



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2024 – 11:06 PM EST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

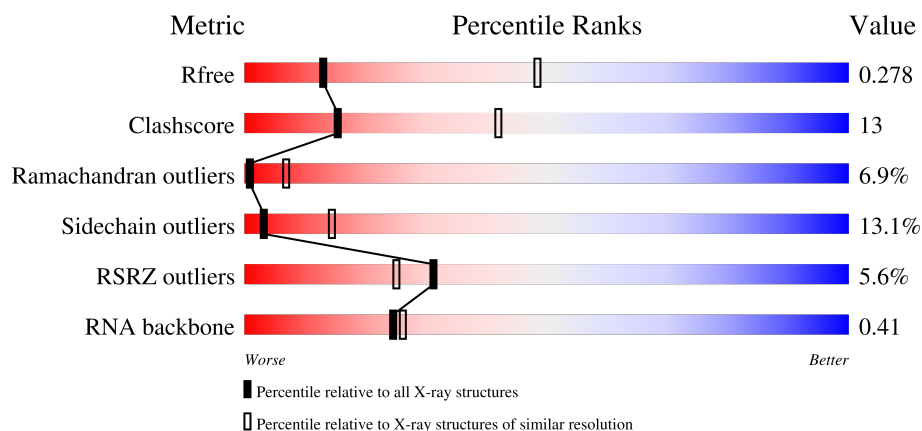
1 Overall quality at a glance

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}	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)
RNA backbone	3690	1014 (3.64-2.96)

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

Mol	Chain	Length	Quality of chain
1	AA	1504	<div> <div>2%</div> <div>51% 39% 10%</div> </div>
1	CA	1504	<div> <div>4%</div> <div>52% 39% 9%</div> </div>
2	AB	234	<div> <div>5%</div> <div>64% 32% .</div> </div>
2	CB	234	<div> <div>12%</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			

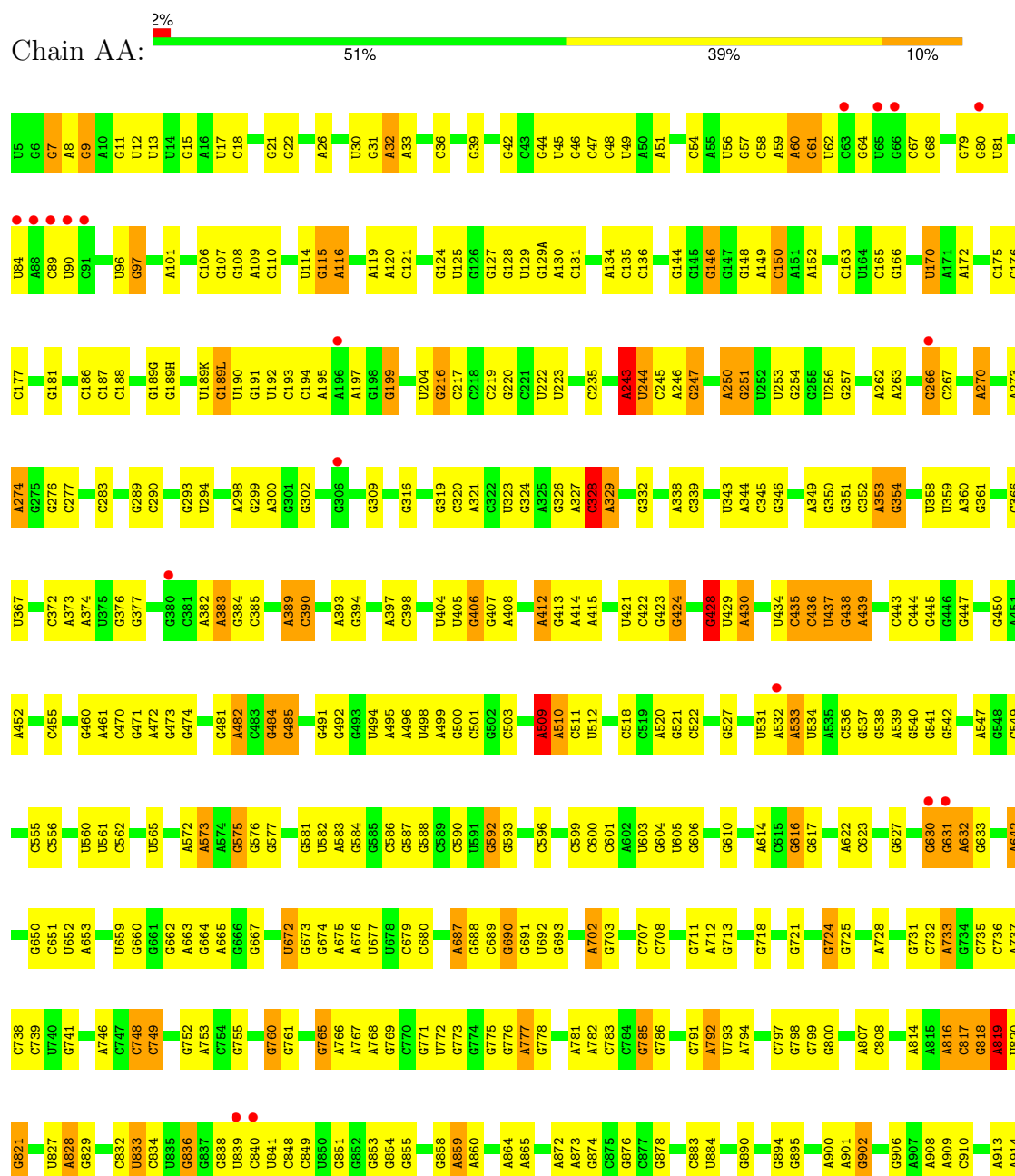
- Molecule 60 is a protein called 50S Ribosomal protein L1.

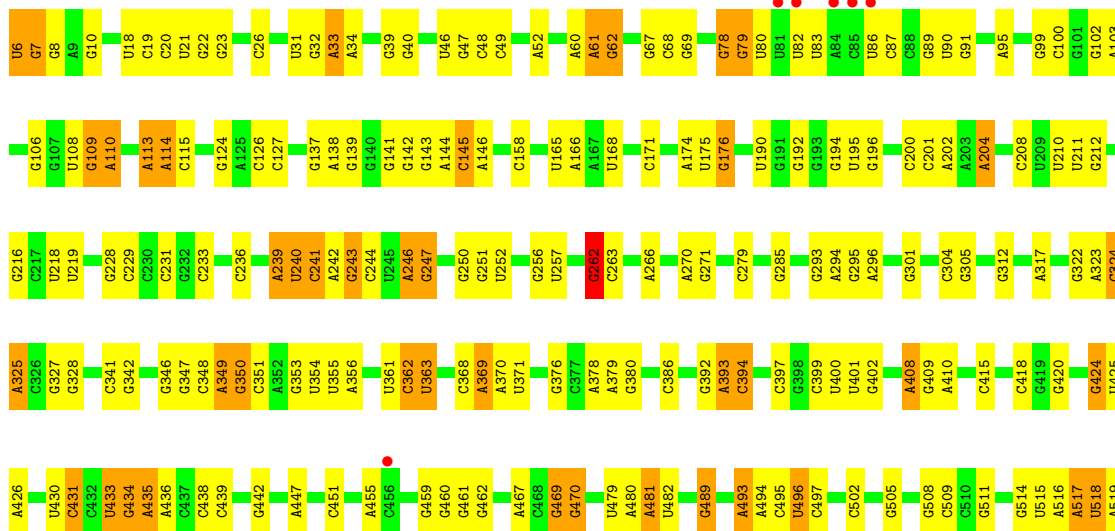
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
60	DC	190	Total	C	N	O	0	0	0
			1157	706	220	231			

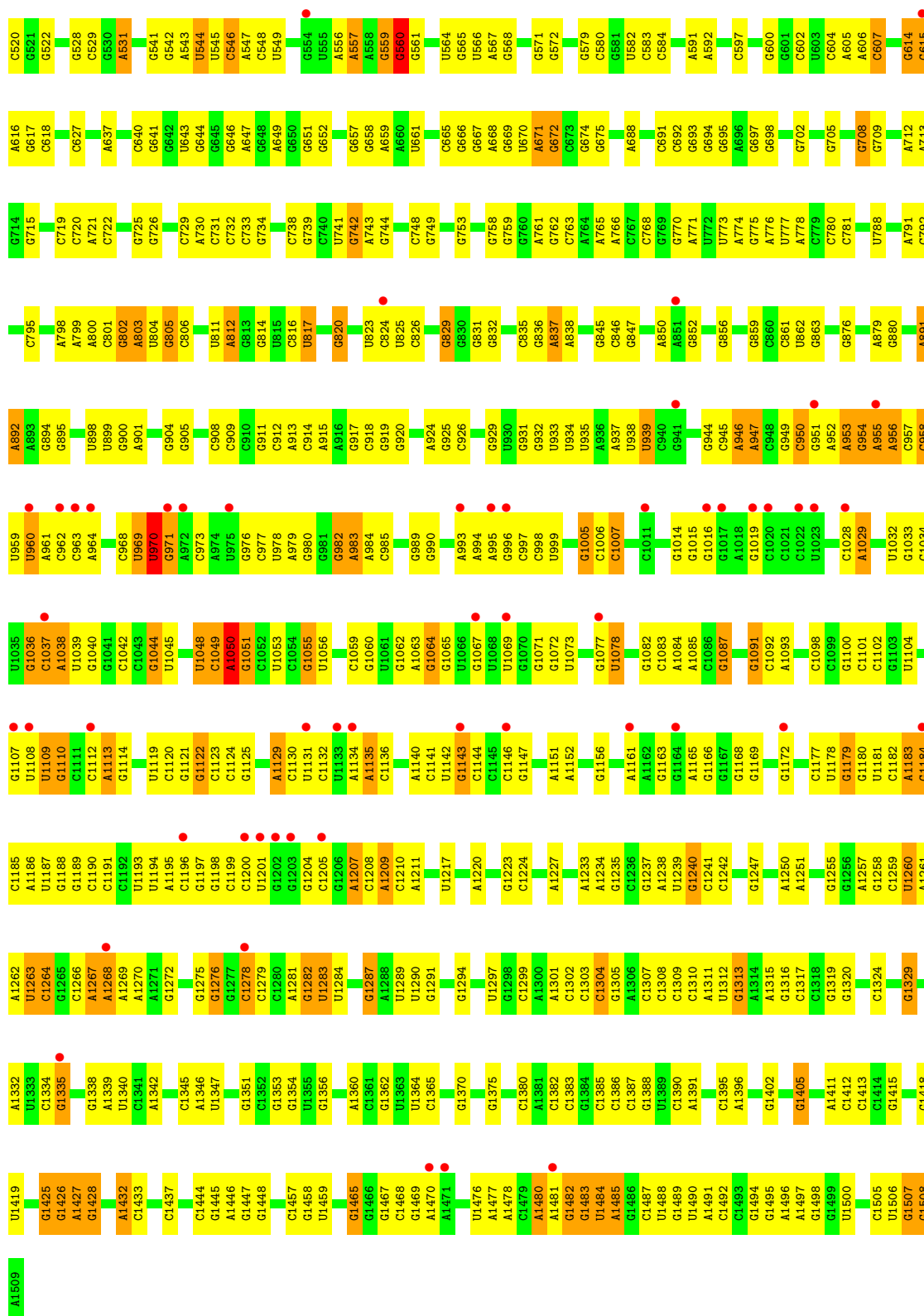
3 Residue-property plots

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

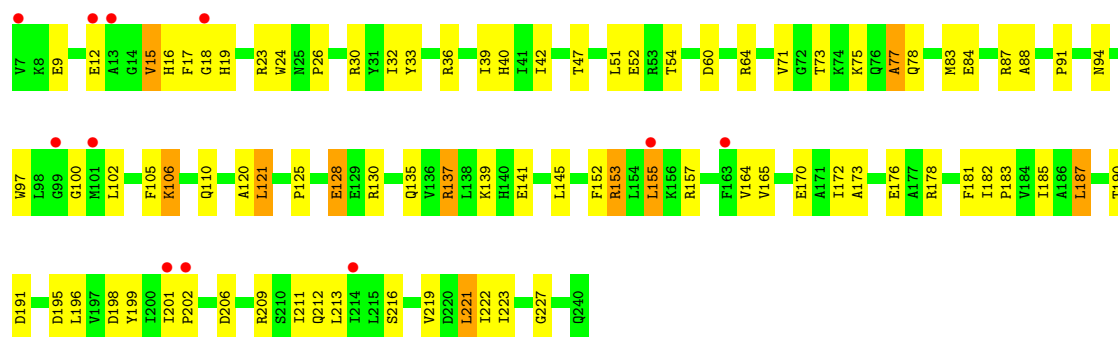




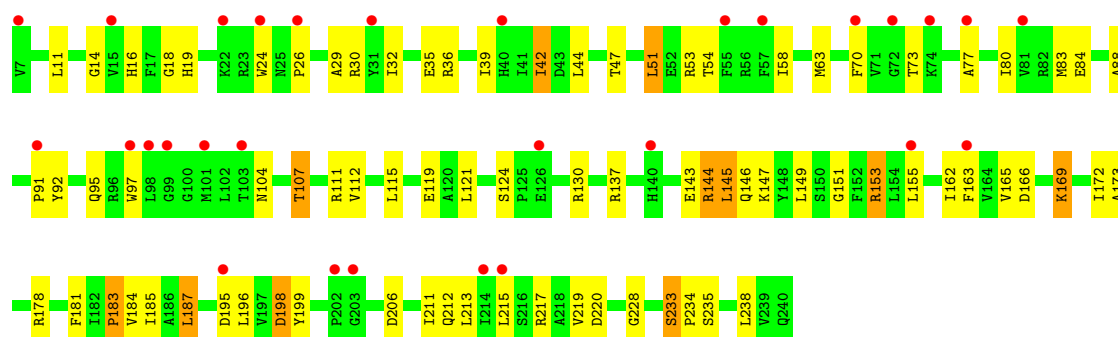


• Molecule 2: 30S Ribosomal protein S2

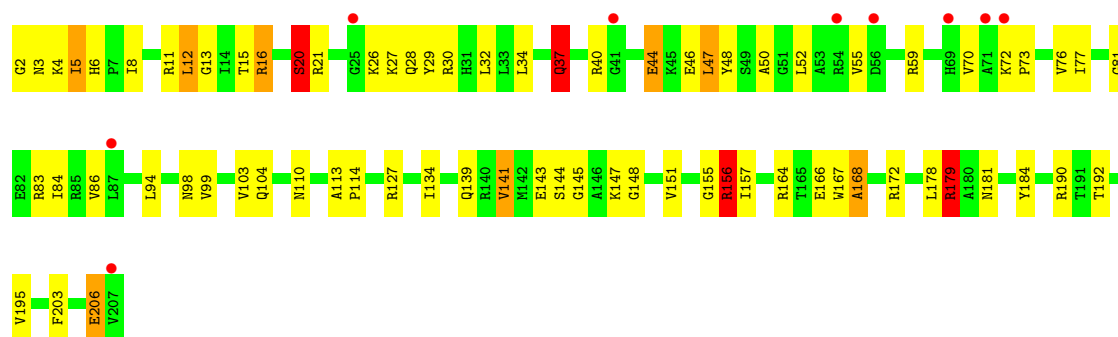




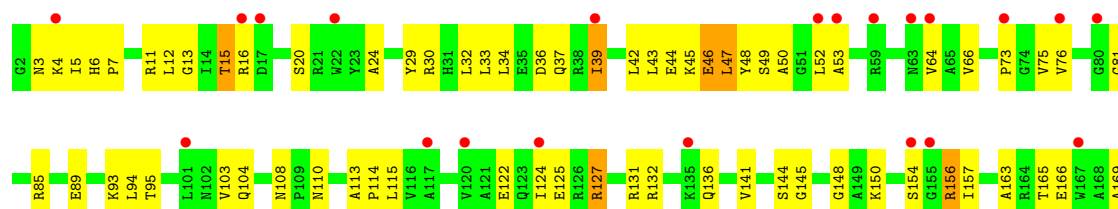
- Molecule 2: 30S Ribosomal protein S2



- Molecule 3: 30S Ribosomal protein S3

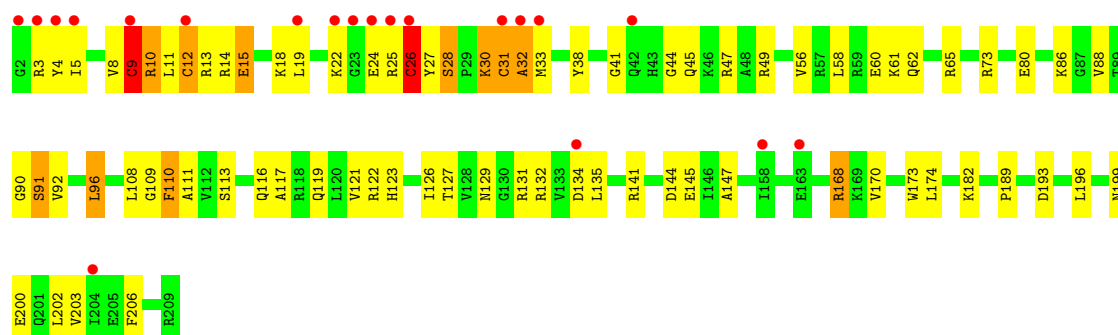


- Molecule 3: 30S Ribosomal protein S3

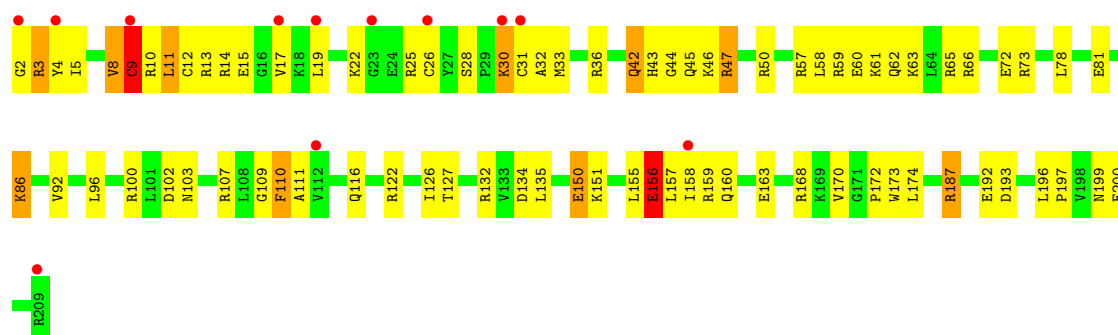




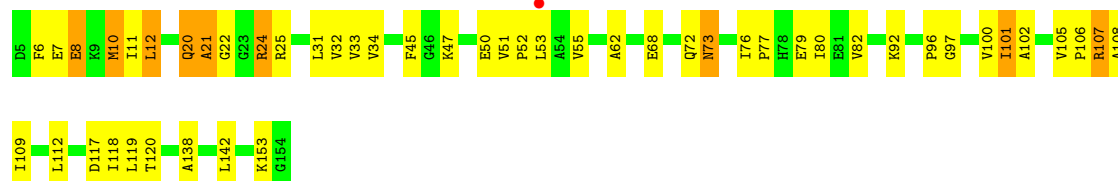
• Molecule 4: 30S Ribosomal protein S4



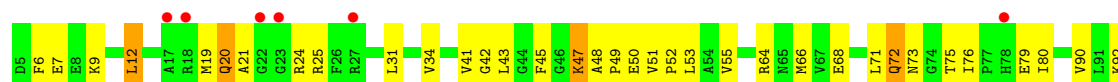
• Molecule 4: 30S Ribosomal protein S4

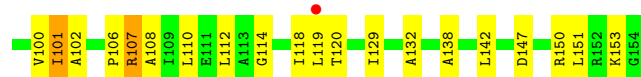


• Molecule 5: 30S Ribosomal protein S5

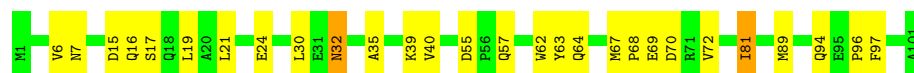


• Molecule 5: 30S Ribosomal protein S5

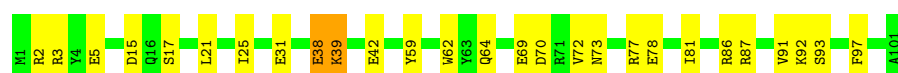




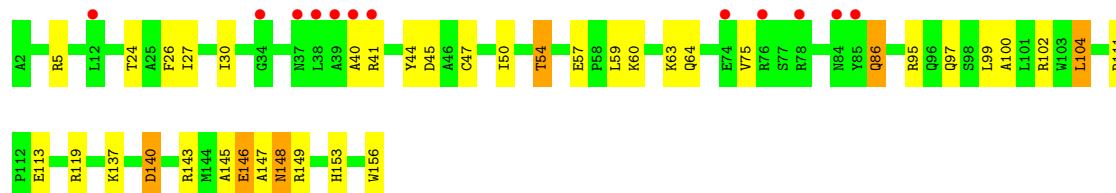
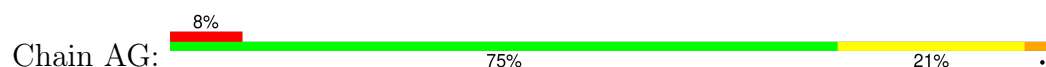
• Molecule 6: 30S Ribosomal protein S6



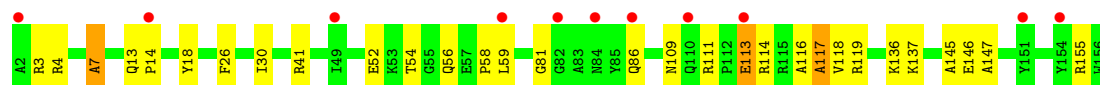
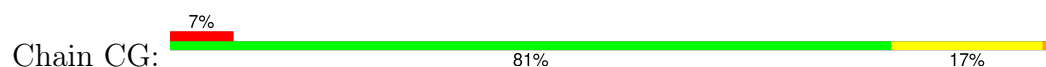
• Molecule 6: 30S Ribosomal protein S6



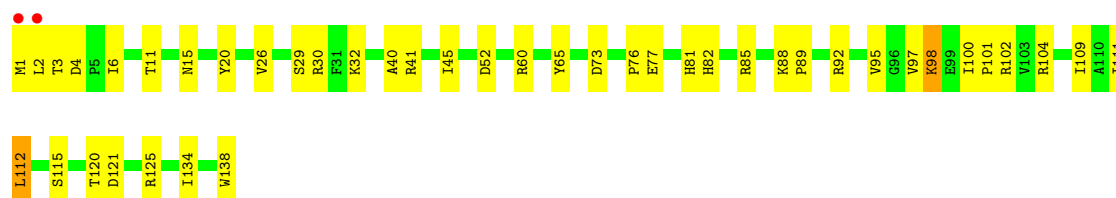
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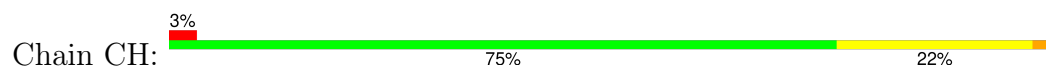
• Molecule 7: 30S Ribosomal protein S7

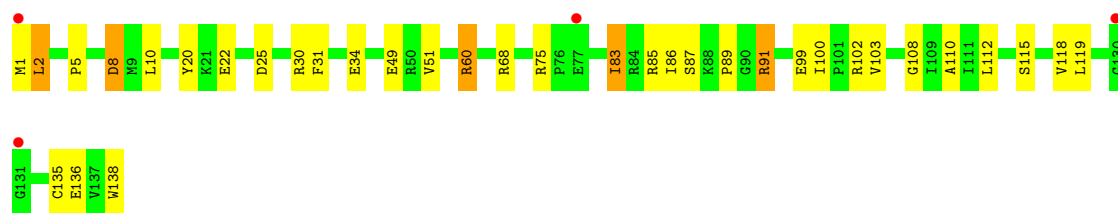


• Molecule 8: 30S Ribosomal protein S8

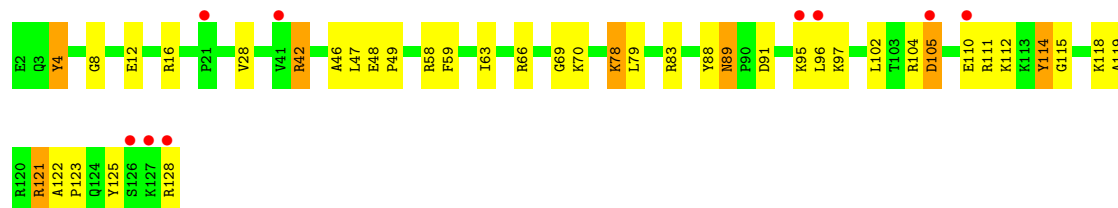


• Molecule 8: 30S Ribosomal protein S8

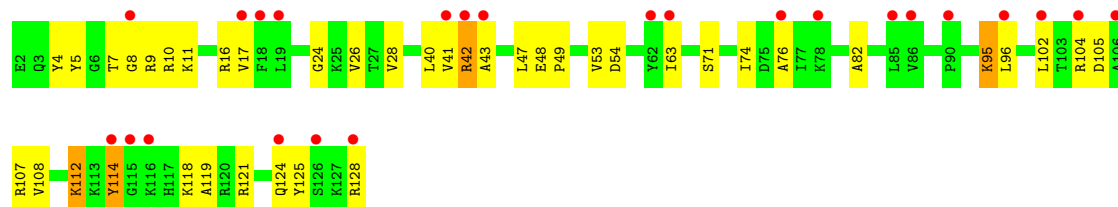




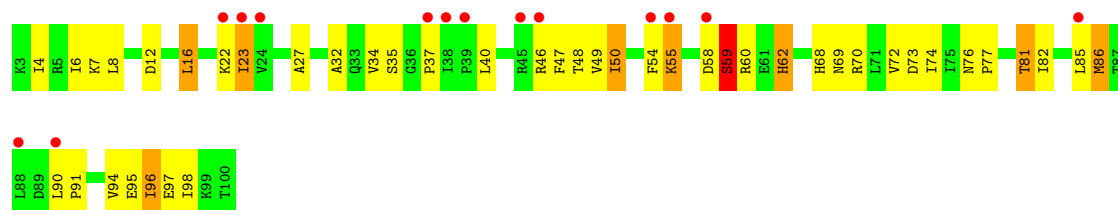
• Molecule 9: 30S Ribosomal protein S9



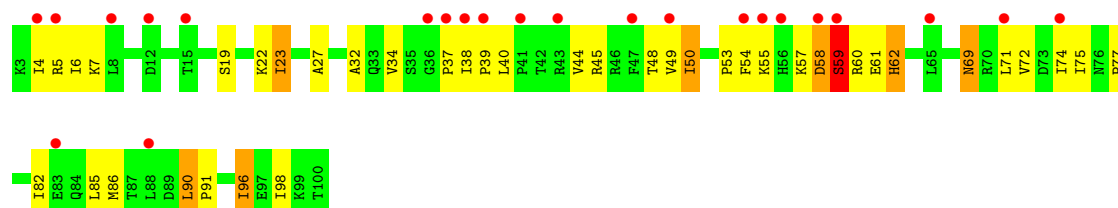
• Molecule 9: 30S Ribosomal protein S9



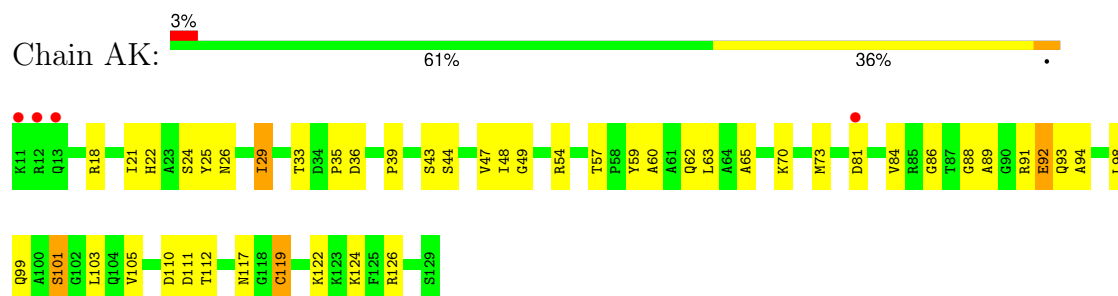
• Molecule 10: 30S Ribosomal protein S10



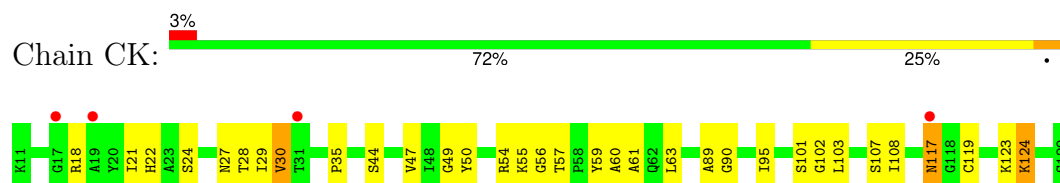
• Molecule 10: 30S Ribosomal protein S10



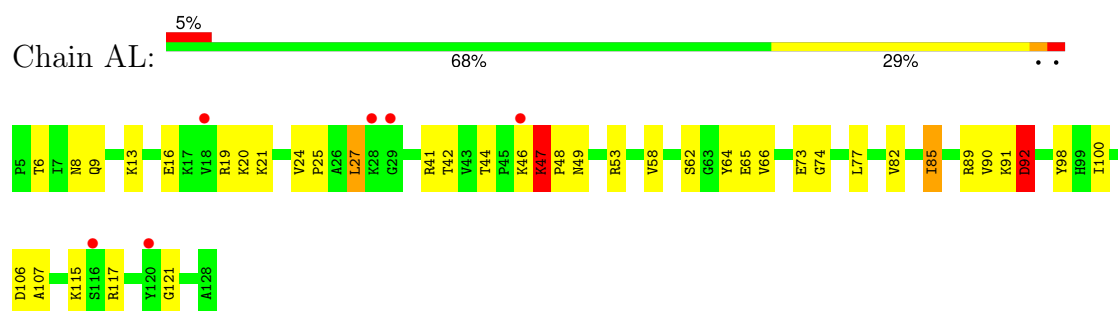
- Molecule 11: 30S Ribosomal protein S11



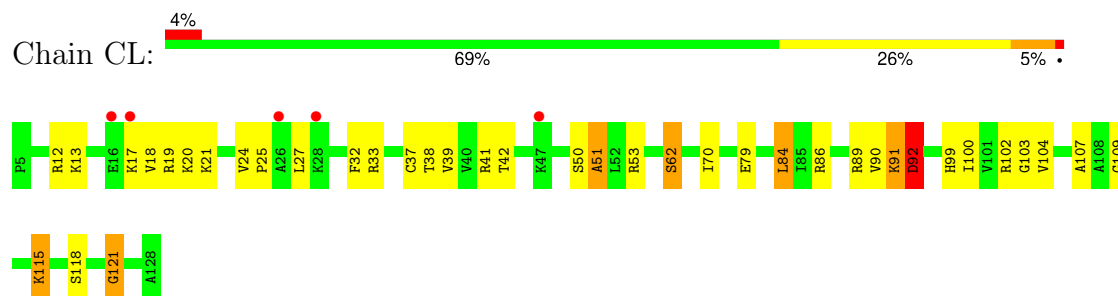
- Molecule 11: 30S Ribosomal protein S11



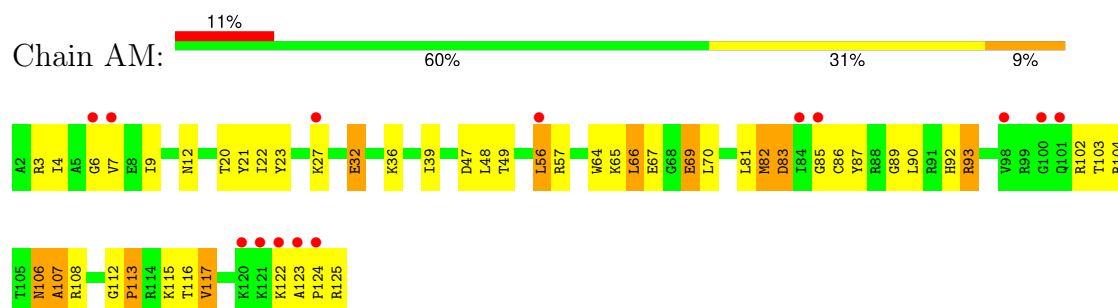
- Molecule 12: 30S Ribosomal protein S12



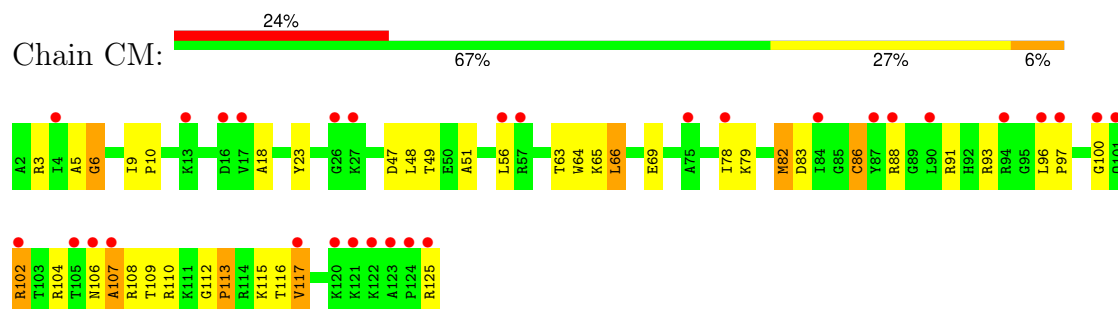
- Molecule 12: 30S Ribosomal protein S12



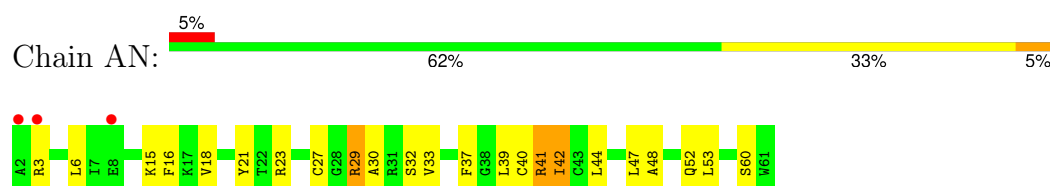
- Molecule 13: 30S Ribosomal protein S13



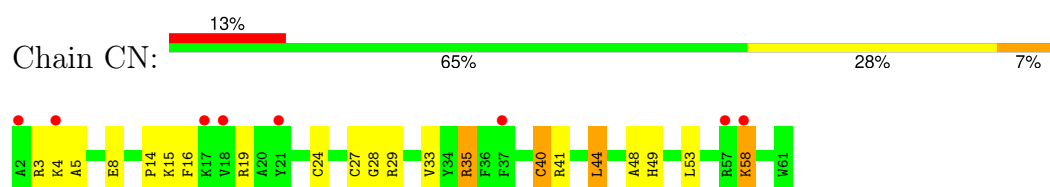
- Molecule 13: 30S Ribosomal protein S13



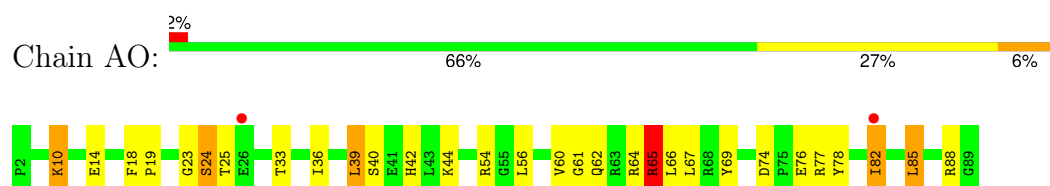
- Molecule 14: 30S Ribosomal protein S14



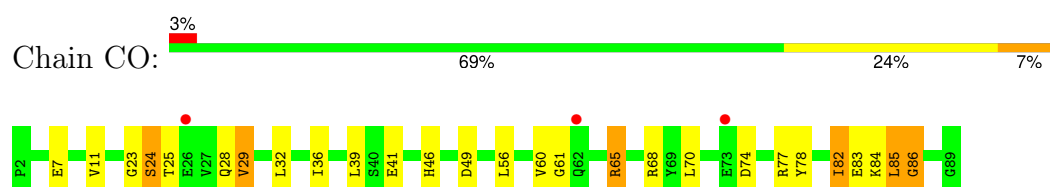
- Molecule 14: 30S Ribosomal protein S14



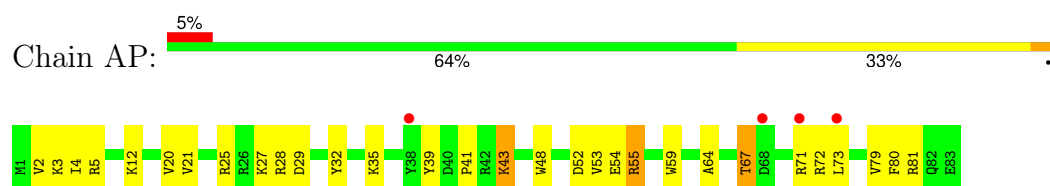
- Molecule 15: 30S Ribosomal protein S15



- Molecule 15: 30S Ribosomal protein S15



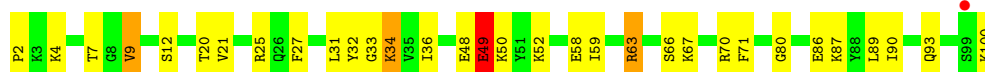
- Molecule 16: 30S Ribosomal protein S16



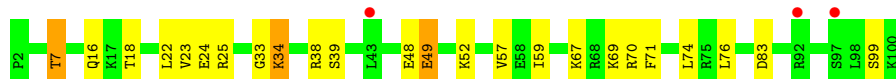
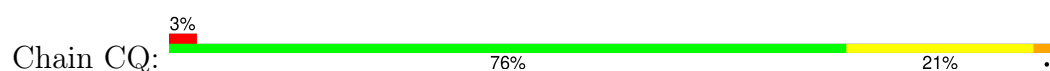
- Molecule 16: 30S Ribosomal protein S16



- Molecule 17: 30S Ribosomal protein S17



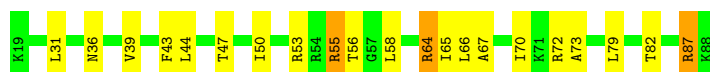
- Molecule 17: 30S Ribosomal protein S17



- Molecule 18: 30S Ribosomal protein S18



- Molecule 18: 30S Ribosomal protein S18



- Molecule 19: 30S Ribosomal protein S19

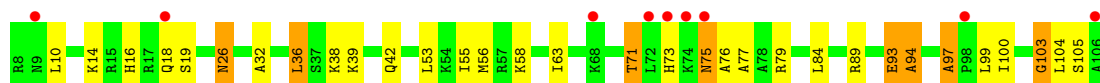


- Molecule 19: 30S Ribosomal protein S19

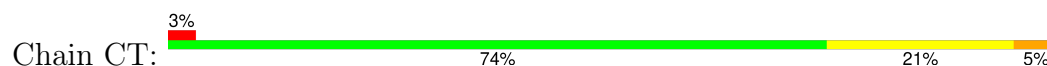




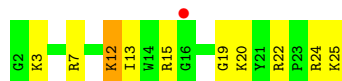
- Molecule 20: 30S Ribosomal protein S20



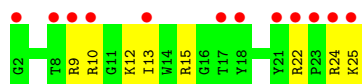
- Molecule 20: 30S Ribosomal protein S20



- Molecule 21: 30S Ribosomal protein THX



- Molecule 21: 30S Ribosomal protein THX



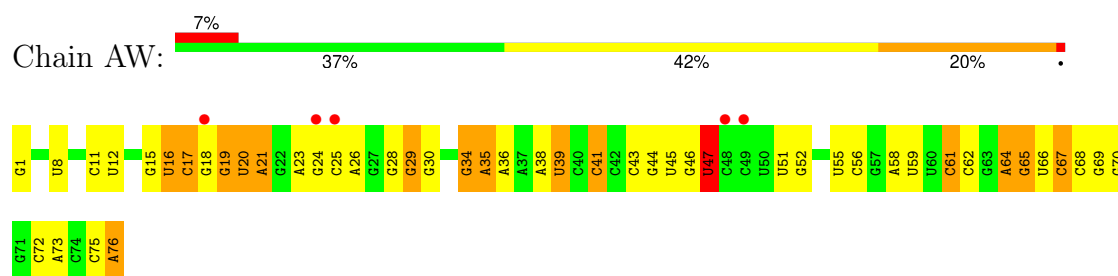
- Molecule 22: P-SITE tRNA



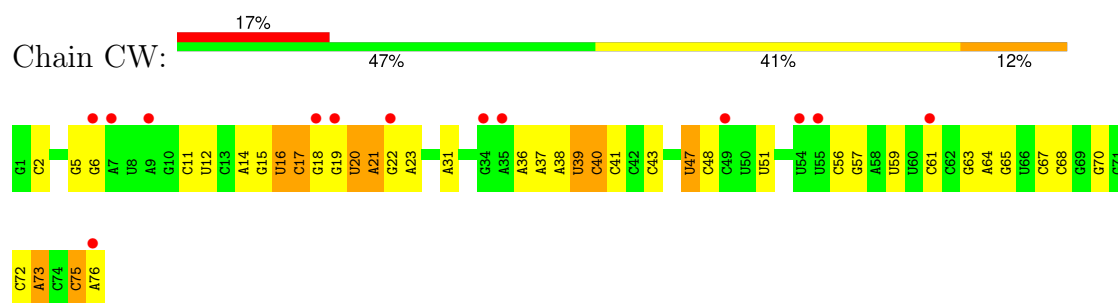
- Molecule 22: P-SITE tRNA



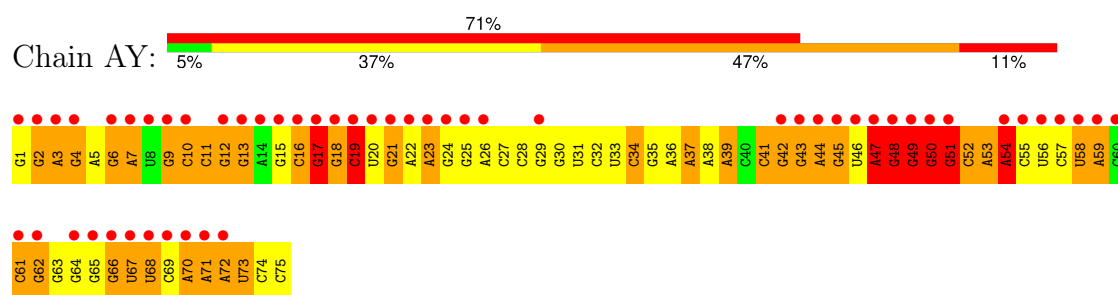
- Molecule 23: E-SITE tRNA



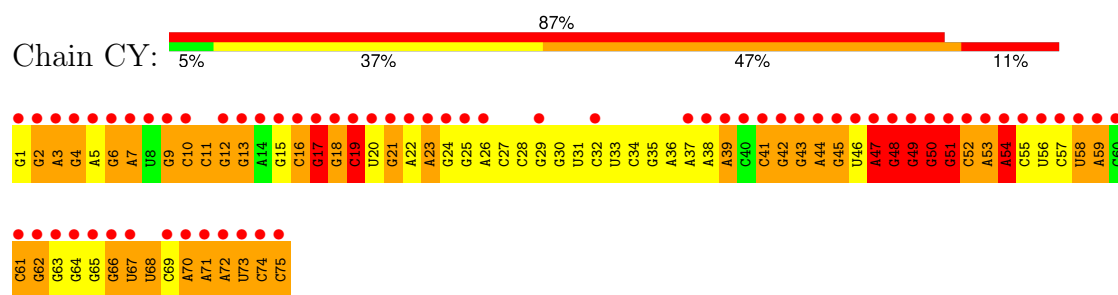
- Molecule 23: E-SITE tRNA



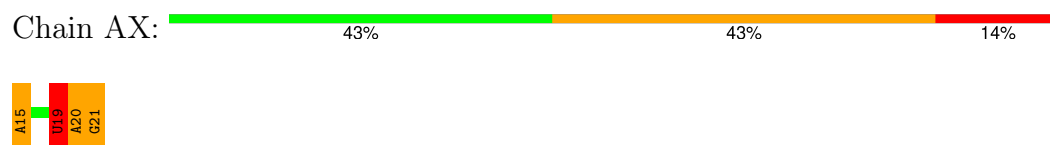
- Molecule 24: A-SITE tRNA



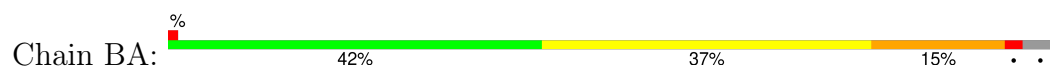
- Molecule 24: A-SITE tRNA



- Molecule 25: mRNA

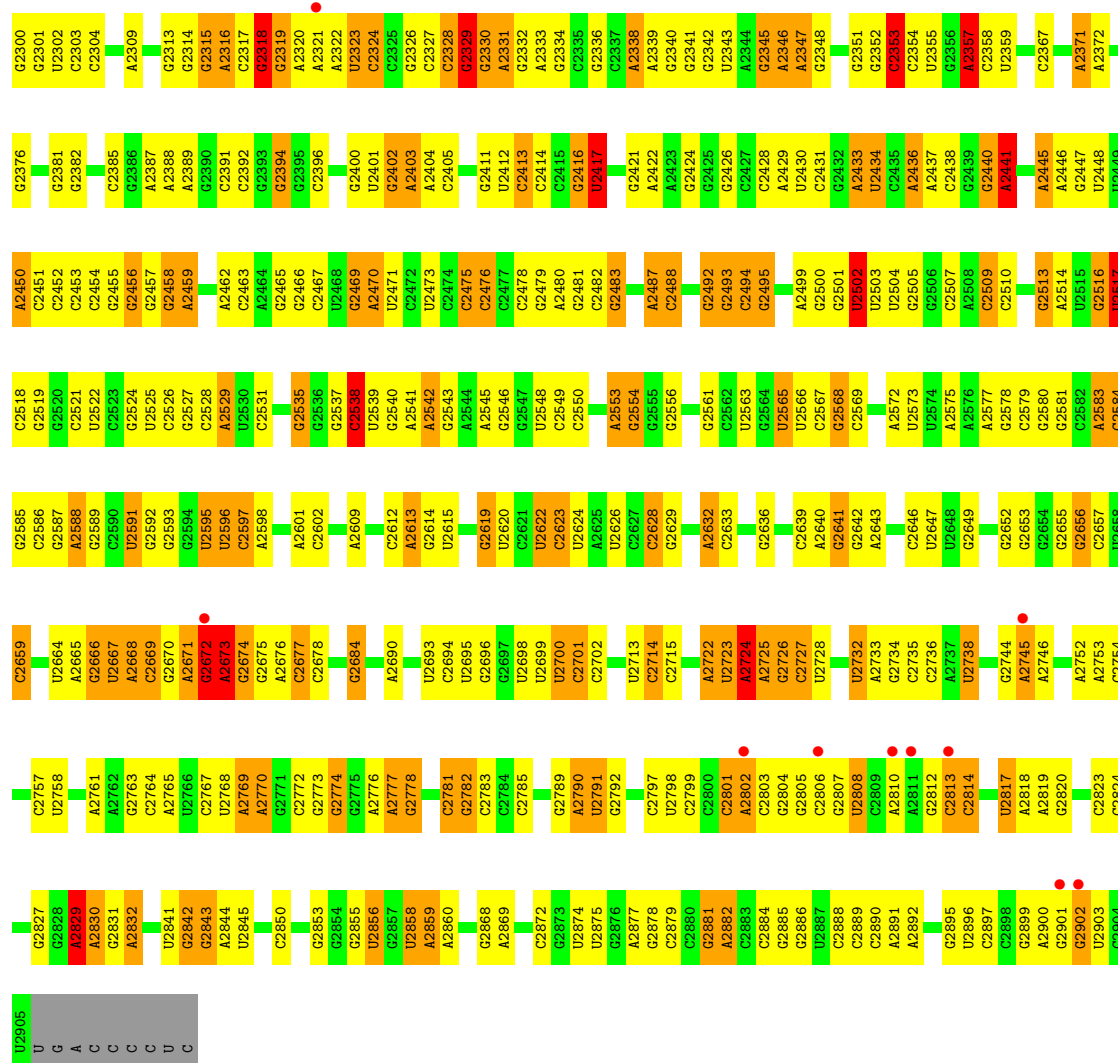


- Molecule 26: 23S ribosomal RNA

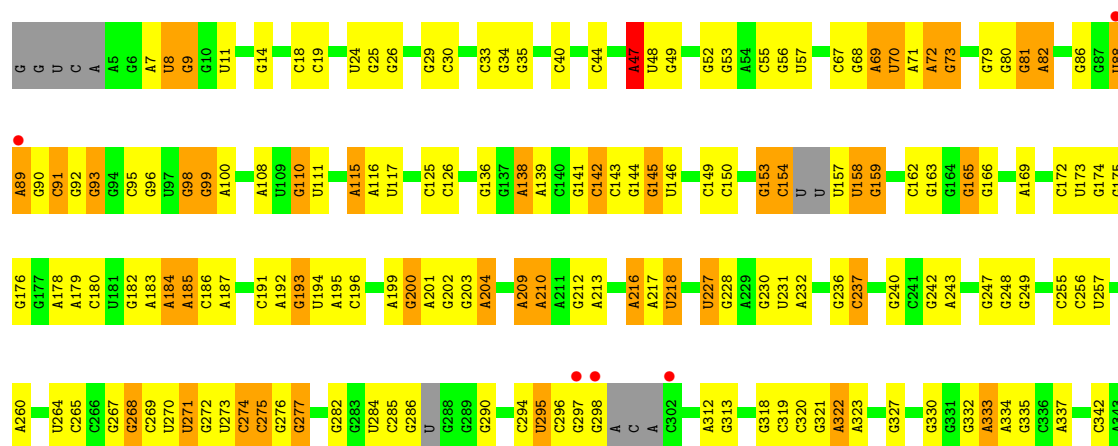


WORLDWIDE
PDB
PROTEIN DATA BANK

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C2223	G2142	C2071	G1985	C1908	C1649	G1743	G1496	G1406	G1324	U1252	A1171
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C2237	A2155	A2083	C2003	A1921	C1662	G1766	G1507	A1425	U1339	G1268	U1186
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G2244	G2169	G2090	G2013	G1930	U1685	G1775	C1595	A1440	A1353	G1281	C1198
G2245	G2170	U2091	U2014	U1931	A1687	G1776	A1600	U1441	G1354	G1282	G1199
G2246	G2171	A2092	C2015	U1932	G1688	G1777	G1526	U1442	U1357	G1284	A1200
G2247	G2180	G2018	G2018	A1934	G1689	A1778	G1527	U1443	U1358	U1285	A1201
U2254	U2096	G2019	G2019	C1935	C1690	G1779	G1528	U1444	C1359	G1286	G1202
U2255	U2097	G2020	C2029	U1936	G1691	G1780	G1529	U1445	U1360	A1287	G1203
U2256	A2098	G2020	G2030	U1937	C1692	G1783	G1530	U1446	C1363	U1204	
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G2187	G2188	G1885	G1885	U1939	C1694	G1789	G1536	U1450	A1291		
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C2196	G2039	C1872	C1872	U1946	C1702	G1794	U1541	G1458	C1296		
C2197	G2040	U1874	U1874	U1947	C1703	G1801	U1542	G1459	G1297		
C2198	A2041	G1875	G1875	A1948	U1705	G1802	U1543	U1460	A1298		
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C2200	U2043	A1877	A1877	G1950	G1716	C1804	G1545	G1462	U1300		
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G2202	G2045	U1879	G1879	G1952	U1717	G1806	U1547	U1465	C1302		
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G2205	G2048	A1889	A1889	C1955	G1724	U1809	C1550	A1387	G1306		
A2284	U2049	C1811	C1811	A1957	U1725	A1810	C1551	U1387	A1307		
G2285	G2050	U1894	U1894	A1958	U1726	A1814	A1552	C1390	G1308		
G2286	A2051	C1895	C1895	A1959	G1727	A1815	C1553	G1391	G1309		
C2287	A2052	C1896	C1896	A1959	G1728	A1816	C1554	G1392	A1310		
G2288	G2053	A1897	A1897	U1967	G1729	A1817	A1555	G1393	G1311		
A2289	A2054	A1898	A1898	C1968	C1730	A1818	A1556	A1394	U1312		
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C2293	G2058	A1975	A1975	C1976	A1739	A1824	G1564	G1401	G1239		
G2294	U2062	U1976	U1976	U1977	C1740	U1824	U1565	U1402	C1245		
A2297	C2063	U1977	U1977	C1983	C1741	U1828	G1570	A1404	A1248		
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• Molecule 26: 23S ribosomal RNA





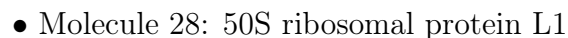
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U2096	U2100	G2101	G2102	C2107	C2108	C2109	U2110	G2111	G2114	C2115	C2116	C2117	C2118	C2119	U2120	C2121	C2122	C2123	C2124	C2125	C2129	U2130	G2131	C2137	A2138	U2139	A2140	G2141	A2147	C2148	C2149	G2152	U2153	C2154	A2155	C2163	C2164	A2079	A2080	A2081	C2082	A2083	C2084	C2085	C2086	C2087	C2088	C2011	U2012	C2013	U2014	C2015	C2094	U2095																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
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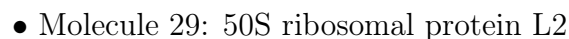
Response	Percentage
Best for the country	49%
Not the best for the country	33%
Don't know	18%

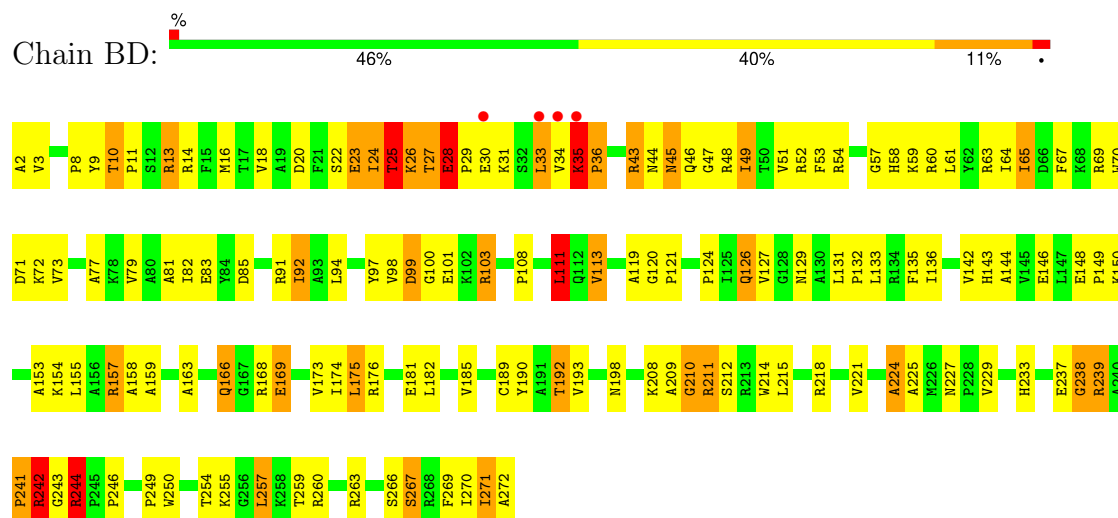


Frequency	Percentage
Very often	3%
Often	47%
Sometimes	43%
Never	10%

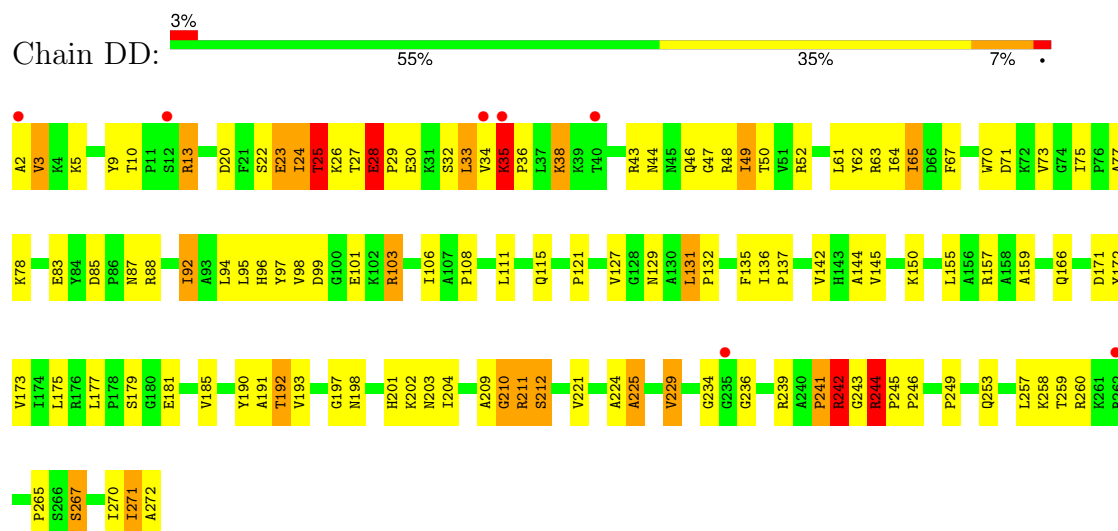


Frequency	Percentage
Very often	15%
Often	65%
Sometimes	23%
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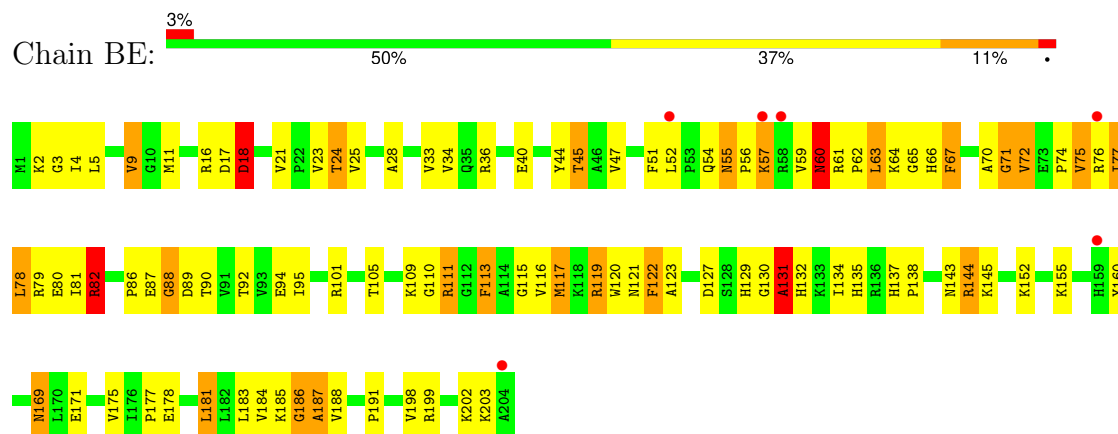




• Molecule 29: 50S ribosomal protein L2

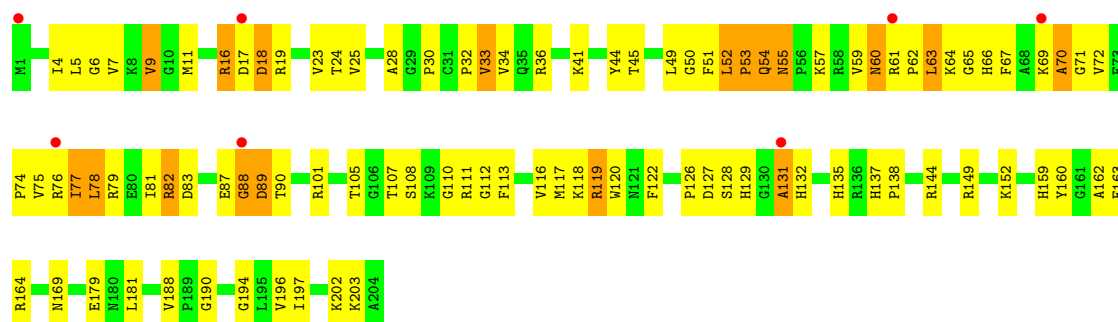


• Molecule 30: 50S ribosomal protein L3

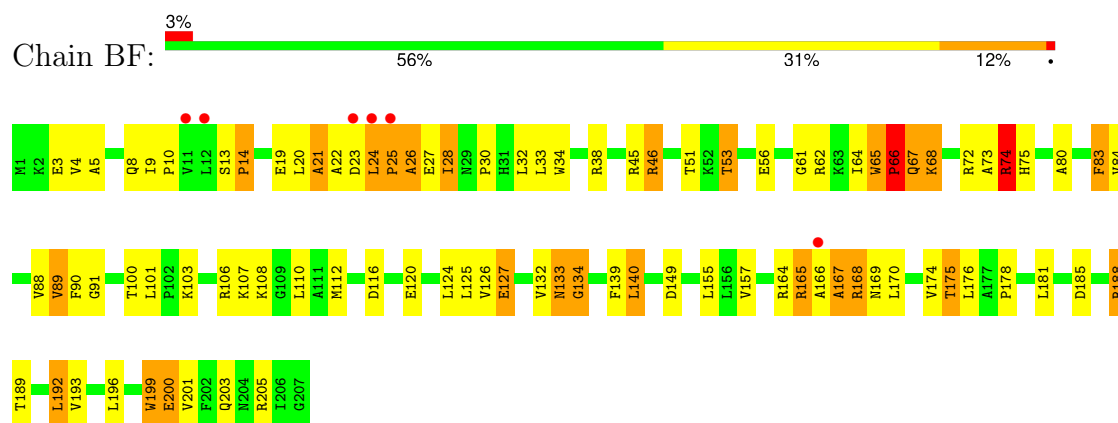


• Molecule 30: 50S ribosomal protein L3

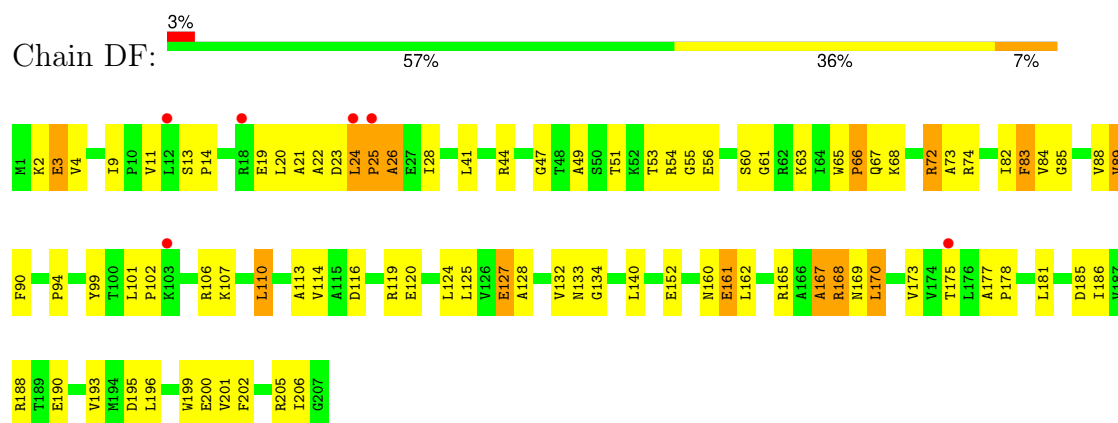




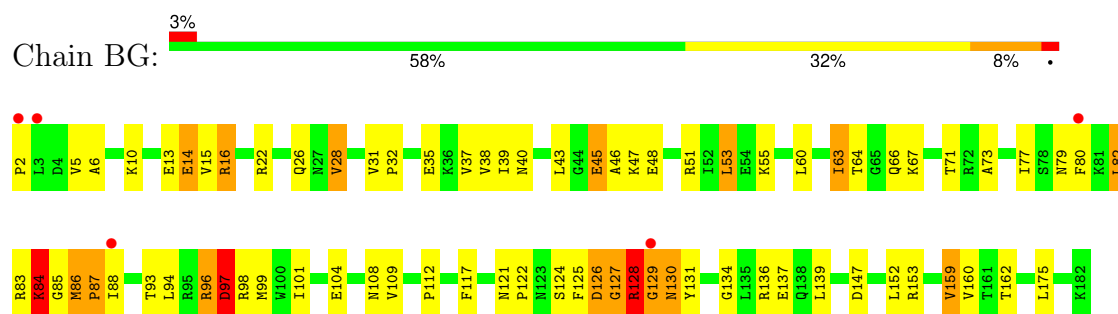
• Molecule 31: 50S ribosomal protein L4



• Molecule 31: 50S ribosomal protein L4

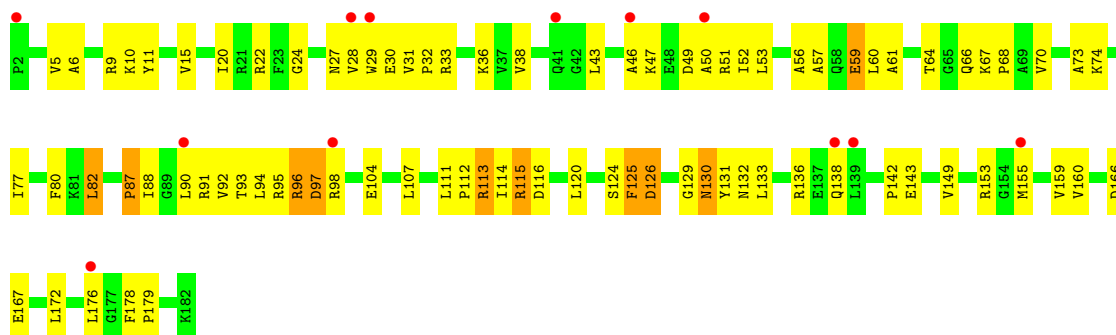


• Molecule 32: 50S ribosomal protein L5



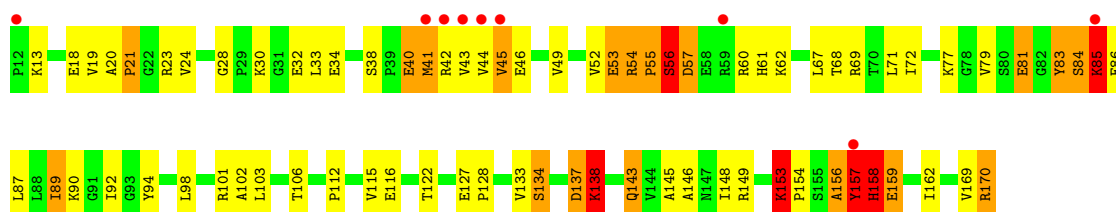
• Molecule 32: 50S ribosomal protein L5

Chain DG: 




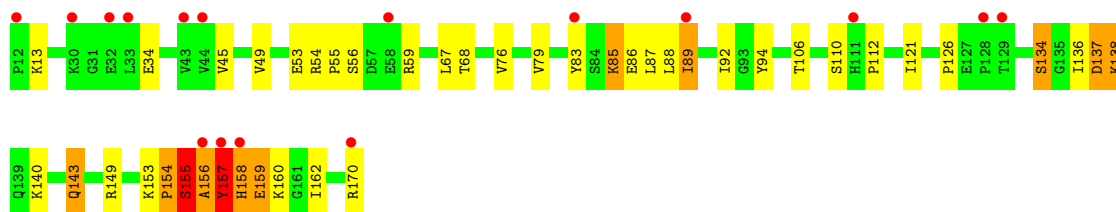
- Molecule 33: 50S ribosomal protein L6

Chain BH: 



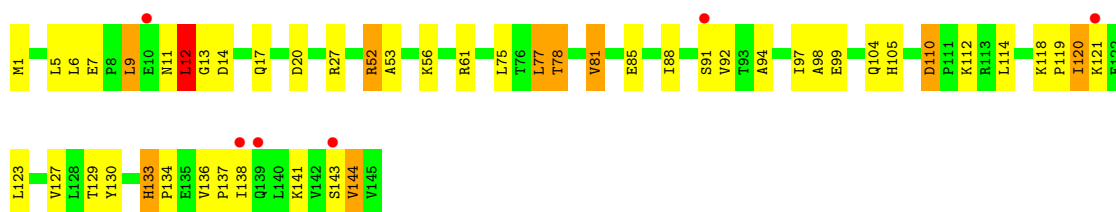
- Molecule 33: 50S ribosomal protein L6

Chain DH: 



- Molecule 34: 50S ribosomal protein L9

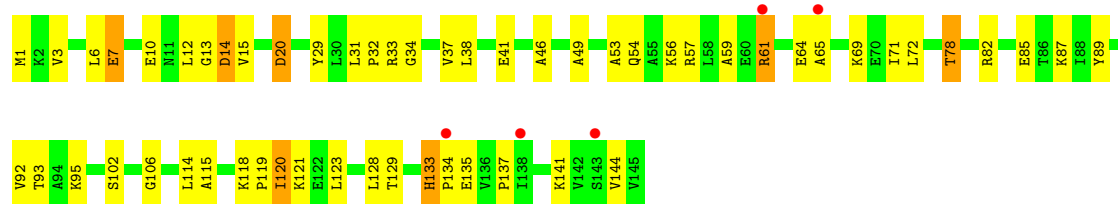
Chain BI: 



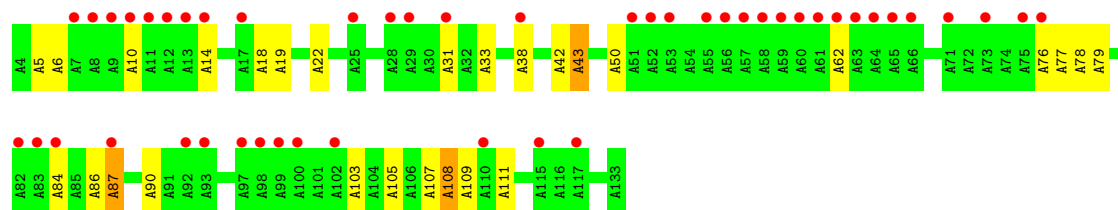
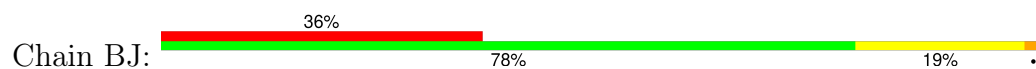
- Molecule 34: 50S ribosomal protein L9

Chain DI: 

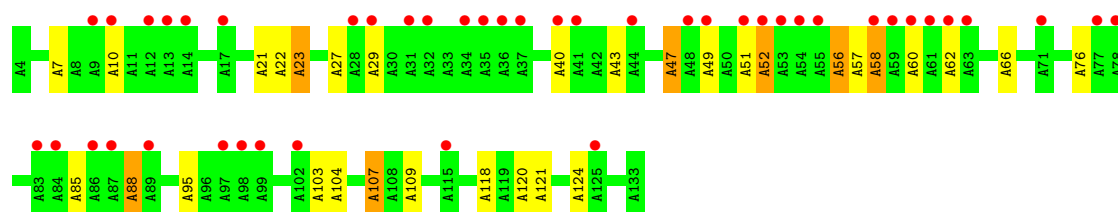
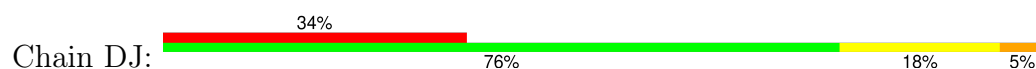




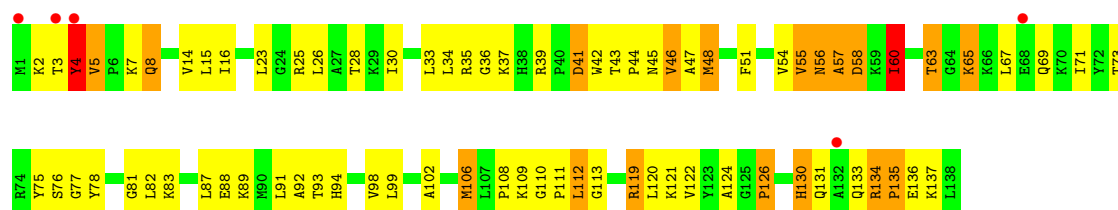
• Molecule 35: 50S ribosomal protein L10



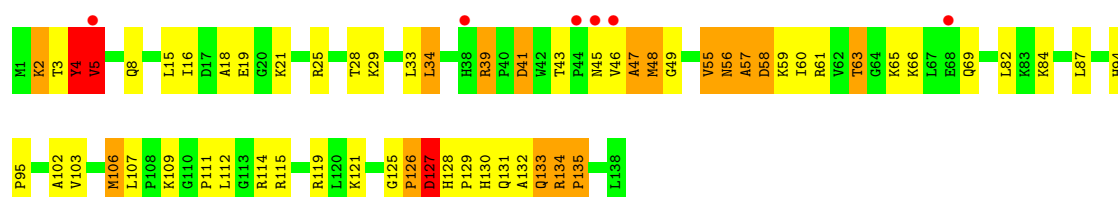
• Molecule 35: 50S ribosomal protein L10



• Molecule 36: 50S ribosomal protein L13



• Molecule 36: 50S ribosomal protein L13



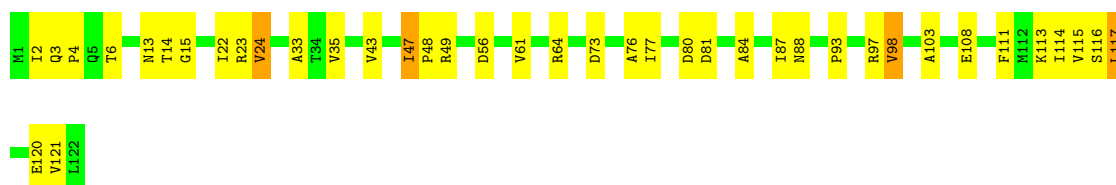
- Molecule 37: 50S ribosomal protein L14

Chain BO:  64% 34% .



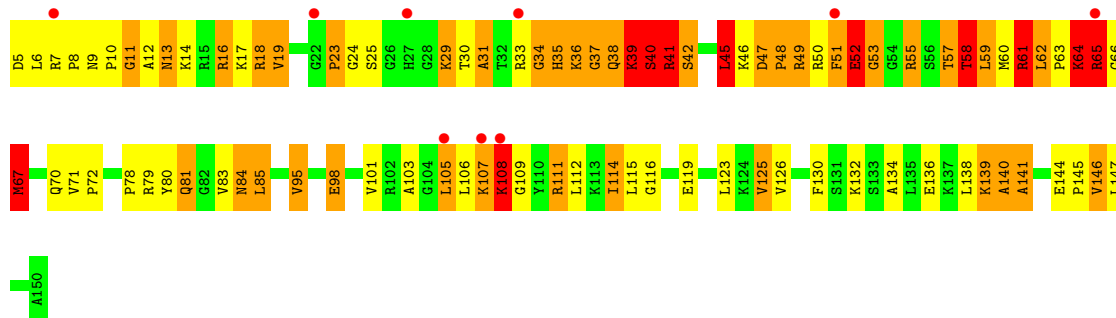
- Molecule 37: 50S ribosomal protein L14

Chain DO:  67% 30% .



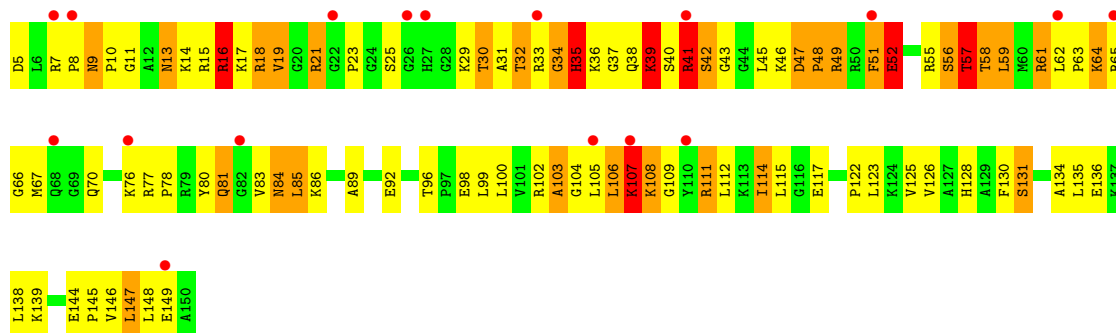
- Molecule 38: 50S ribosomal protein L15

Chain BP:  6% 38% 29% 25% 8%

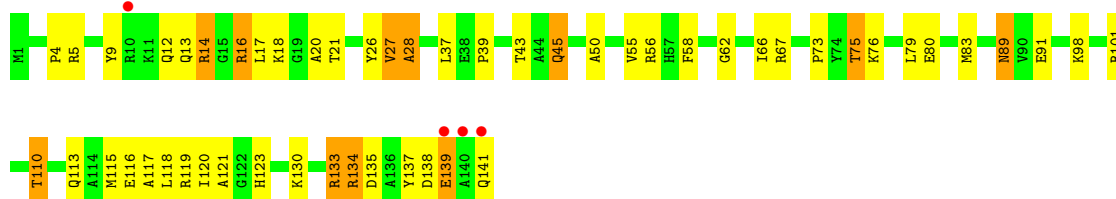


- Molecule 38: 50S ribosomal protein L15

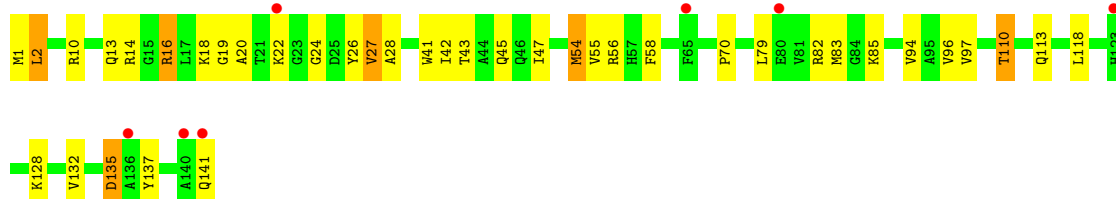
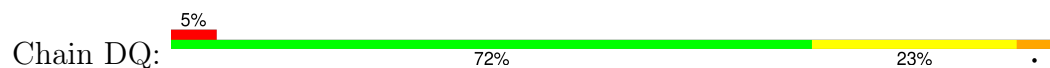
Chain DP:  12% 34% 42% 19% 5%



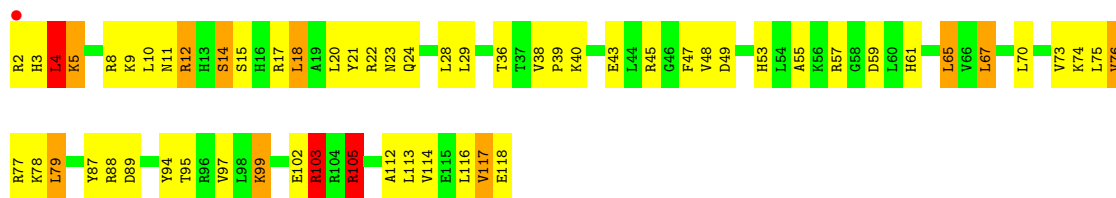
- Molecule 39: 50S ribosomal protein L16



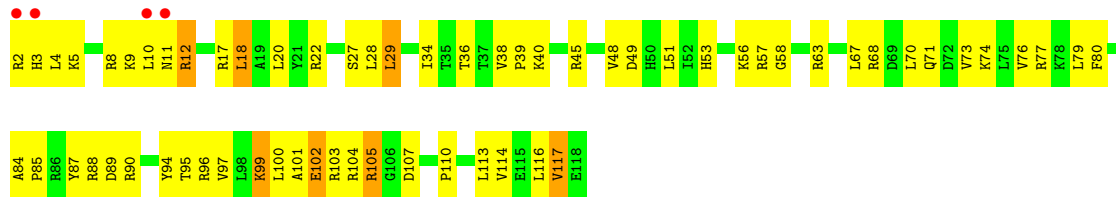
- Molecule 39: 50S ribosomal protein L16



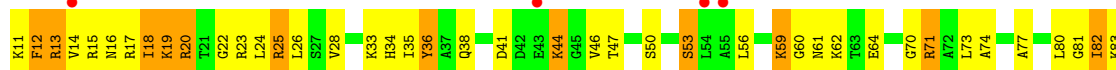
- Molecule 40: 50S ribosomal protein L17



- Molecule 40: 50S ribosomal protein L17

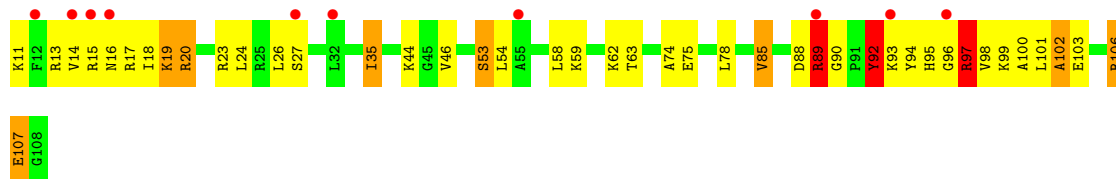


- Molecule 41: 50S ribosomal protein L18

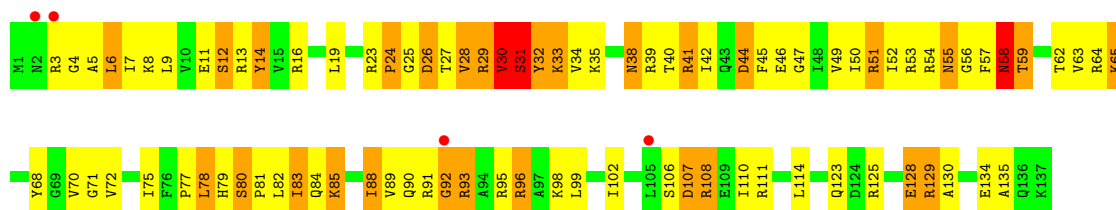




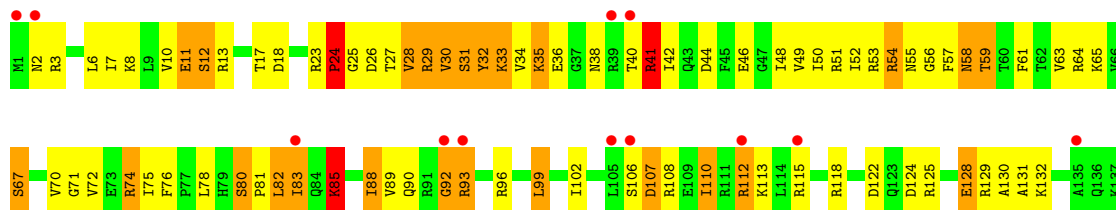
- Molecule 41: 50S ribosomal protein L18



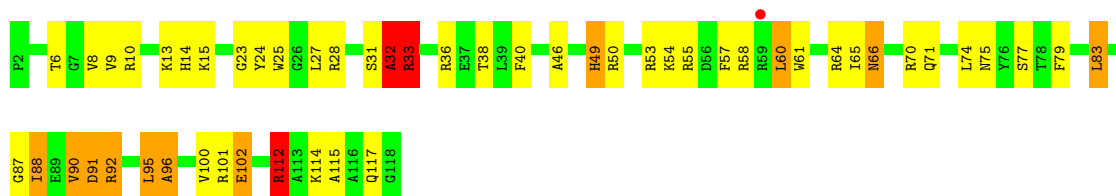
- Molecule 42: 50S ribosomal protein L19



- Molecule 42: 50S ribosomal protein L19

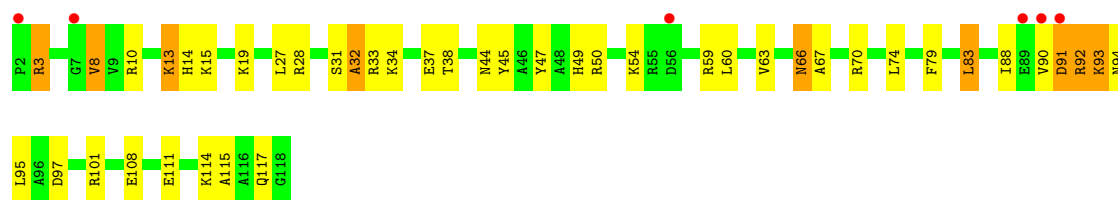


- Molecule 43: 50S ribosomal protein L20

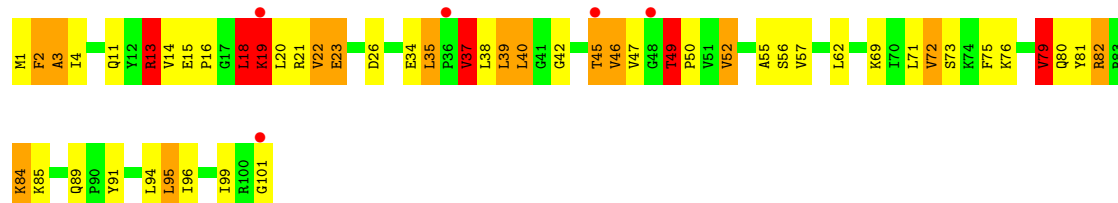


- Molecule 43: 50S ribosomal protein L20

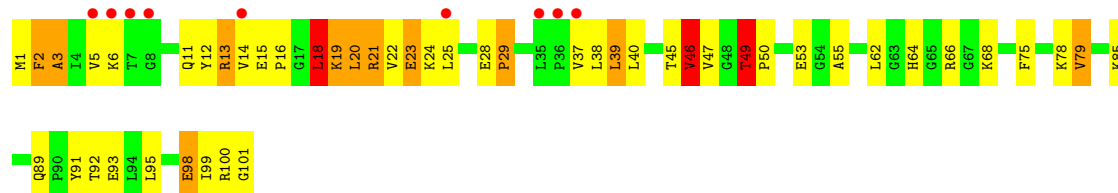




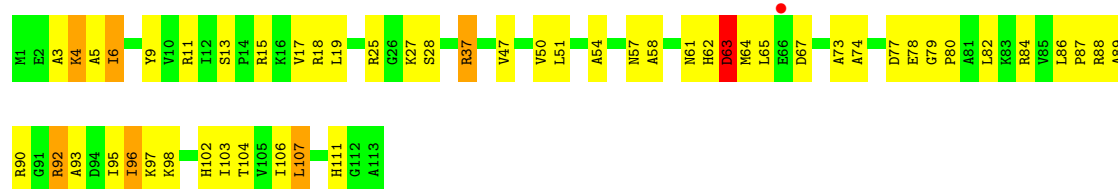
• Molecule 44: 50S ribosomal protein L21



• Molecule 44: 50S ribosomal protein L21



• Molecule 45: 50S ribosomal protein L22

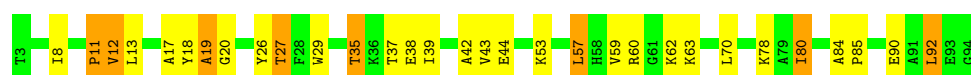


• Molecule 45: 50S ribosomal protein L22



• Molecule 46: 50S ribosomal protein L23

Chain BX: 



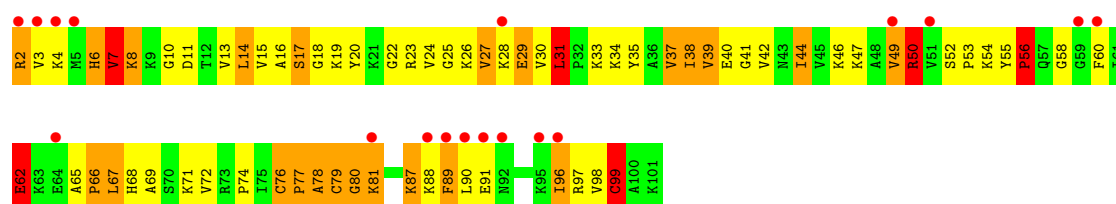
- Molecule 46: 50S ribosomal protein L23

Chain DX: 



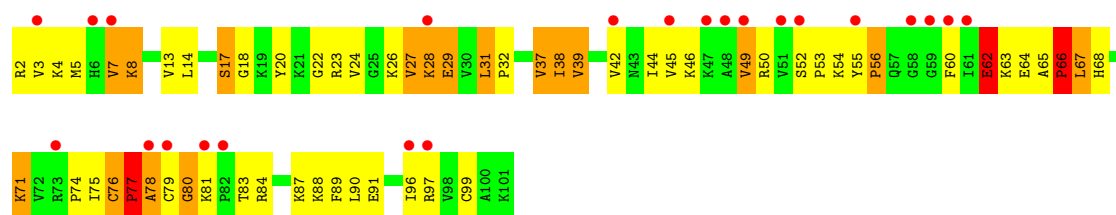
- Molecule 47: 50S ribosomal protein L24

Chain BY: 




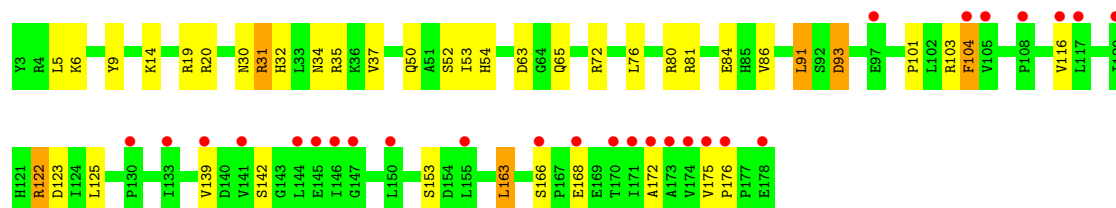
- Molecule 47: 50S ribosomal protein L24

Chain DY: 



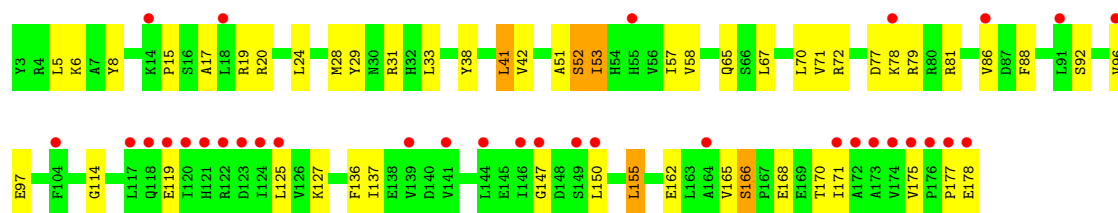
- Molecule 48: 50S ribosomal protein L25

Chain BZ: 



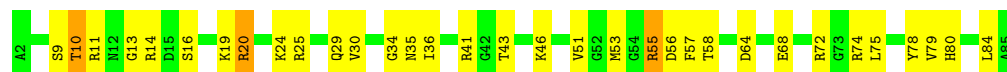
- Molecule 48: 50S ribosomal protein L25

Chain DZ: 



- Molecule 49: 50S ribosomal protein L27

Chain B0: 61% 36%



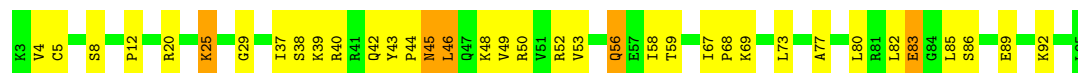
- Molecule 49: 50S ribosomal protein L27

Chain D0: 4% 62% 37%



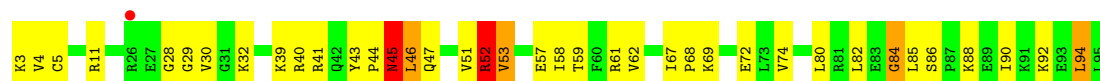
- Molecule 50: 50S ribosomal protein L28

Chain B1: 61% 33% 5%



- Molecule 50: 50S ribosomal protein L28

Chain D1: 59% 34% 7%



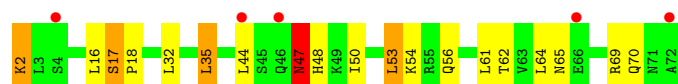
- Molecule 51: 50S ribosomal protein L29

Chain B2: 3% 51% 35% 13%

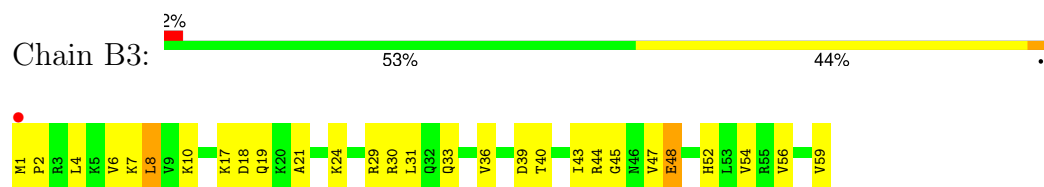


- Molecule 51: 50S ribosomal protein L29

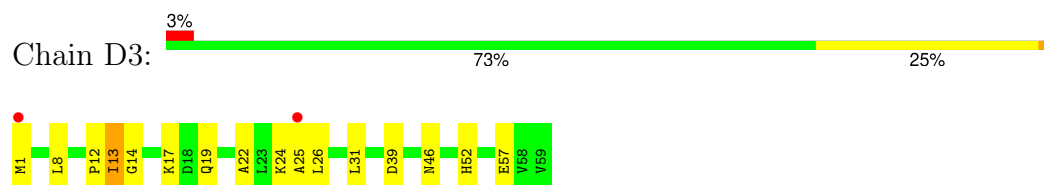
Chain D2: 7% 73% 20% 6%



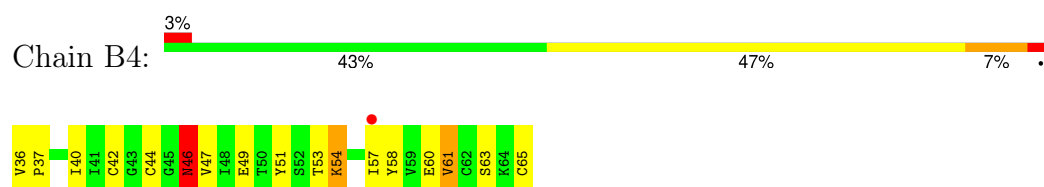
• Molecule 52: 50S ribosomal protein L30



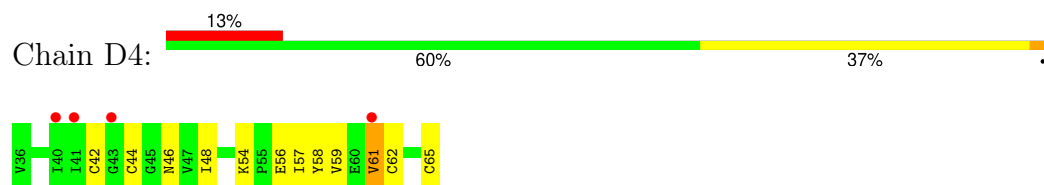
• Molecule 52: 50S ribosomal protein L30



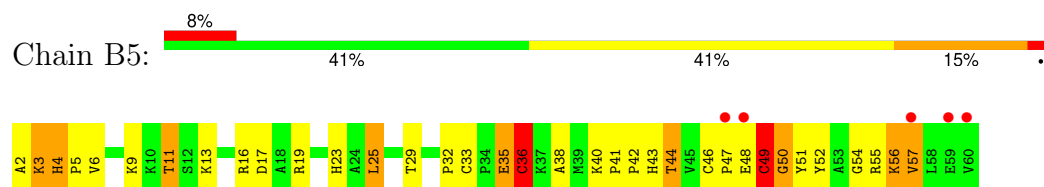
• Molecule 53: 50S ribosomal protein L31



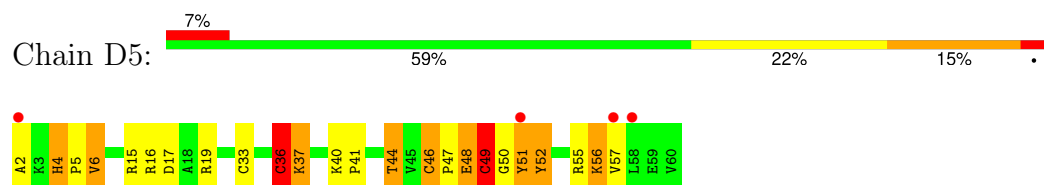
• Molecule 53: 50S ribosomal protein L31



• Molecule 54: 50S ribosomal protein L32



• Molecule 54: 50S ribosomal protein L32

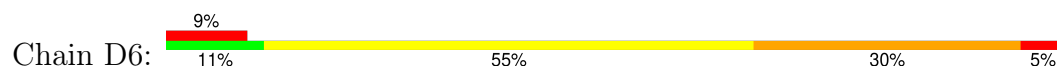


• Molecule 55: 50S ribosomal protein L33





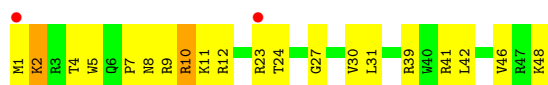
- Molecule 55: 50S ribosomal protein L33



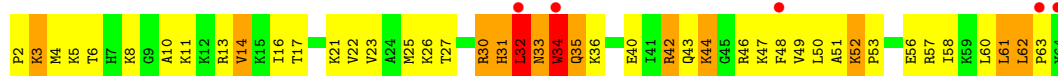
- Molecule 56: 50S ribosomal protein L34



- Molecule 56: 50S ribosomal protein L34



- Molecule 57: 50S ribosomal protein L35



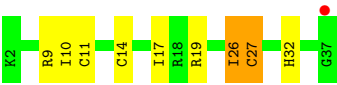
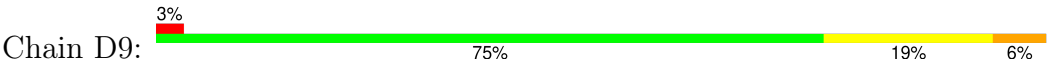
- Molecule 57: 50S ribosomal protein L35



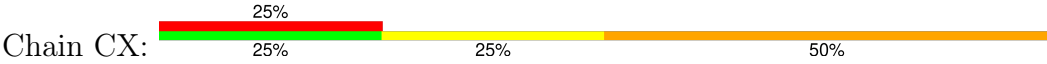
- Molecule 58: 50S ribosomal protein L36



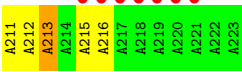
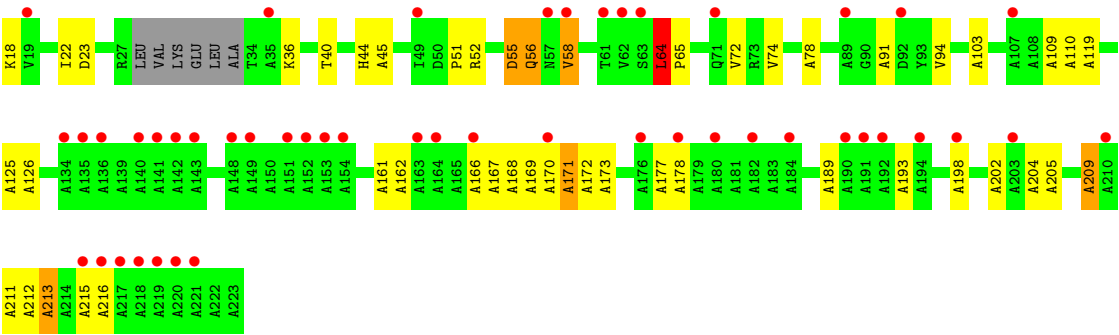
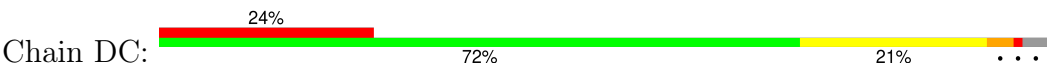
- Molecule 58: 50S ribosomal protein L36



• Molecule 59: mRNA



• Molecule 60: 50S Ribosomal protein L1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0031	Depositor
R, R_{free}	0.225 , 0.279 0.230 , 0.278	Depositor DCC
R_{free} test set	41956 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU

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	C4',C3',C1'

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:C'Y:7:A:N1	24:C'Y:66:G:N2	1.61	1.48
24:AY:7:A:N1	24:AY:66:G:N2	1.61	1.46
24:C'Y:10:C:H41	24:C'Y:45:G:N2	1.03	1.46
24:C'Y:9:G:H21	24:C'Y: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	13
2	CB	232/234 (99%)	181 (78%)	41 (18%)	10 (4%)	2	14
3	AC	204/206 (99%)	150 (74%)	40 (20%)	14 (7%)	1	7
3	CC	204/206 (99%)	159 (78%)	32 (16%)	13 (6%)	1	8
4	AD	206/208 (99%)	155 (75%)	37 (18%)	14 (7%)	1	7
4	CD	206/208 (99%)	160 (78%)	36 (18%)	10 (5%)	2	12
5	AE	148/150 (99%)	129 (87%)	15 (10%)	4 (3%)	4	22
5	CE	148/150 (99%)	130 (88%)	16 (11%)	2 (1%)	9	34
6	AF	99/101 (98%)	89 (90%)	7 (7%)	3 (3%)	3	21
6	CF	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	6	28
7	AG	153/155 (99%)	133 (87%)	18 (12%)	2 (1%)	10	36
7	CG	153/155 (99%)	130 (85%)	18 (12%)	5 (3%)	3	19
8	AH	136/138 (99%)	119 (88%)	14 (10%)	3 (2%)	5	26
8	CH	136/138 (99%)	115 (85%)	18 (13%)	3 (2%)	5	26
9	AI	125/127 (98%)	96 (77%)	25 (20%)	4 (3%)	3	20
9	CI	125/127 (98%)	101 (81%)	21 (17%)	3 (2%)	5	25
10	AJ	96/98 (98%)	76 (79%)	17 (18%)	3 (3%)	3	21
10	CJ	96/98 (98%)	73 (76%)	18 (19%)	5 (5%)	1	11
11	AK	117/119 (98%)	96 (82%)	19 (16%)	2 (2%)	7	31
11	CK	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	4	23
12	AL	122/124 (98%)	95 (78%)	18 (15%)	9 (7%)	1	6

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	DI	143/145 (99%)	110 (77%)	25 (18%)	8 (6%)	1	10
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	5
36	DN	136/138 (99%)	108 (79%)	15 (11%)	13 (10%)	0	3
37	BO	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	7	31
37	DO	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	16	46
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	18
39	DQ	139/141 (99%)	116 (84%)	19 (14%)	4 (3%)	3	22
40	BR	115/117 (98%)	93 (81%)	16 (14%)	6 (5%)	1	11
40	DR	115/117 (98%)	92 (80%)	17 (15%)	6 (5%)	1	11
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	1
43	BU	115/117 (98%)	90 (78%)	19 (16%)	6 (5%)	1	11
43	DU	115/117 (98%)	92 (80%)	19 (16%)	4 (4%)	3	19
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%)	4	22
45	DW	111/113 (98%)	96 (86%)	7 (6%)	8 (7%)	1	6
46	BX	90/92 (98%)	80 (89%)	7 (8%)	3 (3%)	3	19
46	DX	90/92 (98%)	75 (83%)	8 (9%)	7 (8%)	1	5
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	0
48	BZ	174/176 (99%)	141 (81%)	26 (15%)	7 (4%)	2	16
48	DZ	174/176 (99%)	130 (75%)	33 (19%)	11 (6%)	1	8
49	B0	82/84 (98%)	75 (92%)	6 (7%)	1 (1%)	11	38
49	D0	82/84 (98%)	72 (88%)	9 (11%)	1 (1%)	11	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	B1	91/93 (98%)	76 (84%)	12 (13%)	3 (3%)	3	19
50	D1	91/93 (98%)	74 (81%)	10 (11%)	7 (8%)	1	5
51	B2	69/71 (97%)	53 (77%)	10 (14%)	6 (9%)	0	4
51	D2	69/71 (97%)	54 (78%)	11 (16%)	4 (6%)	1	9
52	B3	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	7	30
52	D3	57/59 (97%)	53 (93%)	3 (5%)	1 (2%)	7	30
53	B4	28/30 (93%)	21 (75%)	4 (14%)	3 (11%)	0	2
53	D4	28/30 (93%)	20 (71%)	5 (18%)	3 (11%)	0	2
54	B5	57/59 (97%)	43 (75%)	9 (16%)	5 (9%)	0	4
54	D5	57/59 (97%)	48 (84%)	4 (7%)	5 (9%)	0	4
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%)	5	26
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	7

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%)	9	30
2	CB	202/202 (100%)	181 (90%)	21 (10%)	5	22
3	AC	160/160 (100%)	142 (89%)	18 (11%)	4	18
3	CC	160/160 (100%)	145 (91%)	15 (9%)	7	25
4	AD	180/180 (100%)	160 (89%)	20 (11%)	5	19
4	CD	180/180 (100%)	160 (89%)	20 (11%)	5	19
5	AE	115/115 (100%)	104 (90%)	11 (10%)	7	25
5	CE	115/115 (100%)	101 (88%)	14 (12%)	4	16
6	AF	90/90 (100%)	82 (91%)	8 (9%)	8	28
6	CF	90/90 (100%)	85 (94%)	5 (6%)	17	45
7	AG	126/126 (100%)	115 (91%)	11 (9%)	8	29
7	CG	126/126 (100%)	115 (91%)	11 (9%)	8	29
8	AH	119/119 (100%)	108 (91%)	11 (9%)	7	26
8	CH	119/119 (100%)	107 (90%)	12 (10%)	6	23
9	AI	98/98 (100%)	88 (90%)	10 (10%)	6	23
9	CI	98/98 (100%)	89 (91%)	9 (9%)	7	26
10	AJ	88/88 (100%)	76 (86%)	12 (14%)	3	14
10	CJ	88/88 (100%)	79 (90%)	9 (10%)	6	23
11	AK	90/90 (100%)	82 (91%)	8 (9%)	8	28
11	CK	90/90 (100%)	84 (93%)	6 (7%)	13	39
12	AL	104/104 (100%)	88 (85%)	16 (15%)	2	10
12	CL	104/104 (100%)	90 (86%)	14 (14%)	3	14
13	AM	99/99 (100%)	88 (89%)	11 (11%)	5	19
13	CM	99/99 (100%)	88 (89%)	11 (11%)	5	19
14	AN	49/49 (100%)	43 (88%)	6 (12%)	4	16
14	CN	49/49 (100%)	44 (90%)	5 (10%)	6	23
15	AO	79/79 (100%)	73 (92%)	6 (8%)	11	34
15	CO	79/79 (100%)	76 (96%)	3 (4%)	28	56
16	AP	72/72 (100%)	65 (90%)	7 (10%)	6	25
16	CP	72/72 (100%)	62 (86%)	10 (14%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AQ	94/94 (100%)	88 (94%)	6 (6%)	14	40
17	CQ	94/94 (100%)	89 (95%)	5 (5%)	19	47
18	AR	61/61 (100%)	54 (88%)	7 (12%)	4	18
18	CR	61/61 (100%)	59 (97%)	2 (3%)	33	60
19	AS	69/69 (100%)	56 (81%)	13 (19%)	1	6
19	CS	69/69 (100%)	58 (84%)	11 (16%)	2	9
20	AT	76/76 (100%)	68 (90%)	8 (10%)	5	21
20	CT	76/76 (100%)	67 (88%)	9 (12%)	4	17
21	AU	19/19 (100%)	15 (79%)	4 (21%)	1	4
21	CU	19/19 (100%)	17 (90%)	2 (10%)	5	21
28	BC	61/66 (92%)	55 (90%)	6 (10%)	6	24
29	BD	213/213 (100%)	180 (84%)	33 (16%)	2	10
29	DD	213/213 (100%)	176 (83%)	37 (17%)	1	7
30	BE	165/165 (100%)	134 (81%)	31 (19%)	1	6
30	DE	165/165 (100%)	139 (84%)	26 (16%)	2	10
31	BF	165/165 (100%)	138 (84%)	27 (16%)	2	9
31	DF	165/165 (100%)	149 (90%)	16 (10%)	6	25
32	BG	155/155 (100%)	128 (83%)	27 (17%)	1	7
32	DG	155/155 (100%)	137 (88%)	18 (12%)	4	18
33	BH	132/132 (100%)	106 (80%)	26 (20%)	1	5
33	DH	132/132 (100%)	120 (91%)	12 (9%)	7	27
34	BI	122/122 (100%)	110 (90%)	12 (10%)	6	24
34	DI	122/122 (100%)	111 (91%)	11 (9%)	8	27
36	BN	117/117 (100%)	90 (77%)	27 (23%)	0	3
36	DN	117/117 (100%)	94 (80%)	23 (20%)	1	5
37	BO	100/100 (100%)	92 (92%)	8 (8%)	10	32
37	DO	100/100 (100%)	93 (93%)	7 (7%)	12	37
38	BP	112/112 (100%)	83 (74%)	29 (26%)	0	2
38	DP	112/112 (100%)	86 (77%)	26 (23%)	0	3
39	BQ	111/111 (100%)	97 (87%)	14 (13%)	3	16
39	DQ	111/111 (100%)	101 (91%)	10 (9%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BR	100/100 (100%)	85 (85%)	15 (15%)	2	11
40	DR	100/100 (100%)	85 (85%)	15 (15%)	2	11
41	BS	77/77 (100%)	60 (78%)	17 (22%)	1	3
41	DS	77/77 (100%)	67 (87%)	10 (13%)	3	14
42	BT	120/120 (100%)	98 (82%)	22 (18%)	1	6
42	DT	120/120 (100%)	93 (78%)	27 (22%)	1	3
43	BU	92/92 (100%)	78 (85%)	14 (15%)	2	10
43	DU	92/92 (100%)	82 (89%)	10 (11%)	5	20
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%)	5	20
45	DW	91/91 (100%)	80 (88%)	11 (12%)	4	16
46	BX	74/74 (100%)	67 (90%)	7 (10%)	7	25
46	DX	74/74 (100%)	65 (88%)	9 (12%)	4	16
47	BY	84/84 (100%)	65 (77%)	19 (23%)	1	3
47	DY	84/84 (100%)	67 (80%)	17 (20%)	1	4
48	BZ	155/155 (100%)	141 (91%)	14 (9%)	8	27
48	DZ	155/155 (100%)	148 (96%)	7 (4%)	23	52
49	B0	66/66 (100%)	55 (83%)	11 (17%)	2	8
49	D0	66/66 (100%)	60 (91%)	6 (9%)	7	27
50	B1	78/78 (100%)	68 (87%)	10 (13%)	3	15
50	D1	78/78 (100%)	62 (80%)	16 (20%)	1	4
51	B2	66/66 (100%)	51 (77%)	15 (23%)	0	3
51	D2	66/66 (100%)	60 (91%)	6 (9%)	7	27
52	B3	51/51 (100%)	47 (92%)	4 (8%)	10	33
52	D3	51/51 (100%)	48 (94%)	3 (6%)	16	43
53	B4	27/27 (100%)	22 (82%)	5 (18%)	1	6
53	D4	27/27 (100%)	24 (89%)	3 (11%)	5	19
54	B5	51/51 (100%)	39 (76%)	12 (24%)	0	3
54	D5	51/51 (100%)	41 (80%)	10 (20%)	1	5
55	B6	43/43 (100%)	33 (77%)	10 (23%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	D6	43/43 (100%)	36 (84%)	7 (16%)	2	9
56	B7	41/41 (100%)	35 (85%)	6 (15%)	2	12
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%)	7	27
60	DC	61/66 (92%)	56 (92%)	5 (8%)	9	31
All	All	9654/9664 (100%)	8391 (87%)	1263 (13%)	3	14

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	24,25	18,21,22	1.55	3 (16%)	21,30,33	1.49	3 (14%)

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	24,25	-	2/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AX	19	PSU	C2-N1	5.10	1.43	1.36
25	AX	19	PSU	C6-C5	2.58	1.38	1.35
25	AX	19	PSU	C4-C5	-2.05	1.38	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AX	19	PSU	C6-C5-C4	4.23	121.03	118.17
25	AX	19	PSU	C6-N1-C2	-3.19	119.73	122.69
25	AX	19	PSU	O2-C2-N1	2.99	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 oligosaccharides 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, 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	1504/1504 (100%)	0.04	33 (2%) 62 47	23, 77, 165, 393	0
1	CA	1504/1504 (100%)	0.20	59 (3%) 44 33	38, 86, 188, 312	0
2	AB	234/234 (100%)	0.50	11 (4%) 37 28	66, 113, 158, 196	0
2	CB	234/234 (100%)	0.89	29 (12%) 9 9	85, 139, 177, 216	0
3	AC	206/206 (100%)	0.41	9 (4%) 39 30	64, 96, 134, 183	0
3	CC	206/206 (100%)	0.94	25 (12%) 10 10	90, 130, 182, 221	0
4	AD	208/208 (100%)	0.46	20 (9%) 15 14	55, 91, 126, 174	0
4	CD	208/208 (100%)	0.17	12 (5%) 30 24	49, 79, 108, 139	0
5	AE	150/150 (100%)	0.06	1 (0%) 84 75	47, 76, 104, 125	0
5	CE	150/150 (100%)	0.31	7 (4%) 37 28	58, 88, 126, 148	0
6	AF	101/101 (100%)	-0.03	0 100 100	52, 80, 108, 124	0
6	CF	101/101 (100%)	0.01	0 100 100	52, 82, 116, 139	0
7	AG	155/155 (100%)	0.39	12 (7%) 21 18	61, 97, 137, 156	0
7	CG	155/155 (100%)	0.61	11 (7%) 23 20	82, 119, 157, 175	0
8	AH	138/138 (100%)	0.01	2 (1%) 73 60	50, 81, 105, 135	0
8	CH	138/138 (100%)	0.36	4 (2%) 54 40	59, 95, 119, 146	0
9	AI	127/127 (100%)	0.63	9 (7%) 23 20	58, 112, 146, 230	0
9	CI	127/127 (100%)	1.13	24 (18%) 4 3	94, 136, 180, 235	0
10	AJ	98/98 (100%)	0.99	14 (14%) 7 7	67, 119, 160, 187	0
10	CJ	98/98 (100%)	1.45	23 (23%) 2 2	94, 158, 190, 226	0
11	AK	119/119 (100%)	0.21	4 (3%) 48 35	45, 79, 108, 165	0
11	CK	119/119 (100%)	0.47	4 (3%) 48 35	55, 95, 132, 161	0
12	AL	124/124 (100%)	0.26	6 (4%) 36 28	47, 71, 105, 155	0
12	CL	124/124 (100%)	0.34	5 (4%) 43 32	50, 81, 115, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	124/124 (100%)	0.79	14 (11%) 11 11	68, 112, 153, 231	0
13	CM	124/124 (100%)	1.44	30 (24%) 2 1	101, 153, 200, 218	0
14	AN	60/60 (100%)	0.38	3 (5%) 35 28	55, 85, 135, 155	0
14	CN	60/60 (100%)	1.09	8 (13%) 8 8	104, 137, 160, 182	0
15	AO	88/88 (100%)	0.24	2 (2%) 61 46	48, 80, 111, 130	0
15	CO	88/88 (100%)	0.14	3 (3%) 48 35	55, 87, 117, 139	0
16	AP	83/83 (100%)	0.61	4 (4%) 36 28	65, 92, 125, 149	0
16	CP	83/83 (100%)	0.05	1 (1%) 76 64	51, 73, 112, 139	0
17	AQ	99/99 (100%)	0.23	1 (1%) 79 68	51, 90, 112, 117	0
17	CQ	99/99 (100%)	0.24	3 (3%) 52 39	63, 87, 115, 126	0
18	AR	70/70 (100%)	0.21	3 (4%) 40 30	48, 76, 108, 138	0
18	CR	70/70 (100%)	0.18	0 100 100	61, 91, 126, 149	0
19	AS	78/78 (100%)	0.76	9 (11%) 11 11	72, 114, 165, 189	0
19	CS	78/78 (100%)	1.20	11 (14%) 7 8	111, 160, 208, 221	0
20	AT	99/99 (100%)	0.59	9 (9%) 16 15	67, 102, 150, 169	0
20	CT	99/99 (100%)	0.38	3 (3%) 52 39	49, 96, 135, 150	0
21	AU	24/24 (100%)	0.88	1 (4%) 41 31	74, 92, 117, 119	0
21	CU	24/24 (100%)	2.40	12 (50%) 0 0	105, 141, 205, 253	0
22	AV	77/77 (100%)	-0.08	1 (1%) 74 61	34, 78, 122, 187	0
22	CV	77/77 (100%)	0.28	1 (1%) 74 61	41, 107, 162, 175	0
23	AW	76/76 (100%)	0.95	5 (6%) 26 21	37, 183, 225, 269	0
23	CW	76/76 (100%)	1.14	13 (17%) 5 4	59, 192, 268, 296	0
24	AY	75/75 (100%)	3.10	53 (70%) 0 0	37, 107, 188, 213	0
24	CY	75/75 (100%)	3.70	65 (86%) 0 0	37, 107, 188, 213	0
25	AX	6/7 (85%)	0.10	0 100 100	50, 53, 106, 116	0
26	BA	2807/2915 (96%)	-0.50	38 (1%) 73 60	9, 38, 151, 312	0
26	DA	2807/2915 (96%)	-0.18	45 (1%) 70 57	24, 64, 168, 297	0
27	BB	119/119 (100%)	-0.30	0 100 100	32, 60, 91, 118	0
27	DB	119/119 (100%)	0.45	3 (2%) 58 43	71, 112, 151, 191	0
28	BC	190/206 (92%)	1.20	31 (16%) 5 5	108, 181, 242, 295	0
29	BD	271/271 (100%)	-0.31	4 (1%) 71 58	18, 36, 76, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	DD	271/271 (100%)	-0.05	7 (2%) 57 42	23, 56, 91, 127	0
30	BE	204/204 (100%)	-0.06	6 (2%) 54 40	18, 48, 92, 134	0
30	DE	204/204 (100%)	0.15	7 (3%) 48 35	28, 65, 120, 165	0
31	BF	207/207 (100%)	-0.12	6 (2%) 54 40	17, 48, 133, 191	0
31	DF	207/207 (100%)	0.24	6 (2%) 54 40	31, 87, 149, 214	0
32	BG	181/181 (100%)	0.20	5 (2%) 55 40	56, 82, 129, 172	0
32	DG	181/181 (100%)	0.77	12 (6%) 26 21	82, 128, 167, 210	0
33	BH	159/159 (100%)	0.17	9 (5%) 30 25	32, 68, 118, 181	0
33	DH	159/159 (100%)	0.69	16 (10%) 14 13	70, 128, 180, 235	0
34	BI	145/145 (100%)	0.29	6 (4%) 42 31	44, 95, 123, 159	0
34	DI	145/145 (100%)	0.31	5 (3%) 48 35	48, 101, 137, 159	0
35	BJ	130/130 (100%)	1.73	47 (36%) 1 1	120, 164, 275, 373	0
35	DJ	130/130 (100%)	1.72	44 (33%) 1 1	122, 193, 233, 284	0
36	BN	138/138 (100%)	-0.10	5 (3%) 46 34	24, 46, 95, 129	0
36	DN	138/138 (100%)	0.38	6 (4%) 40 30	54, 90, 120, 133	0
37	BO	122/122 (100%)	-0.40	0 100 100	26, 49, 75, 91	0
37	DO	122/122 (100%)	-0.22	0 100 100	39, 64, 85, 92	0
38	BP	146/146 (100%)	0.48	9 (6%) 28 22	21, 65, 115, 159	0
38	DP	146/146 (100%)	0.76	17 (11%) 11 11	39, 92, 134, 174	0
39	BQ	141/141 (100%)	-0.11	4 (2%) 55 40	27, 51, 85, 188	0
39	DQ	141/141 (100%)	0.41	7 (4%) 35 28	58, 92, 125, 161	0
40	BR	117/117 (100%)	-0.26	1 (0%) 81 70	21, 42, 78, 93	0
40	DR	117/117 (100%)	0.08	4 (3%) 48 35	40, 65, 100, 131	0
41	BS	98/98 (100%)	0.31	5 (5%) 34 27	35, 64, 105, 136	0
41	DS	98/98 (100%)	0.84	10 (10%) 13 13	72, 110, 151, 181	0
42	BT	137/137 (100%)	0.15	4 (2%) 54 40	34, 64, 139, 181	0
42	DT	137/137 (100%)	0.43	12 (8%) 17 16	43, 77, 135, 170	0
43	BU	117/117 (100%)	-0.29	1 (0%) 81 70	15, 37, 73, 98	0
43	DU	117/117 (100%)	0.31	6 (5%) 34 27	40, 80, 135, 155	0
44	BV	101/101 (100%)	-0.09	5 (4%) 35 28	24, 51, 85, 119	0
44	DV	101/101 (100%)	0.60	9 (8%) 17 16	60, 110, 143, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	BW	113/113 (100%)	-0.36	1 (0%) 81 70	25, 37, 75, 137	0
45	DW	113/113 (100%)	0.13	3 (2%) 56 41	49, 66, 103, 147	0
46	BX	92/92 (100%)	-0.36	0 100 100	25, 44, 73, 82	0
46	DX	92/92 (100%)	0.16	2 (2%) 62 47	43, 77, 98, 114	0
47	BY	100/100 (100%)	0.78	18 (18%) 4 4	34, 66, 163, 201	0
47	DY	100/100 (100%)	1.10	23 (23%) 2 2	56, 100, 175, 209	0
48	BZ	176/176 (100%)	0.82	27 (15%) 6 6	43, 119, 275, 309	0
48	DZ	176/176 (100%)	1.18	33 (18%) 4 3	92, 149, 299, 353	0
49	B0	84/84 (100%)	-0.29	0 100 100	25, 43, 78, 110	0
49	D0	84/84 (100%)	0.43	3 (3%) 46 34	58, 84, 105, 128	0
50	B1	93/93 (100%)	-0.19	0 100 100	26, 48, 94, 131	0
50	D1	93/93 (100%)	-0.01	1 (1%) 77 66	39, 62, 111, 153	0
51	B2	71/71 (100%)	-0.05	2 (2%) 55 40	34, 61, 101, 164	0
51	D2	71/71 (100%)	0.41	5 (7%) 24 20	60, 90, 131, 150	0
52	B3	59/59 (100%)	-0.24	1 (1%) 69 55	29, 48, 92, 149	0
52	D3	59/59 (100%)	0.36	2 (3%) 48 35	65, 101, 135, 253	0
53	B4	30/30 (100%)	0.44	1 (3%) 49 36	69, 116, 141, 154	0
53	D4	30/30 (100%)	0.80	4 (13%) 8 8	121, 142, 163, 173	0
54	B5	59/59 (100%)	0.21	5 (8%) 18 17	21, 42, 139, 213	0
54	D5	59/59 (100%)	0.55	4 (6%) 25 20	42, 67, 130, 179	0
55	B6	44/44 (100%)	0.83	5 (11%) 11 11	30, 60, 93, 118	0
55	D6	44/44 (100%)	0.85	4 (9%) 16 15	51, 90, 113, 121	0
56	B7	48/48 (100%)	-0.25	2 (4%) 41 31	20, 30, 63, 124	0
56	D7	48/48 (100%)	-0.05	2 (4%) 41 31	31, 49, 80, 98	0
57	B8	63/63 (100%)	0.16	5 (7%) 20 18	30, 44, 64, 129	0
57	D8	63/63 (100%)	0.71	9 (14%) 7 7	50, 77, 112, 154	0
58	B9	36/36 (100%)	0.11	1 (2%) 55 40	34, 49, 63, 78	0
58	D9	36/36 (100%)	0.67	1 (2%) 55 40	63, 91, 115, 125	0
59	CX	4/4 (100%)	0.30	1 (25%) 2 1	70, 87, 90, 158	0
60	DC	190/196 (96%)	1.45	48 (25%) 2 1	109, 188, 240, 265	0
All	All	21440/21679 (98%)	0.19	1194 (5%) 31 25	9, 77, 180, 393	0

The worst 5 of 1194 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
48	DZ	172	ALA	10.1
9	AI	126	SER	8.2
24	AY	18	G	7.9
24	CY	66	G	7.7
35	DJ	36	ALA	7.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	PSU	AX	19	20/21	0.92	0.08	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.