



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 11:27 AM EDT

PDB ID : 4V9I  
Title : Crystal structure of thermus thermophilus 70S in complex with tRNAs and mRNA containing a pseudouridine in a stop codon  
Authors : Fernandez, I.S.; Ng, C.L.; Kelley, A.C.; Guowei, W.; Yu, Y.T.; Ramakrishnan, V.  
Deposited on : 2013-04-04  
Resolution : 3.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

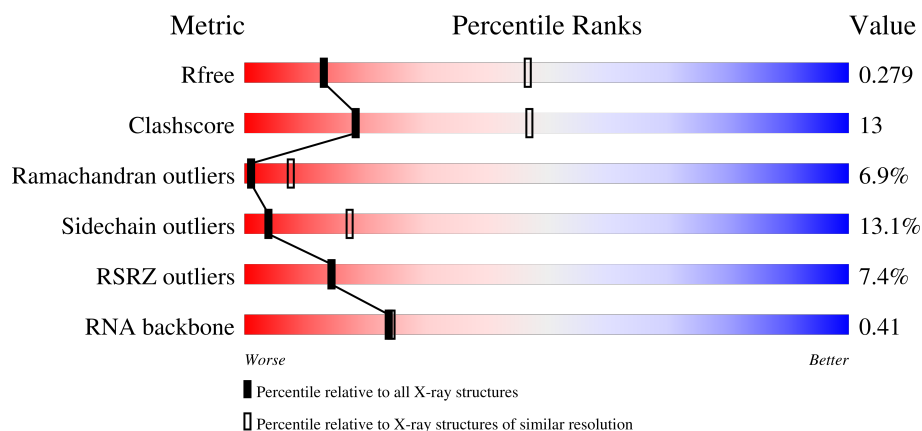
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1504	<div> <div>4%</div> <div>51% 39% 10%</div> </div>
1	CA	1504	<div> <div>6%</div> <div>52% 39% 9%</div> </div>
2	AB	234	<div> <div>5%</div> <div>64% 32% .</div> </div>
2	CB	234	<div> <div>15%</div> <div>65% 30% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	CC	206	
4	AD	208	
4	CD	208	
5	AE	150	
5	CE	150	
6	AF	101	
6	CF	101	
7	AG	155	
7	CG	155	
8	AH	138	
8	CH	138	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	119	
11	CK	119	
12	AL	124	
12	CL	124	
13	AM	124	
13	CM	124	
14	AN	60	
14	CN	60	
15	AO	88	



















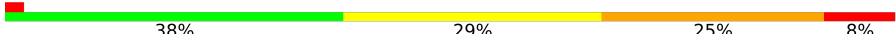






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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	83	
16	CP	83	
17	AQ	99	
17	CQ	99	
18	AR	70	
18	CR	70	
19	AS	78	
19	CS	78	
20	AT	99	
20	CT	99	
21	AU	24	
21	CU	24	
22	AV	77	
22	CV	77	
23	AW	76	
23	CW	76	
24	AY	75	
24	CY	75	
25	AX	7	
26	BA	2915	
26	DA	2915	
27	BB	119	
27	DB	119	
28	BC	206	

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Mol	Chain	Length	Quality of chain
29	BD	271	
29	DD	271	
30	BE	204	
30	DE	204	
31	BF	207	
31	DF	207	
32	BG	181	
32	DG	181	
33	BH	159	
33	DH	159	
34	BI	145	
34	DI	145	
35	BJ	130	
35	DJ	130	
36	BN	138	
36	DN	138	
37	BO	122	
37	DO	122	
38	BP	146	
38	DP	146	
39	BQ	141	
39	DQ	141	
40	BR	117	
40	DR	117	
41	BS	98	

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Mol	Chain	Length	Quality of chain
41	DS	98	
42	BT	137	
42	DT	137	
43	BU	117	
43	DU	117	
44	BV	101	
44	DV	101	
45	BW	113	
45	DW	113	
46	BX	92	
46	DX	92	
47	BY	100	
47	DY	100	
48	BZ	176	
48	DZ	176	
49	B0	84	
49	D0	84	
50	B1	93	
50	D1	93	
51	B2	71	
51	D2	71	
52	B3	59	
52	D3	59	
53	B4	30	
53	D4	30	

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Mol	Chain	Length	Quality of chain
54	B5	59	
54	D5	59	
55	B6	44	
55	D6	44	
56	B7	48	
56	D7	48	
57	B8	63	
57	D8	63	
58	B9	36	
58	D9	36	
59	CX	4	
60	DC	196	

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
25	PSU	AX	19	-	-	X	-

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 295724 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- 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
			1901	1213	341	342	5			
2	CB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	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
			1613	1016	314	282	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	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
			1147	724	217	202	4			
5	CE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	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
			1011	639	198	174			
9	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	CONFLICT	UNP P80374
CI	58	ARG	HIS	CONFLICT	UNP P80374

- 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
			795	499	156	139	1			
10	CJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	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
			971	611	195	164	1			
12	CL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	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
			988	611	205	170	2			
13	CM	124	Total	C	N	O	S	0	0	0
			988	611	205	170	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
			701	443	139	118	1			
16	CP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	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
			824	528	151	143	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			824	528	151	143	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
			630	403	114	111	2			
19	CS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			209	128	50	31			
21	CU	24	Total	C	N	O	0	0	0
			209	128	50	31			

- Molecule 22 is a RNA chain called P-SITE tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	CV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called E-SITE tRNA.

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

- Molecule 24 is a RNA chain called A-SITE tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	75	Total	C	N	O	P	0	0	0
			1619	722	309	514	74			
24	CY	75	Total	C	N	O	P	0	0	0
			1619	722	309	514	74			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	?	-	C	DELETION	GB 443419838
CY	?	-	C	DELETION	GB 443419838

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AX	7	Total	C	N	O	P	0	0	0
			151	68	29	47	7			

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			
26	DA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1151	A	G	CONFLICT	GB 55771382
DA	1151	A	G	CONFLICT	GB 55771382

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 28 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	BC	190	Total	C	N	O	0	0	0
			1157	706	220	231			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BD	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			
29	DD	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BE	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
30	DE	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BF	207	Total	C	N	O	S	0	0	0
			1624	1035	303	283	3			
31	DF	207	Total	C	N	O	S	0	0	0
			1624	1035	303	283	3			

- Molecule 32 is a protein called 50S ribosomal protein L5.

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

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BH	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
33	DH	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BI	145	Total	C	N	O	S	0	0	0
			1132	723	200	208	1			
34	DI	145	Total	C	N	O	S	0	0	0
			1132	723	200	208	1			

- Molecule 35 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BJ	130	Total	C	N	O		0	0	0
			651	390	130	131				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	DJ	130	Total	C	N	O	0	0	0
			651	390	130	131			

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BN	138	Total	C	N	O	S	0	0	0
			1105	712	206	183	4			
36	DN	138	Total	C	N	O	S	0	0	0
			1105	712	206	183	4			

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

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

- Molecule 39 is a protein called 50S ribosomal protein L16.

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

- Molecule 40 is a protein called 50S ribosomal protein L17.

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

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	BS	98	Total	C	N	O	0	0	0
			771	486	154	131			
41	DS	98	Total	C	N	O	0	0	0
			771	486	154	131			

- Molecule 42 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BT	137	Total	C	N	O	S	0	0	0
			1142	710	234	197	1			
42	DT	137	Total	C	N	O	S	0	0	0
			1142	710	234	197	1			

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	32	ALA	PHE	CONFLICT	UNP P60491
DU	32	ALA	PHE	CONFLICT	UNP P60491

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	113	ALA	LYS	CONFLICT	UNP Q5SHP3
DW	113	ALA	LYS	CONFLICT	UNP Q5SHP3

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BX	92	Total	C	N	O		0	0	0
			726	471	131	124				
46	DX	92	Total	C	N	O		0	0	0
			726	471	131	124				

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
47	DY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 48 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	176	Total	C	N	O	S	0	0	0
			1404	897	252	253	2			
48	DZ	176	Total	C	N	O	S	0	0	0
			1404	897	252	253	2			

- Molecule 49 is a protein called 50S ribosomal protein L27.

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

- Molecule 50 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B1	93	Total	C	N	O	S	0	0	0
			734	460	147	126	1			
50	D1	93	Total	C	N	O	S	0	0	0
			734	460	147	126	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	ARG	LYS	CONFLICT	UNP P60494
D1	81	ARG	LYS	CONFLICT	UNP P60494

- Molecule 51 is a protein called 50S ribosomal protein L29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B3	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
52	D3	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B4	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
53	D4	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
54	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B6	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			
55	D6	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 56 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
56	D7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 57 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	B8	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
57	D8	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 58 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
58	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 59 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	CX	4	Total	C	N	O	P	0	0	0
			85	38	14	29	4			

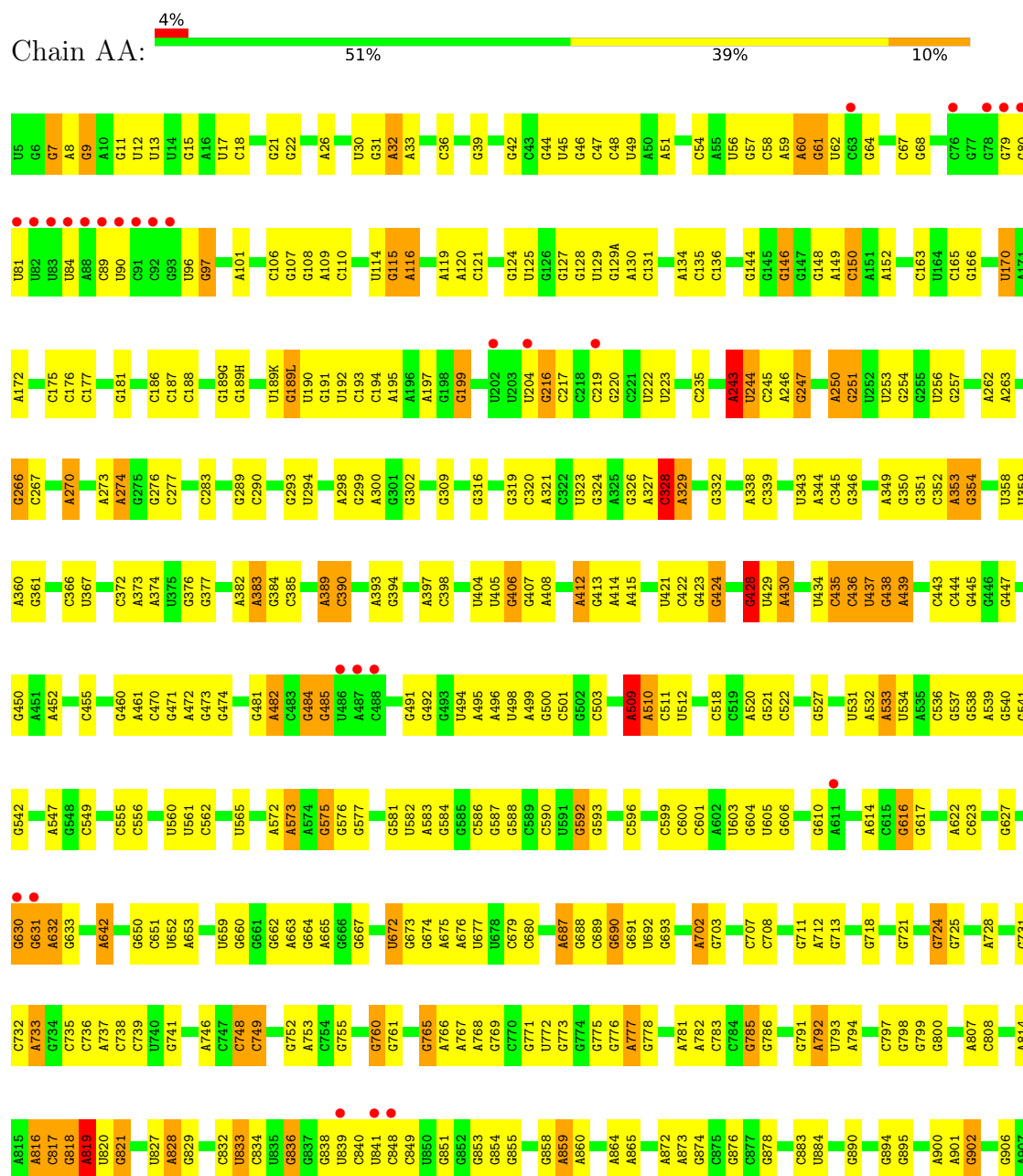
- Molecule 60 is a protein called 50S Ribosomal protein L1.

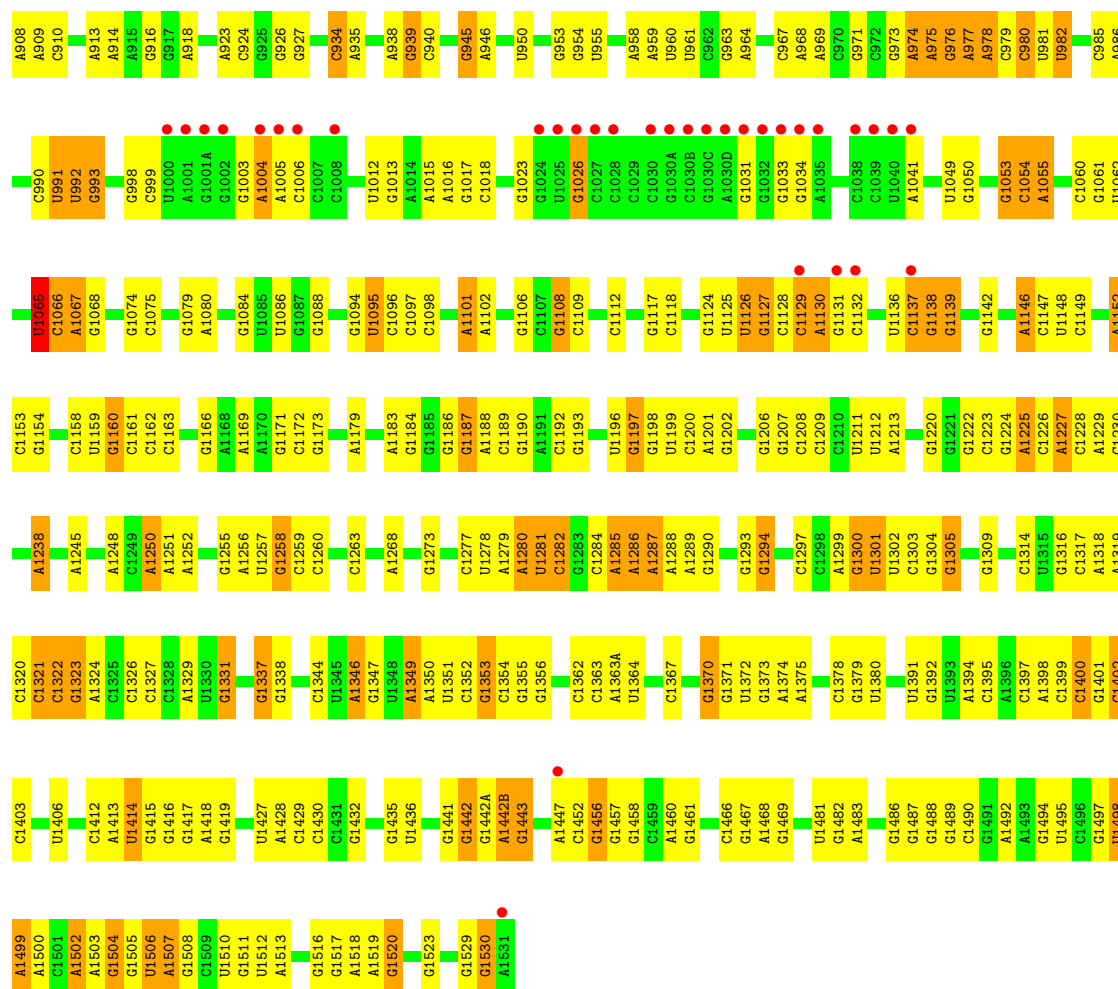
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
60	DC	190	Total	C	N	O	0	0	0
			1157	706	220	231			

### 3 Residue-property plots

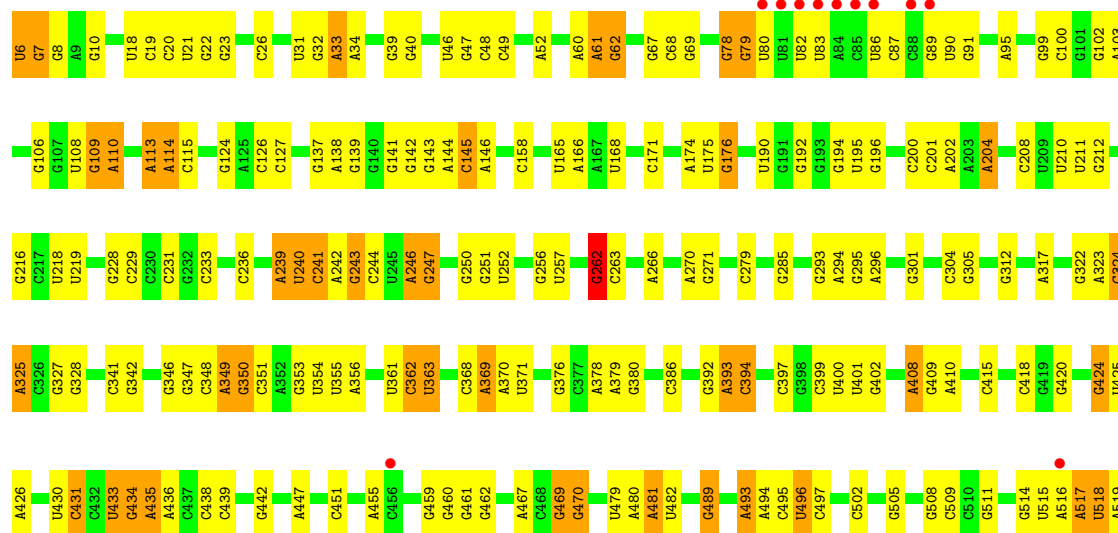
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

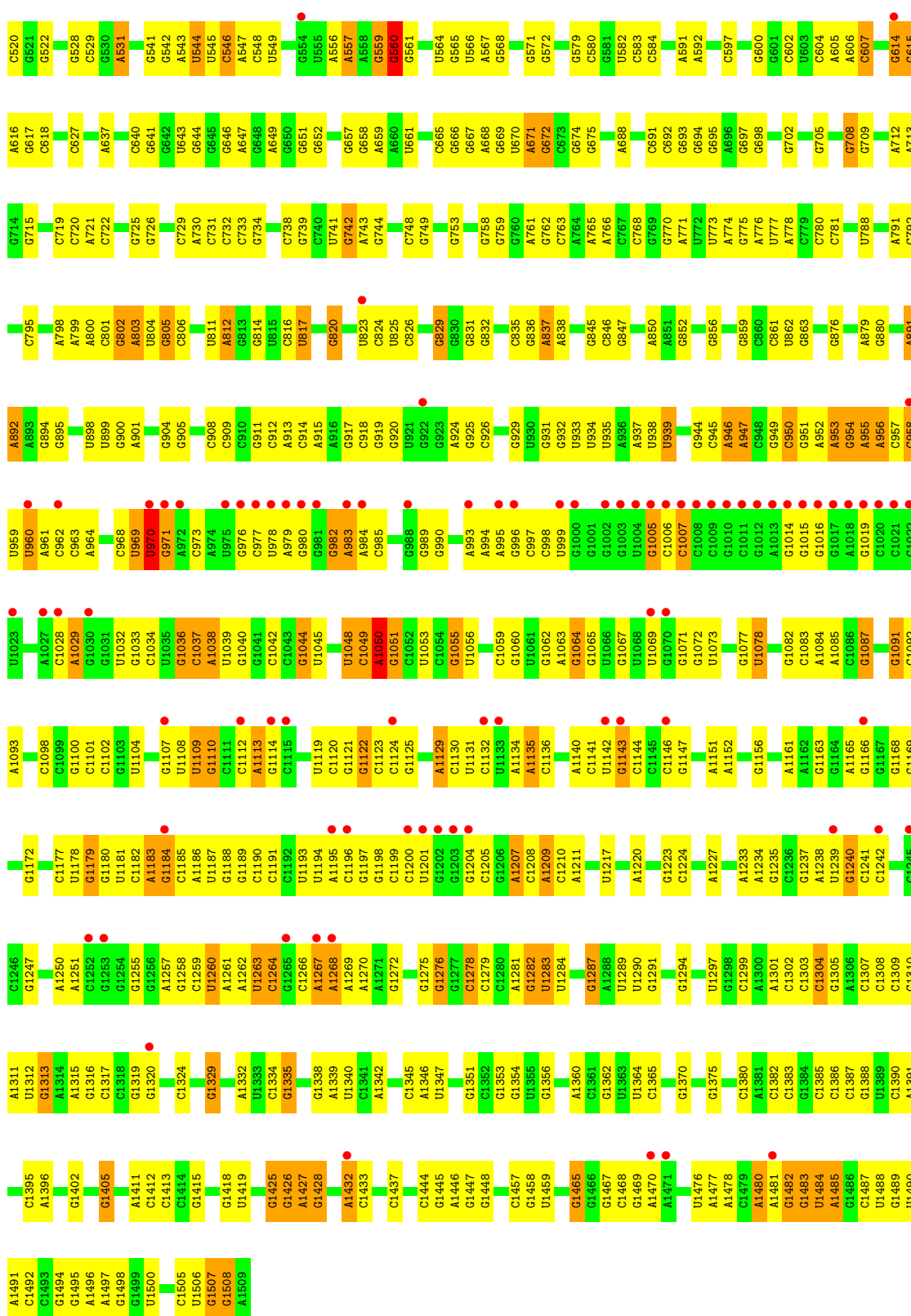
- Molecule 1: 16S ribosomal RNA





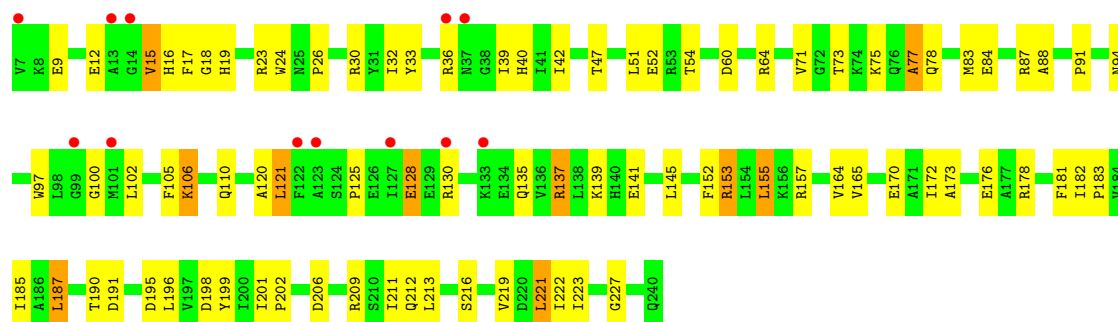
• Molecule 1: 16S ribosomal RNA





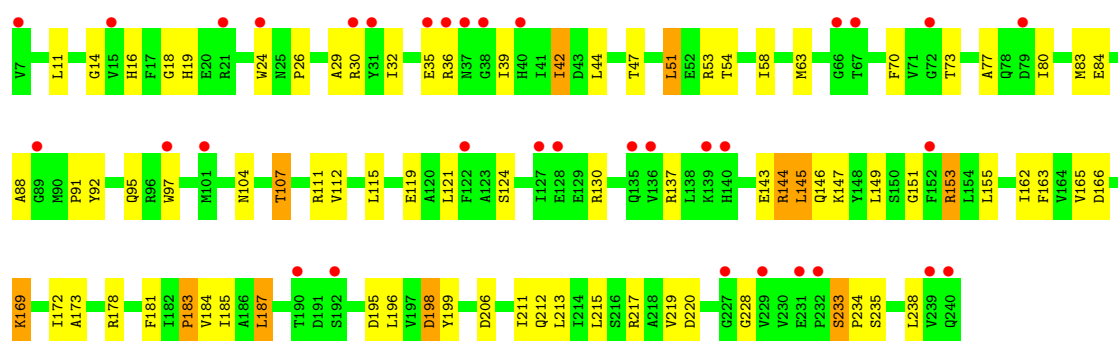
• Molecule 2: 30S Ribosomal protein S2





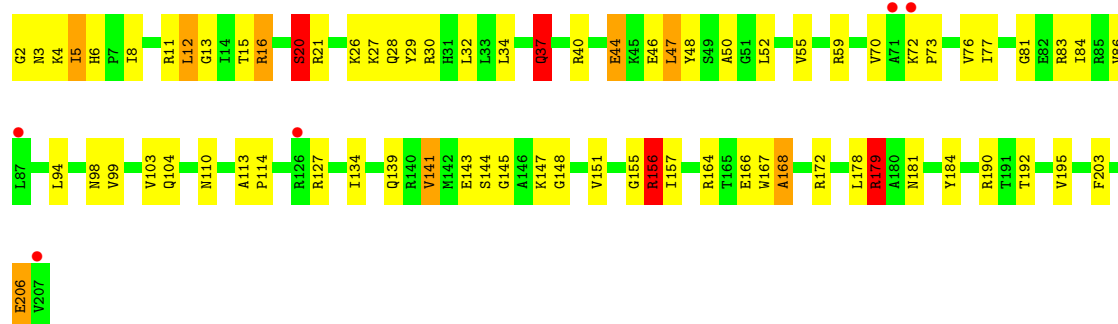
• Molecule 2: 30S Ribosomal protein S2

Chain CB: 15% 65% 30% 5%



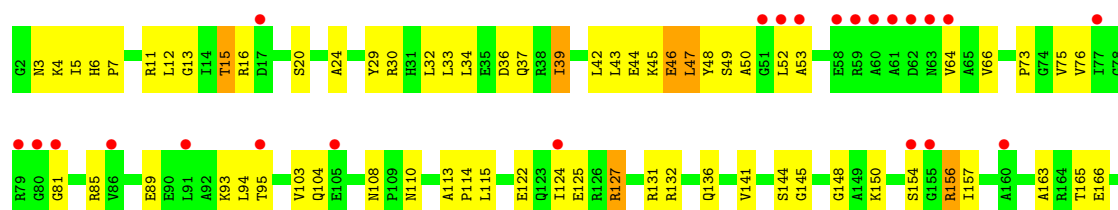
• Molecule 3: 30S Ribosomal protein S3

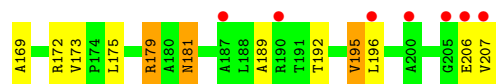
Chain AC: 2% 64% 30% 2%



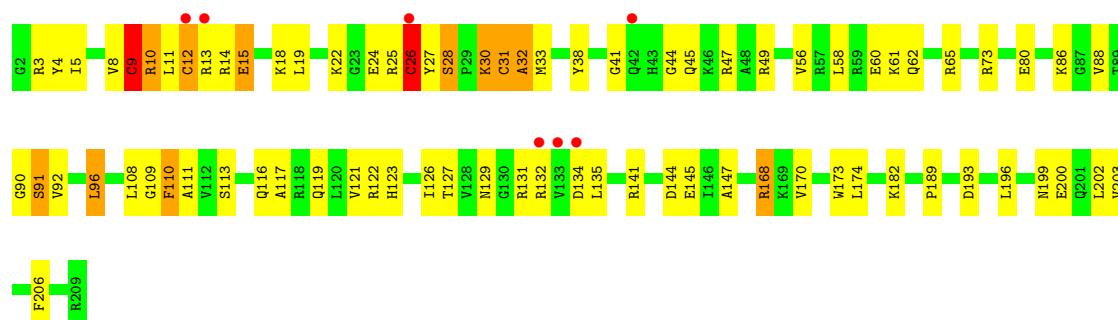
• Molecule 3: 30S Ribosomal protein S3

Chain CC: 15% 62% 34% 1%

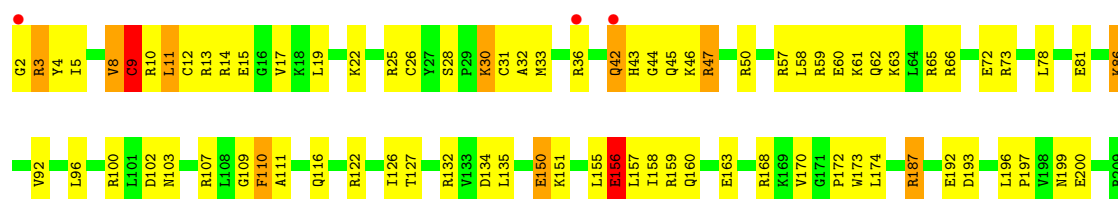




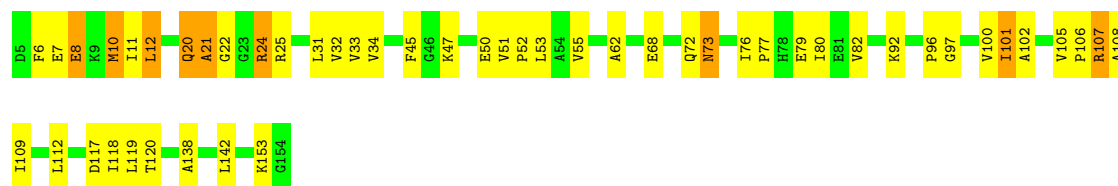
• Molecule 4: 30S Ribosomal protein S4



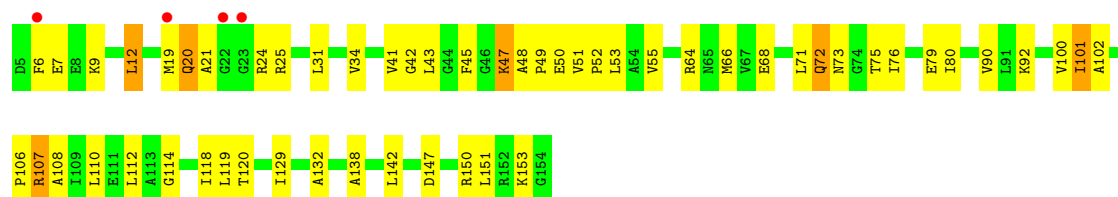
• Molecule 4: 30S Ribosomal protein S4



• Molecule 5: 30S Ribosomal protein S5

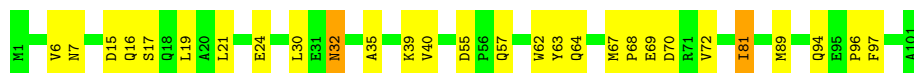


• Molecule 5: 30S Ribosomal protein S5




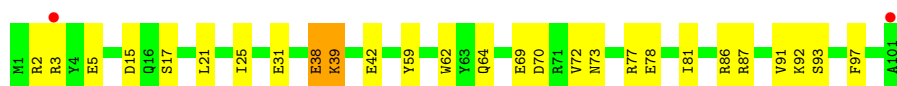
• Molecule 6: 30S Ribosomal protein S6

Chain AF:  72% 26% .




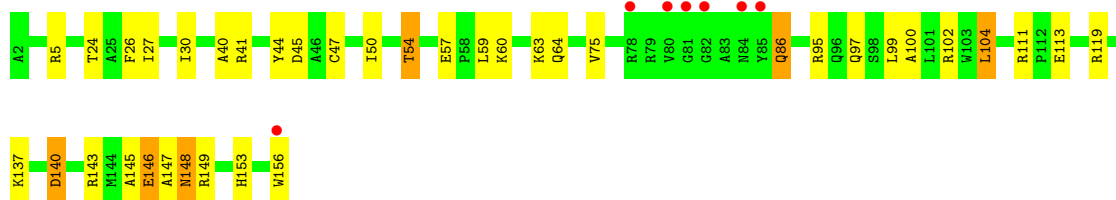
- Molecule 6: 30S Ribosomal protein S6

Chain CF:  73% 25% .




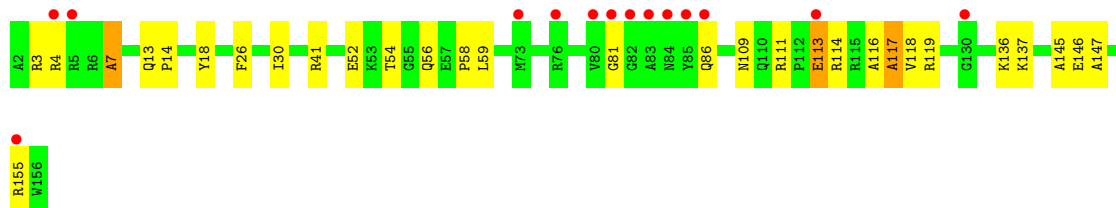
- Molecule 7: 30S Ribosomal protein S7

Chain AG:  75% 21% .



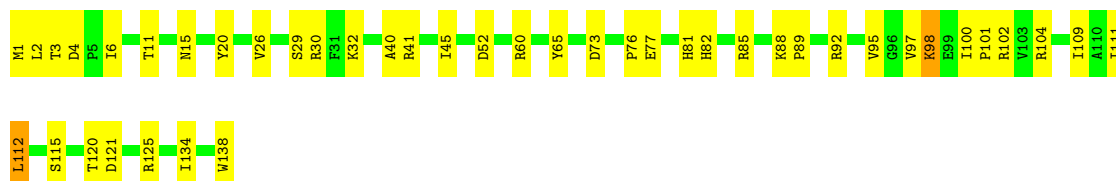
- Molecule 7: 30S Ribosomal protein S7

Chain CG:  81% 17% .




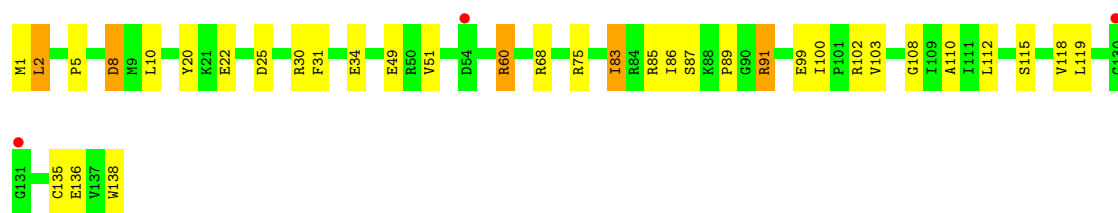
- Molecule 8: 30S Ribosomal protein S8

Chain AH:  69% 30% .

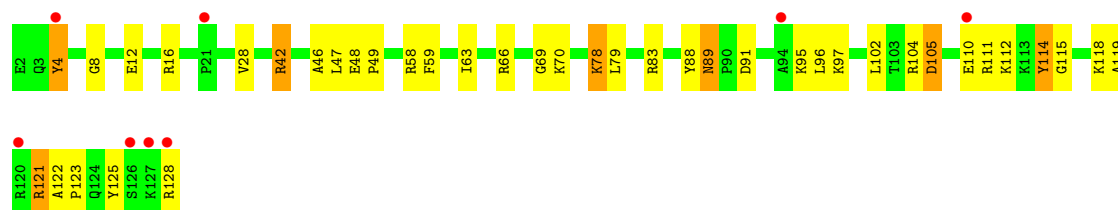


- Molecule 8: 30S Ribosomal protein S8

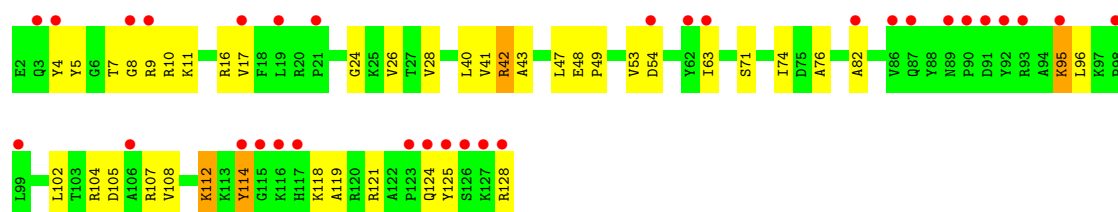
Chain CH:  75% 22% .



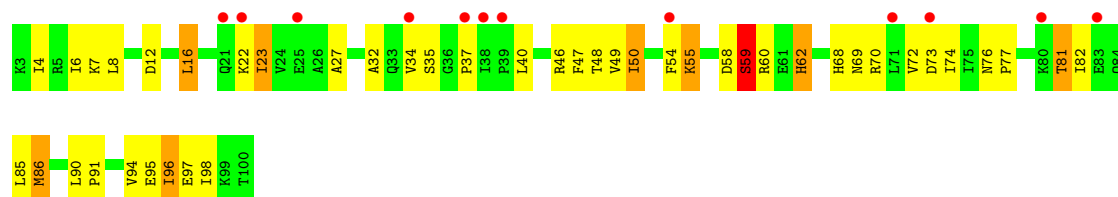
● Molecule 9: 30S Ribosomal protein S9



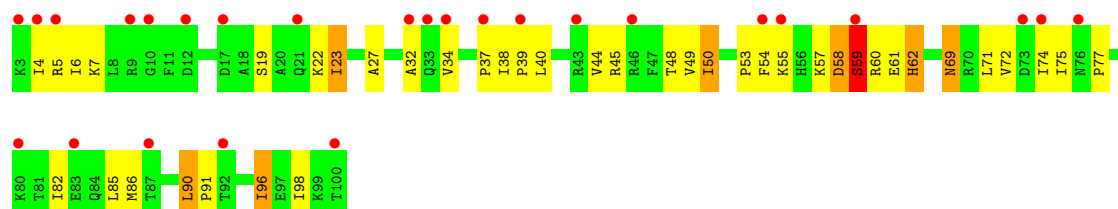
● Molecule 9: 30S Ribosomal protein S9



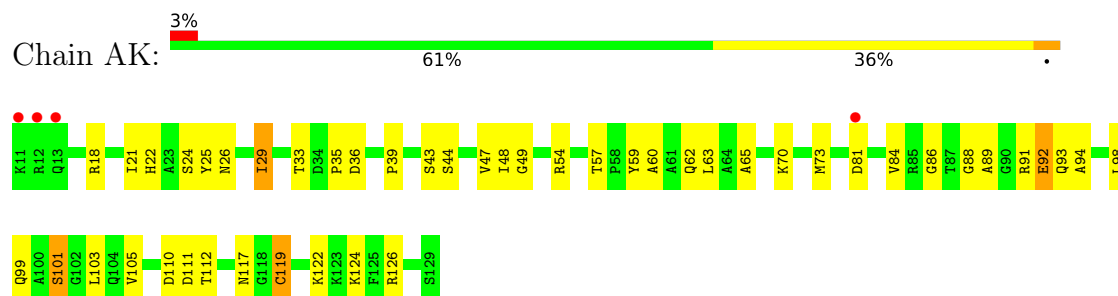
● Molecule 10: 30S Ribosomal protein S10



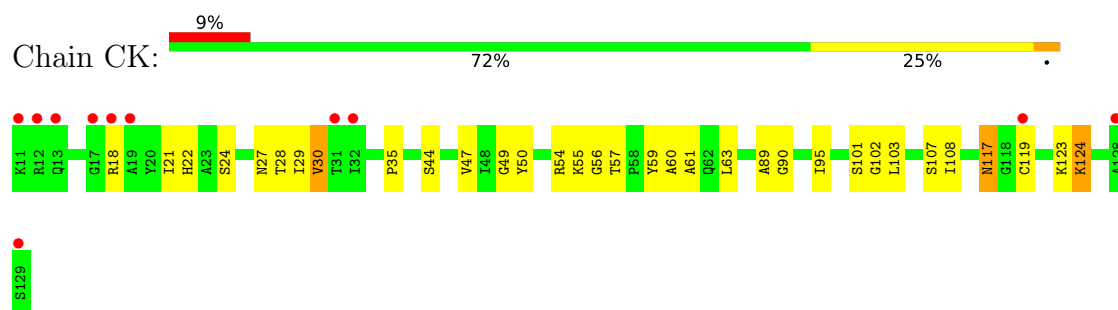
● Molecule 10: 30S Ribosomal protein S10



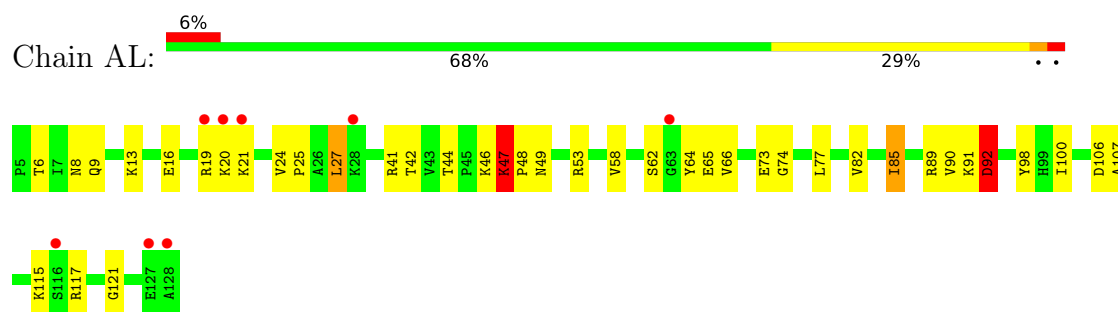
- Molecule 11: 30S Ribosomal protein S11



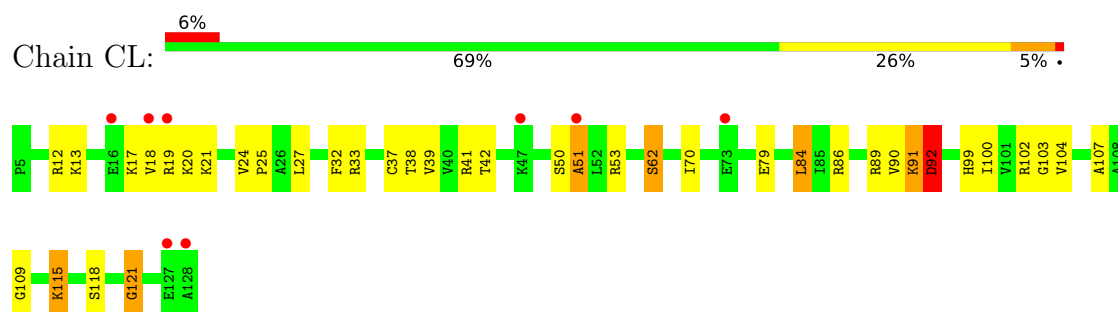
- Molecule 11: 30S Ribosomal protein S11



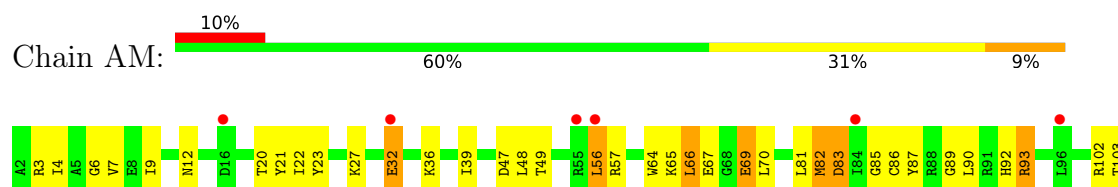
- Molecule 12: 30S Ribosomal protein S12



- Molecule 12: 30S Ribosomal protein S12

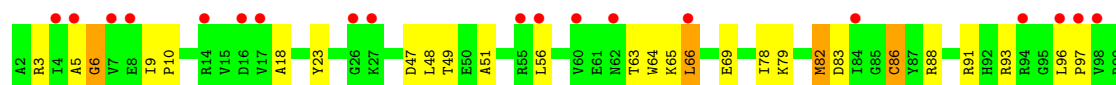


- Molecule 13: 30S Ribosomal protein S13





• Molecule 13: 30S Ribosomal protein S13



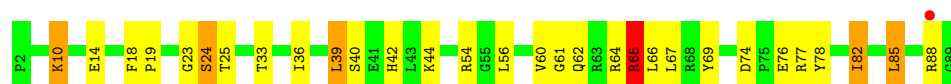
• Molecule 14: 30S Ribosomal protein S14



• Molecule 14: 30S Ribosomal protein S14



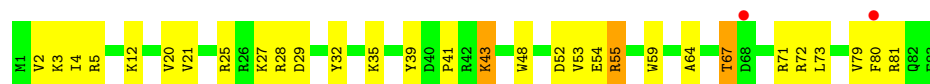
• Molecule 15: 30S Ribosomal protein S15



• Molecule 15: 30S Ribosomal protein S15

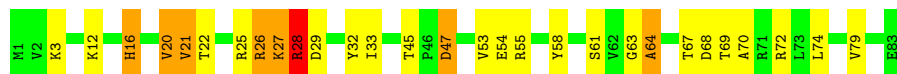


• Molecule 16: 30S Ribosomal protein S16



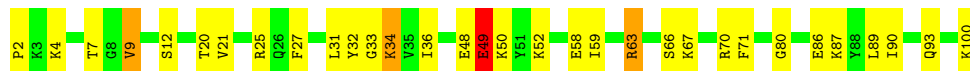
- Molecule 16: 30S Ribosomal protein S16

Chain CP:  65% 25% 8% .




- Molecule 17: 30S Ribosomal protein S17

Chain AQ:  68% 28% . .



- Molecule 17: 30S Ribosomal protein S17

Chain CQ:  2% 76% 21% .



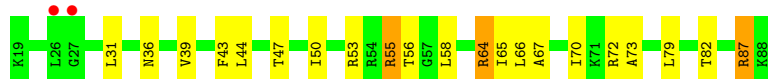
- Molecule 18: 30S Ribosomal protein S18

Chain AR:  % 69% 26% . .



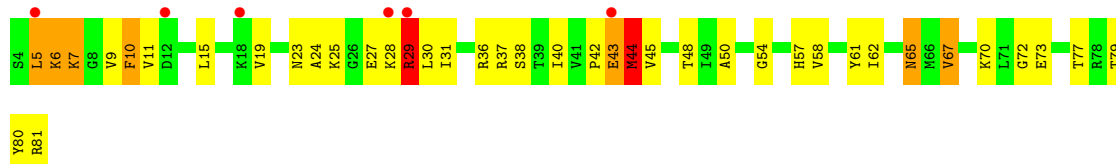
- Molecule 18: 30S Ribosomal protein S18

Chain CR:  3% 70% 26% .



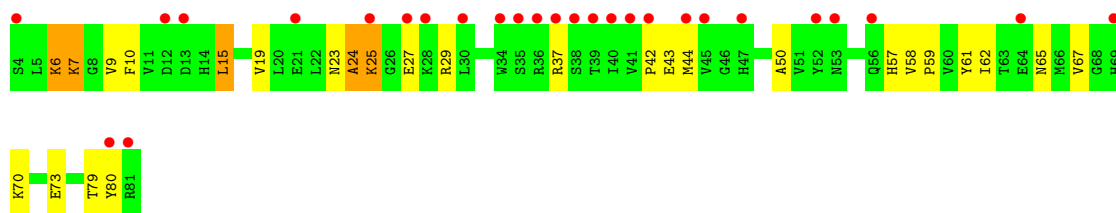
- Molecule 19: 30S Ribosomal protein S19

Chain AS:  8% 49% 40% 9% .



- Molecule 19: 30S Ribosomal protein S19

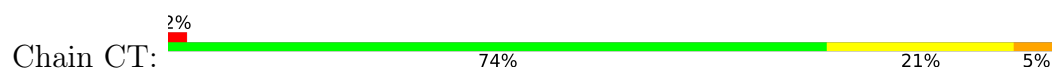
Chain CS:  35% 65% 28% 6%



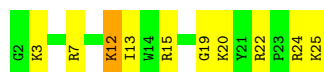
• Molecule 20: 30S Ribosomal protein S20



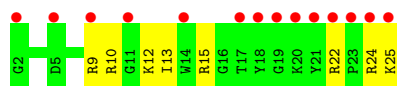
• Molecule 20: 30S Ribosomal protein S20



• Molecule 21: 30S Ribosomal protein THX



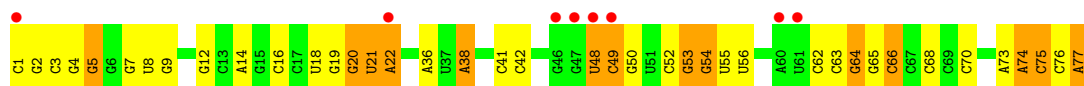
• Molecule 21: 30S Ribosomal protein THX



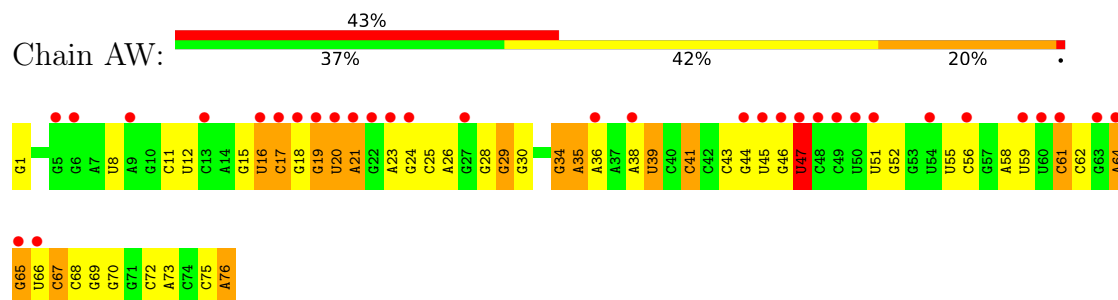
• Molecule 22: P-SITE tRNA



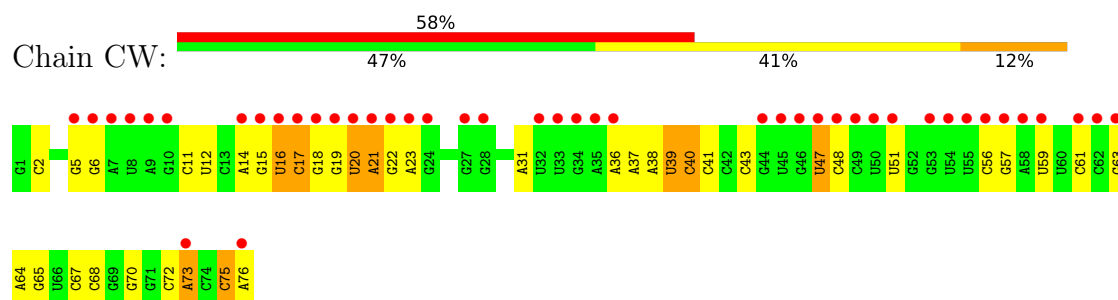
• Molecule 22: P-SITE tRNA



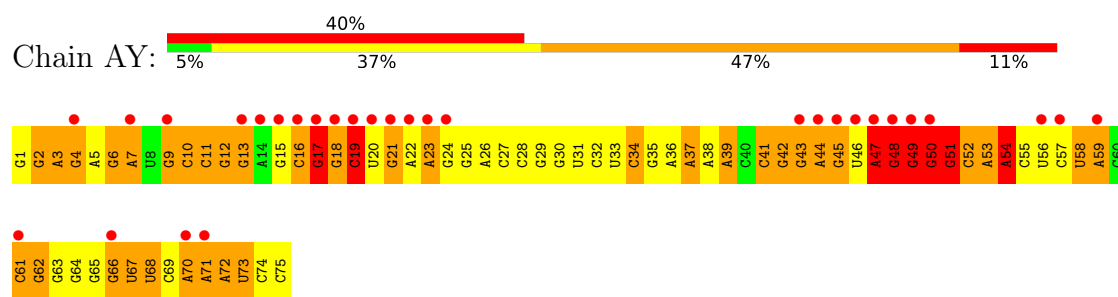
- Molecule 23: E-SITE tRNA



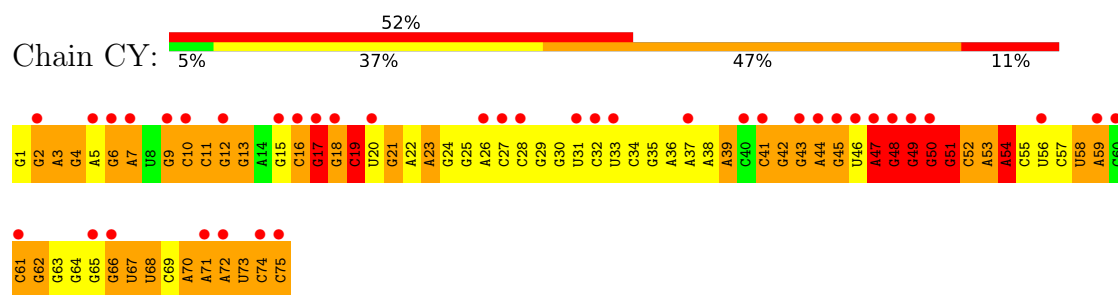
- Molecule 23: E-SITE tRNA



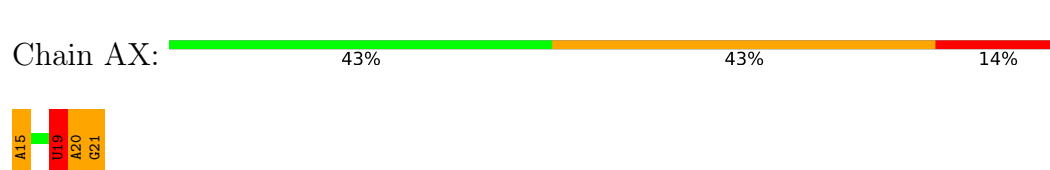
- Molecule 24: A-SITE tRNA



- Molecule 24: A-SITE tRNA

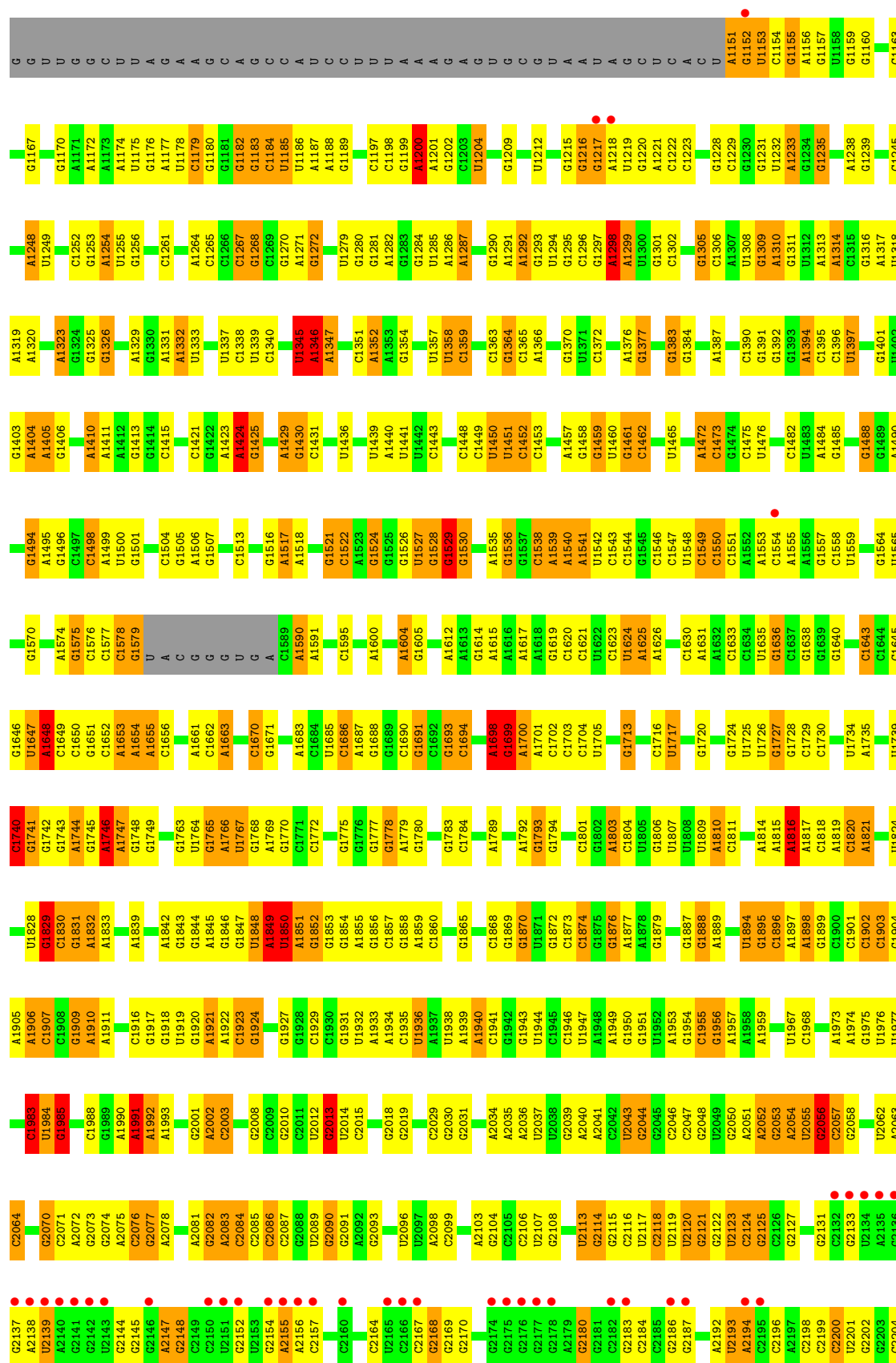


- Molecule 25: mRNA



- Molecule 26: 23S ribosomal RNA

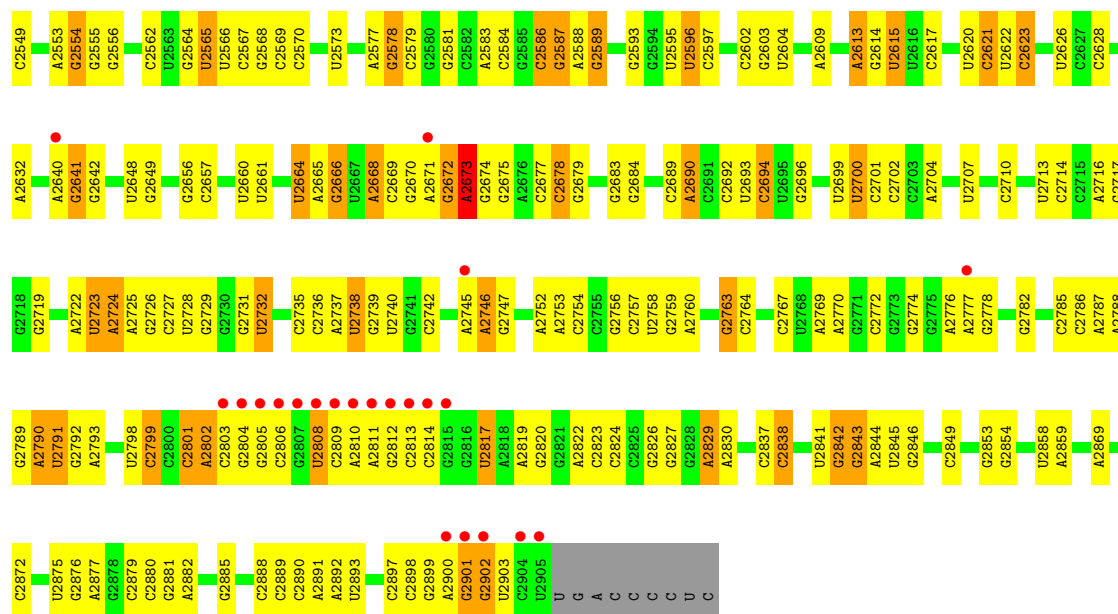






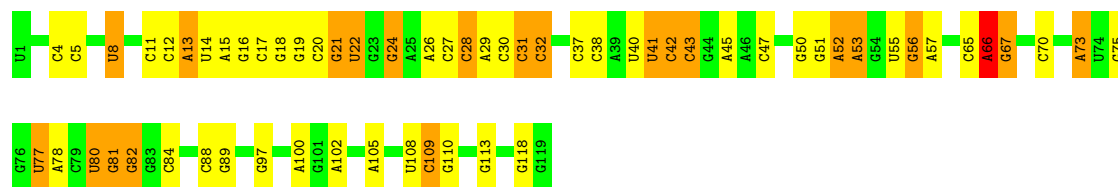
U1374	U1294	A1200	A1065	G988	A916	A929	A752	G675	G599	G519	G433	C342	A260
C1375	G1295	A1201	A1066	A989	A916	A930	A752	C676	A600	G520	G434	A343	U284
A1376	C1296	G1205	U1067	G990	G920	G831	G753	A	G601	U524	G435	G344	C265
C1378	A1298	G1206	U1068	G991	G920	C832	C754	A	C602	U524	G436	A345	G266
G1379	G1297	U1207	G1069	G992	A924	U833	U755	G	C603	A526	G437	G346	G267
U1380	G1301	G1208	U1070	G996	G925	A834	G763	C	G604	A527	A438	A347	G268
A1381	C1302	U1209	U1071	G996	G925	A835	A764	G	G605	U528	C439	C350	C269
G1382	G1303	U1210	A1072	U1002	G928	C836	A768	G	A609	A529	G440	U351	U270
G1383	U1211	U1211	G1075	A1003	G929	C837	A768	C	C609	U529	G444	G352	U271
G1392	U1212	U1212	U1076	A1004	C930	A839	G769	C	U610	U532	A445	A353	G272
G1393	G1213	G1213	A1077	G1005	C931	G940	U770	G	C611	C533	C446	A354	U273
A1394	U1312	U1312	G1083	U1007	C932	C841	G771	C	U611	C534	U447	A355	C274
G1399	A1314	G1216	C1084	U1008	A833	C841	G772	A	G620	U535	A448	G356	C275
G1400	C1315	G1217	U1085	C1008	G934	A948	A773	C	G621	G536	A449	C357	G276
G1401	U1316	G1218	C1086	G1010	C935	G851	G775	G	G622	A537	U454	C360	G282
G1402	A1317	U1219	U1087	G1011	A936	C852	G776	C	G623	U545	A455	G361	G283
U1403	U1318	A1221	C1088	U1013	G937	U853	C776	G	A625	U546	G456	U362	U284
A1404	G1323	C1222	U1089	C1014	C938	C852	G779	C	G626	C547	C459	G365	C285
A1405	G1324	C1223	A1090	A1017	U940	C860	G780	C	G627	U548	U460	C366	U286
G1409	U1325	A1226	G1091	G1018	C942	C860	G782	G	U629	U550	U466	G374	U
A1410	G1326	U1232	A1093	C1021	C943	C863	G783	A	C551	C551	U466	G375	G288
G1413	U1327	A1233	U1094	G1022	A944	G864	G785	A	A553	U553	C469	G376	G289
G1414	G1328	G1239	A1095	A1025	A945	A865	G786	A	G634	U554	C470	G376	G290
C1415	U1329	U1244	G1096	A1026	C948	A866	G787	G	G635	C555	C471	G379	C294
G1420	A1330	C1244	C1098	C1027	C949	A867	G791	U703	U636	A556	U472	G390	U295
C1421	C1331	G1161	A	A1028	U952	U873	A792	G705	G638	U557	U473	U381	C296
G1422	U1332	C1161	G	G1032	C953	U874	U793	G706	A639	U563	C480	U385	G297
A1423	G1333	G1162	A	G1033	A954	A875	G794	C707	G640	C564	C481	C386	A
G1424	C1334	C1163	G	C1036	A955	G876	G794	G708	G641	C566	A482	A387	C
G1425	U1335	U1167	U	U1037	C959	U877	A797	G709	G642	C567	G483	G388	C302
U1429	U1336	G1168	U	G1038	G961	U879	G798	C710	G644	G	G488	G389	C303
G1430	A1346	A1173	G	C1039	A962	C880	C800	G711	A645	C	U489	C390	G304
A1431	G1347	U1174	C	C1040	A963	A881	C801	A716	G646	A570	A312	U391	A
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U1439	G1351	C1179	A	U1044	G966	U885	C804	C719	G649	U575	G493	C394	G319
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U1442	G1354	U1182	G	G1047	G972	G891	G809	A722	G655	A497	A497	G412	A323
C1443	U1355	G1183	A	U1048	G973	C892	A810	C724	A655	U581	G498	U413	G327
G1447	C1356	C1184	C	C1050	U974	U893	G811	G725	G656	U584	G499	G414	G328
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U1451	A1367	G1189	U	G1056	U981	C903	U819	G732	A667	U591	G506	C418	G332
C1452	G1368	U1190	C	U1057	U982	U904	A820	A735	A668	G592	A507	C419	A333
G1453	U1369	G1191	U	C1058	G982	G905	G821	G736	G669	A594	A508	A420	A334
C1454	G1370	C1195	U	U1059	A885	U906	G822	C737	A670	G595	G515	U421	G335
G1455	U1371	C1198	U	G1060	G886	A907	G826	G746	G671	C596	A516	G422	C336
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A1457	G1373	G1293					A828			U598	G518	G432	

G2468	G2469	G2470	G2471	G2472	G2473	G2474	G2475	G2476	G2477	G2478	G2479	G2480	G2481	G2482	G2483	G2484	G2485	G2486	G2487	G2488	G2489	G2490	G2491	G2492	G2493	G2494	G2495	G2496	G2497	G2498	G2499	G2500	G2501	G2502	G2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	G2513	G2514	G2515	G2516	G2517	G2518	G2519	G2520	G2521	G2522	G2523	G2524	G2525	G2526	G2527	G2528	G2529	G2530	G2531	G2532	G2533	G2534	G2535	G2536	G2537	G2538	G2539	G2540	G2541	G2542	G2543	G2544	G2545	G2546	G2547	G2548																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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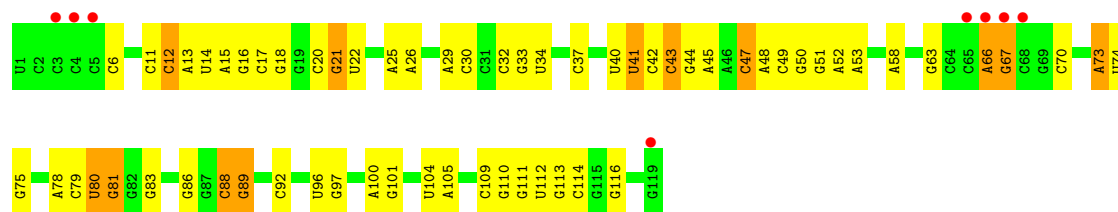
• Molecule 27: 5S ribosomal RNA

Chain BB: 49% 33% 18%



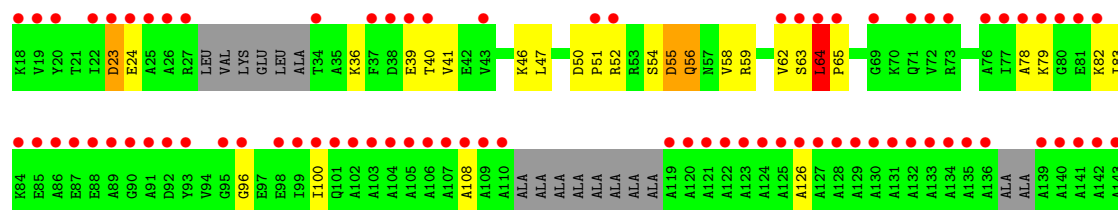
• Molecule 27: 5S ribosomal RNA

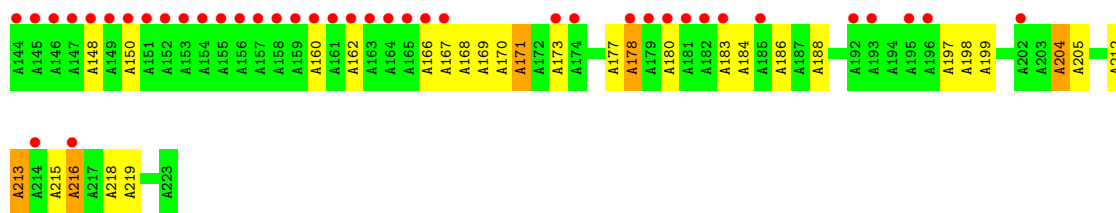
Chain DB: 7% 47% 43% 10%



• Molecule 28: 50S ribosomal protein L1

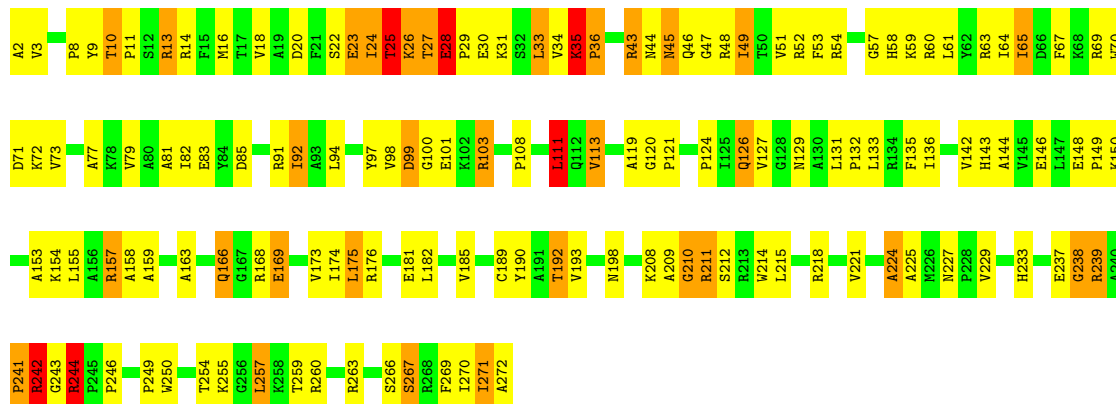
Chain BC: 58% 65% 23% 8%





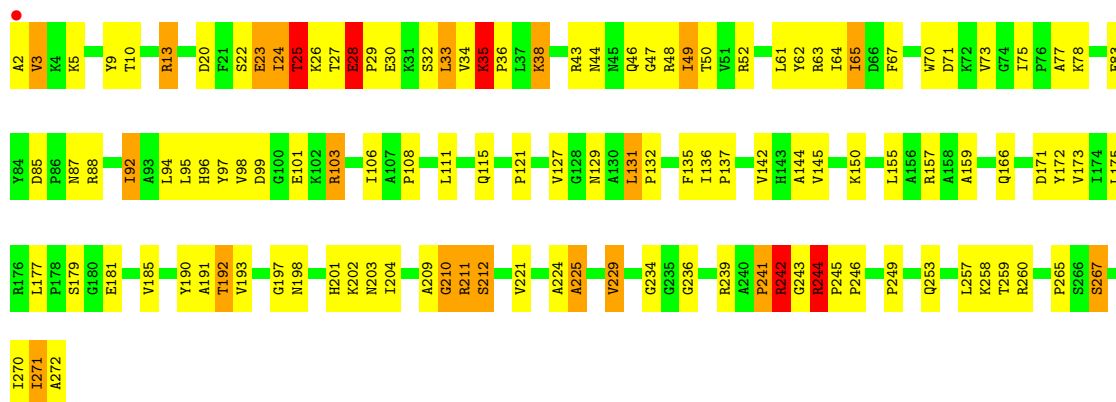
• Molecule 29: 50S ribosomal protein L2

Chain BD: 46% 40% 11% .



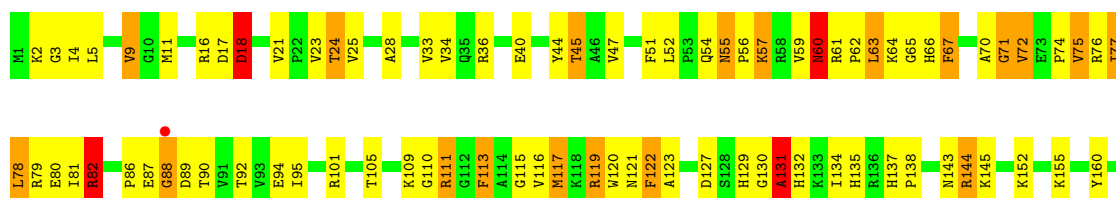
• Molecule 29: 50S ribosomal protein L2

Chain DD: 55% 35% 7% .



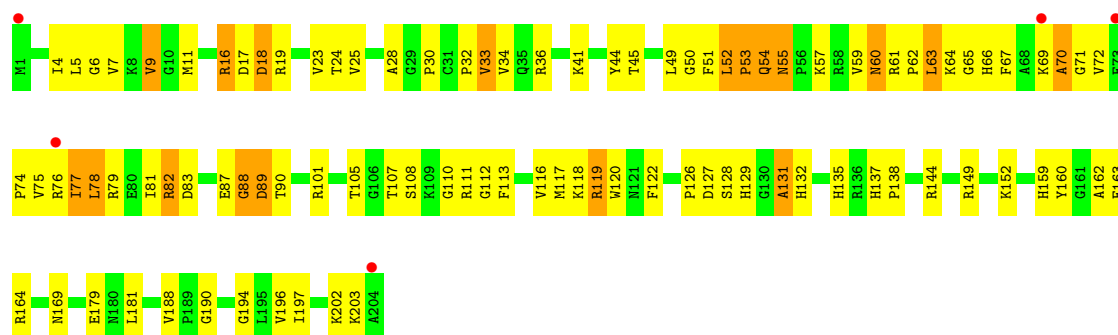
• Molecule 30: 50S ribosomal protein L3

Chain BE: 50% 37% 11% .

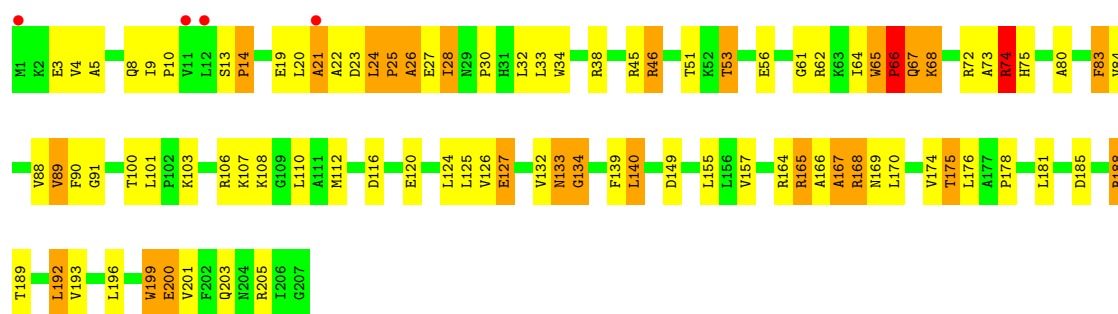




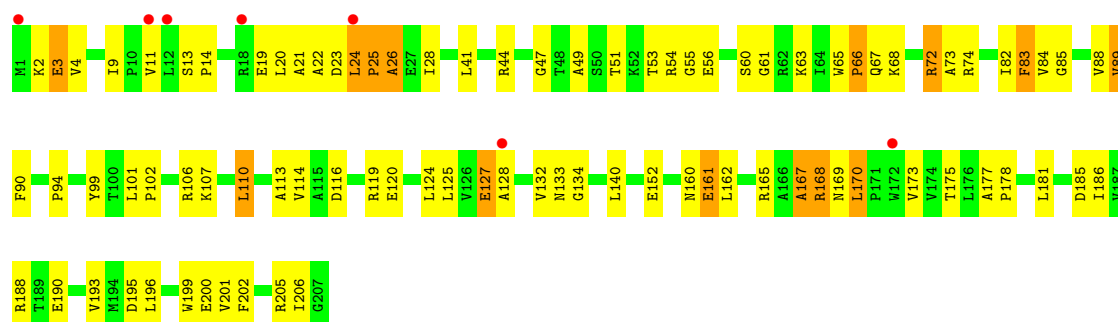
• Molecule 30: 50S ribosomal protein L3



• Molecule 31: 50S ribosomal protein L4

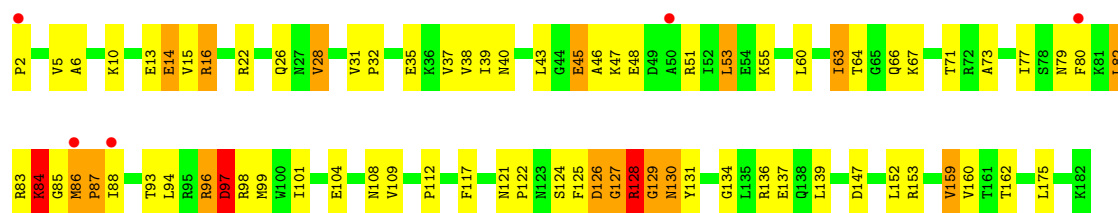


• Molecule 31: 50S ribosomal protein L4

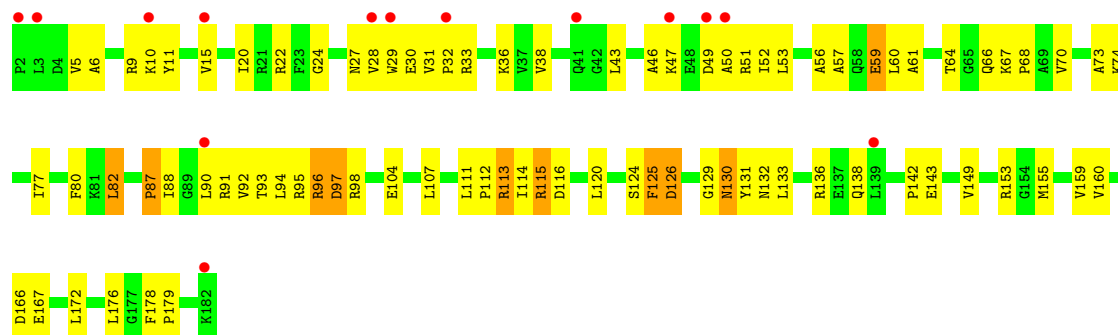


• Molecule 32: 50S ribosomal protein L5

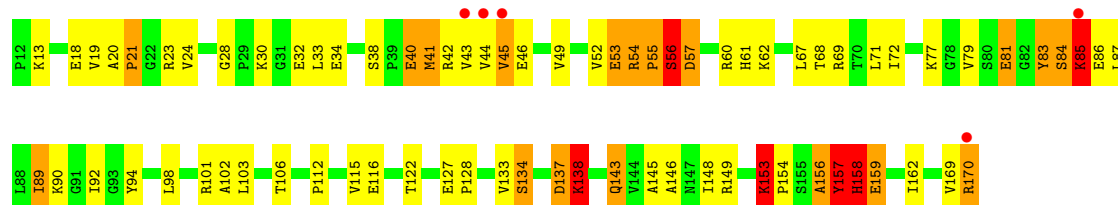




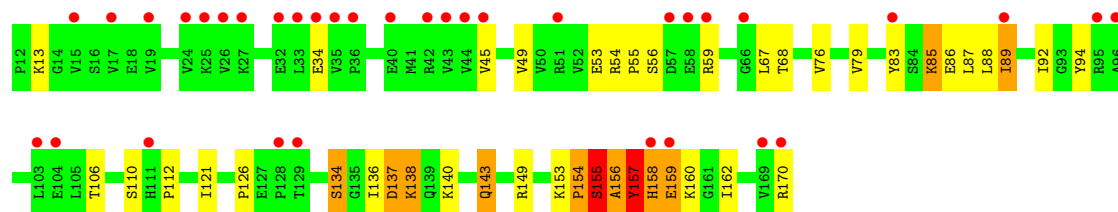
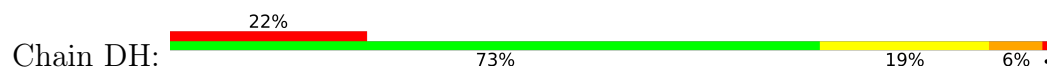
• Molecule 32: 50S ribosomal protein L5



• Molecule 33: 50S ribosomal protein L6

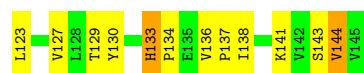


• Molecule 33: 50S ribosomal protein L6



• Molecule 34: 50S ribosomal protein L9

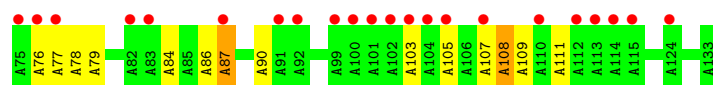
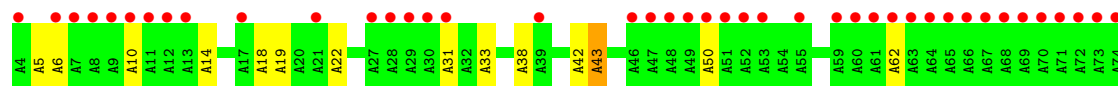
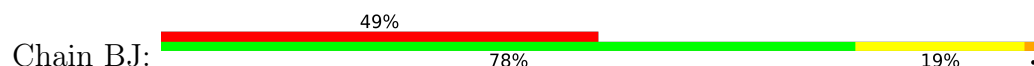




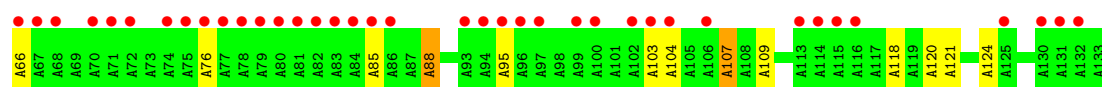
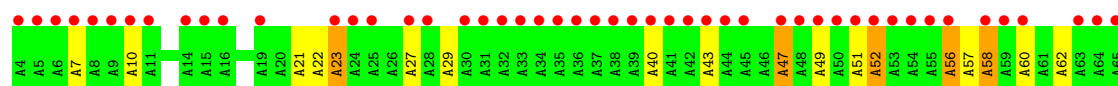
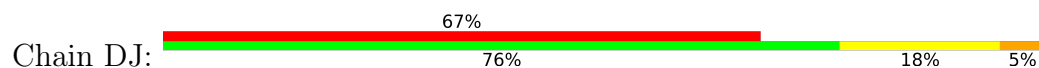
- Molecule 34: 50S ribosomal protein L9



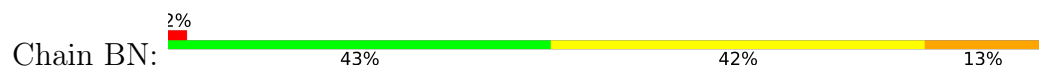
- Molecule 35: 50S ribosomal protein L10



- Molecule 35: 50S ribosomal protein L10

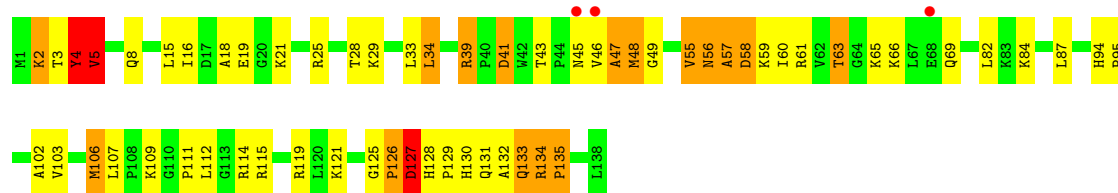


- Molecule 36: 50S ribosomal protein L13



- Molecule 36: 50S ribosomal protein L13





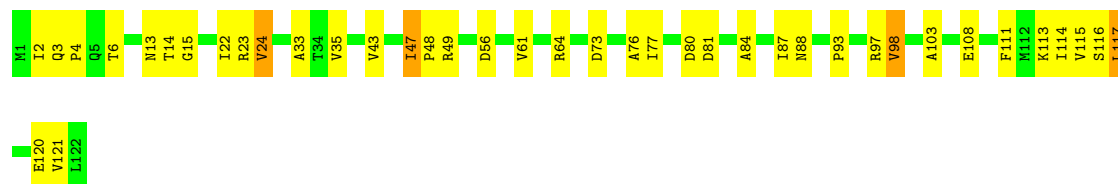
• Molecule 37: 50S ribosomal protein L14

Chain BO: 64% 34%



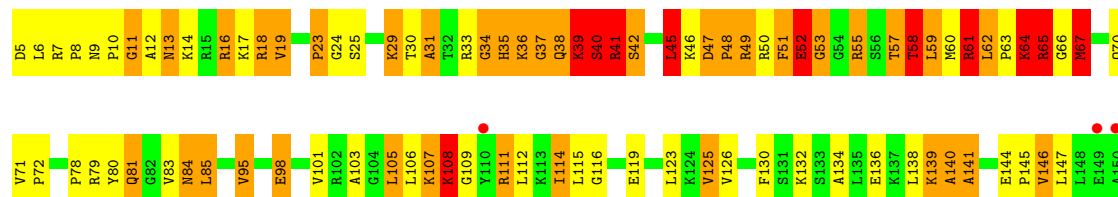
• Molecule 37: 50S ribosomal protein L14

Chain DO: 67% 30%



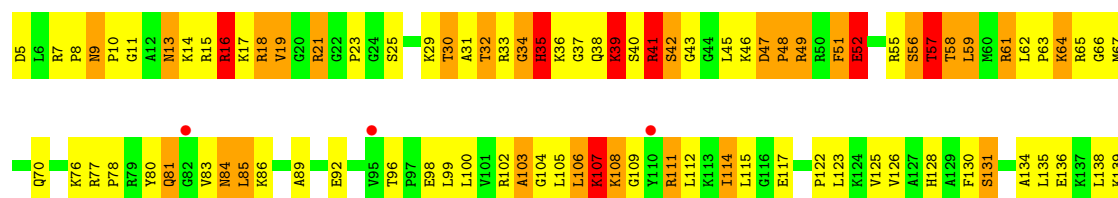
• Molecule 38: 50S ribosomal protein L15

Chain BP: 38% 29% 25% 8%



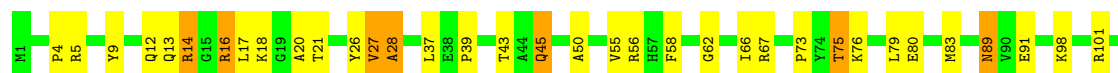
• Molecule 38: 50S ribosomal protein L15

Chain DP: 34% 42% 19% 5%

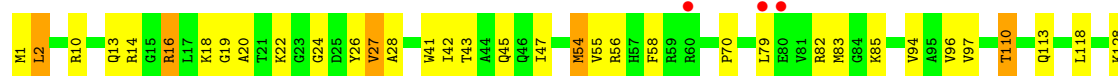
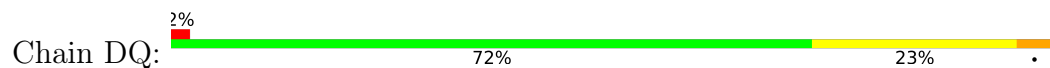




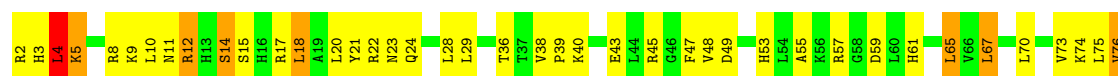
• Molecule 39: 50S ribosomal protein L16



• Molecule 39: 50S ribosomal protein L16



• Molecule 40: 50S ribosomal protein L17

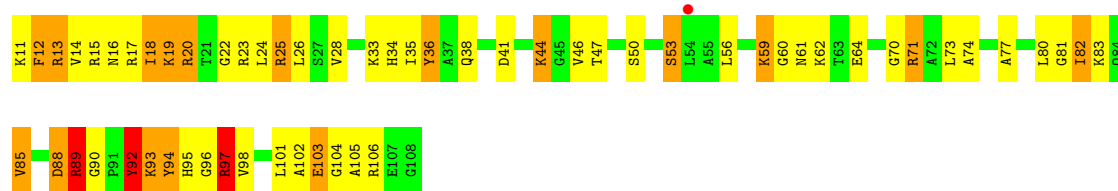


• Molecule 40: 50S ribosomal protein L17

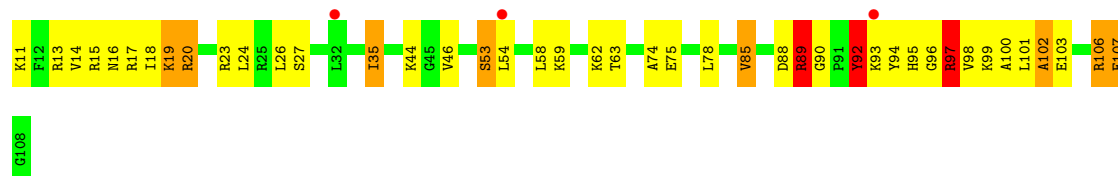


• Molecule 41: 50S ribosomal protein L18

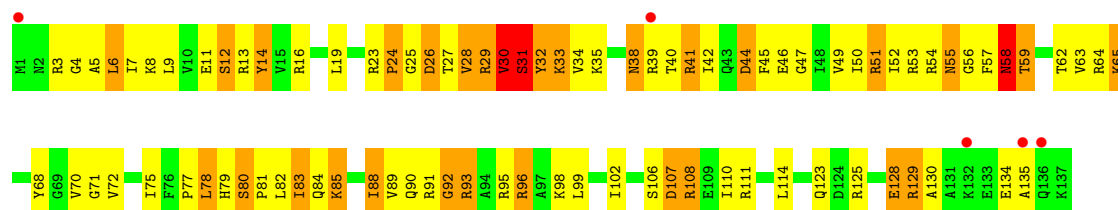




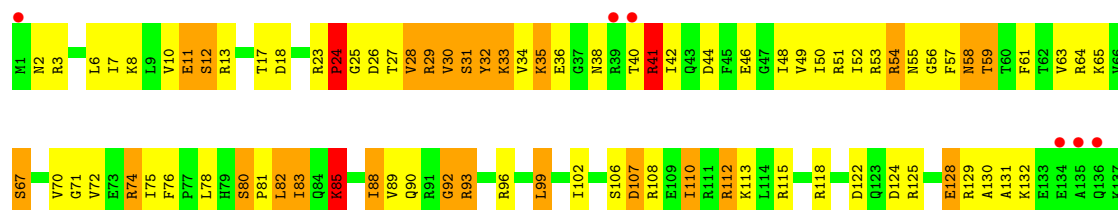
• Molecule 41: 50S ribosomal protein L18



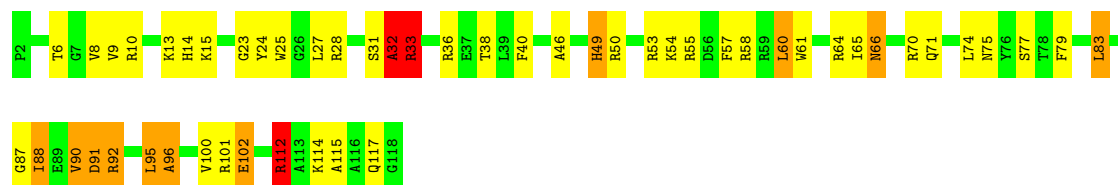
• Molecule 42: 50S ribosomal protein L19



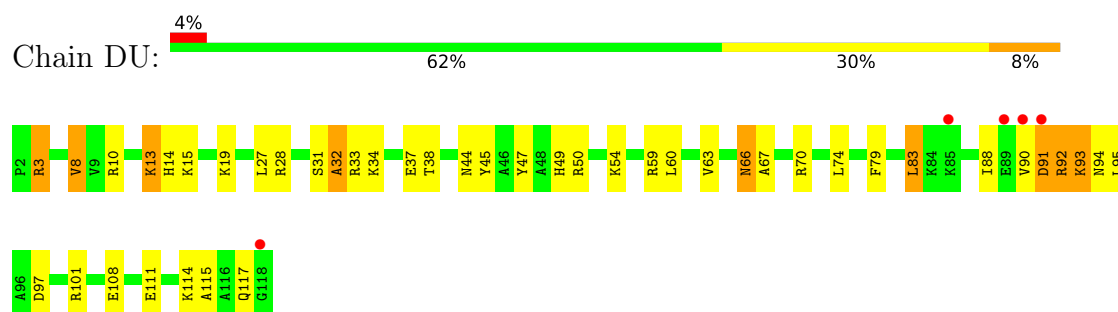
• Molecule 42: 50S ribosomal protein L19



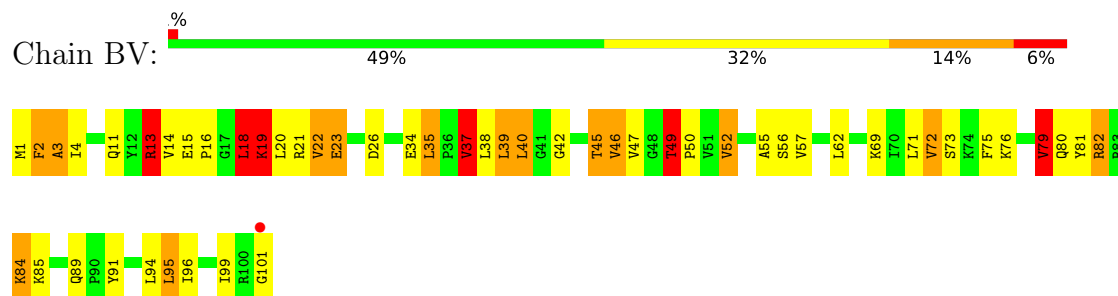
• Molecule 43: 50S ribosomal protein L20



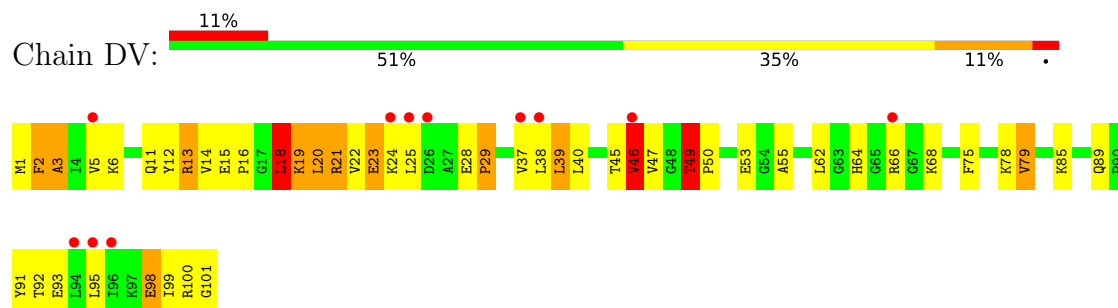
• Molecule 43: 50S ribosomal protein L20



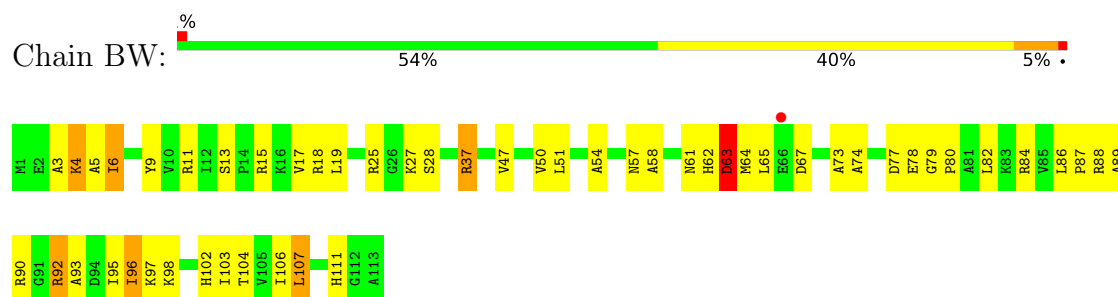
- Molecule 44: 50S ribosomal protein L21



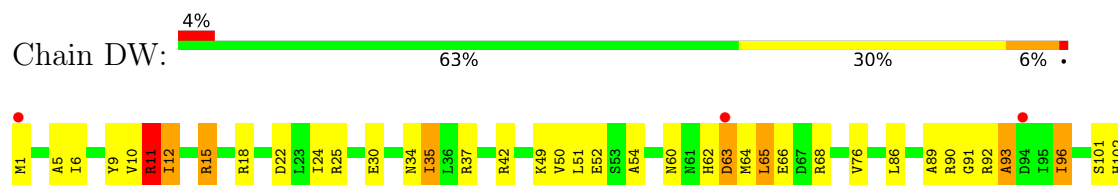
- Molecule 44: 50S ribosomal protein L21



- Molecule 45: 50S ribosomal protein L22



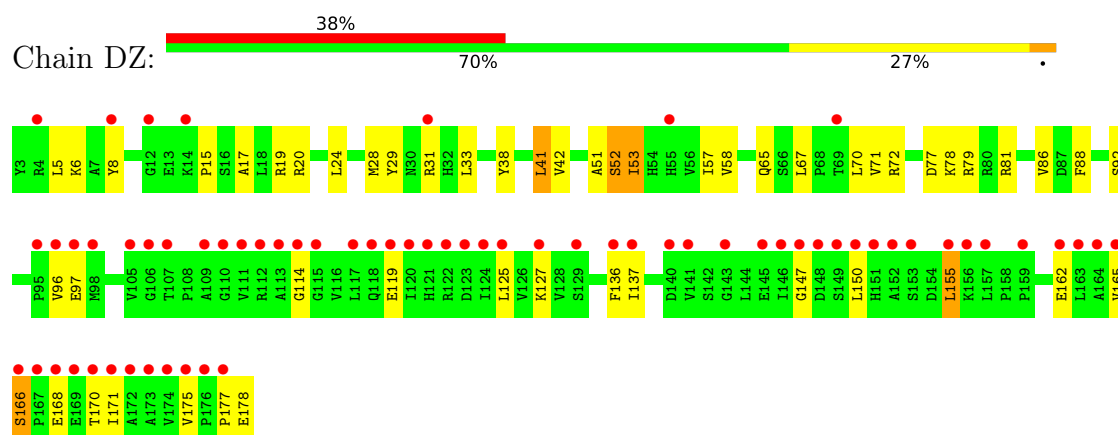
- Molecule 45: 50S ribosomal protein L22



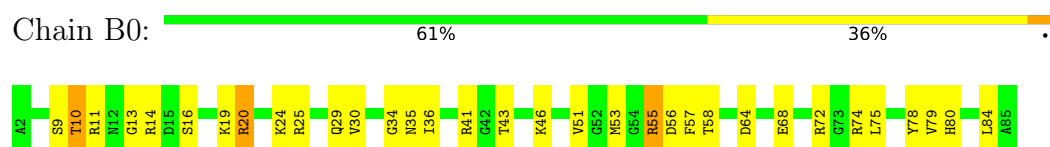




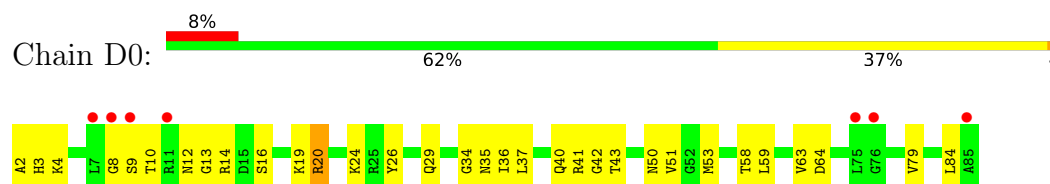
• Molecule 48: 50S ribosomal protein L25



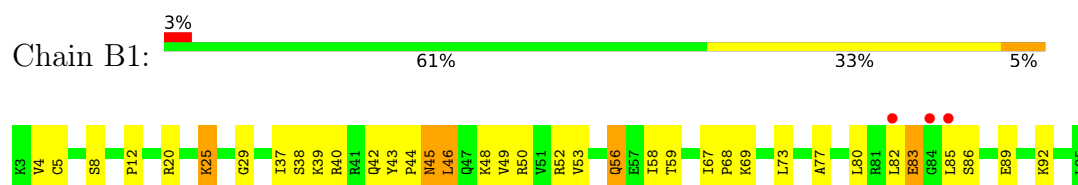
• Molecule 49: 50S ribosomal protein L27



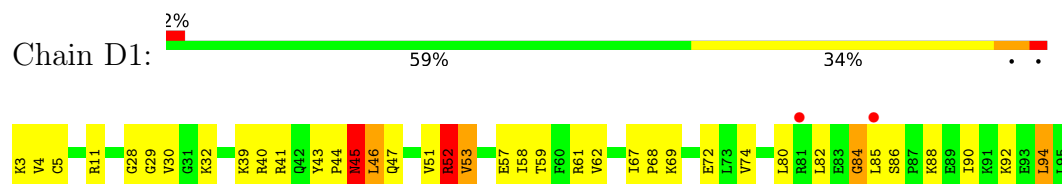
• Molecule 49: 50S ribosomal protein L27



• Molecule 50: 50S ribosomal protein L28

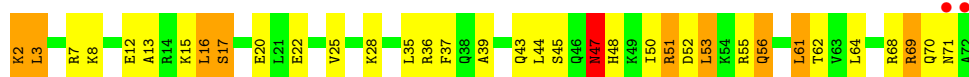


• Molecule 50: 50S ribosomal protein L28

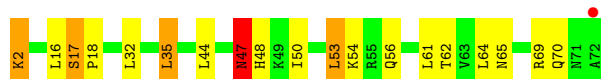
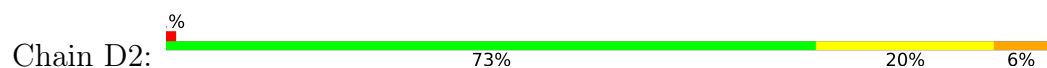


• Molecule 51: 50S ribosomal protein L29

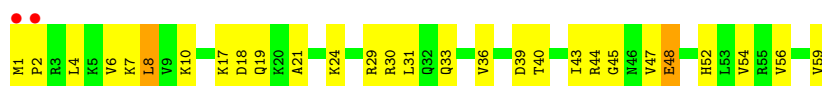




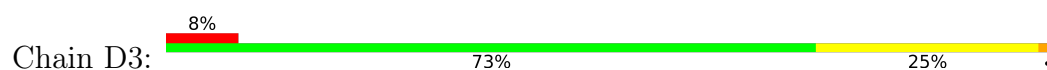
- Molecule 51: 50S ribosomal protein L29



- Molecule 52: 50S ribosomal protein L30



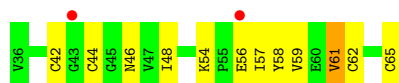
- Molecule 52: 50S ribosomal protein L30



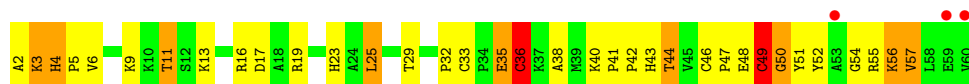
- Molecule 53: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L31



- Molecule 54: 50S ribosomal protein L32



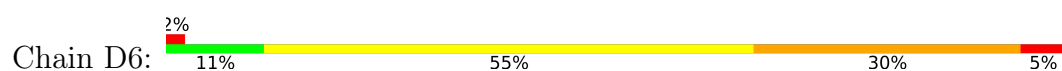
- Molecule 54: 50S ribosomal protein L32



- Molecule 55: 50S ribosomal protein L33



- Molecule 55: 50S ribosomal protein L33



- Molecule 56: 50S ribosomal protein L34



- Molecule 56: 50S ribosomal protein L34



- Molecule 57: 50S ribosomal protein L35



- Molecule 57: 50S ribosomal protein L35




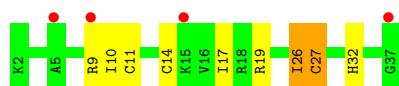
- Molecule 58: 50S ribosomal protein L36

Chain B9:  47% 42% 8% 3%




- Molecule 58: 50S ribosomal protein L36

Chain D9:  11% 75% 19% 6%




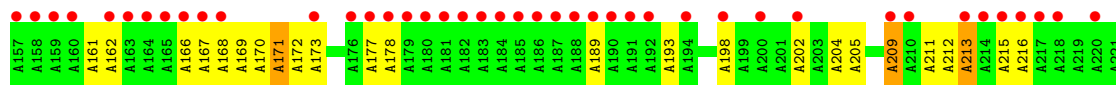
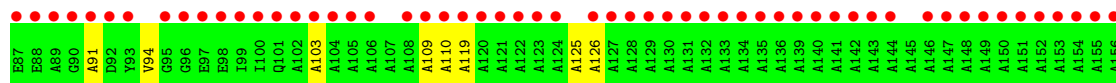
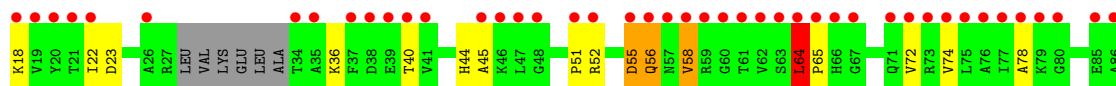
- Molecule 59: mRNA

Chain CX:  25% 25% 25% 50%



- Molecule 60: 50S Ribosomal protein L1

Chain DC:  73% 72% 21% 4%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.92Å 449.90Å 624.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.57 – 3.30 39.57 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.6 (39.57-3.30) 95.6 (39.57-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0031	Depositor
R, $R_{free}$	0.225 , 0.279 0.230 , 0.279	Depositor DCC
$R_{free}$ test set	41956 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 66.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	295724	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	4/36190 (0.0%)	0.75	26/56486 (0.0%)
1	CA	0.40	1/36190 (0.0%)	0.73	17/56486 (0.0%)
2	AB	0.43	0/1936	0.67	0/2609
2	CB	0.44	0/1936	0.64	0/2609
3	AC	0.49	0/1637	0.71	0/2205
3	CC	0.44	0/1637	0.67	0/2205
4	AD	0.54	0/1733	0.84	4/2318 (0.2%)
4	CD	0.52	0/1733	0.77	1/2318 (0.0%)
5	AE	0.45	0/1163	0.76	0/1564
5	CE	0.46	0/1163	0.72	0/1564
6	AF	0.49	0/856	0.77	1/1154 (0.1%)
6	CF	0.48	0/856	0.75	0/1154
7	AG	0.43	0/1276	0.65	0/1709
7	CG	0.40	0/1276	0.64	0/1709
8	AH	0.47	0/1136	0.72	0/1527
8	CH	0.45	0/1136	0.69	0/1527
9	AI	0.48	0/1029	0.71	0/1378
9	CI	0.42	0/1029	0.68	0/1378
10	AJ	0.47	0/808	0.76	0/1085
10	CJ	0.46	0/808	0.68	0/1085
11	AK	0.49	0/900	0.71	0/1213
11	CK	0.45	0/900	0.70	0/1213
12	AL	0.55	0/987	0.81	0/1320
12	CL	0.50	0/987	0.77	0/1320
13	AM	0.45	0/999	0.78	0/1336
13	CM	0.43	0/999	0.68	0/1336
14	AN	0.50	0/501	0.88	1/664 (0.2%)
14	CN	0.46	0/501	0.74	0/664
15	AO	0.46	0/745	0.70	0/992
15	CO	0.40	0/745	0.64	0/992
16	AP	0.47	0/717	0.74	0/963
16	CP	0.50	0/717	0.78	1/963 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.44	0/837	0.70	0/1117
17	CQ	0.46	0/837	0.72	0/1117
18	AR	0.47	0/579	0.79	0/768
18	CR	0.47	0/579	0.69	0/768
19	AS	0.47	0/643	0.68	0/865
19	CS	0.43	0/643	0.61	0/865
20	AT	0.45	0/765	0.70	0/1007
20	CT	0.43	0/765	0.71	0/1007
21	AU	0.52	0/213	0.71	0/277
21	CU	0.53	0/213	0.68	0/277
22	AV	0.40	0/1832	0.75	1/2855 (0.0%)
22	CV	0.38	0/1832	0.72	0/2855
23	AW	0.29	0/1809	0.68	2/2819 (0.1%)
23	CW	0.27	0/1809	0.70	1/2819 (0.0%)
24	AY	0.86	17/1815 (0.9%)	0.94	1/2833 (0.0%)
24	CY	0.86	17/1815 (0.9%)	0.94	1/2833 (0.0%)
25	AX	0.31	0/147	0.72	0/227
26	BA	0.57	22/67709 (0.0%)	0.91	196/105690 (0.2%)
26	DA	0.45	5/67709 (0.0%)	0.80	93/105690 (0.1%)
27	BB	0.45	0/2853	0.81	3/4451 (0.1%)
27	DB	0.35	0/2853	0.72	0/4451
28	BC	0.46	0/1160	0.59	0/1584
29	BD	0.71	0/2155	0.95	1/2905 (0.0%)
29	DD	0.60	0/2155	0.85	0/2905
30	BE	0.70	1/1597 (0.1%)	0.91	1/2153 (0.0%)
30	DE	0.56	1/1597 (0.1%)	0.83	2/2153 (0.1%)
31	BF	0.68	0/1659	0.88	1/2244 (0.0%)
31	DF	0.52	0/1659	0.75	0/2244
32	BG	0.49	0/1499	0.74	0/2016
32	DG	0.44	0/1499	0.67	0/2016
33	BH	0.64	1/1246 (0.1%)	0.88	2/1682 (0.1%)
33	DH	0.47	0/1246	0.67	1/1682 (0.1%)
34	BI	0.48	0/1147	0.75	1/1551 (0.1%)
34	DI	0.47	0/1147	0.72	0/1551
35	BJ	0.51	0/650	0.55	0/907
35	DJ	0.44	0/650	0.53	0/907
36	BN	0.70	0/1132	0.96	0/1525
36	DN	0.49	0/1132	0.77	0/1525
37	BO	0.57	0/943	0.81	0/1269
37	DO	0.53	0/943	0.78	0/1269
38	BP	0.71	0/1131	1.09	3/1504 (0.2%)
38	DP	0.57	0/1131	0.98	2/1504 (0.1%)
39	BQ	0.58	0/1143	0.85	1/1527 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	DQ	0.46	0/1143	0.68	0/1527
40	BR	0.70	0/974	0.98	1/1302 (0.1%)
40	DR	0.54	0/974	0.87	0/1302
41	BS	0.60	0/779	0.98	0/1036
41	DS	0.48	0/779	0.79	0/1036
42	BT	0.59	0/1156	0.97	1/1542 (0.1%)
42	DT	0.58	0/1156	0.95	0/1542
43	BU	0.76	0/975	0.98	1/1297 (0.1%)
43	DU	0.50	0/975	0.75	0/1297
44	BV	0.69	0/790	1.03	4/1057 (0.4%)
44	DV	0.47	0/790	0.76	0/1057
45	BW	0.65	0/907	0.95	1/1216 (0.1%)
45	DW	0.52	0/907	0.77	0/1216
46	BX	0.67	0/740	0.94	1/993 (0.1%)
46	DX	0.52	0/740	0.74	0/993
47	BY	0.68	0/789	0.99	3/1051 (0.3%)
47	DY	0.53	0/789	0.83	0/1051
48	BZ	0.49	0/1436	0.72	0/1949
48	DZ	0.44	0/1436	0.66	0/1949
49	B0	0.61	0/671	0.85	0/892
49	D0	0.51	0/671	0.76	0/892
50	B1	0.62	0/741	0.84	0/984
50	D1	0.53	0/741	0.84	1/984 (0.1%)
51	B2	0.57	0/600	0.86	0/793
51	D2	0.48	0/600	0.79	0/793
52	B3	0.55	0/473	0.87	0/634
52	D3	0.44	0/473	0.70	0/634
53	B4	0.53	0/229	0.79	0/309
53	D4	0.49	0/229	0.75	0/309
54	B5	0.73	0/473	1.08	0/639
54	D5	0.57	0/473	0.88	0/639
55	B6	0.96	1/388 (0.3%)	2.06	4/518 (0.8%)
55	D6	0.83	0/388	1.06	2/518 (0.4%)
56	B7	0.73	0/427	0.96	0/561
56	D7	0.58	0/427	0.85	0/561
57	B8	0.75	0/516	1.12	2/679 (0.3%)
57	D8	0.54	0/516	0.88	1/679 (0.1%)
58	B9	0.69	0/302	1.00	2/397 (0.5%)
58	D9	0.45	0/302	0.73	0/397
59	CX	0.52	0/94	0.72	0/144
60	DC	0.48	0/1160	0.55	0/1584
All	All	0.50	70/321233 (0.0%)	0.81	388/480213 (0.1%)

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	1	0
1	CA	1	0
2	AB	0	1
13	AM	0	1
13	CM	0	1
23	AW	1	0
23	CW	1	0
26	BA	22	0
26	DA	20	0
29	BD	0	3
29	DD	0	2
30	BE	0	2
30	DE	0	1
33	BH	0	1
38	BP	0	10
38	DP	0	4
40	BR	0	2
40	DR	0	1
41	BS	0	1
42	BT	0	3
43	BU	0	3
44	BV	0	2
47	BY	0	1
55	B6	0	1
55	D6	0	1
57	B8	0	1
All	All	46	42

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	B6	47	THR	C-N	8.32	1.53	1.34
24	AY	50	G	C1'-N9	-6.96	1.37	1.46
24	CY	50	G	C1'-N9	-6.95	1.37	1.46
26	BA	1816	A	O3'-P	6.86	1.69	1.61
24	CY	66	G	C1'-N9	-6.73	1.37	1.46

The worst 5 of 388 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	B6	45	LYS	O-C-N	-30.98	73.14	122.70
55	B6	45	LYS	CA-C-N	22.24	166.13	117.20
26	BA	2513	G	O5'-P-OP1	-13.46	93.59	105.70
26	BA	1850	U	O5'-P-OP1	-12.67	94.30	105.70
26	BA	1955	C	C2'-C3'-O3'	12.16	136.24	109.50

5 of 46 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	412	A	C1'
23	AW	47	U	C1'
26	BA	98	G	C1'
26	BA	497	A	C3'
26	BA	715	G	C1',C4',C3'

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	23	ARG	Peptide
13	AM	69	GLU	Peptide
29	BD	224	ALA	Peptide
29	BD	244	ARG	Peptide
29	BD	36	PRO	Peptide

## 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	32329	0	16318	494	1
1	CA	32329	0	16318	469	0
2	AB	1901	0	1951	42	0
2	CB	1901	0	1951	43	0
3	AC	1613	0	1677	43	0
3	CC	1613	0	1677	46	0
4	AD	1703	0	1763	64	0
4	CD	1703	0	1763	50	0
5	AE	1147	0	1207	44	0
5	CE	1147	0	1207	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AF	843	0	857	14	0
6	CF	843	0	857	18	0
7	AG	1257	0	1296	20	0
7	CG	1257	0	1296	12	0
8	AH	1116	0	1177	28	0
8	CH	1116	0	1177	17	0
9	AI	1011	0	1043	31	0
9	CI	1011	0	1043	27	0
10	AJ	795	0	840	36	0
10	CJ	795	0	840	36	0
11	AK	885	0	904	31	0
11	CK	885	0	904	17	0
12	AL	971	0	1057	16	0
12	CL	971	0	1057	19	0
13	AM	988	0	1059	35	0
13	CM	988	0	1059	26	0
14	AN	492	0	529	14	0
14	CN	492	0	529	21	0
15	AO	734	0	771	17	0
15	CO	734	0	771	21	0
16	AP	701	0	720	22	0
16	CP	701	0	720	17	0
17	AQ	824	0	891	23	0
17	CQ	824	0	891	13	0
18	AR	574	0	644	16	0
18	CR	574	0	644	16	0
19	AS	630	0	652	30	0
19	CS	630	0	652	12	0
20	AT	763	0	861	26	0
20	CT	763	0	861	14	0
21	AU	209	0	221	4	0
21	CU	209	0	221	3	0
22	AV	1640	0	837	29	0
22	CV	1640	0	837	27	0
23	AW	1619	0	822	58	0
23	CW	1619	0	822	21	0
24	AY	1619	0	792	222	0
24	CY	1619	0	792	241	0
25	AX	151	0	76	15	0
26	BA	60459	0	30488	1163	0
26	DA	60459	0	30487	1024	0
27	BB	2551	0	1295	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	DB	2551	0	1295	35	0
28	BC	1157	0	1160	27	0
29	BD	2105	0	2182	126	0
29	DD	2105	0	2182	89	0
30	BE	1564	0	1629	97	0
30	DE	1564	0	1629	66	0
31	BF	1624	0	1677	72	0
31	DF	1624	0	1677	63	0
32	BG	1474	0	1535	53	0
32	DG	1474	0	1535	49	0
33	BH	1223	0	1282	48	0
33	DH	1223	0	1282	22	0
34	BI	1132	0	1218	30	0
34	DI	1132	0	1218	29	1
35	BJ	651	0	649	10	0
35	DJ	651	0	649	14	0
36	BN	1105	0	1180	62	0
36	DN	1105	0	1180	42	0
37	BO	933	0	996	33	0
37	DO	933	0	996	30	0
38	BP	1114	0	1187	141	0
38	DP	1114	0	1187	82	0
39	BQ	1122	0	1179	35	0
39	DQ	1122	0	1179	31	0
40	BR	960	0	1021	47	0
40	DR	960	0	1021	46	0
41	BS	771	0	832	46	0
41	DS	771	0	832	33	0
42	BT	1142	0	1202	92	0
42	DT	1142	0	1202	72	0
43	BU	958	0	1018	57	0
43	DU	958	0	1018	52	0
44	BV	779	0	852	54	0
44	DV	779	0	852	39	0
45	BW	896	0	956	40	0
45	DW	896	0	956	23	0
46	BX	726	0	778	26	0
46	DX	726	0	778	20	0
47	BY	776	0	868	79	0
47	DY	776	0	870	45	0
48	BZ	1404	0	1432	20	0
48	DZ	1404	0	1432	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	B0	662	0	688	18	0
49	D0	662	0	688	20	0
50	B1	734	0	808	22	0
50	D1	734	0	808	21	0
51	B2	598	0	653	24	0
51	D2	598	0	653	13	0
52	B3	468	0	523	20	0
52	D3	468	0	523	12	0
53	B4	226	0	229	8	0
53	D4	226	0	229	4	0
54	B5	459	0	477	48	0
54	D5	459	0	478	21	0
55	B6	381	0	390	52	0
55	D6	381	0	391	30	0
56	B7	419	0	467	12	0
56	D7	419	0	467	15	0
57	B8	508	0	576	58	0
57	D8	508	0	576	33	0
58	B9	299	0	324	19	0
58	D9	299	0	324	7	0
59	CX	85	0	43	7	0
60	DC	1157	0	1160	22	0
All	All	295724	0	201402	6566	1

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 13.

The worst 5 of 6566 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)
24:AY:10:C:H41	24:AY:45:G:N2	1.03	1.51
24:CY:7:A:N1	24:CY:66:G:N2	1.61	1.48
24:AY:7:A:N1	24:AY:66:G:N2	1.61	1.46
24:CY:10:C:H41	24:CY:45:G:N2	1.03	1.46
24:CY:9:G:H21	24:CY:11:C:N4	1.02	1.45

All (1) 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)
1:AA:358:U:OP1	34:DI:87:LYS:NZ[4_455]	2.03	0.17

## 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	232/234 (99%)	170 (73%)	51 (22%)	11 (5%)	2	14
2	CB	232/234 (99%)	181 (78%)	41 (18%)	10 (4%)	2	16
3	AC	204/206 (99%)	150 (74%)	40 (20%)	14 (7%)	1	8
3	CC	204/206 (99%)	159 (78%)	32 (16%)	13 (6%)	1	9
4	AD	206/208 (99%)	155 (75%)	37 (18%)	14 (7%)	1	8
4	CD	206/208 (99%)	160 (78%)	36 (18%)	10 (5%)	2	14
5	AE	148/150 (99%)	129 (87%)	15 (10%)	4 (3%)	5	26
5	CE	148/150 (99%)	130 (88%)	16 (11%)	2 (1%)	11	38
6	AF	99/101 (98%)	89 (90%)	7 (7%)	3 (3%)	4	24
6	CF	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	7	32
7	AG	153/155 (99%)	133 (87%)	18 (12%)	2 (1%)	12	40
7	CG	153/155 (99%)	130 (85%)	18 (12%)	5 (3%)	4	22
8	AH	136/138 (99%)	119 (88%)	14 (10%)	3 (2%)	6	30
8	CH	136/138 (99%)	115 (85%)	18 (13%)	3 (2%)	6	30
9	AI	125/127 (98%)	96 (77%)	25 (20%)	4 (3%)	4	22
9	CI	125/127 (98%)	101 (81%)	21 (17%)	3 (2%)	6	28
10	AJ	96/98 (98%)	76 (79%)	17 (18%)	3 (3%)	4	23
10	CJ	96/98 (98%)	73 (76%)	18 (19%)	5 (5%)	2	13
11	AK	117/119 (98%)	96 (82%)	19 (16%)	2 (2%)	9	35
11	CK	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	5	27
12	AL	122/124 (98%)	95 (78%)	18 (15%)	9 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	CL	122/124 (98%)	95 (78%)	20 (16%)	7 (6%)	1	11
13	AM	122/124 (98%)	87 (71%)	23 (19%)	12 (10%)	0	3
13	CM	122/124 (98%)	90 (74%)	23 (19%)	9 (7%)	1	7
14	AN	58/60 (97%)	43 (74%)	11 (19%)	4 (7%)	1	8
14	CN	58/60 (97%)	46 (79%)	8 (14%)	4 (7%)	1	8
15	AO	86/88 (98%)	62 (72%)	19 (22%)	5 (6%)	1	11
15	CO	86/88 (98%)	71 (83%)	10 (12%)	5 (6%)	1	11
16	AP	81/83 (98%)	68 (84%)	13 (16%)	0	100	100
16	CP	81/83 (98%)	64 (79%)	12 (15%)	5 (6%)	1	10
17	AQ	97/99 (98%)	85 (88%)	8 (8%)	4 (4%)	3	17
17	CQ	97/99 (98%)	89 (92%)	5 (5%)	3 (3%)	4	23
18	AR	68/70 (97%)	55 (81%)	8 (12%)	5 (7%)	1	7
18	CR	68/70 (97%)	58 (85%)	6 (9%)	4 (6%)	1	10
19	AS	76/78 (97%)	57 (75%)	11 (14%)	8 (10%)	0	3
19	CS	76/78 (97%)	64 (84%)	8 (10%)	4 (5%)	2	12
20	AT	97/99 (98%)	71 (73%)	22 (23%)	4 (4%)	3	17
20	CT	97/99 (98%)	72 (74%)	21 (22%)	4 (4%)	3	17
21	AU	22/24 (92%)	13 (59%)	7 (32%)	2 (9%)	1	4
21	CU	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	2	15
28	BC	182/206 (88%)	111 (61%)	50 (28%)	21 (12%)	0	2
29	BD	269/271 (99%)	214 (80%)	34 (13%)	21 (8%)	1	6
29	DD	269/271 (99%)	217 (81%)	31 (12%)	21 (8%)	1	6
30	BE	202/204 (99%)	138 (68%)	47 (23%)	17 (8%)	1	5
30	DE	202/204 (99%)	152 (75%)	35 (17%)	15 (7%)	1	7
31	BF	205/207 (99%)	163 (80%)	28 (14%)	14 (7%)	1	8
31	DF	205/207 (99%)	163 (80%)	28 (14%)	14 (7%)	1	8
32	BG	179/181 (99%)	140 (78%)	27 (15%)	12 (7%)	1	8
32	DG	179/181 (99%)	137 (76%)	31 (17%)	11 (6%)	1	10
33	BH	157/159 (99%)	113 (72%)	24 (15%)	20 (13%)	0	1
33	DH	157/159 (99%)	116 (74%)	25 (16%)	16 (10%)	0	3
34	BI	143/145 (99%)	107 (75%)	29 (20%)	7 (5%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	DI	143/145 (99%)	110 (77%)	25 (18%)	8 (6%)	2	11
35	BJ	128/130 (98%)	70 (55%)	42 (33%)	16 (12%)	0	1
35	DJ	128/130 (98%)	72 (56%)	42 (33%)	14 (11%)	0	2
36	BN	136/138 (99%)	100 (74%)	25 (18%)	11 (8%)	1	6
36	DN	136/138 (99%)	108 (79%)	15 (11%)	13 (10%)	0	4
37	BO	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	9	35
37	DO	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	19	51
38	BP	144/146 (99%)	82 (57%)	37 (26%)	25 (17%)	0	1
38	DP	144/146 (99%)	87 (60%)	28 (19%)	29 (20%)	0	0
39	BQ	139/141 (99%)	109 (78%)	25 (18%)	5 (4%)	3	20
39	DQ	139/141 (99%)	116 (84%)	19 (14%)	4 (3%)	4	24
40	BR	115/117 (98%)	93 (81%)	16 (14%)	6 (5%)	2	13
40	DR	115/117 (98%)	92 (80%)	17 (15%)	6 (5%)	2	13
41	BS	96/98 (98%)	58 (60%)	22 (23%)	16 (17%)	0	1
41	DS	96/98 (98%)	63 (66%)	20 (21%)	13 (14%)	0	1
42	BT	135/137 (98%)	95 (70%)	23 (17%)	17 (13%)	0	1
42	DT	135/137 (98%)	89 (66%)	30 (22%)	16 (12%)	0	2
43	BU	115/117 (98%)	90 (78%)	19 (16%)	6 (5%)	2	13
43	DU	115/117 (98%)	92 (80%)	19 (16%)	4 (4%)	3	21
44	BV	99/101 (98%)	74 (75%)	14 (14%)	11 (11%)	0	2
44	DV	99/101 (98%)	72 (73%)	17 (17%)	10 (10%)	0	3
45	BW	111/113 (98%)	92 (83%)	16 (14%)	3 (3%)	5	26
45	DW	111/113 (98%)	96 (86%)	7 (6%)	8 (7%)	1	7
46	BX	90/92 (98%)	80 (89%)	7 (8%)	3 (3%)	4	22
46	DX	90/92 (98%)	75 (83%)	8 (9%)	7 (8%)	1	6
47	BY	98/100 (98%)	53 (54%)	22 (22%)	23 (24%)	0	0
47	DY	98/100 (98%)	60 (61%)	19 (19%)	19 (19%)	0	1
48	BZ	174/176 (99%)	141 (81%)	26 (15%)	7 (4%)	3	18
48	DZ	174/176 (99%)	130 (75%)	33 (19%)	11 (6%)	1	9
49	B0	82/84 (98%)	75 (92%)	6 (7%)	1 (1%)	13	42
49	D0	82/84 (98%)	72 (88%)	9 (11%)	1 (1%)	13	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	B1	91/93 (98%)	76 (84%)	12 (13%)	3 (3%)	4	22
50	D1	91/93 (98%)	74 (81%)	10 (11%)	7 (8%)	1	6
51	B2	69/71 (97%)	53 (77%)	10 (14%)	6 (9%)	1	5
51	D2	69/71 (97%)	54 (78%)	11 (16%)	4 (6%)	1	11
52	B3	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	8	35
52	D3	57/59 (97%)	53 (93%)	3 (5%)	1 (2%)	8	35
53	B4	28/30 (93%)	21 (75%)	4 (14%)	3 (11%)	0	3
53	D4	28/30 (93%)	20 (71%)	5 (18%)	3 (11%)	0	3
54	B5	57/59 (97%)	43 (75%)	9 (16%)	5 (9%)	1	5
54	D5	57/59 (97%)	48 (84%)	4 (7%)	5 (9%)	1	5
55	B6	42/44 (96%)	21 (50%)	8 (19%)	13 (31%)	0	0
55	D6	42/44 (96%)	23 (55%)	7 (17%)	12 (29%)	0	0
56	B7	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
56	D7	46/48 (96%)	45 (98%)	0	1 (2%)	6	30
57	B8	61/63 (97%)	44 (72%)	10 (16%)	7 (12%)	0	2
57	D8	61/63 (97%)	47 (77%)	8 (13%)	6 (10%)	0	3
58	B9	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
58	D9	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
60	DC	182/196 (93%)	115 (63%)	47 (26%)	20 (11%)	0	2
All	All	11898/12136 (98%)	9181 (77%)	1900 (16%)	817 (7%)	1	8

5 of 817 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	106	LYS
2	AB	165	VAL
3	AC	12	LEU
3	AC	20	SER
3	AC	47	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	202/202 (100%)	185 (92%)	17 (8%)	11	35
2	CB	202/202 (100%)	181 (90%)	21 (10%)	7	25
3	AC	160/160 (100%)	142 (89%)	18 (11%)	6	22
3	CC	160/160 (100%)	145 (91%)	15 (9%)	8	30
4	AD	180/180 (100%)	160 (89%)	20 (11%)	6	23
4	CD	180/180 (100%)	160 (89%)	20 (11%)	6	23
5	AE	115/115 (100%)	104 (90%)	11 (10%)	8	29
5	CE	115/115 (100%)	101 (88%)	14 (12%)	5	20
6	AF	90/90 (100%)	82 (91%)	8 (9%)	9	32
6	CF	90/90 (100%)	85 (94%)	5 (6%)	21	52
7	AG	126/126 (100%)	115 (91%)	11 (9%)	10	34
7	CG	126/126 (100%)	115 (91%)	11 (9%)	10	34
8	AH	119/119 (100%)	108 (91%)	11 (9%)	9	31
8	CH	119/119 (100%)	107 (90%)	12 (10%)	7	27
9	AI	98/98 (100%)	88 (90%)	10 (10%)	7	27
9	CI	98/98 (100%)	89 (91%)	9 (9%)	9	31
10	AJ	88/88 (100%)	76 (86%)	12 (14%)	3	16
10	CJ	88/88 (100%)	79 (90%)	9 (10%)	7	27
11	AK	90/90 (100%)	82 (91%)	8 (9%)	9	32
11	CK	90/90 (100%)	84 (93%)	6 (7%)	16	45
12	AL	104/104 (100%)	88 (85%)	16 (15%)	2	12
12	CL	104/104 (100%)	90 (86%)	14 (14%)	4	16
13	AM	99/99 (100%)	88 (89%)	11 (11%)	6	23
13	CM	99/99 (100%)	88 (89%)	11 (11%)	6	23
14	AN	49/49 (100%)	43 (88%)	6 (12%)	5	20
14	CN	49/49 (100%)	44 (90%)	5 (10%)	7	27
15	AO	79/79 (100%)	73 (92%)	6 (8%)	13	39
15	CO	79/79 (100%)	76 (96%)	3 (4%)	33	62
16	AP	72/72 (100%)	65 (90%)	7 (10%)	8	29
16	CP	72/72 (100%)	62 (86%)	10 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AQ	94/94 (100%)	88 (94%)	6 (6%)	17	46
17	CQ	94/94 (100%)	89 (95%)	5 (5%)	22	53
18	AR	61/61 (100%)	54 (88%)	7 (12%)	5	22
18	CR	61/61 (100%)	59 (97%)	2 (3%)	38	66
19	AS	69/69 (100%)	56 (81%)	13 (19%)	1	6
19	CS	69/69 (100%)	58 (84%)	11 (16%)	2	11
20	AT	76/76 (100%)	68 (90%)	8 (10%)	7	25
20	CT	76/76 (100%)	67 (88%)	9 (12%)	5	21
21	AU	19/19 (100%)	15 (79%)	4 (21%)	1	4
21	CU	19/19 (100%)	17 (90%)	2 (10%)	7	25
28	BC	61/66 (92%)	55 (90%)	6 (10%)	8	29
29	BD	213/213 (100%)	180 (84%)	33 (16%)	2	12
29	DD	213/213 (100%)	176 (83%)	37 (17%)	2	8
30	BE	165/165 (100%)	134 (81%)	31 (19%)	1	6
30	DE	165/165 (100%)	139 (84%)	26 (16%)	2	11
31	BF	165/165 (100%)	138 (84%)	27 (16%)	2	10
31	DF	165/165 (100%)	149 (90%)	16 (10%)	8	29
32	BG	155/155 (100%)	128 (83%)	27 (17%)	2	8
32	DG	155/155 (100%)	137 (88%)	18 (12%)	5	22
33	BH	132/132 (100%)	106 (80%)	26 (20%)	1	5
33	DH	132/132 (100%)	120 (91%)	12 (9%)	9	31
34	BI	122/122 (100%)	110 (90%)	12 (10%)	8	29
34	DI	122/122 (100%)	111 (91%)	11 (9%)	9	32
36	BN	117/117 (100%)	90 (77%)	27 (23%)	1	3
36	DN	117/117 (100%)	94 (80%)	23 (20%)	1	5
37	BO	100/100 (100%)	92 (92%)	8 (8%)	12	37
37	DO	100/100 (100%)	93 (93%)	7 (7%)	15	43
38	BP	112/112 (100%)	83 (74%)	29 (26%)	0	2
38	DP	112/112 (100%)	86 (77%)	26 (23%)	1	3
39	BQ	111/111 (100%)	97 (87%)	14 (13%)	4	19
39	DQ	111/111 (100%)	101 (91%)	10 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BR	100/100 (100%)	85 (85%)	15 (15%)	3	13
40	DR	100/100 (100%)	85 (85%)	15 (15%)	3	13
41	BS	77/77 (100%)	60 (78%)	17 (22%)	1	3
41	DS	77/77 (100%)	67 (87%)	10 (13%)	4	17
42	BT	120/120 (100%)	98 (82%)	22 (18%)	1	7
42	DT	120/120 (100%)	93 (78%)	27 (22%)	1	3
43	BU	92/92 (100%)	78 (85%)	14 (15%)	3	13
43	DU	92/92 (100%)	82 (89%)	10 (11%)	6	24
44	BV	82/82 (100%)	60 (73%)	22 (27%)	0	1
44	DV	82/82 (100%)	65 (79%)	17 (21%)	1	4
45	BW	91/91 (100%)	81 (89%)	10 (11%)	6	24
45	DW	91/91 (100%)	80 (88%)	11 (12%)	5	20
46	BX	74/74 (100%)	67 (90%)	7 (10%)	8	29
46	DX	74/74 (100%)	65 (88%)	9 (12%)	5	20
47	BY	84/84 (100%)	65 (77%)	19 (23%)	1	3
47	DY	84/84 (100%)	67 (80%)	17 (20%)	1	5
48	BZ	155/155 (100%)	141 (91%)	14 (9%)	9	32
48	DZ	155/155 (100%)	148 (96%)	7 (4%)	27	58
49	B0	66/66 (100%)	55 (83%)	11 (17%)	2	10
49	D0	66/66 (100%)	60 (91%)	6 (9%)	9	31
50	B1	78/78 (100%)	68 (87%)	10 (13%)	4	18
50	D1	78/78 (100%)	62 (80%)	16 (20%)	1	4
51	B2	66/66 (100%)	51 (77%)	15 (23%)	1	3
51	D2	66/66 (100%)	60 (91%)	6 (9%)	9	31
52	B3	51/51 (100%)	47 (92%)	4 (8%)	12	38
52	D3	51/51 (100%)	48 (94%)	3 (6%)	19	49
53	B4	27/27 (100%)	22 (82%)	5 (18%)	1	7
53	D4	27/27 (100%)	24 (89%)	3 (11%)	6	23
54	B5	51/51 (100%)	39 (76%)	12 (24%)	1	3
54	D5	51/51 (100%)	41 (80%)	10 (20%)	1	5
55	B6	43/43 (100%)	33 (77%)	10 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	D6	43/43 (100%)	36 (84%)	7 (16%)	2	10
56	B7	41/41 (100%)	35 (85%)	6 (15%)	3	14
56	D7	41/41 (100%)	32 (78%)	9 (22%)	1	3
57	B8	53/53 (100%)	41 (77%)	12 (23%)	1	3
57	D8	53/53 (100%)	43 (81%)	10 (19%)	1	6
58	B9	33/33 (100%)	26 (79%)	7 (21%)	1	4
58	D9	33/33 (100%)	30 (91%)	3 (9%)	9	31
60	DC	61/66 (92%)	56 (92%)	5 (8%)	11	36
All	All	9654/9664 (100%)	8391 (87%)	1263 (13%)	4	17

5 of 1263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	DE	55	ASN
45	DW	1	MET
31	DF	140	LEU
30	DE	52	LEU
38	DP	45	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
18	CR	36	ASN
41	DS	34	HIS
20	CT	73	HIS
31	DF	169	ASN
43	DU	66	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504 (99%)	300 (19%)	43 (2%)
1	CA	1504/1504 (100%)	296 (19%)	53 (3%)
22	AV	76/77 (98%)	18 (23%)	4 (5%)
22	CV	76/77 (98%)	22 (28%)	1 (1%)
23	AW	75/76 (98%)	22 (29%)	2 (2%)
23	CW	75/76 (98%)	19 (25%)	2 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	AY	74/75 (98%)	38 (51%)	4 (5%)
24	CY	74/75 (98%)	38 (51%)	4 (5%)
25	AX	6/7 (85%)	3 (50%)	1 (16%)
26	BA	2800/2915 (96%)	779 (27%)	151 (5%)
26	DA	2799/2915 (96%)	754 (26%)	122 (4%)
27	BB	118/119 (99%)	36 (30%)	4 (3%)
27	DB	118/119 (99%)	27 (22%)	4 (3%)
59	CX	3/4 (75%)	2 (66%)	0
All	All	9301/9543 (97%)	2354 (25%)	395 (4%)

5 of 2354 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	22	G

5 of 395 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	495	C
26	DA	355	A
1	CA	671	A
1	CA	1476	U
26	DA	715	G

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

1 non-standard protein/DNA/RNA residue is 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
25	PSU	AX	19	25,24	18,21,22	1.48	2 (11%)	22,30,33	1.37	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PSU	AX	19	25,24	-	2/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AX	19	PSU	C2-N1	4.86	1.43	1.36
25	AX	19	PSU	C6-C5	2.42	1.38	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AX	19	PSU	C6-C5-C4	4.04	121.03	118.20
25	AX	19	PSU	C6-N1-C2	-2.89	119.73	122.68
25	AX	19	PSU	O2-C2-N1	2.79	125.87	122.79

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	AX	19	PSU	O4'-C4'-C5'-O5'
25	AX	19	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	AX	19	PSU	7	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
60	DC	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DC	110:ALA	C	119:ALA	N	13.98
1	DC	136:ALA	C	139:ALA	N	11.93

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1504/1504 (100%)	0.11	60 (3%) 38 36	23, 77, 165, 393	0
1	CA	1504/1504 (100%)	0.26	95 (6%) 20 20	38, 86, 188, 312	0
2	AB	234/234 (100%)	0.26	12 (5%) 28 26	66, 113, 158, 196	0
2	CB	234/234 (100%)	0.67	34 (14%) 2 2	85, 139, 177, 216	0
3	AC	206/206 (100%)	-0.05	5 (2%) 59 56	64, 96, 134, 183	0
3	CC	206/206 (100%)	0.87	30 (14%) 2 2	90, 130, 182, 221	0
4	AD	208/208 (100%)	0.12	7 (3%) 45 43	55, 91, 126, 174	0
4	CD	208/208 (100%)	-0.08	3 (1%) 75 75	49, 79, 108, 139	0
5	AE	150/150 (100%)	-0.02	0 100 100	47, 76, 104, 125	0
5	CE	150/150 (100%)	0.14	4 (2%) 54 52	58, 88, 126, 148	0
6	AF	101/101 (100%)	-0.21	0 100 100	52, 80, 108, 124	0
6	CF	101/101 (100%)	-0.08	2 (1%) 65 64	52, 82, 116, 139	0
7	AG	155/155 (100%)	-0.01	7 (4%) 33 32	61, 97, 137, 156	0
7	CG	155/155 (100%)	0.58	14 (9%) 9 9	82, 119, 157, 175	0
8	AH	138/138 (100%)	-0.20	0 100 100	50, 81, 105, 135	0
8	CH	138/138 (100%)	-0.02	3 (2%) 62 60	59, 95, 119, 146	0
9	AI	127/127 (100%)	0.32	8 (6%) 20 20	58, 112, 146, 230	0
9	CI	127/127 (100%)	1.17	32 (25%) 0 0	94, 136, 180, 235	0
10	AJ	98/98 (100%)	0.72	12 (12%) 4 3	67, 119, 160, 187	0
10	CJ	98/98 (100%)	1.36	26 (26%) 0 0	94, 158, 190, 226	0
11	AK	119/119 (100%)	-0.01	4 (3%) 45 43	45, 79, 108, 165	0
11	CK	119/119 (100%)	0.48	11 (9%) 9 9	55, 95, 132, 161	0
12	AL	124/124 (100%)	0.03	8 (6%) 18 18	47, 71, 105, 155	0
12	CL	124/124 (100%)	0.14	8 (6%) 18 18	50, 81, 115, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	124/124 (100%)	0.70	13 (10%) 6 6	68, 112, 153, 231	0
13	CM	124/124 (100%)	1.50	30 (24%) 0 0	101, 153, 200, 218	0
14	AN	60/60 (100%)	0.07	0 100 100	55, 85, 135, 155	0
14	CN	60/60 (100%)	0.86	7 (11%) 4 4	104, 137, 160, 182	0
15	AO	88/88 (100%)	0.02	1 (1%) 80 81	48, 80, 111, 130	0
15	CO	88/88 (100%)	0.02	2 (2%) 60 59	55, 87, 117, 139	0
16	AP	83/83 (100%)	0.20	2 (2%) 59 56	65, 92, 125, 149	0
16	CP	83/83 (100%)	-0.11	0 100 100	51, 73, 112, 139	0
17	AQ	99/99 (100%)	0.12	0 100 100	51, 90, 112, 117	0
17	CQ	99/99 (100%)	0.02	2 (2%) 65 64	63, 87, 115, 126	0
18	AR	70/70 (100%)	-0.10	1 (1%) 75 75	48, 76, 108, 138	0
18	CR	70/70 (100%)	0.06	2 (2%) 51 50	61, 91, 126, 149	0
19	AS	78/78 (100%)	0.38	6 (7%) 13 12	72, 114, 165, 189	0
19	CS	78/78 (100%)	1.54	27 (34%) 0 0	111, 160, 208, 221	0
20	AT	99/99 (100%)	0.24	4 (4%) 38 36	67, 102, 150, 169	0
20	CT	99/99 (100%)	0.05	2 (2%) 65 64	49, 96, 135, 150	0
21	AU	24/24 (100%)	0.34	0 100 100	74, 92, 117, 119	0
21	CU	24/24 (100%)	2.84	14 (58%) 0 0	105, 141, 205, 253	0
22	AV	77/77 (100%)	-0.08	1 (1%) 77 77	34, 78, 122, 187	0
22	CV	77/77 (100%)	0.40	8 (10%) 6 6	41, 107, 162, 175	0
23	AW	76/76 (100%)	1.93	33 (43%) 0 0	37, 183, 225, 269	0
23	CW	76/76 (100%)	2.60	44 (57%) 0 0	59, 192, 268, 296	0
24	AY	75/75 (100%)	1.76	30 (40%) 0 0	37, 107, 188, 213	0
24	CY	75/75 (100%)	2.48	39 (52%) 0 0	37, 107, 188, 213	0
25	AX	6/7 (85%)	0.13	0 100 100	50, 53, 106, 116	0
26	BA	2807/2915 (96%)	-0.20	75 (2%) 54 52	9, 38, 151, 312	0
26	DA	2807/2915 (96%)	0.01	114 (4%) 37 35	24, 64, 168, 297	0
27	BB	119/119 (100%)	-0.25	0 100 100	32, 60, 91, 118	0
27	DB	119/119 (100%)	0.42	8 (6%) 17 17	71, 112, 151, 191	0
28	BC	190/206 (92%)	3.56	120 (63%) 0 0	108, 181, 242, 295	0
29	BD	271/271 (100%)	-0.45	0 100 100	18, 36, 76, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	DD	271/271 (100%)	-0.26	1 (0%) 92 93	23, 56, 91, 127	0
30	BE	204/204 (100%)	-0.28	2 (0%) 82 82	18, 48, 92, 134	0
30	DE	204/204 (100%)	-0.13	5 (2%) 57 54	28, 65, 120, 165	0
31	BF	207/207 (100%)	-0.29	4 (1%) 66 65	17, 48, 133, 191	0
31	DF	207/207 (100%)	0.04	7 (3%) 45 43	31, 87, 149, 214	0
32	BG	181/181 (100%)	0.03	5 (2%) 53 51	56, 82, 129, 172	0
32	DG	181/181 (100%)	0.49	14 (7%) 13 12	82, 128, 167, 210	0
33	BH	159/159 (100%)	-0.10	5 (3%) 49 48	32, 68, 118, 181	0
33	DH	159/159 (100%)	0.91	35 (22%) 0 1	70, 128, 180, 235	0
34	BI	145/145 (100%)	-0.04	1 (0%) 87 88	44, 95, 123, 159	0
34	DI	145/145 (100%)	0.26	5 (3%) 45 43	48, 101, 137, 159	0
35	BJ	130/130 (100%)	2.98	64 (49%) 0 0	120, 164, 275, 373	0
35	DJ	130/130 (100%)	3.50	87 (66%) 0 0	122, 193, 233, 284	0
36	BN	138/138 (100%)	-0.32	3 (2%) 62 60	24, 46, 95, 129	0
36	DN	138/138 (100%)	-0.01	3 (2%) 62 60	54, 90, 120, 133	0
37	BO	122/122 (100%)	-0.48	0 100 100	26, 49, 75, 91	0
37	DO	122/122 (100%)	-0.35	0 100 100	39, 64, 85, 92	0
38	BP	146/146 (100%)	-0.08	3 (2%) 63 62	21, 65, 115, 159	0
38	DP	146/146 (100%)	0.29	5 (3%) 45 43	39, 92, 134, 174	0
39	BQ	141/141 (100%)	-0.34	2 (1%) 75 75	27, 51, 85, 188	0
39	DQ	141/141 (100%)	0.14	3 (2%) 63 62	58, 92, 125, 161	0
40	BR	117/117 (100%)	-0.36	0 100 100	21, 42, 78, 93	0
40	DR	117/117 (100%)	-0.14	1 (0%) 84 84	40, 65, 100, 131	0
41	BS	98/98 (100%)	-0.06	1 (1%) 82 82	35, 64, 105, 136	0
41	DS	98/98 (100%)	0.34	3 (3%) 49 48	72, 110, 151, 181	0
42	BT	137/137 (100%)	-0.13	5 (3%) 42 40	34, 64, 139, 181	0
42	DT	137/137 (100%)	0.01	6 (4%) 34 33	43, 77, 135, 170	0
43	BU	117/117 (100%)	-0.43	0 100 100	15, 37, 73, 98	0
43	DU	117/117 (100%)	0.10	5 (4%) 35 34	40, 80, 135, 155	0
44	BV	101/101 (100%)	-0.32	1 (0%) 82 82	24, 51, 85, 119	0
44	DV	101/101 (100%)	0.58	11 (10%) 5 5	60, 110, 143, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	BW	113/113 (100%)	-0.35	1 (0%) 84 84	25, 37, 75, 137	0
45	DW	113/113 (100%)	0.01	4 (3%) 44 42	49, 66, 103, 147	0
46	BX	92/92 (100%)	-0.45	0 100 100	25, 44, 73, 82	0
46	DX	92/92 (100%)	-0.11	0 100 100	43, 77, 98, 114	0
47	BY	100/100 (100%)	0.25	10 (10%) 7 7	34, 66, 163, 201	0
47	DY	100/100 (100%)	0.66	13 (13%) 3 3	56, 100, 175, 209	0
48	BZ	176/176 (100%)	1.75	54 (30%) 0 0	43, 119, 275, 309	0
48	DZ	176/176 (100%)	2.37	66 (37%) 0 0	92, 149, 299, 353	0
49	B0	84/84 (100%)	-0.15	0 100 100	25, 43, 78, 110	0
49	D0	84/84 (100%)	0.51	7 (8%) 11 11	58, 84, 105, 128	0
50	B1	93/93 (100%)	-0.17	3 (3%) 47 46	26, 48, 94, 131	0
50	D1	93/93 (100%)	-0.04	2 (2%) 62 60	39, 62, 111, 153	0
51	B2	71/71 (100%)	-0.01	2 (2%) 53 51	34, 61, 101, 164	0
51	D2	71/71 (100%)	-0.01	1 (1%) 75 75	60, 90, 131, 150	0
52	B3	59/59 (100%)	-0.16	2 (3%) 45 43	29, 48, 92, 149	0
52	D3	59/59 (100%)	0.56	5 (8%) 10 10	65, 101, 135, 253	0
53	B4	30/30 (100%)	0.00	1 (3%) 46 44	69, 116, 141, 154	0
53	D4	30/30 (100%)	0.83	2 (6%) 17 17	121, 142, 163, 173	0
54	B5	59/59 (100%)	0.05	3 (5%) 28 26	21, 42, 139, 213	0
54	D5	59/59 (100%)	-0.06	3 (5%) 28 26	42, 67, 130, 179	0
55	B6	44/44 (100%)	0.12	2 (4%) 33 32	30, 60, 93, 118	0
55	D6	44/44 (100%)	0.54	1 (2%) 60 59	51, 90, 113, 121	0
56	B7	48/48 (100%)	-0.31	1 (2%) 63 62	20, 30, 63, 124	0
56	D7	48/48 (100%)	-0.19	1 (2%) 63 62	31, 49, 80, 98	0
57	B8	63/63 (100%)	-0.26	0 100 100	30, 44, 64, 129	0
57	D8	63/63 (100%)	-0.01	2 (3%) 47 46	50, 77, 112, 154	0
58	B9	36/36 (100%)	-0.03	0 100 100	34, 49, 63, 78	0
58	D9	36/36 (100%)	0.58	4 (11%) 5 5	63, 91, 115, 125	0
59	CX	4/4 (100%)	0.37	1 (25%) 0 0	70, 87, 90, 158	0
60	DC	190/196 (96%)	3.98	143 (75%) 0 0	109, 188, 240, 265	0
All	All	21440/21679 (98%)	0.24	1591 (7%) 14 14	9, 77, 180, 393	0

The worst 5 of 1591 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BJ	52	ALA	25.7
48	DZ	172	ALA	20.9
35	BJ	51	ALA	20.7
26	DA	2812	G	20.5
48	DZ	151	HIS	15.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
25	PSU	AX	19	20/21	0.93	0.15	83,95,104,110	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.