



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:52 PM 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

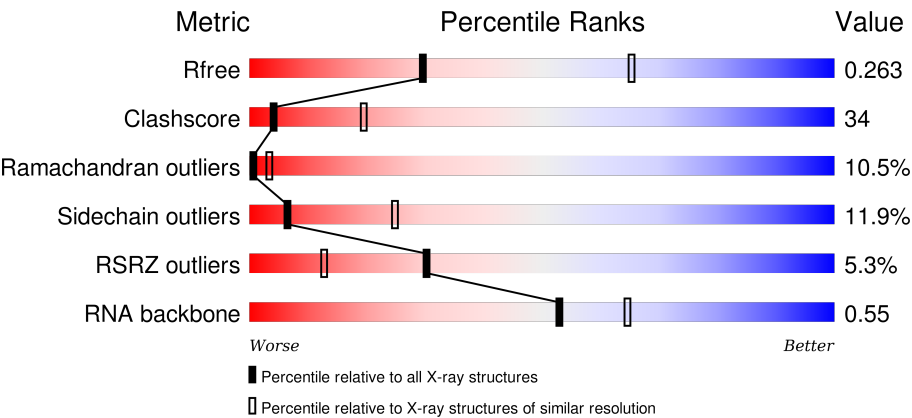
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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 ≥ 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>%</div><div><div></div><div>38%</div><div>48%</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>•</div><div>9%</div></div></div>
2	CB	256	<div><div>%</div><div><div></div><div>33%</div><div>46%</div><div>11%</div><div>•</div><div>9%</div></div></div>



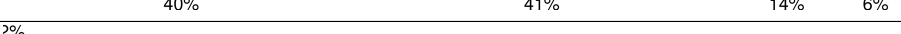
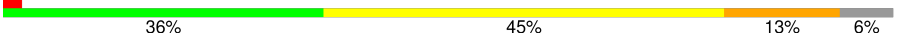

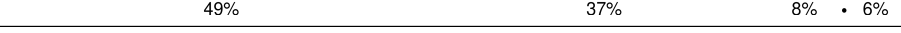

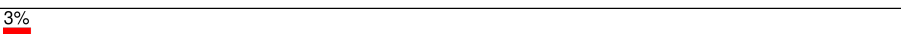

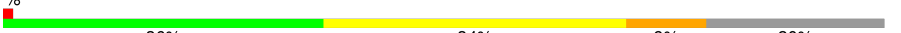
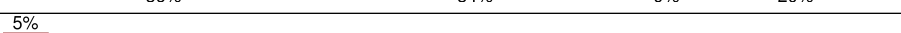


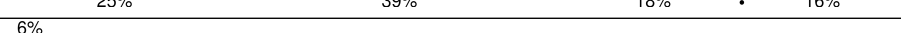
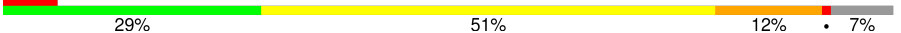

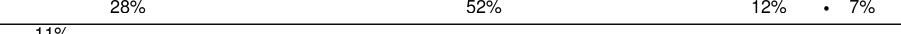


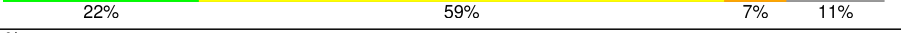
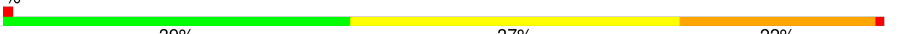

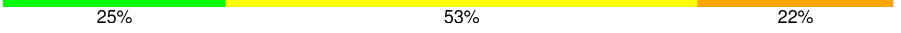


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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	131	
12	CL	131	
13	AM	126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

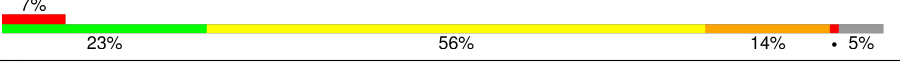
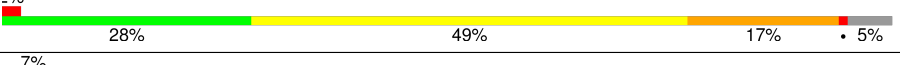
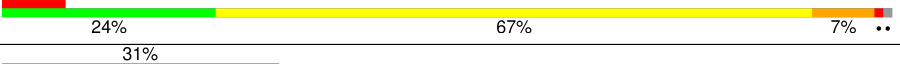
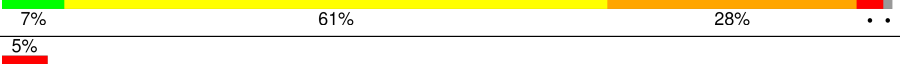
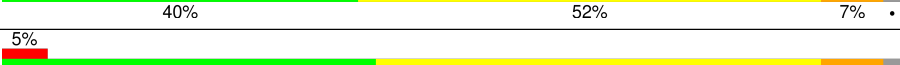

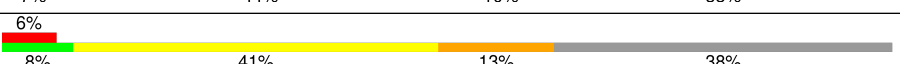
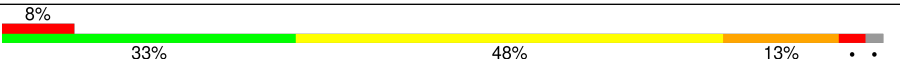





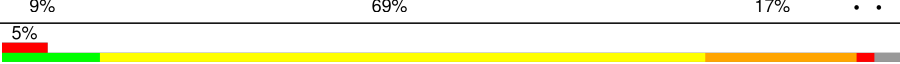
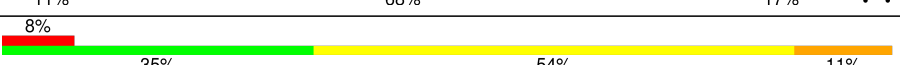
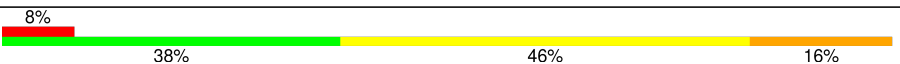

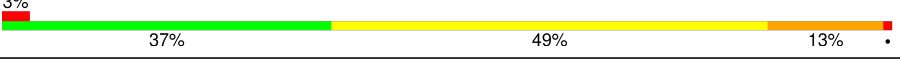
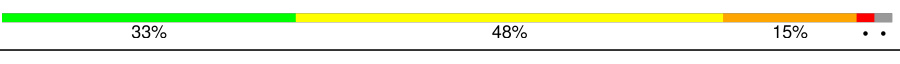


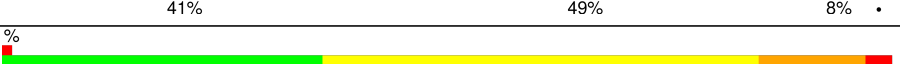



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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	AW	76	
22	CV	76	
22	CW	76	
23	AX	27	
23	CX	27	
24	AY	77	
24	CY	77	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

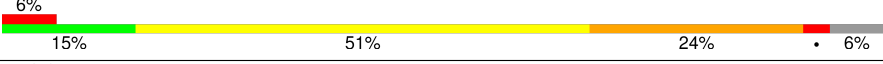
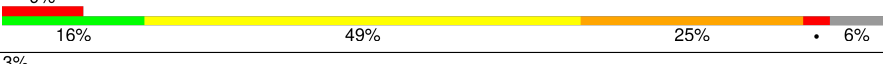
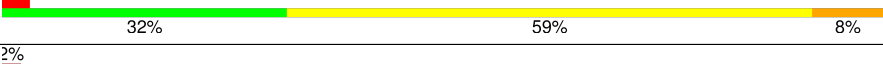
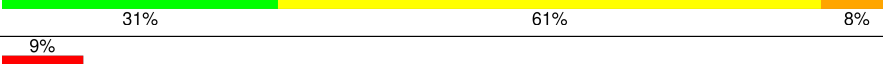
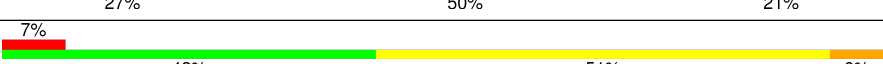
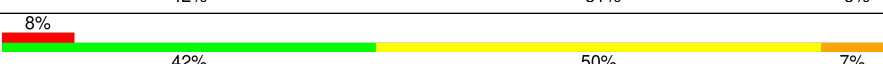
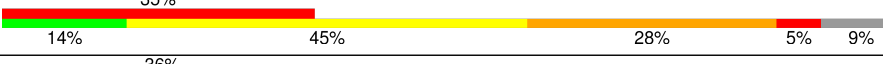
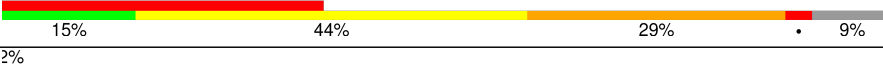
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Mol	Chain	Length	Quality of chain
39	DD	276	
40	BE	206	
40	DE	206	
41	BF	210	
41	DF	210	
42	BG	182	
42	DG	182	
43	BH	180	
43	DH	180	
44	BJ	173	
44	DJ	173	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ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

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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			

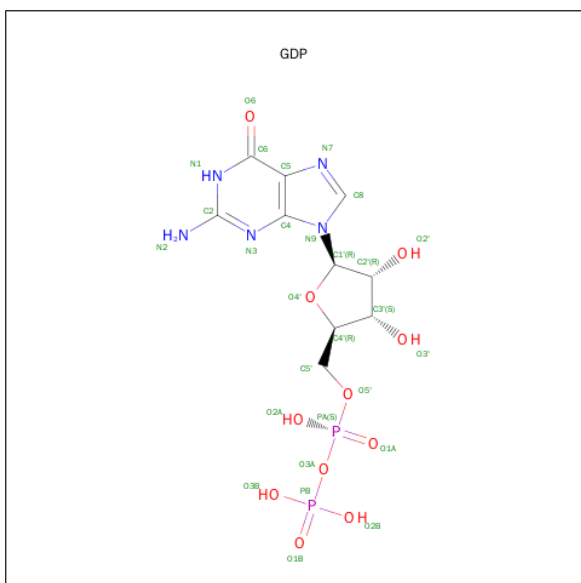
- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

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).

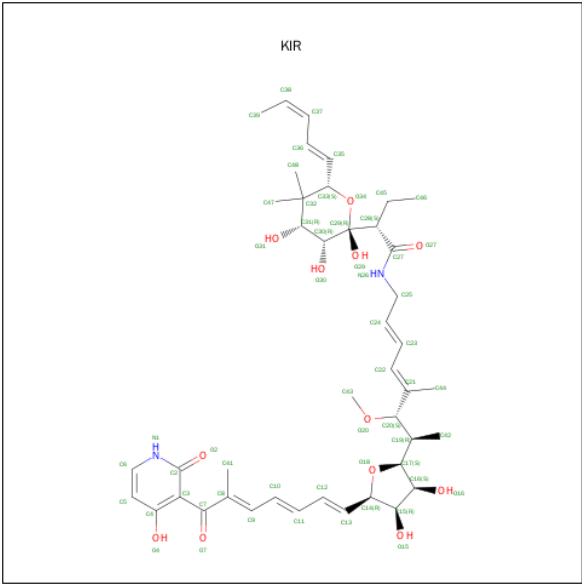
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 61 is KIRROMYCIN (three-letter code: KIR) (formula: C₄₃H₆₀N₂O₁₂).

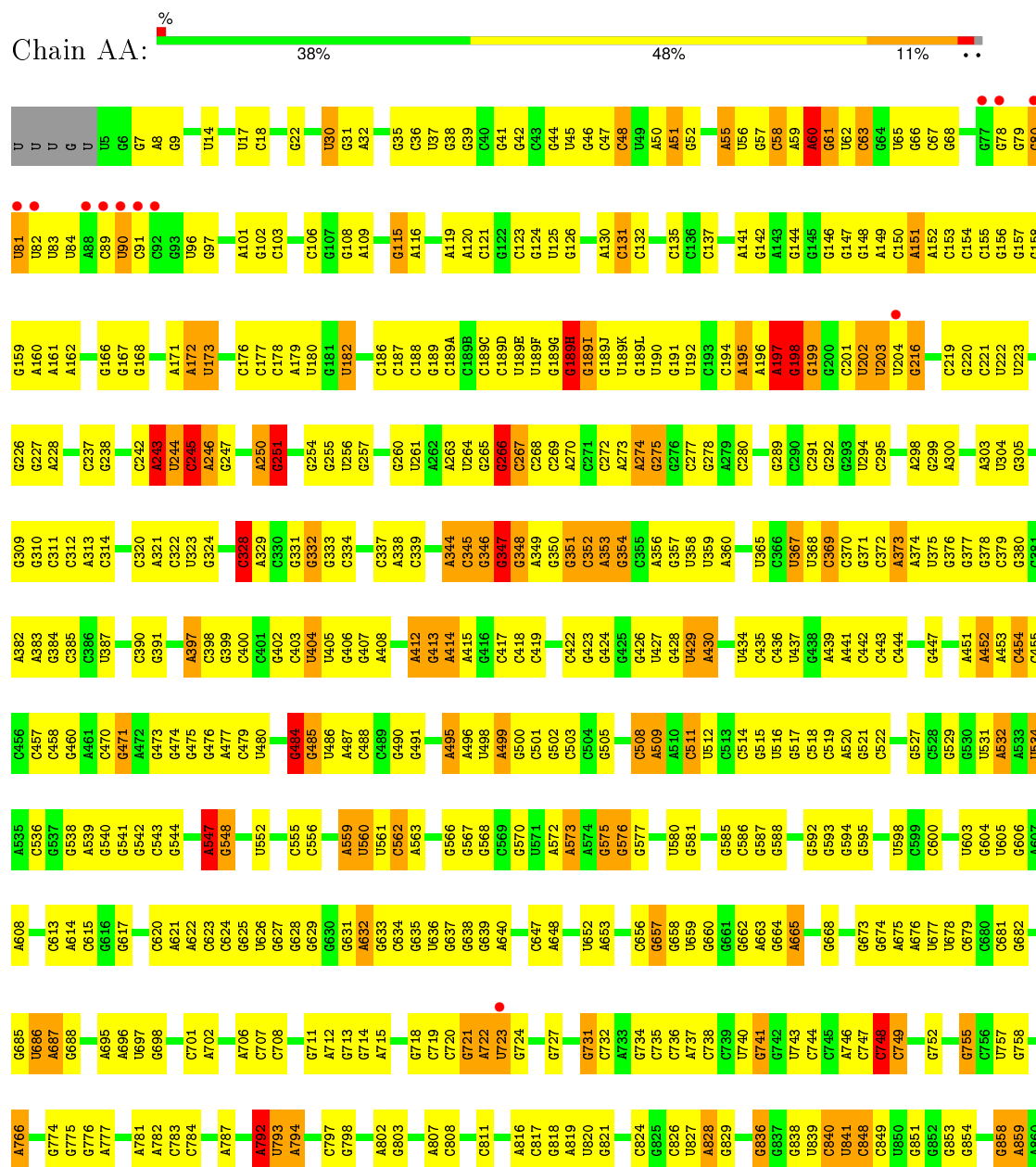


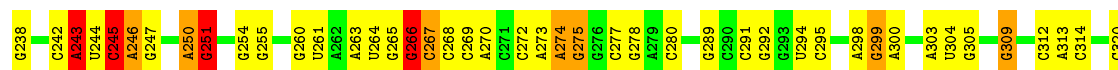
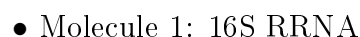
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AZ	1	Total	C	N	O		0	0
			57	43	2	12			
61	CZ	1	Total	C	N	O		0	0
			57	43	2	12			

3 Residue-property plots

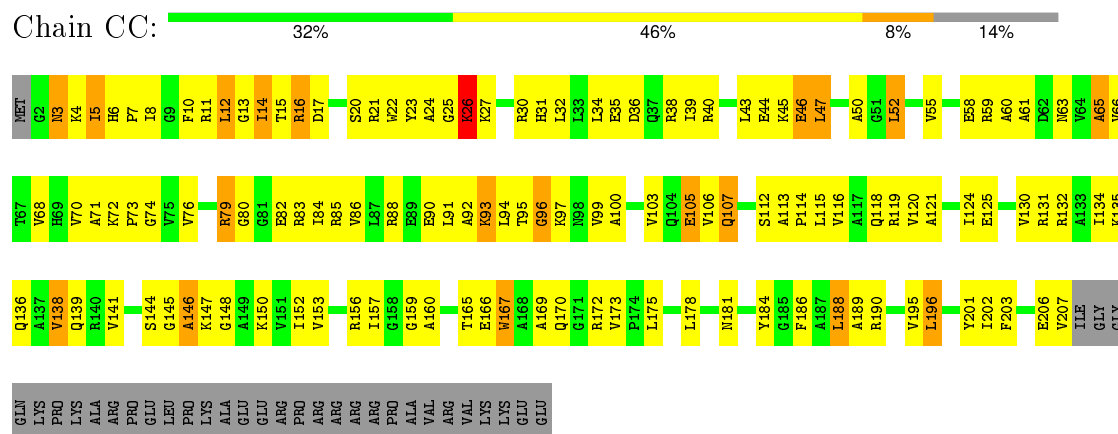
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S rRNA

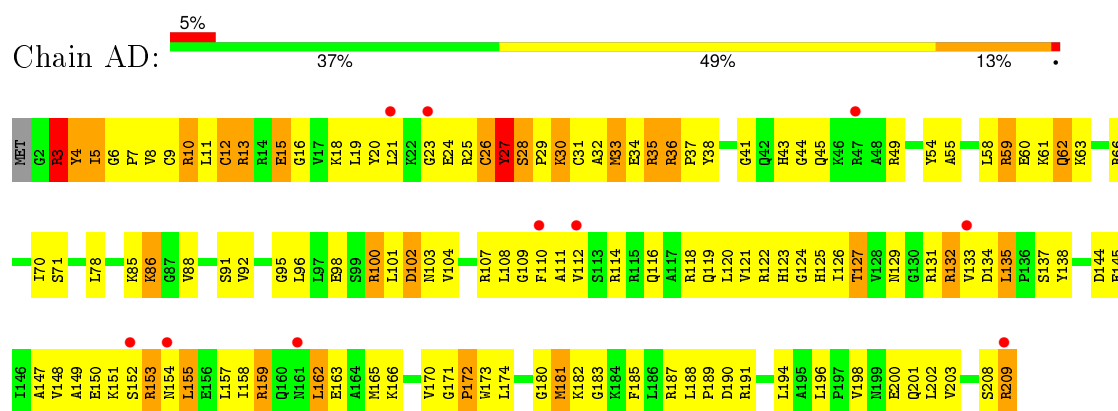




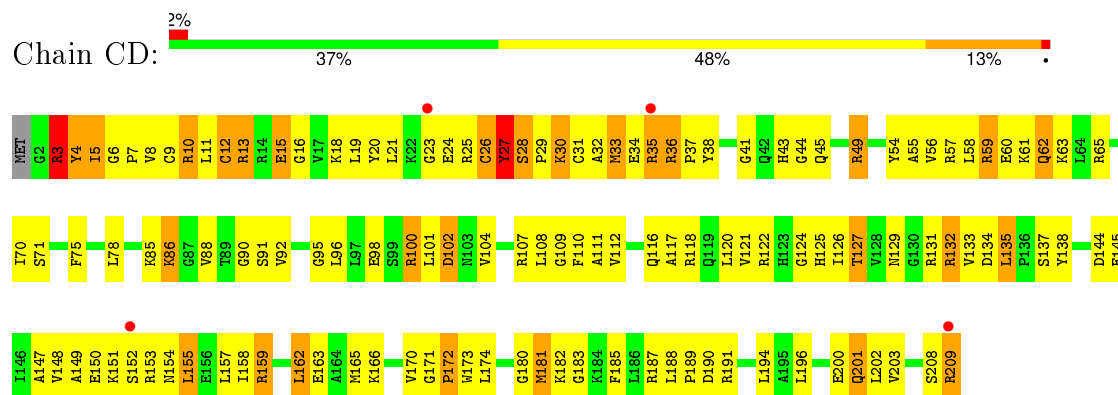




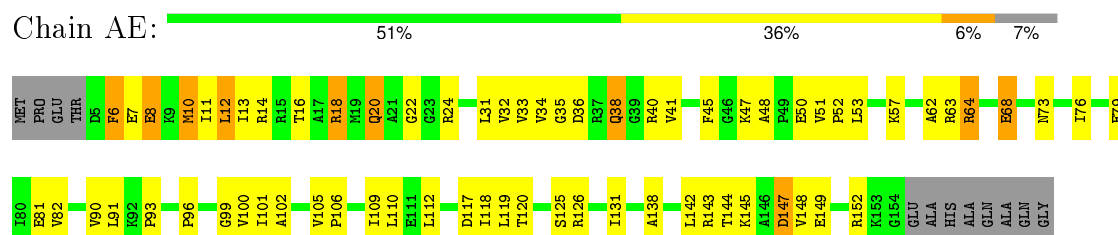
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



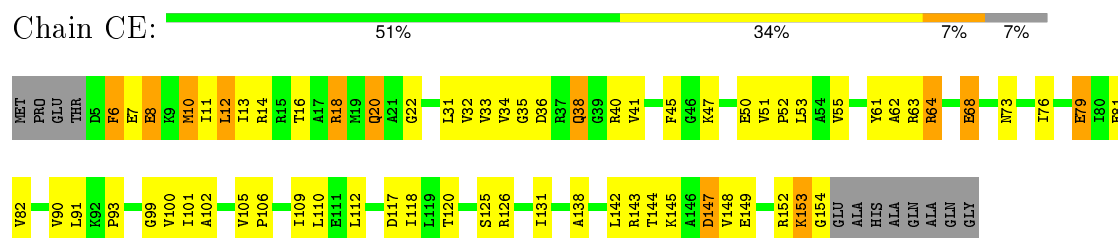
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



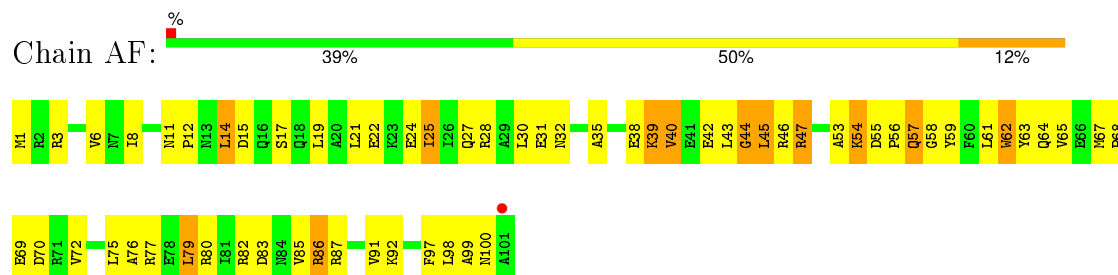
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



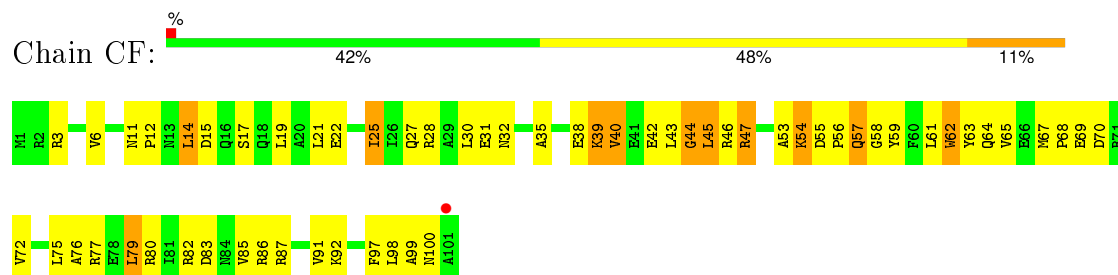
- Molecule 5: 30S RIBOSOMAL PROTEIN S5



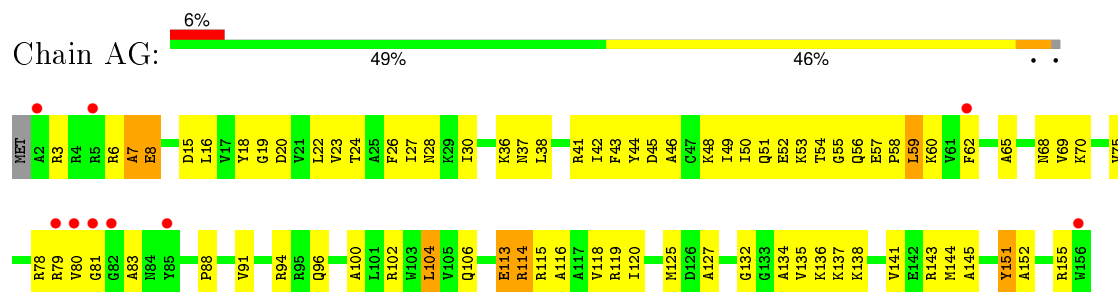
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



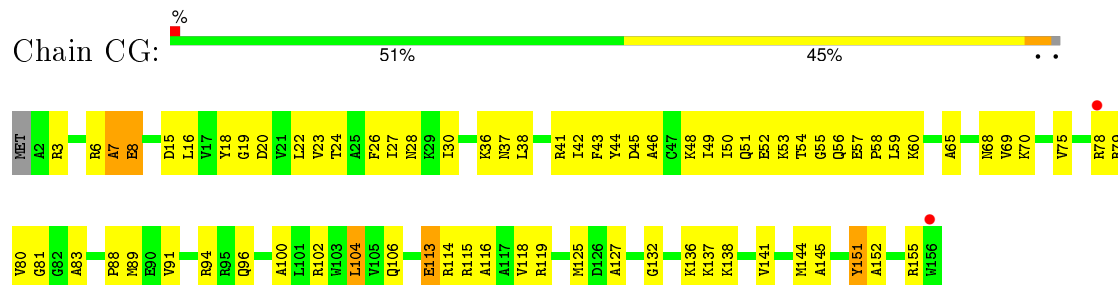
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



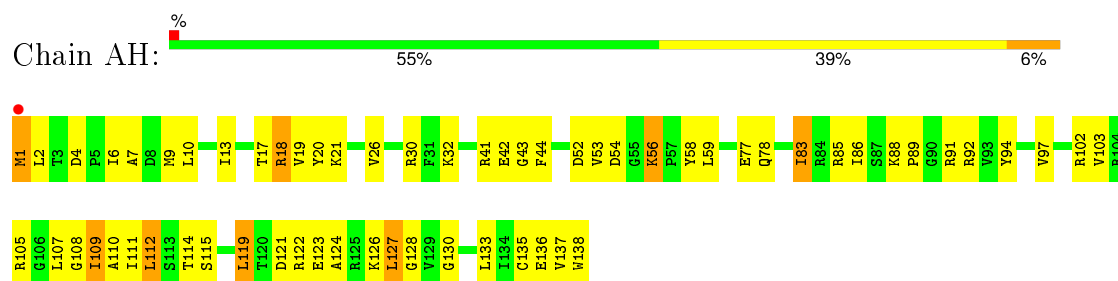
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



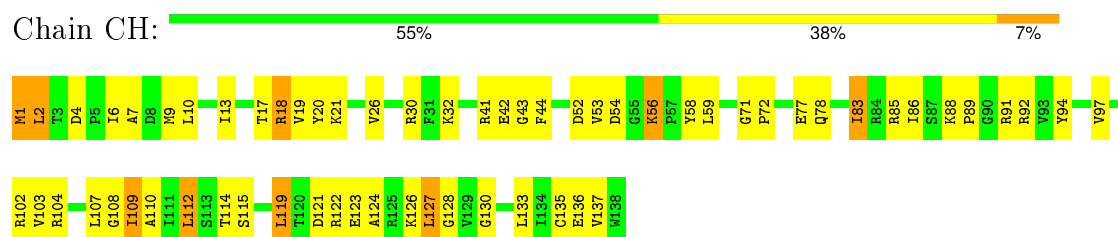
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



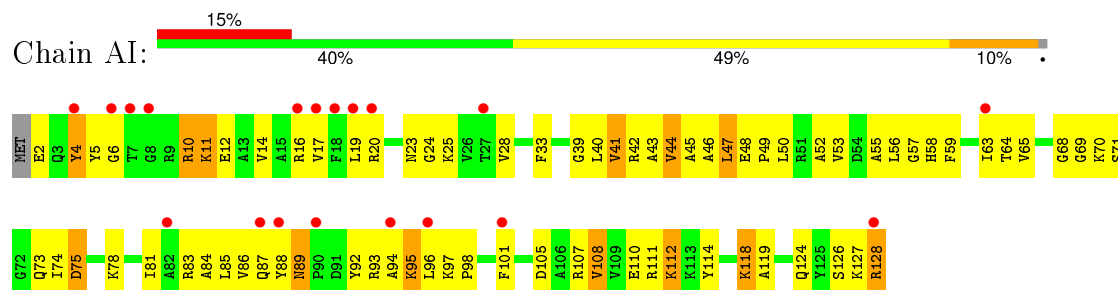
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



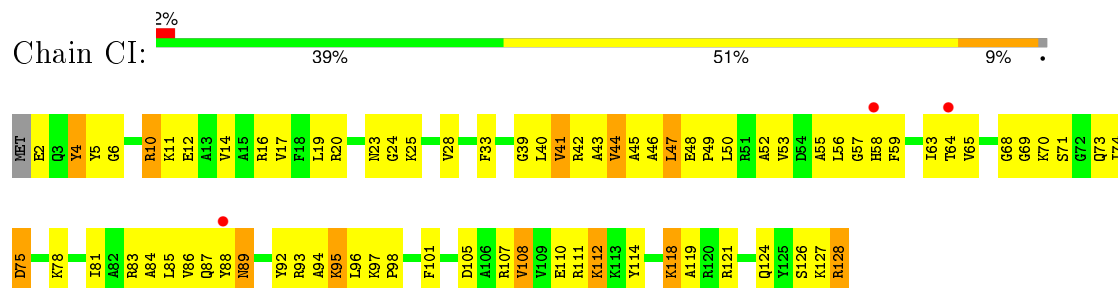
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



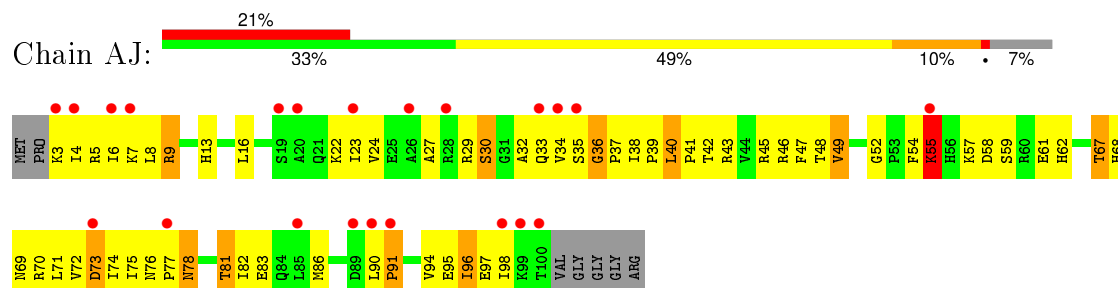
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



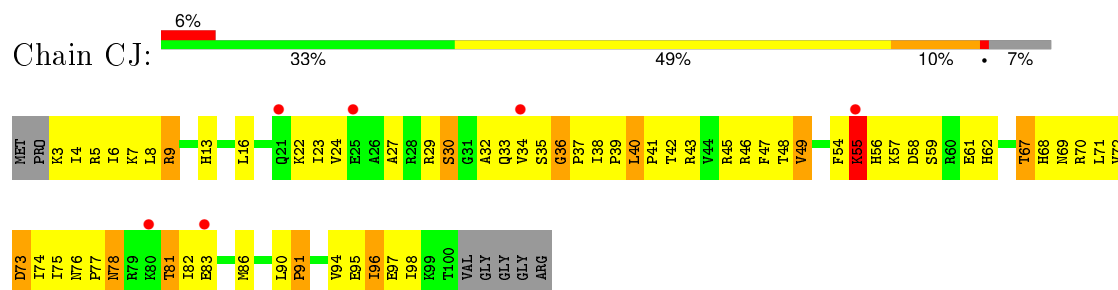
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



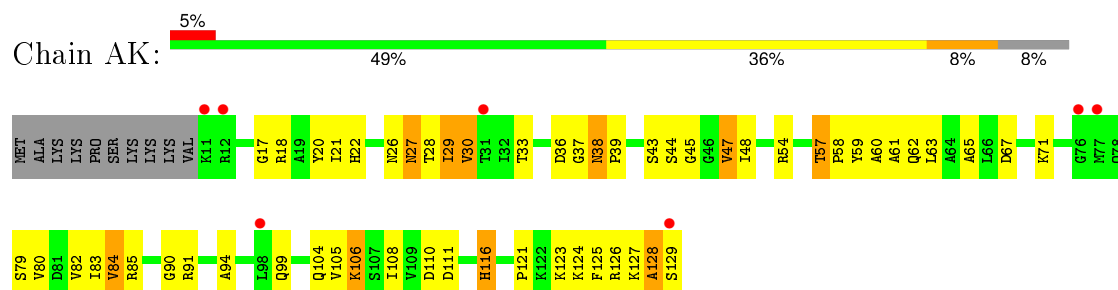
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



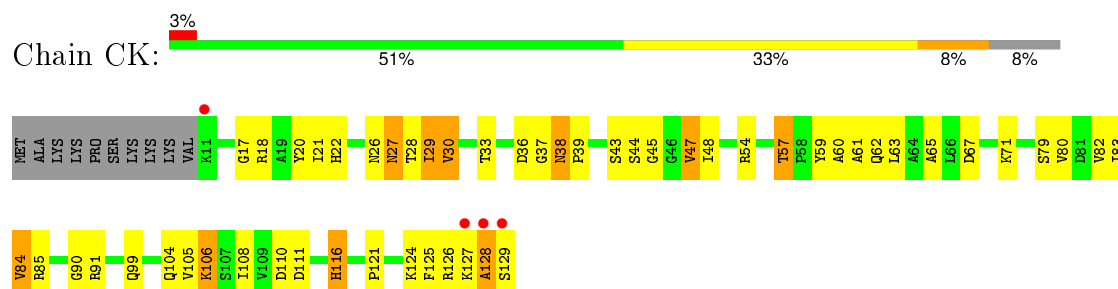
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



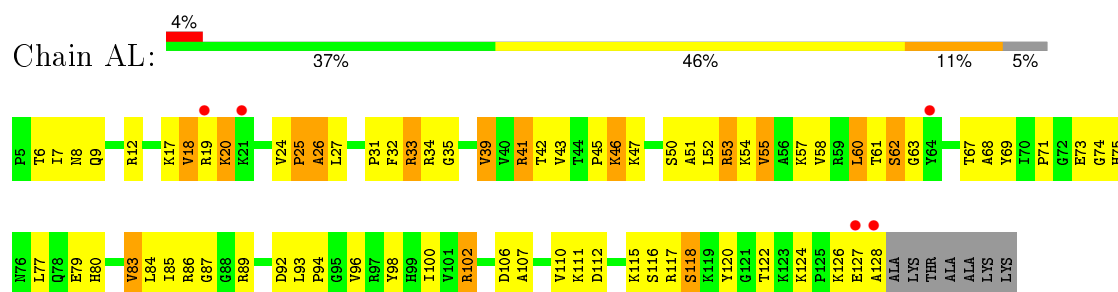
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



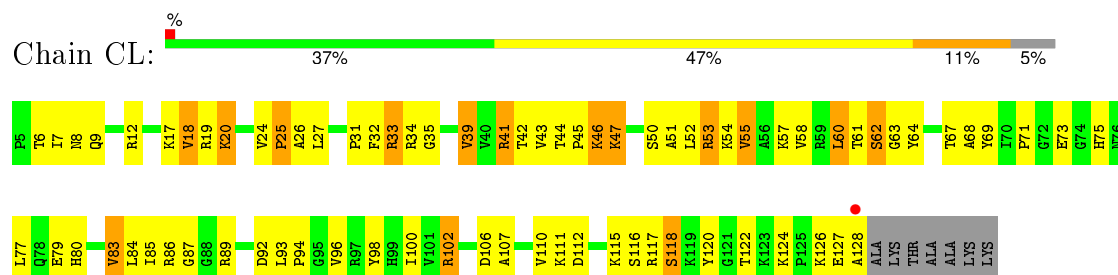
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



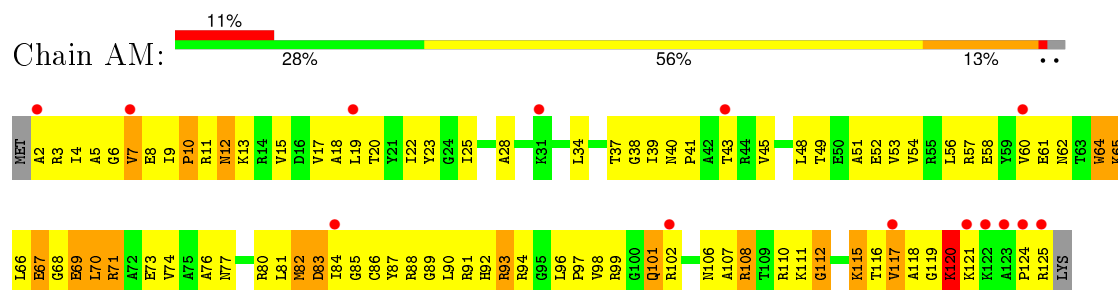
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



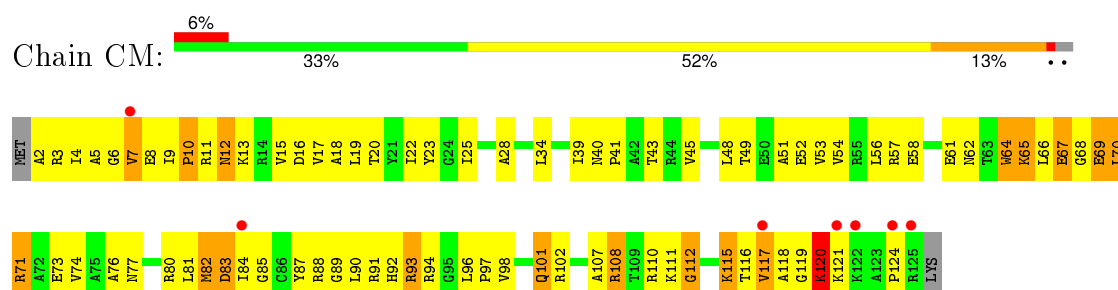
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



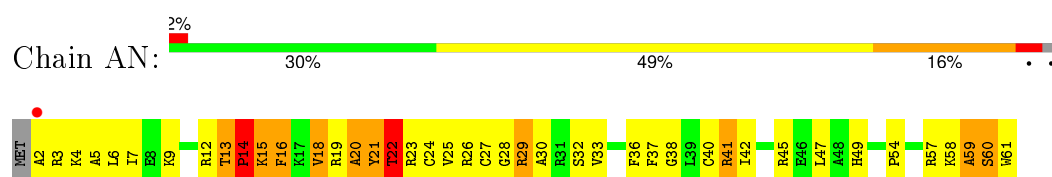
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



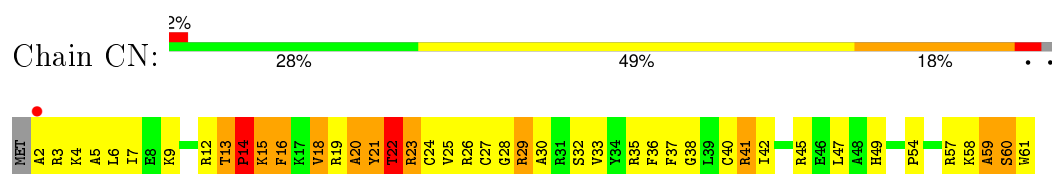
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



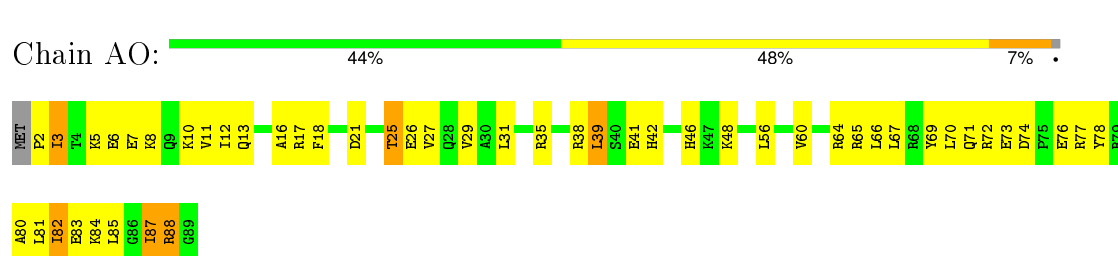
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



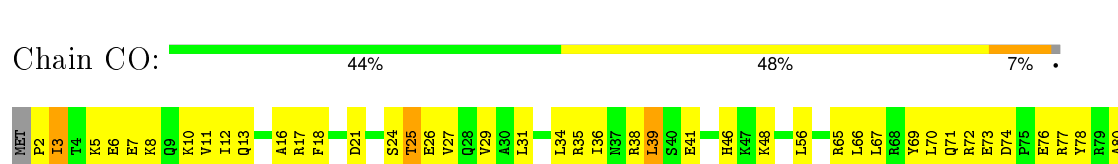
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

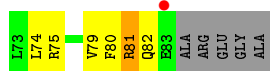
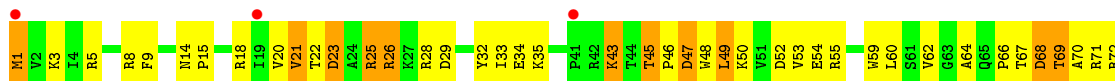
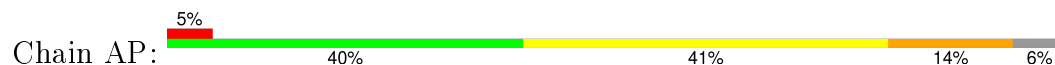


- Molecule 15: 30S RIBOSOMAL PROTEIN S15

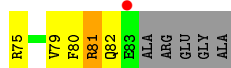
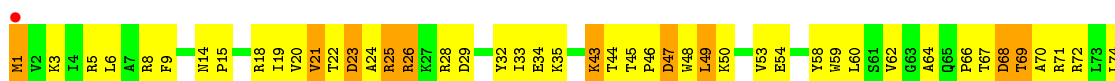




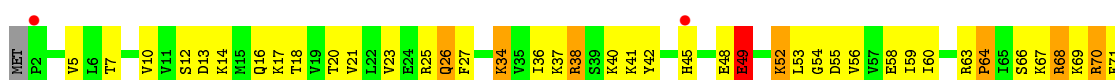
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



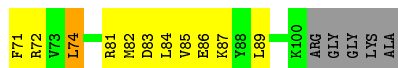
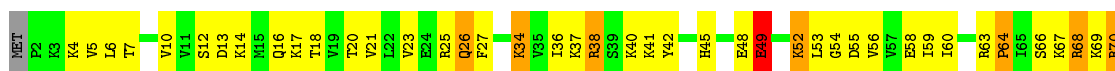
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



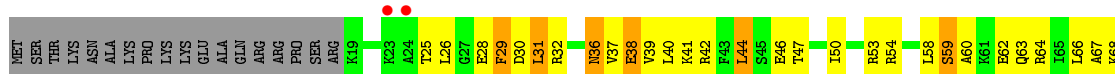
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



• Molecule 17: 30S RIBOSOMAL PROTEIN S17

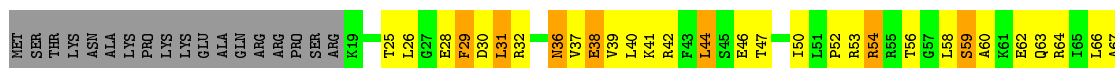


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

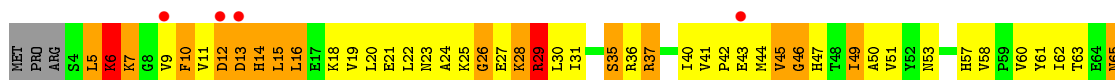
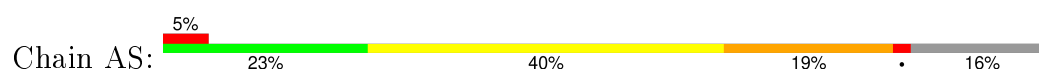




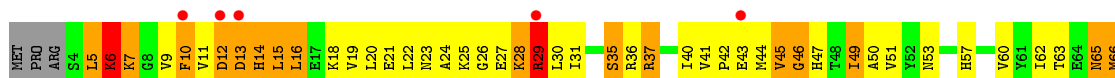
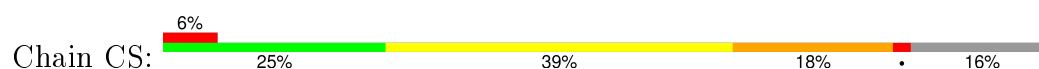
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

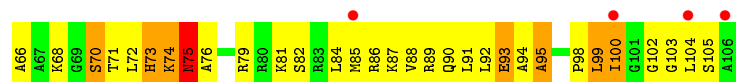


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

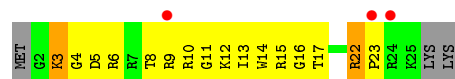


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

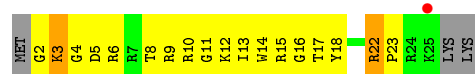




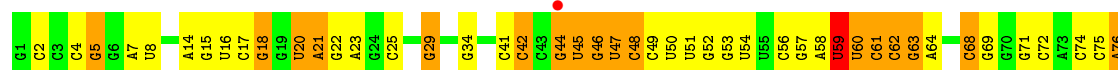
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



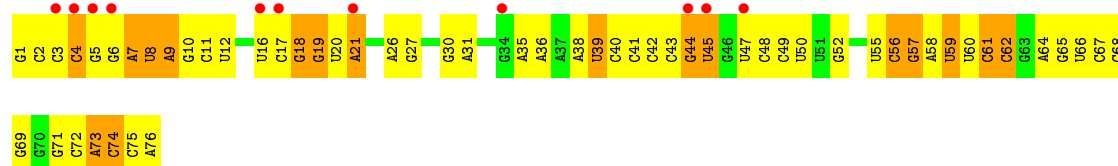
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



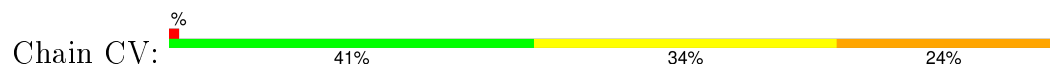
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



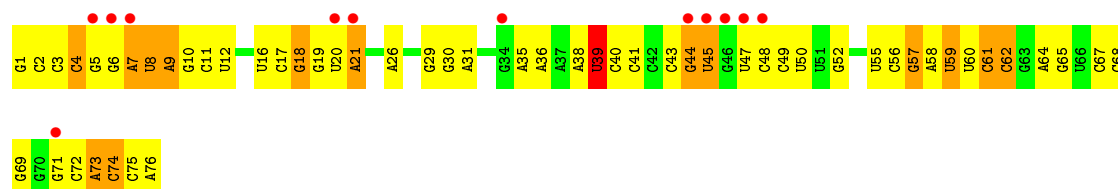
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



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



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



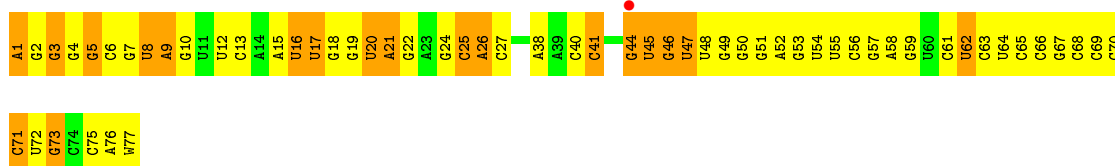
● Molecule 23: MRNA



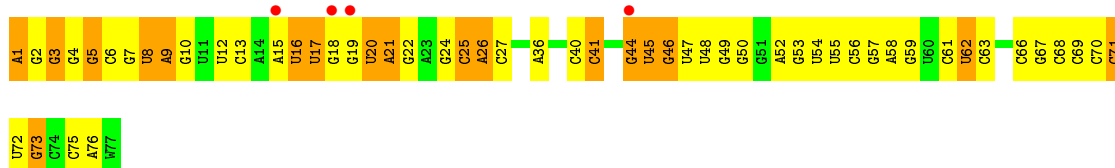
● Molecule 23: MRNA



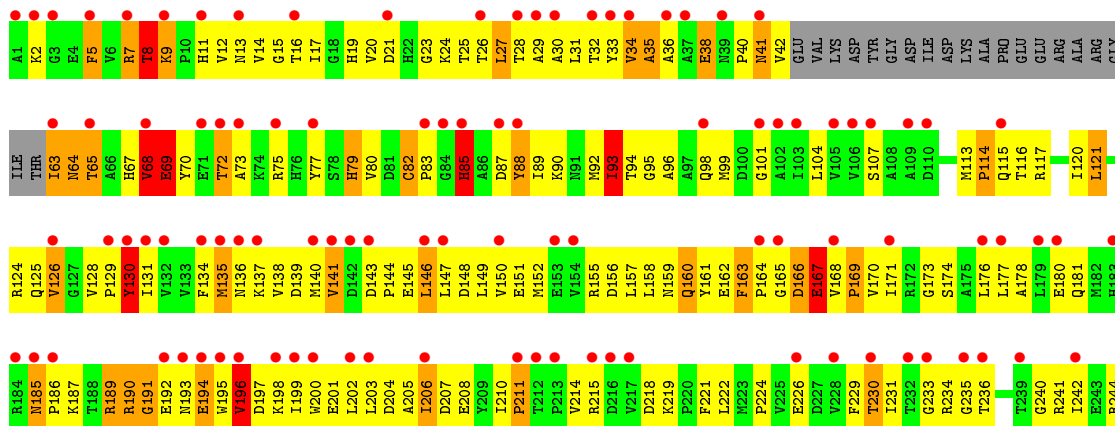
● Molecule 24: A-SITE TRNA TRP-TRNA TRP

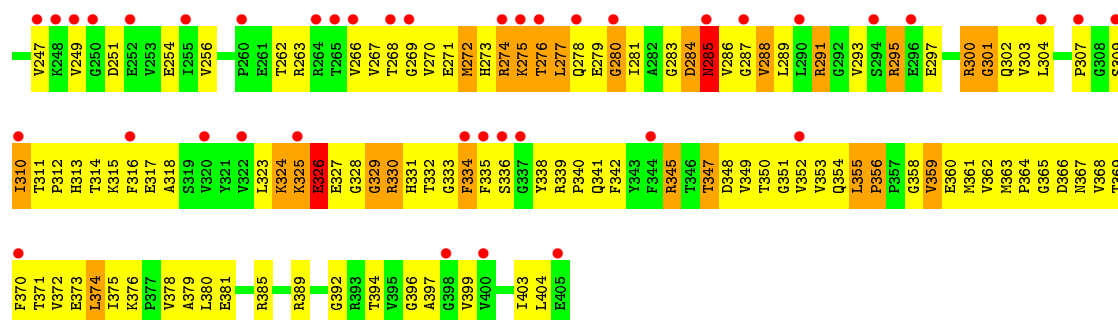


● Molecule 24: A-SITE TRNA TRP-TRNA TRP

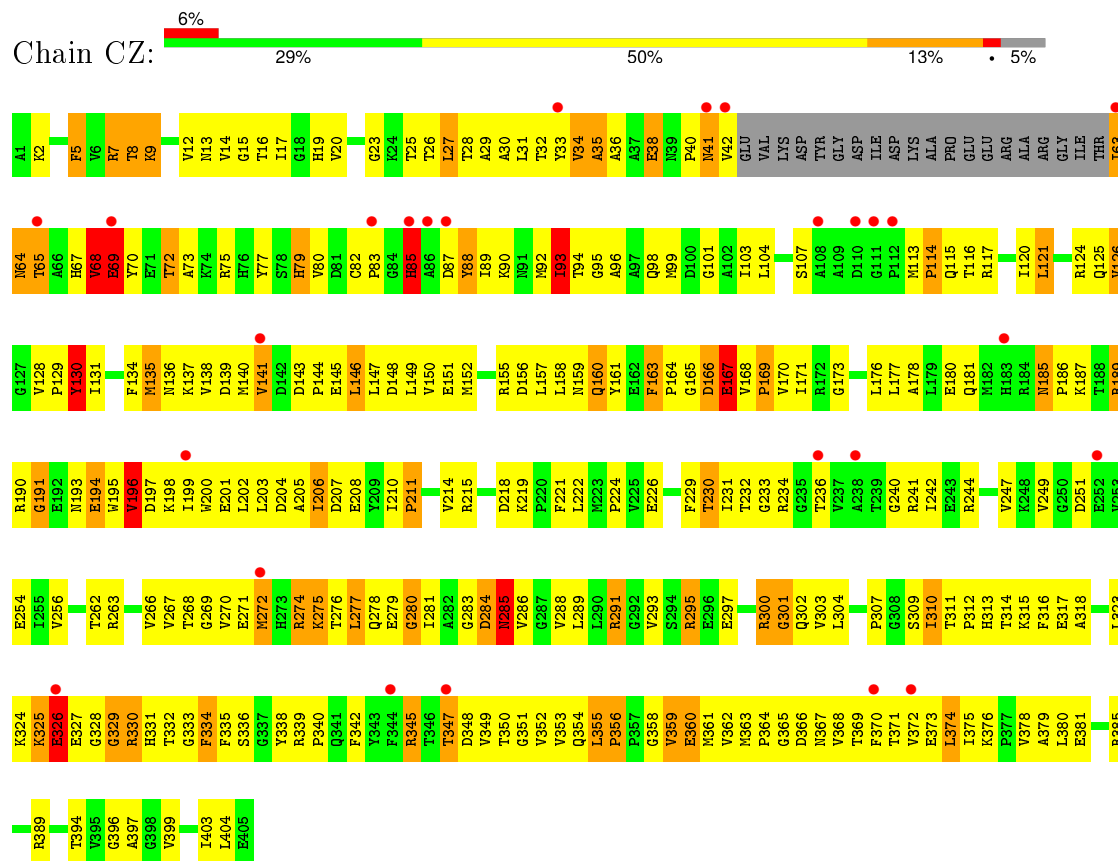


● Molecule 25: ELONGATION FACTOR TU

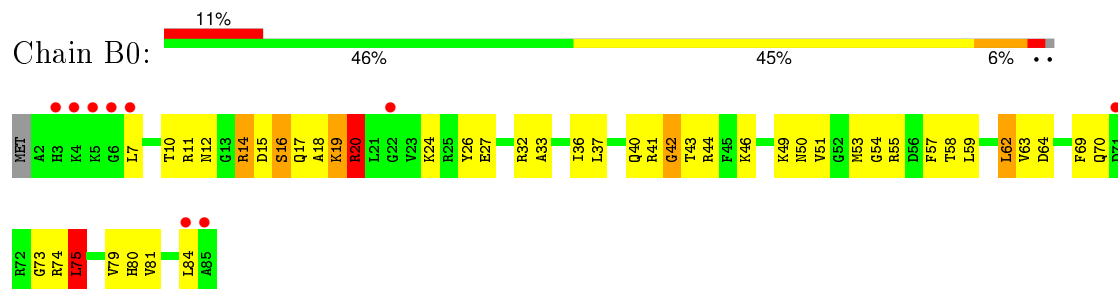




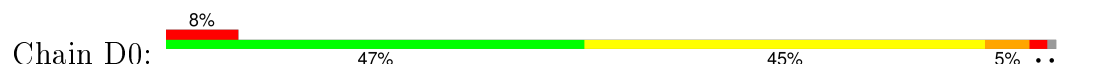
• Molecule 25: ELONGATION FACTOR TU

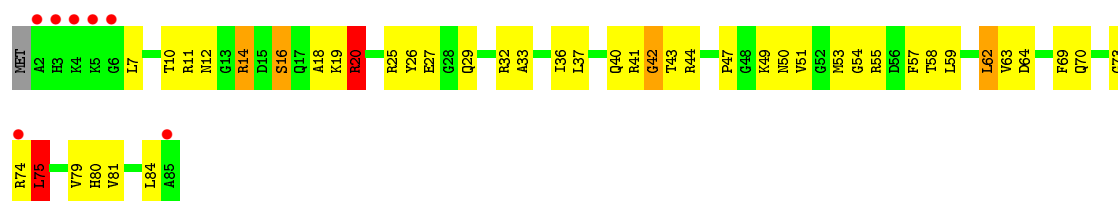


• Molecule 26: 50S RIBOSOMAL PROTEIN L27

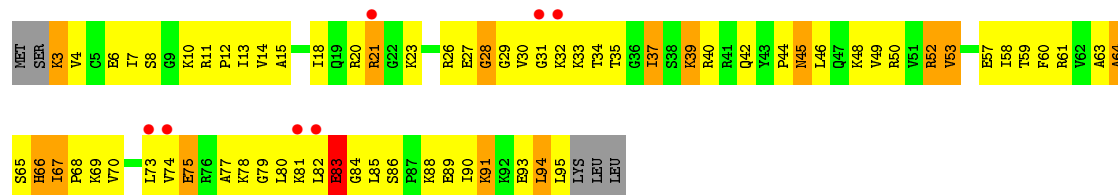


• Molecule 26: 50S RIBOSOMAL PROTEIN L27

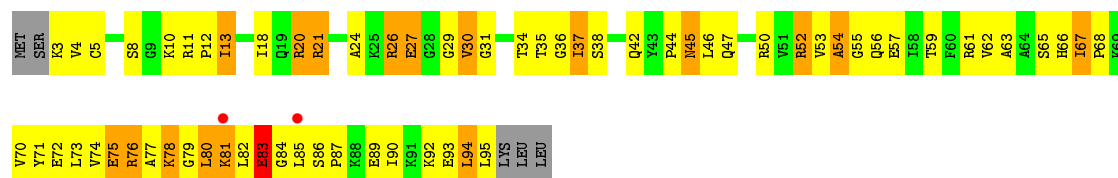




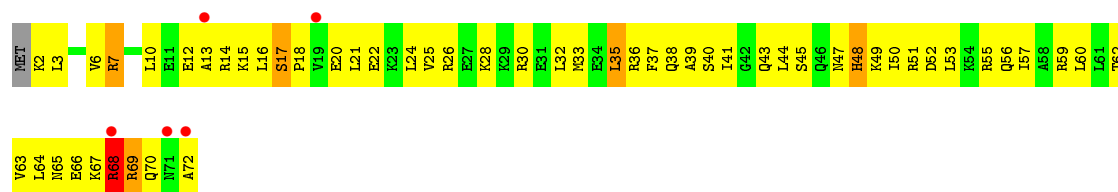
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



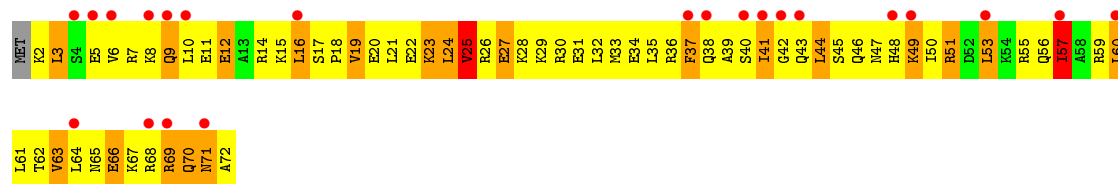
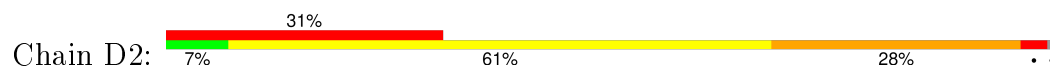
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



• Molecule 28: 50S RIBOSOMAL PROTEIN L29

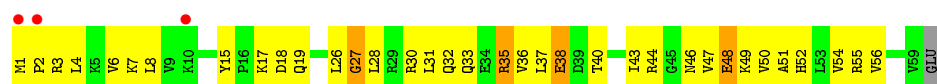


• Molecule 28: 50S RIBOSOMAL PROTEIN L29

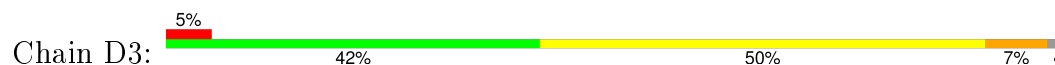


• Molecule 29: 50S RIBOSOMAL PROTEIN L30

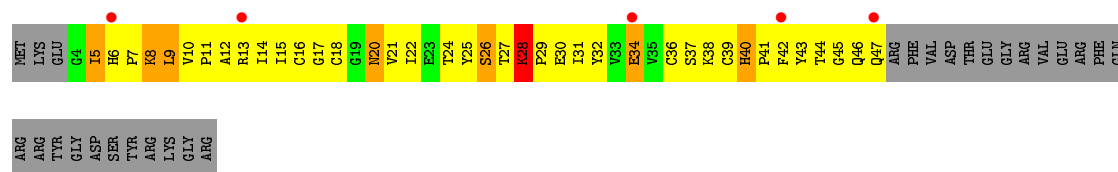
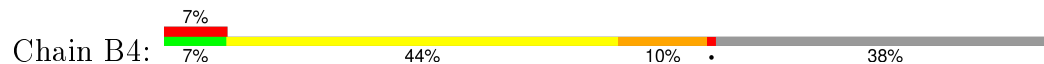




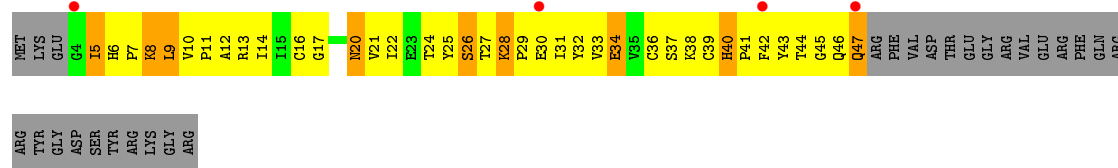
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



• Molecule 30: 50S RIBOSOMAL PROTEIN L31



• Molecule 30: 50S RIBOSOMAL PROTEIN L31



• Molecule 31: 50S RIBOSOMAL PROTEIN L32



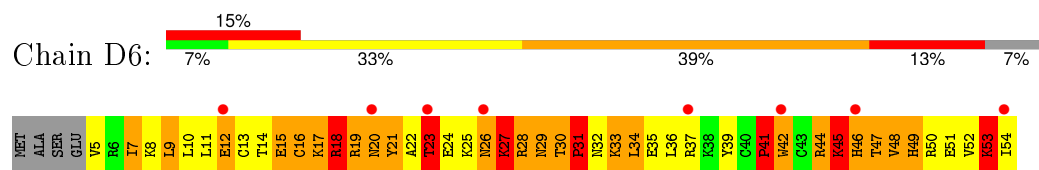
• Molecule 31: 50S RIBOSOMAL PROTEIN L32



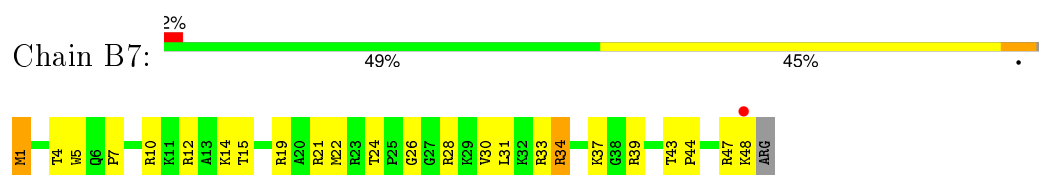
• Molecule 32: 50S RIBOSOMAL PROTEIN L33



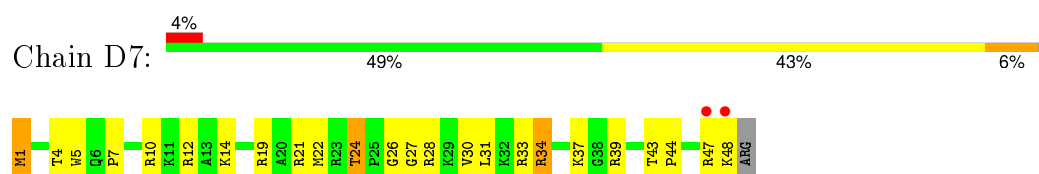
- Molecule 32: 50S RIBOSOMAL PROTEIN L33



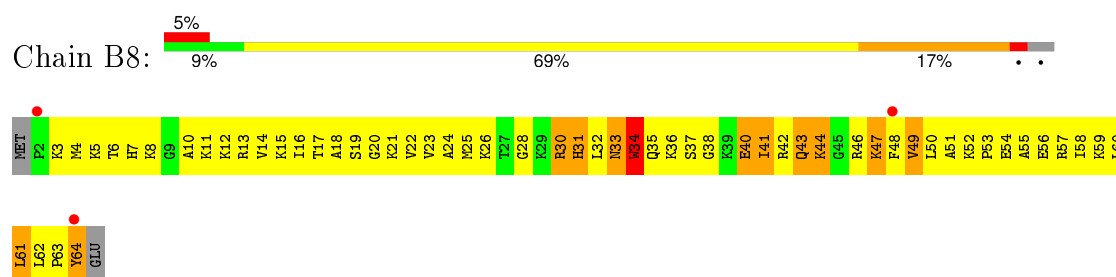
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



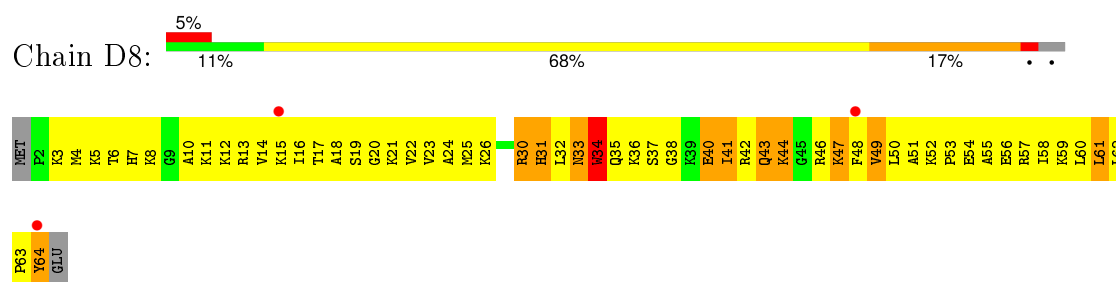
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



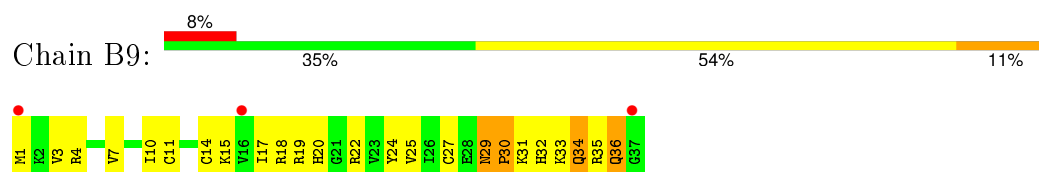
- Molecule 34: 50S RIBOSOMAL PROTEIN L35



- Molecule 34: 50S RIBOSOMAL PROTEIN L35

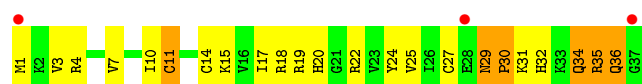


- Molecule 35: 50S RIBOSOMAL PROTEIN L36

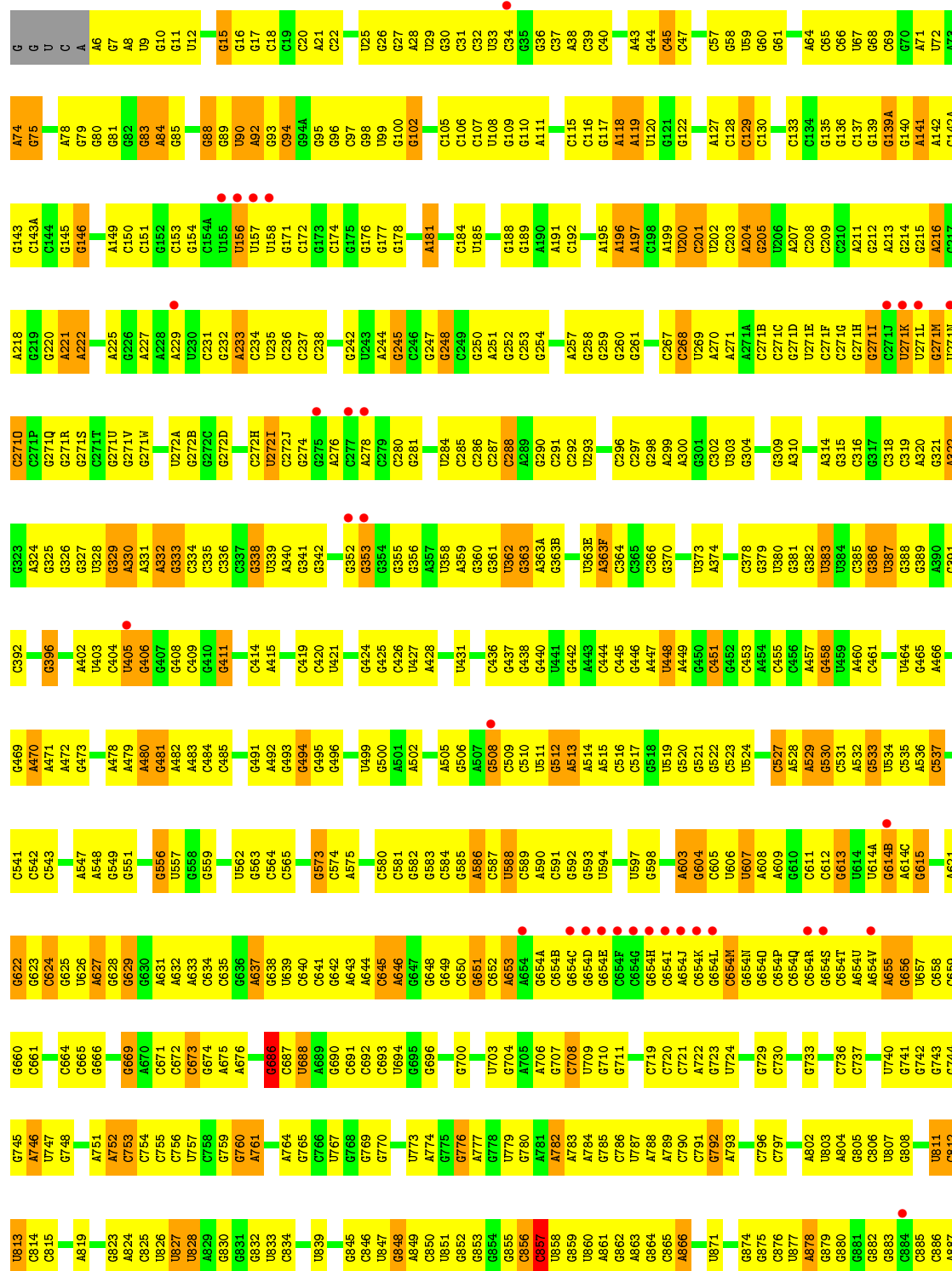


- Molecule 35: 50S RIBOSOMAL PROTEIN L36

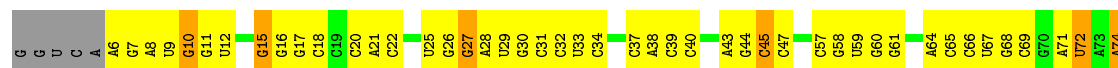


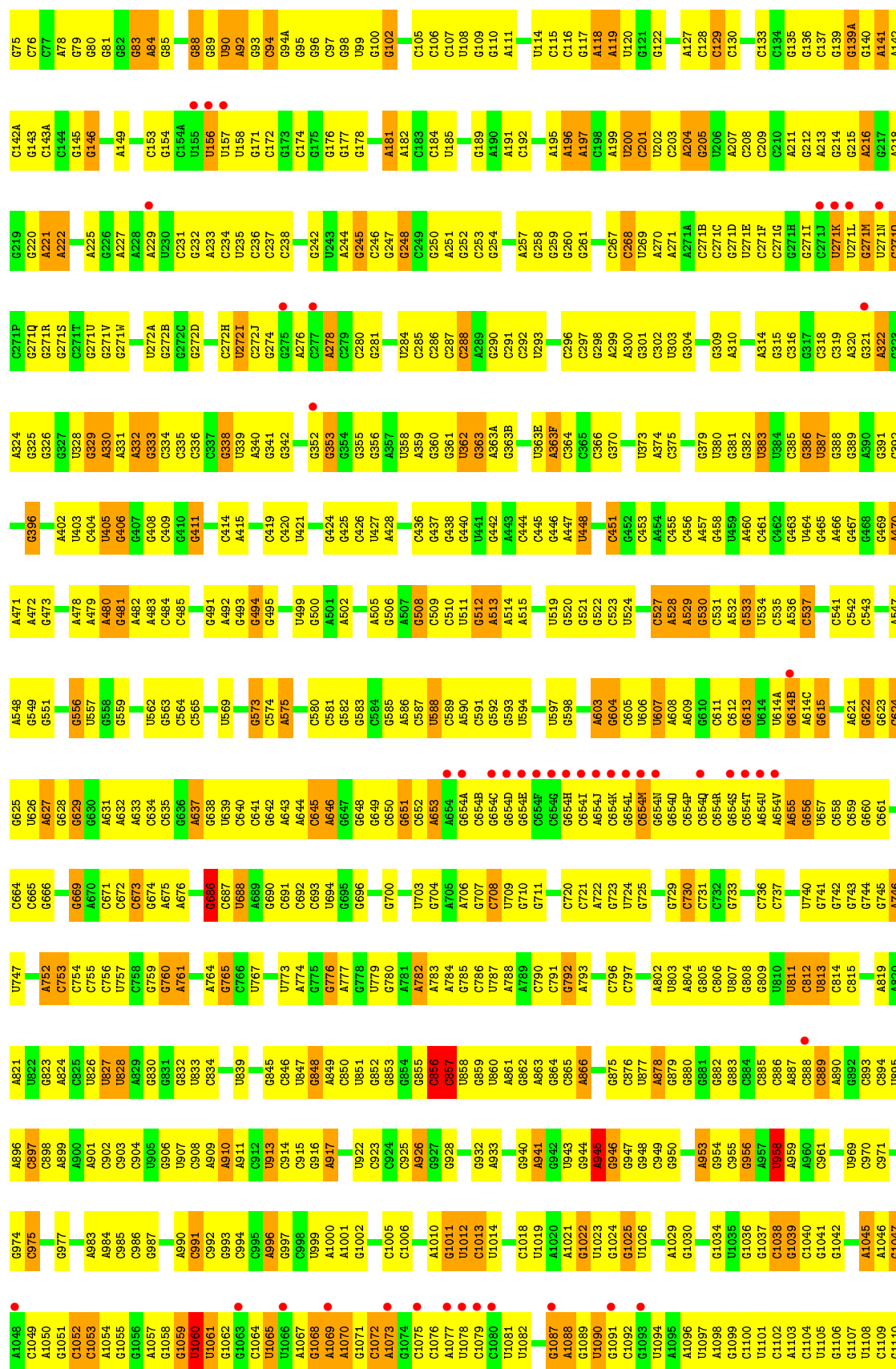


• Molecule 36: 23S RIBOSOMAL RNA

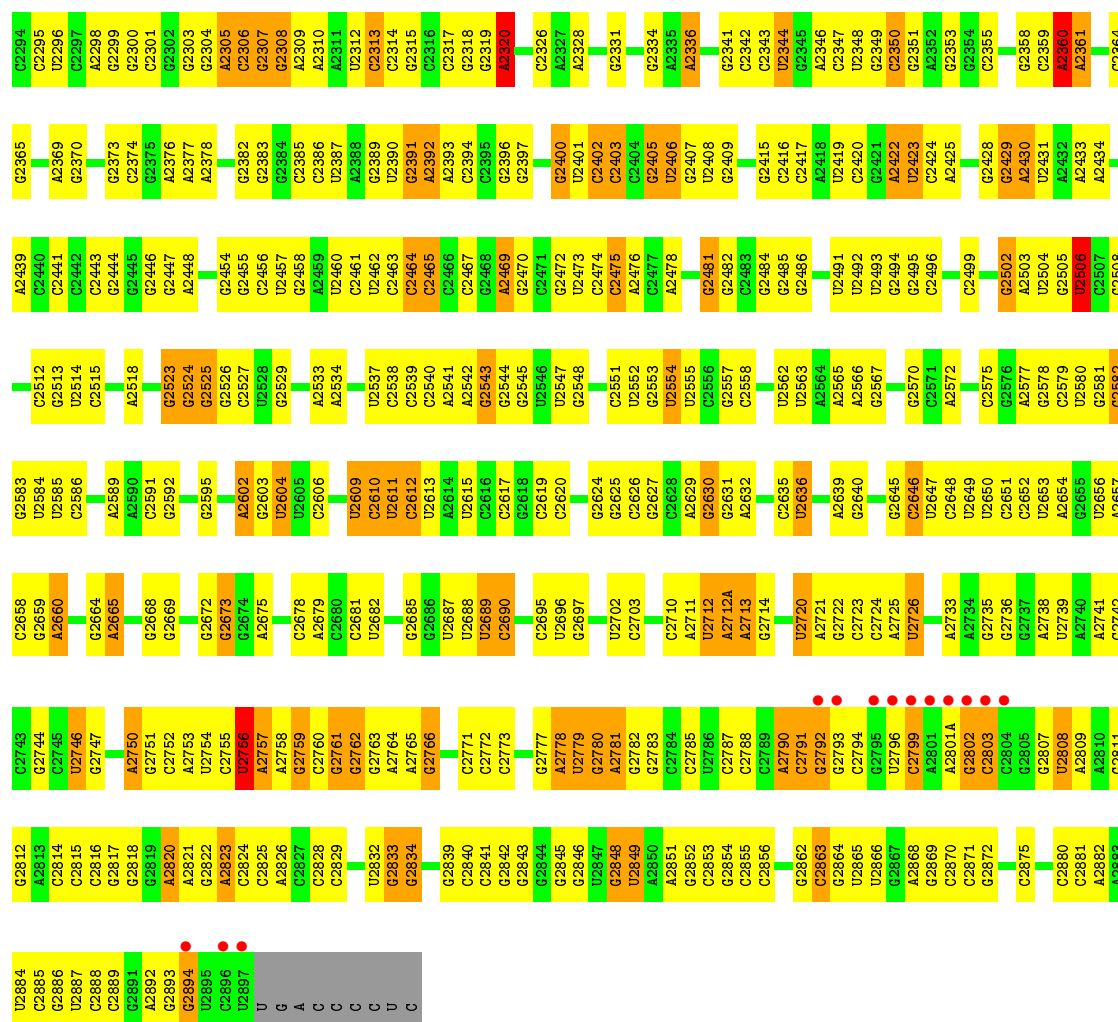


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C1882	G1804	U1720	A1544	G1478	G1337	G1259	C1180	G1106	G1042	U969	C889
G1883	U1805	G1721	C1545	G1479	G1338	G1260	G1186	G1107	C1043	G970	A890
A1884	G1806	A1722	C1546	G1480	G1339	C1261	G1187	U1108	G1044	C971	G892
C1885	G1807	U1739	C1547	U1481	U1340	G1264	U1188	G1109	A1045	G972	C893
C1886	G1838	G1740	C1548	G1482	U1341	A1265	U1189	G1110	A1046	G973	C894
A1887	U1839	A1741	C1549	G1484	G1344	G1268	A1417	G1111	G1047	A973	U895
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C1744	G1642	A1841	A1554	U1420	A1349	G1192	G1193	G1114	G1050	C976	A898
C1745	G1643	C1745	A1554	G1424	G1348	G1193	G1193	G1115	G1051	A989	A899
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				G1491	U1352	A1272	U1199		A1052	A984	A901
				G1492	A1352	U1273	C1200		C1053	C985	A902
				G1493	A1353	A1274	G1203		A1054	C986	C902
				A1495	G1355	G1279	U1205		G1055	G987	C903
				A1496	G1356	G1286			G1056	A990	U905
				A1497	U1357	A1287	C1208		A1057	A991	G906
				U1498	G1358	U1288	G1209		G1058	C992	U907
				C1499	A1359	C1289	U1210		G1059	G993	C908
				G1500	G1360	U1288	G1211		U1060	C994	C909
				C1501	G1361	C1289	U1211		G1061	C995	A910
				U1502	G1362	C1290	G1212		G1062	A996	A911
				U1503	C1363	C1291	G1213		G1064	G997	G912
				C1504	G1364	U1292	A1214		G1065	C998	U913
				G1505	A1365	U1292	G1215		U1066	U999	C914
				C1506	A1366	U1293	G1215		A1067	A1000	C915
				A1507	A1367	U1294	C1221		G1068	A1001	G916
				C1507	G1440	U1294	C1222		A1069	G1002	A917
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				U1512	G1448	A1378	G1232		C1076	U1012	
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				G1524	G1459	G1388	G1238		G1087	U1019	A941
				G1525	A1460	G1389	G1239		A1088	A1020	G942
				U1526	G1461	U1390	U1240		G1089	G1022	U943
				G1527		A1393	A1241		U1090	U1023	A945
				A1528	C1464	U1396	G1242		G1091	G1024	G946
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					C1468	G1401	A1246		A1095	A1029	G950
					A1469	C1402	A1247		A1096	G1030	
					A1470	G1403	G1248		U1097		A953
					A1471	C1404	G1251		A1098	G1034	G954
					A1472	U1405	G1252		G1099	U1035	C955
					G1473	U1406	A1253		C1100	G1036	G956
					G1474	U1407	A1253		U1101	G1037	A957
					G1475	C1407	G1256		C1102	G1038	U958
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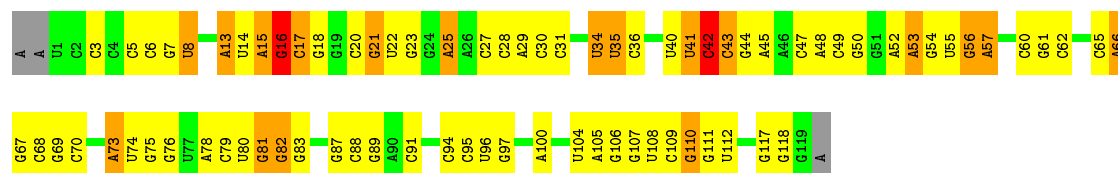






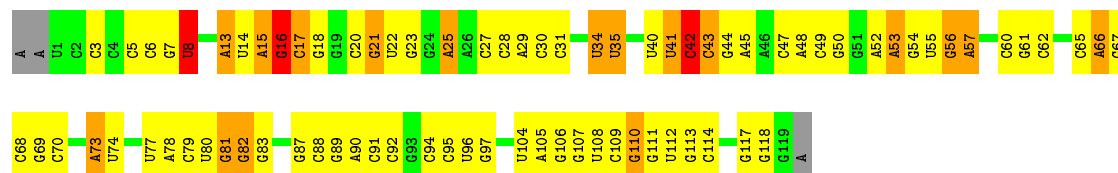
• Molecule 37: 5S RIBOSOMAL RNA

Chain BB: 33% 48% 15%



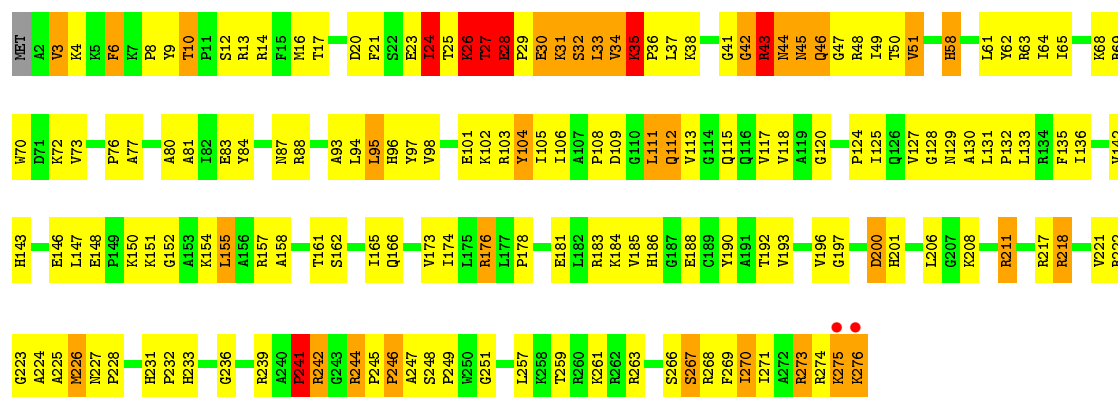
• Molecule 37: 5S RIBOSOMAL RNA

Chain DB: 32% 49% 14%

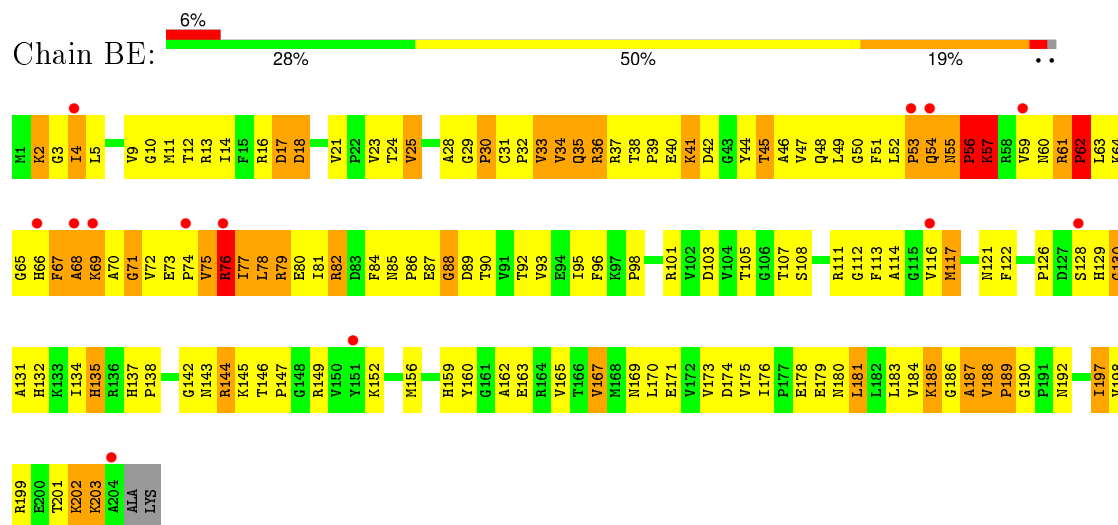


• Molecule 38: 50S RIBOSOMAL PROTEIN L1

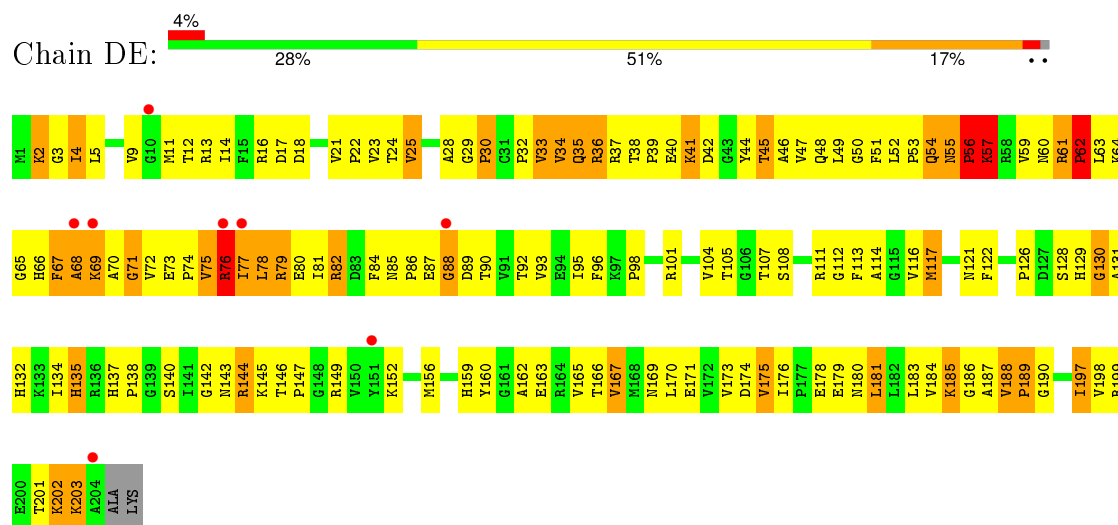




• Molecule 40: 50S RIBOSOMAL PROTEIN L3

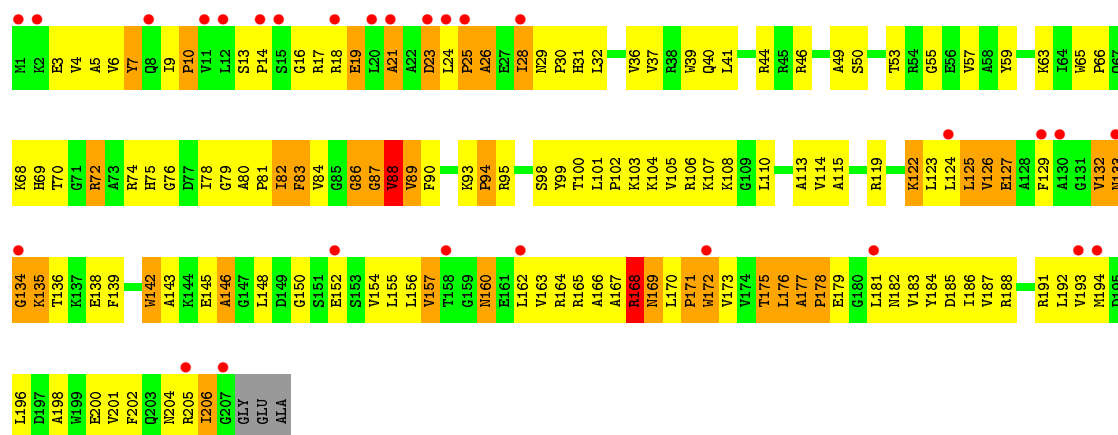


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

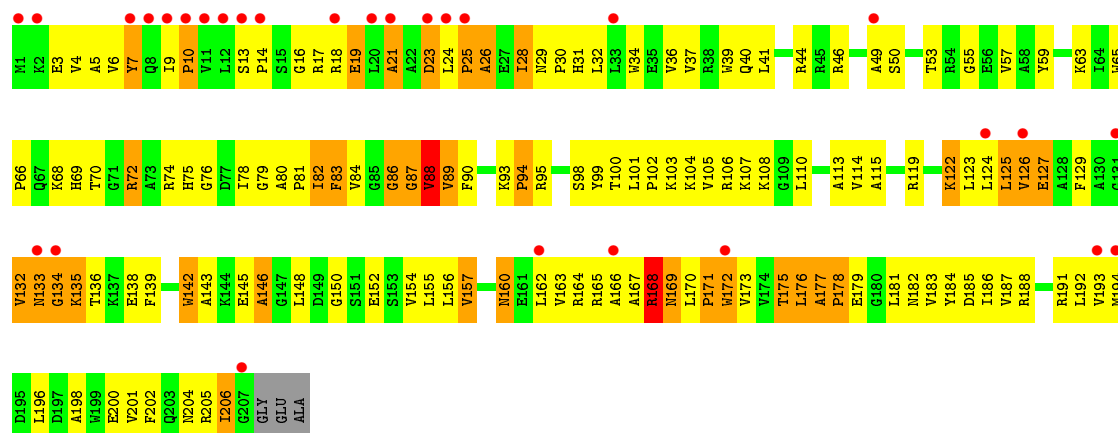


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

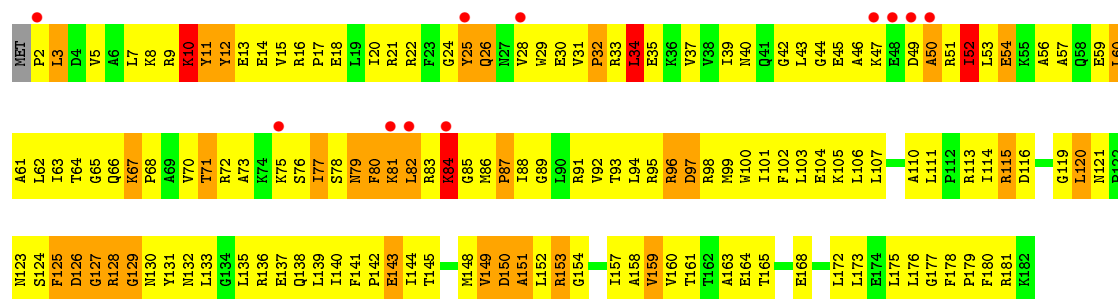




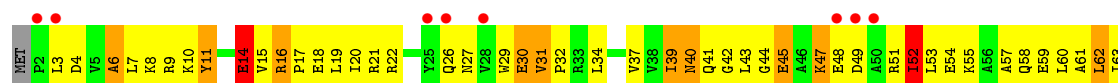
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

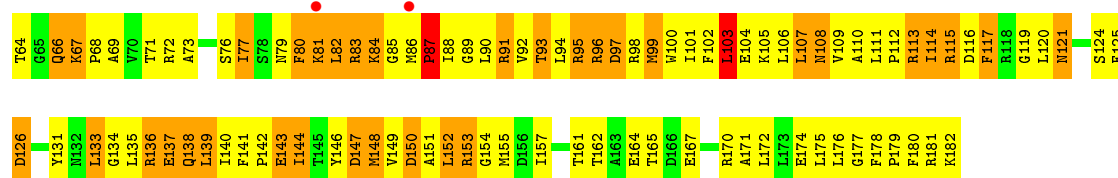


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

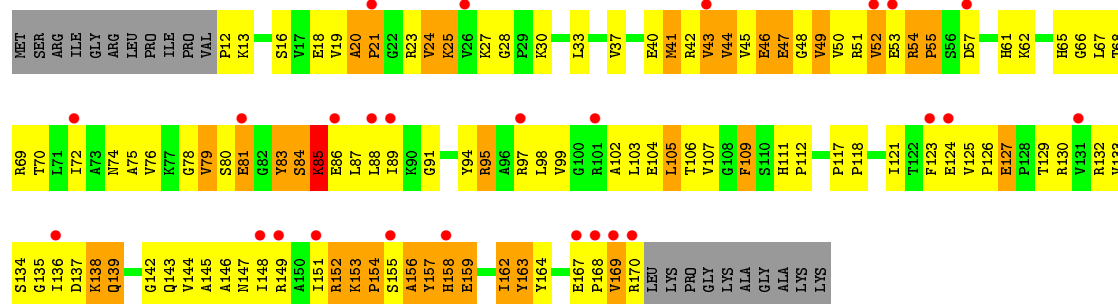


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

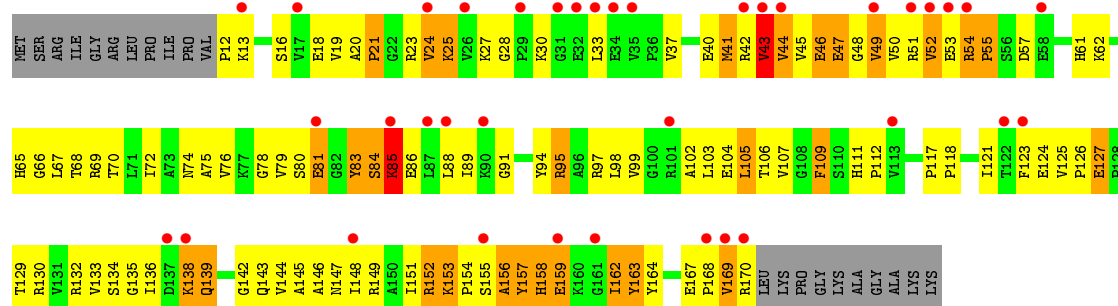




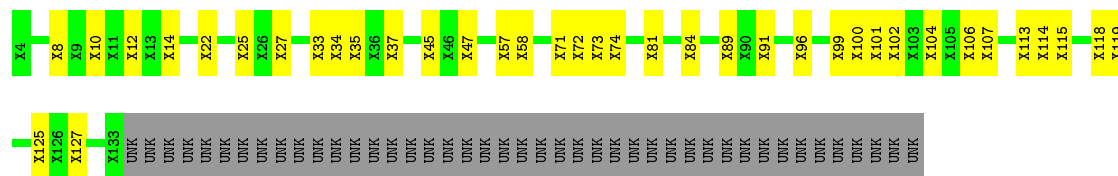
• Molecule 43: 50S RIBOSOMAL PROTEIN L6



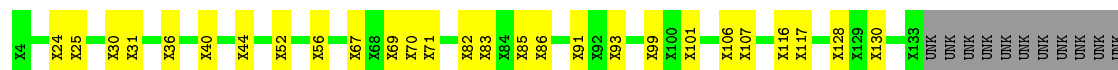
• Molecule 43: 50S RIBOSOMAL PROTEIN L6



• Molecule 44: 50S RIBOSOMAL PROTEIN L10



• Molecule 44: 50S RIBOSOMAL PROTEIN L10





• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK: 83% 12% 5%



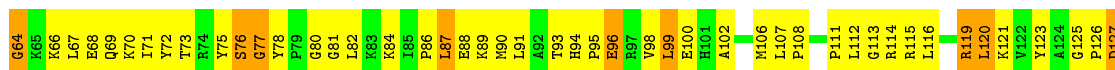
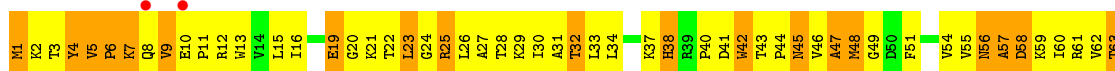
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain DK: 83% 12% 5%



• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN: 20% 56% 23%



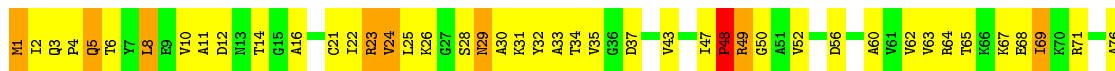
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN: 19% 58% 21%



• Molecule 47: 50S RIBOSOMAL PROTEIN L14

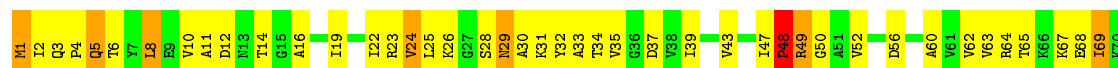
Chain BO: 42% 50% 7%





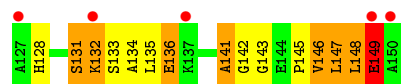
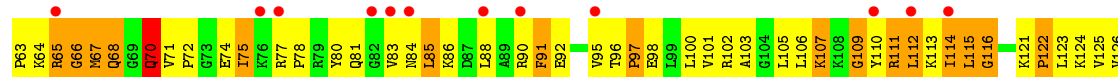
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO: 41% 52% 7% •



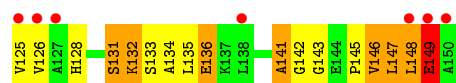
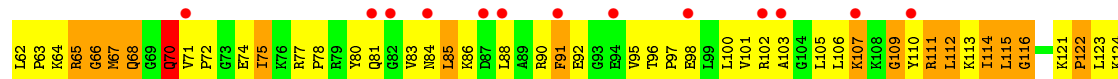
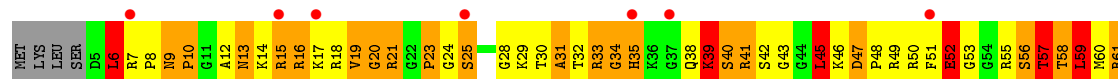
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP: 17% 23% 40% 29% 5% •



• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP: 18% 23% 41% 28% 5% •

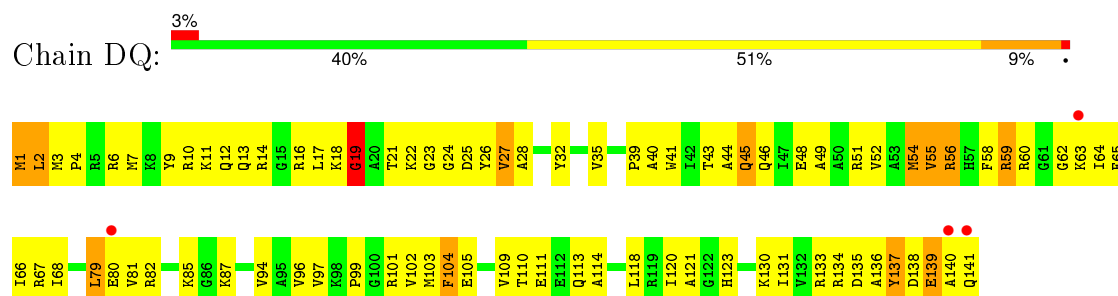


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

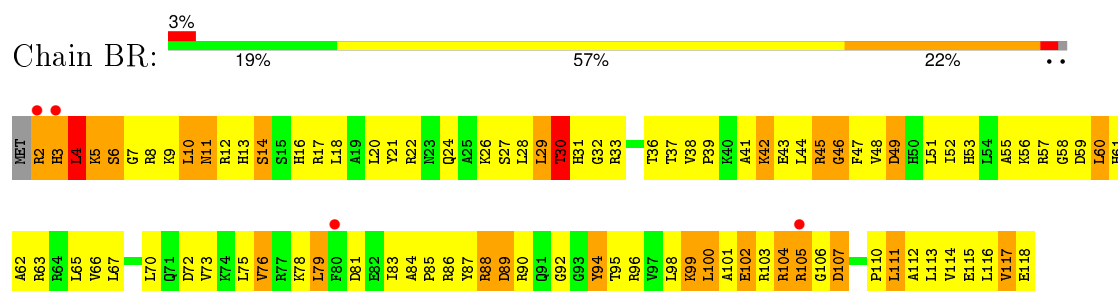
Chain BQ: 43% 48% 9% •



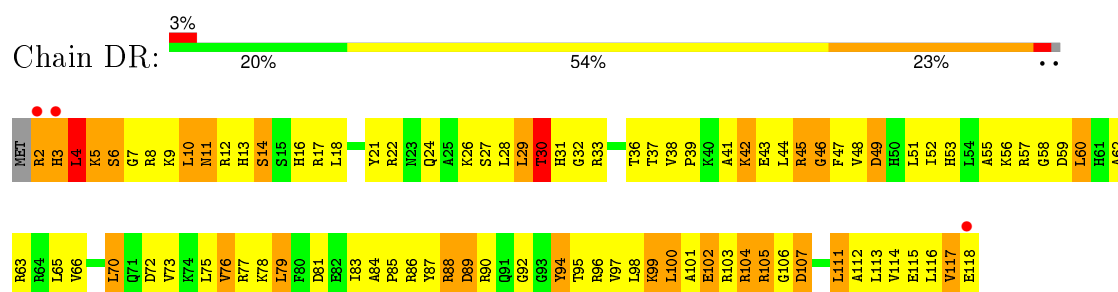
- Molecule 49: 50S RIBOSOMAL PROTEIN L16



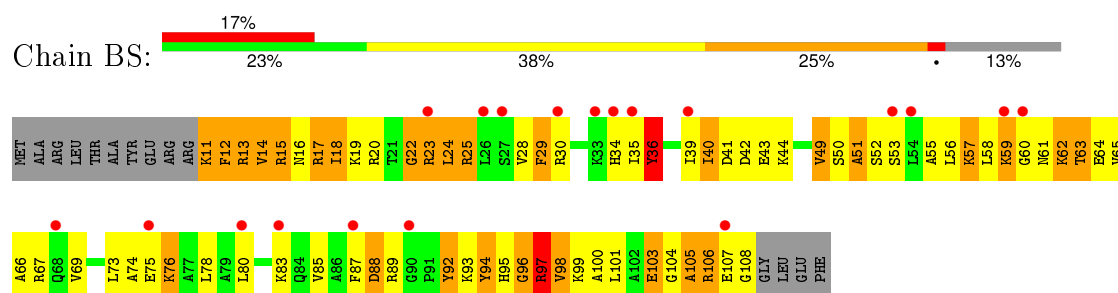
- Molecule 50: 50S RIBOSOMAL PROTEIN L17



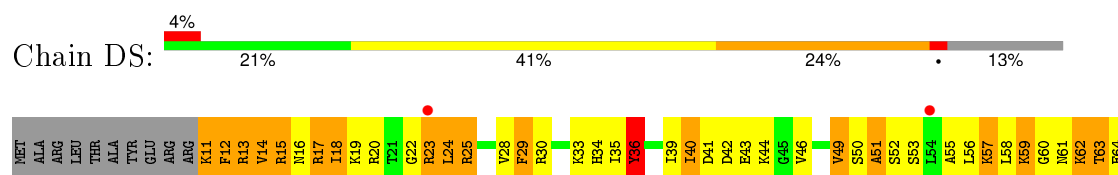
- Molecule 50: 50S RIBOSOMAL PROTEIN L17

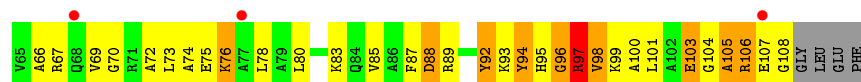


- Molecule 51: 50S RIBOSOMAL PROTEIN L18

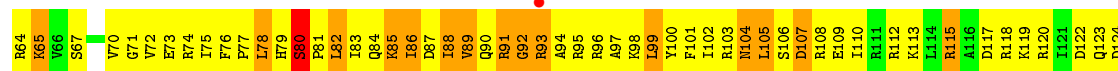
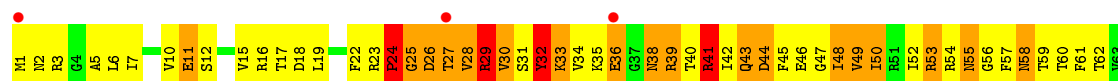
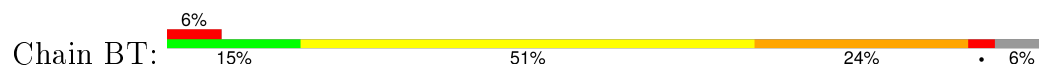


- Molecule 51: 50S RIBOSOMAL PROTEIN L18

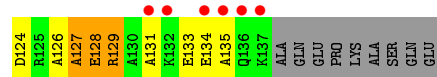
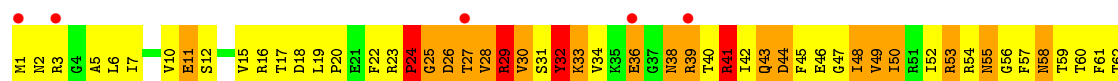
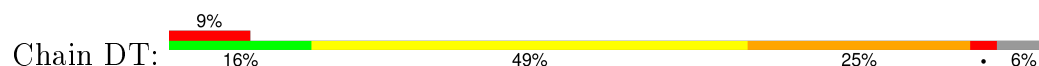




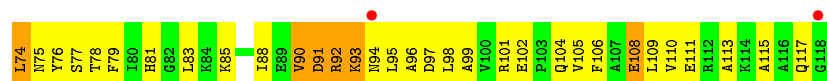
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



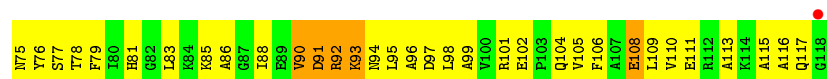
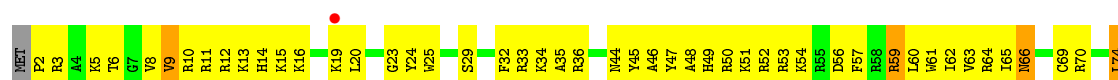
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



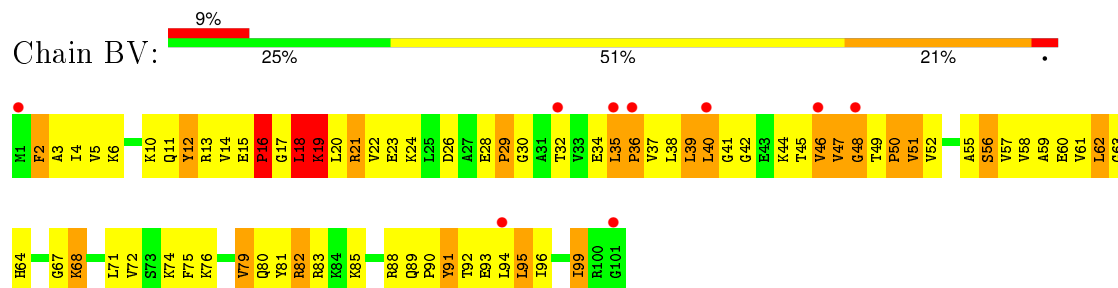
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



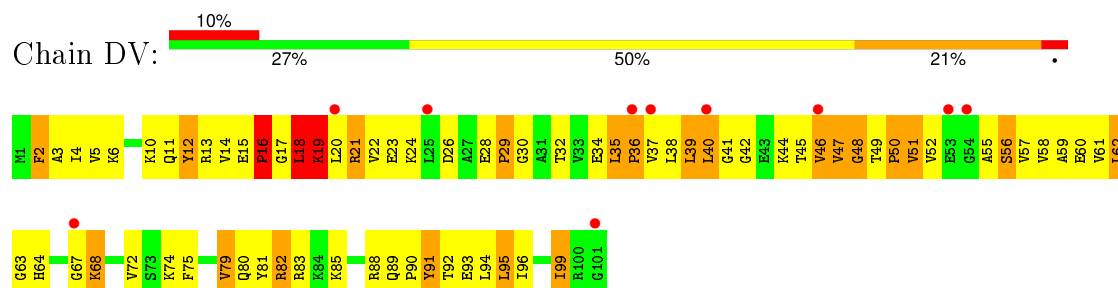
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



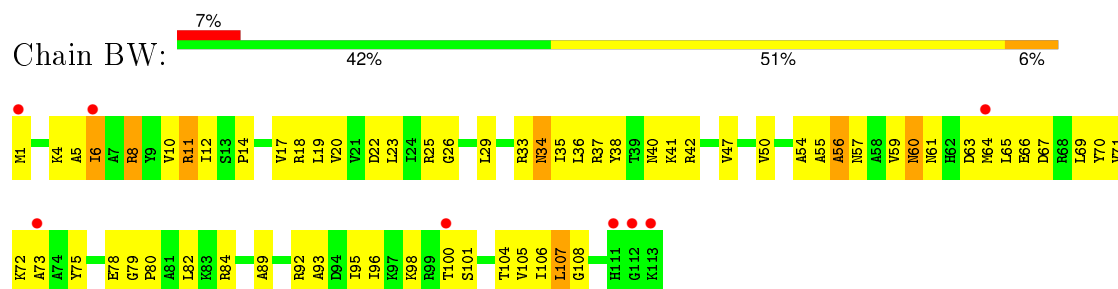
- Molecule 54: 50S RIBOSOMAL PROTEIN L21



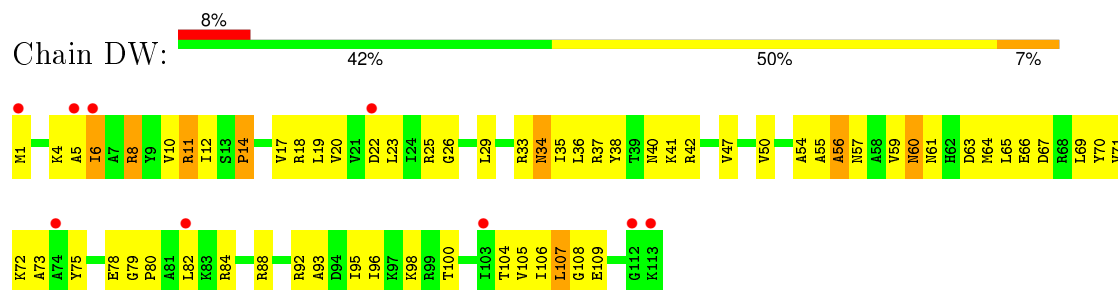
- Molecule 54: 50S RIBOSOMAL PROTEIN L21



- Molecule 55: 50S RIBOSOMAL PROTEIN L22



- Molecule 55: 50S RIBOSOMAL PROTEIN L22



- Molecule 56: 50S RIBOSOMAL PROTEIN L23

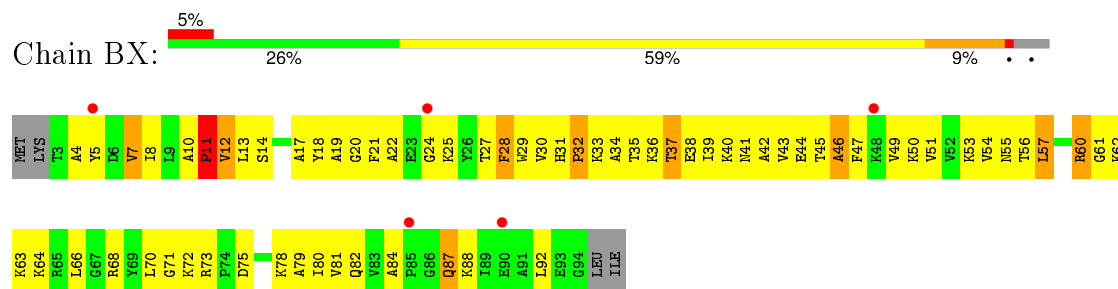
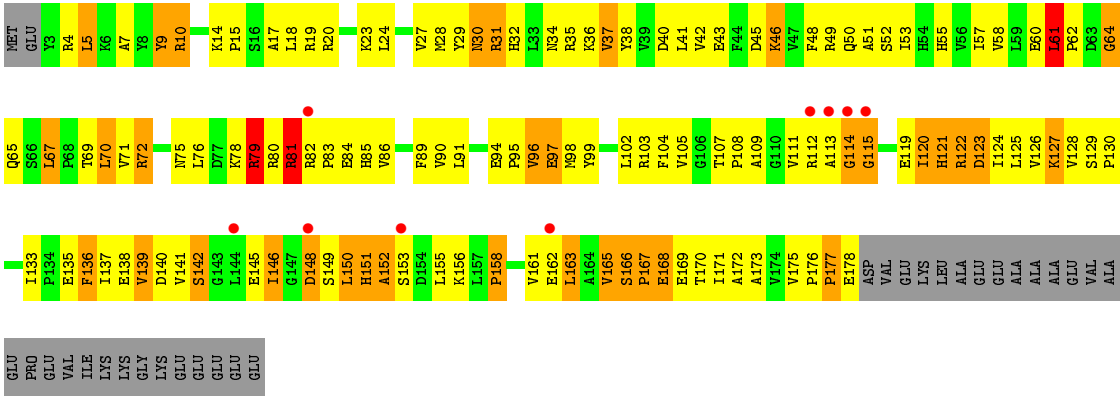


Figure 1: A bar chart showing the number of genes in each of the 20 clusters. The clusters are labeled MET, LYS, T3, A4, Y5, D6, V7, T8, L9, A10, P11, V12, L13, S14, A17, Y18, A19, G20, F21, G24, K25, Y26, T27, F28, W29, V30, H31, P32, K33, A34, T35, K36, T37, E38, L39, K40, N41, A42, V43, E44, T45, A46, V49, K50, V51, V52, K53, V54, N55, T56, E57, R60, G61, K62, K63, K64, R65, L66, G67, R68, Y69, L70, G71, K72, R73, P74, D75, K78, A79, I80, V81, Q82, R83, A84, P85, G86, Q87, R88, L92, E93, G94, LEU, and ILE. The chart shows the distribution of genes across these clusters, with some clusters having a significantly higher number of genes than others.

[illegible][illegible]

Q65	S66	L67	P68	T69	L70	V71	R72	Q73	V74	L75	R76	L77	D77	R78	R79	R80	R81	R82	P83	E84	H85	V86	D87	F88	F89	V90	L91	V96	E97	M98	V99	V100	P101	I102	F103	R104	G106	T107	P108	A109	G110	V111	R112	A113	G114	G115	V116	H121	R122	D123	I124	L125	V126	K127	V128	E129	P130
Q65	S66	L67	P68	T69	L70	V71	R72	Q73	V74	L75	R76	L77	D77	R78	R79	R80	R81	R82	P83	E84	H85	V86	D87	F88	F89	V90	L91	V96	E97	M98	V99	V100	P101	I102	F103	R104	G106	T107	P108	A109	G110	V111	R112	A113	G114	G115	V116	H121	R122	D123	I124	L125	V126	K127	V128	E129	P130
Q65	S66	L67	P68	T69	L70	V71	R72	Q73	V74	L75	R76	L77	D77	R78	R79	R80	R81	R82	P83	E84	H85	V86	D87	F88	F89	V90	L91	V96	E97	M98	V99	V100	P101	I102	F103	R104	G106	T107	P108	A109	G110	V111	R112	A113	G114	G115	V116	H121	R122	D123	I124	L125	V126	K127	V128	E129	P130
Q65	S66	L67	P68	T69	L70	V71	R72	Q73	V74	L75	R76	L77	D77	R78	R79	R80	R81	R82	P83	E84	H85	V86	D87	F88	F89	V90	L91	V96	E97	M98	V99	V100	P101	I102	F103	R104	G106	T107	P108	A109	G110	V111	R112	A113	G114	G115	V116	H121	R122	D123	I124	L125	V126	K127	V128	E129	P130
Q65	S66	L67	P68	T69	L70	V71	R72	Q73	V74	L75	R76	L77	D77	R78	R79	R80	R81	R82	P83	E84	H85	V86	D87	F88	F89	V90	L91	V96	E97	M98	V99	V100	P101	I102	F103	R104	G106	T107	P108	A109	G110	V111	R112	A113	G114	G115	V116	H121	R122	D123	I124	L125	V126	K127	V128	E129	P130
Q65	S66	L67	P68	T69	L70	V71	R72	Q73	V74	L75	R76	L77	D77	R78	R79	R80	R81	R82	P83	E84	H85	V86	D87	F88	F89	V90	L91	V96	E97	M98	V99	V100	P101	I102	F103	R104	G106	T107	P108	A109	G110	V111	R112	A113	G114	G115	V116	H121	R122	D123	I124	L125	V126	K127	V128	E129	P130
Q65	S66	L67	P68	T69	L70	V71	R72	Q73	V74	L75	R76	L77	D77	R78	R79	R80	R81	R82	P83	E84	H85	V86	D87	F88	F89	V90	L91	V96	E97	M98	V99	V100	P101	I102	F103	R104	G106	T107	P108	A109	G110	V111	R112	A113	G114	G115	V116	H121	R122	D123	I124	L125	V126	K127	V128	E129	P130
Q65	S66	L67	P68	T69	L70	V71	R72	Q73	V74	L75	R76	L77	D77	R78	R79	R80	R81	R82	P83	E84	H85	V86	D87	F88	F89	V90	L91	V96	E97	M98	V99	V100	P101	I102	F103	R104	G106	T107	P108	A109	G110	V111	R112	A113	G114	G115	V116	H121	R122	D123	I124	L125	V126	K127	V128	E129	P130
Q65	S66	L67	P68	T69	L70	V71	R72	Q73	V74	L75	R76	L77	D77	R78	R79	R80	R81	R82	P83	E84	H85	V86	D87	F88	F89	V90	L91	V96	E97	M98	V99	V100	P101	I102	F103	R104	G106	T107	P108	A109	G110	V111	R112	A113	G114	G115	V116	H121	R122	D123	I124	L125	V126	K127	V128	E129	P130
Q65	S66	L67	P68	T69	L70	V71	R72	Q73	V74	L75	R76	L77	D77	R78	R79	R80	R81																																								



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	290.20Å 269.20Å 404.00Å 90.00° 91.54° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.10) 92.4 (49.51-2.90)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.237 , 0.264 0.237 , 0.263	Depositor DCC
R_{free} test set	55683 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 68.2	EDS
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 1263345 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	307330	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

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%)	2	10
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%)	14	48
5	CE	148/162 (91%)	136 (92%)	9 (6%)	3 (2%)	9	38
6	AF	99/101 (98%)	72 (73%)	18 (18%)	9 (9%)	1	5
6	CF	99/101 (98%)	73 (74%)	17 (17%)	9 (9%)	1	5
7	AG	153/156 (98%)	127 (83%)	22 (14%)	4 (3%)	7	32
7	CG	153/156 (98%)	129 (84%)	21 (14%)	3 (2%)	9	38
8	AH	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	13	46
8	CH	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	13	46
9	AI	125/128 (98%)	83 (66%)	34 (27%)	8 (6%)	2	10
9	CI	125/128 (98%)	83 (66%)	35 (28%)	7 (6%)	2	13
10	AJ	96/105 (91%)	69 (72%)	21 (22%)	6 (6%)	2	10
10	CJ	96/105 (91%)	71 (74%)	19 (20%)	6 (6%)	2	10
11	AK	117/129 (91%)	98 (84%)	18 (15%)	1 (1%)	21	61
11	CK	117/129 (91%)	99 (85%)	17 (14%)	1 (1%)	21	61

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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%)	8	35
15	CO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	8	35
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	15
17	CQ	97/105 (92%)	85 (88%)	7 (7%)	5 (5%)	2	15
18	AR	68/88 (77%)	55 (81%)	11 (16%)	2 (3%)	6	29
18	CR	68/88 (77%)	56 (82%)	10 (15%)	2 (3%)	6	29
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%)	3	16
26	D0	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	3	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	19
49	DQ	139/141 (99%)	108 (78%)	25 (18%)	6 (4%)	3	19

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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	19
53	DU	115/118 (98%)	82 (71%)	28 (24%)	5 (4%)	3	19
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%)	1	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%)	9	32
2	CB	202/220 (92%)	180 (89%)	22 (11%)	8	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	34
4	CD	180/181 (99%)	162 (90%)	18 (10%)	9	34
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%)	8	29
6	CF	90/90 (100%)	80 (89%)	10 (11%)	8	29
7	AG	126/127 (99%)	118 (94%)	8 (6%)	22	58
7	CG	126/127 (99%)	118 (94%)	8 (6%)	22	58
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%)	14	47
9	CI	98/99 (99%)	89 (91%)	9 (9%)	11	40
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	6	22
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	6	22
11	AK	90/99 (91%)	80 (89%)	10 (11%)	8	29
11	CK	90/99 (91%)	80 (89%)	10 (11%)	8	29
12	AL	104/108 (96%)	92 (88%)	12 (12%)	7	27
12	CL	104/108 (96%)	92 (88%)	12 (12%)	7	27
13	AM	99/101 (98%)	88 (89%)	11 (11%)	8	29
13	CM	99/101 (98%)	88 (89%)	11 (11%)	8	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	28
15	CO	79/80 (99%)	70 (89%)	9 (11%)	7	28
16	AP	72/74 (97%)	64 (89%)	8 (11%)	8	29
16	CP	72/74 (97%)	65 (90%)	7 (10%)	10	36
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	22	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	22	57
18	AR	61/77 (79%)	51 (84%)	10 (16%)	3	12
18	CR	61/77 (79%)	51 (84%)	10 (16%)	3	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%)	28	64
21	CU	19/22 (86%)	18 (95%)	1 (5%)	28	64
25	AZ	322/338 (95%)	279 (87%)	43 (13%)	5	20
25	CZ	322/338 (95%)	281 (87%)	41 (13%)	5	22
26	B0	66/67 (98%)	59 (89%)	7 (11%)	8	31
26	D0	66/67 (98%)	59 (89%)	7 (11%)	8	31
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%)	48	81
28	D2	66/67 (98%)	57 (86%)	9 (14%)	5	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	10
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%)	17	52
33	D7	41/42 (98%)	38 (93%)	3 (7%)	17	52
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	43
35	D9	34/34 (100%)	31 (91%)	3 (9%)	12	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BC	180/181 (99%)	172 (96%)	8 (4%)	35	71
38	DC	180/181 (99%)	172 (96%)	8 (4%)	35	71
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%)	5	20
41	BF	165/166 (99%)	152 (92%)	13 (8%)	15	49
41	DF	165/166 (99%)	152 (92%)	13 (8%)	15	49
42	BG	155/156 (99%)	135 (87%)	20 (13%)	5	21
42	DG	155/156 (99%)	124 (80%)	31 (20%)	1	7
43	BH	132/148 (89%)	118 (89%)	14 (11%)	8	31
43	DH	132/148 (89%)	118 (89%)	14 (11%)	8	31
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%)	19	54
47	DO	100/100 (100%)	93 (93%)	7 (7%)	19	54
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%)	12	41
49	DQ	111/111 (100%)	101 (91%)	10 (9%)	12	41
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	14
51	DS	77/88 (88%)	65 (84%)	12 (16%)	3	14
52	BT	120/127 (94%)	97 (81%)	23 (19%)	2	8
52	DT	120/127 (94%)	97 (81%)	23 (19%)	2	8
53	BU	92/94 (98%)	86 (94%)	6 (6%)	21	57
53	DU	92/94 (98%)	86 (94%)	6 (6%)	21	57
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%)	35	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	DW	91/92 (99%)	86 (94%)	5 (6%)	27 63
56	BX	74/78 (95%)	67 (90%)	7 (10%)	11 38
56	DX	74/78 (95%)	68 (92%)	6 (8%)	15 47
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 13
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%)	43 (2%)
1	CA	1509/1522 (99%)	222 (14%)	46 (3%)
22	AV	75/76 (98%)	22 (29%)	1 (1%)
22	AW	75/76 (98%)	21 (28%)	2 (2%)
22	CV	75/76 (98%)	23 (30%)	1 (1%)
22	CW	75/76 (98%)	21 (28%)	3 (4%)
23	AX	16/27 (59%)	6 (37%)	1 (6%)

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

5 of 1627 RNA backbone outliers are listed below:

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

5 of 200 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2689	U
1	CA	353	A
36	DA	2033	A
36	BA	2762	G
1	CA	115	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	H2U	AY	16	24	17,21,22	1.15	2 (11%)	23,30,33	1.88	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	H2U	AY	17	24	17,21,22	1.10	2 (11%)	23,30,33	1.95	5 (21%)
24	H2U	AY	20	24	17,21,22	0.88	1 (5%)	23,30,33	1.92	4 (17%)
24	OMC	AY	32	24	13,22,23	0.76	0	20,31,34	1.02	2 (10%)
24	MIA	AY	37	24	21,31,32	0.96	0	26,44,47	1.66	4 (15%)
24	7MG	AY	46	24	19,26,27	1.68	3 (15%)	24,39,42	2.29	3 (12%)
24	5MU	AY	54	24	12,22,23	1.38	3 (25%)	14,32,35	4.53	3 (21%)
24	PSU	AY	55	24	13,21,22	1.16	2 (15%)	18,30,33	3.80	8 (44%)
24	4SU	AY	8	24	11,21,22	1.53	4 (36%)	13,30,33	2.30	1 (7%)
24	H2U	CY	16	24	17,21,22	1.15	2 (11%)	23,30,33	1.86	4 (17%)
24	H2U	CY	17	24	17,21,22	1.11	2 (11%)	23,30,33	1.95	5 (21%)
24	H2U	CY	20	24	17,21,22	0.87	1 (5%)	23,30,33	1.93	5 (21%)
24	OMC	CY	32	24	13,22,23	0.73	0	20,31,34	1.03	2 (10%)
24	MIA	CY	37	24	21,31,32	1.08	2 (9%)	26,44,47	1.68	4 (15%)
24	7MG	CY	46	24	19,26,27	1.67	3 (15%)	24,39,42	2.28	3 (12%)
24	5MU	CY	54	24	12,22,23	1.40	3 (25%)	14,32,35	4.52	3 (21%)
24	PSU	CY	55	24	13,21,22	1.13	2 (15%)	18,30,33	3.72	8 (44%)
24	4SU	CY	8	24	11,21,22	1.46	3 (27%)	13,30,33	2.28	1 (7%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 35 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	-2.77	1.30	1.43
24	AY	46	7MG	C8-N7	-2.75	1.30	1.43
24	CY	54	5MU	C6-C5	-2.18	1.34	1.40

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	55	PSU	N1-C2-N3	-12.87	120.12	128.33
24	CY	55	PSU	N1-C2-N3	-12.54	120.33	128.33
24	CY	54	5MU	C5-C4-N3	-8.99	115.13	125.14
24	AY	54	5MU	C5-C4-N3	-8.97	115.16	125.14
24	AY	8	4SU	C5-C4-N3	-8.14	115.66	123.63

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	-	23,30,30	1.61	4 (17%)	30,47,47	1.45	4 (13%)
61	KIR	AZ	502	-	55,59,59	3.69	21 (38%)	53,84,84	1.68	13 (24%)
60	GDP	CZ	501	-	23,30,30	1.51	4 (17%)	30,47,47	1.92	5 (16%)
61	KIR	CZ	502	-	55,59,59	3.69	23 (41%)	53,84,84	1.71	13 (24%)

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 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CZ	502	KIR	O18-C17	-14.40	1.22	1.44
61	AZ	502	KIR	O18-C17	-14.12	1.23	1.44
61	AZ	502	KIR	O30-C30	-11.98	1.17	1.42
61	CZ	502	KIR	O30-C30	-11.66	1.18	1.42
61	CZ	502	KIR	O34-C33	-11.06	1.29	1.44

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AZ	502	KIR	O29-C29-O34	-5.14	101.68	110.18
61	CZ	502	KIR	O29-C29-O34	-5.07	101.79	110.18
60	CZ	501	GDP	N3-C2-N1	-4.81	120.11	127.44
60	CZ	501	GDP	C5-C6-N1	-4.48	117.46	123.59
60	CZ	501	GDP	PA-O3A-PB	-4.35	118.08	132.67

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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1510/1522 (99%)	-0.28	21 (1%) 78 60	44, 78, 160, 200	0
1	CA	1510/1522 (99%)	-0.05	33 (2%) 65 42	37, 73, 161, 200	0
2	AB	234/256 (91%)	-0.08	6 (2%) 59 35	58, 88, 152, 164	0
2	CB	234/256 (91%)	-0.17	3 (1%) 79 62	54, 86, 151, 164	0
3	AC	206/239 (86%)	-0.29	1 (0%) 91 83	52, 75, 101, 110	0
3	CC	206/239 (86%)	-0.28	0 100 100	46, 70, 100, 109	0
4	AD	208/209 (99%)	0.14	10 (4%) 34 15	71, 97, 124, 132	0
4	CD	208/209 (99%)	0.07	4 (1%) 70 48	67, 96, 123, 131	0
5	AE	150/162 (92%)	-0.33	0 100 100	53, 65, 89, 110	0
5	CE	150/162 (92%)	-0.34	0 100 100	49, 63, 88, 109	0
6	AF	101/101 (100%)	0.07	1 (0%) 84 69	71, 99, 115, 122	0
6	CF	101/101 (100%)	-0.13	1 (0%) 84 69	68, 97, 114, 121	0
7	AG	155/156 (99%)	0.21	9 (5%) 26 11	66, 89, 113, 130	0
7	CG	155/156 (99%)	-0.09	2 (1%) 79 62	59, 86, 112, 129	0
8	AH	138/138 (100%)	-0.27	1 (0%) 89 78	54, 70, 87, 95	0
8	CH	138/138 (100%)	-0.28	0 100 100	52, 67, 87, 94	0
9	AI	127/128 (99%)	0.69	19 (14%) 3 1	62, 96, 128, 139	0
9	CI	127/128 (99%)	0.26	3 (2%) 62 39	54, 93, 127, 139	0
10	AJ	98/105 (93%)	0.85	22 (22%) 1 0	59, 99, 141, 145	0
10	CJ	98/105 (93%)	0.39	6 (6%) 25 10	54, 95, 140, 144	0
11	AK	119/129 (92%)	0.07	7 (5%) 26 11	55, 73, 107, 134	0
11	CK	119/129 (92%)	-0.02	4 (3%) 49 24	51, 68, 108, 133	0
12	AL	124/131 (94%)	0.04	5 (4%) 42 20	55, 70, 94, 132	0
12	CL	124/131 (94%)	-0.10	1 (0%) 87 75	51, 68, 93, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	124/126 (98%)	0.38	14 (11%) 7 2	71, 97, 124, 152	0
13	CM	124/126 (98%)	0.15	7 (5%) 28 11	67, 95, 123, 152	0
14	AN	60/61 (98%)	-0.15	1 (1%) 73 52	57, 72, 93, 96	0
14	CN	60/61 (98%)	0.01	1 (1%) 73 52	49, 66, 91, 96	0
15	AO	88/89 (98%)	-0.06	0 100 100	57, 75, 99, 105	0
15	CO	88/89 (98%)	-0.02	0 100 100	56, 74, 98, 104	0
16	AP	83/88 (94%)	0.44	4 (4%) 34 15	74, 91, 109, 135	0
16	CP	83/88 (94%)	0.41	2 (2%) 62 39	72, 89, 108, 136	0
17	AQ	99/105 (94%)	0.02	3 (3%) 54 29	60, 79, 95, 108	0
17	CQ	99/105 (94%)	-0.04	0 100 100	57, 78, 93, 107	0
18	AR	70/88 (79%)	-0.02	3 (4%) 39 18	58, 82, 106, 119	0
18	CR	70/88 (79%)	-0.28	1 (1%) 78 60	56, 79, 105, 118	0
19	AS	78/93 (83%)	0.46	5 (6%) 23 9	75, 99, 137, 139	0
19	CS	78/93 (83%)	0.49	6 (7%) 16 5	71, 99, 136, 139	0
20	AT	99/106 (93%)	0.47	6 (6%) 25 10	75, 97, 131, 135	0
20	CT	99/106 (93%)	0.47	5 (5%) 32 13	71, 96, 132, 135	0
21	AU	24/27 (88%)	0.83	3 (12%) 5 2	66, 84, 103, 115	0
21	CU	24/27 (88%)	0.41	1 (4%) 40 19	64, 78, 99, 115	0
22	AV	76/76 (100%)	-0.27	1 (1%) 79 62	56, 91, 128, 148	0
22	AW	76/76 (100%)	0.83	11 (14%) 3 1	103, 172, 200, 200	0
22	CV	76/76 (100%)	-0.20	1 (1%) 79 62	50, 89, 128, 147	0
22	CW	76/76 (100%)	0.75	12 (15%) 3 1	100, 172, 200, 200	0
23	AX	17/27 (62%)	0.63	2 (11%) 6 2	50, 97, 156, 157	0
23	CX	17/27 (62%)	0.58	1 (5%) 26 11	45, 95, 156, 157	0
24	AY	68/77 (88%)	0.07	1 (1%) 76 58	61, 140, 171, 190	0
24	CY	68/77 (88%)	0.02	4 (5%) 26 11	57, 140, 170, 190	0
25	AZ	385/405 (95%)	1.83	140 (36%) 0 0	116, 142, 165, 183	0
25	CZ	385/405 (95%)	0.47	26 (6%) 20 7	113, 141, 165, 183	0
26	B0	84/85 (98%)	0.66	9 (10%) 8 3	77, 91, 118, 131	0
26	D0	84/85 (98%)	0.59	7 (8%) 14 5	76, 90, 119, 131	0
27	B1	93/98 (94%)	0.46	7 (7%) 17 6	74, 95, 134, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D1	93/98 (94%)	0.27	2 (2%) 65 42	56, 76, 130, 142	0
28	B2	71/72 (98%)	0.49	5 (7%) 19 7	110, 133, 148, 157	0
28	D2	71/72 (98%)	1.45	22 (30%) 1 0	134, 154, 174, 175	0
29	B3	59/60 (98%)	0.70	3 (5%) 32 13	81, 99, 120, 142	0
29	D3	59/60 (98%)	0.58	3 (5%) 32 13	80, 97, 120, 142	0
30	B4	44/71 (61%)	0.24	5 (11%) 7 2	124, 149, 160, 163	0
30	D4	44/71 (61%)	0.41	4 (9%) 11 4	123, 147, 158, 163	0
31	B5	59/60 (98%)	0.34	5 (8%) 13 4	73, 105, 158, 176	0
31	D5	59/60 (98%)	0.17	4 (6%) 20 7	72, 104, 158, 176	0
32	B6	50/54 (92%)	0.86	7 (14%) 4 2	74, 106, 116, 125	0
32	D6	50/54 (92%)	0.90	8 (16%) 3 1	73, 104, 115, 123	0
33	B7	48/49 (97%)	0.47	1 (2%) 67 44	70, 79, 119, 139	0
33	D7	48/49 (97%)	0.62	2 (4%) 40 19	68, 78, 119, 140	0
34	B8	63/65 (96%)	0.53	3 (4%) 34 15	80, 90, 104, 131	0
34	D8	63/65 (96%)	0.45	3 (4%) 34 15	78, 88, 104, 131	0
35	B9	37/37 (100%)	0.68	3 (8%) 15 5	76, 90, 104, 108	0
35	D9	37/37 (100%)	0.32	3 (8%) 15 5	76, 90, 104, 107	0
36	BA	2901/2915 (99%)	-0.08	78 (2%) 58 34	49, 95, 190, 200	0
36	DA	2901/2915 (99%)	0.00	76 (2%) 59 35	46, 93, 190, 200	0
37	BB	119/122 (97%)	-0.45	0 100 100	78, 108, 134, 157	0
37	DB	119/122 (97%)	-0.36	0 100 100	75, 107, 133, 157	0
38	BC	228/229 (99%)	0.75	34 (14%) 3 1	69, 99, 177, 187	0
38	DC	228/229 (99%)	0.36	21 (9%) 11 4	67, 97, 177, 187	0
39	BD	275/276 (99%)	-0.13	3 (1%) 82 66	50, 68, 98, 123	0
39	DD	275/276 (99%)	-0.14	2 (0%) 89 78	47, 66, 97, 123	0
40	BE	204/206 (99%)	0.31	13 (6%) 23 9	64, 93, 141, 152	0
40	DE	204/206 (99%)	0.28	8 (3%) 43 21	64, 93, 141, 152	0
41	BF	207/210 (98%)	0.81	28 (13%) 4 2	73, 128, 176, 184	0
41	DF	207/210 (98%)	0.73	29 (14%) 4 2	71, 127, 176, 184	0
42	BG	181/182 (99%)	0.28	11 (6%) 25 10	97, 125, 147, 157	0
42	DG	181/182 (99%)	0.10	10 (5%) 29 12	75, 96, 125, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BH	159/180 (88%)	0.83	26 (16%) 2 1	106, 142, 163, 165	0
43	DH	159/180 (88%)	1.22	37 (23%) 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%)	0.23	2 (1%) 78 60	78, 104, 145, 148	0
46	DN	138/140 (98%)	0.20	3 (2%) 65 42	77, 104, 144, 147	0
47	BO	122/122 (100%)	-0.14	1 (0%) 87 75	58, 76, 90, 97	0
47	DO	122/122 (100%)	-0.04	0 100 100	57, 76, 89, 97	0
48	BP	146/150 (97%)	0.99	25 (17%) 2 1	73, 121, 146, 162	0
48	DP	146/150 (97%)	1.01	27 (18%) 2 1	72, 120, 145, 162	0
49	BQ	141/141 (100%)	0.05	2 (1%) 78 60	61, 78, 107, 138	0
49	DQ	141/141 (100%)	0.08	4 (2%) 56 32	60, 77, 107, 139	0
50	BR	117/118 (99%)	0.35	4 (3%) 49 24	76, 98, 114, 129	0
50	DR	117/118 (99%)	0.34	3 (2%) 59 35	75, 98, 115, 129	0
51	BS	98/112 (87%)	0.91	19 (19%) 1 1	89, 112, 137, 141	0
51	DS	98/112 (87%)	0.50	5 (5%) 32 13	88, 111, 136, 140	0
52	BT	137/146 (93%)	0.16	9 (6%) 22 8	74, 97, 155, 179	0
52	DT	137/146 (93%)	0.26	13 (9%) 10 4	73, 97, 154, 179	0
53	BU	117/118 (99%)	0.17	4 (3%) 49 24	81, 98, 125, 142	0
53	DU	117/118 (99%)	0.16	2 (1%) 73 52	78, 97, 125, 142	0
54	BV	101/101 (100%)	0.59	9 (8%) 12 4	79, 130, 146, 150	0
54	DV	101/101 (100%)	0.54	10 (9%) 9 3	79, 129, 146, 150	0
55	BW	113/113 (100%)	0.51	8 (7%) 19 7	85, 100, 133, 165	0
55	DW	113/113 (100%)	0.42	9 (7%) 15 5	82, 100, 133, 165	0
56	BX	92/96 (95%)	0.52	5 (5%) 29 12	83, 109, 125, 134	0
56	DX	92/96 (95%)	0.44	8 (8%) 13 4	83, 108, 124, 134	0
57	BY	100/110 (90%)	1.88	39 (39%) 0 0	127, 146, 179, 187	0
57	DY	100/110 (90%)	1.83	40 (40%) 0 0	126, 146, 179, 187	0
58	BZ	176/206 (85%)	0.12	5 (2%) 56 32	75, 103, 135, 144	0
58	DZ	176/206 (85%)	0.08	9 (5%) 32 13	64, 94, 140, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	21994/23368 (94%)	0.16	1167 (5%) 30 13	37, 93, 162, 200	0

The worst 5 of 1167 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	DQ	141	GLN	14.5
49	BQ	141	GLN	12.9
38	BC	1	PRO	11.9
43	DH	170	ARG	11.9
53	DU	118	GLY	11.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	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	1.30	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.