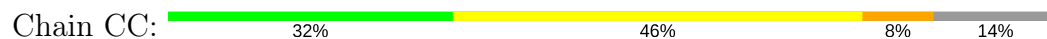
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



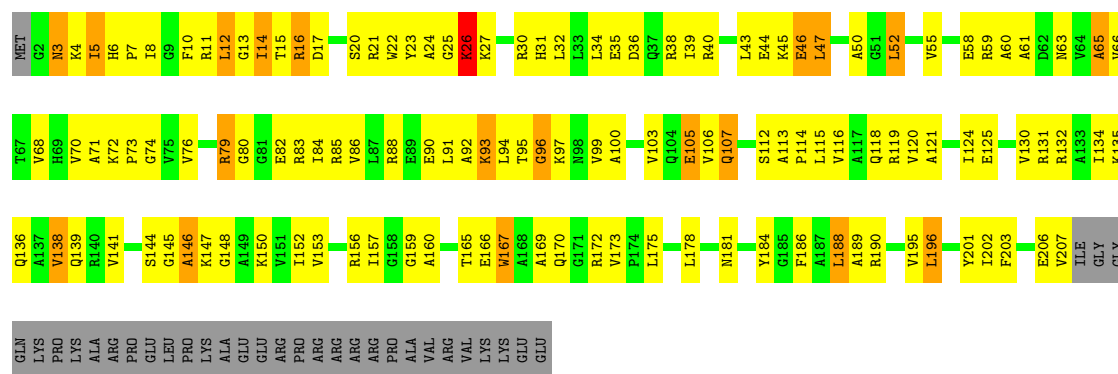
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



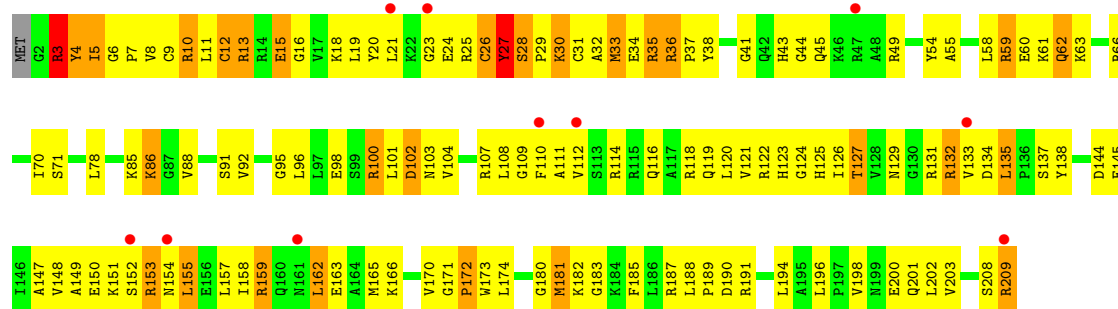
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



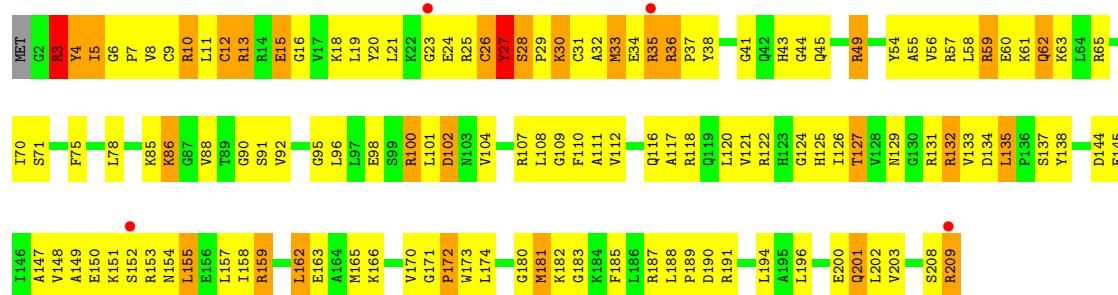




### • Molecule 4: 30S RIBOSOMAL PROTEIN S4



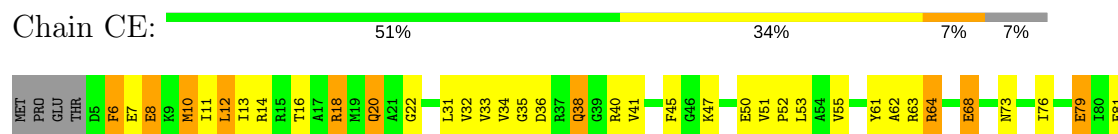
### • Molecule 4: 30S RIBOSOMAL PROTEIN S4



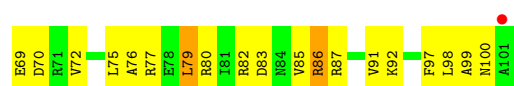
### • Molecule 5: 30S RIBOSOMAL PROTEIN S5



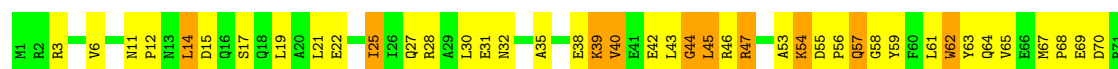
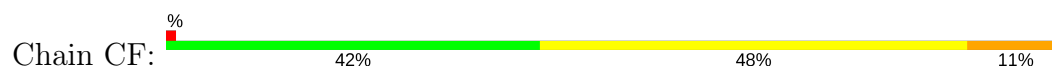
### • Molecule 5: 30S RIBOSOMAL PROTEIN S5



• Molecule 6: 30S RIBOSOMAL PROTEIN S6



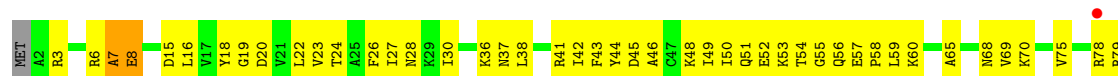
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



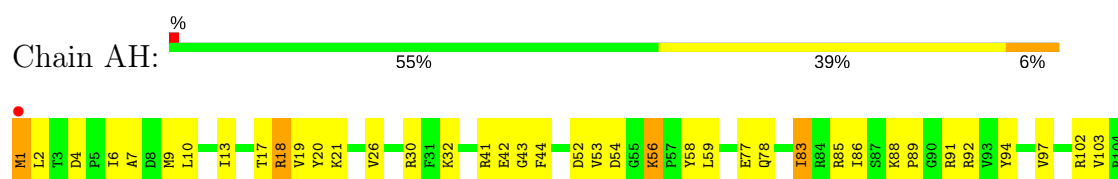
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



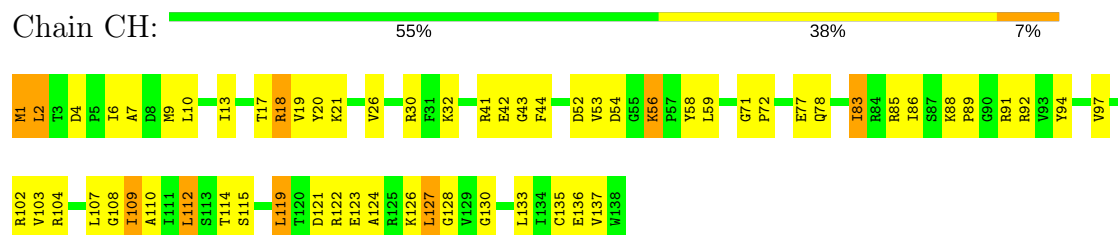
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



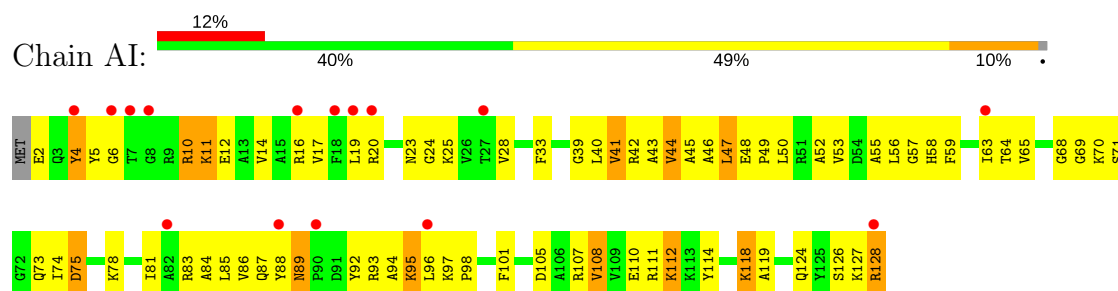
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



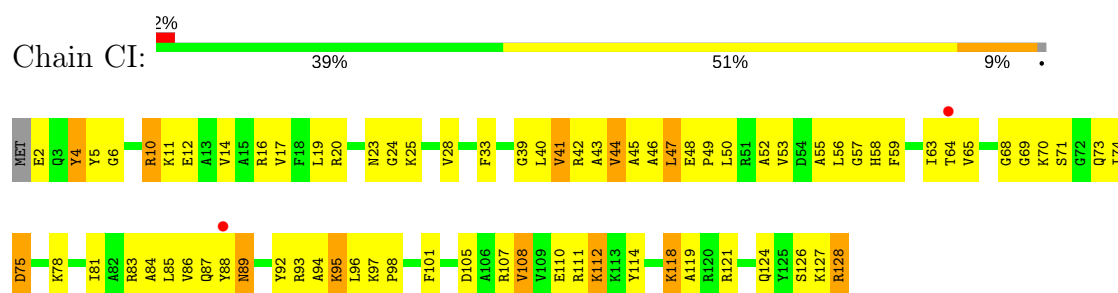
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



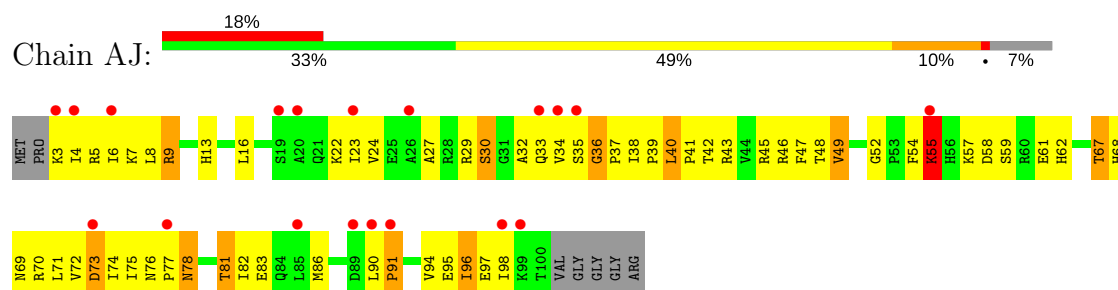
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



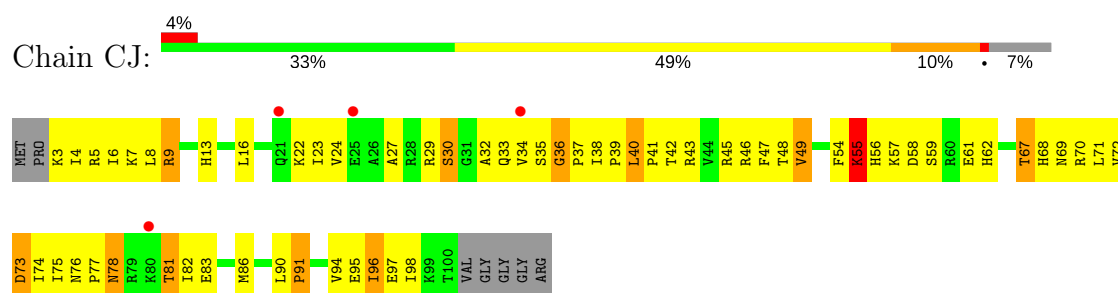
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



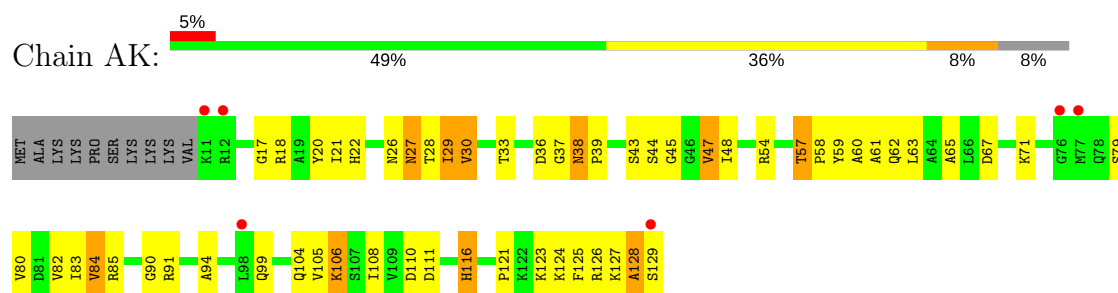
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



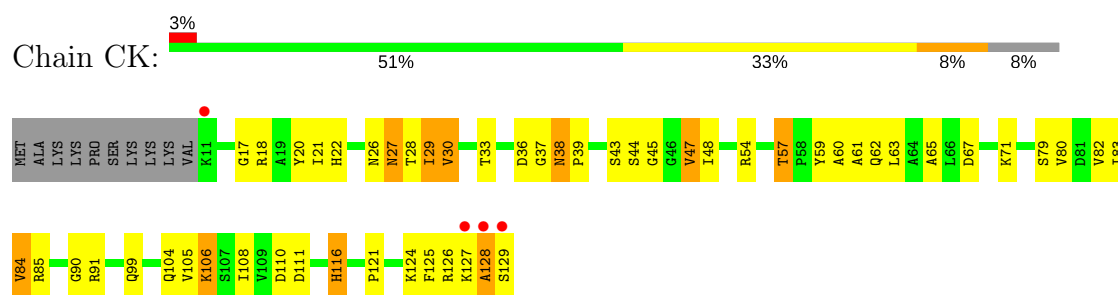
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



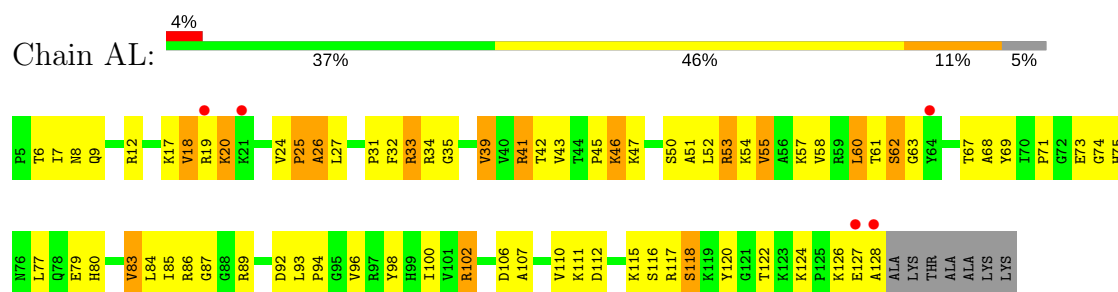
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



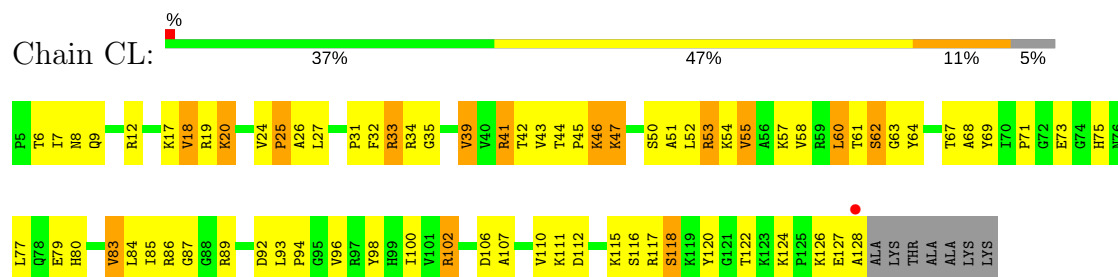
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



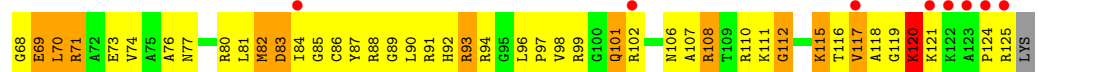
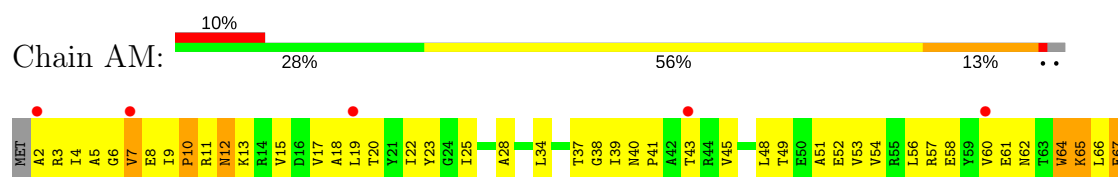
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



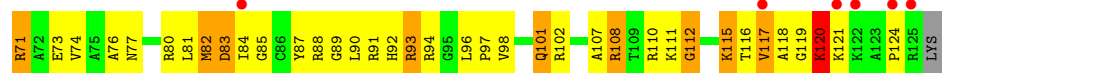
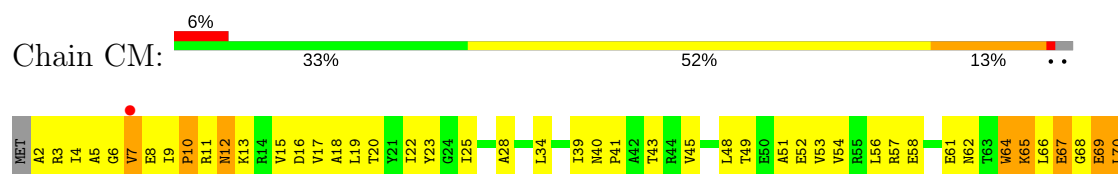
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



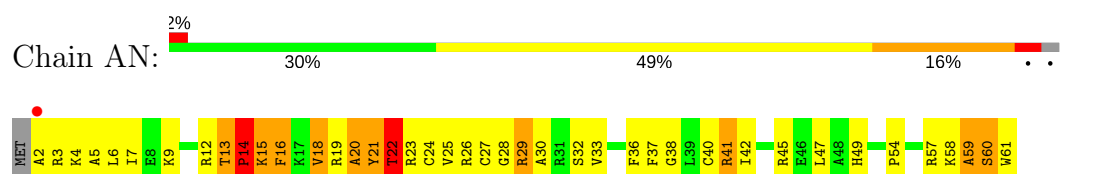
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



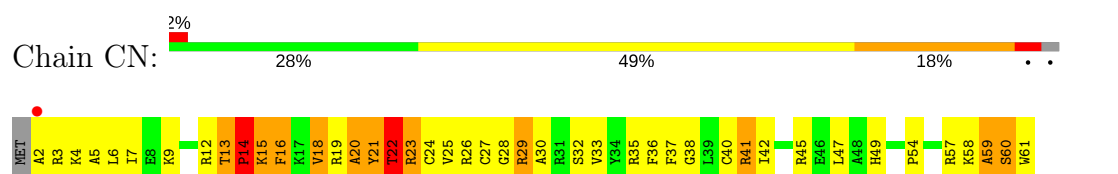
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



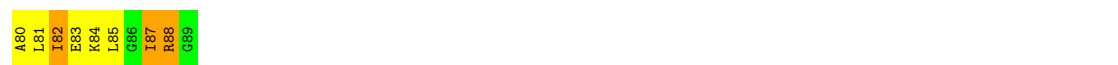
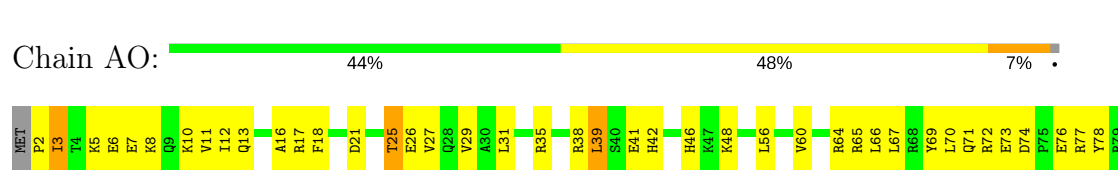
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



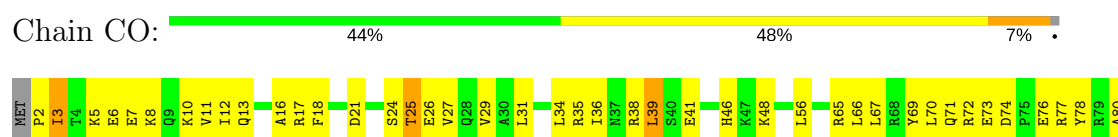
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

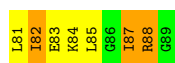


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

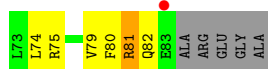
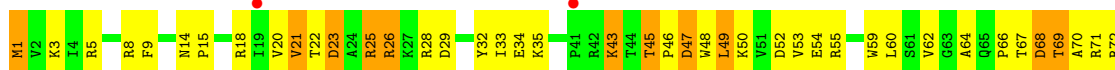
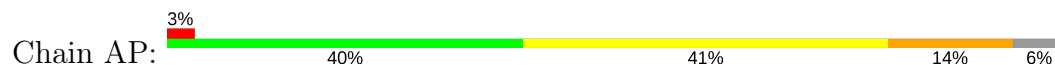


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

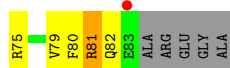




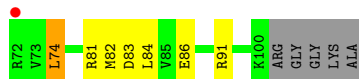
## • Molecule 16: 30S RIBOSOMAL PROTEIN S16



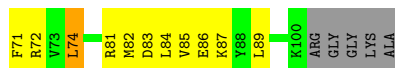
## • Molecule 16: 30S RIBOSOMAL PROTEIN S16



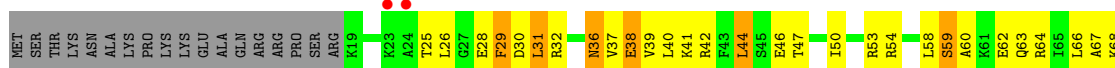
## • Molecule 17: 30S RIBOSOMAL PROTEIN S17



## • Molecule 17: 30S RIBOSOMAL PROTEIN S17

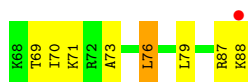
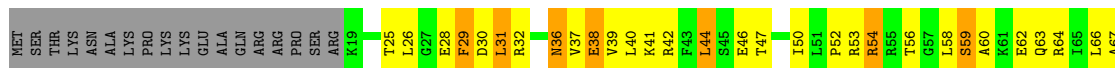


## • Molecule 18: 30S RIBOSOMAL PROTEIN S18

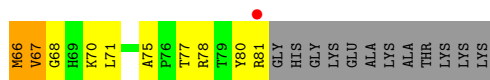
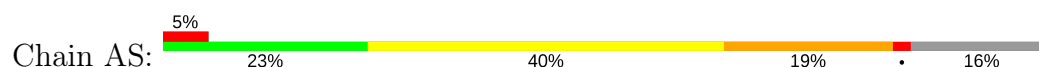




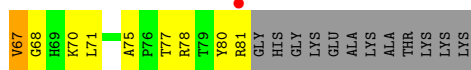
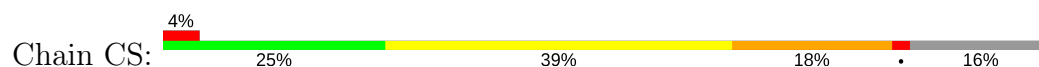
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



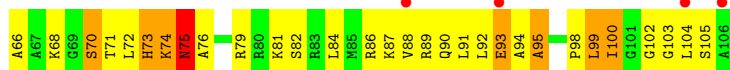
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

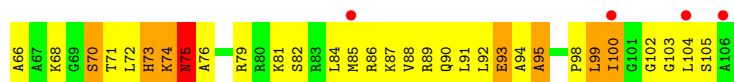


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

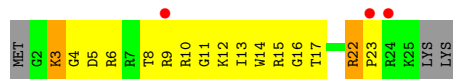


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

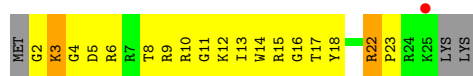




- Molecule 21: 30S RIBOSOMAL PROTEIN THX



- Molecule 21: 30S RIBOSOMAL PROTEIN THX



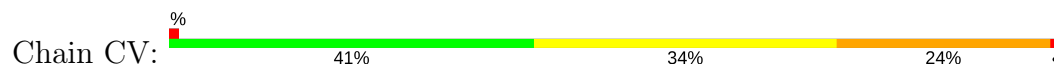
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



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



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

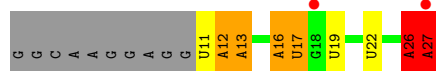
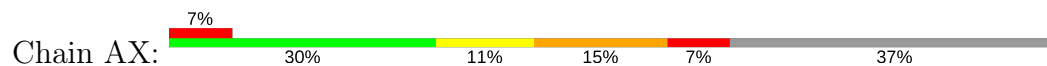


- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

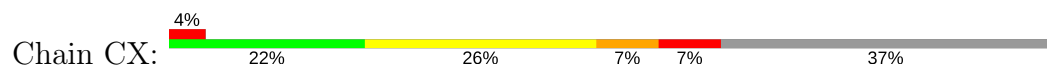




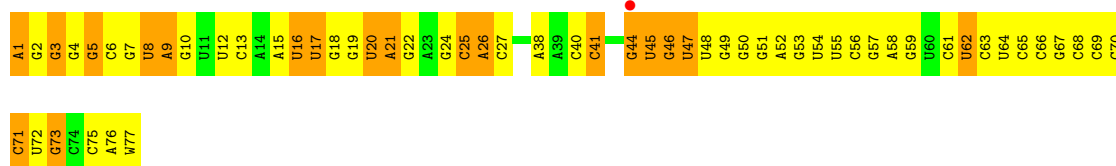
- Molecule 23: MRNA



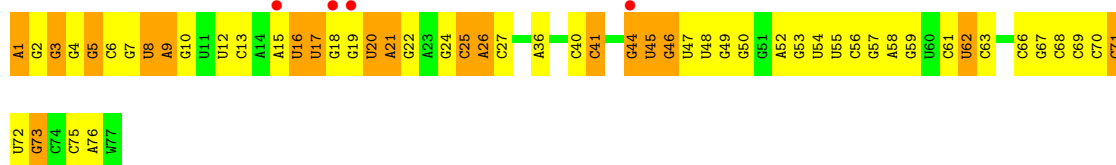
- Molecule 23: MRNA



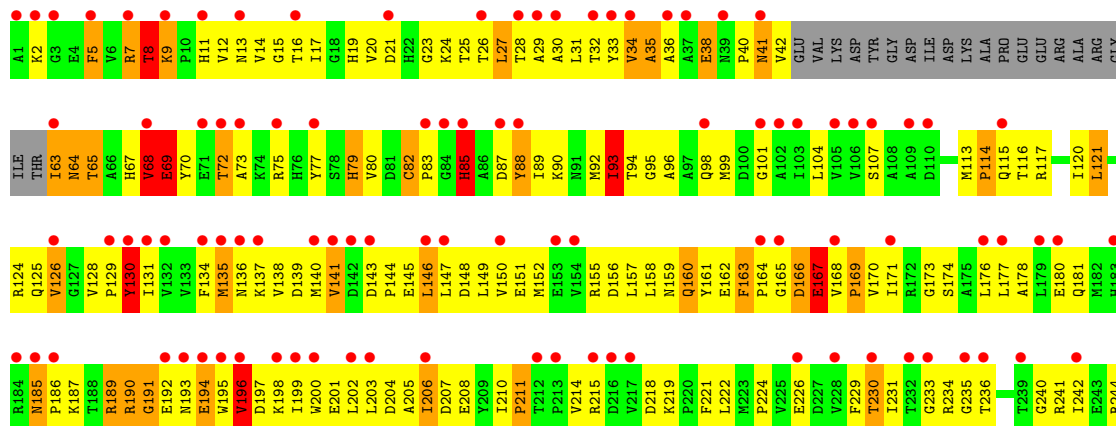
- Molecule 24: A-SITE TRNA TRP-TRNA TRP

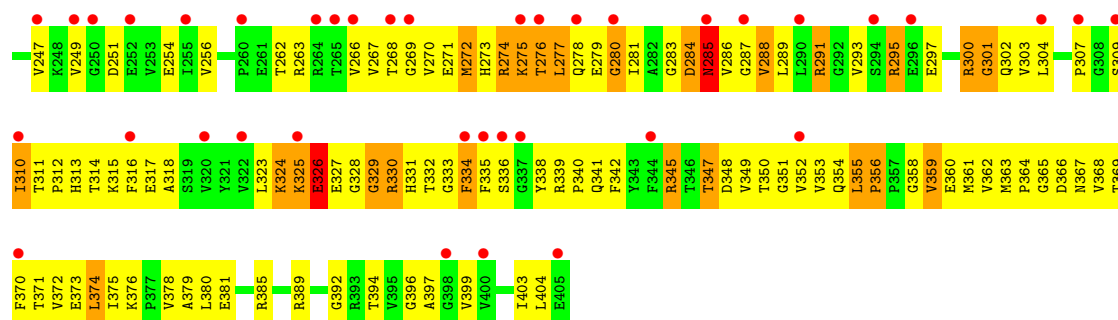


- Molecule 24: A-SITE TRNA TRP-TRNA TRP

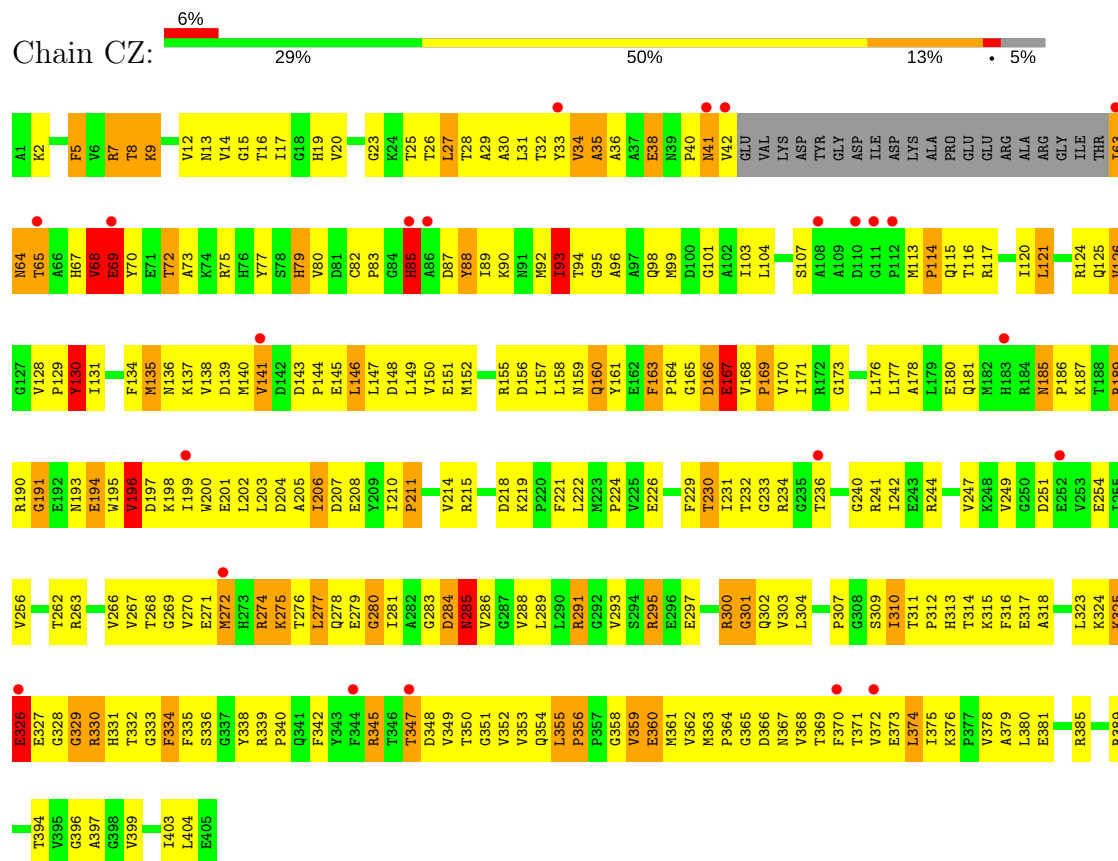


- Molecule 25: ELONGATION FACTOR TU

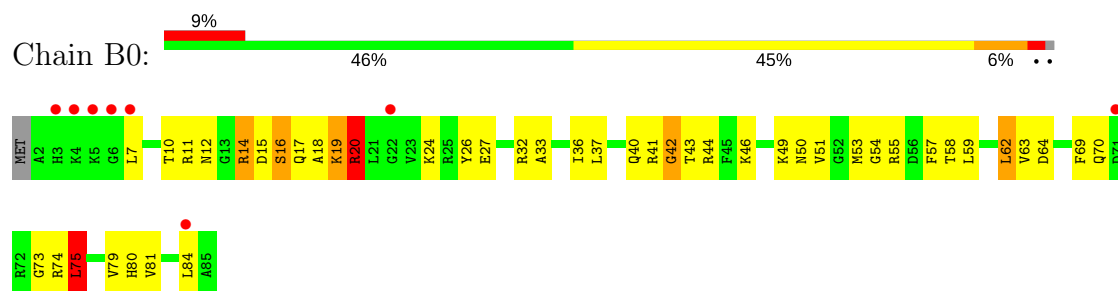




• Molecule 25: ELONGATION FACTOR TU

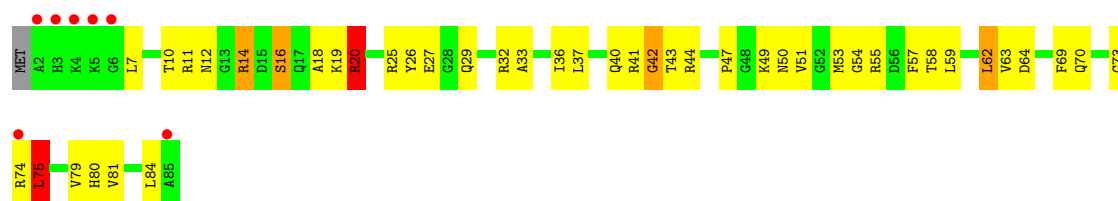


• Molecule 26: 50S RIBOSOMAL PROTEIN L27

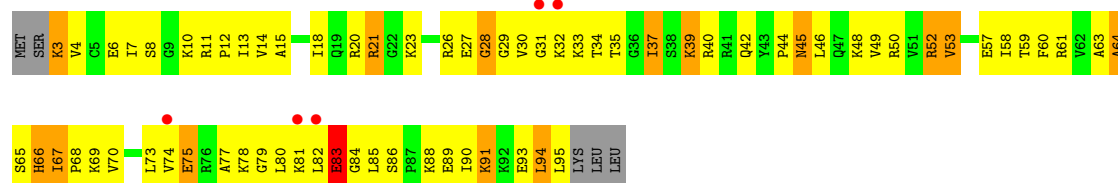


• Molecule 26: 50S RIBOSOMAL PROTEIN L27

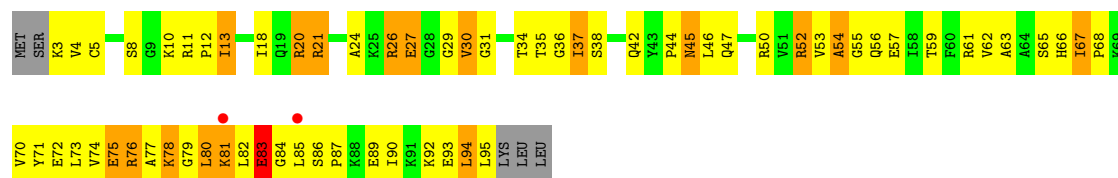




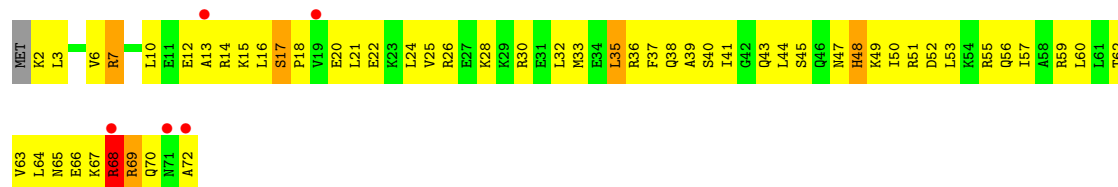
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



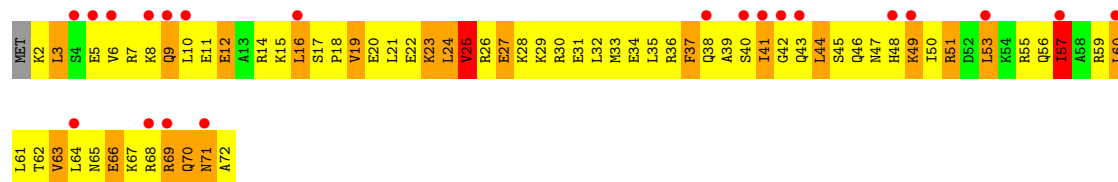
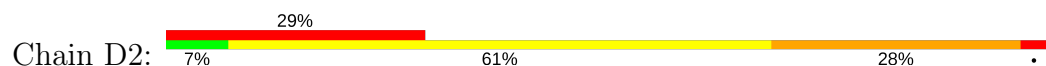
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



• Molecule 28: 50S RIBOSOMAL PROTEIN L29

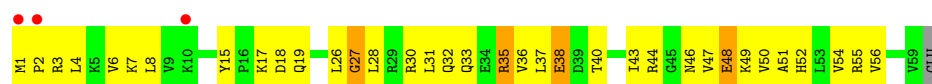


• Molecule 28: 50S RIBOSOMAL PROTEIN L29

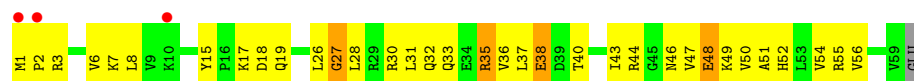


• Molecule 29: 50S RIBOSOMAL PROTEIN L30

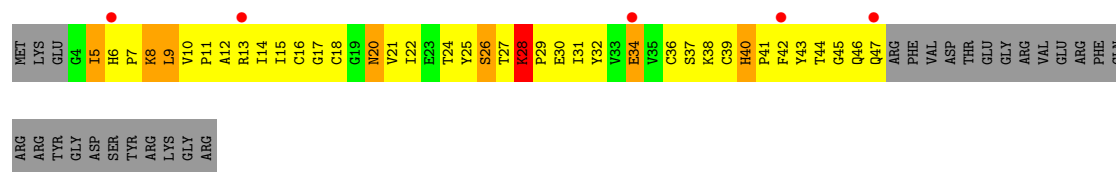




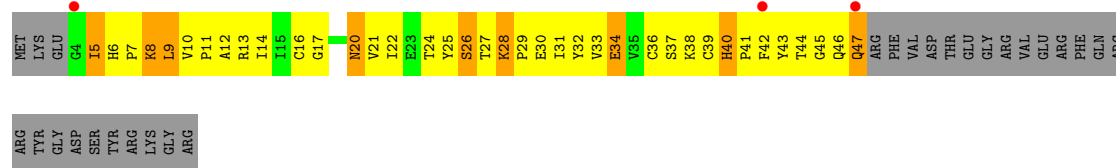
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



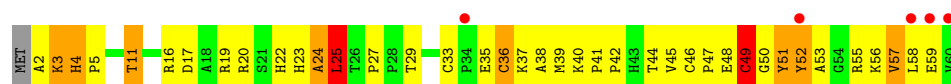
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



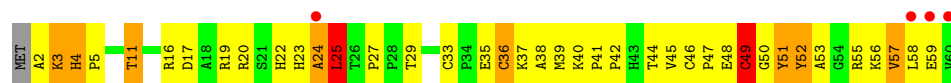
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



• Molecule 31: 50S RIBOSOMAL PROTEIN L32



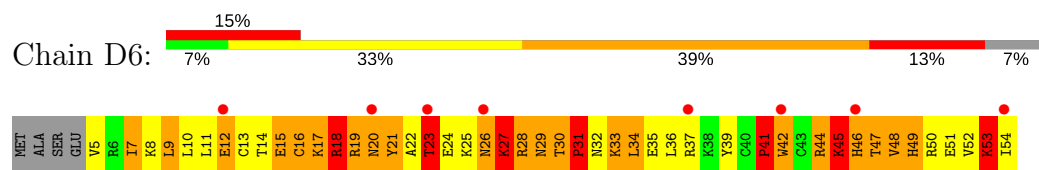
• Molecule 31: 50S RIBOSOMAL PROTEIN L32



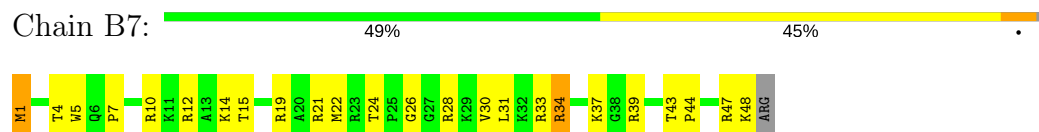
• Molecule 32: 50S RIBOSOMAL PROTEIN L33



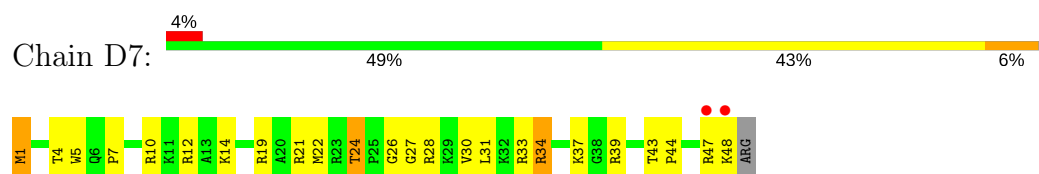
- Molecule 32: 50S RIBOSOMAL PROTEIN L33



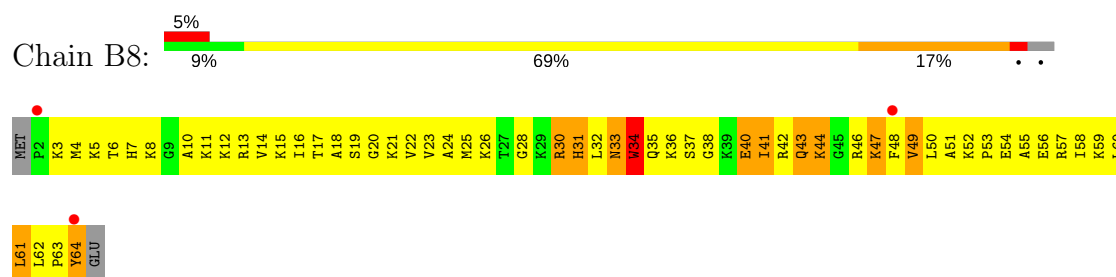
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



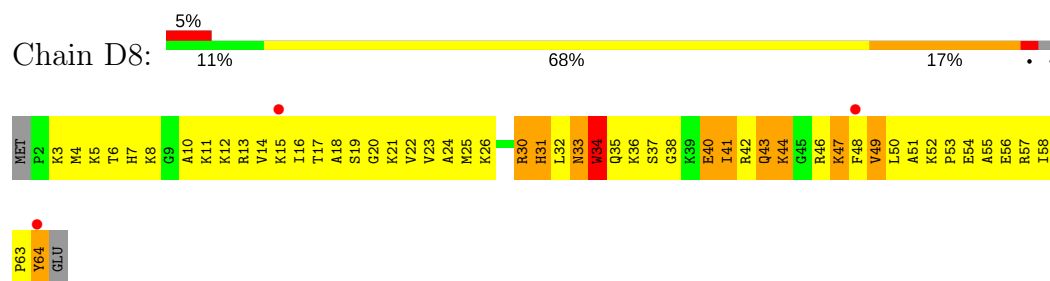
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



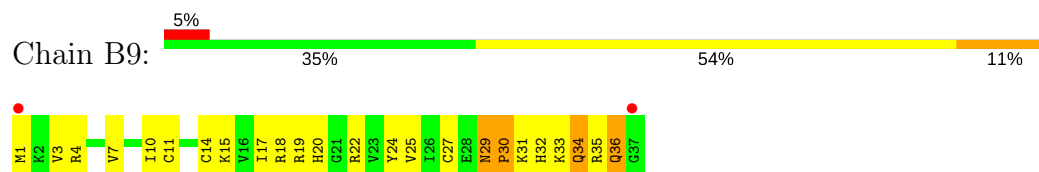
- Molecule 34: 50S RIBOSOMAL PROTEIN L35



- Molecule 34: 50S RIBOSOMAL PROTEIN L35



- Molecule 35: 50S RIBOSOMAL PROTEIN L36

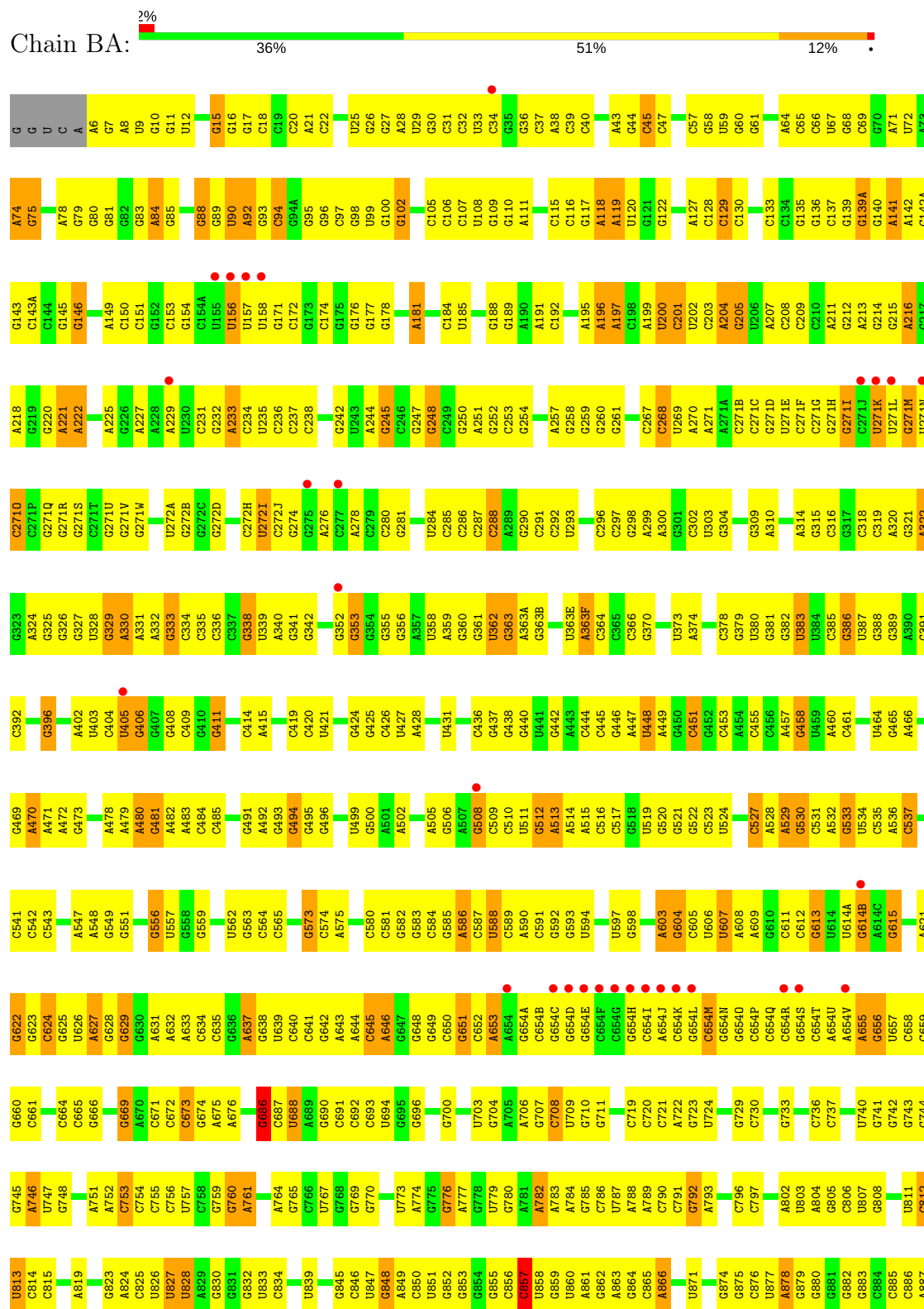


- Molecule 35: 50S RIBOSOMAL PROTEIN L36

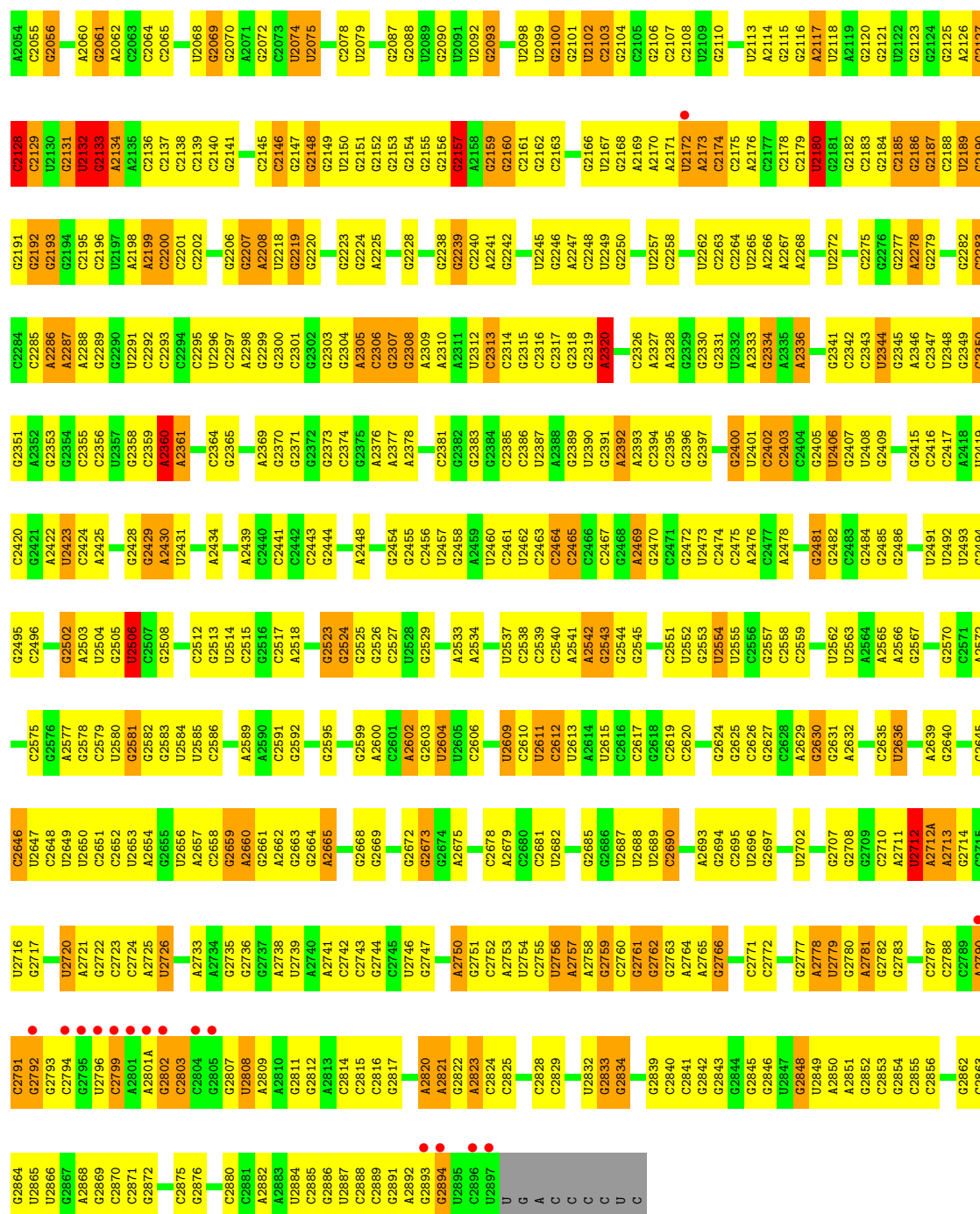




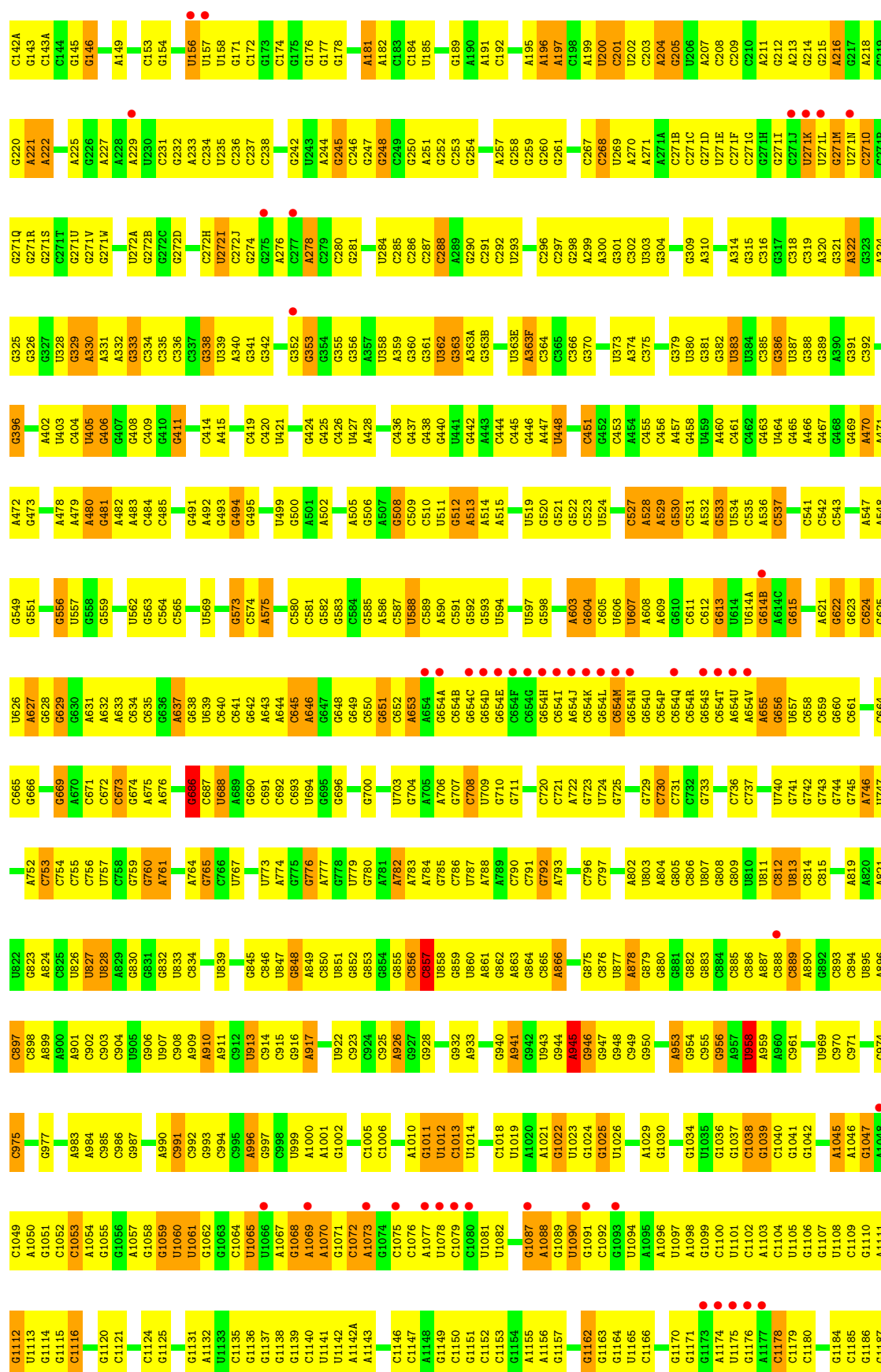
• Molecule 36: 23S RIBOSOMAL RNA



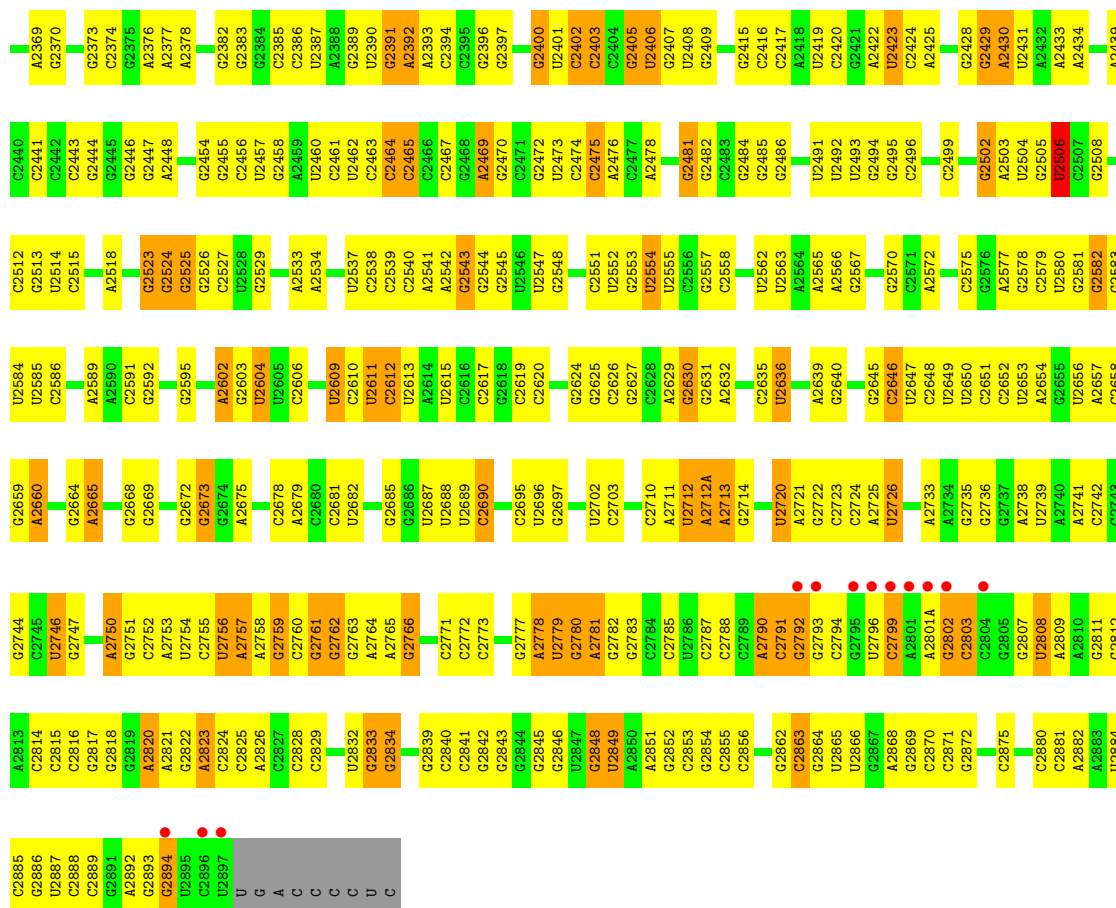
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A1972	C1882	C1804	U1720	A1544	G1478	C1411	G1337	G1259	C1180	G1106	G1042	U969	C889
A1981	C1883	U1805	G1721	C1545	G1479	A1412	G1338	C1261	G1186	G1107	C1043	U970	A890
C1982	A1884	C1806	A1722	C1546	G1480	G1413	G1339	C1261	U1187	C1108	C1044	C971	G892
C1983	C1885	G1807	U1739	C1547	U1481	G1414	U1340	G1264	U1188	C1109	A1045	C972	C893
G1984	C1886	C1638	G1740	C1548	G1482	G1416	U1341	A1265	U1189	G1110	A1046	A973	C894
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	G1899	G1813	G1642	A1554	U1490	U1420	A1349	A1270	G1192	G1114	G1051	C977	A898
	A1900		G1643	A1555	A1491	U1421		A1271	G1193	C1116	C1052	A983	A900
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	C1902	U1818	C1648	A1558	C1493	G1426	A1353	U1273	C1200	G1120	A1054	C985	A902
		A1819	G1649	G1559	A1494	A1427	A1354	A1274		C1121	G1055	C986	C902
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	G1906	A1821	G1651	A1567	U1496	G1436	U1357	A1278	A1204	C1124	A1057	A990	U905
	G1907	G1822	G1652	A1568	U1497	C1430	G1358	A1279	U1205	G1125	G1058	C991	U907
	C1908		G1653	A1569	C1498	U1431	A1359				U1061	C992	C908
	C1909	G1826	A1654	A1570	C1499	C1432		A1286	C1208	G1131	U1062	C993	C908
	G1910	G1827	C1657	A1571	G1500	U1433	A1360	A1287	G1209	A1132	C1063	C994	A909
	U1911	G1828	C1658	U1578	C1501	A1434	G1361	U1288	A1210	U1133	G1064	C995	A910
	A1912			A1579	C1502	G1435	C1362	C1289	U1211	C1135	C1065	C996	A911
	C1914	G1831		A1580	U1503	G1437	C1363	C1290	G1212	G1136	C1066	C997	C912
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		C1837	G1667	A1583	U1507	G1440	A1367	U1294		C1140	G1068	A1001	G916
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	G1932	C1843	A1677	U1590	U1512	G1448	A1378	A1302		C1147	C1075	G1011	G928
	C1933	G1845	C1678	G1591	C1513	A1449	A1379	G1303	G1231	G1148	C1076	U1012	
			G1679	C1592	U1514	G1450	G1380	C1304	G1232	G1149	U1077	C1013	
	C1936	G1846	U1680	G1593	G1515	C1450A		C1305	C1233	C1150	U1078	U1014	G932
	U1937	A1847	G1681	G1594	C1516		A1384	C1306	U1234	G1151	C1079		A933
	A1938	A1848	G1682	G1595	G1517	U1453	G1385		G1235	G1152			
			C1683	A1596	U1518	G1455	C1387	G1311	G1236	C1153	A1084	C1018	G940
	U1946	U1851	C1684	C1598	U1523	C1458	G1388	U1312	A1237	G1154		U1019	A941
	C1947	A1854	U1688	C1599	G1524	G1459	G1389	C1313	G1238	A1155	G1087	A1020	G942
	G1948	C1855	A1689	G1600	G1525	A1460	U1390	C1314	G1239	A1156	A1088	U1021	U943
		G1856	A1689	C1601	U1526	G1461		C1315	U1240	G1157	G1089	G1022	G944
	C1952	G1857	G1697	U1602	G1527		A1393	U1316	A1241		U1090	U1023	A945
	A1953	G1858	A1698	A1603	A1528	C1464		C1317	G1243	G1162	G1091	G1024	G946
	G1954	G1860	G1699	C1607	A1528A	G1465	U1396	G1318	G1244	G1163	C1092	U1025	G947
	U1955	G1861	A1700	A1608	G1529	G1466		C1320	G1245	G1164	G1093	U1026	G948
		G1862	A1701	A1609		C1467	G1400		G1246	U1165	U1094		C949
	C1959	G1863	U1709	A1610	U1534	C1468	G1401	C1327	A1247	C1166	A1095	A1029	G950
	A1960	U1817	C1710	A1614	A1535	A1469	C1402	G1328	G1248		U1096	G1030	
	U1963	G1865	C1711	G1615	C1536	G1470	C1403	U1329		G1171	U1097	U1034	A953
		A1876	C1712	A1616	G1537	A1471	C1404	C1330	C1251	G1173	G1098	U1035	C955
		U1798	C1713	C1617	G1538	A1472	U1405	A1331	G1252	A1174	G1100	G1036	G956
	C1967	G1877	U1713	G1618	G1539	G1473	U1406	G1332	A1253	U1175	U1101	G1037	A957
	G1968	G1878	G1714	A1619	U1540	G1474	C1407	C1333		G1176	C1102	C1038	U958
	A2051	C1879	G1717	G1619	G1541	G1475	A1408	G1334	G1256	A1177	A1103	G1039	A959
	G2053	A1802		G1620	A1542	C1476	C1409	U1335	C1257	C1178	C1104	C1040	A960



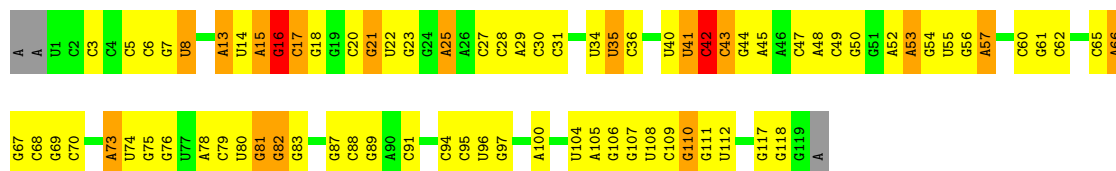




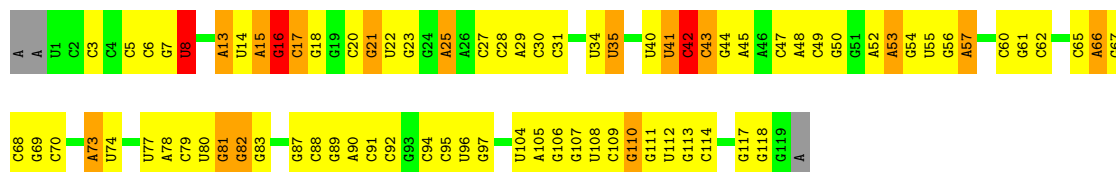
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G2207	U2144	A2208	U2218	C2146	G2219	G2219	G2220	G2223	G2224	A2225	G2228	C2230	C2231	G2238	C2239	A2310	G2238	C2240	A2241	G2242	U2245	G2246	A2247	C2248	U2249	G2250	U2257	C2258	U2262	C2263	C2264	U2265	A2266	A2267	A2268	U2272	C2275	G2276	C2277	A2278	G2279	G2282	C2283	C2284	C2285	A2286	C2287	A2288	C2289	G2290	U2291	C2292	C2293	C2294					
U1993	C1993	C1996	C1997	C1998	C1999	G2000	A2001	C2006	C2007	C2008	G2009	G2010	U2011	U2012	C2013	G2104	U2105	A2170	U2171	U2172	C2175	A2176	C2177	C2178	C2179	A2180	G2181	C2182	G2120	C2183	C2184	C2185	C2186	G2187	C2188	U2189	C2190	G2191	C2192	C2193	C2194	C2195	U2196	U2197	A2198	C2199	C2200	C2201	C2202	C2203	C2204								
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C1902	G1906	G1907	C1908	C1909	G1910	U1911	C1914	U1915	A1916	U1917	G1921	G1922	A1928	G1929	G1930	U1931	A1932	G1933	A1936	A1937	U1938	U1939	U1940	U1946	U1947	G1948	A1952	A1953	G1954	U1955	G1959	A1960	U1963	C1967	G1968	A1969	A1970	A1971	A1972	A1981	C1982	A1986	A1987	A1989	C1993	G1998	G1999	G1992											
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C1648	G1649	G1650	G1651	G1652	G1653	A1654	C1657	C1658	U1659	A1665	G1666	G1667	A1668	A1669	C1670	G1674	A1677	G1678	U1679	U1680	G1681	G1682	C1683	C1684	U1688	A1689	C1697	A1698	A1699	A1700	A1701	U1709	C1710	C1711	C1712	U1713	G1717	G1718	G1719	U1720	G1721	A1722	U1739	G1740	G1741	G1742	G1743	G1744	G1745	G1747A									
A1567	G1568	A1569	G1573	G1574	U1578	A1579	A1580	G1581	C1582	A1583	C1584	A1586	A1587	C1588	C1589	U1590	G1591	G1592	G1593	G1594	G1595	A1596	A1597	C1598	C1599	C1600	G1601	U1602	A1603	C1607	A1608	A1609	A1610	A1614	C1615	A1616	C1617	A1618	G1619	G1620	G1630	A1634	G1635	C1636	A1637	C1638	U1639	A1640	A1641	G1642	G1643	G1647							
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A1419	U1420	G1425	A1427	C1428	C1429	C1430	U1431	C1432	U1433	A1434	G1435	C1436	C1437	U1438	A1439	A1445	A1445A	C1446	C1447	G1448	A1449	C1450	U1453	C1455	C1458	C1459	A1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	A1469	C1470	A1471	C1472	C1473	C1474	C1475	C1476	C1477	C1478	C1479	G1480	C1481	C1482	C1484	C1485	A1486	A1490							
G1348	A1349	U1352	A1353	C1354	G1355	G1356	U1357	C1358	A1359	A1360	C1361	C1362	C1363	G1364	A1365	A1366	A1367	G1368	C1374	C1375	C1376	C1377	A1378	C1379	G1380	A1384	C1385	C1386	C1387	G1388	C1389	U1390	A1393	U1396	G1400	C1401	C1402	C1403	C1404	U1405	U1406	C1407	C1408	C1409	C1410	C1411	A1412	C1413	G1416	C1417	C1418								
A1268	A1269	G1270	G1271	U1272	U1273	A1274	A1278	G1279	A1286	A1287	U1288	C1289	C1290	C1291	U1292	C1293	U1294	C1297	G1299	U1300	A1301	A1302	G1303	C1304	C1305	C1306	G1311	U1312	U1313	C1314	C1315	U1316	A1317	C1318	C1320	C1327	G1328	U1329	C1330	A1331	A1332	C1333	G1334	U1335	A1336	G1337	C1338	G1339	U1340	U1341	A1344	A1345	C1346						
U1188	A1189	G1190	G1191	G1192	G1193	U1199	C1200	G1203	A1204	U1205	C1208	C1209	A1210	U1211	U1212	A1213	A1214	G1215	C1221	U1221A	C1222	G1223	G1227	G1231	G1232	G1235	G1236	U1240	A1241	A1242	G1243	G1244	G1245	A1246	G1248	C1251	G1252	A1253	G1256	C1257	G1258	G1259	G1260	C1261	A1264	A1265	G1266	C1267											



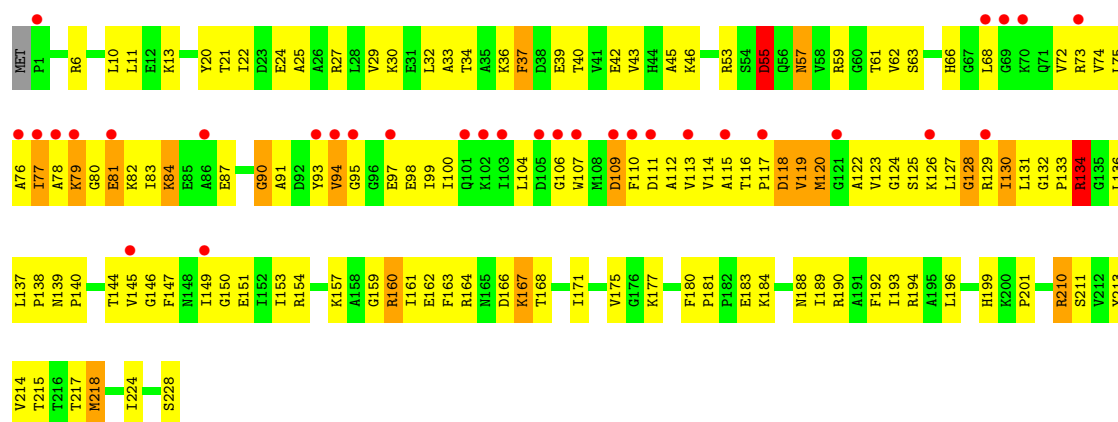
Chain BB: 33% 50% 13%



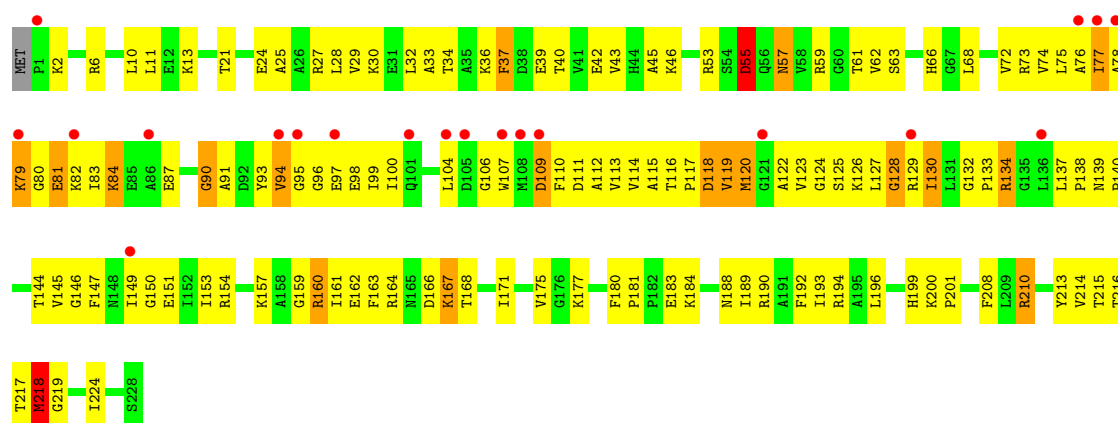
Chain DB: 32% 51% 12%



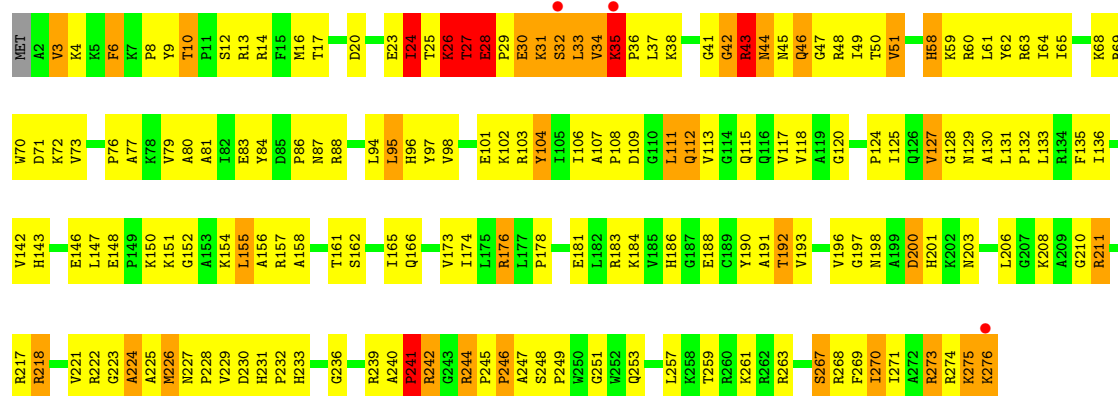
Chain BC: 14% 42% 49% 8%



• Molecule 38: 50S RIBOSOMAL PROTEIN L1

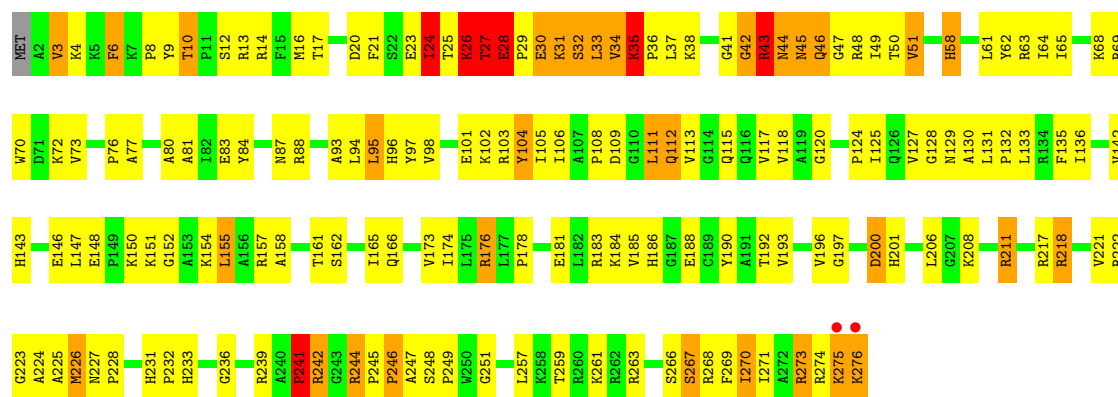


• Molecule 39: 50S RIBOSOMAL PROTEIN L2

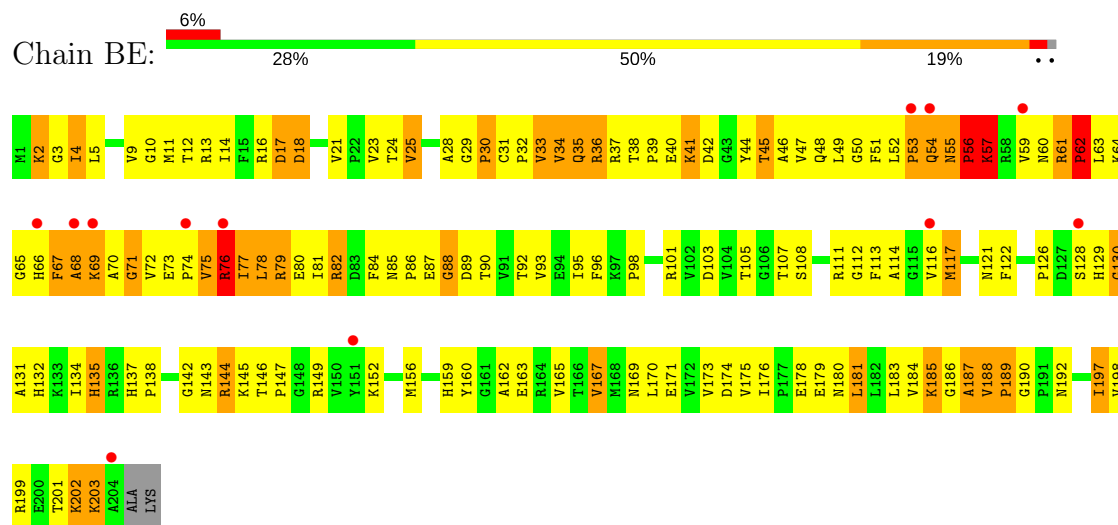


• Molecule 39: 50S RIBOSOMAL PROTEIN L2

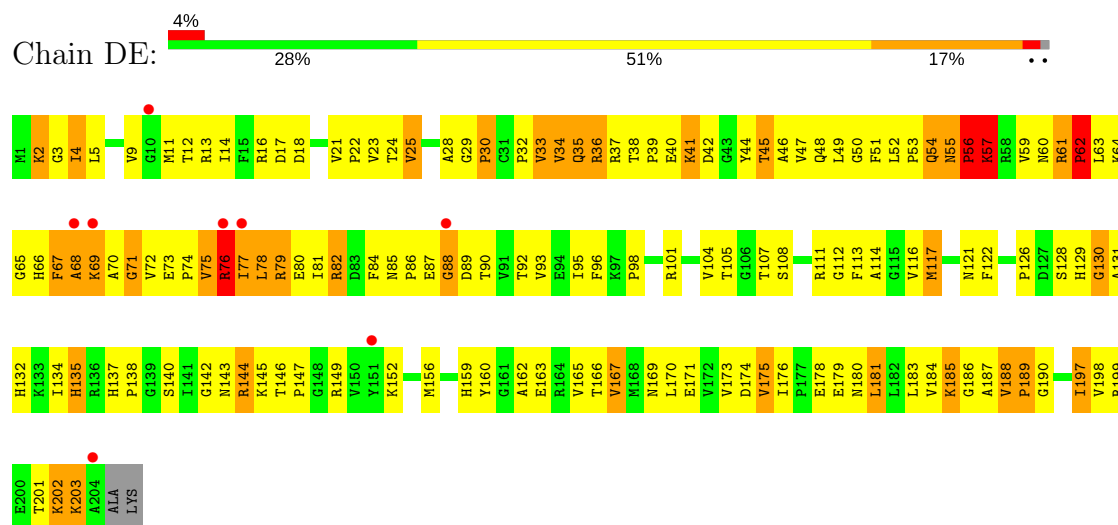




• Molecule 40: 50S RIBOSOMAL PROTEIN L3

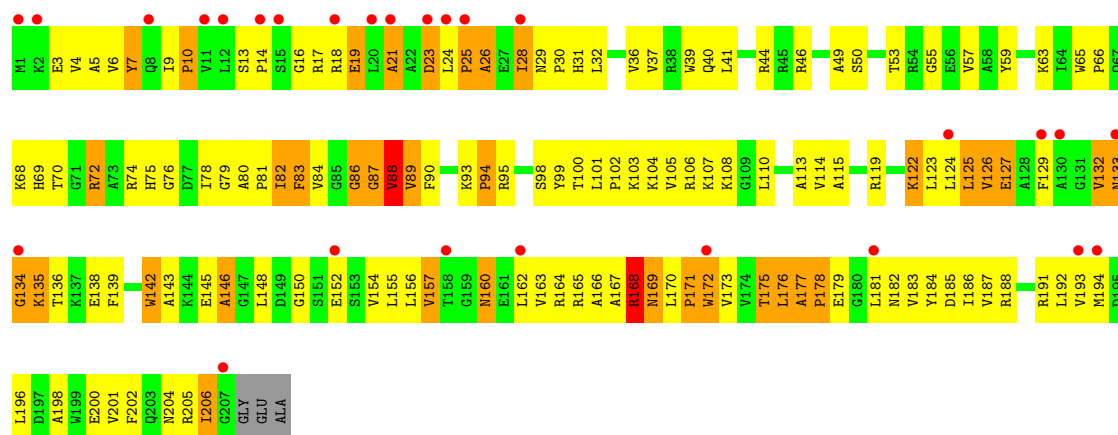


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

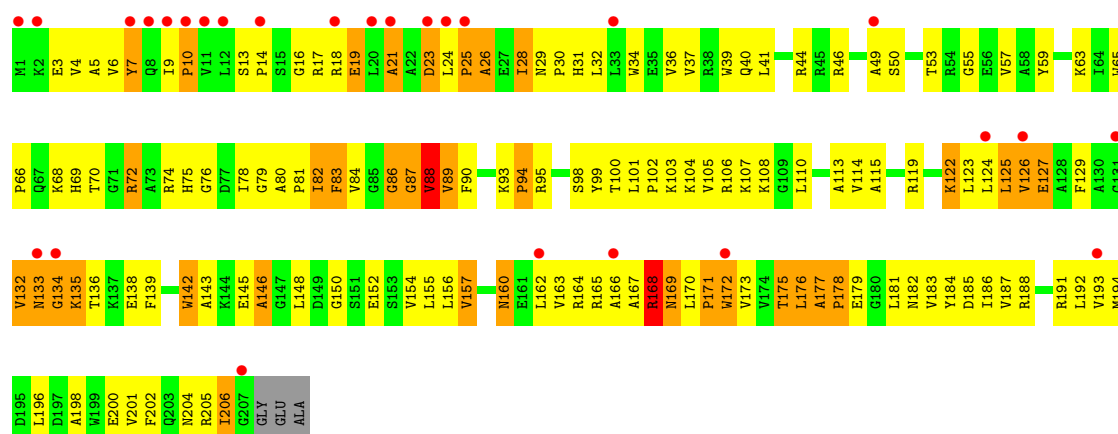


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

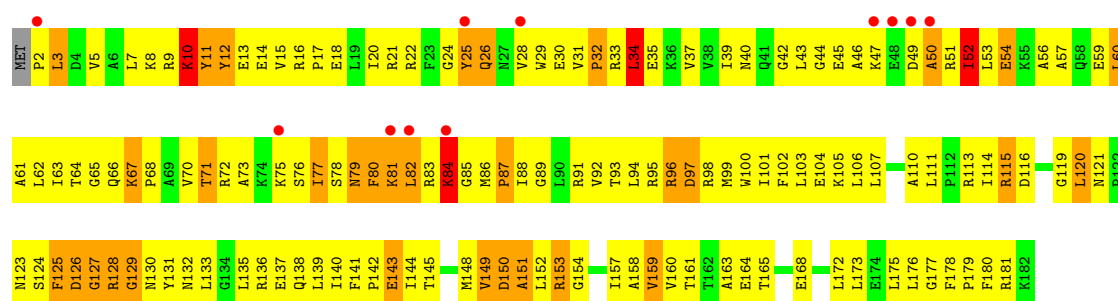




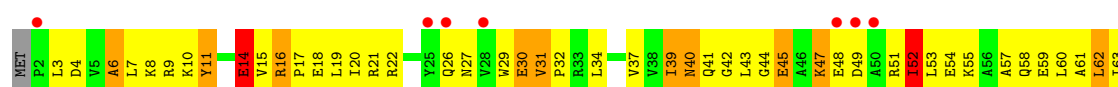
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

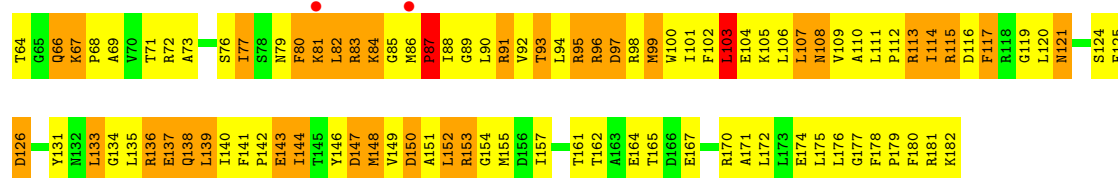


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

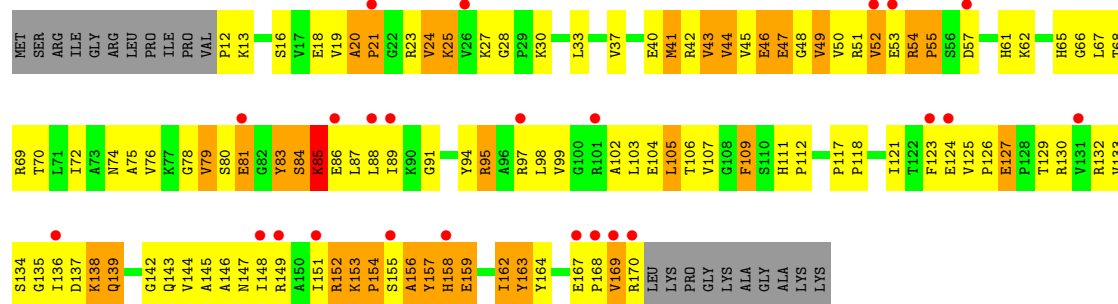


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

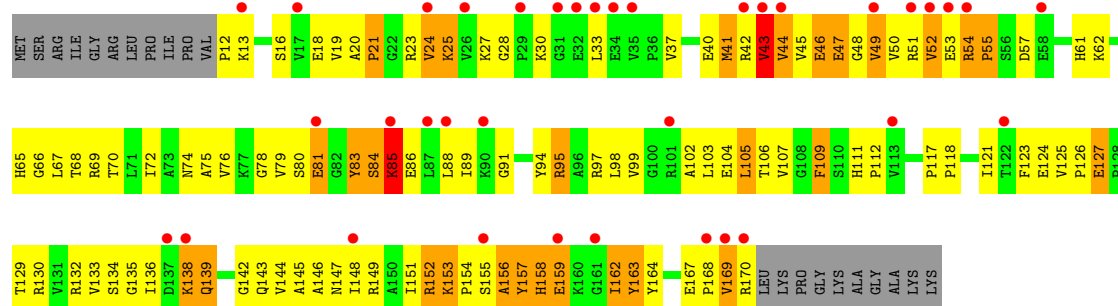




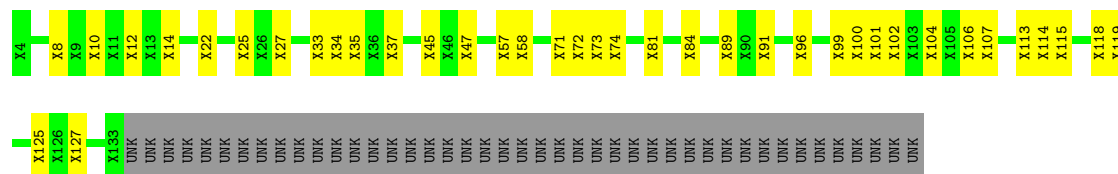
• Molecule 43: 50S RIBOSOMAL PROTEIN L6



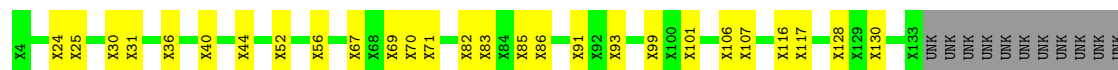
• Molecule 43: 50S RIBOSOMAL PROTEIN L6



• Molecule 44: 50S RIBOSOMAL PROTEIN L10

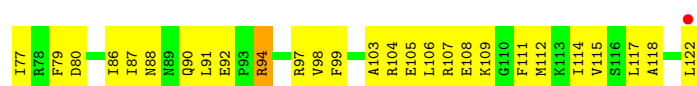


• Molecule 44: 50S RIBOSOMAL PROTEIN L10



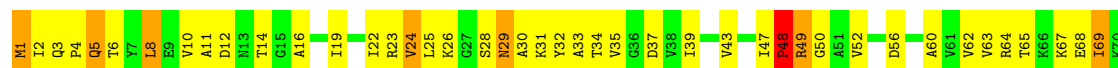






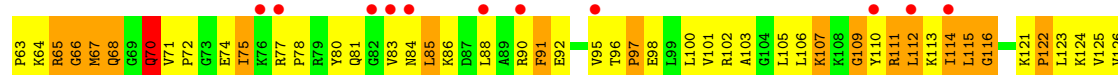
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO: 41% 52% 7% •



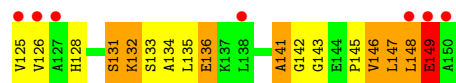
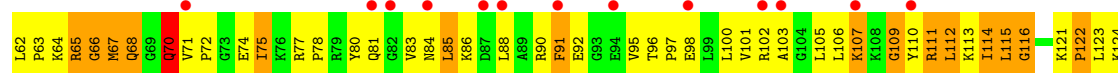
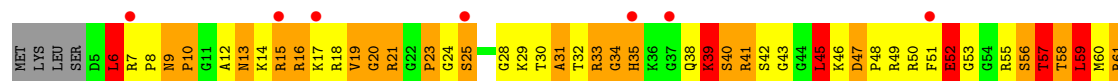
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP: 14% 23% 40% 29% 5% •



• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP: 18% 23% 41% 28% 5% •

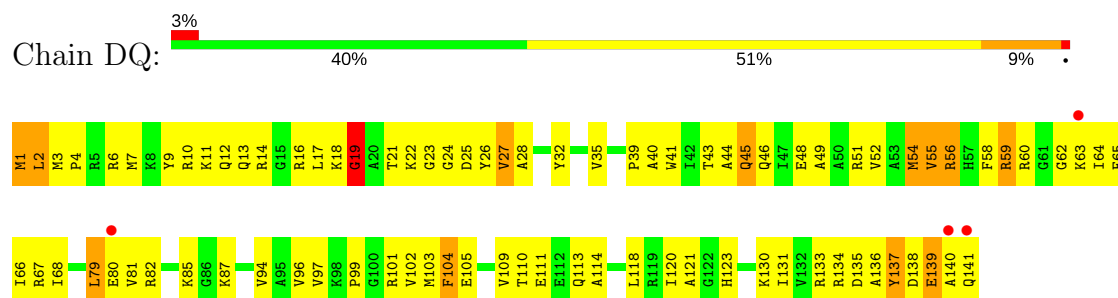


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

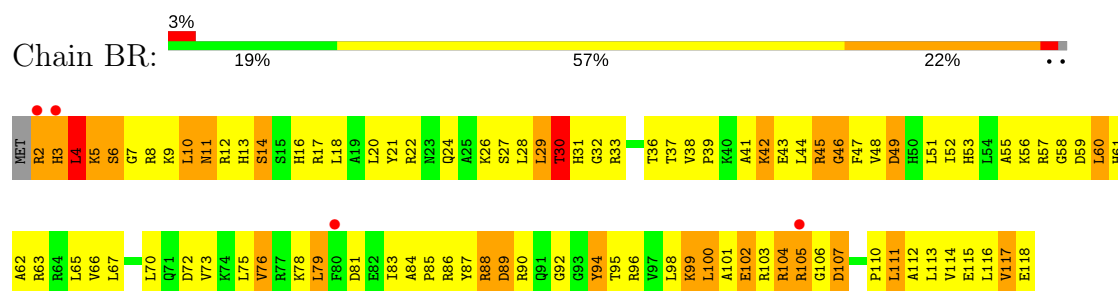
Chain BQ: 43% 48% 9% •



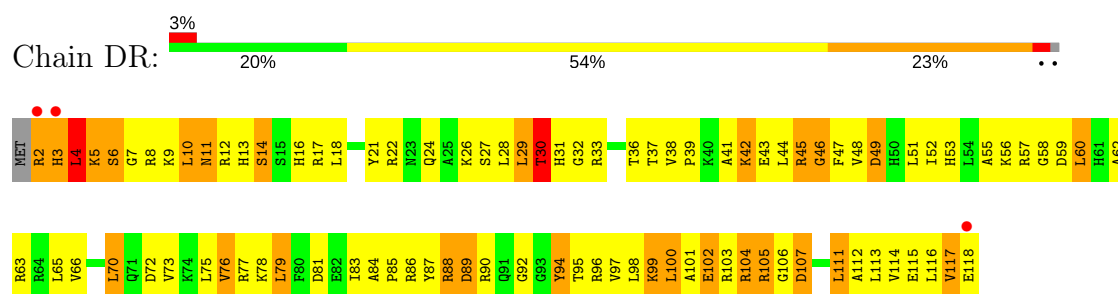
- Molecule 49: 50S RIBOSOMAL PROTEIN L16



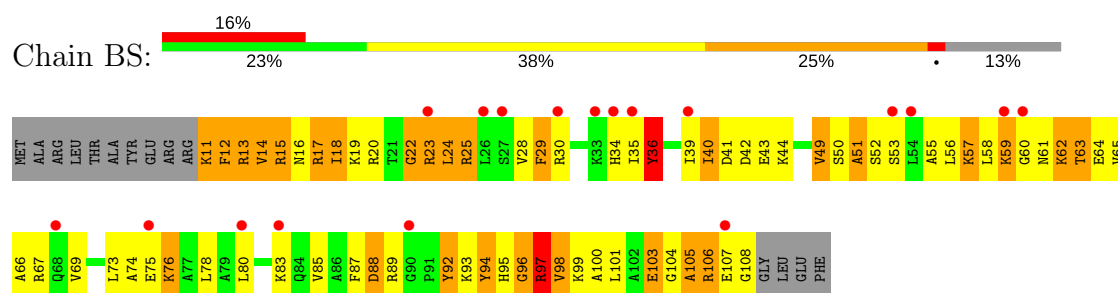
- Molecule 50: 50S RIBOSOMAL PROTEIN L17



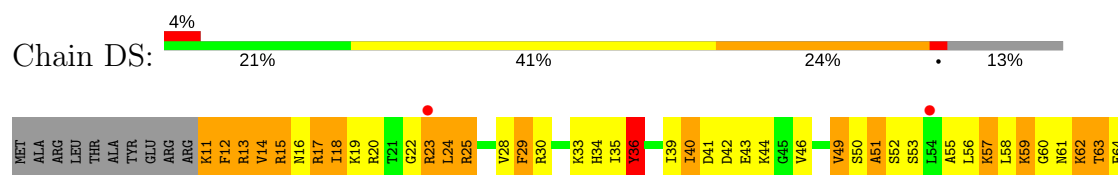
- Molecule 50: 50S RIBOSOMAL PROTEIN L17



- Molecule 51: 50S RIBOSOMAL PROTEIN L18

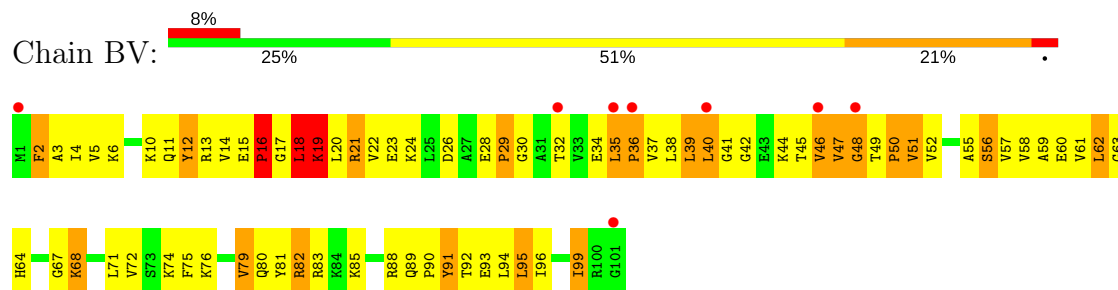


- Molecule 51: 50S RIBOSOMAL PROTEIN L18

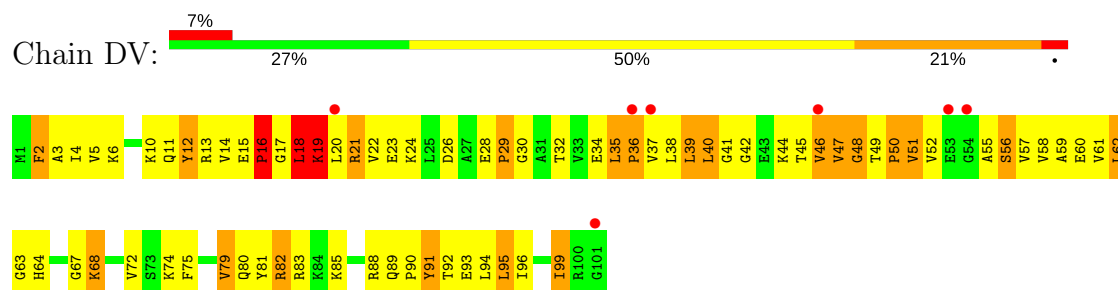




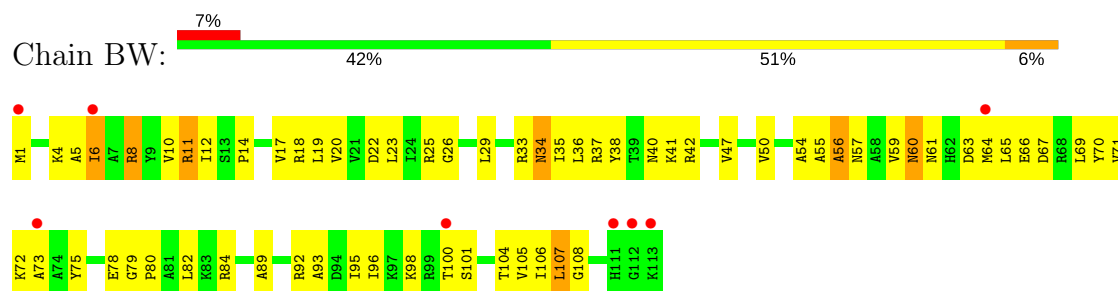
- Molecule 54: 50S RIBOSOMAL PROTEIN L21



- Molecule 54: 50S RIBOSOMAL PROTEIN L21



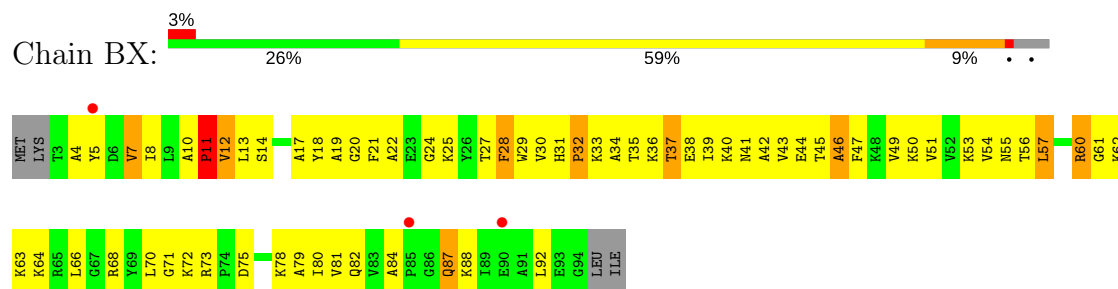
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



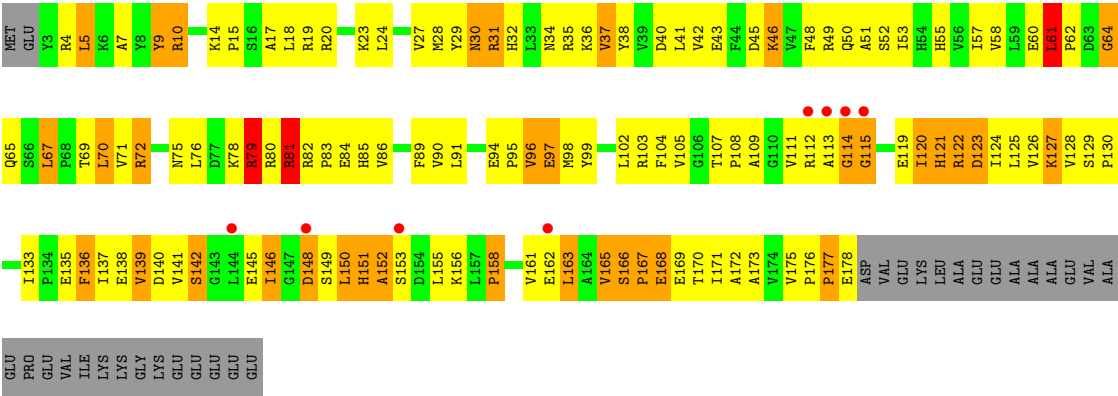
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



- Molecule 56: 50S RIBOSOMAL PROTEIN L23







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	290.20Å 269.20Å 404.00Å 90.00° 91.54° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.10) 92.4 (49.51-2.90)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.237 , 0.264 0.237 , 0.263	Depositor DCC
$R_{free}$ test set	55683 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	79.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 67.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	307330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

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

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OMC, GDP, ZN, H2U, KIR, MIA, 4SU, 7MG, 5MU, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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



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

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	4	59
1	CA	4	49
22	AV	0	3
22	CV	0	2
23	AX	0	2
23	CX	0	1
36	BA	2	63
36	DA	2	72
37	BB	0	2
37	DB	0	2
49	BQ	0	1
49	DQ	0	1
All	All	12	257

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

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

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

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

5 of 12 chirality outliers are listed below:

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

5 of 257 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	14	U	Sidechain
1	AA	189(G)	G	Sidechain
1	AA	30	U	Sidechain
1	AA	37	U	Sidechain
1	AA	60	A	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32451	0	16382	929	0
1	CA	32451	0	16382	850	0
2	AB	1900	0	1951	185	2
2	CB	1900	0	1951	176	2
3	AC	1612	0	1677	145	0
3	CC	1612	0	1677	141	0
4	AD	1703	0	1765	168	0
4	CD	1703	0	1765	156	0
5	AE	1146	0	1207	69	0
5	CE	1146	0	1207	69	0
6	AF	843	0	857	64	0
6	CF	843	0	857	59	0
7	AG	1257	0	1296	70	0
7	CG	1257	0	1296	63	0
8	AH	1116	0	1177	55	0
8	CH	1116	0	1177	49	0
9	AI	1010	0	1037	109	0
9	CI	1010	0	1037	109	0
10	AJ	794	0	840	116	0
10	CJ	794	0	840	116	0
11	AK	885	0	904	58	0
11	CK	885	0	904	57	0
12	AL	970	0	1057	99	0
12	CL	970	0	1057	97	0
13	AM	987	0	1059	116	0
13	CM	987	0	1059	116	0
14	AN	492	0	530	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	530	62	0
15	AO	734	0	771	44	0
15	CO	734	0	771	43	0
16	AP	700	0	720	75	0
16	CP	700	0	720	80	0
17	AQ	823	0	891	60	0
17	CQ	823	0	891	62	0
18	AR	574	0	644	46	0
18	CR	574	0	644	50	0
19	AS	629	0	652	76	0
19	CS	629	0	652	73	0
20	AT	763	0	861	97	0
20	CT	763	0	861	99	0
21	AU	208	0	221	25	0
21	CU	208	0	221	29	0
22	AV	1619	0	822	59	0
22	AW	1619	0	822	82	0
22	CV	1619	0	822	58	0
22	CW	1619	0	822	76	0
23	AX	362	0	184	15	0
23	CX	362	0	184	14	0
24	AY	1645	0	853	132	0
24	CY	1645	0	853	89	0
25	AZ	2984	0	2997	475	0
25	CZ	2984	0	2997	384	0
26	B0	662	0	688	66	0
26	D0	662	0	688	65	0
27	B1	731	0	808	84	0
27	D1	731	0	808	80	0
28	B2	598	0	653	87	0
28	D2	598	0	653	215	0
29	B3	467	0	523	35	0
29	D3	467	0	523	35	0
30	B4	340	0	337	53	0
30	D4	340	0	336	58	0
31	B5	459	0	480	84	0
31	D5	459	0	480	76	0
32	B6	433	0	461	123	0
32	D6	433	0	461	121	0
33	B7	418	0	467	38	0
33	D7	418	0	467	37	0
34	B8	507	0	576	130	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	DW	896	0	953	84	0
56	BX	725	0	778	100	0
56	DX	725	0	778	92	0
57	BY	775	0	870	177	0
57	DY	775	0	870	169	0
58	BZ	1403	0	1432	211	0
58	DZ	1403	0	1432	189	0
59	AD	1	0	0	1	0
59	AN	1	0	0	1	0
59	B4	1	0	0	1	0
59	B9	1	0	0	1	0
59	CD	1	0	0	1	0
59	CN	1	0	0	1	0
59	D4	1	0	0	0	0
59	D9	1	0	0	0	0
60	AZ	28	0	12	15	0
60	CZ	28	0	12	8	0
61	AZ	57	0	58	13	0
61	CZ	57	0	58	9	0
All	All	307330	0	208699	17315	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

The worst 5 of 17315 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	232/256 (91%)	161 (69%)	48 (21%)	23 (10%)	1	4
2	CB	232/256 (91%)	164 (71%)	45 (19%)	23 (10%)	1	4
3	AC	204/239 (85%)	169 (83%)	22 (11%)	13 (6%)	1	9
3	CC	204/239 (85%)	171 (84%)	21 (10%)	12 (6%)	2	12
4	AD	206/209 (99%)	149 (72%)	39 (19%)	18 (9%)	1	5
4	CD	206/209 (99%)	149 (72%)	38 (18%)	19 (9%)	1	4
5	AE	148/162 (91%)	136 (92%)	10 (7%)	2 (1%)	13	47
5	CE	148/162 (91%)	136 (92%)	9 (6%)	3 (2%)	9	37
6	AF	99/101 (98%)	72 (73%)	18 (18%)	9 (9%)	1	4
6	CF	99/101 (98%)	73 (74%)	17 (17%)	9 (9%)	1	4
7	AG	153/156 (98%)	127 (83%)	22 (14%)	4 (3%)	6	31
7	CG	153/156 (98%)	129 (84%)	21 (14%)	3 (2%)	9	37
8	AH	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	12	45
8	CH	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	12	45
9	AI	125/128 (98%)	83 (66%)	34 (27%)	8 (6%)	1	9
9	CI	125/128 (98%)	83 (66%)	35 (28%)	7 (6%)	2	12
10	AJ	96/105 (91%)	69 (72%)	21 (22%)	6 (6%)	1	10
10	CJ	96/105 (91%)	71 (74%)	19 (20%)	6 (6%)	1	10
11	AK	117/129 (91%)	98 (84%)	18 (15%)	1 (1%)	20	60
11	CK	117/129 (91%)	99 (85%)	17 (14%)	1 (1%)	20	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AL	122/131 (93%)	104 (85%)	10 (8%)	8 (7%)	1	9
12	CL	122/131 (93%)	104 (85%)	10 (8%)	8 (7%)	1	9
13	AM	122/126 (97%)	85 (70%)	27 (22%)	10 (8%)	1	6
13	CM	122/126 (97%)	85 (70%)	28 (23%)	9 (7%)	1	7
14	AN	58/61 (95%)	42 (72%)	9 (16%)	7 (12%)	0	2
14	CN	58/61 (95%)	43 (74%)	7 (12%)	8 (14%)	0	1
15	AO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	7	33
15	CO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	7	33
16	AP	81/88 (92%)	58 (72%)	17 (21%)	6 (7%)	1	7
16	CP	81/88 (92%)	59 (73%)	16 (20%)	6 (7%)	1	7
17	AQ	97/105 (92%)	85 (88%)	7 (7%)	5 (5%)	2	14
17	CQ	97/105 (92%)	85 (88%)	7 (7%)	5 (5%)	2	14
18	AR	68/88 (77%)	55 (81%)	11 (16%)	2 (3%)	5	28
18	CR	68/88 (77%)	56 (82%)	10 (15%)	2 (3%)	5	28
19	AS	76/93 (82%)	48 (63%)	15 (20%)	13 (17%)	0	0
19	CS	76/93 (82%)	47 (62%)	16 (21%)	13 (17%)	0	0
20	AT	97/106 (92%)	67 (69%)	22 (23%)	8 (8%)	1	6
20	CT	97/106 (92%)	67 (69%)	21 (22%)	9 (9%)	1	4
21	AU	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	3	17
21	CU	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	3	17
25	AZ	381/405 (94%)	263 (69%)	80 (21%)	38 (10%)	1	4
25	CZ	381/405 (94%)	266 (70%)	77 (20%)	38 (10%)	1	4
26	B0	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	2	16
26	D0	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	2	16
27	B1	91/98 (93%)	68 (75%)	13 (14%)	10 (11%)	0	3
27	D1	91/98 (93%)	63 (69%)	10 (11%)	18 (20%)	0	0
28	B2	69/72 (96%)	46 (67%)	17 (25%)	6 (9%)	1	5
28	D2	69/72 (96%)	37 (54%)	16 (23%)	16 (23%)	0	0
29	B3	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	1	5
29	D3	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	1	5
30	B4	42/71 (59%)	24 (57%)	11 (26%)	7 (17%)	0	0

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

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

5 of 1283 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	181 (90%)	21 (10%)	8	31
2	CB	202/220 (92%)	180 (89%)	22 (11%)	7	30
3	AC	160/188 (85%)	141 (88%)	19 (12%)	6	25
3	CC	160/188 (85%)	142 (89%)	18 (11%)	7	28
4	AD	180/181 (99%)	162 (90%)	18 (10%)	9	33
4	CD	180/181 (99%)	162 (90%)	18 (10%)	9	33
5	AE	115/123 (94%)	102 (89%)	13 (11%)	7	28
5	CE	115/123 (94%)	102 (89%)	13 (11%)	7	28
6	AF	90/90 (100%)	80 (89%)	10 (11%)	7	29
6	CF	90/90 (100%)	80 (89%)	10 (11%)	7	29
7	AG	126/127 (99%)	118 (94%)	8 (6%)	21	56
7	CG	126/127 (99%)	118 (94%)	8 (6%)	21	56
8	AH	119/119 (100%)	107 (90%)	12 (10%)	9	33
8	CH	119/119 (100%)	107 (90%)	12 (10%)	9	33
9	AI	98/99 (99%)	90 (92%)	8 (8%)	13	45
9	CI	98/99 (99%)	89 (91%)	9 (9%)	11	39
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	5	22
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	5	22
11	AK	90/99 (91%)	80 (89%)	10 (11%)	7	29
11	CK	90/99 (91%)	80 (89%)	10 (11%)	7	29
12	AL	104/108 (96%)	92 (88%)	12 (12%)	6	27
12	CL	104/108 (96%)	92 (88%)	12 (12%)	6	27
13	AM	99/101 (98%)	88 (89%)	11 (11%)	7	29
13	CM	99/101 (98%)	88 (89%)	11 (11%)	7	29
14	AN	49/50 (98%)	42 (86%)	7 (14%)	4	17
14	CN	49/50 (98%)	42 (86%)	7 (14%)	4	17
15	AO	79/80 (99%)	70 (89%)	9 (11%)	7	27
15	CO	79/80 (99%)	70 (89%)	9 (11%)	7	27
16	AP	72/74 (97%)	64 (89%)	8 (11%)	7	29
16	CP	72/74 (97%)	65 (90%)	7 (10%)	9	35
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	20	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	20	56
18	AR	61/77 (79%)	51 (84%)	10 (16%)	2	12
18	CR	61/77 (79%)	51 (84%)	10 (16%)	2	12
19	AS	69/80 (86%)	56 (81%)	13 (19%)	2	8
19	CS	69/80 (86%)	56 (81%)	13 (19%)	2	8
20	AT	76/82 (93%)	68 (90%)	8 (10%)	8	31
20	CT	76/82 (93%)	68 (90%)	8 (10%)	8	31
21	AU	19/22 (86%)	18 (95%)	1 (5%)	26	63
21	CU	19/22 (86%)	18 (95%)	1 (5%)	26	63
25	AZ	322/338 (95%)	279 (87%)	43 (13%)	4	19
25	CZ	322/338 (95%)	281 (87%)	41 (13%)	5	21
26	B0	66/67 (98%)	59 (89%)	7 (11%)	8	30
26	D0	66/67 (98%)	59 (89%)	7 (11%)	8	30
27	B1	78/83 (94%)	67 (86%)	11 (14%)	4	18
27	D1	78/83 (94%)	68 (87%)	10 (13%)	5	21
28	B2	66/67 (98%)	64 (97%)	2 (3%)	46	79
28	D2	66/67 (98%)	57 (86%)	9 (14%)	4	19
29	B3	51/52 (98%)	45 (88%)	6 (12%)	6	25
29	D3	51/52 (98%)	45 (88%)	6 (12%)	6	25
30	B4	39/63 (62%)	32 (82%)	7 (18%)	2	9
30	D4	39/63 (62%)	33 (85%)	6 (15%)	3	14
31	B5	51/52 (98%)	45 (88%)	6 (12%)	6	25
31	D5	51/52 (98%)	45 (88%)	6 (12%)	6	25
32	B6	49/52 (94%)	32 (65%)	17 (35%)	0	0
32	D6	49/52 (94%)	31 (63%)	18 (37%)	0	0
33	B7	41/42 (98%)	38 (93%)	3 (7%)	16	50
33	D7	41/42 (98%)	38 (93%)	3 (7%)	16	50
34	B8	53/55 (96%)	44 (83%)	9 (17%)	2	11
34	D8	53/55 (96%)	44 (83%)	9 (17%)	2	11
35	B9	34/34 (100%)	31 (91%)	3 (9%)	12	42
35	D9	34/34 (100%)	31 (91%)	3 (9%)	12	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BC	180/181 (99%)	172 (96%)	8 (4%)	33	69
38	DC	180/181 (99%)	172 (96%)	8 (4%)	33	69
39	BD	217/218 (100%)	186 (86%)	31 (14%)	4	17
39	DD	217/218 (100%)	187 (86%)	30 (14%)	4	19
40	BE	165/166 (99%)	145 (88%)	20 (12%)	6	24
40	DE	165/166 (99%)	143 (87%)	22 (13%)	4	20
41	BF	165/166 (99%)	152 (92%)	13 (8%)	14	47
41	DF	165/166 (99%)	152 (92%)	13 (8%)	14	47
42	BG	155/156 (99%)	135 (87%)	20 (13%)	5	21
42	DG	155/156 (99%)	124 (80%)	31 (20%)	1	6
43	BH	132/148 (89%)	118 (89%)	14 (11%)	8	30
43	DH	132/148 (89%)	118 (89%)	14 (11%)	8	30
46	BN	117/119 (98%)	101 (86%)	16 (14%)	4	19
46	DN	117/119 (98%)	101 (86%)	16 (14%)	4	19
47	BO	100/100 (100%)	93 (93%)	7 (7%)	18	52
47	DO	100/100 (100%)	93 (93%)	7 (7%)	18	52
48	BP	112/116 (97%)	93 (83%)	19 (17%)	2	11
48	DP	112/116 (97%)	93 (83%)	19 (17%)	2	11
49	BQ	111/111 (100%)	101 (91%)	10 (9%)	11	40
49	DQ	111/111 (100%)	101 (91%)	10 (9%)	11	40
50	BR	100/101 (99%)	87 (87%)	13 (13%)	5	21
50	DR	100/101 (99%)	85 (85%)	15 (15%)	3	15
51	BS	77/88 (88%)	65 (84%)	12 (16%)	3	13
51	DS	77/88 (88%)	65 (84%)	12 (16%)	3	13
52	BT	120/127 (94%)	97 (81%)	23 (19%)	1	7
52	DT	120/127 (94%)	97 (81%)	23 (19%)	1	7
53	BU	92/94 (98%)	86 (94%)	6 (6%)	20	55
53	DU	92/94 (98%)	86 (94%)	6 (6%)	20	55
54	BV	82/82 (100%)	67 (82%)	15 (18%)	2	9
54	DV	82/82 (100%)	67 (82%)	15 (18%)	2	9
55	BW	91/92 (99%)	87 (96%)	4 (4%)	33	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	DW	91/92 (99%)	86 (94%)	5 (6%)	25 61
56	BX	74/78 (95%)	67 (90%)	7 (10%)	10 37
56	DX	74/78 (95%)	68 (92%)	6 (8%)	14 45
57	BY	84/91 (92%)	71 (84%)	13 (16%)	3 14
57	DY	84/91 (92%)	72 (86%)	12 (14%)	4 17
58	BZ	155/179 (87%)	130 (84%)	25 (16%)	3 12
58	DZ	155/179 (87%)	131 (84%)	24 (16%)	3 14
All	All	10338/10854 (95%)	9112 (88%)	1226 (12%)	6 25

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

Mol	Chain	Res	Type
54	BV	95	LEU
7	CG	24	THR
51	DS	97	ARG
57	BY	7	VAL
2	CB	187	LEU

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

Mol	Chain	Res	Type
53	BU	49	HIS
5	CE	20	GLN
49	DQ	141	GLN
55	BW	57	ASN
2	CB	45	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1509/1522 (99%)	227 (15%)	0
1	CA	1509/1522 (99%)	222 (14%)	0
22	AV	75/76 (98%)	22 (29%)	0
22	AW	75/76 (98%)	21 (28%)	0
22	CV	75/76 (98%)	23 (30%)	0
22	CW	75/76 (98%)	21 (28%)	0
23	AX	16/27 (59%)	6 (37%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	CX	16/27 (59%)	5 (31%)	0
24	AY	74/77 (96%)	25 (33%)	0
24	CY	74/77 (96%)	25 (33%)	0
36	BA	2900/2915 (99%)	494 (17%)	0
36	DA	2900/2915 (99%)	492 (16%)	0
37	BB	118/122 (96%)	22 (18%)	0
37	DB	118/122 (96%)	22 (18%)	0
All	All	9534/9630 (99%)	1627 (17%)	0

5 of 1627 RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

## 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	16	24	17,21,22	1.01	1 (5%)	21,30,33	1.88	4 (19%)
24	H2U	AY	17	24	17,21,22	1.10	2 (11%)	21,30,33	1.97	5 (23%)
24	H2U	AY	20	24	17,21,22	0.85	1 (5%)	21,30,33	1.94	5 (23%)
24	OMC	AY	32	24	15,22,23	0.73	0	19,31,34	0.76	1 (5%)
24	MIA	AY	37	24	23,31,32	0.97	0	25,44,47	1.63	3 (12%)
24	7MG	AY	46	24	20,26,27	1.67	3 (15%)	22,39,42	2.23	2 (9%)
24	5MU	AY	54	24	14,22,23	1.23	2 (14%)	16,32,35	4.27	3 (18%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	PSU	AY	55	24	16,21,22	1.11	2 (12%)	20,30,33	3.73	8 (40%)
24	4SU	AY	8	24	14,21,22	1.41	4 (28%)	15,30,33	2.65	2 (13%)
24	H2U	CY	16	24	17,21,22	1.00	1 (5%)	21,30,33	1.86	4 (19%)
24	H2U	CY	17	24	17,21,22	1.11	2 (11%)	21,30,33	1.96	5 (23%)
24	H2U	CY	20	24	17,21,22	0.85	1 (5%)	21,30,33	1.95	5 (23%)
24	OMC	CY	32	24	15,22,23	0.73	0	19,31,34	0.77	1 (5%)
24	MIA	CY	37	24	23,31,32	1.09	2 (8%)	25,44,47	1.66	3 (12%)
24	7MG	CY	46	24	20,26,27	1.78	4 (20%)	22,39,42	2.23	2 (9%)
24	5MU	CY	54	24	14,22,23	1.28	3 (21%)	16,32,35	4.27	3 (18%)
24	PSU	CY	55	24	16,21,22	1.09	2 (12%)	20,30,33	3.66	8 (40%)
24	4SU	CY	8	24	14,21,22	1.36	3 (21%)	15,30,33	2.63	2 (13%)

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

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	46	7MG	C8-N9	-5.04	1.38	1.45
24	AY	46	7MG	C8-N9	-4.99	1.38	1.45
24	CY	46	7MG	C8-N7	-2.83	1.30	1.43
24	AY	46	7MG	C8-N7	-2.81	1.30	1.43
24	CY	54	5MU	C6-C5	-2.23	1.34	1.40

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	55	PSU	N1-C2-N3	-11.51	120.12	128.40
24	CY	55	PSU	N1-C2-N3	-11.22	120.33	128.40
24	CY	54	5MU	C5-C4-N3	-9.17	115.13	125.24
24	AY	54	5MU	C5-C4-N3	-9.15	115.16	125.24
24	AY	46	7MG	C5-C6-N1	-7.57	111.50	123.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	17	H2U	P-O5'-C5'-C4'
24	CY	17	H2U	P-O5'-C5'-C4'

There are no ring outliers.

14 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	16	H2U	3	0
24	AY	17	H2U	3	0
24	AY	20	H2U	1	0
24	AY	46	7MG	3	0
24	AY	54	5MU	1	0
24	AY	55	PSU	1	0
24	AY	8	4SU	1	0
24	CY	16	H2U	4	0
24	CY	17	H2U	4	0
24	CY	20	H2U	1	0
24	CY	46	7MG	3	0
24	CY	54	5MU	1	0
24	CY	55	PSU	1	0
24	CY	8	4SU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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$
60	GDP	AZ	501	-	25,30,30	1.54	5 (20%)	26,47,47	1.48	4 (15%)
61	KIR	AZ	502	-	53,59,59	3.43	19 (35%)	57,84,84	1.70	12 (21%)
60	GDP	CZ	501	-	25,30,30	1.44	4 (16%)	26,47,47	2.15	5 (19%)
61	KIR	CZ	502	-	53,59,59	3.42	21 (39%)	57,84,84	1.74	13 (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
60	GDP	AZ	501	-	-	0/12/32/32	0/3/3/3
61	KIR	AZ	502	-	-	0/54/98/98	0/3/3/3
60	GDP	CZ	501	-	-	0/12/32/32	0/3/3/3
61	KIR	CZ	502	-	-	0/54/98/98	0/3/3/3

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CZ	502	KIR	O18-C17	-14.49	1.22	1.44
61	AZ	502	KIR	O18-C17	-14.22	1.23	1.44
61	AZ	502	KIR	O30-C30	-12.35	1.17	1.42
61	CZ	502	KIR	O30-C30	-12.02	1.18	1.42
60	CZ	501	GDP	C6-C5	-2.92	1.35	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AZ	502	KIR	O29-C29-O34	-5.04	101.68	110.22
60	CZ	501	GDP	N3-C2-N1	-5.03	120.11	127.46
61	CZ	502	KIR	O29-C29-O34	-4.98	101.79	110.22
60	CZ	501	GDP	C5-C6-N1	-4.23	117.46	123.48
61	CZ	502	KIR	C48-C32-C47	-4.11	101.43	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 45 short contacts:

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1510/1522 (99%)	-0.29	19 (1%) 77 59	44, 78, 160, 200	0
1	CA	1510/1522 (99%)	-0.07	31 (2%) 64 43	37, 73, 161, 200	0
2	AB	234/256 (91%)	-0.10	6 (2%) 56 33	58, 88, 152, 164	0
2	CB	234/256 (91%)	-0.19	3 (1%) 77 59	54, 86, 151, 164	0
3	AC	206/239 (86%)	-0.30	1 (0%) 90 80	52, 75, 101, 110	0
3	CC	206/239 (86%)	-0.30	0 100 100	46, 70, 100, 109	0
4	AD	208/209 (99%)	0.11	10 (4%) 31 14	71, 97, 124, 132	0
4	CD	208/209 (99%)	0.05	4 (1%) 67 46	67, 96, 123, 131	0
5	AE	150/162 (92%)	-0.35	0 100 100	53, 65, 89, 110	0
5	CE	150/162 (92%)	-0.35	0 100 100	49, 63, 88, 109	0
6	AF	101/101 (100%)	0.04	1 (0%) 82 67	71, 99, 115, 122	0
6	CF	101/101 (100%)	-0.15	1 (0%) 82 67	68, 97, 114, 121	0
7	AG	155/156 (99%)	0.18	7 (4%) 34 16	66, 89, 113, 130	0
7	CG	155/156 (99%)	-0.11	2 (1%) 77 59	59, 86, 112, 129	0
8	AH	138/138 (100%)	-0.28	1 (0%) 87 75	54, 70, 87, 95	0
8	CH	138/138 (100%)	-0.30	0 100 100	52, 67, 87, 94	0
9	AI	127/128 (99%)	0.65	15 (11%) 5 2	62, 96, 128, 139	0
9	CI	127/128 (99%)	0.23	2 (1%) 72 51	54, 93, 127, 139	0
10	AJ	98/105 (93%)	0.81	19 (19%) 1 0	59, 99, 141, 145	0
10	CJ	98/105 (93%)	0.36	4 (4%) 38 18	54, 95, 140, 144	0
11	AK	119/129 (92%)	0.04	6 (5%) 30 13	55, 73, 107, 134	0
11	CK	119/129 (92%)	-0.04	4 (3%) 46 23	51, 68, 108, 133	0
12	AL	124/131 (94%)	0.02	5 (4%) 39 19	55, 70, 94, 132	0
12	CL	124/131 (94%)	-0.12	1 (0%) 86 71	51, 68, 93, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	124/126 (98%)	0.34	13 (10%) 7 2	71, 97, 124, 152	0
13	CM	124/126 (98%)	0.13	7 (5%) 25 11	67, 95, 123, 152	0
14	AN	60/61 (98%)	-0.17	1 (1%) 70 49	57, 72, 93, 96	0
14	CN	60/61 (98%)	-0.02	1 (1%) 70 49	49, 66, 91, 96	0
15	AO	88/89 (98%)	-0.08	0 100 100	57, 75, 99, 105	0
15	CO	88/89 (98%)	-0.05	0 100 100	56, 74, 98, 104	0
16	AP	83/88 (94%)	0.41	3 (3%) 43 21	74, 91, 109, 135	0
16	CP	83/88 (94%)	0.38	2 (2%) 59 37	72, 89, 108, 136	0
17	AQ	99/105 (94%)	-0.00	3 (3%) 51 27	60, 79, 95, 108	0
17	CQ	99/105 (94%)	-0.06	0 100 100	57, 78, 93, 107	0
18	AR	70/88 (79%)	-0.04	3 (4%) 36 17	58, 82, 106, 119	0
18	CR	70/88 (79%)	-0.30	1 (1%) 75 57	56, 79, 105, 118	0
19	AS	78/93 (83%)	0.43	5 (6%) 20 7	75, 99, 137, 139	0
19	CS	78/93 (83%)	0.46	4 (5%) 29 13	71, 99, 136, 139	0
20	AT	99/106 (93%)	0.44	5 (5%) 29 13	75, 97, 131, 135	0
20	CT	99/106 (93%)	0.43	5 (5%) 29 13	71, 96, 132, 135	0
21	AU	24/27 (88%)	0.77	3 (12%) 4 2	66, 84, 103, 115	0
21	CU	24/27 (88%)	0.37	1 (4%) 37 18	64, 78, 99, 115	0
22	AV	76/76 (100%)	-0.29	1 (1%) 77 59	56, 91, 128, 148	0
22	AW	76/76 (100%)	0.79	10 (13%) 4 2	103, 172, 200, 200	0
22	CV	76/76 (100%)	-0.22	1 (1%) 77 59	50, 89, 128, 147	0
22	CW	76/76 (100%)	0.70	11 (14%) 3 1	100, 172, 200, 200	0
23	AX	17/27 (62%)	0.58	2 (11%) 5 2	50, 97, 156, 157	0
23	CX	17/27 (62%)	0.53	1 (5%) 23 10	45, 95, 156, 157	0
24	AY	68/77 (88%)	0.04	1 (1%) 74 54	61, 140, 171, 190	0
24	CY	68/77 (88%)	-0.01	4 (5%) 23 10	57, 140, 170, 190	0
25	AZ	385/405 (95%)	1.76	136 (35%) 0 0	116, 142, 165, 183	0
25	CZ	385/405 (95%)	0.44	23 (5%) 23 9	113, 141, 165, 183	0
26	B0	84/85 (98%)	0.62	8 (9%) 9 3	77, 91, 118, 131	0
26	D0	84/85 (98%)	0.55	7 (8%) 12 4	76, 90, 119, 131	0
27	B1	93/98 (94%)	0.43	5 (5%) 26 12	74, 95, 134, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	D1	93/98 (94%)	0.24	2 (2%) 62 41	56, 76, 130, 142	0
28	B2	71/72 (98%)	0.46	5 (7%) 17 7	110, 133, 148, 157	0
28	D2	71/72 (98%)	1.39	21 (29%) 1 0	134, 154, 174, 175	0
29	B3	59/60 (98%)	0.66	3 (5%) 29 13	81, 99, 120, 142	0
29	D3	59/60 (98%)	0.54	3 (5%) 29 13	80, 97, 120, 142	0
30	B4	44/71 (61%)	0.21	5 (11%) 6 2	124, 149, 160, 163	0
30	D4	44/71 (61%)	0.38	3 (6%) 18 7	123, 147, 158, 163	0
31	B5	59/60 (98%)	0.31	5 (8%) 11 4	73, 105, 158, 176	0
31	D5	59/60 (98%)	0.14	4 (6%) 18 7	72, 104, 158, 176	0
32	B6	50/54 (92%)	0.82	7 (14%) 3 1	74, 106, 116, 125	0
32	D6	50/54 (92%)	0.86	8 (16%) 2 1	73, 104, 115, 123	0
33	B7	48/49 (97%)	0.43	0 100 100	70, 79, 119, 139	0
33	D7	48/49 (97%)	0.58	2 (4%) 37 18	68, 78, 119, 140	0
34	B8	63/65 (96%)	0.49	3 (4%) 31 14	80, 90, 104, 131	0
34	D8	63/65 (96%)	0.41	3 (4%) 31 14	78, 88, 104, 131	0
35	B9	37/37 (100%)	0.63	2 (5%) 26 12	76, 90, 104, 108	0
35	D9	37/37 (100%)	0.29	3 (8%) 13 5	76, 90, 104, 107	0
36	BA	2901/2915 (99%)	-0.10	71 (2%) 59 37	49, 95, 190, 200	0
36	DA	2901/2915 (99%)	-0.02	71 (2%) 59 37	46, 93, 190, 200	0
37	BB	119/122 (97%)	-0.46	0 100 100	78, 108, 134, 157	0
37	DB	119/122 (97%)	-0.37	0 100 100	75, 107, 133, 157	0
38	BC	228/229 (99%)	0.71	32 (14%) 3 1	69, 99, 177, 187	0
38	DC	228/229 (99%)	0.33	20 (8%) 11 4	67, 97, 177, 187	0
39	BD	275/276 (99%)	-0.15	3 (1%) 80 65	50, 68, 98, 123	0
39	DD	275/276 (99%)	-0.16	2 (0%) 87 75	47, 66, 97, 123	0
40	BE	204/206 (99%)	0.28	12 (5%) 23 10	64, 93, 141, 152	0
40	DE	204/206 (99%)	0.25	8 (3%) 40 19	64, 93, 141, 152	0
41	BF	207/210 (98%)	0.77	27 (13%) 4 2	73, 128, 176, 184	0
41	DF	207/210 (98%)	0.69	27 (13%) 4 2	71, 127, 176, 184	0
42	BG	181/182 (99%)	0.25	11 (6%) 22 9	97, 125, 147, 157	0
42	DG	181/182 (99%)	0.08	9 (4%) 30 13	75, 96, 125, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BH	159/180 (88%)	0.79	24 (15%) 3 1	106, 142, 163, 165	0
43	DH	159/180 (88%)	1.16	36 (22%) 1 0	106, 142, 163, 165	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	138/140 (98%)	0.20	2 (1%) 75 57	78, 104, 145, 148	0
46	DN	138/140 (98%)	0.17	3 (2%) 62 41	77, 104, 144, 147	0
47	BO	122/122 (100%)	-0.16	1 (0%) 86 71	58, 76, 90, 97	0
47	DO	122/122 (100%)	-0.06	0 100 100	57, 76, 89, 97	0
48	BP	146/150 (97%)	0.94	21 (14%) 3 1	73, 121, 146, 162	0
48	DP	146/150 (97%)	0.96	27 (18%) 1 1	72, 120, 145, 162	0
49	BQ	141/141 (100%)	0.02	2 (1%) 75 57	61, 78, 107, 138	0
49	DQ	141/141 (100%)	0.05	4 (2%) 53 29	60, 77, 107, 139	0
50	BR	117/118 (99%)	0.31	4 (3%) 46 23	76, 98, 114, 129	0
50	DR	117/118 (99%)	0.31	3 (2%) 56 33	75, 98, 115, 129	0
51	BS	98/112 (87%)	0.87	18 (18%) 1 1	89, 112, 137, 141	0
51	DS	98/112 (87%)	0.46	5 (5%) 29 13	88, 111, 136, 140	0
52	BT	137/146 (93%)	0.13	9 (6%) 19 7	74, 97, 155, 179	0
52	DT	137/146 (93%)	0.23	12 (8%) 11 4	73, 97, 154, 179	0
53	BU	117/118 (99%)	0.14	3 (2%) 56 33	81, 98, 125, 142	0
53	DU	117/118 (99%)	0.13	2 (1%) 70 49	78, 97, 125, 142	0
54	BV	101/101 (100%)	0.56	8 (7%) 13 5	79, 130, 146, 150	0
54	DV	101/101 (100%)	0.50	7 (6%) 18 7	79, 129, 146, 150	0
55	BW	113/113 (100%)	0.47	8 (7%) 17 6	85, 100, 133, 165	0
55	DW	113/113 (100%)	0.38	9 (7%) 13 5	82, 100, 133, 165	0
56	BX	92/96 (95%)	0.49	3 (3%) 47 24	83, 109, 125, 134	0
56	DX	92/96 (95%)	0.40	7 (7%) 15 5	83, 108, 124, 134	0
57	BY	100/110 (90%)	1.81	38 (38%) 0 0	127, 146, 179, 187	0
57	DY	100/110 (90%)	1.76	40 (40%) 0 0	126, 146, 179, 187	0
58	BZ	176/206 (85%)	0.09	5 (2%) 53 29	75, 103, 135, 144	0
58	DZ	176/206 (85%)	0.06	8 (4%) 34 16	64, 94, 140, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	21994/23368 (94%)	0.13	1090 (4%) 30 13	37, 93, 162, 200	0

The worst 5 of 1090 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	DQ	141	GLN	14.2
49	BQ	141	GLN	12.6
38	BC	1	PRO	11.6
43	DH	170	ARG	11.5
53	DU	118	GLY	11.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
24	MIA	CY	37	29/30	0.93	0.28	-	60,80,107,108	0
24	5MU	AY	54	21/22	0.92	0.20	-	143,153,153,156	0
24	H2U	CY	20	20/21	0.79	0.38	-	185,186,187,187	0
24	MIA	AY	37	29/30	0.94	0.26	-	63,84,108,108	0
24	7MG	AY	46	24/25	0.65	0.39	-	166,169,171,171	0
24	4SU	CY	8	20/21	0.85	0.24	-	140,141,142,142	0
24	PSU	AY	55	20/21	0.80	0.19	-	157,166,168,168	0
24	7MG	CY	46	24/25	0.84	0.23	-	166,168,170,170	0
24	OMC	AY	32	21/22	0.92	0.29	-	98,106,112,113	0
24	H2U	AY	20	20/21	0.74	0.34	-	186,186,188,188	0
24	5MU	CY	54	21/22	0.89	0.15	-	142,153,154,156	0
24	PSU	CY	55	20/21	0.79	0.18	-	158,166,168,168	0
24	H2U	CY	17	20/21	0.80	0.58	-	194,195,195,195	0
24	OMC	CY	32	21/22	0.90	0.17	-	96,103,108,109	0
24	H2U	AY	16	20/21	0.58	0.66	-	181,191,192,193	0
24	H2U	AY	17	20/21	0.80	0.54	-	194,195,195,195	0
24	H2U	CY	16	20/21	0.56	0.70	-	181,191,191,193	0
24	4SU	AY	8	20/21	0.76	0.30	-	140,143,144,144	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
61	KIR	AZ	502	57/57	0.74	0.57	1.45	139,147,150,150	0
59	ZN	CD	301	1/1	0.99	0.31	1.31	85,85,85,85	0
61	KIR	CZ	502	57/57	0.84	0.34	0.89	139,145,150,151	0
59	ZN	AD	301	1/1	0.99	0.29	0.64	99,99,99,99	0
60	GDP	CZ	501	28/28	0.81	0.25	0.04	141,145,153,153	0
59	ZN	AN	101	1/1	0.99	0.16	-0.12	84,84,84,84	0
59	ZN	D4	101	1/1	0.99	0.14	-0.60	129,129,129,129	0
60	GDP	AZ	501	28/28	0.83	0.23	-0.67	151,157,158,158	0
59	ZN	D9	101	1/1	0.97	0.10	-0.73	133,133,133,133	0
59	ZN	CN	101	1/1	1.00	0.17	-0.93	63,63,63,63	0
59	ZN	B4	101	1/1	0.88	0.08	-1.02	200,200,200,200	0
59	ZN	B9	101	1/1	0.94	0.14	-1.31	200,200,200,200	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.