



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 11:56 PM UTC

PDB ID : 4V9M / pdb_00004v9m
Title : 70S Ribosome translocation intermediate FA-4.2A containing elongation factor EFG/FUSIDIC ACID/GDP, mRNA, and tRNA bound in the pe^{*}/E state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-25
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

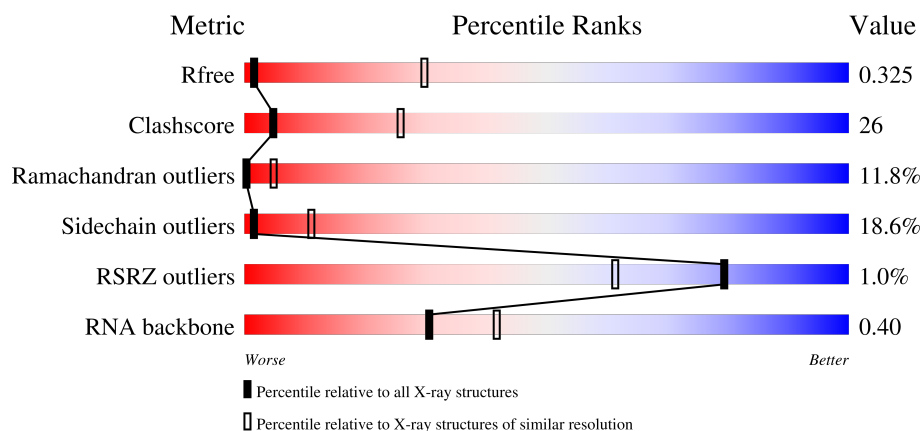
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)

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	AB	235	36% 41% 20% •
1	CB	235	35% 44% 17% •
2	AC	207	2% 41% 47% 12%
2	CC	207	2% 46% 42% 12%

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Mol	Chain	Length	Quality of chain
3	AD	208	
3	CD	208	
4	AE	151	
4	CE	151	
5	AF	101	
5	CF	101	
6	AG	155	
6	CG	155	
7	AH	138	
7	CH	138	
8	AI	127	
8	CI	127	
9	AJ	99	
9	CJ	99	
10	AK	119	
10	CK	119	
11	AL	125	
11	CL	125	
12	AM	125	
12	CM	125	
13	AN	60	
13	CN	60	
14	AO	88	
14	CO	88	
15	AP	84	

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Mol	Chain	Length	Quality of chain
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AA	1511	
20	CA	1511	
21	AW	77	
21	CW	77	
22	AV	23	
22	CV	23	
23	AY	687	
23	CY	687	
24	BC	228	
24	DC	228	
25	BD	275	
25	DD	275	
26	BE	205	
26	DE	205	
27	BF	208	
27	DF	208	

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Mol	Chain	Length	Quality of chain
28	BG	181	
28	DG	181	
29	BH	167	
29	DH	167	
30	BJ	170	
30	DJ	170	
31	BK	140	
31	DK	140	
32	BN	138	
32	DN	138	
33	BO	122	
33	DO	122	
34	BP	146	
34	DP	146	
35	BQ	141	
35	DQ	141	
36	BR	117	
36	DR	117	
37	BS	99	
37	DS	99	
38	BT	138	
38	DT	138	
39	BU	117	
39	DU	117	
40	BV	101	

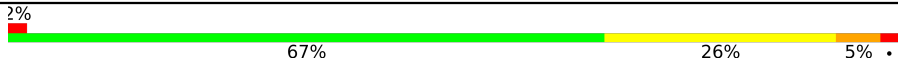
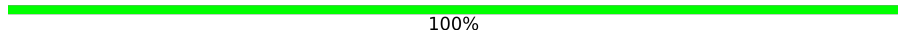
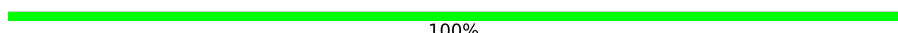
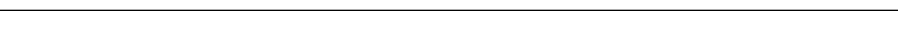
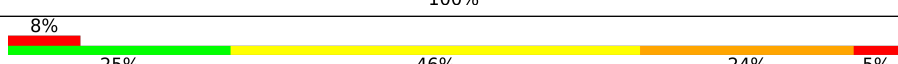
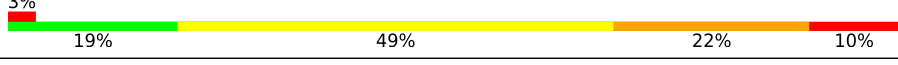
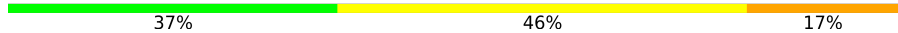
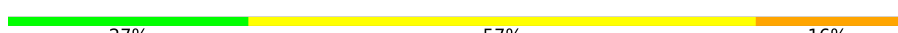
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Mol	Chain	Length	Quality of chain
40	DV	101	
41	BW	113	
41	DW	113	
42	BX	93	
42	DX	93	
43	BY	107	
43	DY	107	
44	BZ	185	
44	DZ	185	
45	B0	84	
45	D0	84	
46	B2	71	
46	D2	71	
47	B3	60	
47	D3	60	
48	B5	59	
48	D5	59	
49	B6	50	
49	D6	50	
50	B7	49	
50	D7	49	
51	B8	64	
51	D8	64	
52	B9	37	
52	D9	37	

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Mol	Chain	Length	Quality of chain
53	Be	102	 2% 67% 26% 5%
53	De	102	 68% 26% 5%
54	Bf	31	 100%
54	Bg	31	 100%
54	Df	31	 90% 10%
54	Dg	31	 97%
55	Bh	30	 100%
55	Dh	30	 100%
56	B1	93	 8% 25% 46% 24% 5%
56	D1	93	 3% 19% 49% 22% 10%
57	B4	35	 37% 46% 14%
57	D4	35	 37% 46% 17%
58	BA	2879	 28% 57% 15%
58	DA	2879	 27% 57% 16%
59	BB	119	 32% 57% 11%
59	DB	119	 26% 66% 8%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 308068 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 protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			
1	CB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			
2	CC	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			
4	CE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	HIS	ARG	conflict	UNP P62669
CI	58	HIS	ARG	conflict	UNP P62669

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			
9	CJ	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			
11	CL	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			
12	CM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			
15	CP	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	100	Total	C	N	O	S	0	0	0
			835	534	155	144	2			
16	CQ	100	Total	C	N	O	S	0	0	0
			835	534	155	144	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	96	GLU	GLN	conflict	UNP P62658
CQ	96	GLU	GLN	conflict	UNP P62658

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			
18	CS	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	41	ILE	VAL	conflict	UNP P62661
CT	41	ILE	VAL	conflict	UNP P62661

- Molecule 20 is a RNA chain called ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AA	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			
20	CA	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			

- Molecule 21 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AW	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			
21	CW	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			

- Molecule 22 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			
22	CV	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AY	667	Total	C	N	O	S	0	0	0
			5219	3318	893	990	18			
23	CY	667	Total	C	N	O	S	0	0	0
			5219	3318	893	990	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	129	LYS	HIS	conflict	UNP Q72I01
AY	226	ASN	HIS	conflict	UNP Q72I01
CY	129	LYS	HIS	conflict	UNP Q72I01

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Chain	Residue	Modelled	Actual	Comment	Reference
CY	226	ASN	HIS	conflict	UNP Q72I01

- Molecule 24 is a protein called 50S ribosomal protein L1.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	20	VAL	ILE	conflict	UNP Q72GV9
BC	28	ARG	HIS	conflict	UNP Q72GV9
DC	20	VAL	ILE	conflict	UNP Q72GV9
DC	28	ARG	HIS	conflict	UNP Q72GV9

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BE	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			
26	DE	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			
27	DF	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	2	LYS	-	insertion	UNP Q72I05
BF	3	GLU	-	insertion	UNP Q72I05
BF	4	VAL	-	insertion	UNP Q72I05
BF	5	ALA	-	insertion	UNP Q72I05
BF	6	VAL	-	insertion	UNP Q72I05
DF	2	LYS	-	insertion	UNP Q72I05
DF	3	GLU	-	insertion	UNP Q72I05
DF	4	VAL	-	insertion	UNP Q72I05
DF	5	ALA	-	insertion	UNP Q72I05
DF	6	VAL	-	insertion	UNP Q72I05

- Molecule 28 is a protein called 50S ribosomal protein L5.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	5	VAL	LEU	conflict	UNP Q72I16
DG	5	VAL	LEU	conflict	UNP Q72I16

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	167	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			
29	DH	167	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			

- Molecule 30 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BJ	170	Total	C	N	O		0	0	0
			851	510	170	171				
30	DJ	170	Total	C	N	O		0	0	0
			851	510	170	171				

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BK	140	Total	C	N	O	S	0	0	0
			1035	659	183	188	5			
31	DK	140	Total	C	N	O	S	0	0	0
			1035	659	183	188	5			

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- Molecule 33 is a protein called 50S ribosomal protein L14.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	69	ILE	VAL	conflict	UNP Q72I14
DO	69	ILE	VAL	conflict	UNP Q72I14

- Molecule 34 is a protein called 50S ribosomal protein L15.

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

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	32	TYR	PHE	conflict	UNP Q72I11
DQ	32	TYR	PHE	conflict	UNP Q72I11

- Molecule 36 is a protein called 50S ribosomal protein L17.

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

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BS	99	Total	C	N	O		0	0	0
			775	488	155	132				
37	DS	99	Total	C	N	O		0	0	0
			775	488	155	132				

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BT	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			
38	DT	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	123	GLN	LYS	conflict	UNP Q72JU9
BT	135	ALA	VAL	conflict	UNP Q72JU9
DT	123	GLN	LYS	conflict	UNP Q72JU9
DT	135	ALA	VAL	conflict	UNP Q72JU9

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
39	DU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
41	DW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BX	93	Total	C	N	O	0	0	0
			734	477	132	125			
42	DX	93	Total	C	N	O	0	0	0
			734	477	132	125			

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BY	107	Total	C	N	O	S	0	0	0
			818	524	155	134	5			
43	DY	107	Total	C	N	O	S	0	0	0
			818	524	155	134	5			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BZ	185	Total	C	N	O	S	0	0	0
			1473	939	262	270	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	DZ	185	Total	C	N	O	S	0	0	0
			1473	939	262	270	2			

- Molecule 45 is a protein called 50S ribosomal protein L27.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B0	11	ARG	LYS	conflict	UNP Q72HR3
D0	11	ARG	LYS	conflict	UNP Q72HR3

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			
47	D3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	29	THR	ILE	conflict	UNP P62652
D5	29	THR	ILE	conflict	UNP P62652

- Molecule 49 is a protein called 50S ribosomal protein L33.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
50	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
51	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	Be	102	Total	C	N	O		0	0	0
			686	430	119	137				
53	De	102	Total	C	N	O		0	0	0
			686	430	119	137				

- Molecule 54 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	Bf	31	Total	C	N	O	0	0	0
			156	93	31	32			
54	Bg	31	Total	C	N	O	0	0	0
			156	93	31	32			
54	Df	31	Total	C	N	O	0	0	0
			156	93	31	32			
54	Dg	31	Total	C	N	O	0	0	0
			156	93	31	32			

- Molecule 55 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	Bh	30	Total	C	N	O	0	0	0
			151	90	30	31			
55	Dh	30	Total	C	N	O	0	0	0
			151	90	30	31			

- Molecule 56 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			
56	D1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	LYS	ARG	conflict	UNP Q72G84
D1	81	LYS	ARG	conflict	UNP Q72G84

- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	B4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			
57	D4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			

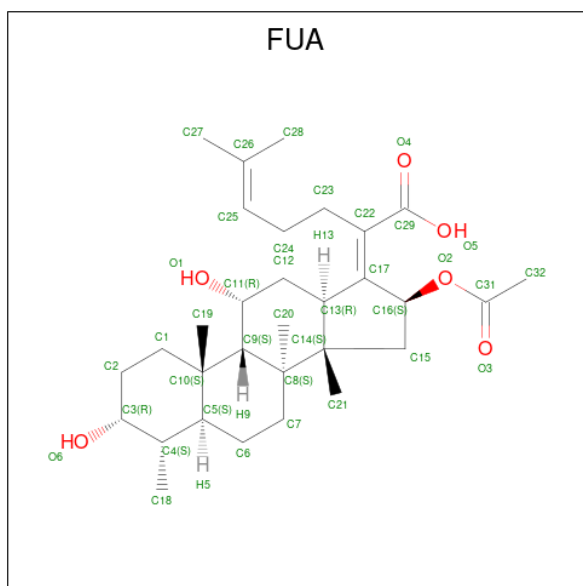
- Molecule 58 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			
58	DA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

- Molecule 59 is a RNA chain called 5S ribosomal RNA.

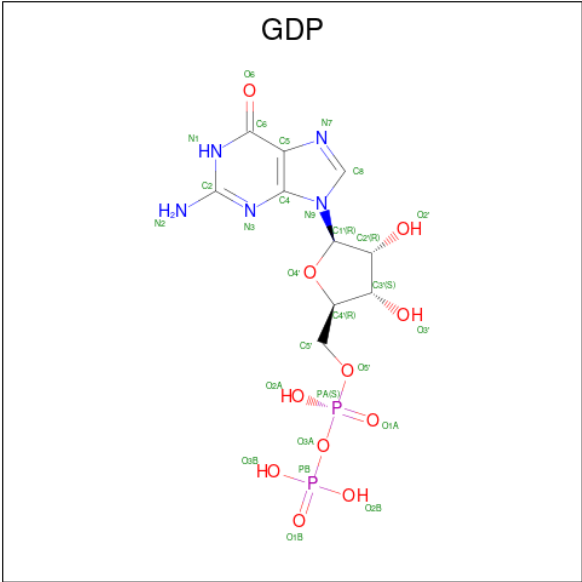
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
59	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 60 is FUSIDIC ACID (CCD ID: FUA) (formula: $C_{31}H_{48}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	AY	1	Total	C	O	0	0
			37	31	6		
60	CY	1	Total	C	O	0	0
			37	31	6		

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

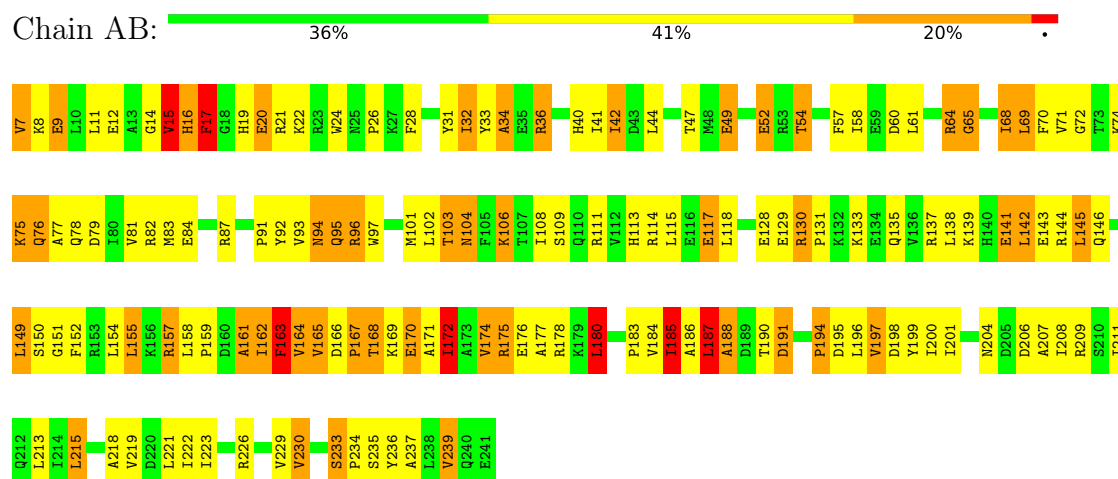


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
61	CY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

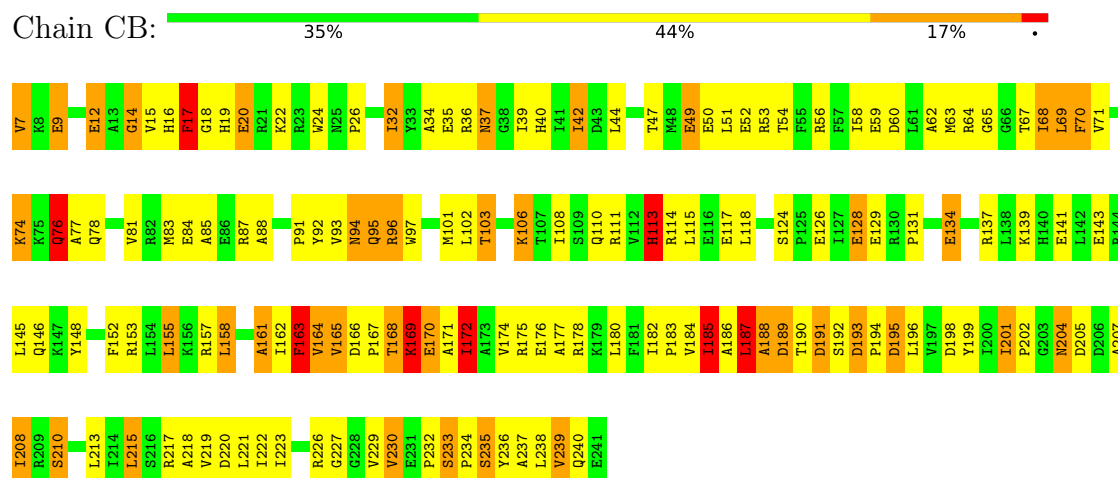
3 Residue-property plots

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.

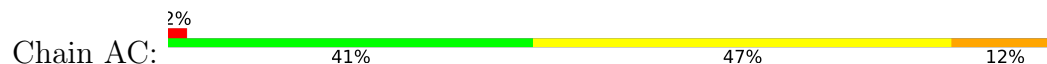
• Molecule 1: 30S ribosomal protein S2

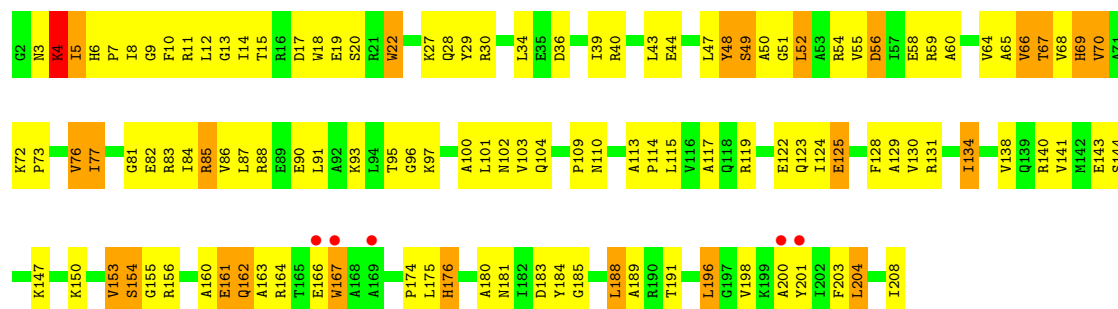


• Molecule 1: 30S ribosomal protein S2

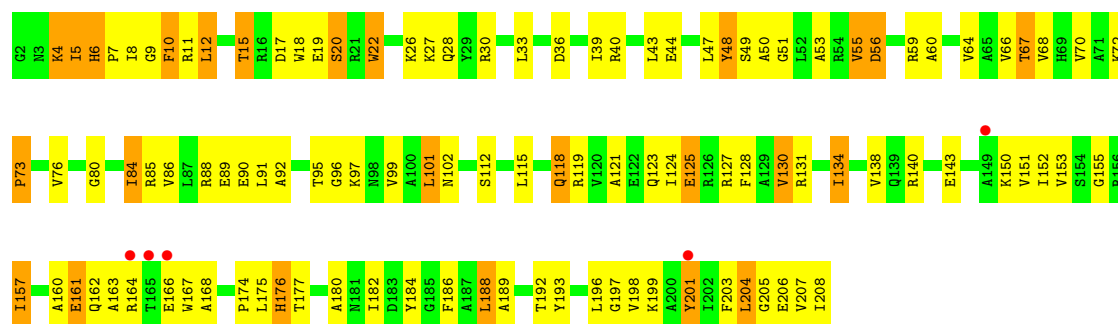


• Molecule 2: 30S ribosomal protein S3

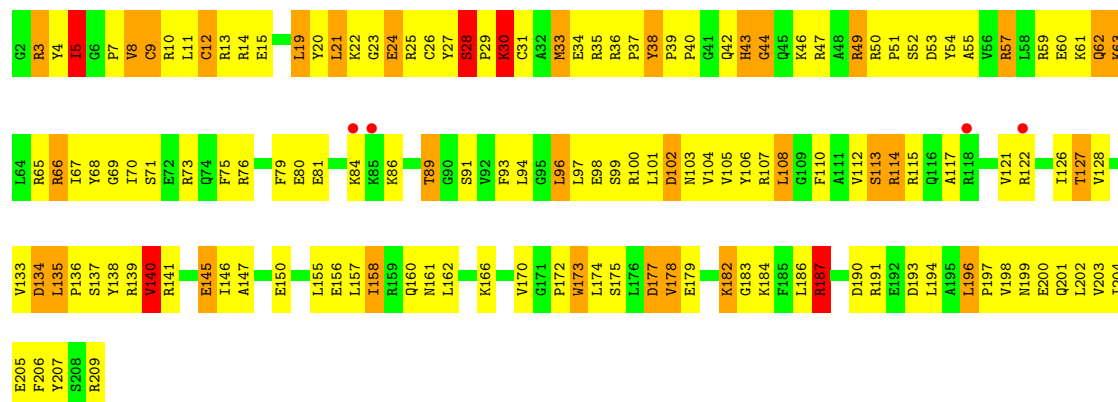




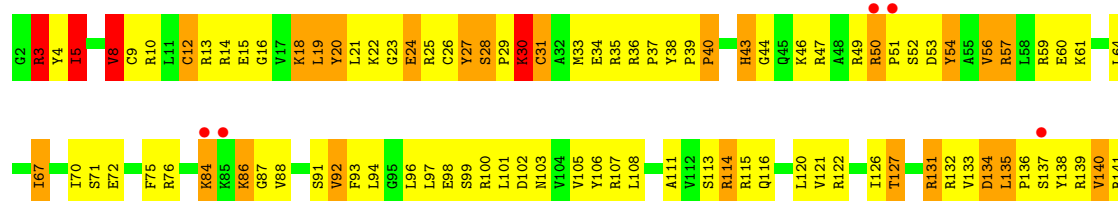
• Molecule 2: 30S ribosomal protein S3

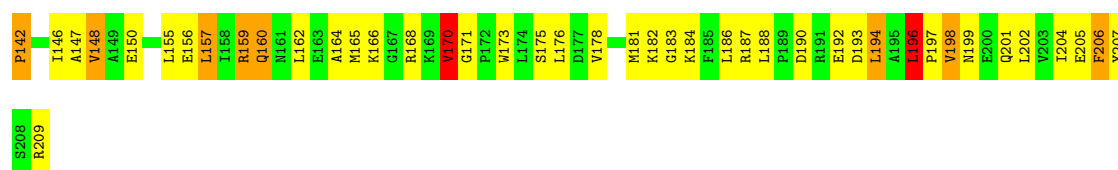


• Molecule 3: 30S ribosomal protein S4

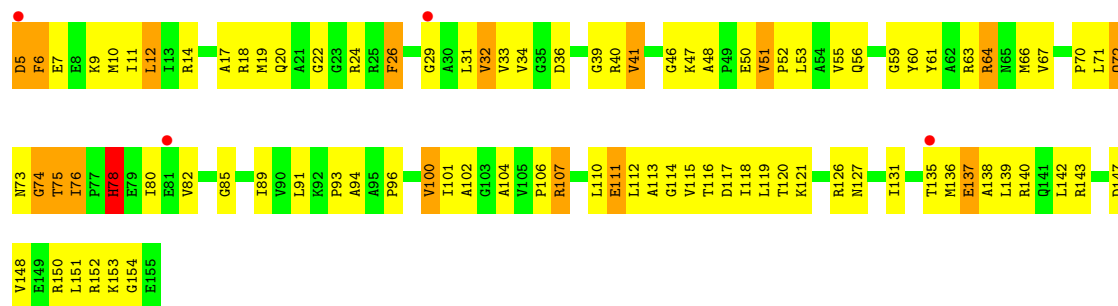


• Molecule 3: 30S ribosomal protein S4

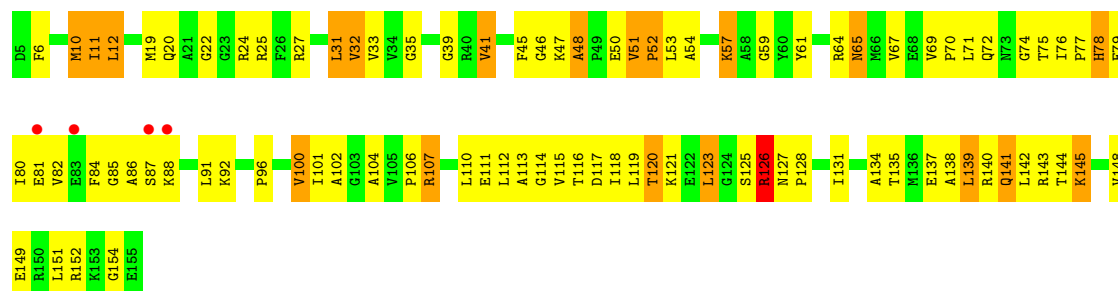




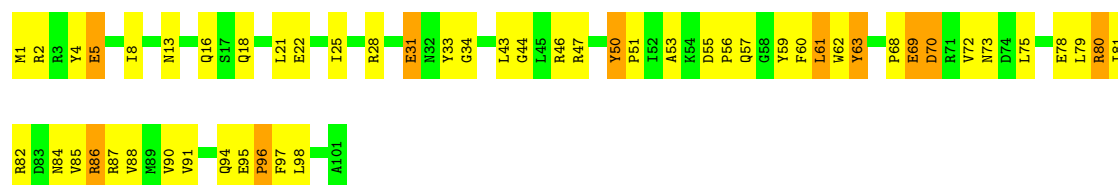
• Molecule 4: 30S ribosomal protein S5



• Molecule 4: 30S ribosomal protein S5

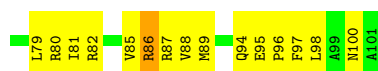


• Molecule 5: 30S ribosomal protein S6



• Molecule 5: 30S ribosomal protein S6

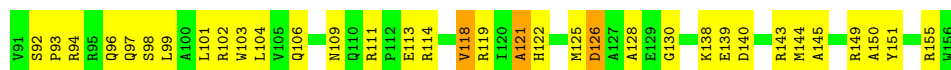




- Molecule 6: 30S ribosomal protein S7



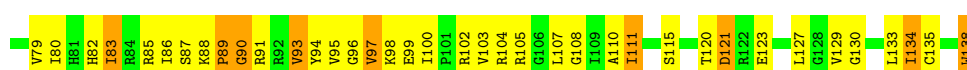
- Molecule 6: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S8

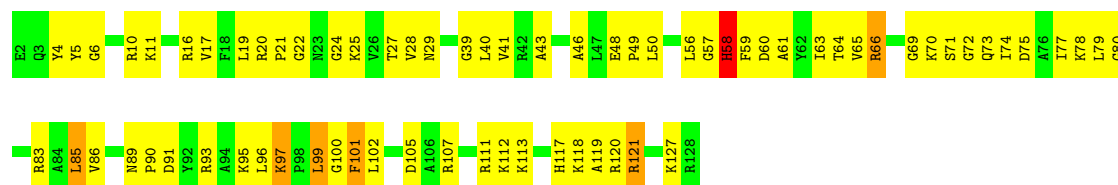


- Molecule 7: 30S ribosomal protein S8

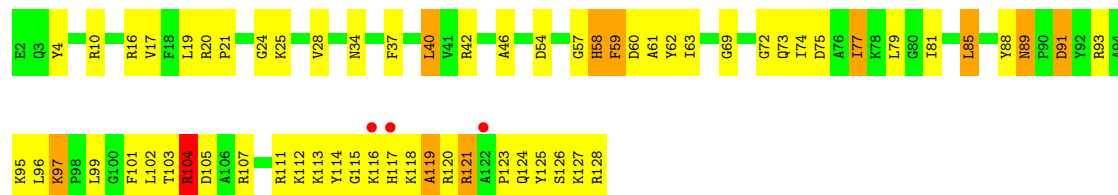


- Molecule 8: 30S ribosomal protein S9

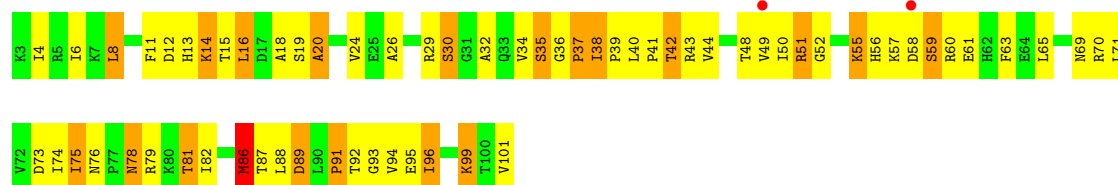




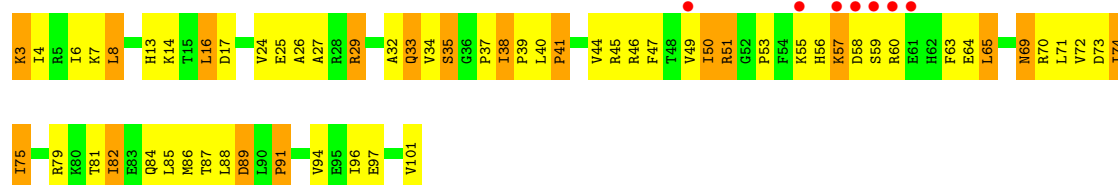
• Molecule 8: 30S ribosomal protein S9



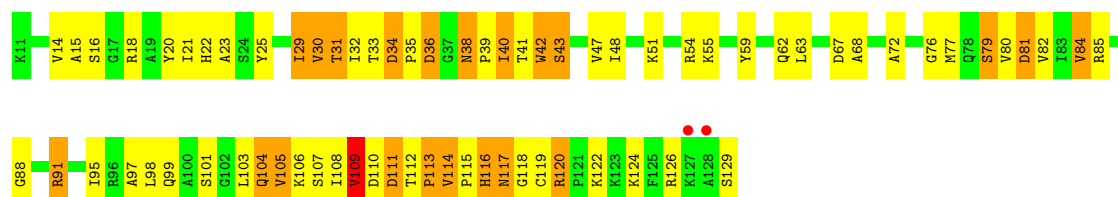
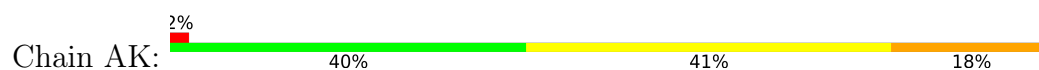
• Molecule 9: 30S ribosomal protein S10



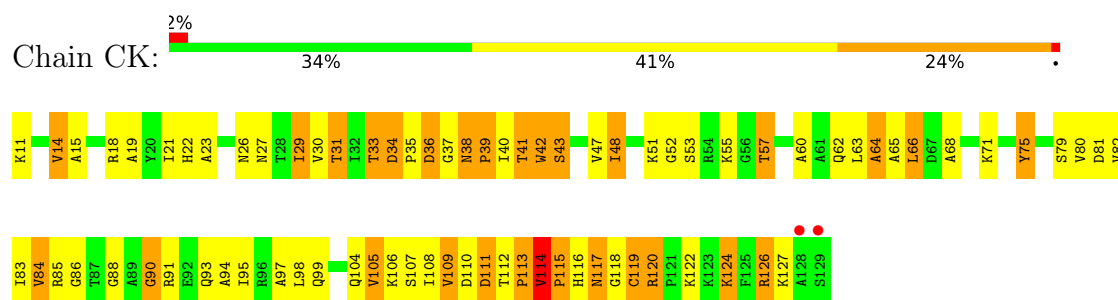
• Molecule 9: 30S ribosomal protein S10



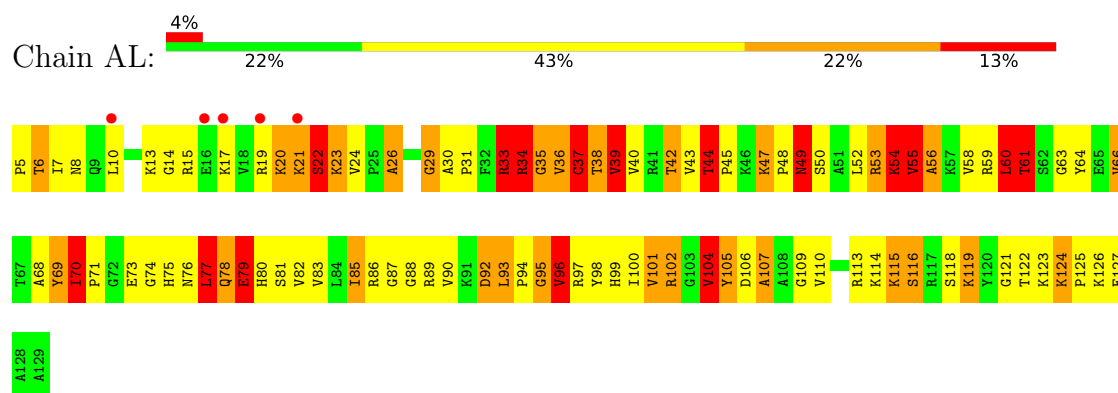
• Molecule 10: 30S ribosomal protein S11



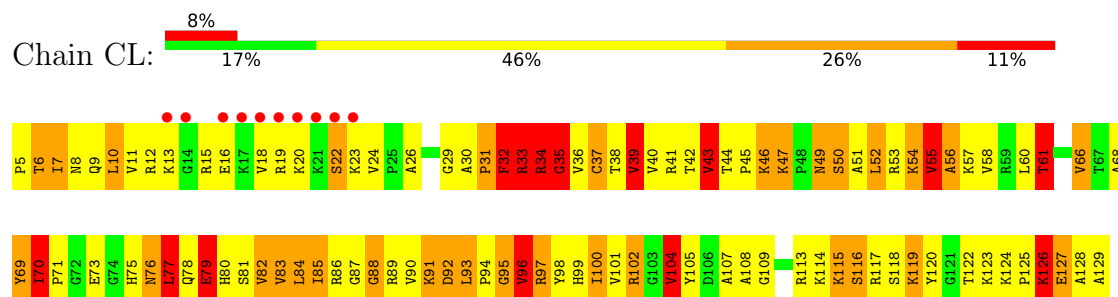
• Molecule 10: 30S ribosomal protein S11



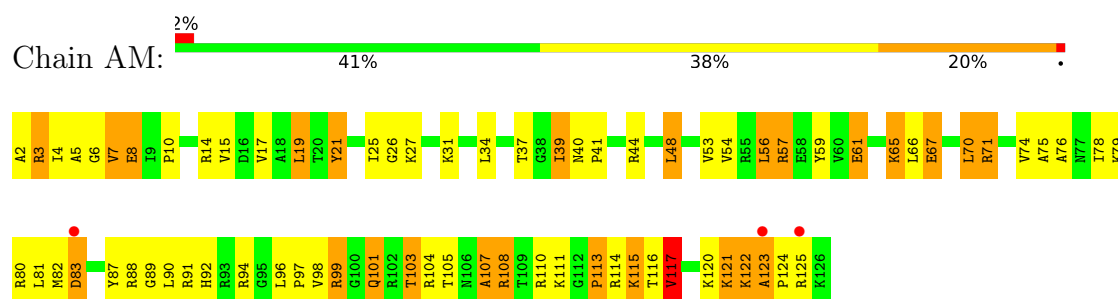
• Molecule 11: 30S ribosomal protein S12



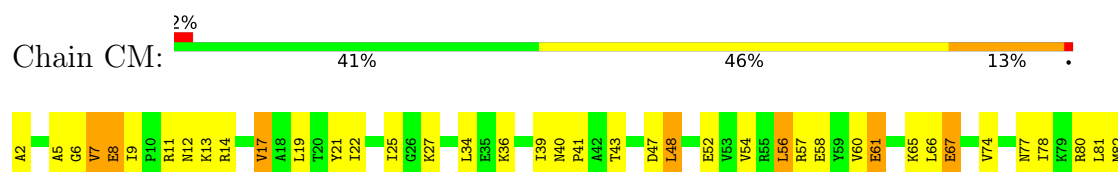
• Molecule 11: 30S ribosomal protein S12

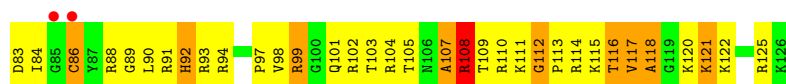


• Molecule 12: 30S ribosomal protein S13

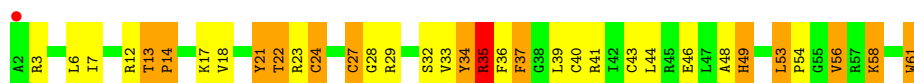
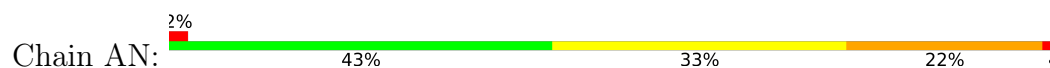


• Molecule 12: 30S ribosomal protein S13

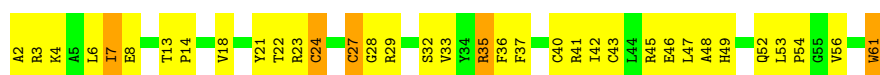




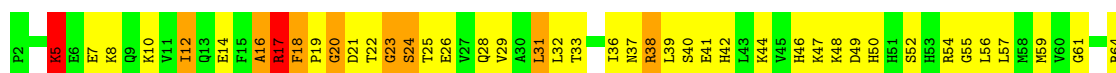
- Molecule 13: 30S ribosomal protein S14 type Z



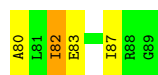
- Molecule 13: 30S ribosomal protein S14 type Z



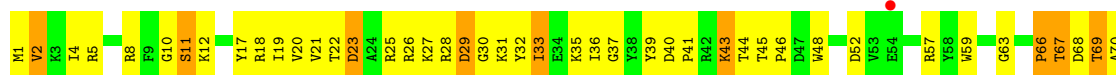
- Molecule 14: 30S ribosomal protein S15



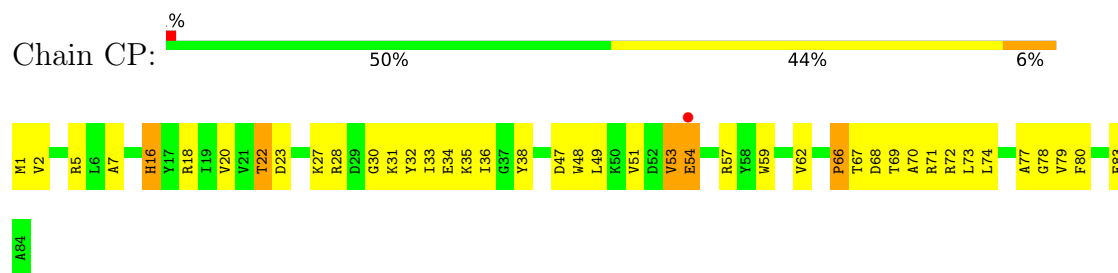
- Molecule 14: 30S ribosomal protein S15



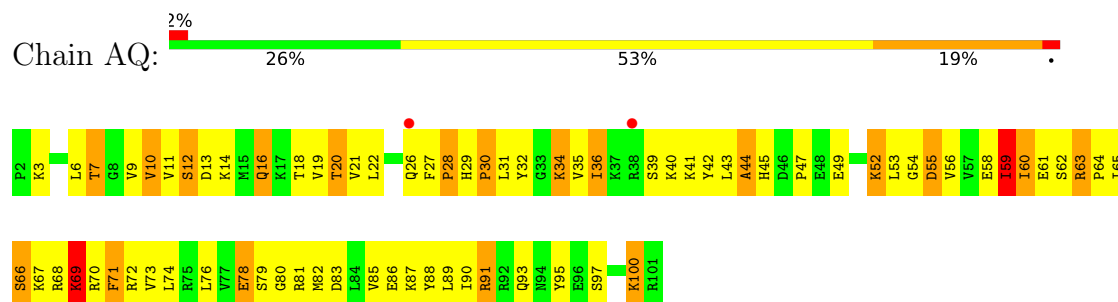
- Molecule 15: 30S ribosomal protein S16



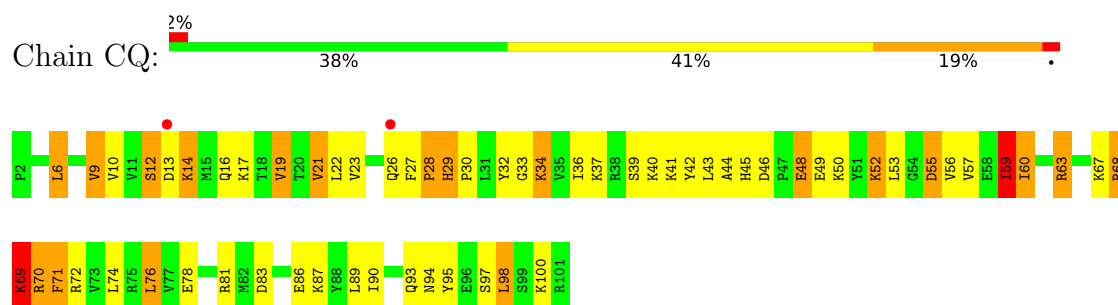
- Molecule 15: 30S ribosomal protein S16



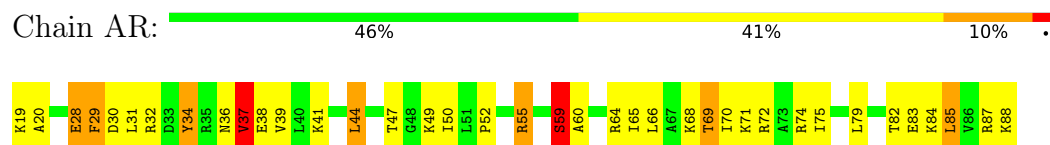
- Molecule 16: 30S ribosomal protein S17



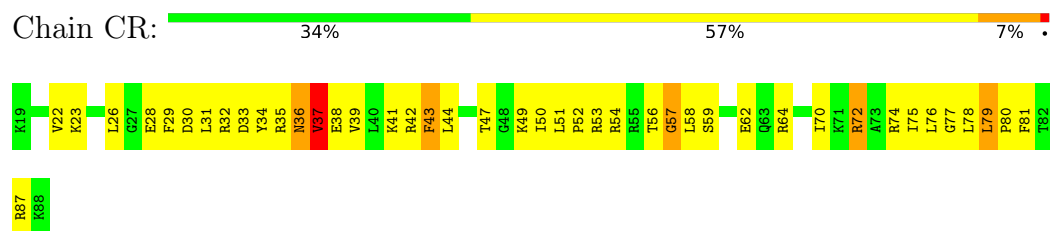
- Molecule 16: 30S ribosomal protein S17



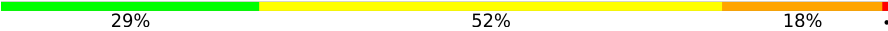
- Molecule 17: 30S ribosomal protein S18

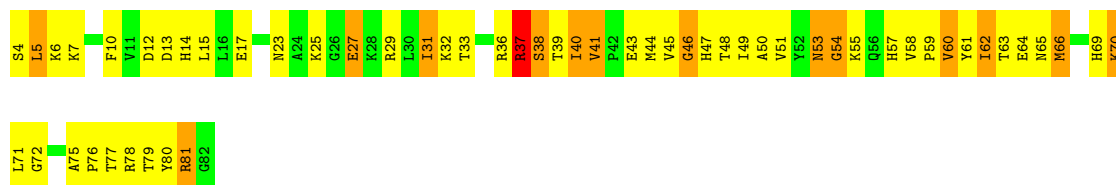


- Molecule 17: 30S ribosomal protein S18

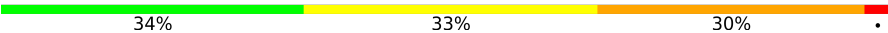


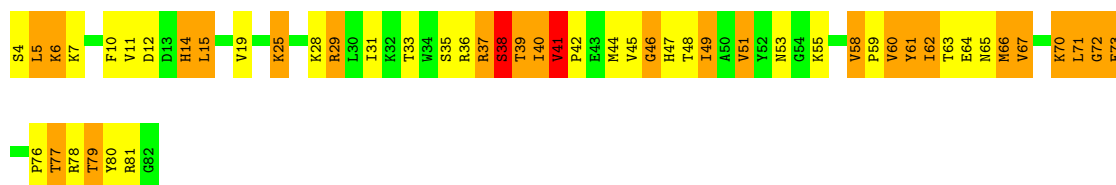
- Molecule 18: 30S ribosomal protein S19

Chain AS:  29% 52% 18% .

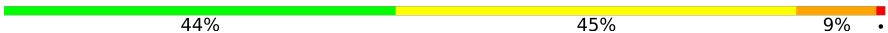


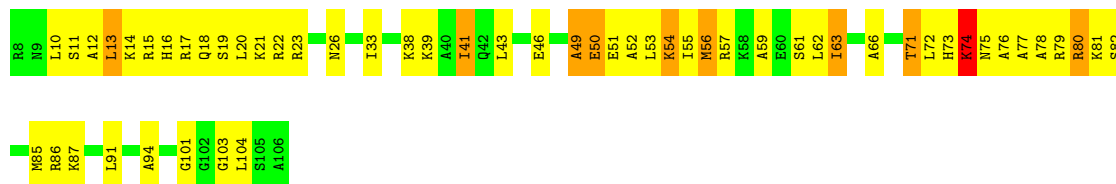
- Molecule 18: 30S ribosomal protein S19

Chain CS:  34% 33% 30% .



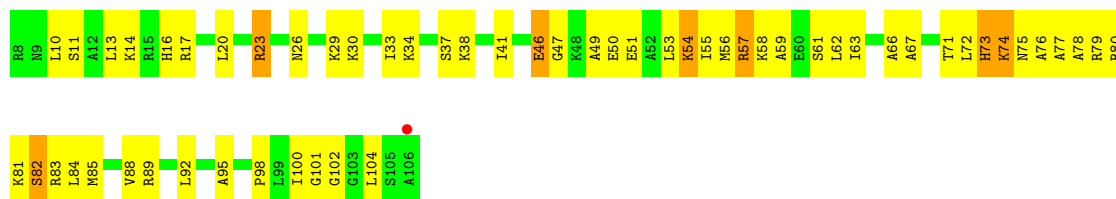
- Molecule 19: 30S ribosomal protein S20

Chain AT:  44% 45% 9% .



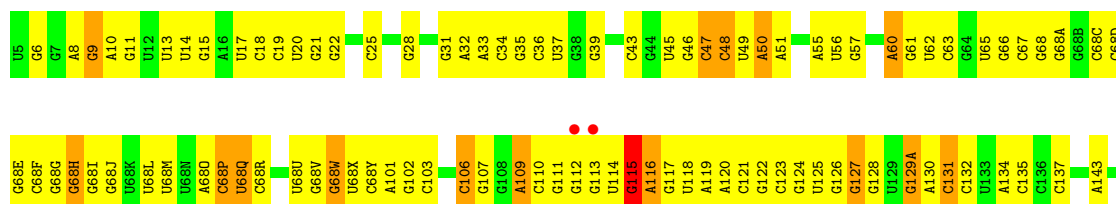
- Molecule 19: 30S ribosomal protein S20

Chain CT:  42% 51% 7% .

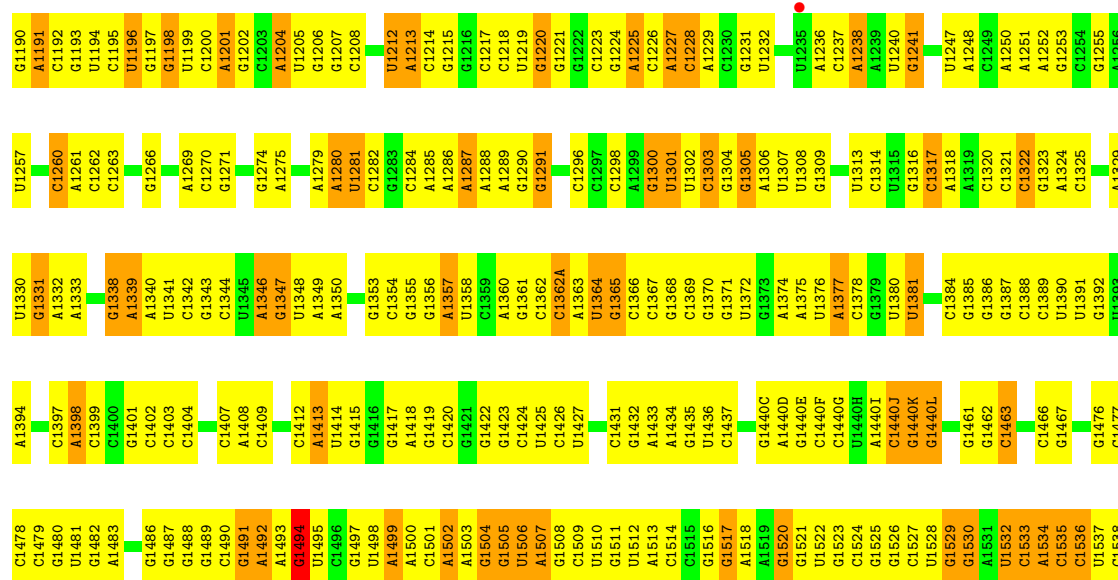


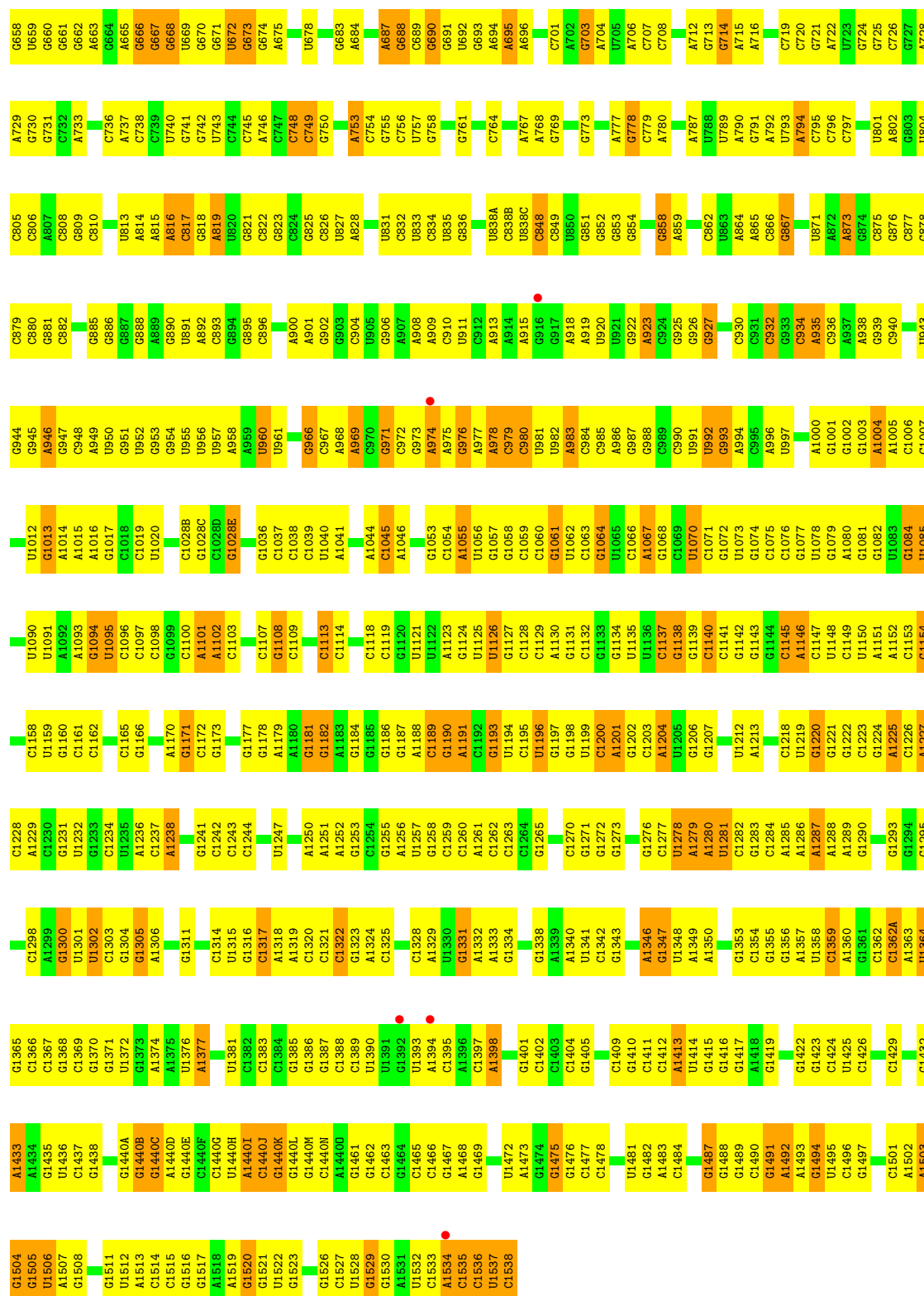
- Molecule 20: ribosomal RNA 16S

Chain AA:  29% 58% 12% .

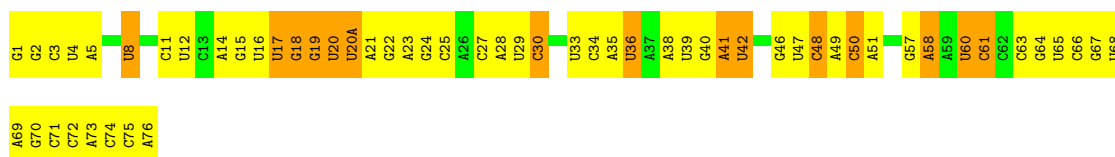


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A1123	G1057	A996	C934	A859	G785	C719	C634	C569	G505	A430	U365	A298	A228	A149
G1124	G1058	U997	A935	A860		G720	G635	G570	A509	A431	C366	G299	U229	C150
U1125	C936	G998	C936	C861	U789	G721		A571	A510	U434	U367	A300	G230	A151
U1126	C937	G998A	A937		A790	A722	A640	A572	C511	U435	U368	G302	G231	A160
G1127	G1061	U999	A938	A864	G791	U723	A642	A574		C435	C369	G302	G232	A161
C1128	U1062	A1000	G939	A865	U792		A643		C514	U437	C370	A303	C233	A162
C1063	G1001	G940	C940	C866	U793	G726	C643	G575	C515	U438	C372	G305	C234	C163
G1064	G1002	G941	G941	C867	U794	G727	G644	G576	C516	U439	A373	G306	C235	U164
U1065	G1003	C968	G942	C868	C795	A728	C645	G577	C517	A440	A374	C307	G236	
C1066	C1004	G869	U943	G869	C796	A729	U646	C578	C518	A441	G375	C307	G237	
A1067	A1005	G944	U943	U870	C797	G730		G579	C519	C442	U376	C308	G238	C169
	G945			U871	G798		A653	U580	C520	C443	G376	C309		U170
U1070	C1006	A946	G947	A872	U799	A733	G657	G581	A520	C444	G377	C310	C241	A171
C1071	C947		G947	A873	U799	G734		G582	C521	C445	G378	C311	C242	A172
G1072	C948	G874		A874	U801	G735	U672	A583	C522	C446	C379	C312	C243	U173
U1073	U1011				A802	C736	A665	G584	A523	C447	G380	A313	U244	C174
G1074	U1012	A949	C977	C877	A803	A737	G666	G585	G524	A448	C381	C314	C245	C175
C1075	G1013	G951	C878	G878	U804	C738	G667	C586	C525	C449	A382	A315	A246	C176
C1076	A1014	C979	C879	C805	U804	C739	G668	C587	C526	G450	A383	G316	G247	
G1077	A1015	C980	U952	C806	G906	U740		G588	C527	A451	G384	G317		A179
U1078	A1016	A881	G953	C807	U807	G741	G671	U591	C528	A452	C385	G318	C251	A185
G1079	G954	C881	U955	C808	U807	G742	U672	G592	C529	A453	C386	G319	U256	C186
C1145	U1078	C882	U955	C809	A814	C743	G673	G593	U531	C454	U387	C320	U257	C186A
A1146	A1080	C983	C962	C810	A815	C749	G674	G594	A532	C455	C388	C321	G257	
C1147	C1019	U864	G963	C811	A816	A746	A675	G594	C533	C456	A389	C322	C257	
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U1085	U1025	C882	U961	A818	A818	C750	A684	U598	C536	G458A	C396	G326	U261	U186H
C1153	G1026	U891	C962	A819	A819	C751	G685	C599	C537	G458B	A397	A327	A262	U186I
G1087	C1027	A892	G963	C817	C817	C752	U686	C600	C538	G458D	C398	C328	A263	G186J
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U1095	G1028H			C825	C825		G693	A609	C545	U480	G406	C339	C271	C194
C1096	G1033	G906	G906	C826	C826		A694	A609	C546	C481	G407	C340	A273	A195
C1097	G1034	A907	A907	C827	C827	C762	A695	G610	A547	A482	A408	U341	A196	A196
C1098	G1035	A908	A908	U827	U827	C763	A696	A611	C548	C483	G409	C342	A279	A197
G1099	G1036	A909	A909	U828	U828	C764	U697	C612	C549	G484	G410		C280	G198
C1100	C1037	C910	C910	A828	A828	C765		C613	C550	G485	A411	C345	G281	G199
A1101	C1038			C829	C829	G766	G700	A614	U551	C488	A412	C346	A282	G200
A1102	C1039			C830	C830	A766	C701	G615	C552	C489	G413	C347	C283	
C1103	U1040	A914	A914	U831	U831	A767	A702	G616	A553	C490	A414		G284	U201B
G1104	A1041	G916	G916	U832	U832	C770	G703	G617	C556	C492	A415	C352	G285	U201C
	A1044			C834	C834	G771	A704	U618	C557	G493	A416	C353	G286	G216
C1107	C1045	A919	A919	U835	U835		C707	C620	C558	C494	C417	C354	U287	C217
G1108	A1046	U920	U920	C836	C836	G775	C708	G621	A559	U495	C418	C355	G288	C218
C1109	G1047	C985	C985	G837	G837	G776	G709	A622	U560	A497		A356	G289	C219
A1110	G1048	A923	A923	C838	C838	A777	G710	C623	U561	U498	C422	C357	C290	G220
A1111	U1049	C924	C924	U838A	U838A	C778	G711	C624	C562	U499	G423	U358	C291	C221
C1112	G987	G987	G987	C838B	C838B	C779		G627	C563	A499	G424	U359	C292	U222
C1113	C988	G988	G988	U838C	U838C	G780	G713	G628	A564	C501	G425	A360	G293	U223
	C989	G926	G926	C848	C848		G714	G629	C565	C502	G426	G361	U294	C224
C1118	U1052	G927	G927			A780	A715	G629	C566	C503	U427	G362	C295	C225
C1119	G1053	C931	C931			A781	A716	G629	C567				U296	G226
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C1189	U1121													

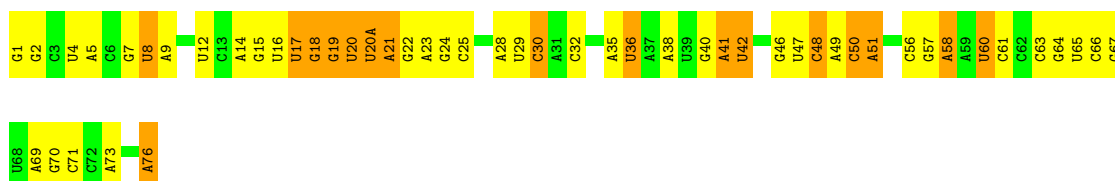




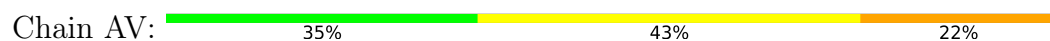
● Molecule 21: transfer RNA



- Molecule 21: transfer RNA



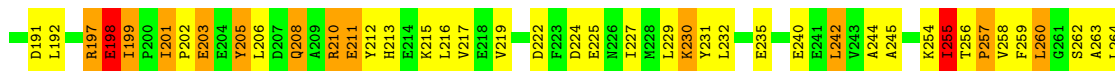
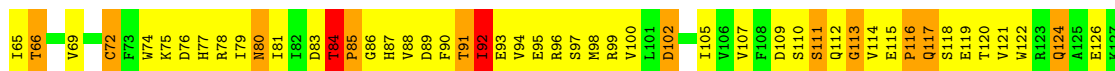
- Molecule 22: messenger RNA

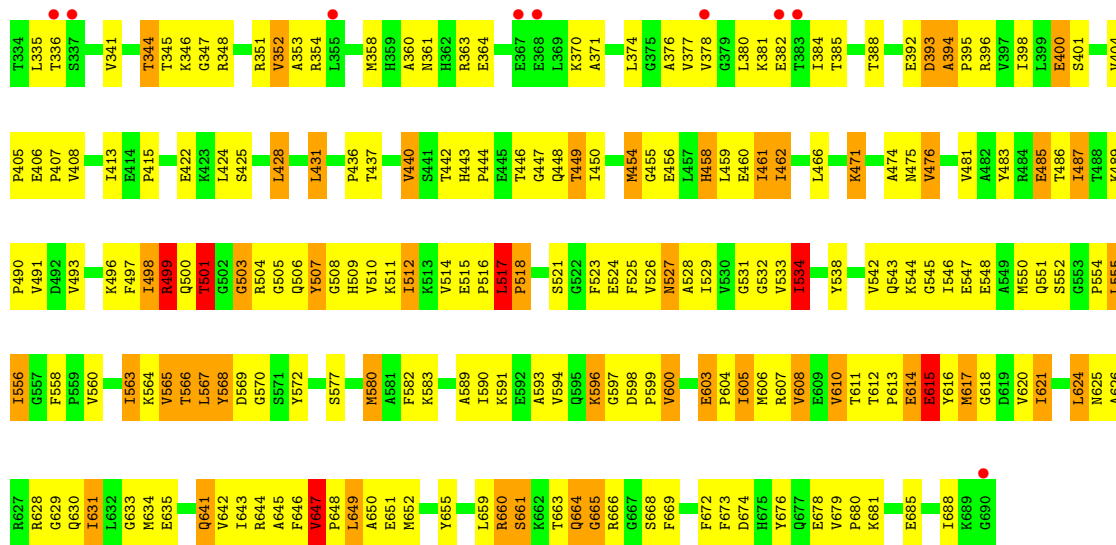


- Molecule 22: messenger RNA

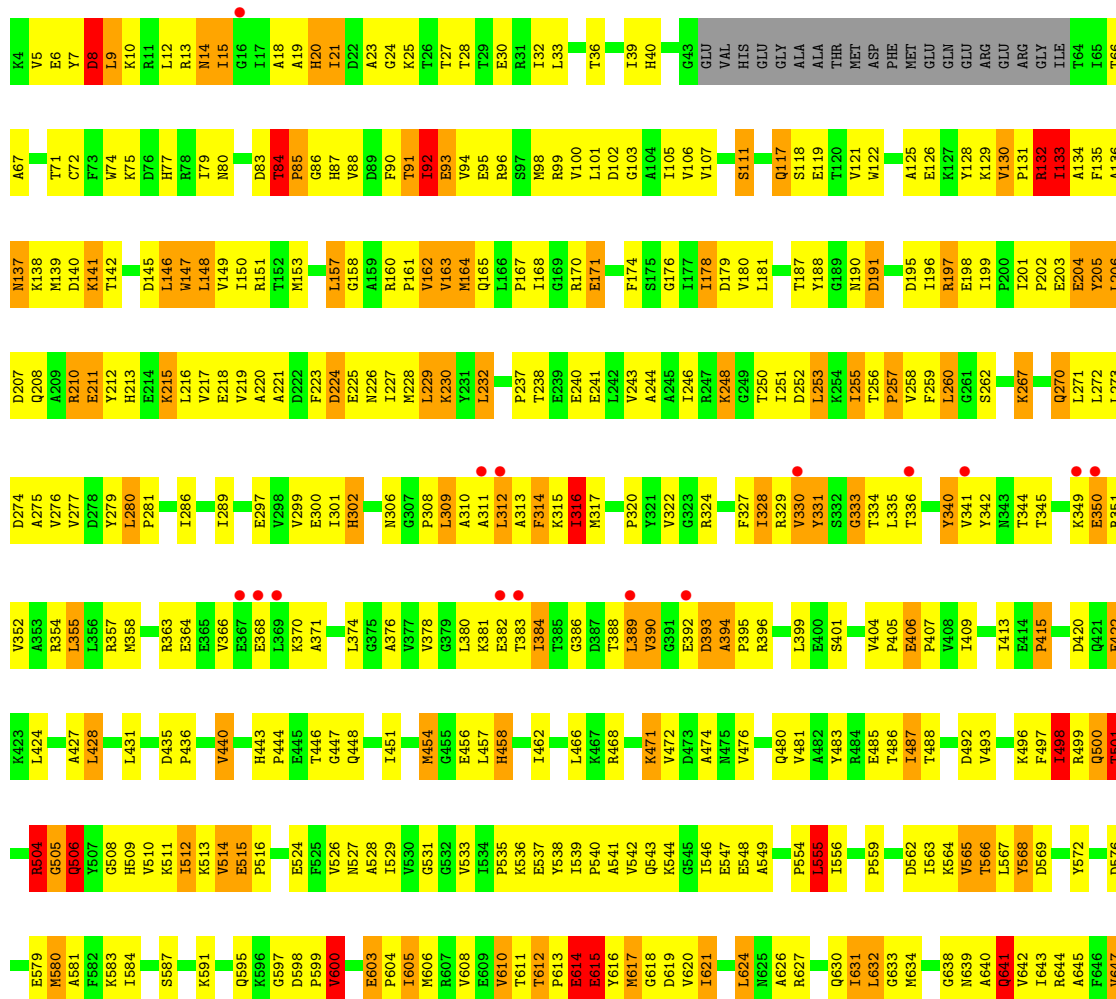


- Molecule 23: Elongation factor G



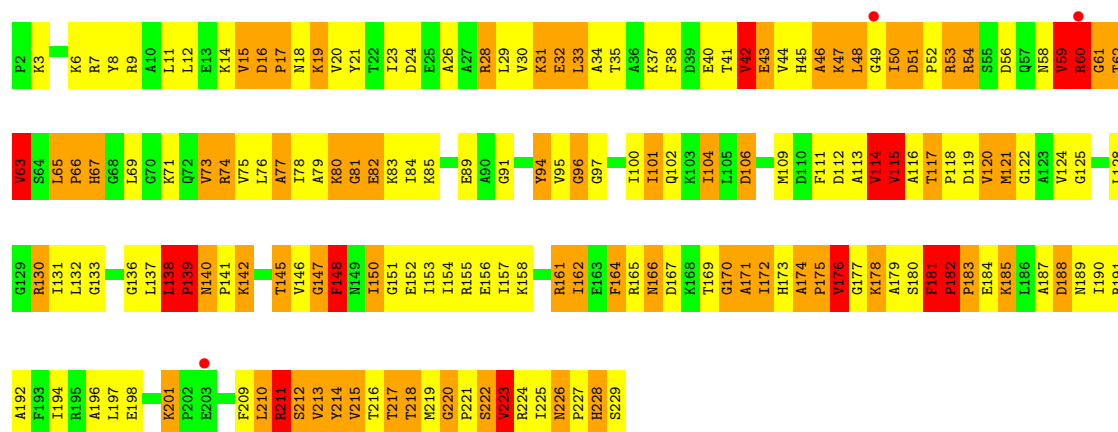
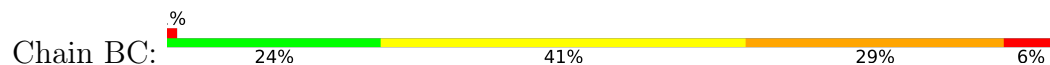


• Molecule 23: Elongation factor G

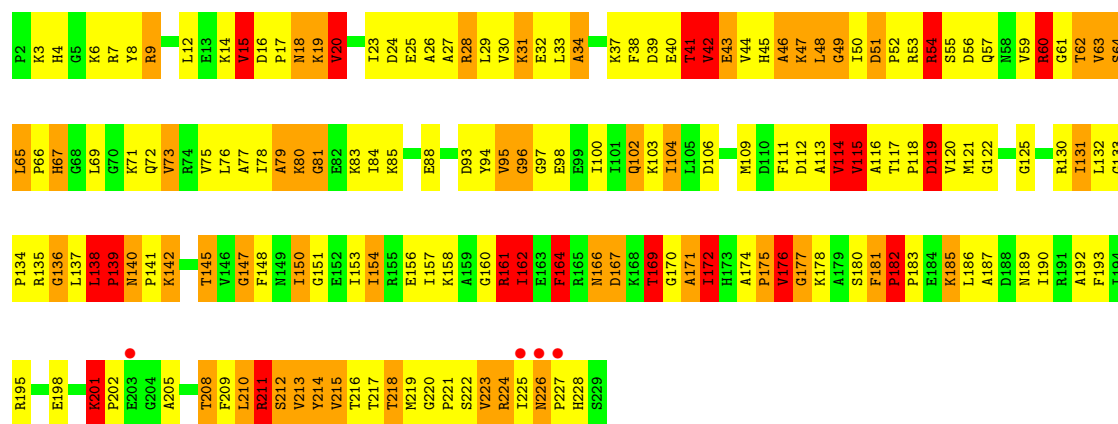




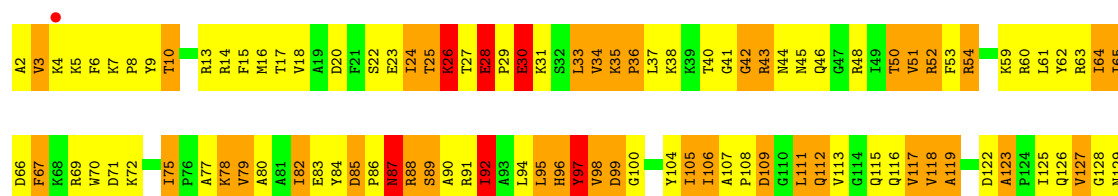
• Molecule 24: 50S ribosomal protein L1

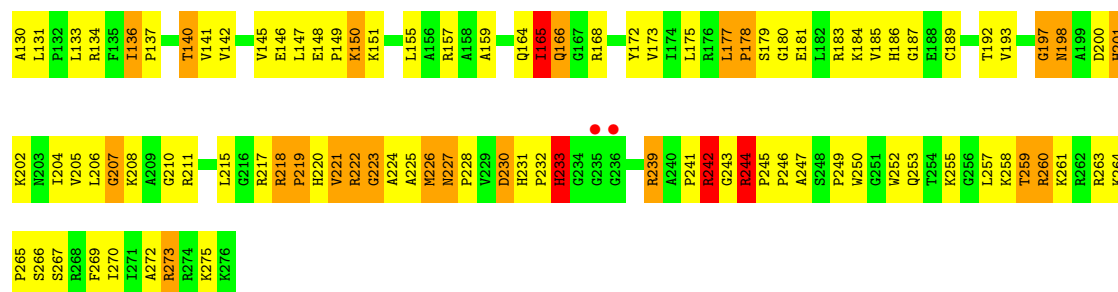


• Molecule 24: 50S ribosomal protein L1

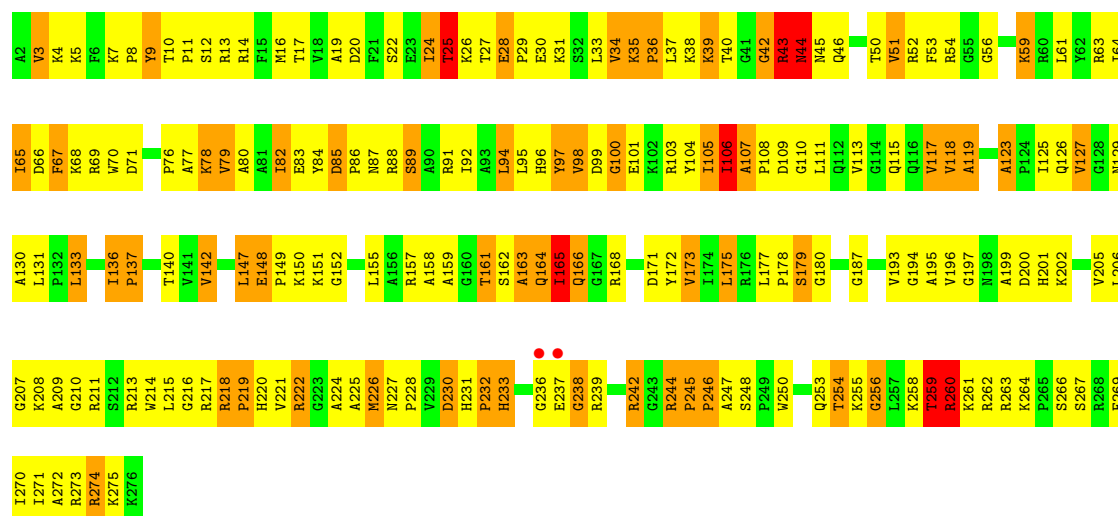


• Molecule 25: 50S ribosomal protein L2

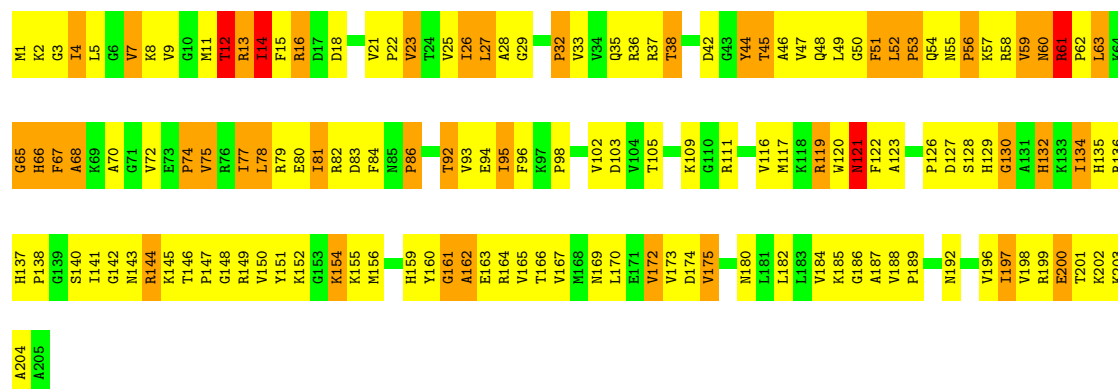




• Molecule 25: 50S ribosomal protein L2

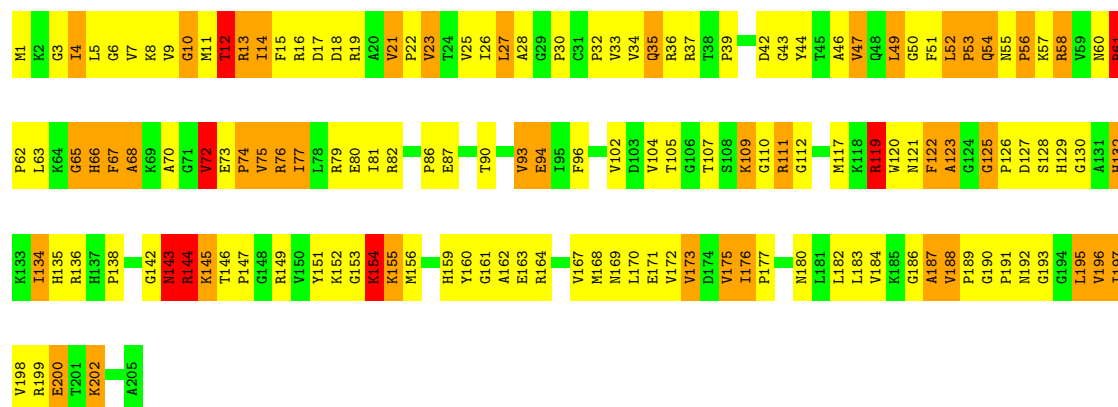


• Molecule 26: 50S ribosomal protein L3

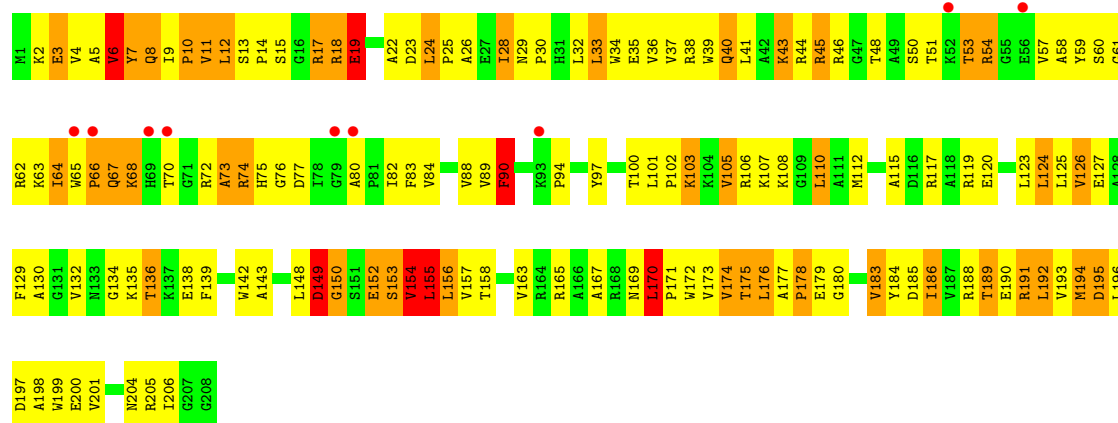


• Molecule 26: 50S ribosomal protein L3

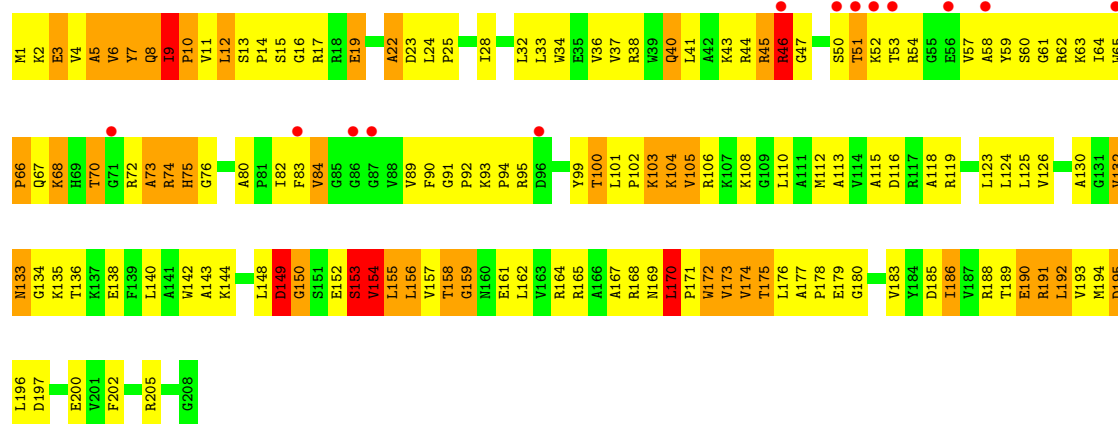




• Molecule 27: 50S ribosomal protein L4

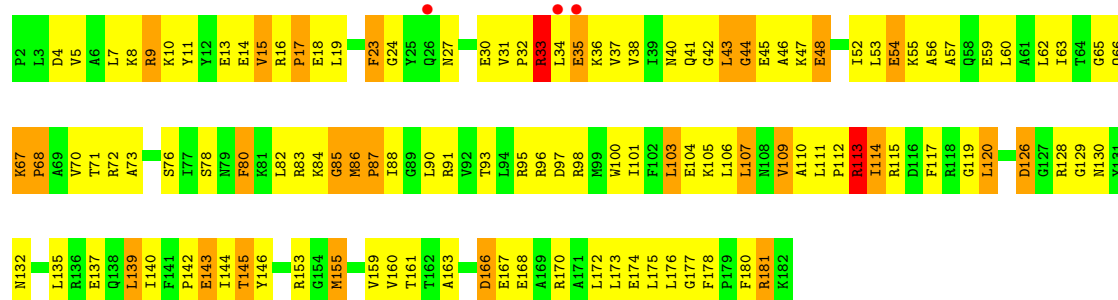


• Molecule 27: 50S ribosomal protein L4



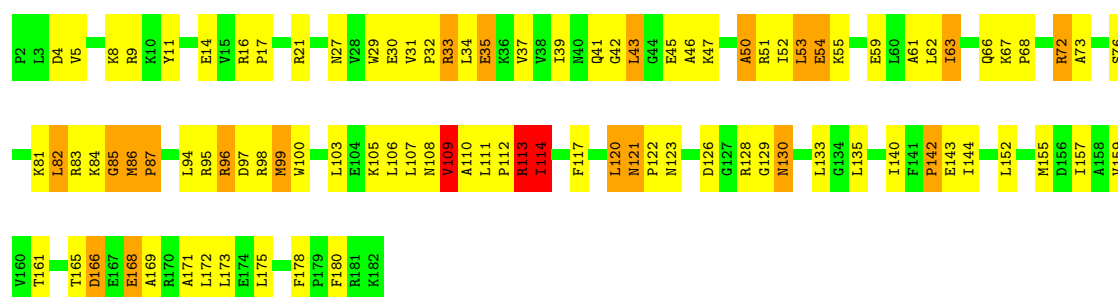
• Molecule 28: 50S ribosomal protein L5





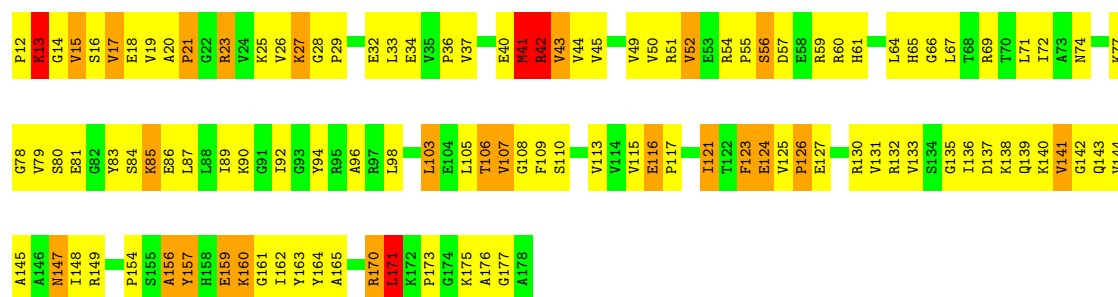
• Molecule 28: 50S ribosomal protein L5

Chain DG: 47% 40% 11% .



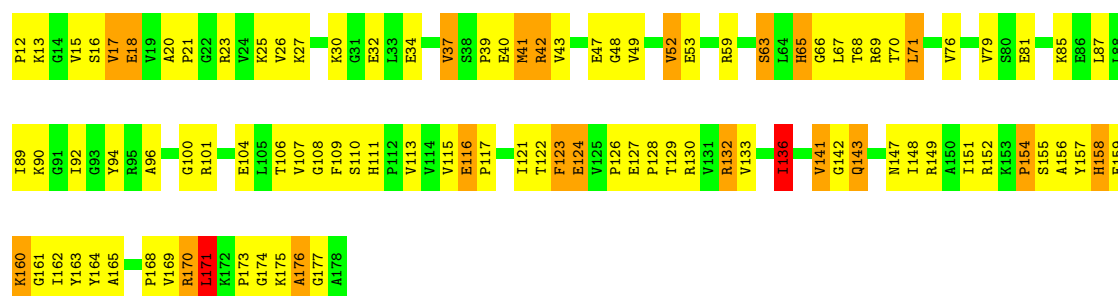
• Molecule 29: 50S ribosomal protein L6

Chain BH: 32% 51% 14% .

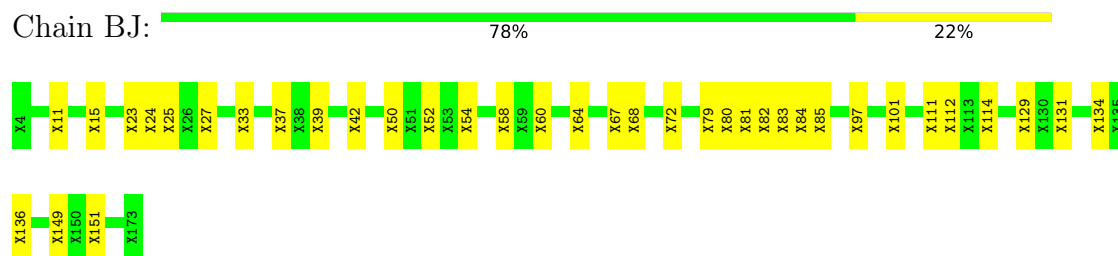


• Molecule 29: 50S ribosomal protein L6

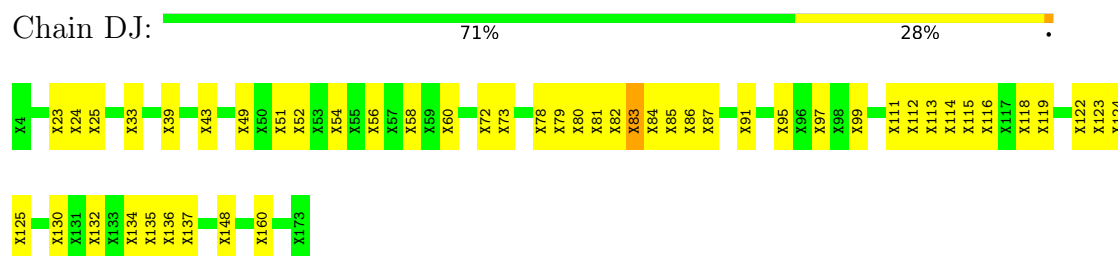
Chain DH: 41% 46% 12% .



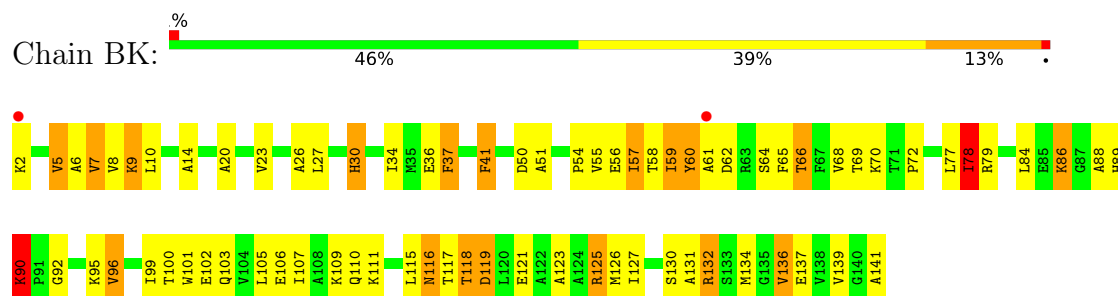
- Molecule 30: 50S ribosomal protein L10



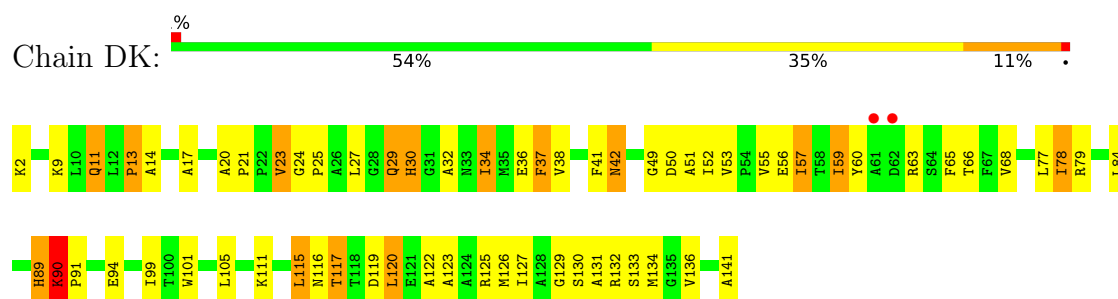
- Molecule 30: 50S ribosomal protein L10



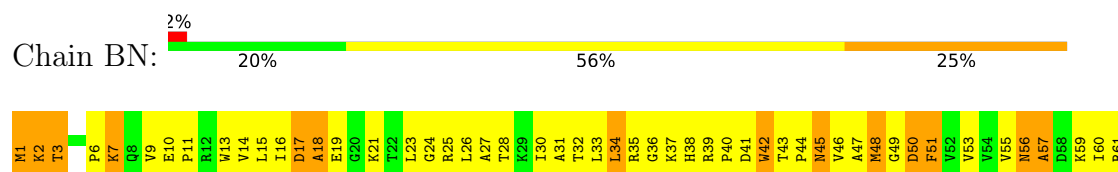
- Molecule 31: 50S ribosomal protein L11

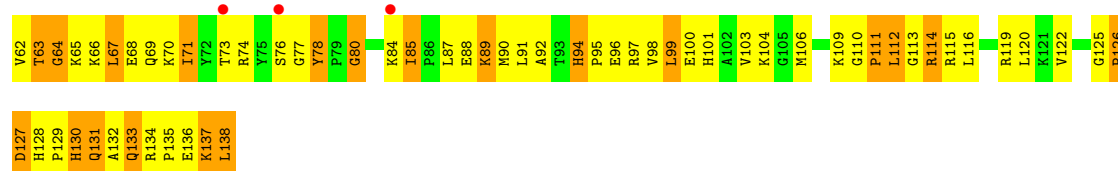


- Molecule 31: 50S ribosomal protein L11

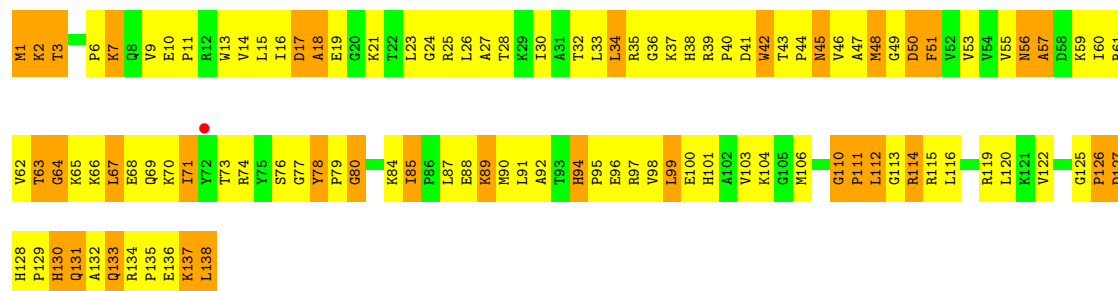


- Molecule 32: 50S ribosomal protein L13

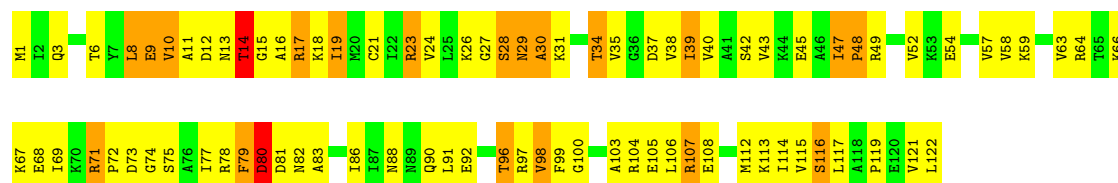




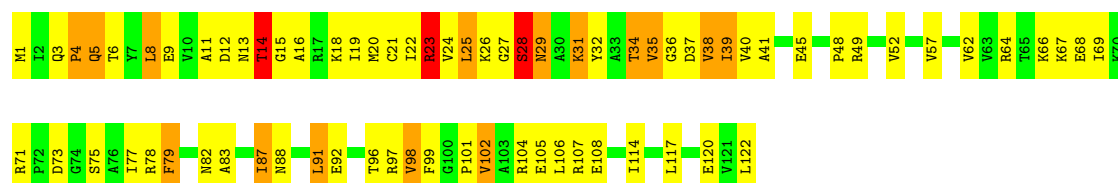
• Molecule 32: 50S ribosomal protein L13



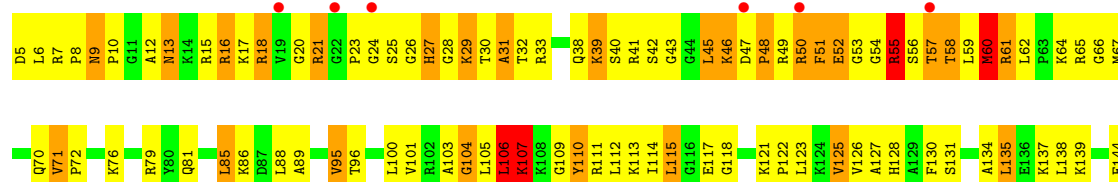
• Molecule 33: 50S ribosomal protein L14



• Molecule 33: 50S ribosomal protein L14

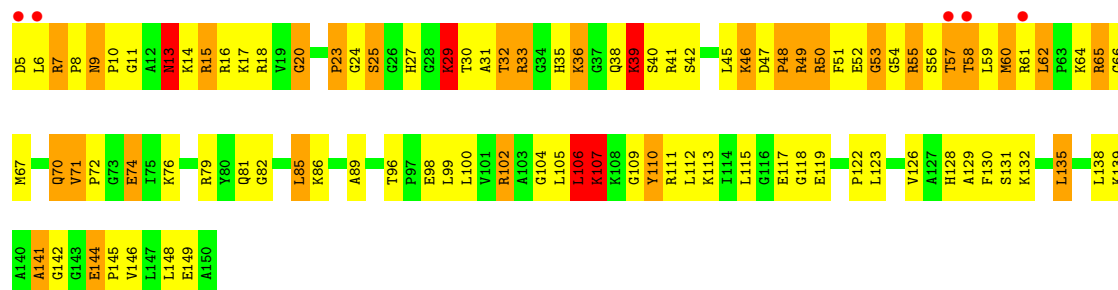


• Molecule 34: 50S ribosomal protein L15





- Molecule 34: 50S ribosomal protein L15



- Molecule 35: 50S ribosomal protein L16

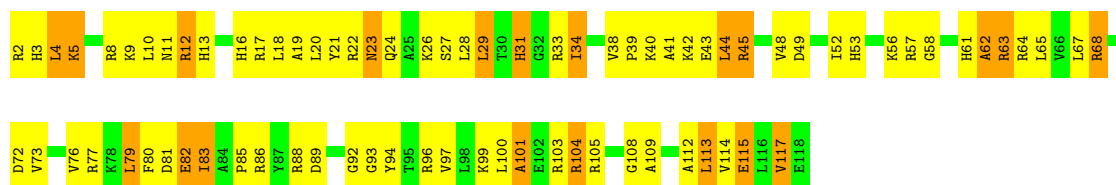


- Molecule 35: 50S ribosomal protein L16

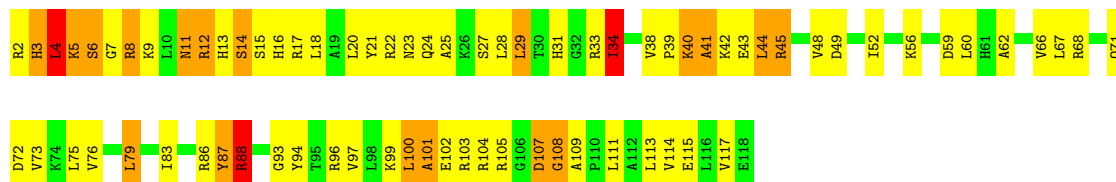


- Molecule 36: 50S ribosomal protein L17

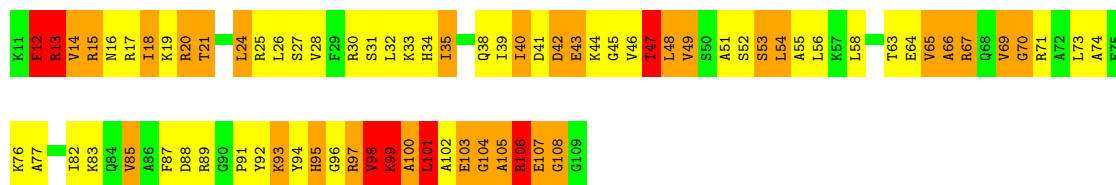
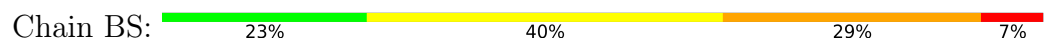




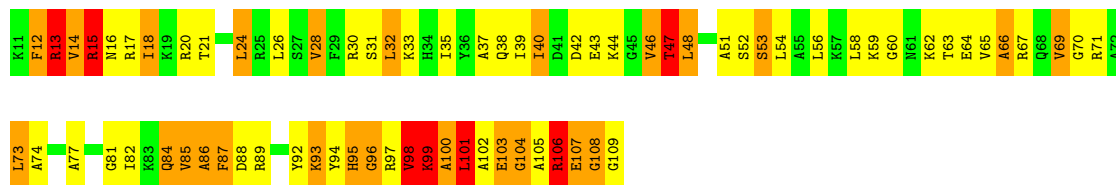
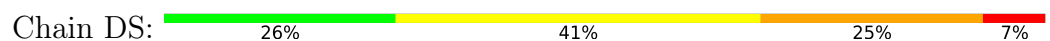
• Molecule 36: 50S ribosomal protein L17



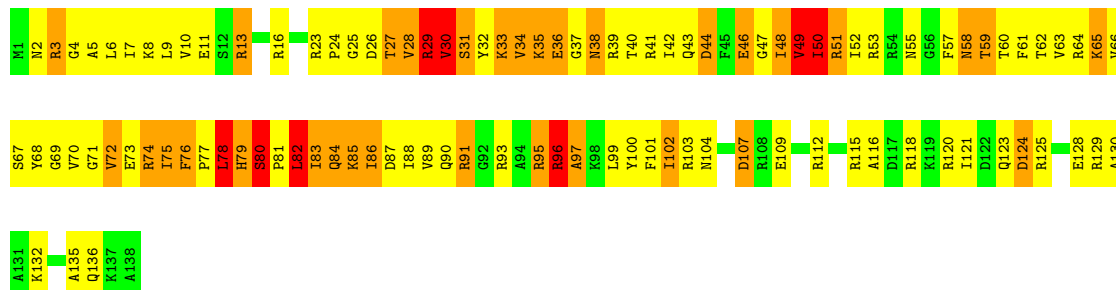
• Molecule 37: 50S ribosomal protein L18



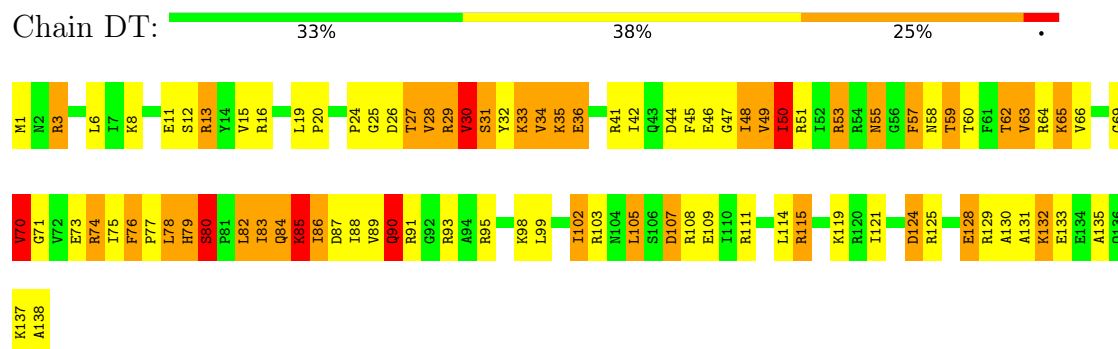
• Molecule 37: 50S ribosomal protein L18



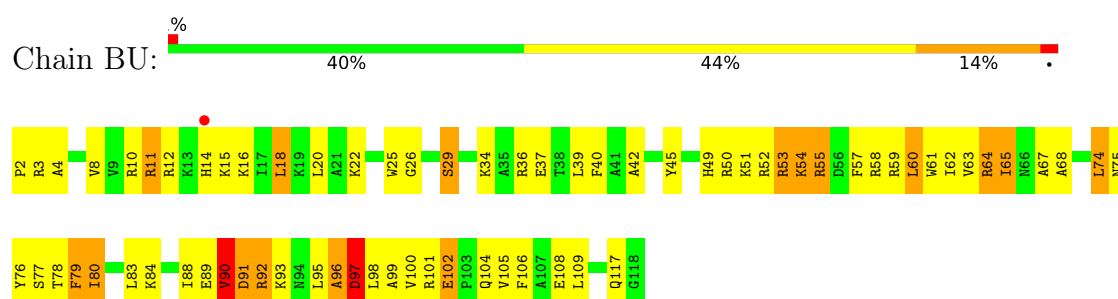
• Molecule 38: 50S ribosomal protein L19



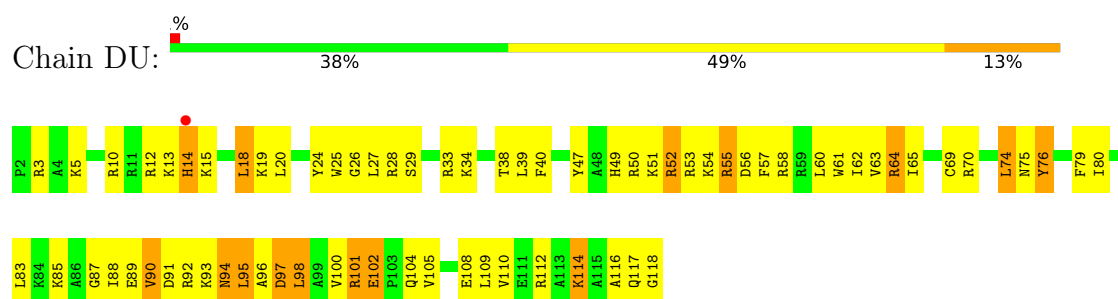
- Molecule 38: 50S ribosomal protein L19



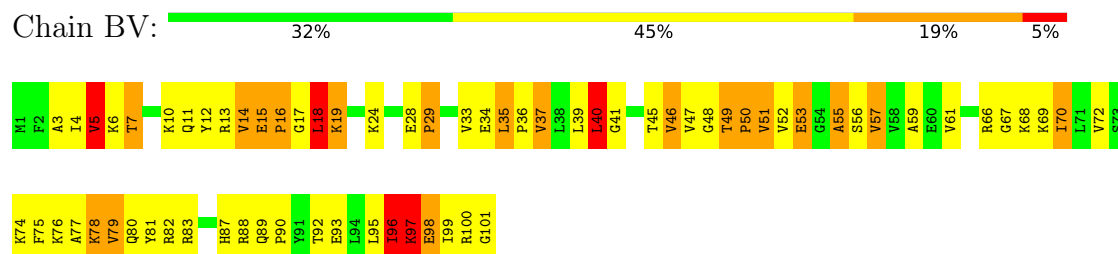
- Molecule 39: 50S ribosomal protein L20



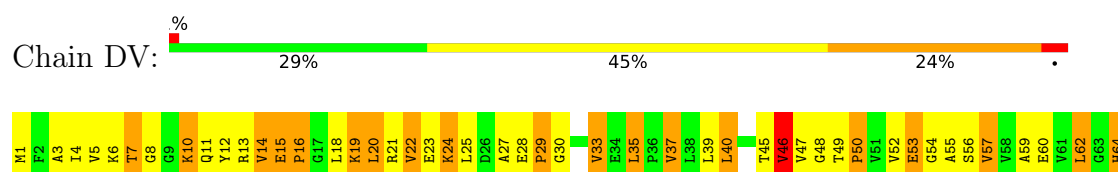
- Molecule 39: 50S ribosomal protein L20

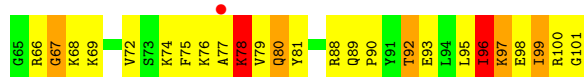


- Molecule 40: 50S ribosomal protein L21



- Molecule 40: 50S ribosomal protein L21





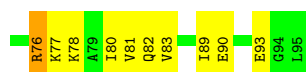
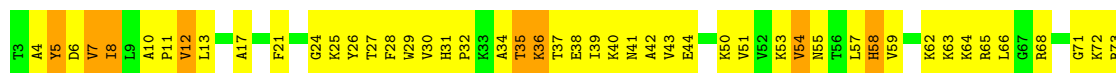
• Molecule 41: 50S ribosomal protein L22



• Molecule 41: 50S ribosomal protein L22



• Molecule 42: 50S ribosomal protein L23



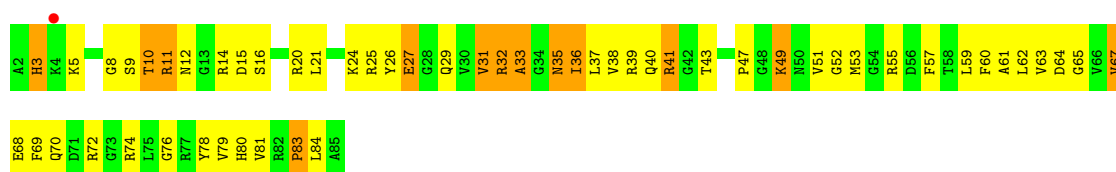
• Molecule 42: 50S ribosomal protein L23



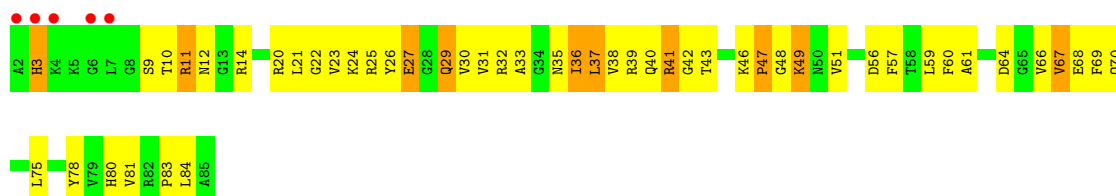
• Molecule 43: 50S ribosomal protein L24



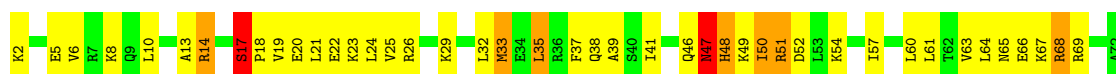




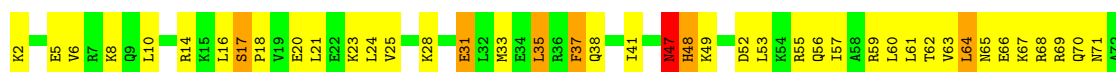
- Molecule 45: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L30



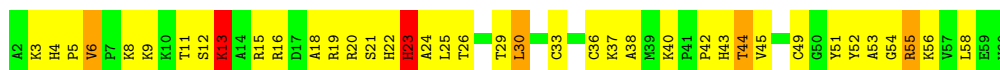
- Molecule 48: 50S ribosomal protein L32





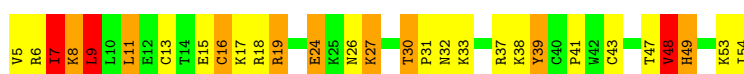
- Molecule 48: 50S ribosomal protein L32

Chain D5: 



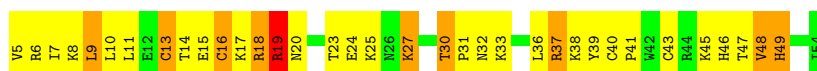
- Molecule 49: 50S ribosomal protein L33

Chain B6: 



- Molecule 49: 50S ribosomal protein L33

Chain D6: 



- Molecule 50: 50S ribosomal protein L34

Chain B7: 

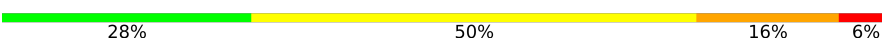


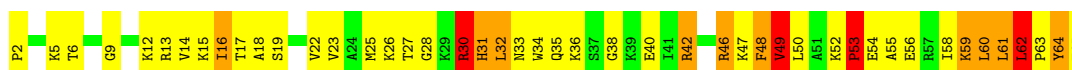
- Molecule 50: 50S ribosomal protein L34

Chain D7: 

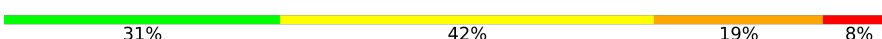


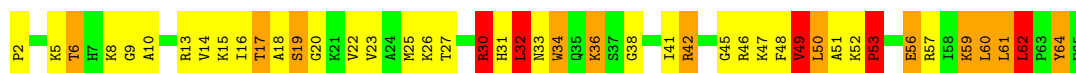
- Molecule 51: 50S ribosomal protein L35

Chain B8: 



- Molecule 51: 50S ribosomal protein L35

Chain D8: 



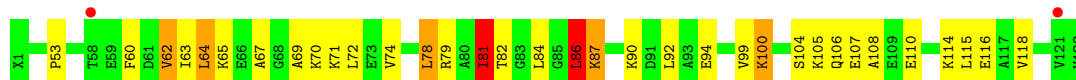
- Molecule 52: 50S ribosomal protein L36



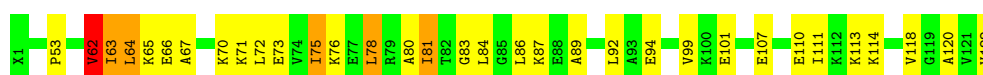
- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L7/L12



- Molecule 53: 50S ribosomal protein L7/L12



- Molecule 54: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 54: 50S ribosomal protein L7/L12

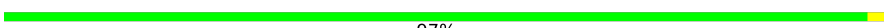


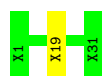
There are no outlier residues recorded for this chain.

- Molecule 54: 50S ribosomal protein L7/L12



- Molecule 54: 50S ribosomal protein L7/L12

Chain Dg:  97%



- Molecule 55: 50S ribosomal protein L7/L12

Chain Bh:  100%

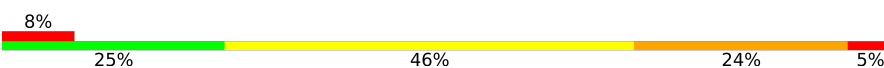
There are no outlier residues recorded for this chain.

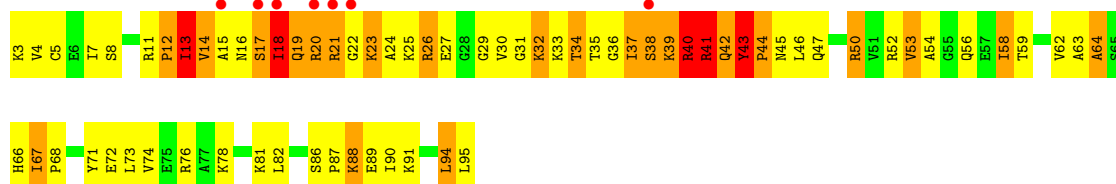
- Molecule 55: 50S ribosomal protein L7/L12

Chain Dh:  100%

There are no outlier residues recorded for this chain.

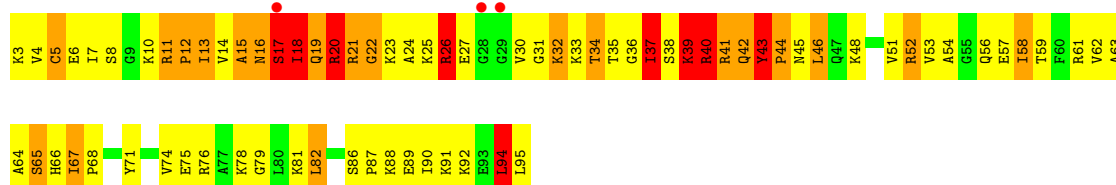
- Molecule 56: 50S ribosomal protein L28

Chain B1:  8% 25% 46% 24% 5%

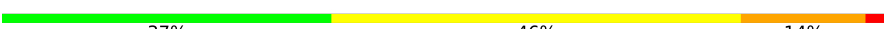


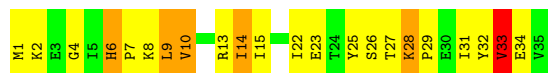
- Molecule 56: 50S ribosomal protein L28

Chain D1:  3% 19% 49% 22% 10%



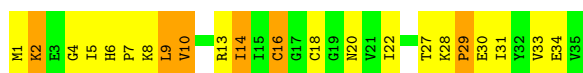
- Molecule 57: 50S ribosomal protein L31

Chain B4:  37% 46% 14%



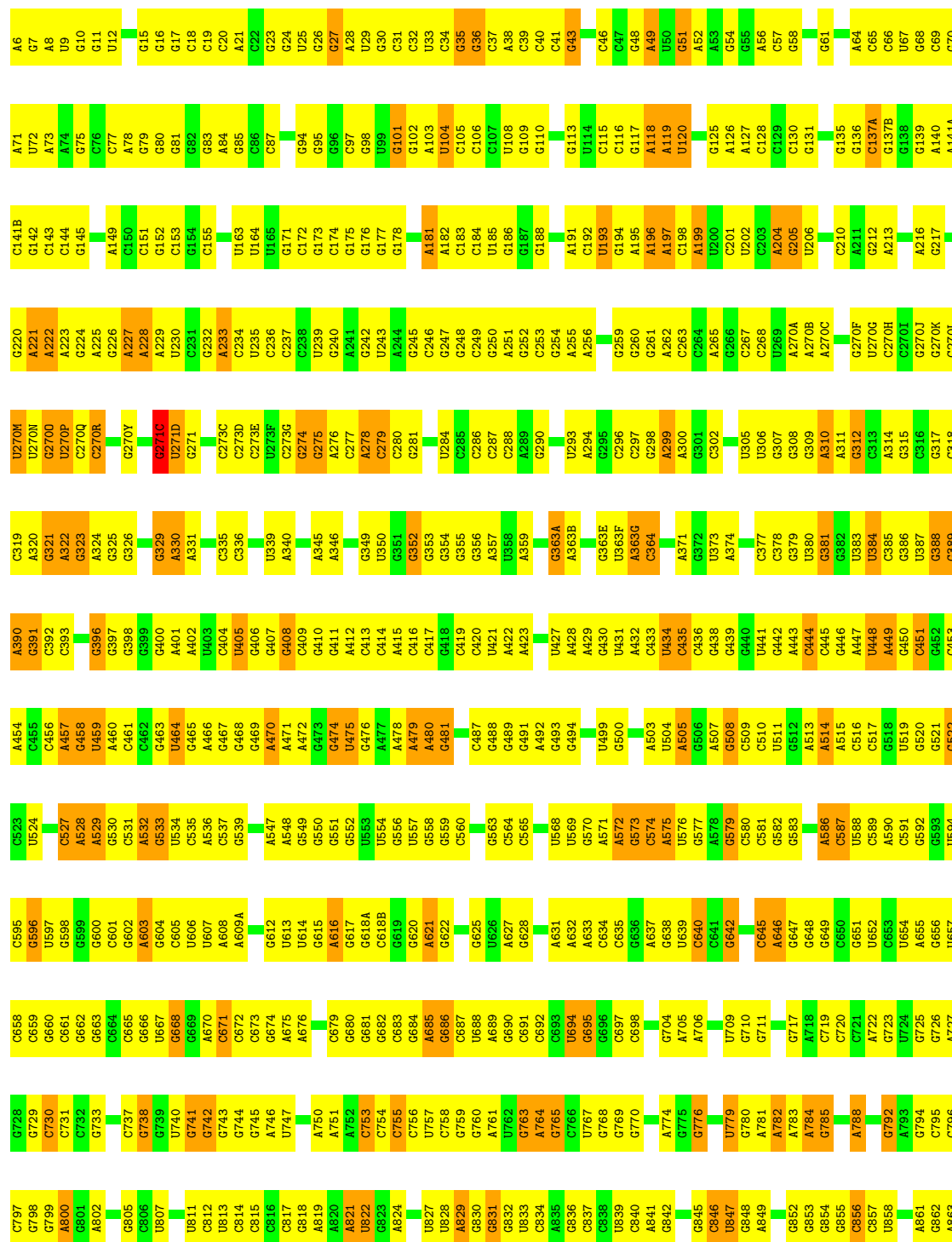
- Molecule 57: 50S ribosomal protein L31

Chain D4:  37% 46% 17%



• Molecule 58: 23S ribosomal RNA

Chain BA: 28% 57% 15%

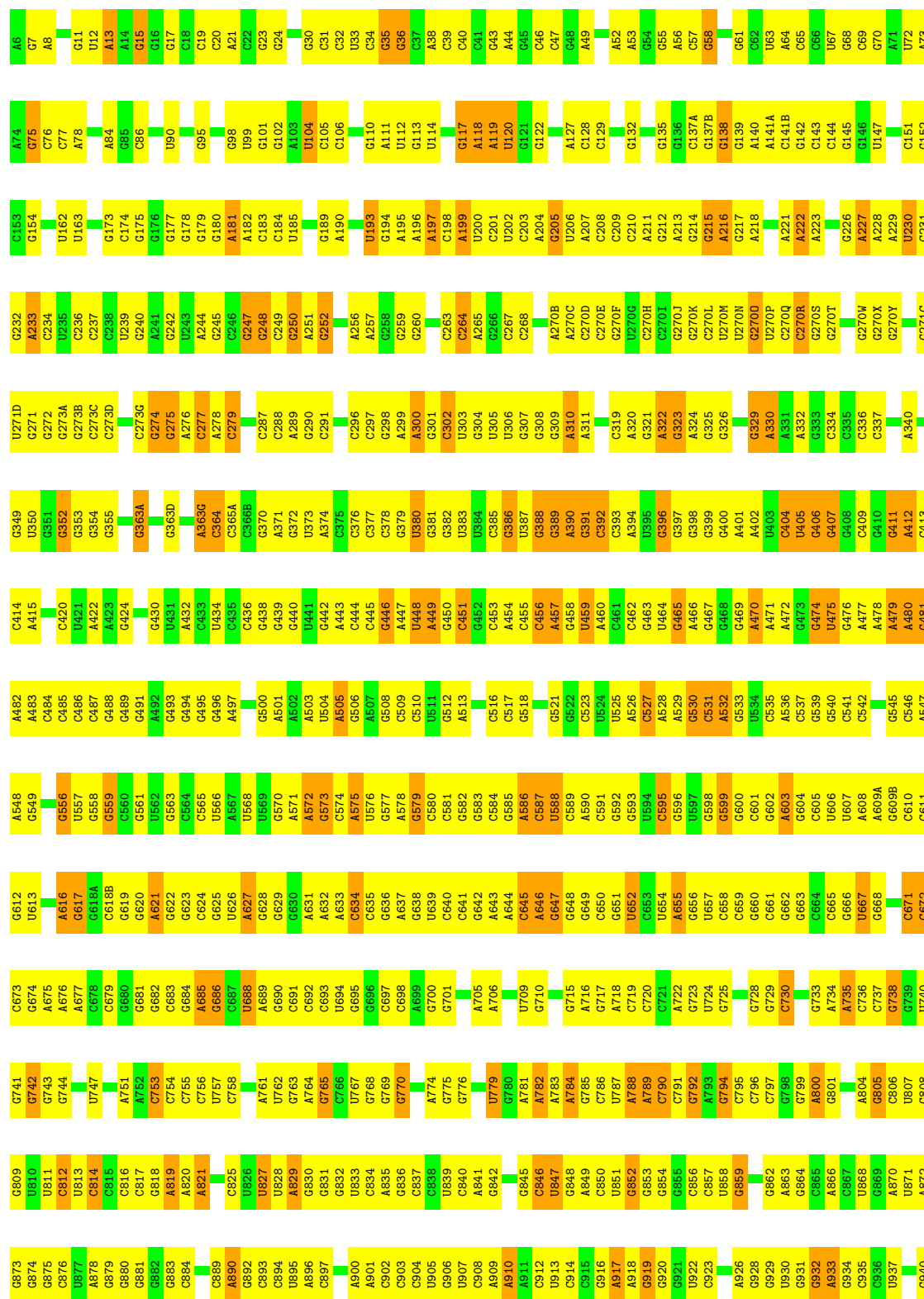


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G1856	G1857	G1858	G1859	G1860	G1623	G1624	G1492	G1422	U1341	U1273	A1143	C1008	A866
G1861	G1862	G1863	G1864	G1865	G1625	G1626	G1493	G1423	A1342	A1274	G1144	C1009	U870
G1866	G1867	G1868	G1869	G1870	G1627	G1628	G1494	G1424	G1343	A1275	C1145	A1010	A871
G1871	G1872	G1873	G1874	G1875	G1629	G1630	G1495	G1425	G1344	A1276	C1146	G1011	A872
G1876	G1877	G1878	G1879	G1880	G1631	G1632	G1496	G1426	C1345	A1277	C1147	C1012	
G1881	G1882	G1883	G1884	G1885	A1633	A1634	U1497	A1427		U1084	U1084	U1014	A878
G1886	G1887	G1888	G1889	G1890	A1635	A1636	C1498	C1428	A1349	G1280	G1150	G1015	A879
G1891	G1892	G1893	G1894	G1895	G1637	G1638	C1499	G1429	U1352	G1281	G1151	G1016	G880
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G1906	G1907	G1908	G1909	G1910	G1643	G1644	C1505		G1355	U1287	A1155	A1020	U959
G1911	G1912	G1913	G1914	G1915	G1645	G1646	G1506		G1356	U1288	A1156	A1021	A890
G1916	G1917	G1918	G1919	G1920	G1647	G1648	G1507		G1357	C1289	G1157	G1022	G892
G1921	G1922	G1923	G1924	G1925	G1649	G1650	G1508		U1358	C1290		G1023	C961
G1926	G1927	G1928	G1929	G1930	G1651	G1652	G1509		A1359	C1291	C1161	G1024	A896
G1931	G1932	G1933	G1934	G1935	G1653	G1654	G1510		A1360	G1292	G1162	G1025	C897
G1936	G1937	G1938	G1939	G1940	G1655	G1656	G1511		G1361	U1294	G1163	U1026	A901
G1941	G1942	G1943	G1944	G1945	G1657	G1658	G1512		G1362	C1295	G1164	A1027	C902
G1946	G1947	G1948	G1949	G1950	G1659	G1660	G1513		A1363	G1296	C1165	A1028	
G1951	G1952	G1953	G1954	G1955	G1661	G1662	G1514		A1364	C1297	C1166	A1029	G906
G1956	G1957	G1958	G1959	G1960	G1663	G1664	G1515		G1365	G1298	U1167	A1032	U907
G1961	G1962	G1963	G1964	G1965	G1665	G1666	G1516		A1366	C1299		U1033	C908
G1966	G1967	G1968	G1969	G1970	G1667	G1668	G1517		A1367	U1300		G1034	C909
G1971	G1972	G1973	G1974	G1975	G1669	G1670	G1518		G1371	A1301	G1171	U1035	A910
G1976	G1977	G1978	G1979	G1980	G1671	G1672	G1519		U1372	A1302	A1174	G1036	A911
G1981	G1982	G1983	G1984	G1985	G1673	G1674	G1520		G1373	G1303	G1175	G1037	A912
G1986	G1987	G1988	G1989	G1990	G1675	G1676	G1521		C1374	C1304	G1176		U913
G1991	G1992	G1993	G1994	G1995	G1677	G1678	G1522		C1375	C1305	A1177	C974B	C914
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G2001	G2002	G2003	G2004	G2005	G1681	G1682	G1524		A1377	U1242	G1179	C976	C916
G2006	G2007	G2008	G2009	G2010	G1683	G1684	G1525		G1378	G1243	C1180	G1044	A917
G2011	G2012	G2013	G2014	G2015	G1685	G1686	G1526		A1379	A1244		A1045	A918
G2016	G2017	G2018	G2019	G2020	G1687	G1688	G1527		G1380	G1245		A1046	G919
G2021	G2022	G2023	G2024	G2025	G1689	G1690	G1528		A1381	A1247	G1183	A1047	G920
G2026	G2027	G2028	G2029	G2030	G1691	G1692	G1529		G1382	G1248	G1184	G1048	G921
G2031	G2032	G2033	G2034	G2035	G1693	G1694	G1530		G1383	U1249	G1185	C1049	U922
G2036	G2037	G2038	G2039	G2040	G1695	G1696	G1531		A1384	G1250	G1186		U923
G2041	G2042	G2043	G2044	G2045	G1697	G1698	G1532		G1385	C1251	G1187		C924
G2046	G2047	G2048	G2049	G2050	G1699	G1700	G1533		A1386	U1252	G1190	C1053	C925
G2051	G2052	G2053	G2054	G2055	G1701	G1702	G1534		A1387	A1253	G1191	A1054	A926
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G2071	G2072	G2073	G2074	G2075	G1709	G1710	G1538		A1391	C1257	G1196	U1060	U930
G2076	G2077	G2078	G2079	G2080	G1711	G1712	G1539		G1392	G1258	G1197	U1061	G931
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G2101	G2102	G2103	G2104	G2105	G1721	G1722	G1544		G1408	A1263	C1202	A1070	C936
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G2126	G2127	G2128	G2129	G2130	G1731	G1732	G1549		G1417	U1269	G1207	G1075	A941
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G2151	G2152	G2153	G2154	G2155	G1741	G1742	G1554						
G2156	G2157	G2158	G2159	G2160	G1743	G1744	G1555						
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G2186	G2187	G2188	G2189	G2190	G1755	G1756	G1561						
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G2196	G2197	G2198	G2199	G2200	G1759	G1760	G1563						
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G2211	G2212	G2213	G2214	G2215	G1765	G1766	G1566						
G2216	G2217	G2218	G2219	G2220	G1767	G1768	G1567						
G2221	G2222	G2223	G2224	G2225	G1769	G1770	G1568						
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G2231	G2232	G2233	G2234	G2235	G1773	G1774	G1570						
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G2431	G2432	G2433	G2434	G2435	G1833	G1834	G1600						
G2441	G2442	G2443	G2444	G2445</									



● Molecule 58: 23S ribosomal RNA

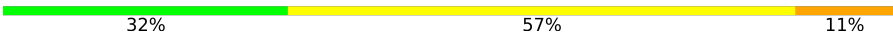
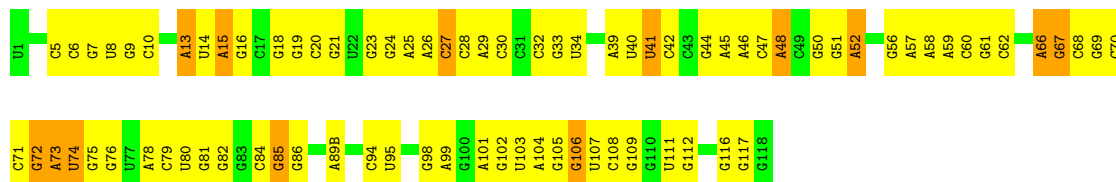
Chain DA:  27% 57% 16%



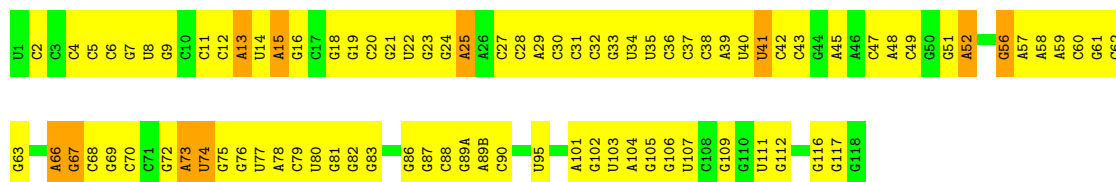
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G1801	A1802	A1803	C1806	G1807	G1808	A1809	A1810	G1811	A1812	G1813	G1814	A1815	G1816	G1817	G1818	G1819	A1820	A1821	G1822	G1823	C1824	A1825	G1826	A1827	G1828	A1829	C1830	G1831	A1832	C1833	A1834	U1841	G1842	G1843	A1844	G1845	G1846	A1847	A1848	G1849	G1850	A1851	A1852	A1853	A1854	G1855	G1856	G1857	A1858	A1859	G1860	G1861	G1862	G1863	U1864	G1865	G1866	G1867	G1868	G1869	G1870	G1871	G1872	U1796	C1797	U1798	G1799	A1871	A1872
C1712	U1716	G1717	G1718	G1725	G1726	U1727	G1728	A1729	U1730	G1731	A1732	G1733	C1741	C1742	G1743	G1746	G1747	G1748	A1749	G1750	C1751	C1752	G1756	U1757	G1758	A1762	G1763	G1764	C1771	G1772	A1773	C1774	U1777	U1778	U1779	A1780	G1781	G1782	A1783	A1784	A1785	A1786	A1787	C1788	A1789	C1790	A1791	G1792	U1796	C1797	U1798	G1799	A1871	A1872															
G1651	A1652	G1653	A1654	A1655	C1656	G1657	C1658	G1659	C1660	G1661	A1664	A1665	G1666	G1667	A1668	A1669	C1670	G1671	C1672	U1673	G1674	C1675	A1676	A1677	G1678	U1679	U1680	G1681	G1682	G1683	C1684	C1685	G1686	U1687	U1688	A1689	A1690	C1691	U1692	U1693	G1694	G1695	G1696	G1697	A1698	A1699	A1700	A1701	G1702	G1703	G1704	G1705	U1706	C1707	U1708	U1709	G1710	C1711											
A1586	A1587	C1588	C1589	A1590	C1591	G1594	G1595	C1598	C1599	G1600	G1601	A1602	A1603	A1604	C1605	A1606	A1608	A1609	A1610	C1611	G1612	G1613	A1614	A1615	A1616	C1617	A1618	G1619	G1622	G1623	G1626	G1627	G1628	U1629	G1630	G1631	A1632	G1633	A1634	G1635	A1636	A1637	G1638	U1639	G1640	A1641	G1642	A1643	G1644	A1510	A1511	A1512	C1645	G1646	G1647	G1648	G1649	G1650											
G1517	C1518	G1519	G1522	U1523	G1524	G1525	G1526	A1529	G1530	C1531	C1532	C1533	G1534	U1535	A1536	C1537	G1538	G1539	U1540	U1541	G1542	A1543	C1544	A1545	A1546	C1547	C1548	C1549	C1550	G1551	G1552	G1555	C1556	C1557	A1558	G1559	G1563	G1568	A1569	A1570	A1571	A1572	C1575	U1576	C1577	U1578	A1579	A1580	G1581	C1582	A1583	C1585																	
G1449	C1450	C1451	A1453	U1454	G1455	C1458	G1459	A1460	A1461	C1462	C1463	C1464	G1465	G1466	C1467	C1468	A1469	G1470	A1471	A1472	G1473	C1474	G1478	G1479	C1480	U1481	G1482	A1483	A1486	G1487	G1488	U1489	A1490	G1491	A1492	C1493	A1494	A1495	A1496	U1497	C1498	C1499	G1500	C1501	C1502	U1503	C1504	C1505	A1509	A1510	A1511	A1512	C1513	C1514	C1515	U1516													
G1389	U1390	U1391	U1394	A1395	U1396	U1397	C1398	C1399	G1400	G1401	C1402	C1403	C1404	U1405	U1406	C1407	C1408	C1409	G1410	C1411	U1414	U1415	G1416	G1417	C1418	A1419	U1420	G1421	G1422	G1423	G1424	G1425	G1426	A1427	C1428	C1429	A1430	U1431	C1432	U1433	U1434	G1435	G1436	C1437	U1438	A1439	G1440	G1441	G1442	G1443	G1444	A1445	C1446	G1447	G1448	A1498													
U1323	G1324	G1325	U1326	C1327	G1328	U1329	C1330	A1331	G1332	U1335	A1336	G1337	G1338	G1339	U1340	U1341	A1342	G1343	G1344	G1345	G1346	G1347	G1348	A1349	C1350	C1351	U1352	A1353	A1354	G1355	G1358	A1359	A1360	C1363	G1364	A1365	A1366	A1367	G1368	U1372	C1375	C1376	G1377	A1378	A1379	G1380	G1381	G1382	C1383	A1384	C1385	C1386	G1388																
U1255	G1256	A1262	U1263	G1264	A1265	A1268	A1269	C1270	G1271	G1271	A1272	U1273	A1274	A1275	A1276	A1277	A1278	G1279	G1280	G1283	A1284	G1285	A1286	A1287	U1288	C1289	C1290	C1291	U1292	C1293	U1294	C1295	G1296	C1297	C1298	G1299	U1300	A1301	A1302	G1303	C1304	C1305	C1306	A1307	A1308	G1309	G1310	G1311	U1312	U1313	C1314	A1315	U1316	A1317	A1321	A1322													
G1193	A1194	G1195	U1133	U1135	G1136	U1137	G1138	G1139	C1140	U1141	U1142	A1143	G1144	C1145	U1146	G1147	U1148	C1150	G1151	C1152	G1153	U1154	A1155	U1156	G1157	C1158	U1159	C1160	G1161	G1162	G1163	U1165	G1164	C1165	U1166	U1167	G1168	G1169	G1170	U1173	A1174	U1175	G1176	A1177	C1178	G1179	C1180	G1183	G1184	C1185	G1186	G1187	U1188	A1189	G1190														
U1066	A1067	G1068	A1069	G1070	A1071	C1072	A1073	G1074	C1075	C1076	U1077	A1078	C1079	C1080	U1081	U1082	U1083	A1084	A1085	A1086	A1087	U1088	U1089	U1090	G1091	C1092	G1093	U1094	A1095	U1096	G1097	G1098	C1102	A1103	U1105	G1106	G1107	U1108	C1109	U1110	A1111	G1112	U1113	G1114	G1115	C1116	G1120	G1121	G1122	C1123	G1124	C1125	A1126	A1127	C1128	A1129													
C1004	C1005	C1006	C1007	C1008	A1009	A1010	G1011	G1012	C1013	G1016	G1017	C1018	U1019	A1020	A1021	G1022	U1023	G1024	G1025	U1026	A1027	A1028	A1029	G1030	G1031	U1032	U1033	G1034	U1035	G1036	G1039	C1040	G1041	C1042	C1043	G1044	A1045	A1046	G1047	A1048	C1049	A1050	G1051	C1052	C1053	A1054	G1055	G1056	A1057	G1058	G1059	C1060	G1061	C1062	G1063	C1064	U1065												
A941	G942	U943	G944	A945	G946	G947	G948	G949	G950	C951	G954	C955	G956	A957	U958	A959	A960	C961	G962	U963	A964	C965	G966	C967	G968	U969	C970	C971	G972	A973	G974A	C974B	G975	G979	A980	A981	C982	A983	C986	C987	A988	C989	A990	C991	C992	C993	C994	C995	A996	C997	C998	U999	A1000	A1001	G1002	G1003													

U2895	C2893	A2765	G2700	G2630	A2565	G2497	U2431	C2368	G2306	G2234	A2158	G2090	G2027	C1962
C2834	G2631	G2766	C2701	G2636	A2566	C2498	A2432	A2369	G2307	G2235	G2159	U2091	A2030	U1963
U2835	G2632	C2767	C2702	C2567	A2567	C2499	A2433	G2370	G2308	C2236	G2162	U2092	A2031	G1964
G2837	G2633	C2768	U2703	C2568	A2568	U2500	A2434	G2371	A2309	G2237		G2093	A2032	C1965
G2838	U2636	C2771	C2704	G2569	G2570	C2501	A2435	G2372	A2310	G2238	G2166	G2094	A2033	A1966
G2839	U2637	C2772	A2705	C2570	G2571	A2503	G2436	C2374	A2311	G2239	U2167	U2096	U2034	C1967
C2840	U2638	C2773	G2706	U2639	A2572	U2504	A2439	G2375	G2312	C2240	G2168	C2097	G2035	G1968
C2841	A2639	C2774	G2707	G2573	C2574	U2505	A2440	A2376	C2313	A2241	A2169		G2036	G1969
C2842	G2640	C2775	G2708	U2574	G2575	U2506	C2441	A2377	G2314	G2242	G2170	G2102	G2037	A1970
G2843	G2641	C2776	G2709	C2576	G2577	U2507	C2442	A2378	G2315	U2243	A2171	U2101	G2038	A1971
G2844	G2642	U2778	C2710	G2577	G2578	G2508		A2379	G2316	U2244	U2172	G2102	G2039	A1972
G2845	G2643	U2779	U2712	A2577	G2579	G2509	G2445	C2380	G2317	U2245	A2173	G2103	G2040	G1973
U2847	C2646	U2780	A2718	G2578	G2580	C2510	G2446	C2381	G2318	A2247	C2174	G2104	U2041	C1974
C2848	U2647	A2781	A2713	U2585	U2581	U2511	A2447	G2382	G2319	A2248	G2175	G2105	A2042	G1975
U2849	G2648	G2782	G2714	U2586	G2582	C2512	A2448	G2383	A2320	G2249	A2176	G2106	A2043	U1976
U2850	U2649	G2783	C2715	G2583	G2581	U2513	U2449	G2384	G2321	U2250	G2177	G2107	C2044	U1977
A2851	U2650	C2784	U2716	U2584	G2582	U2514	A2450	C2385	A2322		C2178	G2108	C2045	A1978
G2852	G2651	U2785	G2717	U2585	G2583	U2515	A2451	C2386	G2323	C2254	C2179	G2109	G2046	C1979
G2853	C2652	U2786	G2718	U2586	U2584	C2516	A2452	U2387	G2324	C2255	U2180	G2110	G1980	
G2854	U2653	G2787	G2719	U2587	U2585	C2517	A2453		G2325	G2256	G2181	G2111	U2047	G1981
G2855	A2654	U2788	U2720	A2587	U2586	U2518	G2454	U2390	C2326	G2257	G2182	G2112	G2049	C1982
G2856	G2655	U2789	A2721	A2587	U2587	U2519	G2455	G2391	A2327	U2257	C2183	U2113	C2050	
G2857	U2656	C2791	G2722	C2656	U2590	C2520	G2456	A2392	G2328	G2259	G2184	G2115	A2051	G1990
A2860	A2657	G2792	C2723	U2656	C2591	C2521	A2459	A2393	G2330	U2262	C2185	G2116	G2052	U1991
G2861	G2658	G2793	A2725	G2659	G2592	U2522		C2394	G2331		G2186	A2117	G2053	G1992
G2862	C2659	U2794	U2726	U2593	G2595	C2525	U2462	C2395	U2332	A2266	U2189	U2118	A2054	U1993
G2863	A2660	G2795	G2727	C2594	G2596	G2526	C2463	C2396	A2333		C2196	U2119	C2055	
G2864	G2661	U2796	U2728	G2595	G2597	C2527	C2464	U2397	G2334	A2267	G2191	G2120	G2056	U1995
U2865	A2662	C2798	G2729	U2598	G2599	U2528	C2465	U2398	A2335	A2268	G2192	G2121	A2057	G1996
U2866	G2663	G2799	C2730	U2598	G2599	C2529	C2466	G2400	U2336	A2269	G2193	U2122	A2058	G1997
U2867	U2664	U2801	G2731	G2599	G2599	G2530	C2467	U2401	G2337	G2271		G2125	G2059	G1998
A2868	A2665	G2802	G2732	G2600	C2601	A2531	G2468	C2402	G2339	U2272	C2196	A2126	A2061	G1999
G2869	C2666		A2733	G2601	G2602	G2532	G2470	C2403	G2340	A2273	C2197	G2127	A2062	G2000
C2870	G2667	G2807	G2736	U2604	G2603	A2534	G2471	C2404	G2341	A2274	A2198	G2128	G2063	G2001
C2871	G2668		G2737	U2605	U2604	G2535	G2472	G2405	G2342	C2275	A2199	C2129	G2064	G2002
G2872	A2671			U2606	U2605	G2536	U2473		G2343			U2130	C2065	G2003
C2873	G2672		C2742	G2606	G2606	U2537		U2408	U2344	A2278	C2207	G2131	C2066	G2004
C2874			C2743	G2607	G2607	U2538	A2476	G2409	G2345	G2282	U2208	U2132	C2067	A2005
C2875	G2678		G2744	G2608	G2608	C2539	C2477	G2410	A2346	C2283	G2209	U2133	U2068	C2006
G2876	A2679		C2745	U2609	U2609	C2540	A2478	A2411	G2347	A2134	G2210	A2134	G2069	C2007
G2877	G2680		U2746	C2610	C2610	A2541	G2479	A2412	U2348	C2284	G2211	A2135	G2070	C2008
U2878	C2681		G2747	U2611	U2611	A2542	C2480	G2415	G2349	C2285	A2212	G2136	A2071	G2010
C2879	U2682		A2748	C2612	C2612	G2543	G2481	C2416	C2350	A2286	U2213	C2137	G2072	U2011
C2880	G2683		A2749	U2613	U2613	G2544	G2482	C2417	G2351	A2287	G2215	C2138	G2073	G2012
C2881	U2684			C2617	C2617	U2545	G2483	A2418	A2352	A2287	G2216	C2139	U2074	A2013
A2882	G2685		U2754	G2618	G2618	U2546	G2484	U2419	G2353	U2290	G2217		U2075	A2014
U2883	U2686		G2755	G2619	G2619	U2547	G2485	C2420	G2354	U2291	G2218	G2145	U2079	U2016
C2885	U2687		U2756	C2620	C2620	G2548	G2486	G2421	C2355	C2292	G2219	C2146	G2080	U2017
U2886	U2688		G2757	C2621	C2621	G2549	G2487	A2422	G2358	C2293	G2224	G2147	G2081	G2018
U2887	C2689		A2758	C2622	C2622	U2554	A2488	U2423	A2361	G2299	A2225	G2148	A2082	A2019
C2888	U2689		G2759	C2623	C2623	U2555	G2489	C2424	G2362	G2300	G2226	G2151	G2083	A2020
C2889	U2690		G2760	C2624	C2624	G2557	G2490	A2425	A2363	G2301	G2228		C2084	C2021
G2891	U2691		G2761	C2625	C2625	G2558	U2493	A2426	G2364	G2302	G2230	G2154	U2086	U2022
A2892	U2692		G2762	C2626	C2626	C2559	G2494	C2427	C2365	G2303	G2231	G2155	G2087	G2023
G2893	U2693		G2763	C2627	C2627	U2564	G2495	G2428	G2366	G2304	U2232	G2156	G2088	C2024
G2894	U2694		A2764	C2628	C2628	A2564	C2496	G2429	A2367	G2305	U2233	G2157	U2089	C2025
				C2629	C2629			A2430	G2367					C2026

● Molecule 59: 5S ribosomal RNA

Chain BB:  32% 57% 11%

● Molecule 59: 5S ribosomal RNA

Chain DB:  26% 66% 8%

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	307.21Å 670.44Å 350.40Å 90.00° 92.37° 90.00°	Depositor
Resolution (Å)	40.00 – 4.00 40.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-4.00) 77.7 (40.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 4.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.281 , 0.329 0.286 , 0.325	Depositor DCC
R_{free} test set	25982 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	74.5	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.24$, $\langle L^2 \rangle = 0.09$	Xtriage
Estimated twinning fraction	0.249 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	308068	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: FUA, GDP

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	AB	0.56	1/1945 (0.1%)	1.11	16/2621 (0.6%)
1	CB	0.54	0/1945	1.09	18/2621 (0.7%)
2	AC	0.38	0/1645	0.87	3/2216 (0.1%)
2	CC	0.38	0/1645	0.93	5/2216 (0.2%)
3	AD	0.38	0/1733	0.93	5/2318 (0.2%)
3	CD	0.38	0/1733	0.94	10/2318 (0.4%)
4	AE	0.41	0/1172	0.97	5/1576 (0.3%)
4	CE	0.45	1/1172 (0.1%)	0.93	2/1576 (0.1%)
5	AF	0.38	0/856	0.90	2/1154 (0.2%)
5	CF	0.38	0/856	0.87	0/1154
6	AG	0.36	0/1276	0.89	1/1709 (0.1%)
6	CG	0.37	0/1276	0.91	3/1709 (0.2%)
7	AH	0.41	0/1136	0.98	3/1527 (0.2%)
7	CH	0.40	0/1136	0.97	4/1527 (0.3%)
8	AI	0.39	0/1029	0.84	0/1379
8	CI	0.35	0/1029	0.84	1/1379 (0.1%)
9	AJ	0.36	0/815	0.86	1/1095 (0.1%)
9	CJ	0.40	0/815	0.92	0/1095
10	AK	0.48	0/900	1.06	6/1213 (0.5%)
10	CK	0.50	0/900	1.08	8/1213 (0.7%)
11	AL	0.57	0/992	1.36	19/1327 (1.4%)
11	CL	0.53	0/992	1.24	10/1327 (0.8%)
12	AM	0.40	0/1008	1.00	5/1347 (0.4%)
12	CM	0.36	0/1008	0.92	3/1347 (0.2%)
13	AN	0.34	0/501	0.92	3/664 (0.5%)
13	CN	0.35	0/501	0.80	0/664
14	AO	0.41	0/745	0.90	2/992 (0.2%)
14	CO	0.36	0/745	0.85	0/992
15	AP	0.37	0/722	0.89	2/970 (0.2%)
15	CP	0.34	0/722	0.86	2/970 (0.2%)
16	AQ	0.53	0/848	1.18	7/1131 (0.6%)
16	CQ	0.49	0/848	1.18	11/1131 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.38	0/579	0.92	1/768 (0.1%)
17	CR	0.36	0/579	0.88	1/768 (0.1%)
18	AS	0.39	0/647	0.91	3/870 (0.3%)
18	CS	0.41	0/647	1.11	6/870 (0.7%)
19	AT	0.41	0/765	0.91	1/1007 (0.1%)
19	CT	0.40	0/765	0.90	0/1007
20	AA	0.19	0/36351	0.43	3/56736 (0.0%)
20	CA	0.18	0/36351	0.41	2/56736 (0.0%)
21	AW	0.19	0/1827	0.45	0/2845
21	CW	0.19	0/1827	0.45	0/2845
22	AV	0.15	0/568	0.35	0/886
22	CV	0.15	0/568	0.38	0/886
23	AY	0.49	4/5317 (0.1%)	1.14	41/7198 (0.6%)
23	CY	0.49	2/5317 (0.0%)	1.12	35/7198 (0.5%)
24	BC	0.59	0/1774	1.25	28/2391 (1.2%)
24	DC	0.61	0/1774	1.25	30/2391 (1.3%)
25	BD	0.46	0/2195	1.09	17/2955 (0.6%)
25	DD	0.46	0/2195	1.04	9/2955 (0.3%)
26	BE	0.47	0/1602	1.11	12/2160 (0.6%)
26	DE	0.44	0/1602	1.08	13/2160 (0.6%)
27	BF	0.48	1/1663 (0.1%)	1.17	18/2249 (0.8%)
27	DF	0.48	0/1663	1.15	13/2249 (0.6%)
28	BG	0.37	0/1499	0.89	2/2016 (0.1%)
28	DG	0.50	3/1499 (0.2%)	1.10	11/2016 (0.5%)
29	BH	0.42	0/1298	0.98	1/1751 (0.1%)
29	DH	0.45	0/1298	0.95	2/1751 (0.1%)
31	BK	0.41	0/1054	0.95	6/1427 (0.4%)
31	DK	0.41	0/1054	0.94	4/1427 (0.3%)
32	BN	0.43	0/1131	1.07	9/1525 (0.6%)
32	DN	0.43	0/1131	1.07	9/1525 (0.6%)
33	BO	0.39	0/943	1.00	6/1269 (0.5%)
33	DO	0.38	0/943	0.93	1/1269 (0.1%)
34	BP	0.44	0/1131	0.99	1/1504 (0.1%)
34	DP	0.41	0/1131	1.03	5/1504 (0.3%)
35	BQ	0.42	0/1143	1.00	2/1527 (0.1%)
35	DQ	0.41	0/1143	1.02	3/1527 (0.2%)
36	BR	0.46	0/974	0.93	1/1302 (0.1%)
36	DR	0.43	0/974	0.96	1/1302 (0.1%)
37	BS	0.47	0/783	1.16	10/1041 (1.0%)
37	DS	0.50	0/783	1.16	8/1041 (0.8%)
38	BT	0.49	0/1161	1.07	7/1549 (0.5%)
38	DT	0.49	0/1161	1.05	8/1549 (0.5%)
39	BU	0.48	0/982	0.91	1/1306 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DU	0.49	0/982	0.91	0/1306
40	BV	0.49	0/790	1.10	5/1057 (0.5%)
40	DV	0.48	0/790	1.05	4/1057 (0.4%)
41	BW	0.44	0/911	0.99	3/1220 (0.2%)
41	DW	0.44	0/911	1.05	2/1220 (0.2%)
42	BX	0.34	0/748	0.87	0/1004
42	DX	0.37	0/748	0.88	1/1004 (0.1%)
43	BY	0.44	0/831	1.13	12/1108 (1.1%)
43	DY	0.43	0/831	1.12	8/1108 (0.7%)
44	BZ	0.39	0/1505	0.99	7/2042 (0.3%)
44	DZ	0.38	0/1505	1.01	11/2042 (0.5%)
45	B0	0.33	0/671	0.79	0/892
45	D0	0.38	0/671	0.83	0/892
46	B2	0.42	0/600	0.99	3/793 (0.4%)
46	D2	0.40	0/600	0.96	2/793 (0.3%)
47	B3	0.37	0/482	1.02	3/646 (0.5%)
47	D3	0.36	0/482	0.98	4/646 (0.6%)
48	B5	0.40	0/473	0.93	2/639 (0.3%)
48	D5	0.39	0/473	1.01	2/639 (0.3%)
49	B6	0.42	0/440	1.04	4/586 (0.7%)
49	D6	0.40	0/440	0.95	2/586 (0.3%)
50	B7	0.41	0/438	0.93	0/575
50	D7	0.38	0/438	0.98	0/575
51	B8	0.44	0/525	1.01	2/691 (0.3%)
51	D8	0.41	0/525	1.06	3/691 (0.4%)
52	B9	0.38	0/310	0.87	0/407
52	D9	0.33	0/310	0.92	0/407
53	Be	0.82	1/538 (0.2%)	1.02	2/715 (0.3%)
53	De	0.38	0/538	0.91	1/715 (0.1%)
56	B1	0.71	1/739 (0.1%)	1.36	15/981 (1.5%)
56	D1	0.75	1/739 (0.1%)	1.48	15/981 (1.5%)
57	B4	0.52	0/276	1.11	2/372 (0.5%)
57	D4	0.51	0/276	1.00	0/372
58	BA	0.20	2/69437 (0.0%)	0.44	5/108401 (0.0%)
58	DA	0.19	0/69437	0.43	0/108401
59	BB	0.18	0/2853	0.41	0/4451
59	DB	0.17	0/2853	0.39	0/4451
All	All	0.30	17/330554 (0.0%)	0.67	608/492202 (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	AB	0	2
1	CB	0	3
11	CL	0	1
23	AY	0	5
23	CY	0	1
24	BC	0	2
24	DC	0	3
25	BD	0	2
27	BF	0	2
27	DF	0	2
30	BJ	0	1
30	DJ	0	1
37	BS	0	2
37	DS	0	4
41	BW	0	1
41	DW	0	1
56	B1	0	1
56	D1	0	2
All	All	0	36

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	Be	87	LYS	C-N	17.11	1.53	1.33
23	CY	500	GLN	C-N	-8.46	1.21	1.33
58	BA	1914	C	O3'-P	-8.40	1.48	1.61
28	DG	109	VAL	N-CA	-8.09	1.36	1.45
23	AY	503	GLY	C-N	-7.92	1.22	1.33

The worst 5 of 608 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CY	500	GLN	CA-C-N	19.32	158.44	121.54
23	CY	500	GLN	C-N-CA	19.32	158.44	121.54
23	AY	503	GLY	O-C-N	-15.78	102.18	122.70
58	BA	1914	C	C4'-C3'-O3'	-15.68	89.48	113.00
23	CY	500	GLN	CA-C-O	-14.33	101.03	122.38

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	163	PHE	Peptide
1	AB	170	GLU	Peptide
23	AY	133	ILE	Peptide
23	AY	135	PHE	Mainchain
23	AY	499	ARG	Mainchain

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	AB	1910	0	1957	140	0
1	CB	1910	0	1957	135	0
2	AC	1621	0	1688	89	0
2	CC	1621	0	1688	72	0
3	AD	1703	0	1763	141	0
3	CD	1703	0	1763	109	0
4	AE	1156	0	1213	69	0
4	CE	1156	0	1213	71	0
5	AF	843	0	857	46	0
5	CF	843	0	857	47	0
6	AG	1257	0	1296	49	0
6	CG	1257	0	1296	53	0
7	AH	1116	0	1177	74	0
7	CH	1116	0	1177	73	0
8	AI	1010	0	1037	59	0
8	CI	1010	0	1037	61	0
9	AJ	802	0	849	54	0
9	CJ	802	0	849	50	0
10	AK	885	0	904	56	0
10	CK	885	0	904	55	0
11	AL	976	0	1062	100	0
11	CL	976	0	1062	112	0
12	AM	997	0	1072	56	0
12	CM	997	0	1072	57	0
13	AN	492	0	529	40	0
13	CN	492	0	529	29	0
14	AO	734	0	771	52	0
14	CO	734	0	771	42	0
15	AP	706	0	725	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CP	706	0	725	37	0
16	AQ	835	0	904	63	0
16	CQ	835	0	904	66	0
17	AR	574	0	644	35	0
17	CR	574	0	644	44	0
18	AS	634	0	655	38	0
18	CS	634	0	655	47	0
19	AT	763	0	861	44	0
19	CT	763	0	861	44	0
20	AA	32474	0	16393	1065	0
20	CA	32474	0	16393	1060	0
21	AW	1635	0	831	69	0
21	CW	1635	0	831	50	0
22	AV	503	0	252	13	0
22	CV	503	0	252	16	0
23	AY	5219	0	5290	348	0
23	CY	5219	0	5290	333	0
24	BC	1742	0	1798	168	0
24	DC	1742	0	1798	179	0
25	BD	2145	0	2234	220	0
25	DD	2145	0	2234	214	0
26	BE	1569	0	1634	136	0
26	DE	1569	0	1634	145	0
27	BF	1628	0	1680	144	0
27	DF	1628	0	1680	145	0
28	BG	1474	0	1535	99	0
28	DG	1474	0	1535	83	0
29	BH	1274	0	1342	81	0
29	DH	1274	0	1342	70	0
30	BJ	851	0	196	31	0
30	DJ	851	0	196	43	0
31	BK	1035	0	1082	56	0
31	DK	1035	0	1082	54	0
32	BN	1104	0	1179	222	0
32	DN	1104	0	1180	232	0
33	BO	933	0	996	65	0
33	DO	933	0	996	69	0
34	BP	1114	0	1187	95	0
34	DP	1114	0	1187	100	0
35	BQ	1122	0	1179	72	0
35	DQ	1122	0	1179	71	0
36	BR	960	0	1021	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DR	960	0	1021	80	0
37	BS	775	0	835	83	0
37	DS	775	0	835	74	0
38	BT	1147	0	1207	109	0
38	DT	1147	0	1207	92	0
39	BU	964	0	1020	95	0
39	DU	964	0	1022	104	1
40	BV	779	0	852	70	0
40	DV	779	0	852	70	0
41	BW	900	0	964	54	0
41	DW	900	0	964	59	0
42	BX	734	0	789	44	0
42	DX	734	0	789	52	0
43	BY	818	0	908	62	0
43	DY	818	0	908	53	0
44	BZ	1473	0	1497	85	0
44	DZ	1473	0	1497	80	0
45	B0	662	0	688	44	0
45	D0	662	0	688	42	0
46	B2	598	0	653	32	0
46	D2	598	0	653	39	0
47	B3	477	0	529	21	0
47	D3	477	0	529	30	0
48	B5	459	0	477	29	0
48	D5	459	0	477	45	0
49	B6	433	0	461	26	0
49	D6	433	0	461	27	0
50	B7	430	0	480	39	0
50	D7	430	0	480	30	0
51	B8	517	0	582	50	0
51	D8	517	0	582	46	0
52	B9	307	0	338	22	0
52	D9	307	0	335	14	0
53	Be	686	0	617	28	0
53	De	686	0	615	15	0
54	Bf	156	0	41	0	0
54	Bg	156	0	38	0	0
54	Df	156	0	42	2	0
54	Dg	156	0	40	1	0
55	Bh	151	0	41	0	0
55	Dh	151	0	40	0	0
56	B1	732	0	808	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	D1	732	0	808	82	0
57	B4	271	0	284	17	0
57	D4	271	0	284	15	0
58	BA	61997	0	31250	2049	1
58	DA	61997	0	31250	2315	0
59	BB	2551	0	1295	94	0
59	DB	2551	0	1295	96	0
60	AY	37	0	47	13	0
60	CY	37	0	47	10	0
61	AY	28	0	12	6	0
61	CY	28	0	12	5	0
All	All	308068	0	213012	13186	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 26.

The worst 5 of 13186 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)
20:CA:1494:G:C5'	58:DA:1913:A:N6	1.79	1.45
32:BN:1:MET:HG2	40:BV:13:ARG:NH1	1.30	1.39
58:BA:2681:C:N4	58:BA:2725:A:H62	1.22	1.35
23:AY:580:MET:CE	58:BA:1913:A:N1	1.91	1.34
32:DN:66:LYS:NZ	58:DA:1140:C:OP2	1.62	1.32

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)
58:BA:1015:G:O2'	39:DU:118:GLY:O[3_545]	2.10	0.10

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	
1	AB	233/235 (99%)	155 (66%)	52 (22%)	26 (11%)	0	6
1	CB	233/235 (99%)	152 (65%)	55 (24%)	26 (11%)	0	6
2	AC	205/207 (99%)	156 (76%)	33 (16%)	16 (8%)	1	12
2	CC	205/207 (99%)	148 (72%)	41 (20%)	16 (8%)	1	12
3	AD	206/208 (99%)	145 (70%)	37 (18%)	24 (12%)	0	5
3	CD	206/208 (99%)	150 (73%)	32 (16%)	24 (12%)	0	5
4	AE	149/151 (99%)	124 (83%)	17 (11%)	8 (5%)	1	18
4	CE	149/151 (99%)	116 (78%)	25 (17%)	8 (5%)	1	18
5	AF	99/101 (98%)	73 (74%)	20 (20%)	6 (6%)	1	15
5	CF	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	1	15
6	AG	153/155 (99%)	122 (80%)	23 (15%)	8 (5%)	1	18
6	CG	153/155 (99%)	116 (76%)	28 (18%)	9 (6%)	1	16
7	AH	136/138 (99%)	93 (68%)	29 (21%)	14 (10%)	0	7
7	CH	136/138 (99%)	101 (74%)	22 (16%)	13 (10%)	0	9
8	AI	125/127 (98%)	93 (74%)	28 (22%)	4 (3%)	3	25
8	CI	125/127 (98%)	97 (78%)	22 (18%)	6 (5%)	2	19
9	AJ	97/99 (98%)	73 (75%)	14 (14%)	10 (10%)	0	7
9	CJ	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	1	15
10	AK	117/119 (98%)	85 (73%)	16 (14%)	16 (14%)	0	3
10	CK	117/119 (98%)	79 (68%)	21 (18%)	17 (14%)	0	3
11	AL	123/125 (98%)	42 (34%)	45 (37%)	36 (29%)	0	0
11	CL	123/125 (98%)	43 (35%)	41 (33%)	39 (32%)	0	0
12	AM	123/125 (98%)	88 (72%)	24 (20%)	11 (9%)	0	10
12	CM	123/125 (98%)	90 (73%)	24 (20%)	9 (7%)	1	13
13	AN	58/60 (97%)	43 (74%)	8 (14%)	7 (12%)	0	4
13	CN	58/60 (97%)	44 (76%)	8 (14%)	6 (10%)	0	7
14	AO	86/88 (98%)	62 (72%)	15 (17%)	9 (10%)	0	7
14	CO	86/88 (98%)	62 (72%)	20 (23%)	4 (5%)	2	19
15	AP	82/84 (98%)	64 (78%)	14 (17%)	4 (5%)	1	19
15	CP	82/84 (98%)	62 (76%)	16 (20%)	4 (5%)	1	19
16	AQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	CQ	98/100 (98%)	68 (69%)	21 (21%)	9 (9%)	0	10
17	AR	68/70 (97%)	52 (76%)	11 (16%)	5 (7%)	1	13
17	CR	68/70 (97%)	47 (69%)	19 (28%)	2 (3%)	3	26
18	AS	77/79 (98%)	41 (53%)	24 (31%)	12 (16%)	0	3
18	CS	77/79 (98%)	50 (65%)	11 (14%)	16 (21%)	0	1
19	AT	97/99 (98%)	81 (84%)	10 (10%)	6 (6%)	1	15
19	CT	97/99 (98%)	76 (78%)	17 (18%)	4 (4%)	2	21
23	AY	663/687 (96%)	436 (66%)	147 (22%)	80 (12%)	0	4
23	CY	663/687 (96%)	454 (68%)	139 (21%)	70 (11%)	0	7
24	BC	226/228 (99%)	106 (47%)	70 (31%)	50 (22%)	0	1
24	DC	226/228 (99%)	114 (50%)	68 (30%)	44 (20%)	0	2
25	BD	273/275 (99%)	177 (65%)	52 (19%)	44 (16%)	0	3
25	DD	273/275 (99%)	171 (63%)	56 (20%)	46 (17%)	0	2
26	BE	203/205 (99%)	127 (63%)	45 (22%)	31 (15%)	0	3
26	DE	203/205 (99%)	128 (63%)	40 (20%)	35 (17%)	0	2
27	BF	206/208 (99%)	132 (64%)	53 (26%)	21 (10%)	0	8
27	DF	206/208 (99%)	131 (64%)	42 (20%)	33 (16%)	0	3
28	BG	179/181 (99%)	126 (70%)	40 (22%)	13 (7%)	1	13
28	DG	179/181 (99%)	131 (73%)	35 (20%)	13 (7%)	1	13
29	BH	165/167 (99%)	113 (68%)	32 (19%)	20 (12%)	0	4
29	DH	165/167 (99%)	102 (62%)	42 (26%)	21 (13%)	0	4
31	BK	138/140 (99%)	98 (71%)	30 (22%)	10 (7%)	1	13
31	DK	138/140 (99%)	100 (72%)	31 (22%)	7 (5%)	1	18
32	BN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	0	5
32	DN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	0	5
33	BO	120/122 (98%)	84 (70%)	20 (17%)	16 (13%)	0	3
33	DO	120/122 (98%)	86 (72%)	24 (20%)	10 (8%)	0	11
34	BP	144/146 (99%)	82 (57%)	36 (25%)	26 (18%)	0	2
34	DP	144/146 (99%)	81 (56%)	35 (24%)	28 (19%)	0	2
35	BQ	139/141 (99%)	94 (68%)	33 (24%)	12 (9%)	0	10
35	DQ	139/141 (99%)	99 (71%)	30 (22%)	10 (7%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BR	115/117 (98%)	80 (70%)	21 (18%)	14 (12%)	0	4
36	DR	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	0	7
37	BS	97/99 (98%)	57 (59%)	18 (19%)	22 (23%)	0	1
37	DS	97/99 (98%)	48 (50%)	26 (27%)	23 (24%)	0	1
38	BT	136/138 (99%)	85 (62%)	22 (16%)	29 (21%)	0	1
38	DT	136/138 (99%)	90 (66%)	22 (16%)	24 (18%)	0	2
39	BU	115/117 (98%)	91 (79%)	18 (16%)	6 (5%)	1	18
39	DU	115/117 (98%)	90 (78%)	21 (18%)	4 (4%)	3	23
40	BV	99/101 (98%)	65 (66%)	16 (16%)	18 (18%)	0	2
40	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	3
41	BW	111/113 (98%)	84 (76%)	17 (15%)	10 (9%)	0	10
41	DW	111/113 (98%)	85 (77%)	14 (13%)	12 (11%)	0	7
42	BX	91/93 (98%)	66 (72%)	19 (21%)	6 (7%)	1	15
42	DX	91/93 (98%)	70 (77%)	15 (16%)	6 (7%)	1	15
43	BY	105/107 (98%)	44 (42%)	38 (36%)	23 (22%)	0	1
43	DY	105/107 (98%)	47 (45%)	28 (27%)	30 (29%)	0	0
44	BZ	183/185 (99%)	129 (70%)	34 (19%)	20 (11%)	0	7
44	DZ	183/185 (99%)	121 (66%)	44 (24%)	18 (10%)	0	9
45	B0	82/84 (98%)	58 (71%)	17 (21%)	7 (8%)	0	11
45	D0	82/84 (98%)	51 (62%)	24 (29%)	7 (8%)	0	11
46	B2	69/71 (97%)	50 (72%)	13 (19%)	6 (9%)	0	10
46	D2	69/71 (97%)	50 (72%)	16 (23%)	3 (4%)	2	20
47	B3	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	1	18
47	D3	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	1	18
48	B5	57/59 (97%)	41 (72%)	12 (21%)	4 (7%)	1	14
48	D5	57/59 (97%)	36 (63%)	18 (32%)	3 (5%)	1	18
49	B6	48/50 (96%)	27 (56%)	13 (27%)	8 (17%)	0	3
49	D6	48/50 (96%)	28 (58%)	11 (23%)	9 (19%)	0	2
50	B7	47/49 (96%)	31 (66%)	14 (30%)	2 (4%)	2	20
50	D7	47/49 (96%)	36 (77%)	6 (13%)	5 (11%)	0	7
51	B8	62/64 (97%)	32 (52%)	22 (36%)	8 (13%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	D8	62/64 (97%)	38 (61%)	14 (23%)	10 (16%)	0	3
52	B9	35/37 (95%)	23 (66%)	7 (20%)	5 (14%)	0	3
52	D9	35/37 (95%)	26 (74%)	8 (23%)	1 (3%)	3	26
53	Be	70/102 (69%)	35 (50%)	28 (40%)	7 (10%)	0	8
53	De	70/102 (69%)	39 (56%)	24 (34%)	7 (10%)	0	8
56	B1	91/93 (98%)	53 (58%)	19 (21%)	19 (21%)	0	1
56	D1	91/93 (98%)	57 (63%)	15 (16%)	19 (21%)	0	1
57	B4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	3
57	D4	33/35 (94%)	15 (46%)	9 (27%)	9 (27%)	0	0
All	All	13256/13564 (98%)	8908 (67%)	2779 (21%)	1569 (12%)	0	5

5 of 1569 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	76	GLN
1	AB	94	ASN
1	AB	95	GLN
1	AB	165	VAL
1	AB	194	PRO

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	
1	AB	203/203 (100%)	159 (78%)	44 (22%)	1	6
1	CB	203/203 (100%)	164 (81%)	39 (19%)	1	10
2	AC	161/161 (100%)	136 (84%)	25 (16%)	2	15
2	CC	161/161 (100%)	134 (83%)	27 (17%)	2	13
3	AD	180/180 (100%)	147 (82%)	33 (18%)	2	12
3	CD	180/180 (100%)	146 (81%)	34 (19%)	1	11
4	AE	116/116 (100%)	96 (83%)	20 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CE	116/116 (100%)	92 (79%)	24 (21%)	1	7
5	AF	90/90 (100%)	83 (92%)	7 (8%)	11	35
5	CF	90/90 (100%)	78 (87%)	12 (13%)	4	18
6	AG	126/126 (100%)	111 (88%)	15 (12%)	5	21
6	CG	126/126 (100%)	115 (91%)	11 (9%)	9	32
7	AH	119/119 (100%)	101 (85%)	18 (15%)	3	16
7	CH	119/119 (100%)	104 (87%)	15 (13%)	4	20
8	AI	98/98 (100%)	85 (87%)	13 (13%)	4	18
8	CI	98/98 (100%)	86 (88%)	12 (12%)	5	21
9	AJ	89/89 (100%)	69 (78%)	20 (22%)	1	6
9	CJ	89/89 (100%)	69 (78%)	20 (22%)	1	6
10	AK	90/90 (100%)	72 (80%)	18 (20%)	1	9
10	CK	90/90 (100%)	68 (76%)	22 (24%)	1	5
11	AL	104/104 (100%)	77 (74%)	27 (26%)	0	4
11	CL	104/104 (100%)	73 (70%)	31 (30%)	0	3
12	AM	100/100 (100%)	79 (79%)	21 (21%)	1	7
12	CM	100/100 (100%)	83 (83%)	17 (17%)	2	13
13	AN	49/49 (100%)	40 (82%)	9 (18%)	1	11
13	CN	49/49 (100%)	42 (86%)	7 (14%)	3	17
14	AO	79/79 (100%)	68 (86%)	11 (14%)	3	17
14	CO	79/79 (100%)	70 (89%)	9 (11%)	5	22
15	AP	72/72 (100%)	63 (88%)	9 (12%)	4	20
15	CP	72/72 (100%)	69 (96%)	3 (4%)	26	49
16	AQ	95/95 (100%)	78 (82%)	17 (18%)	2	12
16	CQ	95/95 (100%)	80 (84%)	15 (16%)	2	15
17	AR	61/61 (100%)	52 (85%)	9 (15%)	3	16
17	CR	61/61 (100%)	49 (80%)	12 (20%)	1	9
18	AS	69/69 (100%)	54 (78%)	15 (22%)	1	6
18	CS	69/69 (100%)	51 (74%)	18 (26%)	0	4
19	AT	76/76 (100%)	65 (86%)	11 (14%)	3	16
19	CT	76/76 (100%)	67 (88%)	9 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	AY	563/579 (97%)	459 (82%)	104 (18%)	1	11
23	CY	563/579 (97%)	448 (80%)	115 (20%)	1	8
24	BC	180/180 (100%)	133 (74%)	47 (26%)	0	4
24	DC	180/180 (100%)	138 (77%)	42 (23%)	1	5
25	BD	217/217 (100%)	174 (80%)	43 (20%)	1	9
25	DD	217/217 (100%)	175 (81%)	42 (19%)	1	10
26	BE	165/165 (100%)	134 (81%)	31 (19%)	1	11
26	DE	165/165 (100%)	131 (79%)	34 (21%)	1	8
27	BF	165/165 (100%)	129 (78%)	36 (22%)	1	6
27	DF	165/165 (100%)	139 (84%)	26 (16%)	2	15
28	BG	155/155 (100%)	127 (82%)	28 (18%)	2	12
28	DG	155/155 (100%)	129 (83%)	26 (17%)	2	13
29	BH	136/136 (100%)	108 (79%)	28 (21%)	1	8
29	DH	136/136 (100%)	113 (83%)	23 (17%)	2	13
31	BK	105/105 (100%)	86 (82%)	19 (18%)	2	12
31	DK	105/105 (100%)	90 (86%)	15 (14%)	3	17
32	BN	117/117 (100%)	101 (86%)	16 (14%)	3	17
32	DN	117/117 (100%)	101 (86%)	16 (14%)	3	17
33	BO	100/100 (100%)	80 (80%)	20 (20%)	1	9
33	DO	100/100 (100%)	82 (82%)	18 (18%)	2	12
34	BP	112/112 (100%)	91 (81%)	21 (19%)	1	11
34	DP	112/112 (100%)	89 (80%)	23 (20%)	1	8
35	BQ	111/111 (100%)	87 (78%)	24 (22%)	1	6
35	DQ	111/111 (100%)	86 (78%)	25 (22%)	1	6
36	BR	100/100 (100%)	83 (83%)	17 (17%)	2	13
36	DR	100/100 (100%)	81 (81%)	19 (19%)	1	10
37	BS	77/77 (100%)	61 (79%)	16 (21%)	1	7
37	DS	77/77 (100%)	61 (79%)	16 (21%)	1	7
38	BT	120/120 (100%)	91 (76%)	29 (24%)	1	5
38	DT	120/120 (100%)	91 (76%)	29 (24%)	1	5
39	BU	93/93 (100%)	73 (78%)	20 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DU	93/93 (100%)	78 (84%)	15 (16%)	2	14
40	BV	82/82 (100%)	64 (78%)	18 (22%)	1	6
40	DV	82/82 (100%)	63 (77%)	19 (23%)	1	5
41	BW	92/92 (100%)	71 (77%)	21 (23%)	1	6
41	DW	92/92 (100%)	77 (84%)	15 (16%)	2	14
42	BX	75/75 (100%)	65 (87%)	10 (13%)	4	18
42	DX	75/75 (100%)	60 (80%)	15 (20%)	1	9
43	BY	88/88 (100%)	63 (72%)	25 (28%)	0	3
43	DY	88/88 (100%)	69 (78%)	19 (22%)	1	6
44	BZ	162/162 (100%)	126 (78%)	36 (22%)	1	6
44	DZ	162/162 (100%)	134 (83%)	28 (17%)	2	13
45	B0	66/66 (100%)	51 (77%)	15 (23%)	1	6
45	D0	66/66 (100%)	54 (82%)	12 (18%)	2	12
46	B2	66/66 (100%)	58 (88%)	8 (12%)	5	21
46	D2	66/66 (100%)	59 (89%)	7 (11%)	6	24
47	B3	52/52 (100%)	44 (85%)	8 (15%)	2	15
47	D3	52/52 (100%)	46 (88%)	6 (12%)	5	22
48	B5	51/51 (100%)	40 (78%)	11 (22%)	1	6
48	D5	51/51 (100%)	42 (82%)	9 (18%)	2	12
49	B6	49/49 (100%)	42 (86%)	7 (14%)	3	17
49	D6	49/49 (100%)	40 (82%)	9 (18%)	1	11
50	B7	42/42 (100%)	35 (83%)	7 (17%)	2	13
50	D7	42/42 (100%)	35 (83%)	7 (17%)	2	13
51	B8	54/54 (100%)	40 (74%)	14 (26%)	0	4
51	D8	54/54 (100%)	39 (72%)	15 (28%)	0	3
52	B9	34/34 (100%)	31 (91%)	3 (9%)	9	32
52	D9	34/34 (100%)	32 (94%)	2 (6%)	18	42
53	Be	54/54 (100%)	46 (85%)	8 (15%)	3	16
53	De	54/54 (100%)	44 (82%)	10 (18%)	1	11
56	B1	78/78 (100%)	62 (80%)	16 (20%)	1	8
56	D1	78/78 (100%)	62 (80%)	16 (20%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	B4	31/31 (100%)	24 (77%)	7 (23%)	1	6
57	D4	31/31 (100%)	26 (84%)	5 (16%)	2	14
All	All	11138/11170 (100%)	9068 (81%)	2070 (19%)	1	11

5 of 2070 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	DT	83	ILE
41	DW	106	ILE
38	DT	80	SER
37	BS	13	ARG
35	BQ	129	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 147 such sidechains are listed below:

Mol	Chain	Res	Type
31	DK	29	GLN
49	D6	49	HIS
32	DN	69	GLN
39	DU	75	ASN
32	BN	133	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	AA	1510/1511 (99%)	291 (19%)	17 (1%)
20	CA	1510/1511 (99%)	294 (19%)	16 (1%)
21	AW	76/77 (98%)	21 (27%)	2 (2%)
21	CW	76/77 (98%)	24 (31%)	2 (2%)
22	AV	22/23 (95%)	11 (50%)	1 (4%)
22	CV	22/23 (95%)	8 (36%)	2 (9%)
58	BA	2878/2879 (99%)	666 (23%)	22 (0%)
58	DA	2878/2879 (99%)	658 (22%)	23 (0%)
59	BB	118/119 (99%)	17 (14%)	2 (1%)
59	DB	118/119 (99%)	14 (11%)	1 (0%)
All	All	9208/9218 (99%)	2004 (21%)	88 (0%)

5 of 2004 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	AA	9	G
20	AA	13	U
20	AA	32	A
20	AA	39	G
20	AA	47	C

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	CA	1532	U
58	DA	971	C
20	CA	1537	U
58	DA	271(C)	G
58	DA	1558	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	GDP	AY	702	-	29,30,30	1.05	1 (3%)	45,47,47	1.71	9 (20%)
60	FUA	AY	701	-	39,40,40	1.67	7 (17%)	50,64,64	2.20	13 (26%)
61	GDP	CY	702	-	29,30,30	1.05	1 (3%)	45,47,47	1.71	9 (20%)
60	FUA	CY	701	-	39,40,40	1.70	6 (15%)	50,64,64	2.30	13 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	GDP	AY	702	-	-	2/16/32/32	0/3/3/3
60	FUA	AY	701	-	-	9/16/92/92	0/4/4/4
61	GDP	CY	702	-	-	2/16/32/32	0/3/3/3
60	FUA	CY	701	-	-	10/16/92/92	0/4/4/4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	CY	701	FUA	C23-C22	-4.46	1.39	1.51
60	CY	701	FUA	C23-C24	-4.45	1.39	1.53
60	AY	701	FUA	C23-C24	-4.39	1.39	1.53
60	AY	701	FUA	C23-C22	-4.36	1.40	1.51
60	CY	701	FUA	C29-C22	4.29	1.53	1.47

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CY	701	FUA	C13-C12-C11	-7.49	101.03	111.90
60	AY	701	FUA	C13-C12-C11	-7.45	101.09	111.90
60	AY	701	FUA	C24-C23-C22	6.26	126.06	112.72
60	CY	701	FUA	C24-C23-C22	5.75	124.96	112.72
61	AY	702	GDP	C2-N3-C4	5.33	121.47	112.30

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

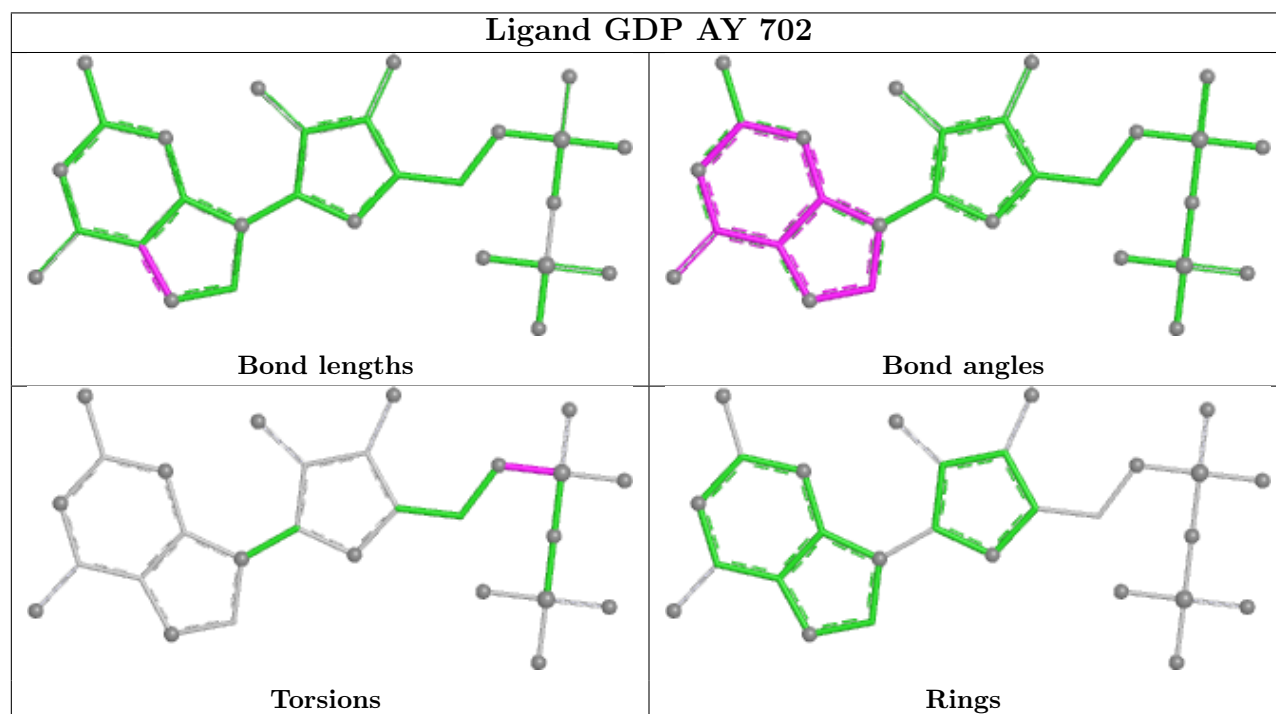
Mol	Chain	Res	Type	Atoms
60	AY	701	FUA	C13-C17-C22-C23
60	AY	701	FUA	C13-C17-C22-C29
60	AY	701	FUA	C29-C22-C23-C24
60	CY	701	FUA	C13-C17-C22-C23
60	CY	701	FUA	C13-C17-C22-C29

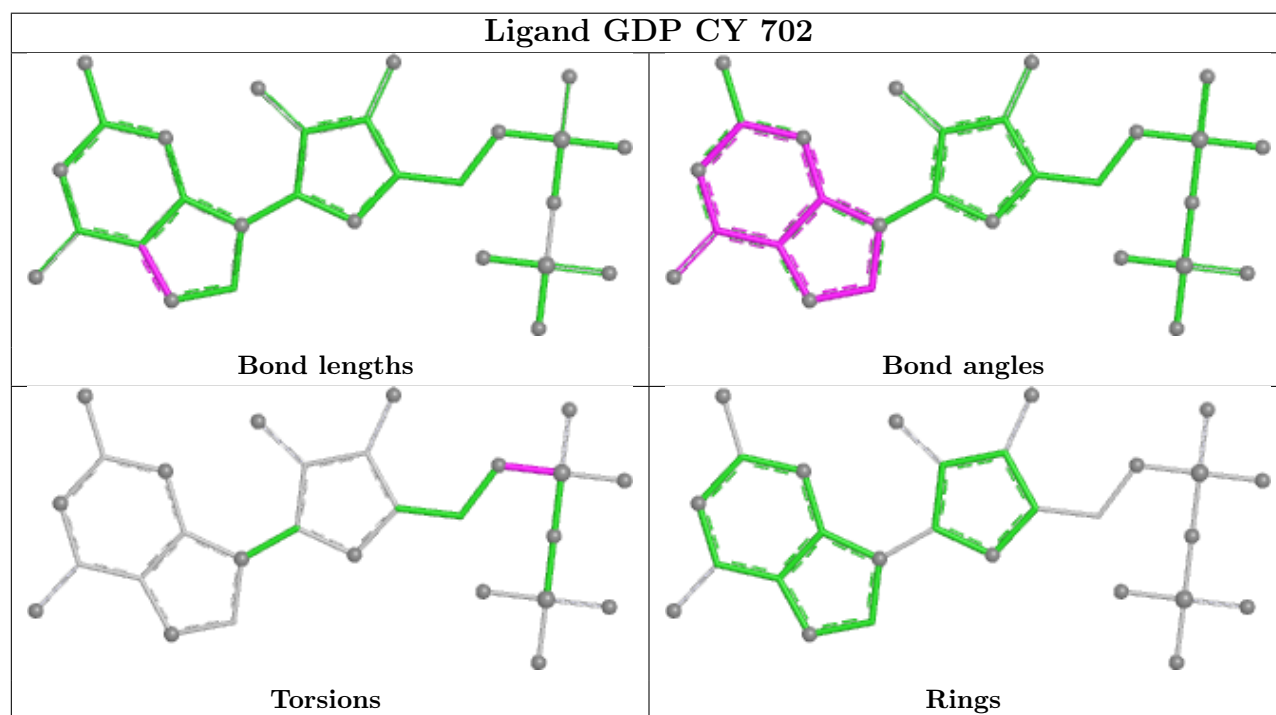
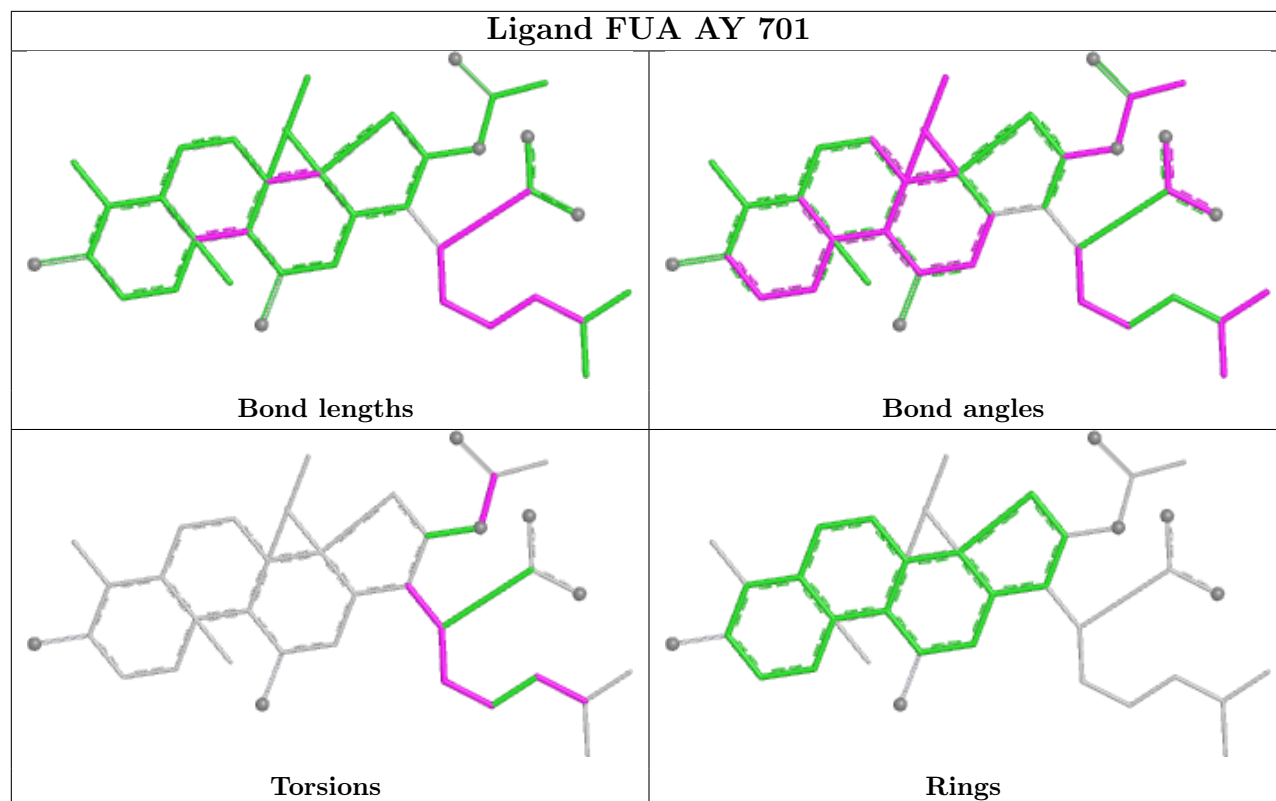
There are no ring outliers.

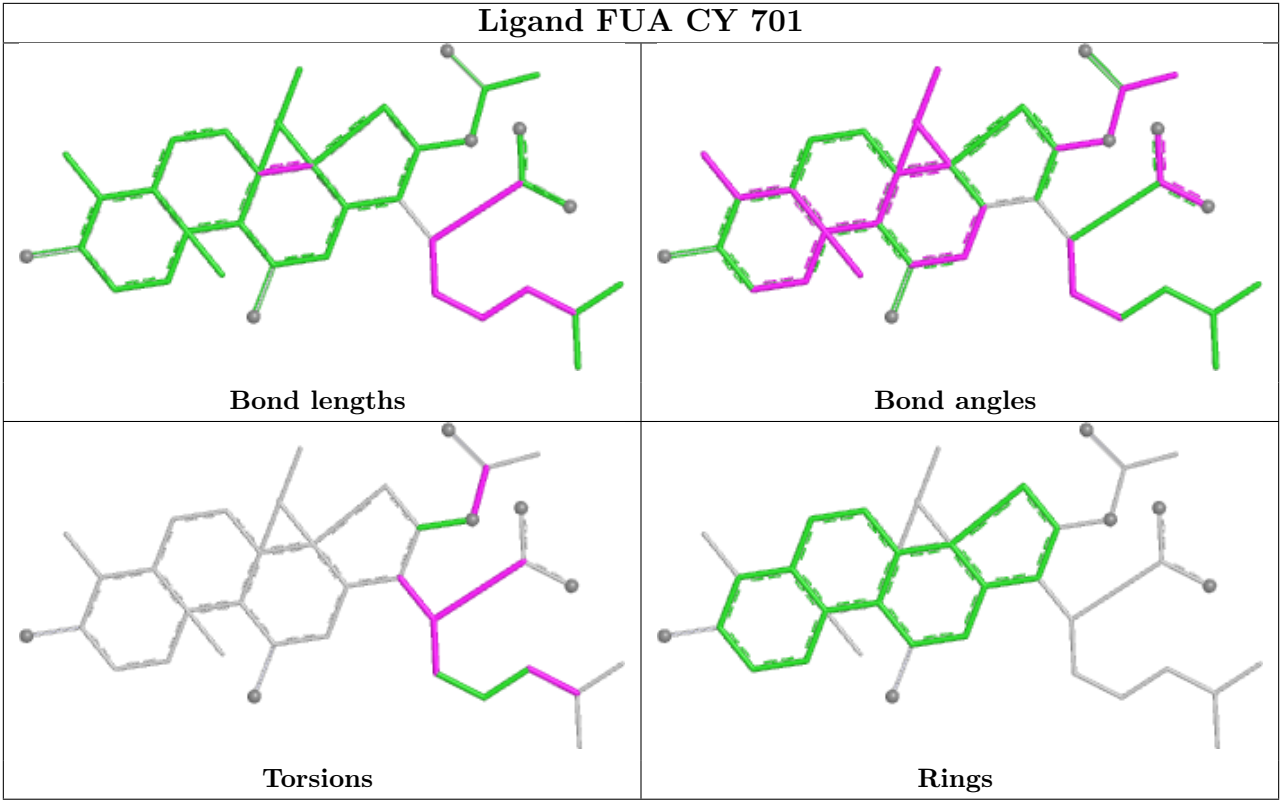
4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AY	702	GDP	6	0
60	AY	701	FUA	13	0
61	CY	702	GDP	5	0
60	CY	701	FUA	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
53	De	1
53	Be	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	De	30:UNK	C	51:ALA	N	37.61
1	Be	30:UNK	C	51:ALA	N	36.82

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	AB	235/235 (100%)	-1.10	0	100	100	41, 81, 119, 159	0
1	CB	235/235 (100%)	-0.99	0	100	100	38, 80, 117, 178	0
2	AC	207/207 (100%)	-0.61	5 (2%)	59	44	34, 76, 116, 152	0
2	CC	207/207 (100%)	-0.59	5 (2%)	59	44	44, 78, 121, 158	0
3	AD	208/208 (100%)	-0.45	4 (1%)	66	49	37, 71, 125, 178	0
3	CD	208/208 (100%)	-0.37	5 (2%)	59	44	51, 83, 120, 165	0
4	AE	151/151 (100%)	-0.31	4 (2%)	57	42	30, 57, 93, 133	0
4	CE	151/151 (100%)	-0.20	4 (2%)	57	42	31, 61, 99, 185	0
5	AF	101/101 (100%)	-1.05	0	100	100	31, 52, 87, 115	0
5	CF	101/101 (100%)	-1.06	1 (0%)	79	61	25, 52, 78, 129	0
6	AG	155/155 (100%)	-0.81	1 (0%)	85	71	54, 100, 147, 204	0
6	CG	155/155 (100%)	-0.78	0	100	100	57, 99, 155, 218	0
7	AH	138/138 (100%)	-1.16	0	100	100	28, 49, 83, 117	0
7	CH	138/138 (100%)	-0.98	0	100	100	29, 57, 101, 142	0
8	AI	127/127 (100%)	-0.85	0	100	100	48, 87, 128, 163	0
8	CI	127/127 (100%)	-0.56	3 (2%)	59	44	51, 91, 136, 195	0
9	AJ	99/99 (100%)	-0.51	2 (2%)	65	48	46, 74, 108, 114	0
9	CJ	99/99 (100%)	-0.49	7 (7%)	22	21	37, 82, 121, 145	0
10	AK	119/119 (100%)	-0.83	2 (1%)	69	51	41, 71, 114, 157	0
10	CK	119/119 (100%)	-0.81	2 (1%)	69	51	22, 59, 106, 135	0
11	AL	125/125 (100%)	-0.43	5 (4%)	42	33	31, 63, 97, 178	0
11	CL	125/125 (100%)	-0.39	10 (8%)	18	19	29, 68, 109, 136	0
12	AM	125/125 (100%)	-0.50	3 (2%)	59	44	61, 101, 139, 150	0
12	CM	125/125 (100%)	-0.59	2 (1%)	70	52	52, 106, 160, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	-0.73	1 (1%) 69 51	42, 64, 97, 106	0
13	CN	60/60 (100%)	-0.94	0 100 100	47, 67, 112, 156	0
14	AO	88/88 (100%)	-0.93	1 (1%) 78 60	32, 61, 102, 172	0
14	CO	88/88 (100%)	-0.83	2 (2%) 61 45	29, 61, 108, 215	0
15	AP	84/84 (100%)	-0.61	1 (1%) 76 59	47, 80, 118, 187	0
15	CP	84/84 (100%)	-0.60	1 (1%) 76 59	53, 81, 118, 174	0
16	AQ	100/100 (100%)	-0.38	2 (2%) 65 48	33, 56, 100, 124	0
16	CQ	100/100 (100%)	-0.42	2 (2%) 65 48	30, 58, 89, 139	0
17	AR	70/70 (100%)	-1.05	0 100 100	30, 55, 101, 156	0
17	CR	70/70 (100%)	-0.93	0 100 100	32, 46, 123, 186	0
18	AS	79/79 (100%)	-0.71	0 100 100	68, 90, 148, 159	0
18	CS	79/79 (100%)	-0.68	0 100 100	59, 92, 146, 215	0
19	AT	99/99 (100%)	-0.75	0 100 100	58, 86, 116, 146	0
19	CT	99/99 (100%)	-0.58	1 (1%) 79 61	42, 81, 114, 147	0
20	AA	1511/1511 (100%)	-0.77	10 (0%) 84 68	25, 78, 180, 324	0
20	CA	1511/1511 (100%)	-0.79	7 (0%) 87 73	19, 82, 182, 332	0
21	AW	77/77 (100%)	-0.88	0 100 100	55, 121, 189, 218	0
21	CW	77/77 (100%)	-1.04	0 100 100	58, 118, 230, 278	0
22	AV	23/23 (100%)	-0.62	0 100 100	70, 138, 188, 222	0
22	CV	23/23 (100%)	-0.14	1 (4%) 40 31	88, 142, 211, 231	0
23	AY	667/687 (97%)	-0.54	10 (1%) 72 54	29, 79, 132, 191	0
23	CY	667/687 (97%)	-0.59	16 (2%) 59 44	32, 84, 131, 188	0
24	BC	228/228 (100%)	-0.71	3 (1%) 75 57	91, 147, 211, 238	0
24	DC	228/228 (100%)	-0.85	4 (1%) 67 50	89, 175, 227, 263	0
25	BD	275/275 (100%)	-0.65	3 (1%) 78 60	24, 52, 90, 160	0
25	DD	275/275 (100%)	-0.76	2 (0%) 84 68	23, 50, 94, 155	0
26	BE	205/205 (100%)	-0.92	0 100 100	25, 52, 97, 202	0
26	DE	205/205 (100%)	-0.85	0 100 100	28, 60, 135, 173	0
27	BF	208/208 (100%)	-0.58	9 (4%) 40 31	32, 67, 126, 195	0
27	DF	208/208 (100%)	-0.26	13 (6%) 26 23	34, 86, 165, 230	0
28	BG	181/181 (100%)	-0.62	3 (1%) 69 51	52, 103, 150, 206	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	181/181 (100%)	-0.87	0 100 100	73, 110, 158, 205	0
29	BH	167/167 (100%)	-0.95	0 100 100	38, 64, 111, 161	0
29	DH	167/167 (100%)	-0.91	0 100 100	40, 74, 130, 167	0
30	BJ	0/170	-	-	-	-
30	DJ	0/170	-	-	-	-
31	BK	140/140 (100%)	-0.57	2 (1%) 73 55	67, 118, 175, 206	0
31	DK	140/140 (100%)	-0.80	2 (1%) 73 55	66, 132, 200, 220	0
32	BN	138/138 (100%)	-0.56	3 (2%) 62 46	58, 85, 106, 118	0
32	DN	138/138 (100%)	-0.57	1 (0%) 84 68	63, 87, 111, 121	0
33	BO	122/122 (100%)	-0.82	0 100 100	24, 49, 67, 114	0
33	DO	122/122 (100%)	-0.72	0 100 100	30, 56, 88, 124	0
34	BP	146/146 (100%)	-0.23	6 (4%) 41 32	28, 73, 113, 171	0
34	DP	146/146 (100%)	-0.26	5 (3%) 48 35	31, 84, 130, 202	0
35	BQ	141/141 (100%)	-0.62	2 (1%) 73 55	40, 66, 100, 164	0
35	DQ	141/141 (100%)	-0.50	2 (1%) 73 55	36, 64, 104, 161	0
36	BR	117/117 (100%)	-0.91	0 100 100	29, 53, 85, 105	0
36	DR	117/117 (100%)	-0.94	0 100 100	21, 53, 88, 156	0
37	BS	99/99 (100%)	-0.68	0 100 100	60, 111, 172, 189	0
37	DS	99/99 (100%)	-0.71	0 100 100	38, 128, 194, 220	0
38	BT	138/138 (100%)	-0.71	0 100 100	36, 64, 106, 201	0
38	DT	138/138 (100%)	-0.66	0 100 100	32, 71, 115, 216	0
39	BU	117/117 (100%)	-0.83	1 (0%) 81 64	26, 44, 83, 132	0
39	DU	117/117 (100%)	-0.63	1 (0%) 81 64	6, 45, 90, 155	0
40	BV	101/101 (100%)	-0.59	0 100 100	31, 51, 79, 104	0
40	DV	101/101 (100%)	-0.70	1 (0%) 79 61	38, 70, 111, 124	0
41	BW	113/113 (100%)	-0.78	4 (3%) 47 35	22, 51, 104, 120	0
41	DW	113/113 (100%)	-0.71	1 (0%) 81 64	30, 49, 105, 202	0
42	BX	93/93 (100%)	-0.68	0 100 100	31, 59, 93, 113	0
42	DX	93/93 (100%)	-0.86	0 100 100	29, 63, 111, 175	0
43	BY	107/107 (100%)	-0.68	3 (2%) 55 40	35, 71, 133, 156	0
43	DY	107/107 (100%)	-0.72	5 (4%) 36 29	55, 87, 133, 209	0
44	BZ	185/185 (100%)	-0.84	1 (0%) 87 73	42, 78, 126, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DZ	185/185 (100%)	-0.78	0 100 100	36, 75, 123, 161	0
45	B0	84/84 (100%)	-0.46	1 (1%) 76 59	38, 70, 99, 162	0
45	D0	84/84 (100%)	-0.33	5 (5%) 27 24	33, 67, 139, 212	0
46	B2	71/71 (100%)	-0.88	0 100 100	44, 71, 114, 167	0
46	D2	71/71 (100%)	-0.82	0 100 100	53, 76, 129, 183	0
47	B3	60/60 (100%)	-0.85	0 100 100	26, 43, 74, 113	0
47	D3	60/60 (100%)	-0.76	0 100 100	27, 57, 99, 111	0
48	B5	59/59 (100%)	-0.74	0 100 100	22, 56, 142, 156	0
48	D5	59/59 (100%)	-0.53	0 100 100	18, 67, 175, 198	0
49	B6	50/50 (100%)	-0.73	0 100 100	65, 91, 124, 176	0
49	D6	50/50 (100%)	-0.54	0 100 100	66, 106, 136, 139	0
50	B7	49/49 (100%)	-0.85	0 100 100	30, 48, 107, 132	0
50	D7	49/49 (100%)	-0.87	0 100 100	38, 51, 125, 168	0
51	B8	64/64 (100%)	-0.67	0 100 100	30, 62, 80, 89	0
51	D8	64/64 (100%)	-0.55	0 100 100	38, 70, 114, 148	0
52	B9	37/37 (100%)	-0.11	0 100 100	41, 63, 116, 166	0
52	D9	37/37 (100%)	-0.57	0 100 100	36, 55, 111, 148	0
53	Be	72/102 (70%)	-0.71	2 (2%) 55 40	69, 117, 170, 201	0
53	De	72/102 (70%)	-1.08	0 100 100	82, 121, 212, 249	0
54	Bf	0/31	-	-	-	-
54	Bg	0/31	-	-	-	-
54	Df	0/31	-	-	-	-
54	Dg	0/31	-	-	-	-
55	Bh	0/30	-	-	-	-
55	Dh	0/30	-	-	-	-
56	B1	93/93 (100%)	-0.18	7 (7%) 20 20	40, 87, 151, 208	0
56	D1	93/93 (100%)	-0.24	3 (3%) 50 37	42, 84, 174, 216	0
57	B4	35/35 (100%)	-1.10	0 100 100	96, 160, 227, 248	0
57	D4	35/35 (100%)	-0.93	0 100 100	116, 170, 265, 282	0
58	BA	2879/2879 (100%)	-0.90	3 (0%) 92 87	17, 60, 166, 304	0
58	DA	2879/2879 (100%)	-0.92	1 (0%) 100 100	17, 62, 182, 341	0
59	BB	119/119 (100%)	-1.05	0 100 100	32, 114, 187, 214	0
59	DB	119/119 (100%)	-0.98	0 100 100	53, 104, 162, 246	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	22682/23306 (97%)	-0.75	219 (0%) 79 61	6, 73, 161, 341	0

The worst 5 of 219 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	DP	5	ASP	8.2
28	BG	26	GLN	6.1
45	D0	3	HIS	6.0
24	DC	203	GLU	5.9
56	D1	28	GLY	5.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

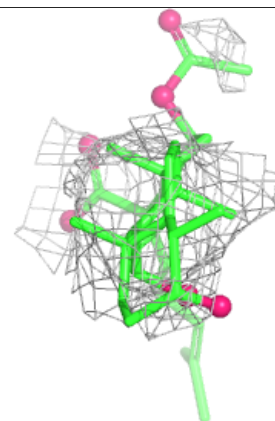
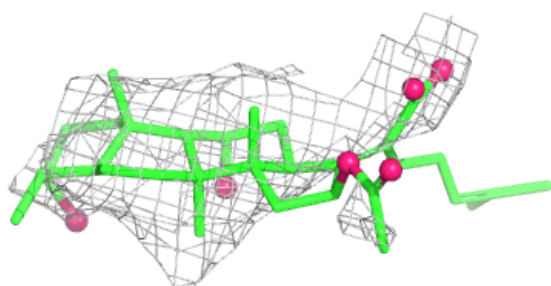
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	FUA	AY	701	37/37	0.96	0.12	119,146,161,162	0
60	FUA	CY	701	37/37	0.98	0.07	125,150,161,166	0
61	GDP	AY	702	28/28	0.99	0.04	58,89,106,121	0
61	GDP	CY	702	28/28	0.99	0.03	58,90,102,118	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

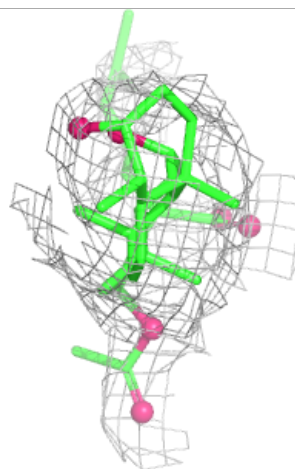
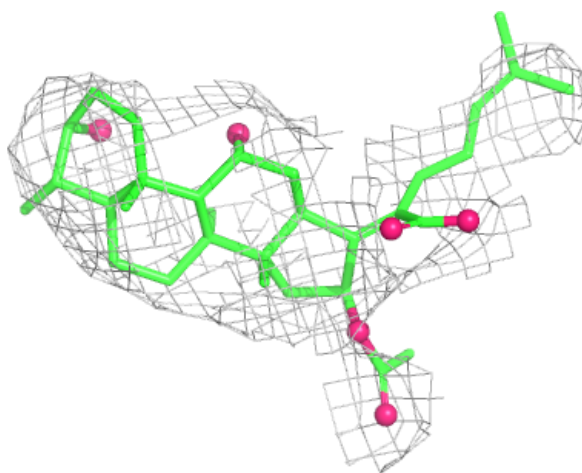
Electron density around FUA AY 701:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



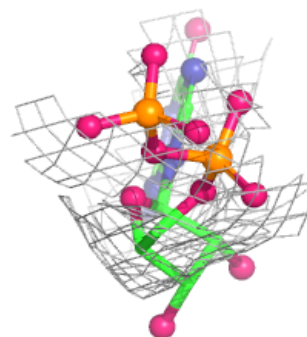
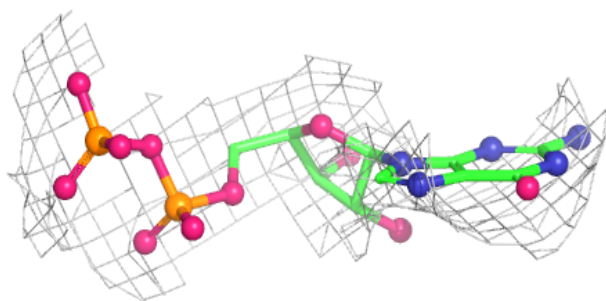
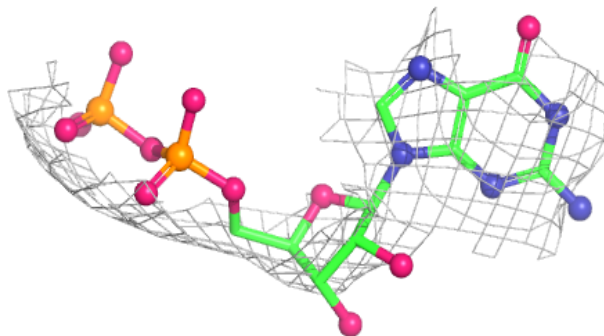
Electron density around FUA CY 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

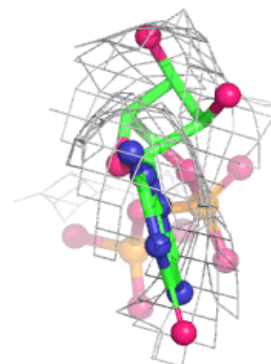
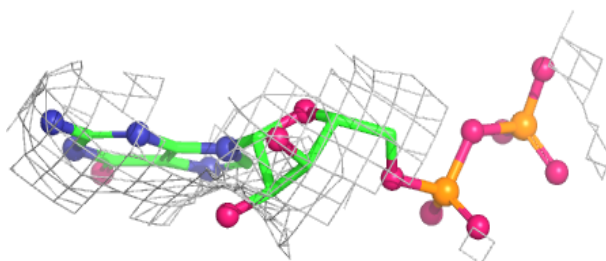
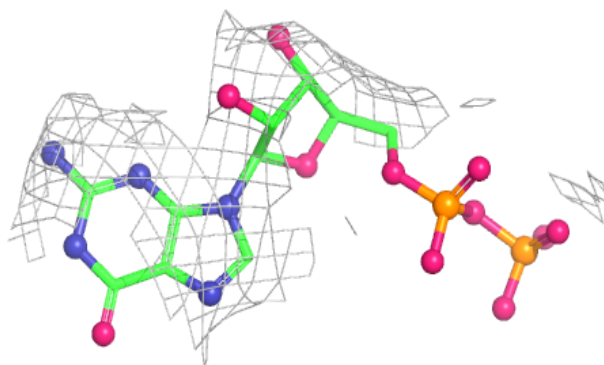


Electron density around GDP AY 702:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GDP CY 702:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.