



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2023 – 11:52 AM EDT

PDB ID : 4V9M
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

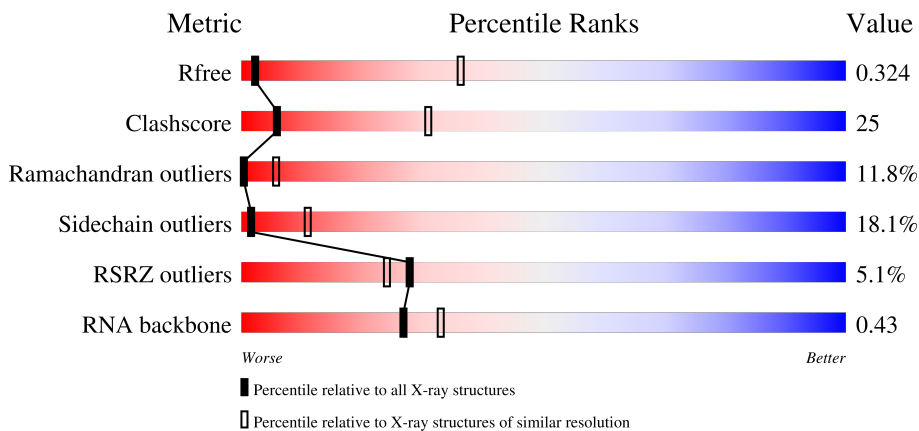
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



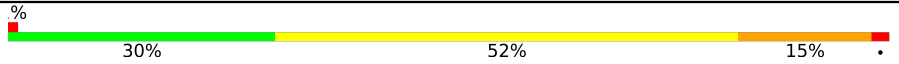

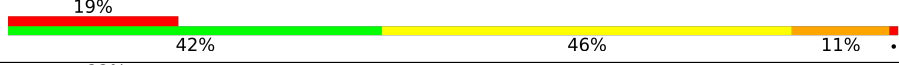
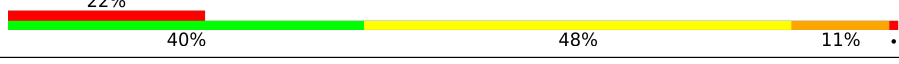

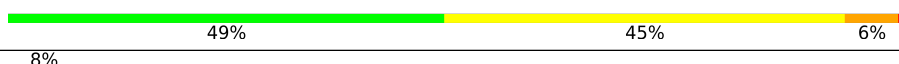
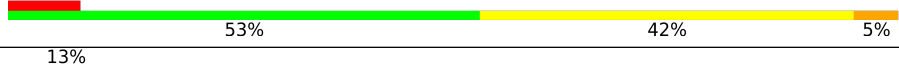
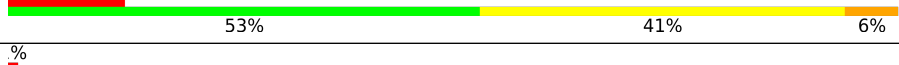
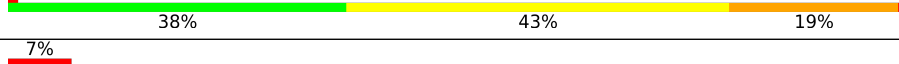
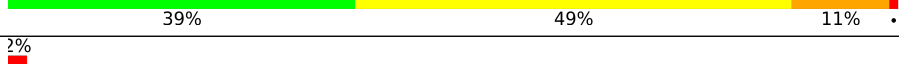

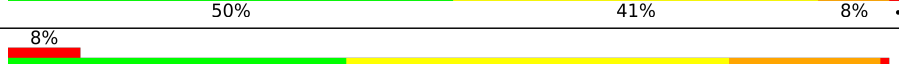
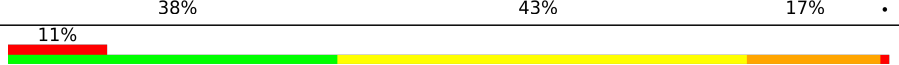
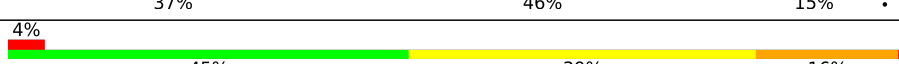
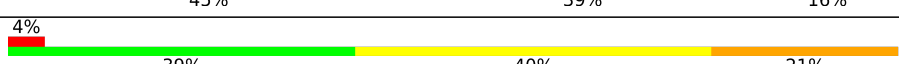
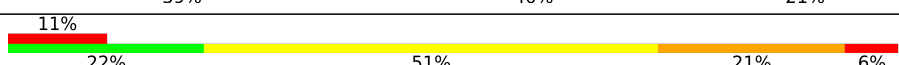
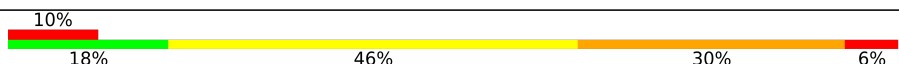
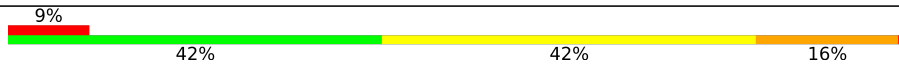
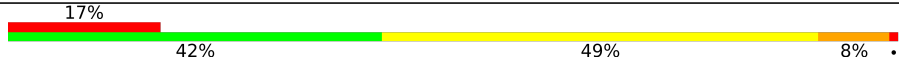


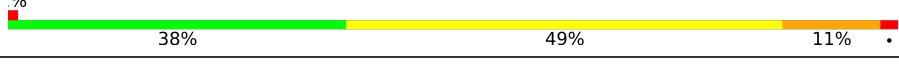

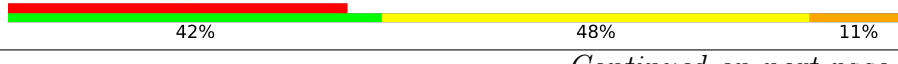

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)
RNA backbone	3102	1048 (5.00-3.00)

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	
1	CB	235	
2	AC	207	
2	CC	207	

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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	

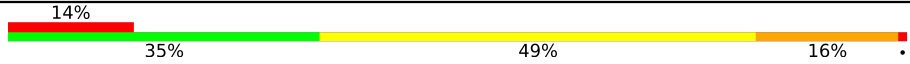

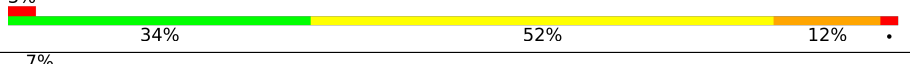
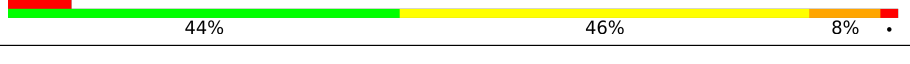


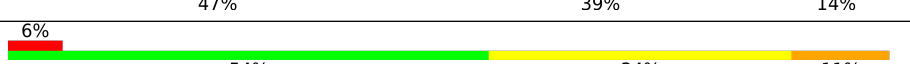
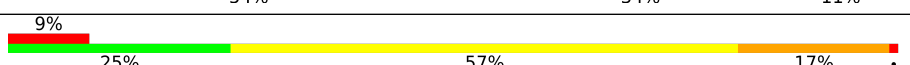
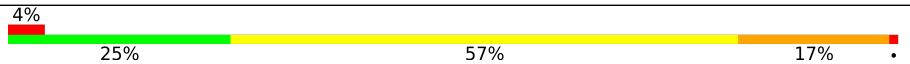

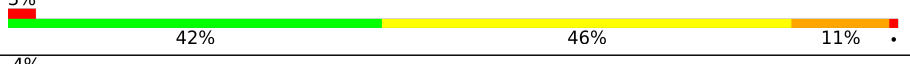
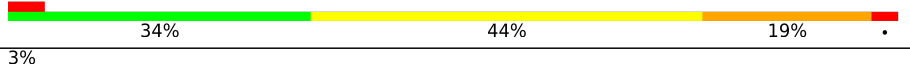
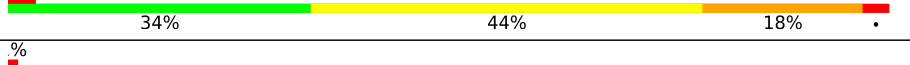

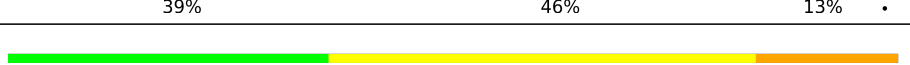
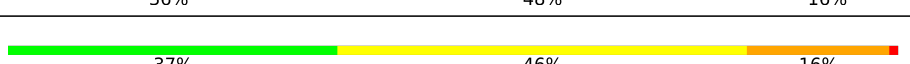
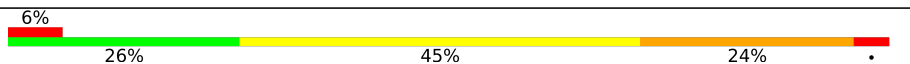
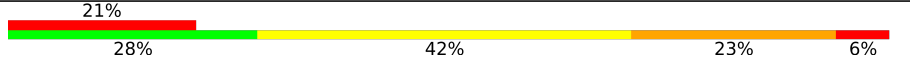
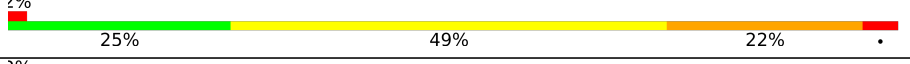
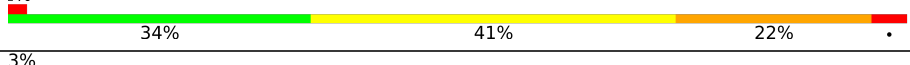


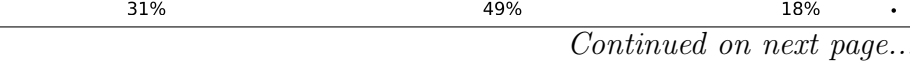


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Mol	Chain	Length	Quality of chain
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AA	1511	
20	CA	1511	
21	AW	77	
21	CW	77	
22	AV	23	
22	CV	23	
23	AY	687	
23	CY	687	
24	BC	228	
24	DC	228	
25	BD	275	
25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

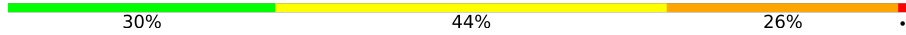


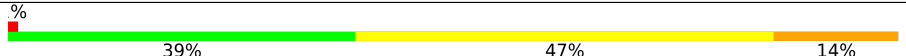
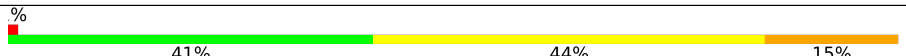
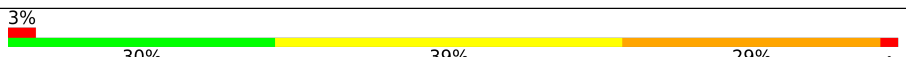
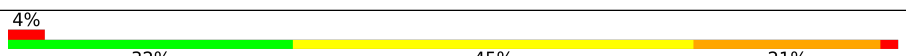
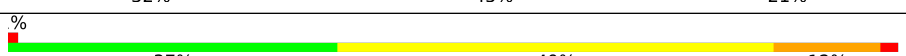
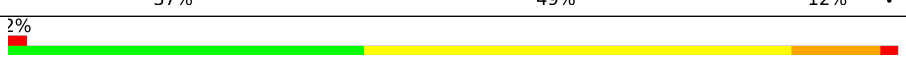
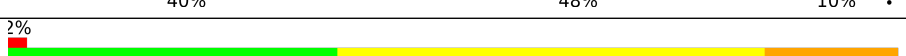
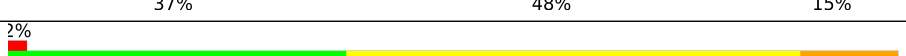
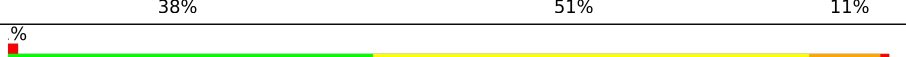

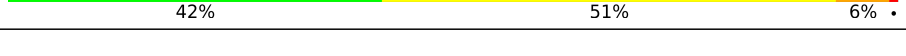

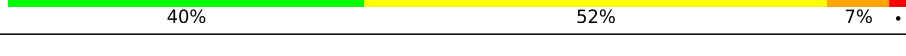


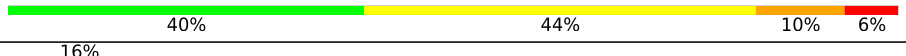
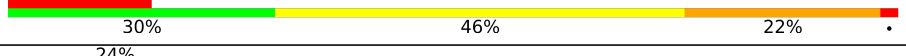
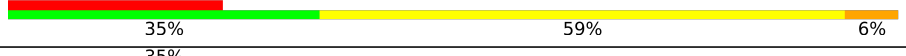

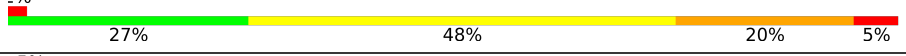
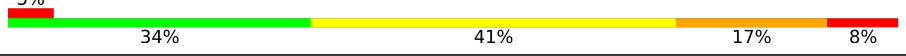

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Mol	Chain	Length	Quality of chain
28	BG	181	
28	DG	181	
29	BH	167	
29	DH	167	
30	BJ	170	
30	DJ	170	
31	BK	140	
31	DK	140	
32	BN	138	
32	DN	138	
33	BO	122	
33	DO	122	
34	BP	146	
34	DP	146	
35	BQ	141	
35	DQ	141	
36	BR	117	
36	DR	117	
37	BS	99	
37	DS	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	 30% 44% 26%
41	BW	113	 7% 34% 57% 9%
41	DW	113	 6% 36% 50% 12%
42	BX	93	 % 39% 47% 14%
42	DX	93	 % 41% 44% 15%
43	BY	107	 3% 30% 39% 29%
43	DY	107	 4% 32% 45% 21%
44	BZ	185	 % 37% 49% 12%
44	DZ	185	 2% 40% 48% 10%
45	B0	84	 2% 37% 48% 15%
45	D0	84	 2% 38% 51% 11%
46	B2	71	 % 41% 49% 8%
46	D2	71	 42% 51% 6%
47	B3	60	 52% 37% 10%
47	D3	60	 2% 40% 52% 7%
48	B5	59	 49% 39% 10%
48	D5	59	 2% 37% 47% 12%
49	B6	50	 40% 44% 10% 6%
49	D6	50	 16% 30% 46% 22%
50	B7	49	 24% 35% 59% 6%
50	D7	49	 35% 47% 43% 8%
51	B8	64	 2% 27% 48% 20% 5%
51	D8	64	 5% 34% 41% 17% 8%
52	B9	37	 38% 32% 51% 11% 5%
52	D9	37	 3% 51% 46%

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Mol	Chain	Length	Quality of chain
53	Be	102	 23% 85% 15%
53	De	102	 16% 87% 11%
54	Bf	31	 100%
54	Bg	31	 100%
54	Df	31	 100%
54	Dg	31	 100%
55	Bh	30	 100%
55	Dh	30	 100%
56	B1	93	 28% 30% 45% 24%
56	D1	93	 28% 20% 52% 23% 5%
57	B4	35	 20% 40% 46% 14%
57	D4	35	 46% 34% 49% 17%
58	BA	2879	 28% 55% 16%
58	DA	2879	 27% 56% 16%
59	BB	119	 32% 54% 14%
59	DB	119	 7% 26% 61% 13%

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	AB	235	1910	1218	342	345	5	0	0	0
1	CB	235	1910	1218	342	345	5	0	0	0

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
28	BG	181	1474	942	268	260	4	0	0	0
28	DG	181	1474	942	268	260	4	0	0	0

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
			Total	C	N	O	S			
29	BH	167	1274	806	238	229	1	0	0	0
29	DH	167	1274	806	238	229	1	0	0	0

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S			
34	BP	146	Total 1114	C 692	N 227	O 193	S 2	0	0	0
34	DP	146	Total 1114	C 692	N 227	O 193	S 2	0	0	0

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

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

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

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
			Total	C	N	O			
36	BR	117	960	599	202	159	0	0	0
36	DR	117	960	599	202	159	0	0	0

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

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

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

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

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
			Total	C	N	O			
54	Bf	31	156	93	31	32	0	0	0
54	Bg	31	156	93	31	32	0	0	0
54	Df	31	156	93	31	32	0	0	0
54	Dg	31	156	93	31	32	0	0	0

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

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

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

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

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
			Total	C	N	O	S			
57	B4	35	271	174	44	50	3	0	0	0
57	D4	35	271	174	44	50	3	0	0	0

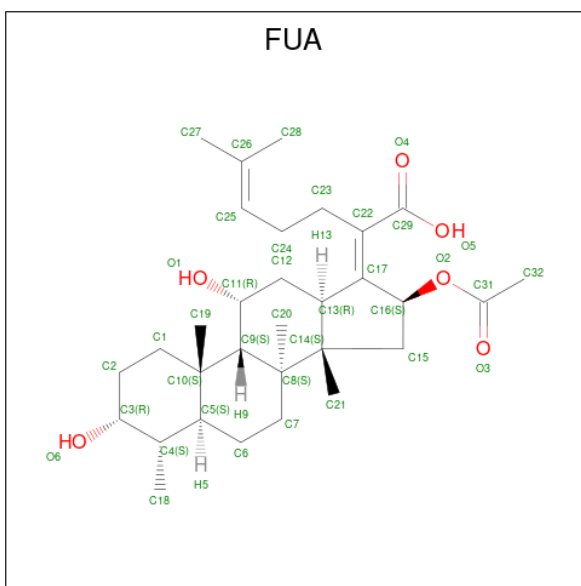
- Molecule 58 is a RNA chain called 23S ribosomal RNA.

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

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

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

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



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

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

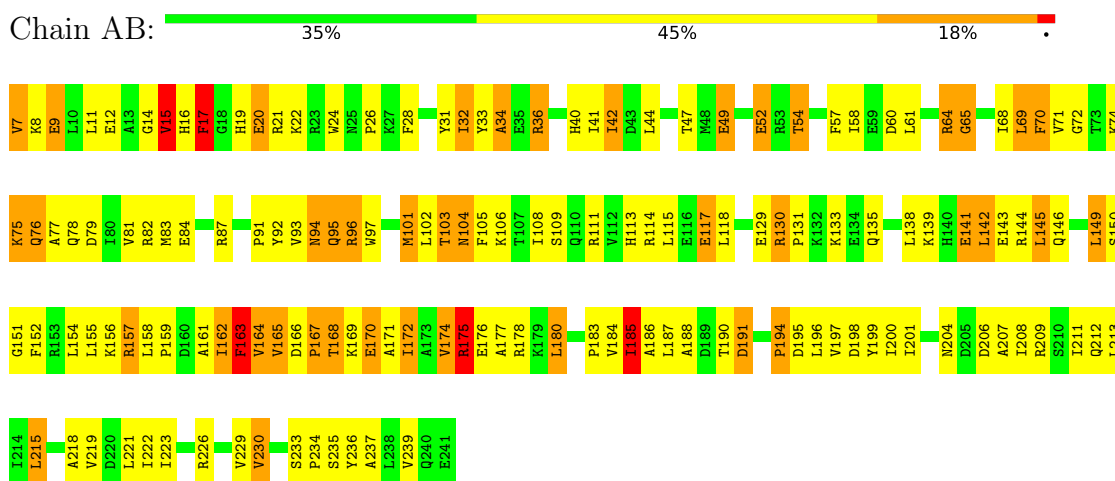


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
61	AY	1	28	10	5	11	2	0	0
61	CY	1	28	10	5	11	2	0	0

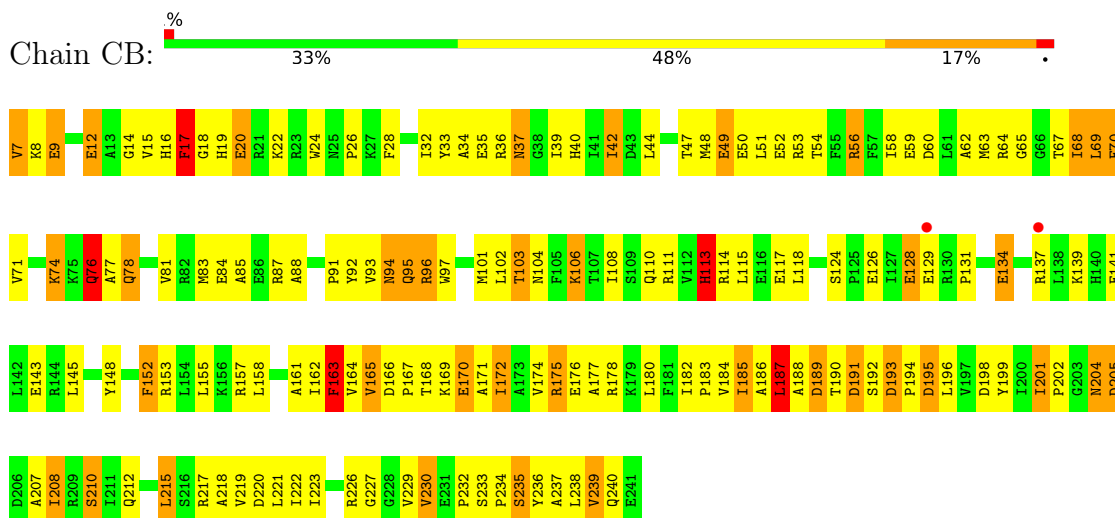
3 Residue-property plots

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.

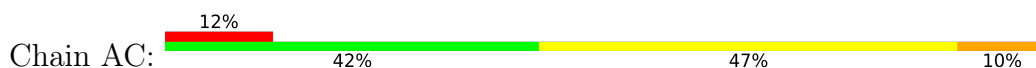
- Molecule 1: 30S ribosomal protein S2

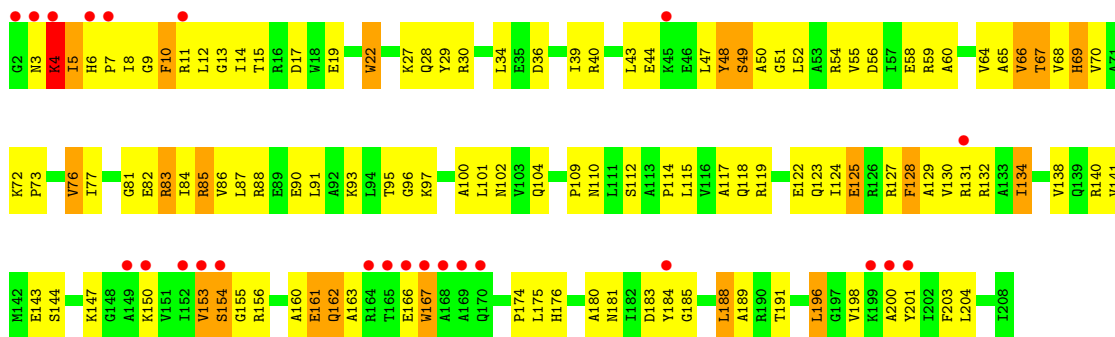


- Molecule 1: 30S ribosomal protein S2

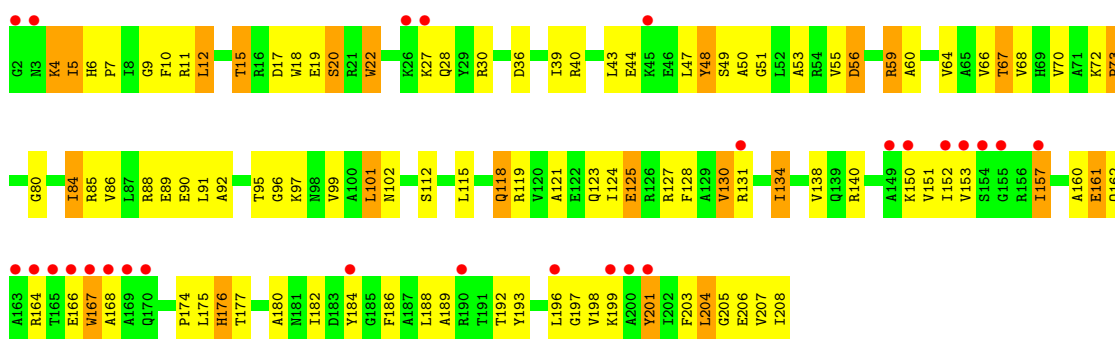


- Molecule 2: 30S ribosomal protein S3

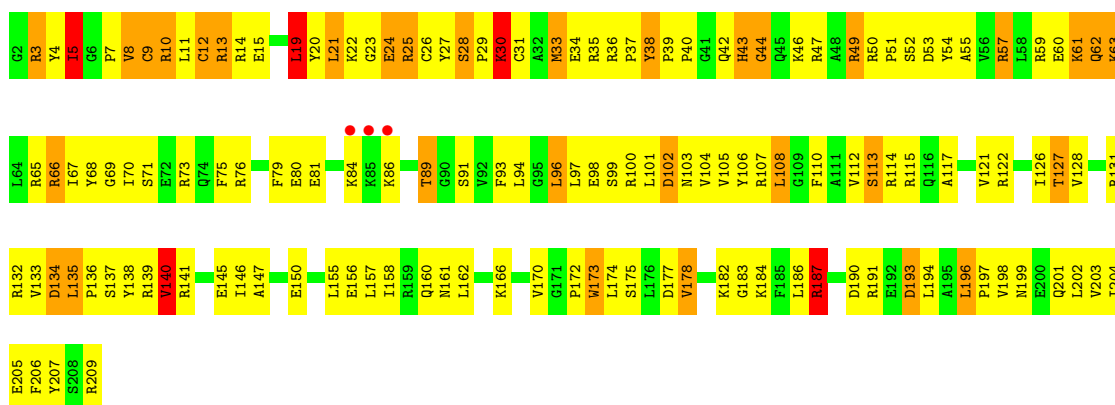




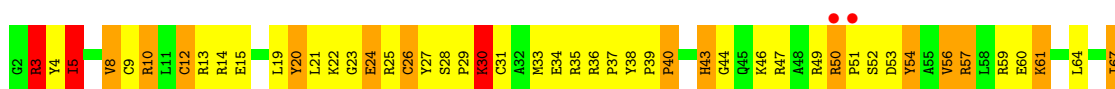
• Molecule 2: 30S ribosomal protein S3

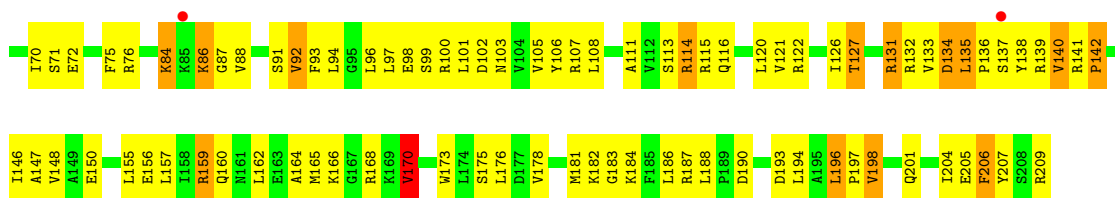


• Molecule 3: 30S ribosomal protein S4

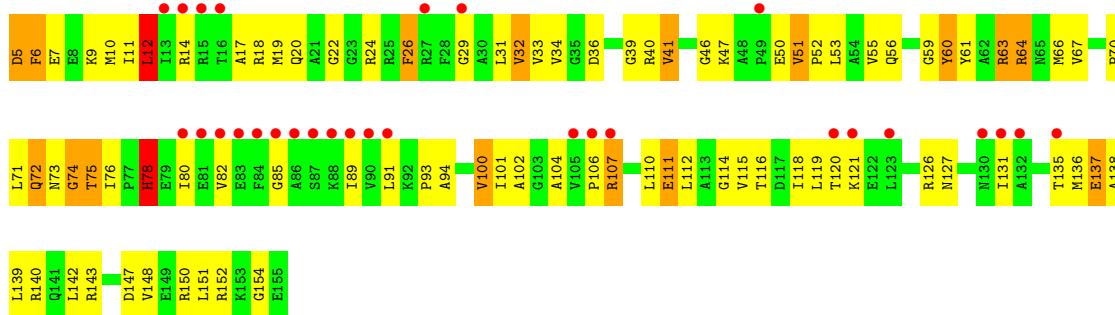
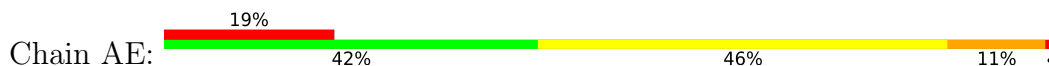


• Molecule 3: 30S ribosomal protein S4

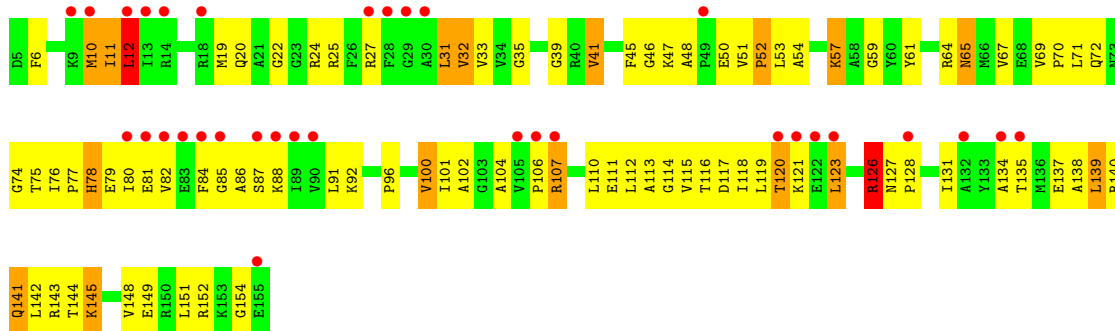




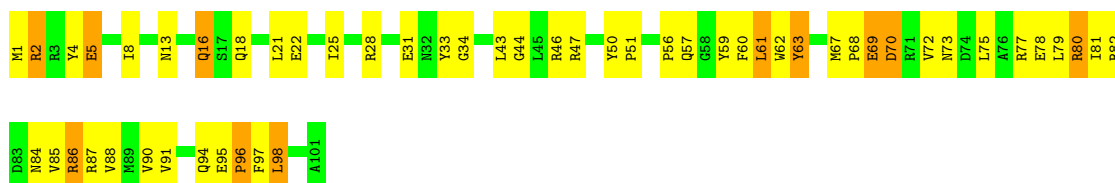
• Molecule 4: 30S ribosomal protein S5



• Molecule 4: 30S ribosomal protein S5

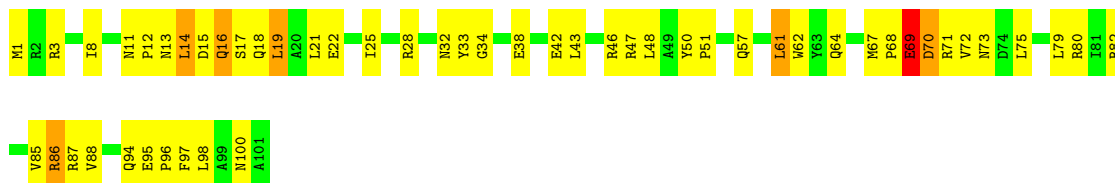


• Molecule 5: 30S ribosomal protein S6

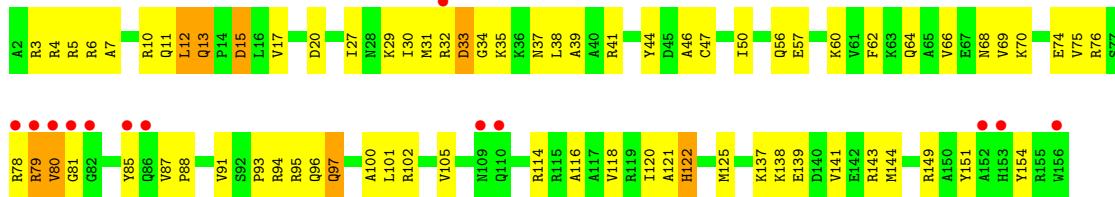


• Molecule 5: 30S ribosomal protein S6

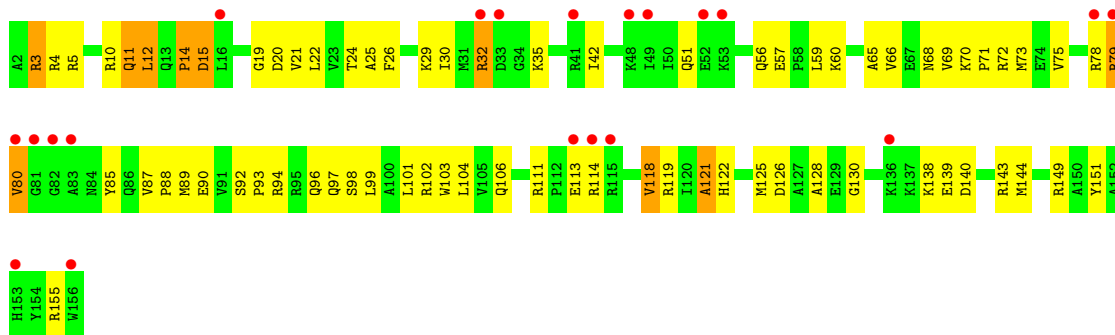




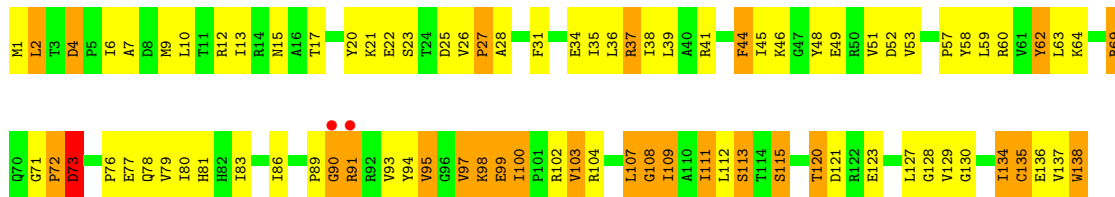
• Molecule 6: 30S ribosomal protein S7



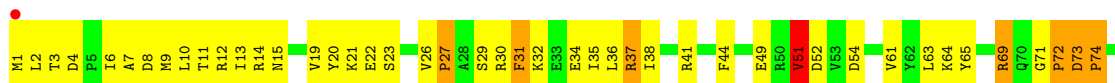
• Molecule 6: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S8

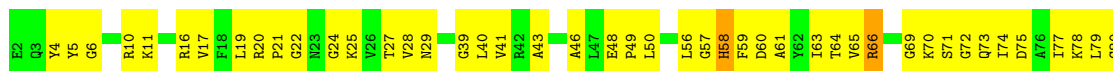


• Molecule 7: 30S ribosomal protein S8

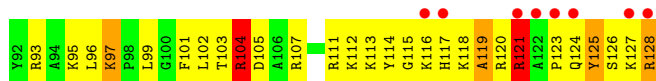




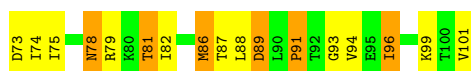
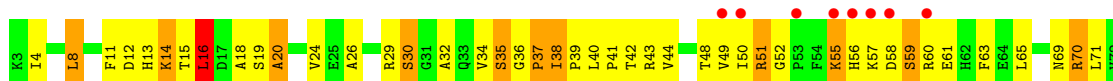
- Molecule 8: 30S ribosomal protein S9



- Molecule 8: 30S ribosomal protein S9



- Molecule 9: 30S ribosomal protein S10

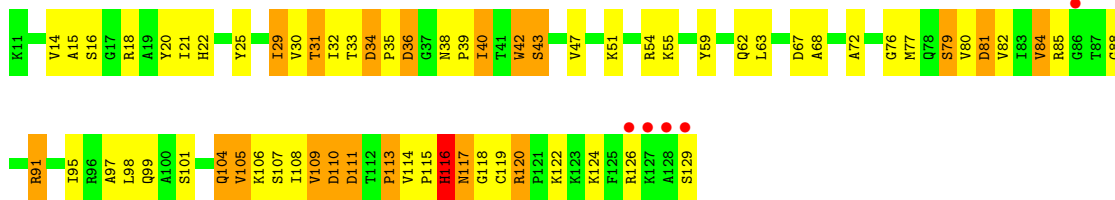


- Molecule 9: 30S ribosomal protein S10

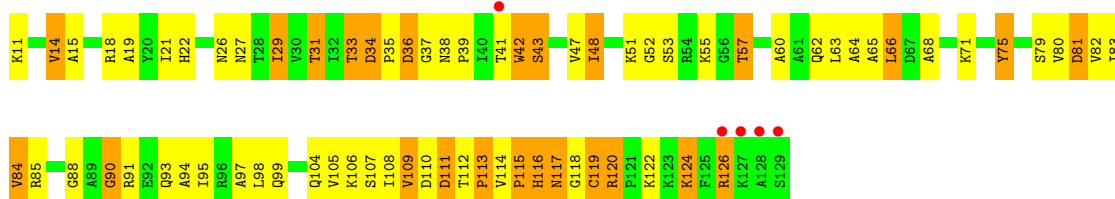


- Molecule 10: 30S ribosomal protein S11

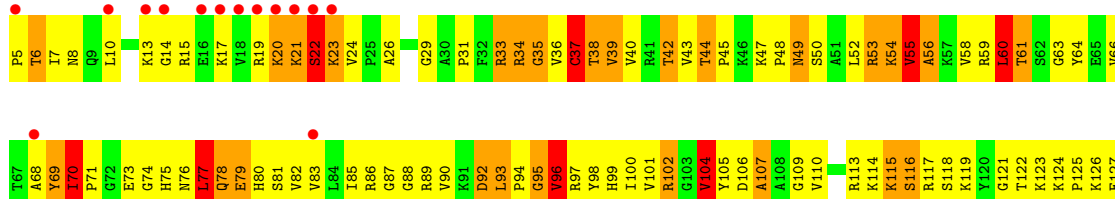




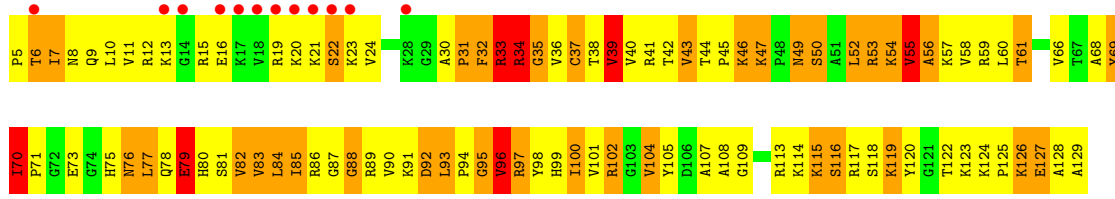
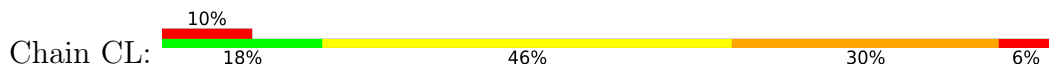
• Molecule 10: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S12

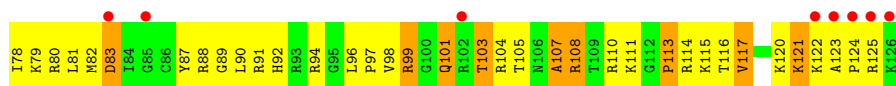


• Molecule 11: 30S ribosomal protein S12

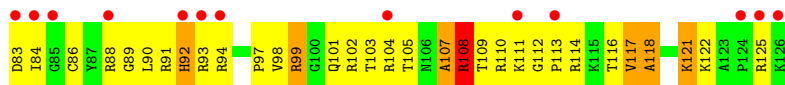
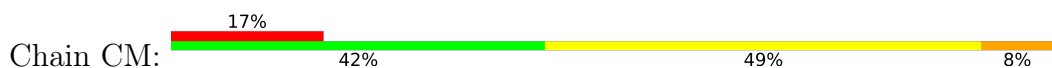


• Molecule 12: 30S ribosomal protein S13

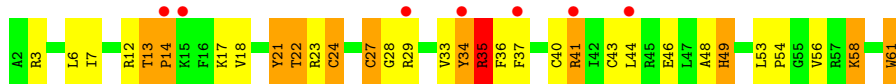




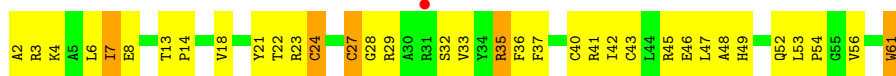
- Molecule 12: 30S ribosomal protein S13



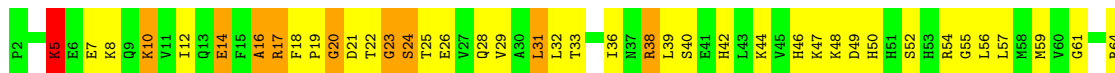
- Molecule 13: 30S ribosomal protein S14 type Z



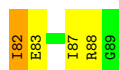
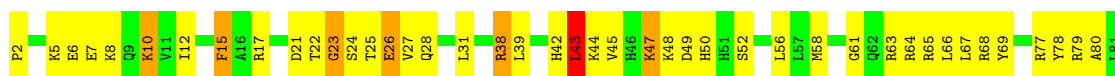
- Molecule 13: 30S ribosomal protein S14 type Z



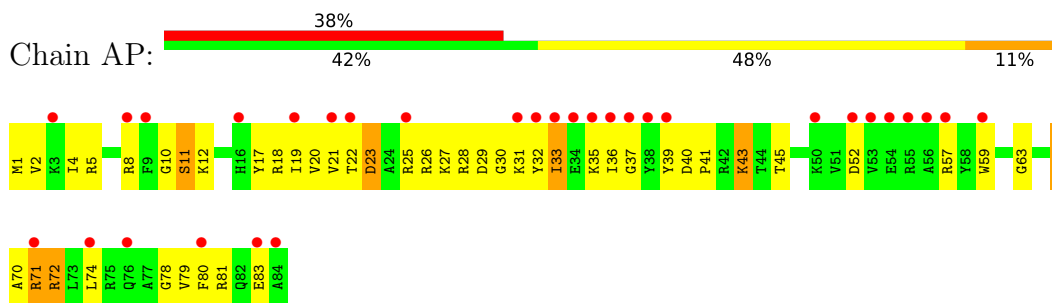
- Molecule 14: 30S ribosomal protein S15



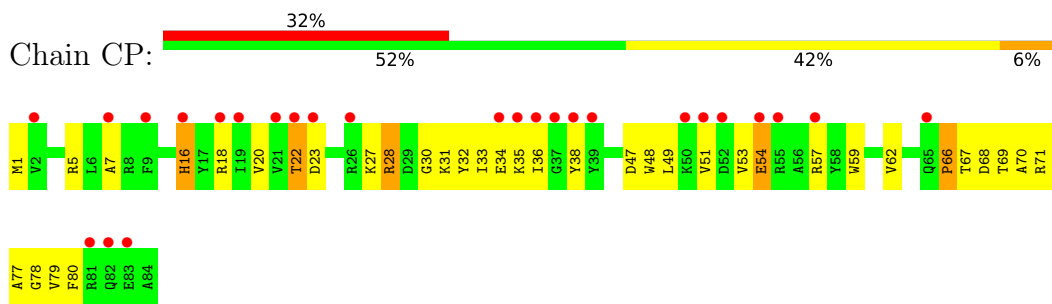
- Molecule 14: 30S ribosomal protein S15



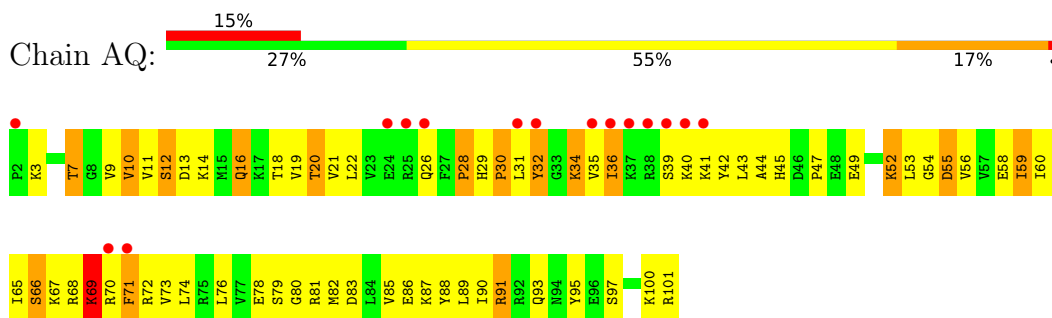
- Molecule 15: 30S ribosomal protein S16



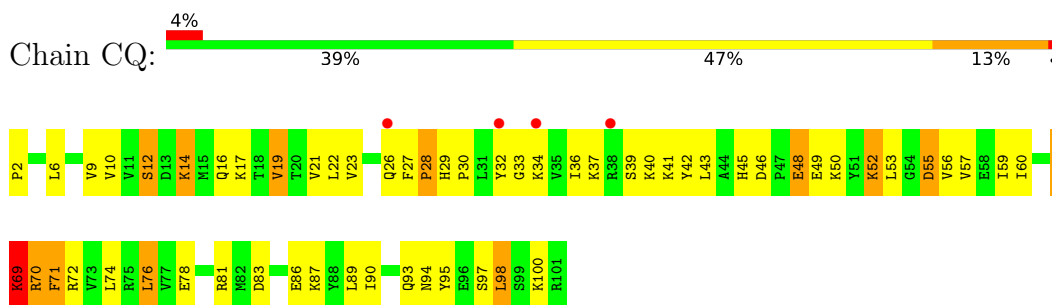
- Molecule 15: 30S ribosomal protein S16



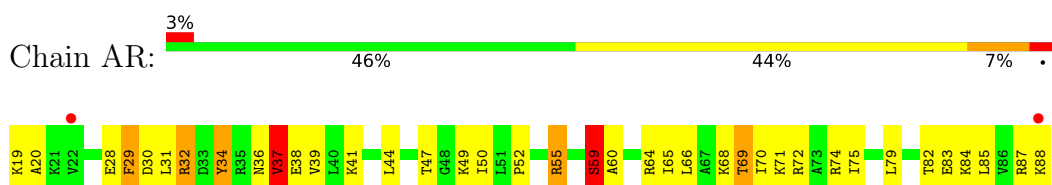
- Molecule 16: 30S ribosomal protein S17



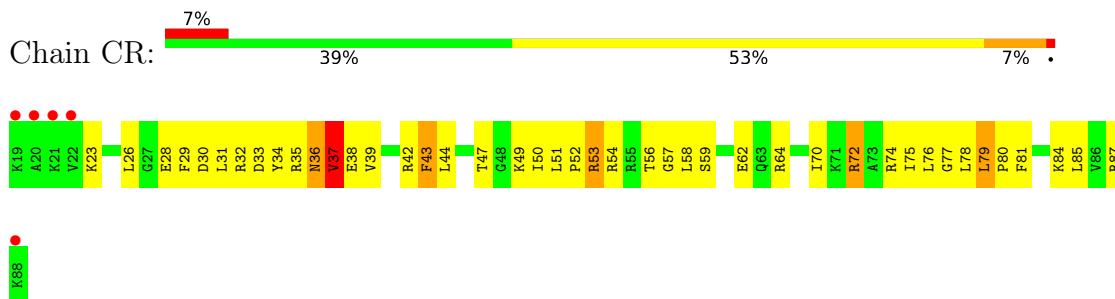
- Molecule 16: 30S ribosomal protein S17



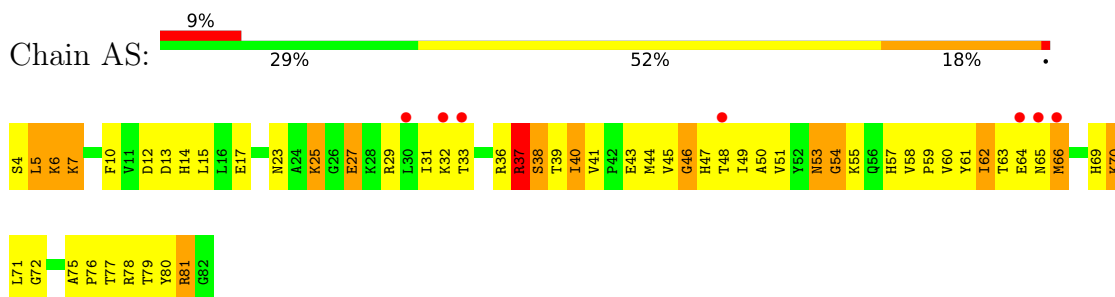
- Molecule 17: 30S ribosomal protein S18



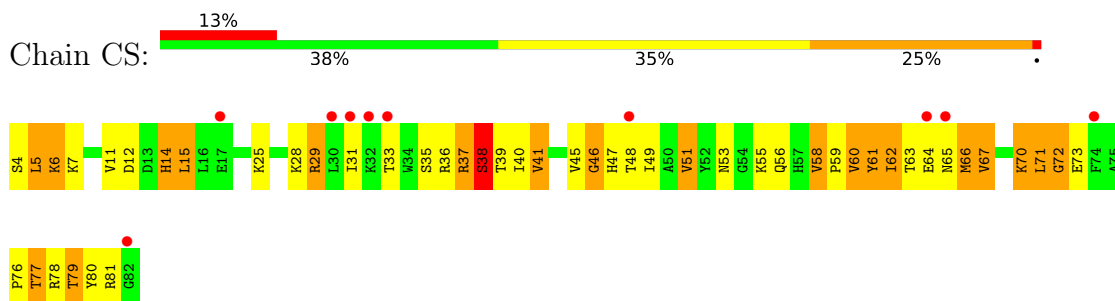
- Molecule 17: 30S ribosomal protein S18



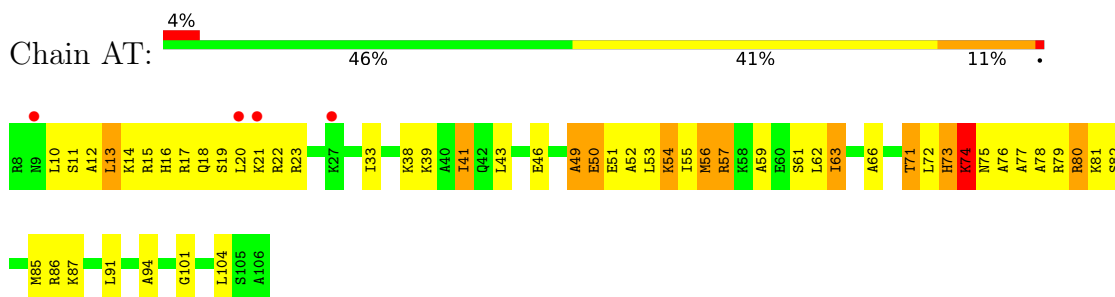
- Molecule 18: 30S ribosomal protein S19



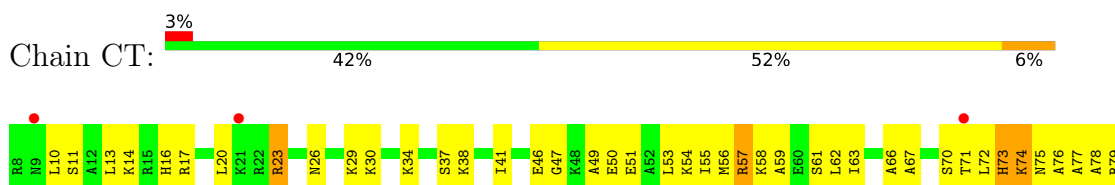
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20

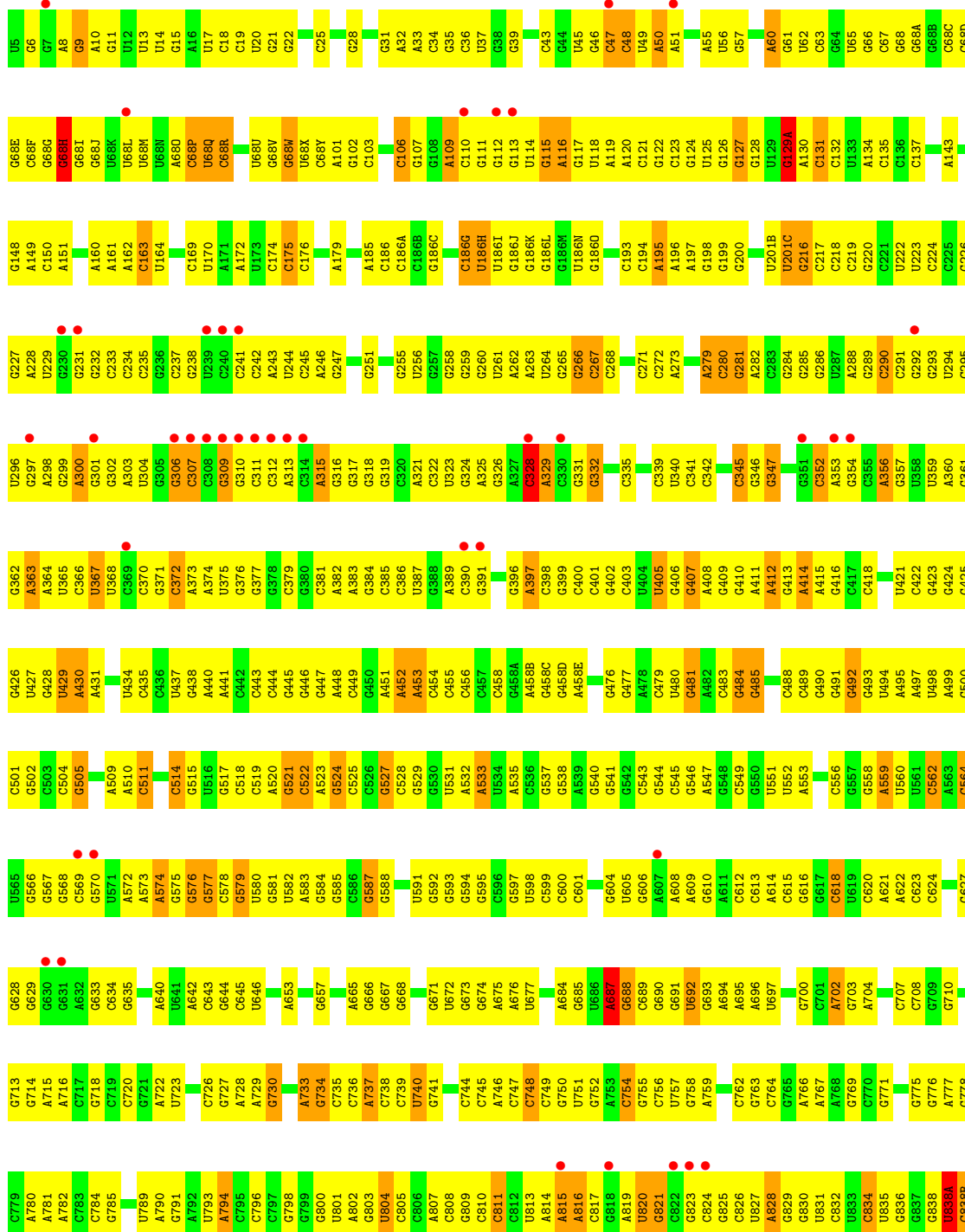


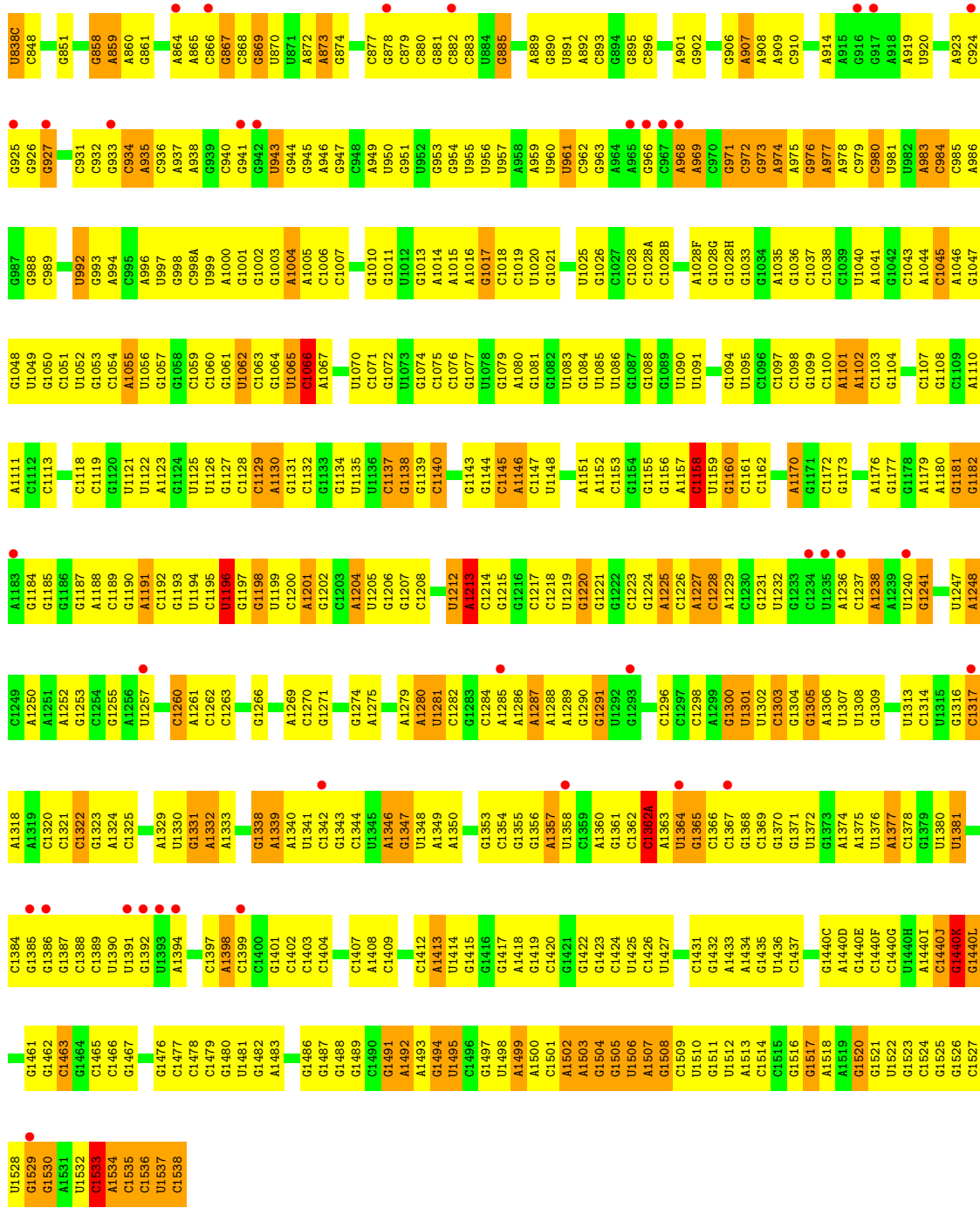
- Molecule 19: 30S ribosomal protein S20



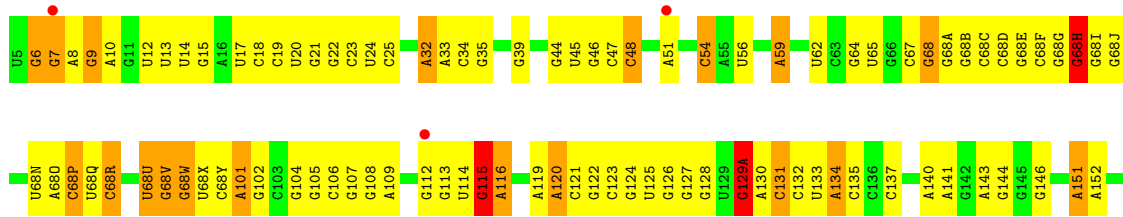
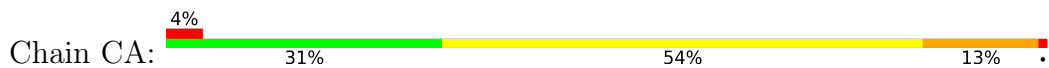


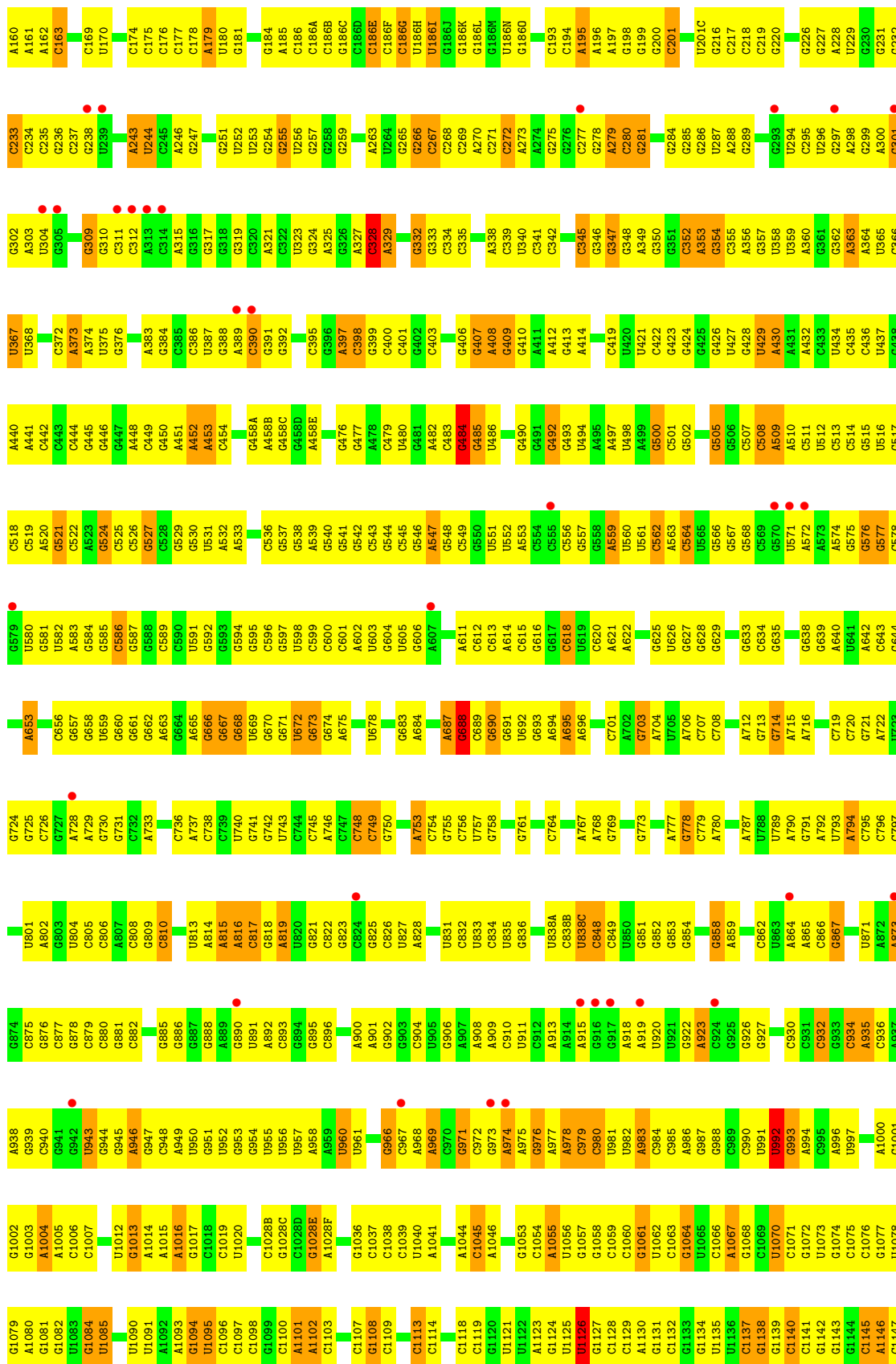
● Molecule 20: ribosomal RNA 16S

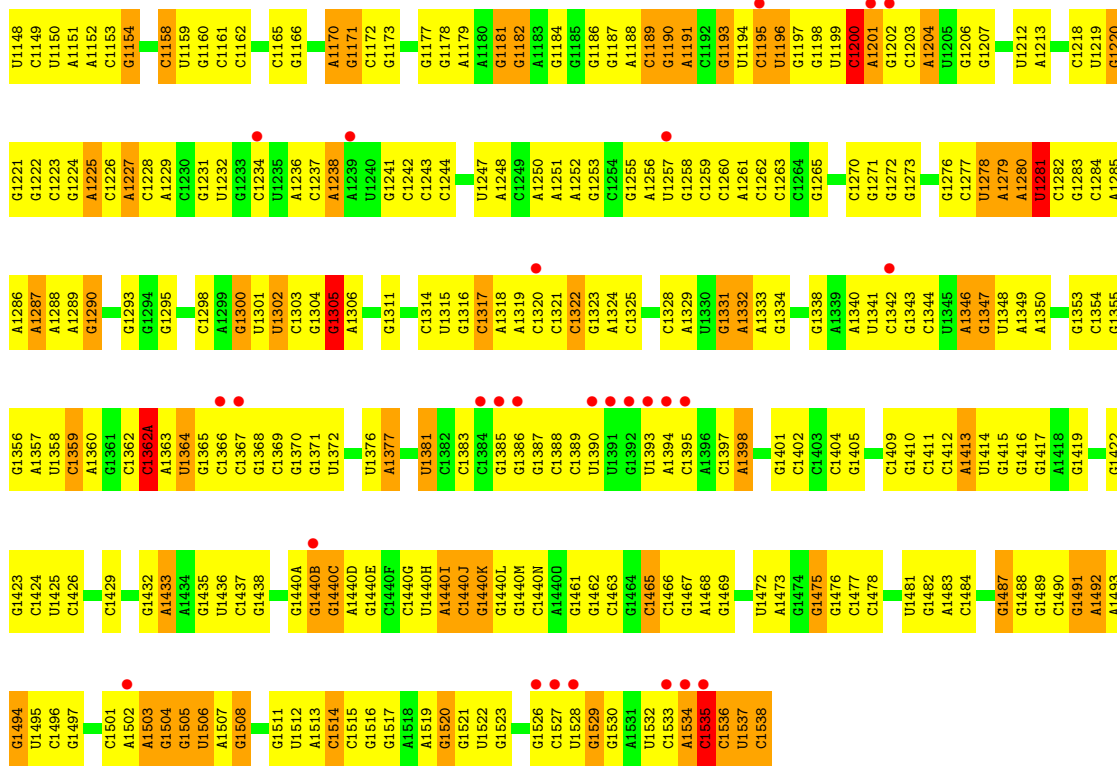




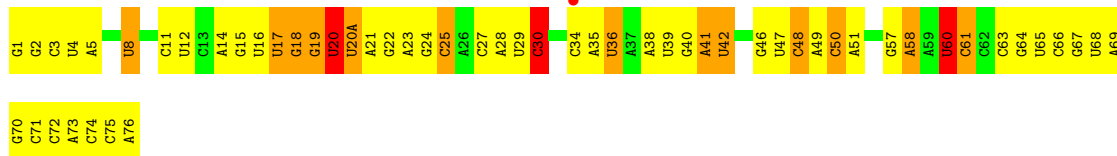
• Molecule 20: ribosomal RNA 16S



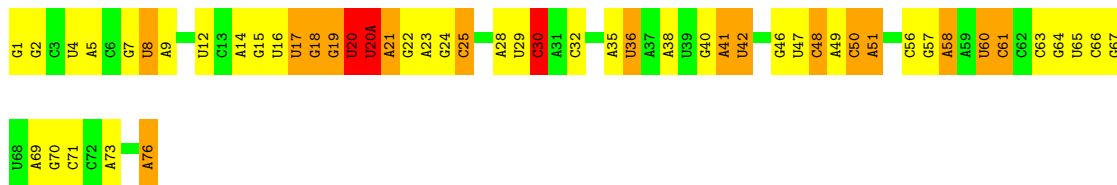




• Molecule 21: transfer RNA



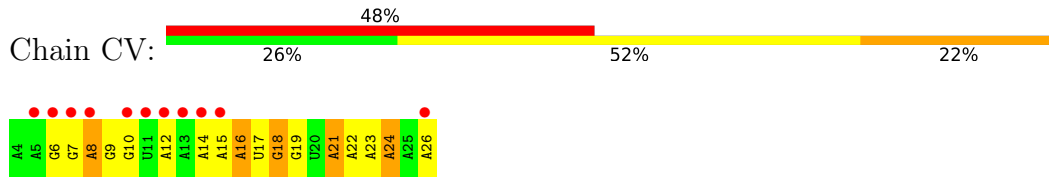
• Molecule 21: transfer RNA



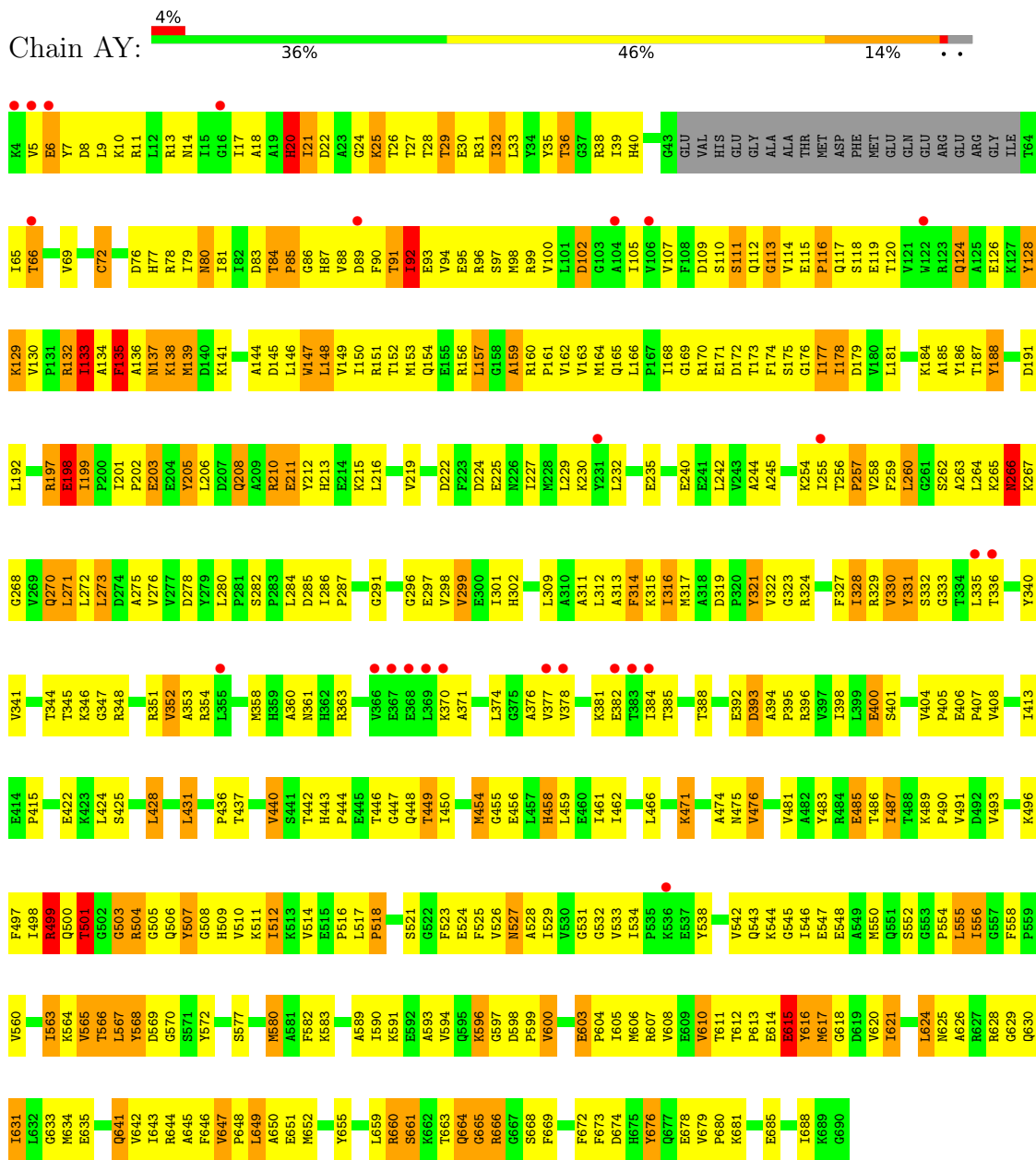
• Molecule 22: messenger RNA



• Molecule 22: messenger RNA

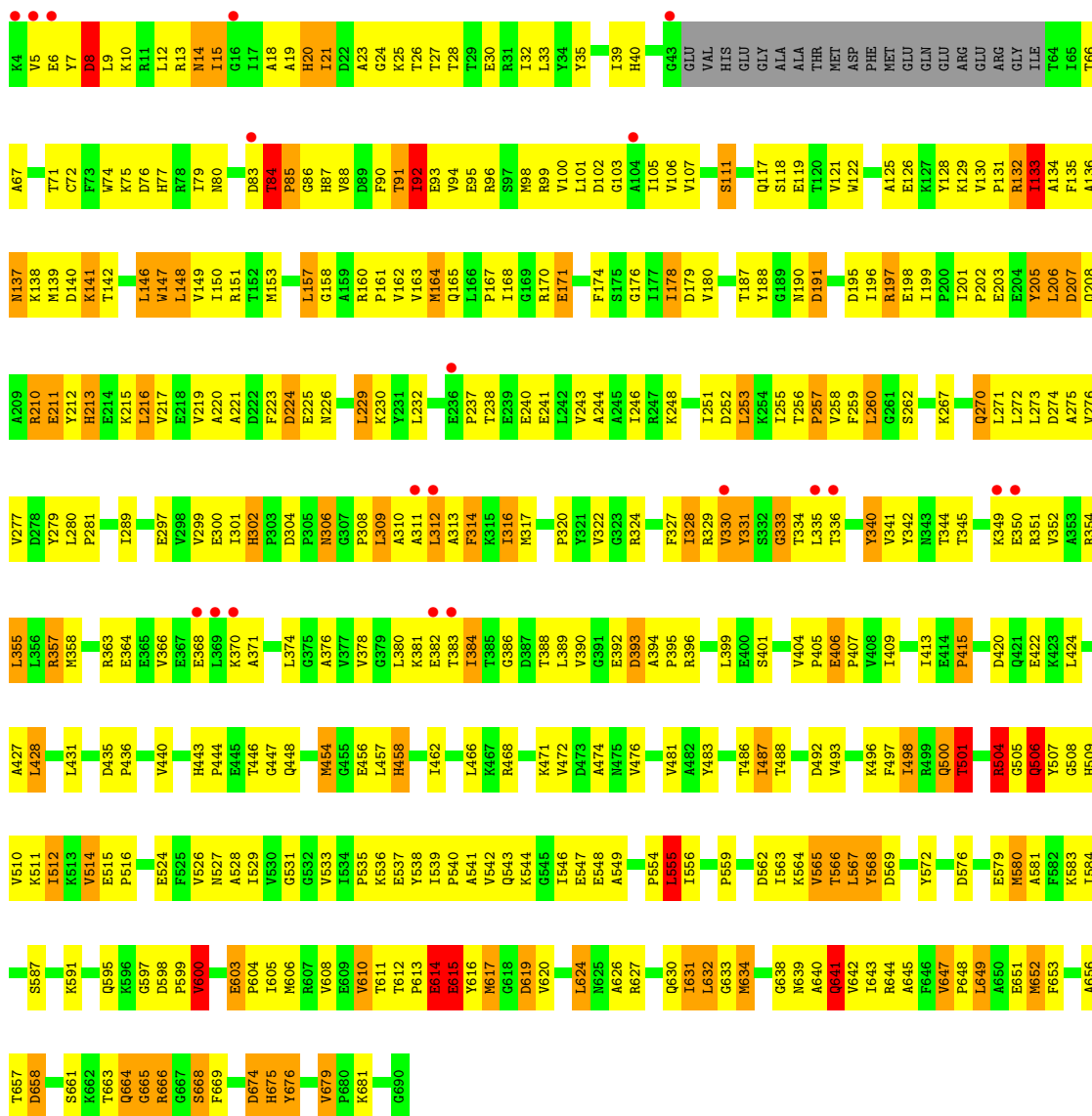


• Molecule 23: Elongation factor G

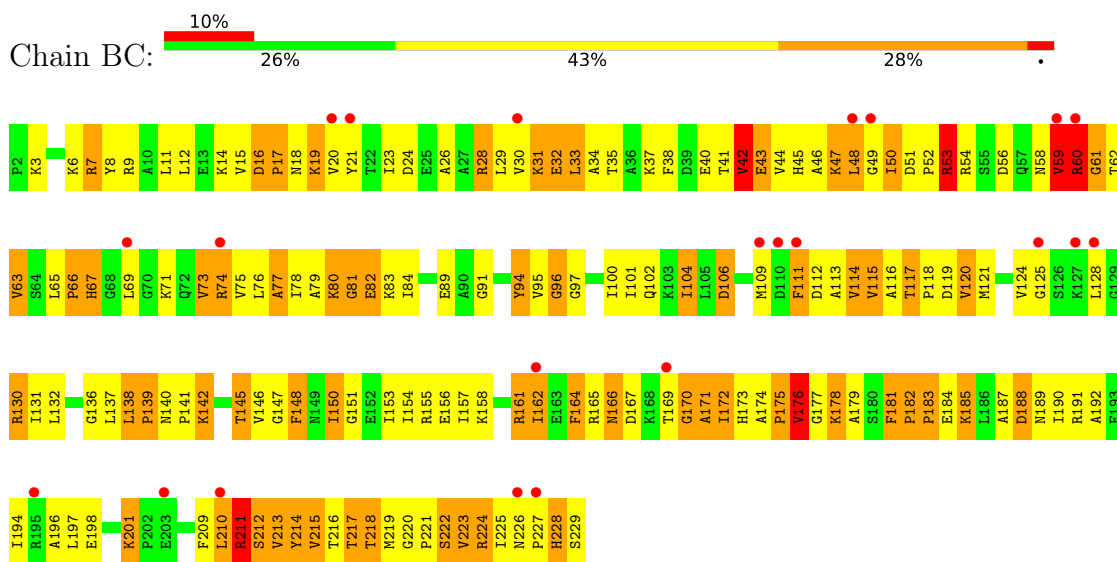


• Molecule 23: Elongation factor G

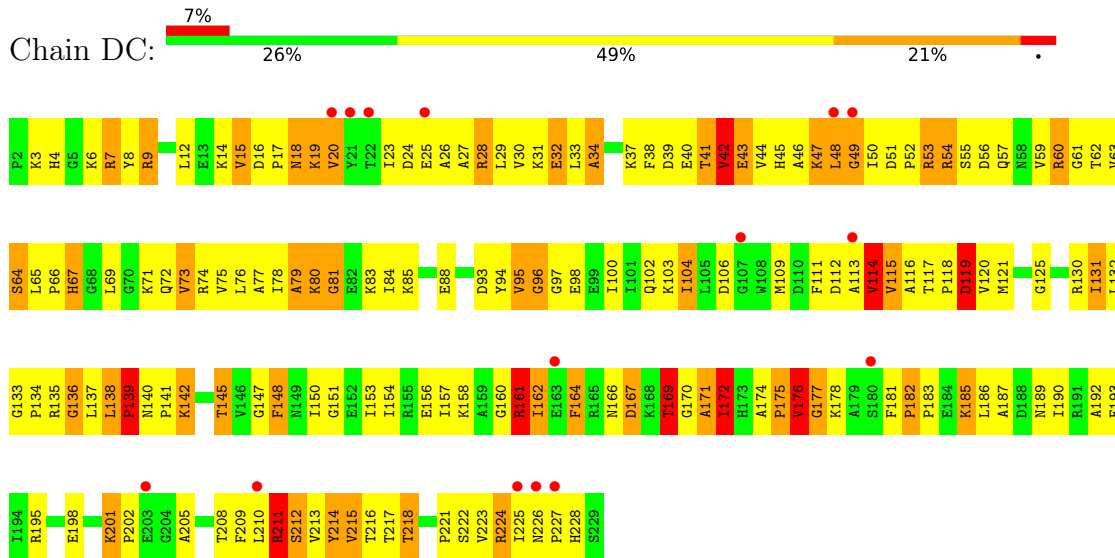




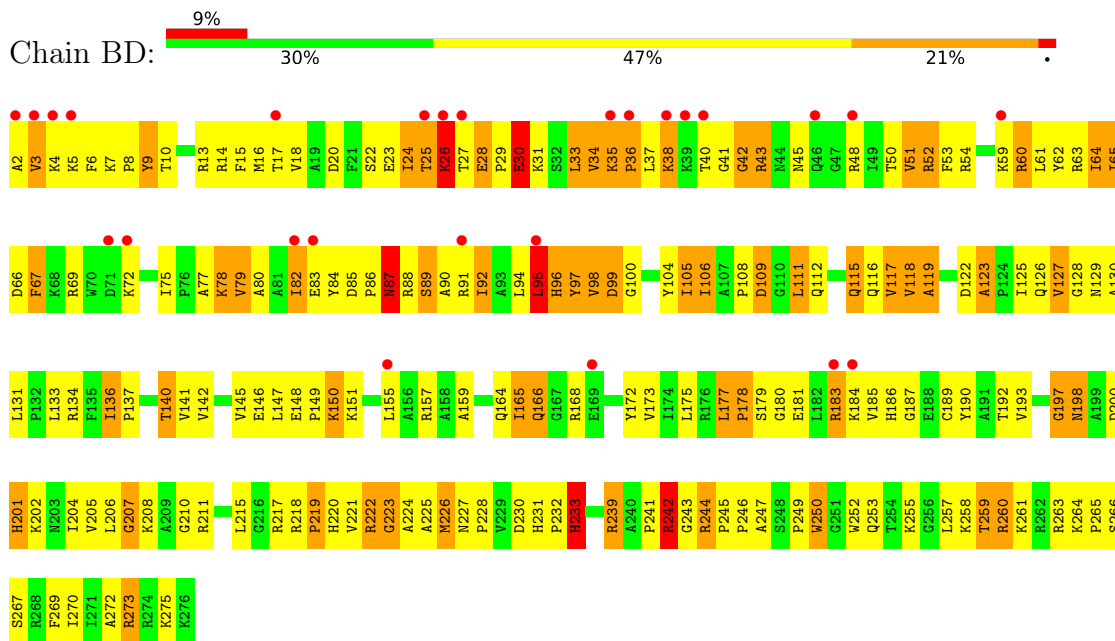
● Molecule 24: 50S ribosomal protein L1



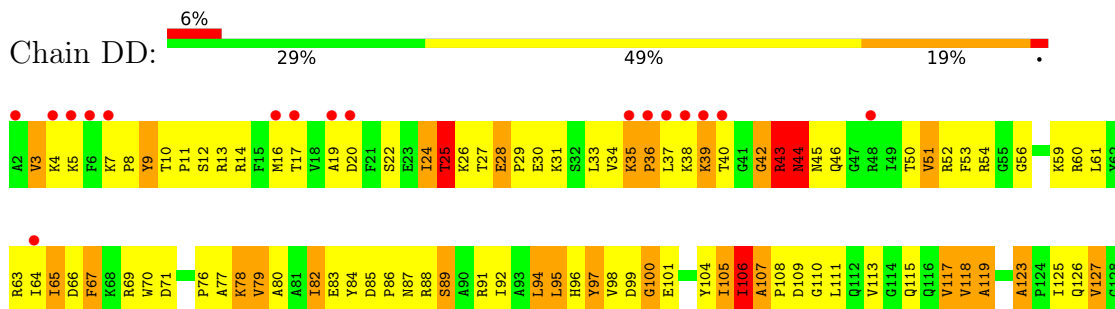
• Molecule 24: 50S ribosomal protein L1

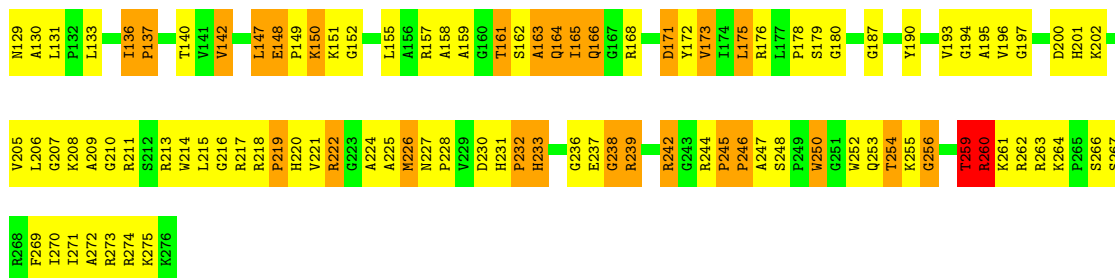


• Molecule 25: 50S ribosomal protein L2

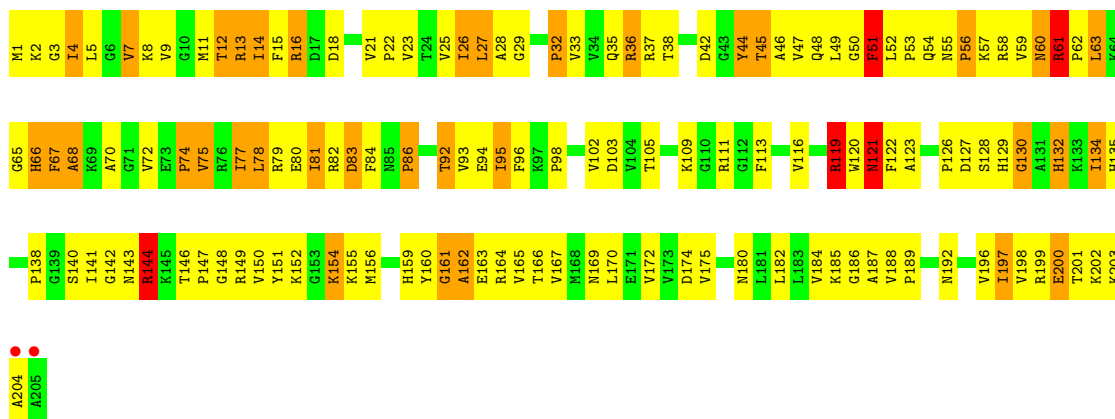


• Molecule 25: 50S ribosomal protein L2

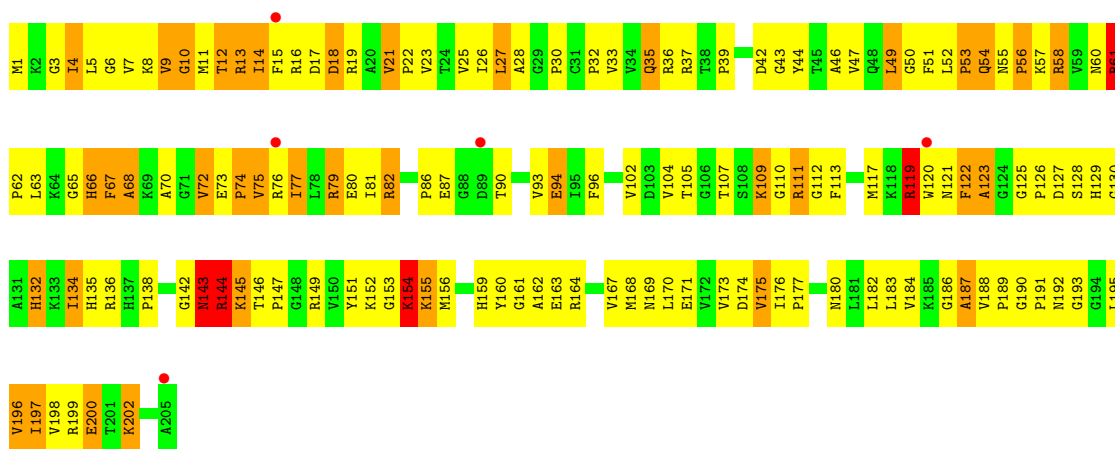




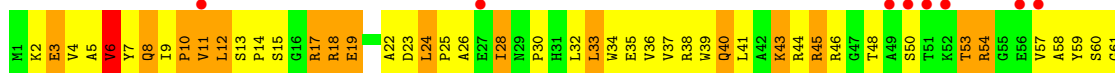
• Molecule 26: 50S ribosomal protein L3

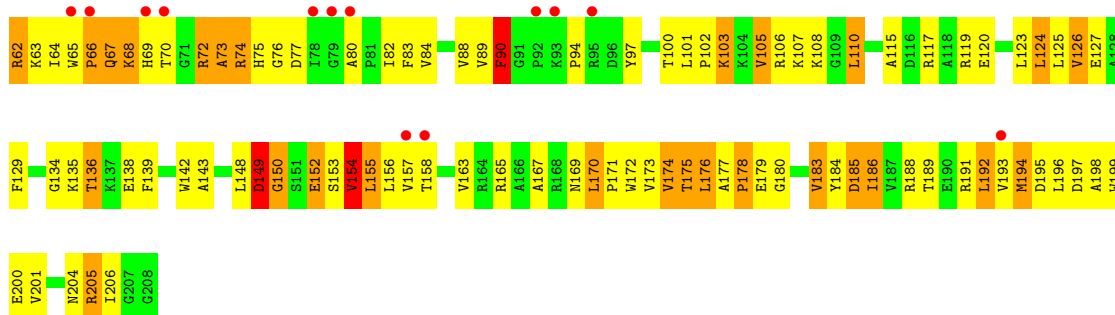


• Molecule 26: 50S ribosomal protein L3

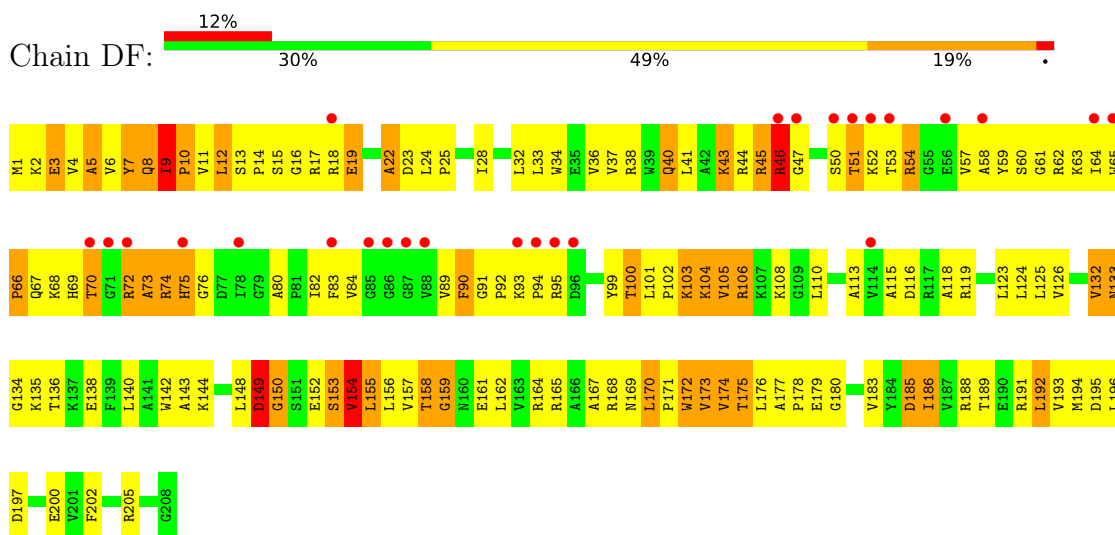


• Molecule 27: 50S ribosomal protein L4

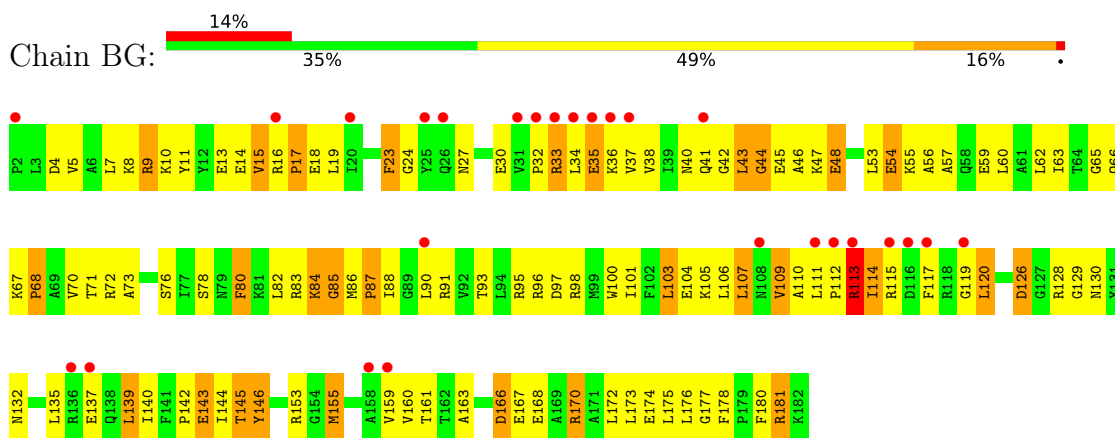




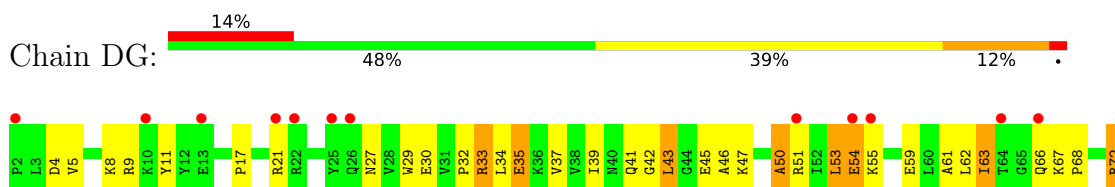
• Molecule 27: 50S ribosomal protein L4

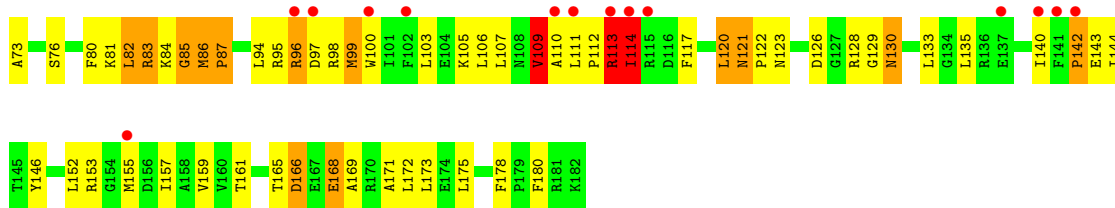


• Molecule 28: 50S ribosomal protein L5

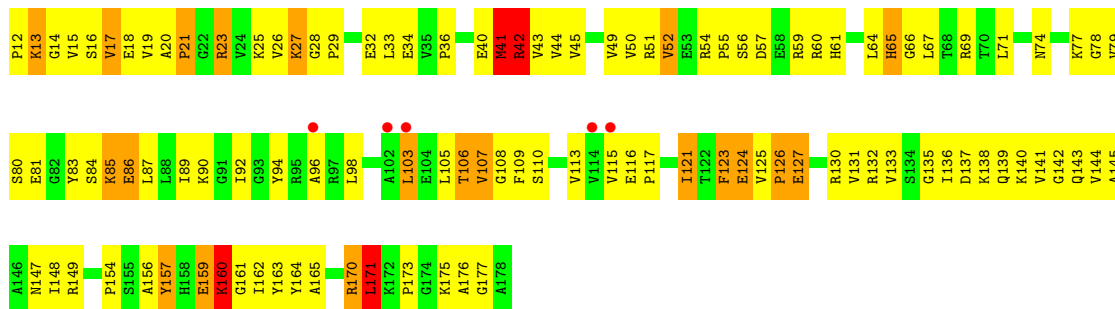


• Molecule 28: 50S ribosomal protein L5

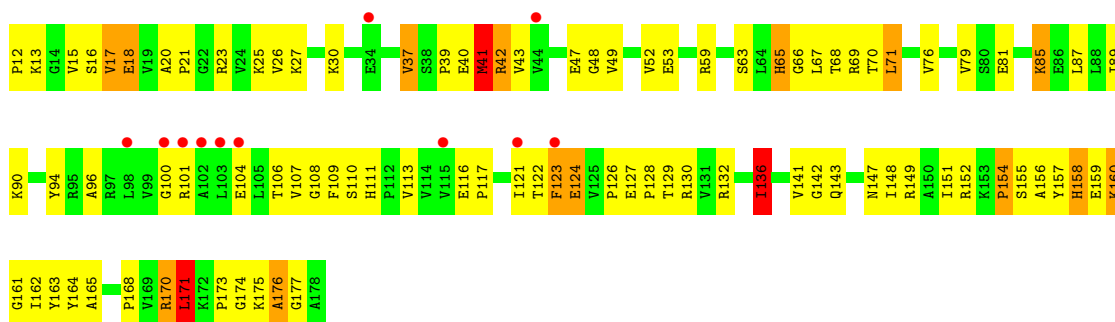




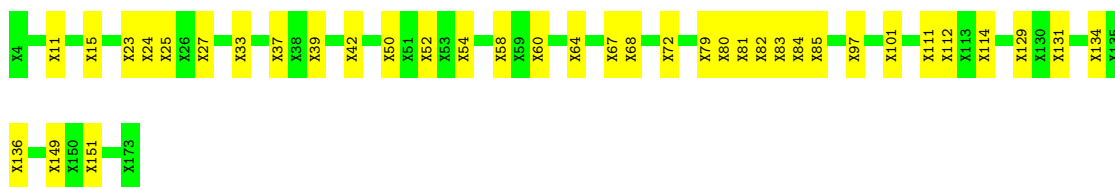
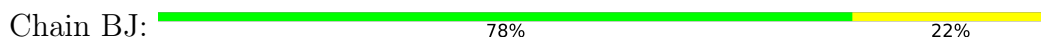
• Molecule 29: 50S ribosomal protein L6



• Molecule 29: 50S ribosomal protein L6

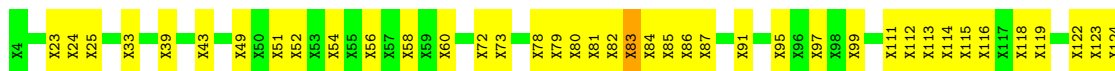


• Molecule 30: 50S ribosomal protein L10

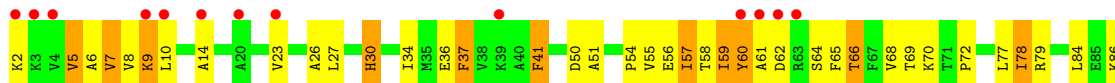


• Molecule 30: 50S ribosomal protein L10





• Molecule 31: 50S ribosomal protein L11



• Molecule 31: 50S ribosomal protein L11

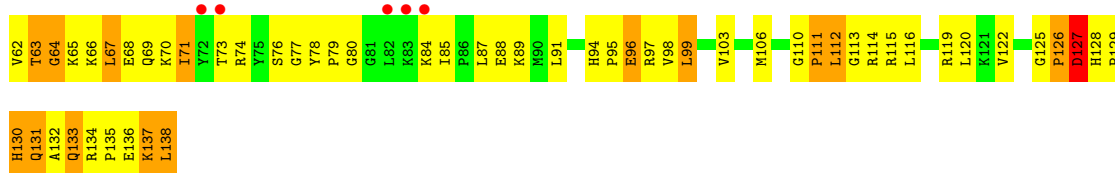


• Molecule 32: 50S ribosomal protein L13

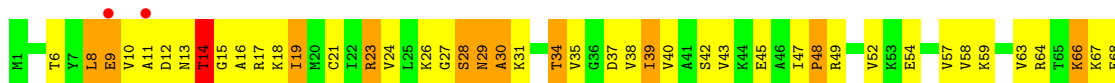


• Molecule 32: 50S ribosomal protein L13

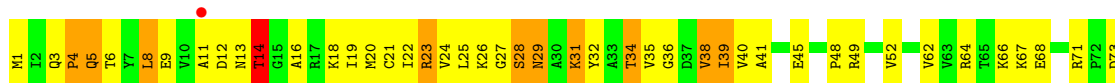
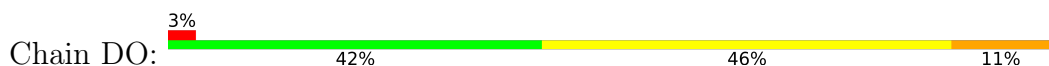




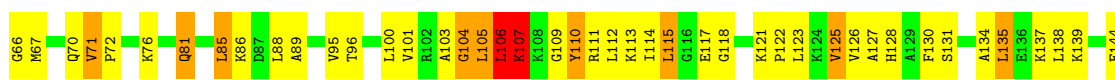
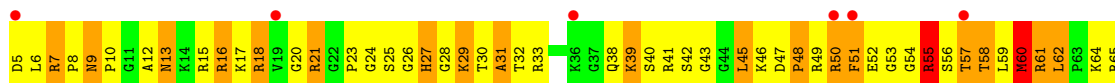
• Molecule 33: 50S ribosomal protein L14



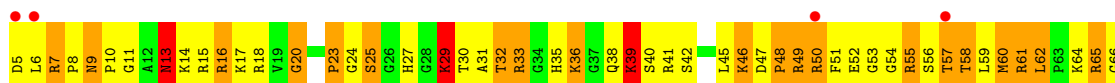
• Molecule 33: 50S ribosomal protein L14



• Molecule 34: 50S ribosomal protein L15

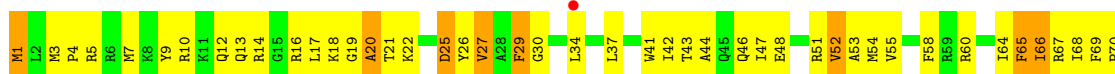
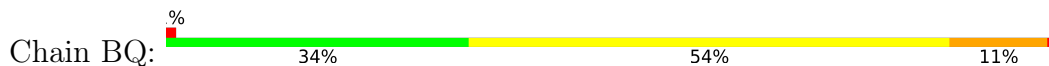


• Molecule 34: 50S ribosomal protein L15

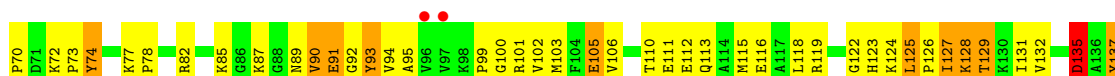




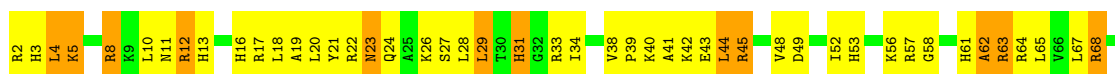
- Molecule 35: 50S ribosomal protein L16



- Molecule 35: 50S ribosomal protein L16

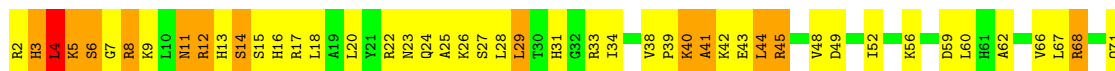


- Molecule 36: 50S ribosomal protein L17

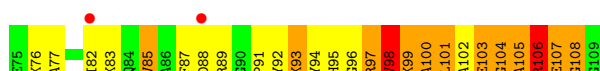
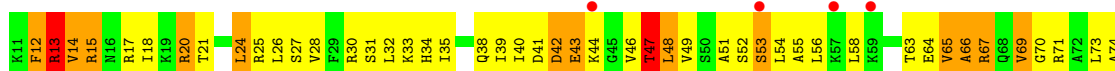
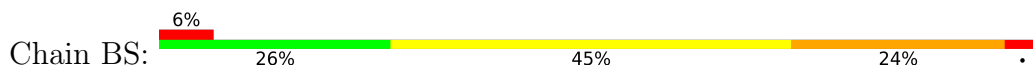


- Molecule 36: 50S ribosomal protein L17

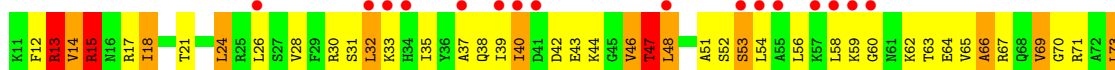




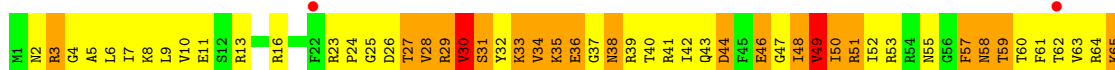
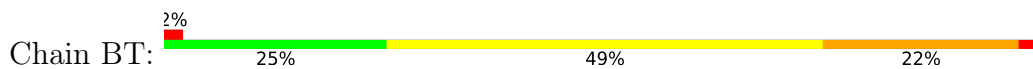
• Molecule 37: 50S ribosomal protein L18



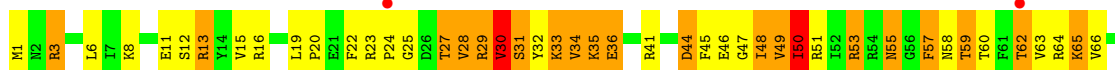
• Molecule 37: 50S ribosomal protein L18

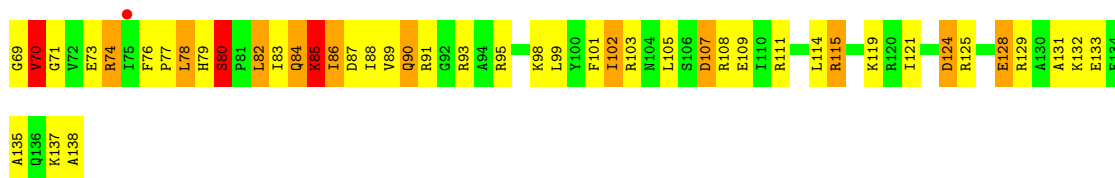


• Molecule 38: 50S ribosomal protein L19

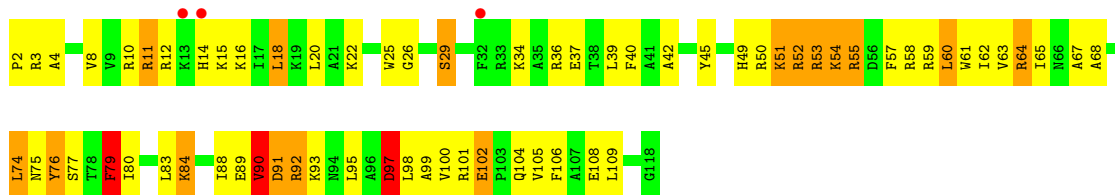
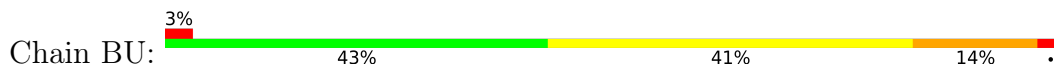


• Molecule 38: 50S ribosomal protein L19

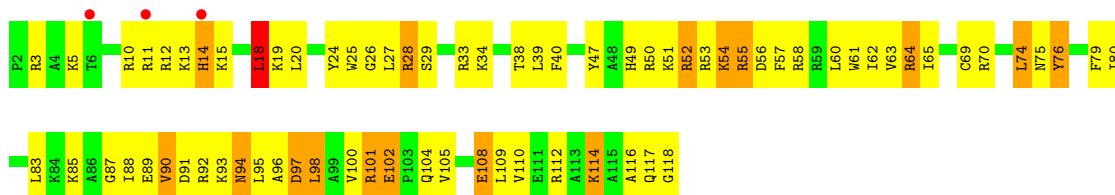




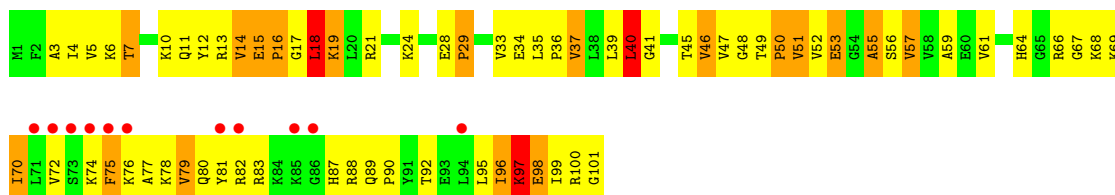
• Molecule 39: 50S ribosomal protein L20



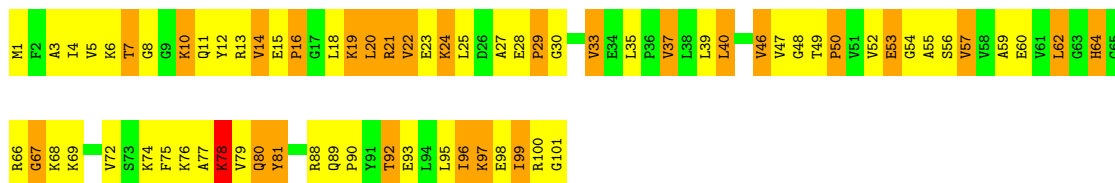
• Molecule 39: 50S ribosomal protein L20



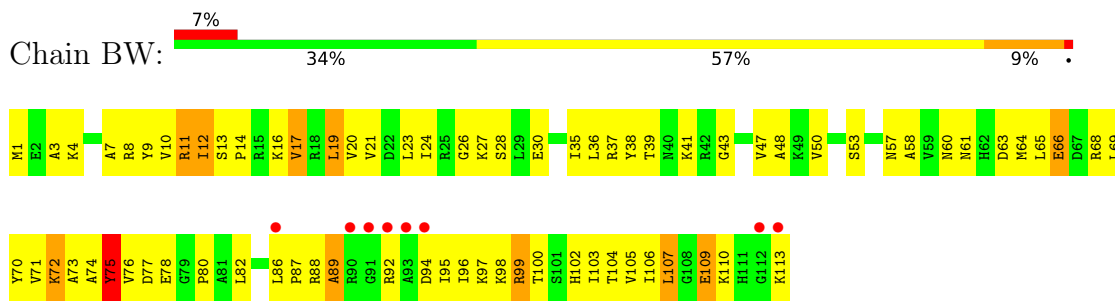
• Molecule 40: 50S ribosomal protein L21



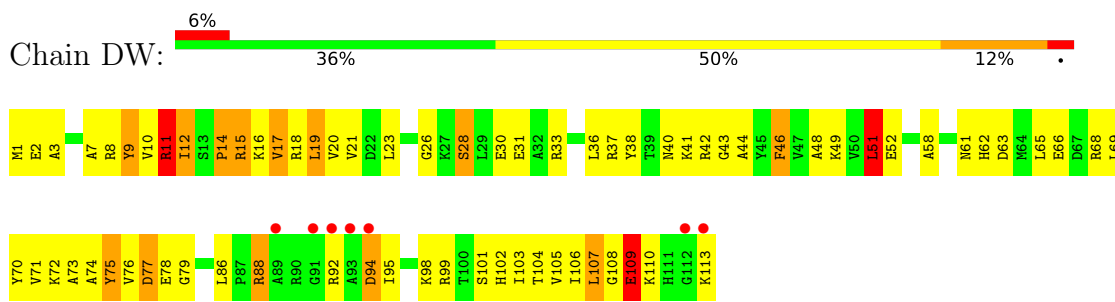
• Molecule 40: 50S ribosomal protein L21



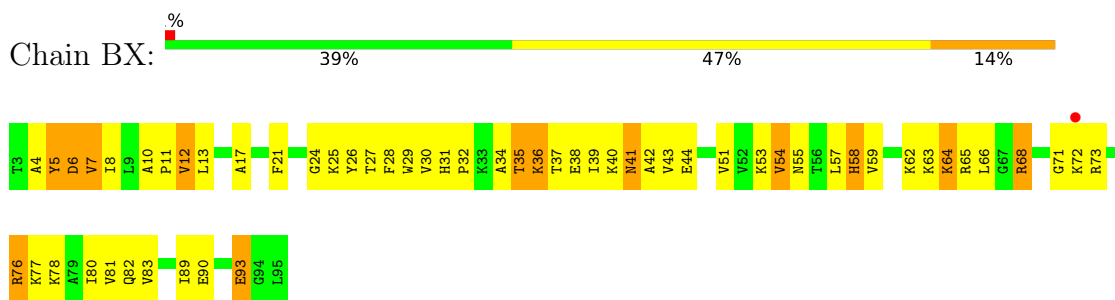
• Molecule 41: 50S ribosomal protein L22



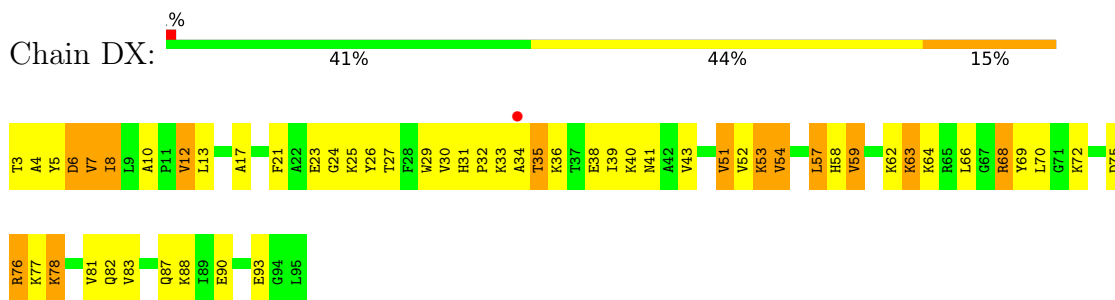
• Molecule 41: 50S ribosomal protein L22



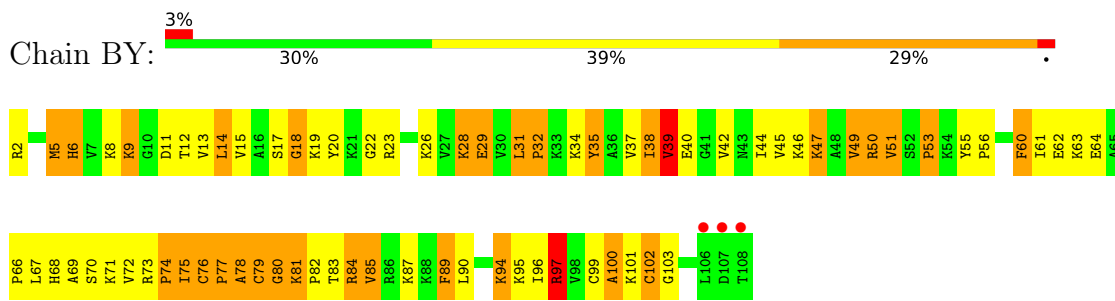
• Molecule 42: 50S ribosomal protein L23



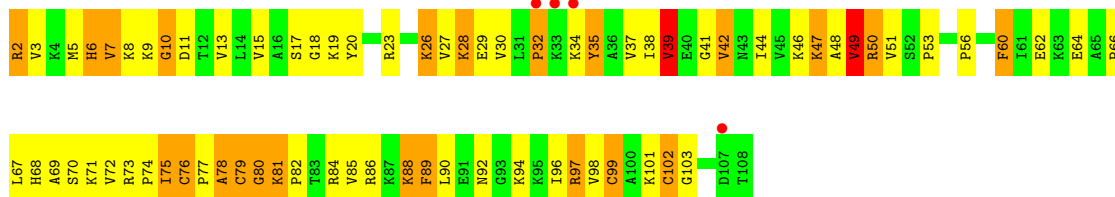
• Molecule 42: 50S ribosomal protein L23



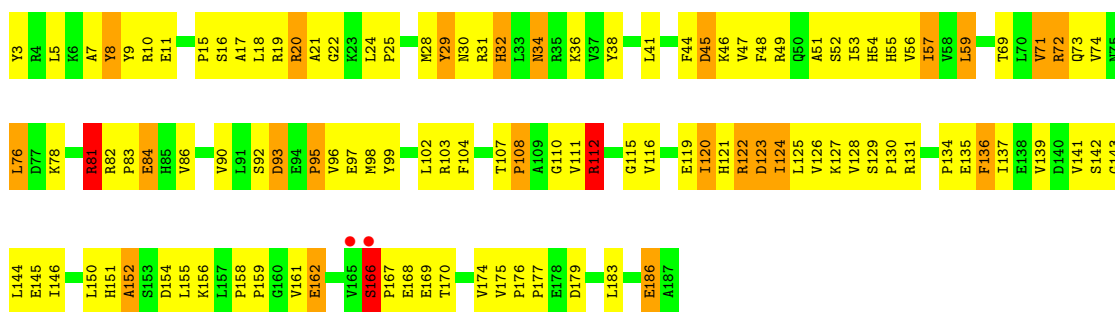
• Molecule 43: 50S ribosomal protein L24



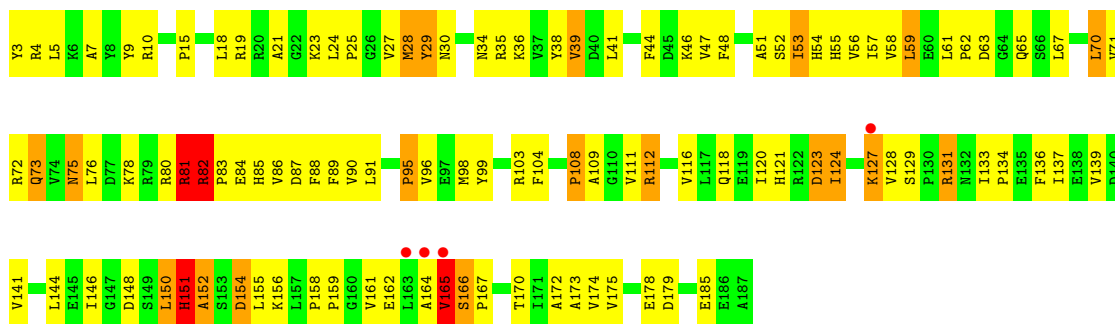
- Molecule 43: 50S ribosomal protein L24



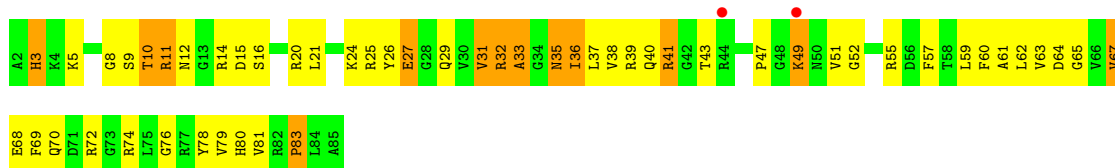
- Molecule 44: 50S ribosomal protein L25



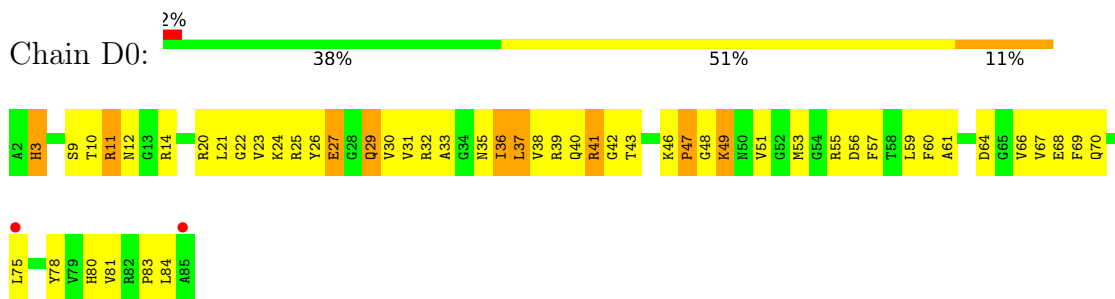
- Molecule 44: 50S ribosomal protein L25



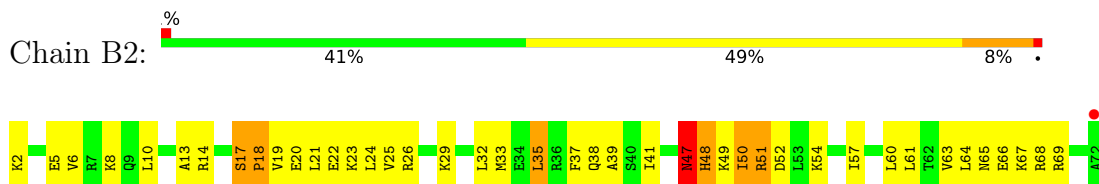
- Molecule 45: 50S ribosomal protein L27



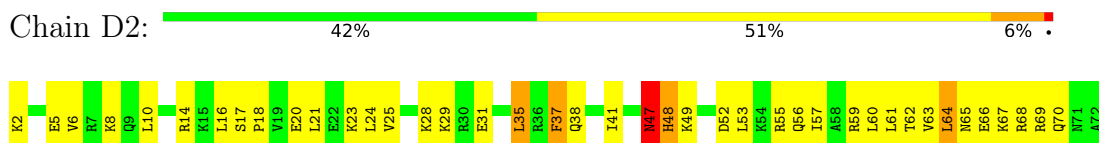
- Molecule 45: 50S ribosomal protein L27



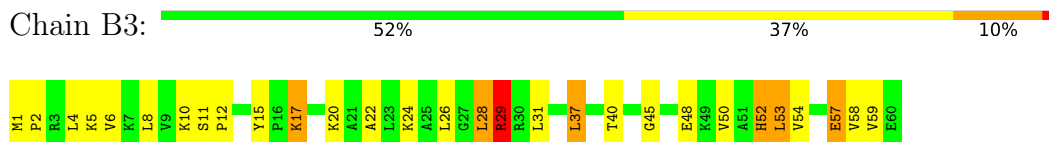
- Molecule 46: 50S ribosomal protein L29



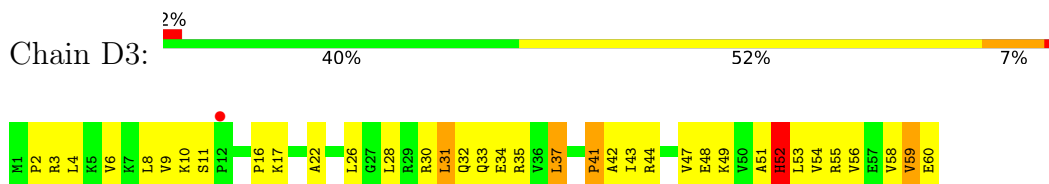
- Molecule 46: 50S ribosomal protein L29



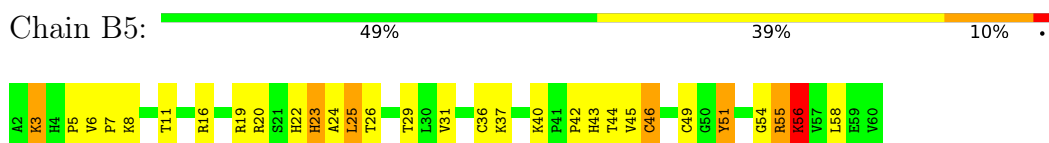
- Molecule 47: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L30



- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32





- Molecule 49: 50S ribosomal protein L33



- Molecule 49: 50S ribosomal protein L33



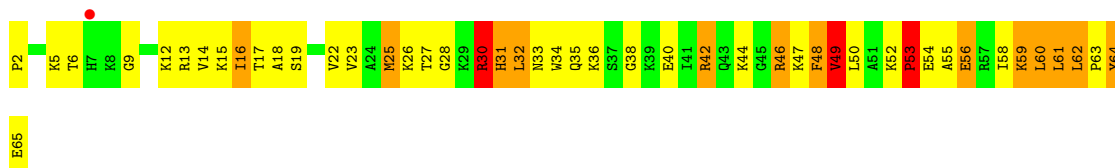
- Molecule 50: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L34



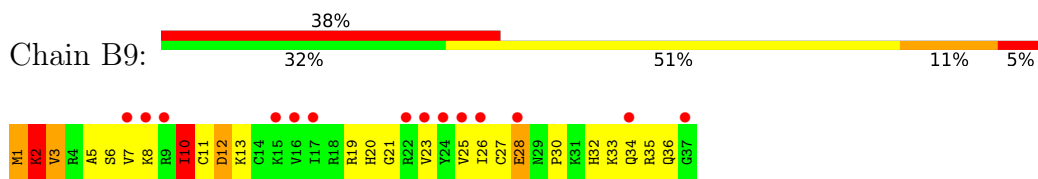
- Molecule 51: 50S ribosomal protein L35



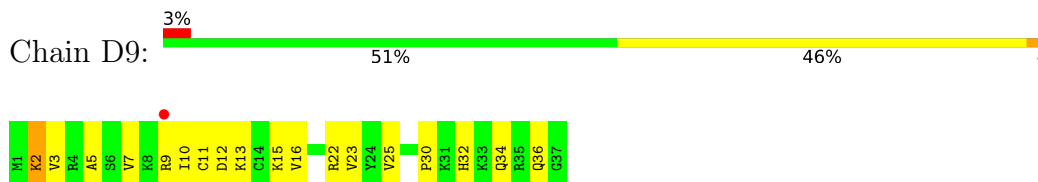
- Molecule 51: 50S ribosomal protein L35



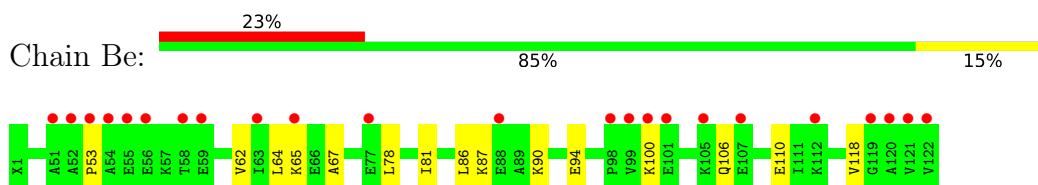
- Molecule 52: 50S ribosomal protein L36



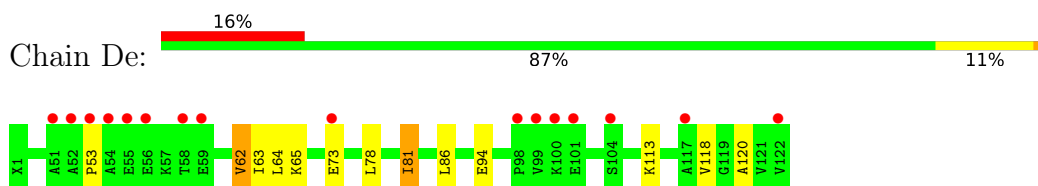
- Molecule 52: 50S ribosomal protein L36



- 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



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 55: 50S ribosomal protein L7/L12

Chain Bh:  100%

There are no outlier residues recorded for this chain.

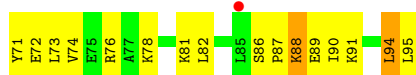
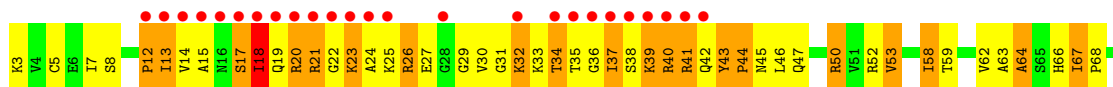
- Molecule 55: 50S ribosomal protein L7/L12

Chain Dh:  100%

There are no outlier residues recorded for this chain.

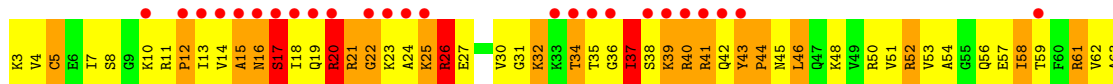
- Molecule 56: 50S ribosomal protein L28

Chain B1:  28%
30% 45% 24%



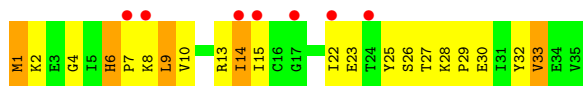
- Molecule 56: 50S ribosomal protein L28

Chain D1:  28%
20% 52% 23% 5%



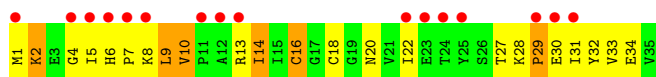
- Molecule 57: 50S ribosomal protein L31

Chain B4:  20%
40% 46% 14%

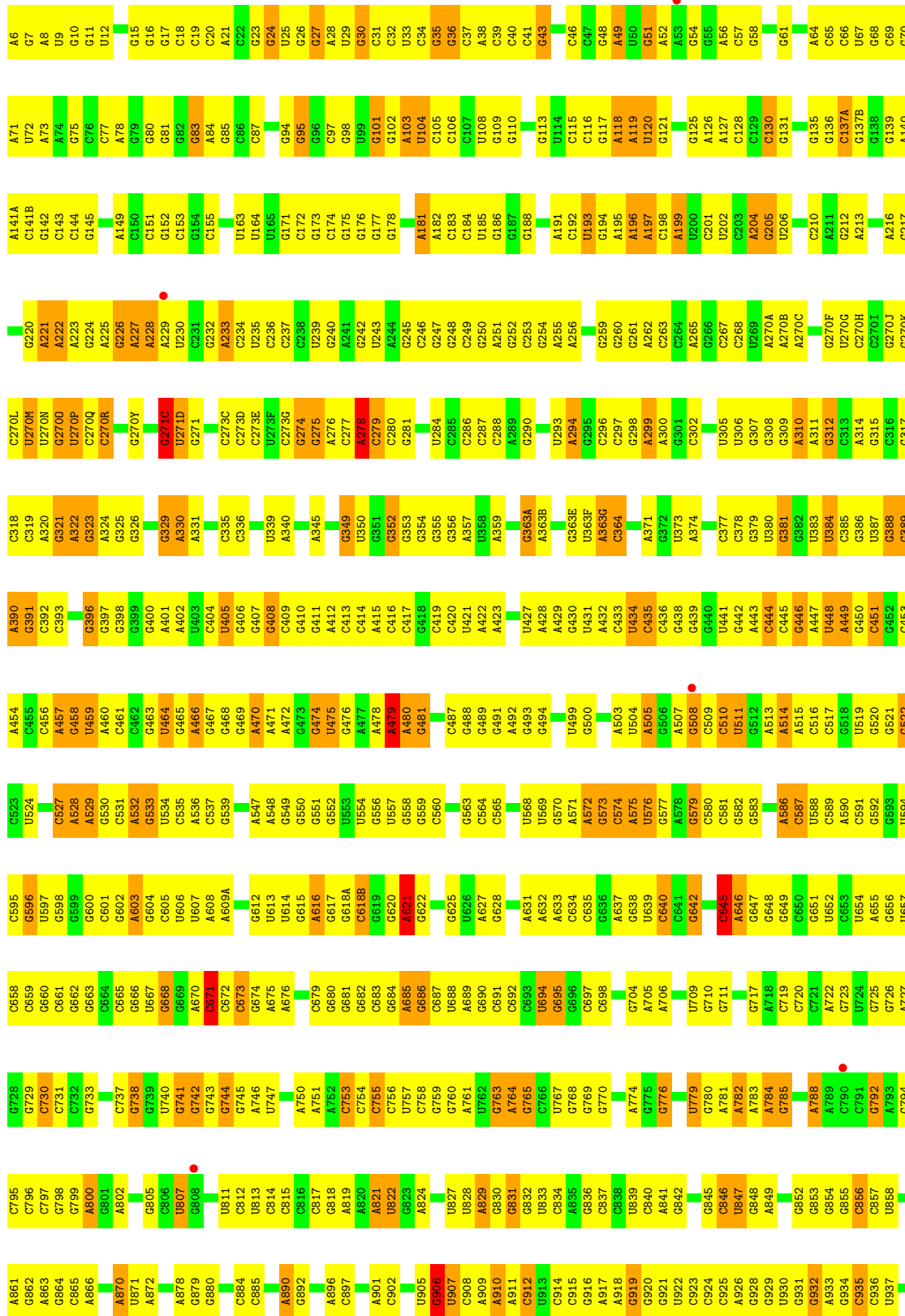


- Molecule 57: 50S ribosomal protein L31

Chain D4:  46%
34% 49% 17%



- Molecule 58: 23S ribosomal RNA



C1838	A1676	G1769	A1546	U1481	G1410	G1366	U1205	G1138	G1071	A1001	G940
G1639	A1677	G1770	C1548	G1483	C1411	U1267	G1206	G1139	C1072	G1002	A941
G1840	G1678	G1771	C1547	A1486	G1416	A1268	C1207	C1140	A1073	G1003	G942
G1842	U1679	U1841	G1514	G1487	C1417	A1269	G1208	U1141	G1074	G1004	U943
G1845	G1681	G1772	G1551	G1488	C1418	G1270	A1209	U1142	C1075	G1005	G944
G1846	G1682	A1773	A1553	U1489	A1419	G1271	A1210	A1145	C1076	G1006	A945
A1847	C1683	G1619	A1584	A1490	U1420	A1272	U1211	A1143	A1077	G1007	G946
	C1684	G1622	G1557	G1491	G1421	A1273	G1212	A1144	U1078	C1008	G947
	G1687	G1623	A1558	G1492	G1422	A1274	A1213	C1145	C1079	A1009	G948
	A1690	G1624	A1559	C1493	G1423	A1275	G1214	A1146	C1080	A1010	C949
	C1691	G1625	G1560	A1494	G1424	A1276	A1215	C1147	U1081	G1011	G950
	U1692	G1626	A1496	A1495	G1425	G1277	G1216	U1082	U1012	G1012	C951
	U1693	G1627	U1497	A1496	G1426	G1278	C1217	A1148	U1083	G1013	G952
	U1694	G1628	C1498	A1497	A1427	G1279	A1220	C1150	A1084	U1014	A953
	G1695	A1631	C1499	U1498	C1428	G1280	C1221	G1151	A1085	G1015	G954
	G1696	A1632	G1500	A1501	A1430	G1281	G1222	C1152	A1086	G1016	C955
	G1697	G1633	G1501	C1502	C1431	G1282	G1223	G1153	G1087	G1017	G956
	A1698	G1634	A1566	A1567	A1432	A1283	C1224	G1154	A1088	G1018	A957
	G1699	G1635	G1568	C1569	A1434	A1284	G1225	A1155	G1089	U1019	U958
	G1700	G1636	A1570	A1571	G1435	U1285	A1226	A1156	U1090	A1020	A959
	A1701	A1637	A1572	A1509	C1437	C1289	G1227	C1161	C1092	G1022	A960
	G1702	C1638	A1572	A1510	U1438	C1290	G1228	U1023	G1093	U1023	C961
	G1703	U1639	C1575	A1511	A1439	C1291	G1229	G1024	G1094	G1024	U963
	G1704	A1640	U1576	A1512	A1440	U1284	G1230	G1163	A1096	G1025	C964
	C1708	G1641	U1577	A1513	G1442	G1285	G1231	G1164	U1091	U1026	G965
	C1800	G1642	U1578	A1514	G1443	G1286	C1232	U1165	A1101	A1027	G966
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	A1802	G1646	G1581	U1516	A1445	U1288	G1234	U1167	A1103	A1029	G968
	G1803	G1647	A1582	G1517	C1446	C1289	G1235	G1171	C1104	U969	U969
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	C1806	G1650	A1584	U1519	U1446	U1291	G1237	A1174	G1106	U1033	C971
	A1810	A1651	U1585	A1520	C1451	U1292	G1238	U1175	U1108	G1034	G972
	G1811	G1652	U1586	G1521	U1452	A1301	U1239	U1176	C1110	U1035	A973
	G1812	A1653	C1588	G1522	U1453	A1302	A1241	G1177	A1111	G1036	G974A
	G1813	G1654	U1589	U1523	U1454	C1305	A1242	A1178	G1112	G1037	C974B
	G1814	A1655	C1590	G1524	G1455	C1306	G1243	C1179	U1113	U975	G975
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	U1818	C1660	G1594	A1528	C1462	G1310	A1247	G1185	A1045	A1045	A980
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	G1823	G1666	C1600	U1533	C1468	A1317	A1254	G1191	A1054	A1054	A988
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	C1765	G1674	A1543	A1544	G1479	G1328	U1263	G1202	U1133	G1063	G997
	A1912	C1675	A1545	C1408	G1480	U1329	U1264	G1203	C1136	A1069	C998
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A1913	A1914	A1915	A1916	A1919	G1922	G1923	G1924	A1928	A1929	G1930	A1931	G1935	A1936	A1937	A1938	U1939	U1940	C1941	G1942	U1943	U1944	U1945	U1946	G1947	G1948	G1949	G1950	U1951	A1952	A1953	G1954	U1955	U1956	C1957	C1958	A1959	A1960	C1961	U1962	U1963	G1964	G1965	A1966	C1967	G1968	A1969	A1970	C2000	A2001	A2002	U2003	G2004	A2005	G2006	C2007	G2010	G2011	G2012	G2013	A2014	A2015	G2018	G2019	U2020	U2021	U2022	G2023	G2024	C2025	A2030	A2031	G2032	A2033	G2034	G2035	A2036	C2037	G2038	A2039	G2110	C2111	G2112	U2041	A2042	C2043	G2044	C2045	A2046	U2047
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● Molecule 58: 23S ribosomal RNA



A6	G7	A8	B9	G10	G11	U12	A13	A14	G15	G16	G17	G18	C19	C20	A21	G22	G23	G24	G30	C31	C32	U33	C34	G35	G36	C37	A38	C39	C40	G41	G42	G43	A44	A45	G46	G47	G48	A49	A50	A51	A52	A53	G54	G55	A56	C57	G58	G61	G62	U63	A64	C65	C66	U67	G68	C69	G70	A71	U72
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C151	G152	G153	G154	U162	U163	G173	G174	G175	G176	G177	G178	G179	A180	G181	G182	C183	C184	U185	G186	G187	G188	G189	A190	U193	G194	A195	C196	G197	C198	A199	U200	C201	U202	C203	A204	G205	U206	A207	C208	C209	C210	G211	G212	G213	G214	G215	A216	G217	A218	A219	A220	A221	A222	A223	G226	A227	A228
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A229	U230	C231	C232	A233	C234	U235	C236	C237	C238	U239	G240	A241	G242	U243	A244	C245	C246	G247	G248	C249	G250	A251	G252	A256	A257	G258	C259	G260	G261	C262	C263	U264	A265	A266	C267	C268	U269	A270A	U270B	A270C	C270D	C270E	U270F	U270G	C270H	C270I	C270J	G270K	C270L	U270M	U270N	U270O	U270P	C270Q	C270R	G270S	G270T	G270U
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G270X	G270Y	G271C	U271D	G271	G272	G273A	G273B	C273C	C273D	U273G	G274	G275	A276	A277	A278	C279	C287	C288	A289	C290	C291	A294	G295	C296	C297	G298	A299	A300	G301	C302	U303	G304	U305	U306	G307	G308	C309	A310	A311	C319	A320	G321	A322	G323	A324	G325	G326	G329	A330	A331	A332	C334
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C335	C336	C337	A340	G349	U350	G351	G352	G353	G354	G355	G363A	G363D	A363G	C364	C365A	C366B	G370	A371	G372	U373	A374	A375	C376	C377	C378	G379	U380	G381	G382	U383	U384	C385	G386	U387	G388	C389	A390	G391	C392	C393	A394	U395	G396	G397	G398	G399	A400	A401	A402	U403	C404	U405	A406	G407
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G408	C409	G410	G411	C412	C413	C414	A415	C420	U421	G422	A423	A424	G424	C430	U431	A432	C433	U434	C435	C436	G437	G438	A439	G440	U441	G442	A443	C444	C445	G446	A447	U448	A449	G450	C451	G452	C453	A454	C455	C456	A457	G458	U459	A460	C461	C462	C463	U464	G465	A466	G467	G468	C469	A470	A471	A472	G473	C474	U475
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G476	A477	A479	A480	C481	A482	A483	C484	C485	C486	C487	C488	G489	A491	A492	G493	G494	G495	A496	G500	U501	A502	A503	U504	C505	A506	C507	U508	U509	C510	G511	G512	A513	C516	C517	G518	G521	G522	G523	U524	G525	U526	A527	A528	A529	G530	C531	G532	G533	C534	U535	A536	G539	G540
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C541	C542	G545	C546	C547	A548	G549	G556	U557	G558	G559	C560	U562	G563	C564	G565	U566	G568	U569	G570	A571	A572	G573	C574	C575	C576	U577	A578	G579	C580	C581	G582	G583	C584	G585	A586	C587	U588	C589	A590	C591	G592	G593	U594	C595	G596	U597	G598	C599	G600	C601	C602	U603	A603	A604	G605	U606
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U607	A608	A609A	G609B	C610	C611	C612	A616	G617	G618A	C618B	G619	G620	A621	G622	G623	C624	G625	U626	A627	G628	G629	G630	A631	A632	A633	C634	C635	C636	C637	A638	C639	G640	A643	A644	C645	A646	C647	C648	C649	C650	G651	U652	U653	C654	A655	G656	U657	C658	C659	C660	C661	C662	G663	A664	G665	C666
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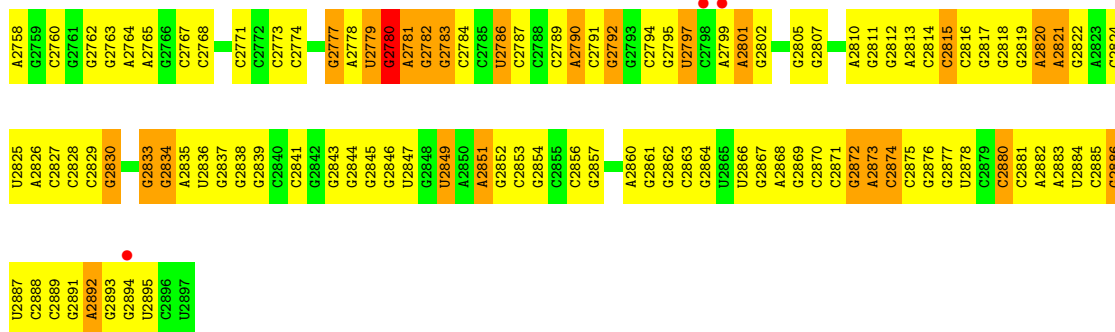
U667	G668	C671	C672	C673	G674	A675	A676	A677	G681	G682	C683	G684	G685	C686	U688	A689	G690	C691	C692	C693	U694	G695	G696	G697	A706	U709	G710	G715	A716	G717	A718	C719	C720	C721	A722	C723	U724	G725	G728	C729	C730	C662	G733	A734	A735	C736	C737
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G738	G739	U740	G741	G742	G743	G744	U747	A751	A752	C753	C754	C755	U757	C758	A761	U762	G763	A764	G765	C766	U767	G768	G769	G770	A774	G775	C776	U779	A781	A782	A783	A784	G785	C786	U787	C788	A789	C790	C791	G792	C793	U794	C795	C796	C797	G798	G799	A800	G801	A804	U805	G805
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C806	U807	C808	C809	U810	U811	C812	U813	C814	C815	C816	C817	C818	A819	A820	A821	C825	U826	U827	U828	A829	C830	C831	C832	U833	C834	A835	C836	C837	C838	C839	C840	A841	C842	G845	C846	U847	C848	A849	C850	U851	C852	G853	C854	G855	C856	C857	U858	C859	C862	A863	G864	C865	A866	C867	U868	C869
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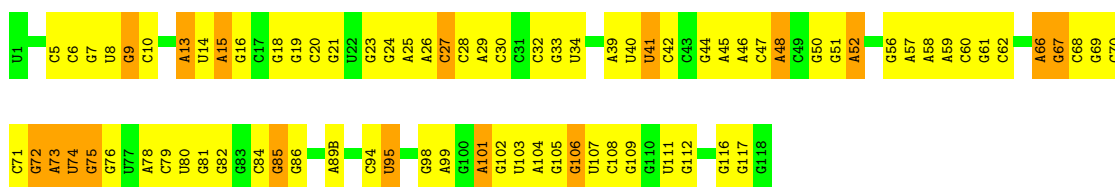
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U1709	C1648	U1514	C1386	A1317	G1248	G1187	G1125	U1061	U999	C936	U871
C1710	A1583	C1515	G1387	A1321	U1249	U1188	A1126	G1082	A1000	U937	A872
C1711	C1585	U1516	G1388	A1322	G1249	U1189	A1127	G1083	A1001		G873
C1712	A1586	C1517	G1389	U1323	G1250	G1190	A1128	C1084	G1002	G940	G874
U1716	A1587	C1518	U1390	G1324	A1253	G1193	A1129	U1065	G1003	G941	G875
G1717	C1588	U1519	U1391	G1325	A1254	G1194	U1130	U1066	G1004	G942	G876
A1684	C1589	A1451	A1451	G1326	U1255	A1194	G1131	A1067	C1005	U943	U877
A1655	U1590	A1454	U1394	C1327	U1256	A1195	A1132	G1068	C1006	U944	A878
G1726	C1591	G1455	U1395	G1328	A1262	C1196	U1133	A1069	C1007	A945	G879
U1727	G1594	C1458	U1396	U1329	A1263	C1197	U1135	A1070	C1008	A946	G880
C1658	G1595	U1459	U1397	C1330	G1264	U1198	G1136	G1071	A1009	G947	G881
A1729	U1659	A1459	A1331	G1331	G1264	U1199	G1137	G1072	G882	G948	G882
U1730	C1660	A1460	G1332	G1332	A1265	C1200	G1138	A1073	G1011	C949	G883
A1731	G1661	G1461	U1335	C1201	C1201	C1201	G1139	G1074	U1012	G950	G884
A1732	C1598	C1462	U1336	G1268	A1268	C1140	G1140	G1075	U1013	C951	
G1733	C1599	G1463	A1336	G1401	A1269	C1141	C1076	A1077	C1013	C951	A887
A1664	C1600	C1464	C1403	A1269	A1270	G1203	U1141	U1078	G1016	G954	C888
G1665	U1602	G1465	G1338	G1337	G1271	U1205	U1142	C1079	G1017	C955	C889
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A1668	C1604	U1406	U1406	U1340	U1273	C1207	G1144	U1081	U1019	G957	G892
A1669	C1605	C1407	C1408	U1341	A1274	A1210	C1145	U1082	A1020	U958	C893
C1670	C1537	A1469	C1409	G1342	A1275	A1211	C1146	U1083	A1021	A959	C894
U1748	A1671	G1470	G1343	G1343	G1276	U1211	C1147	U1084	U1022	A960	U895
A1749	U1609	A1471	G1410	G1344	G1277	G1212	A1148	A1084	G1023	C961	A896
G1750	A1673	A1472	C1411	C1345	A1278	A1213	G1149	A1085	G1024	G962	C897
C1751	G1674	G1473	G1346	G1346	G1279	A1214	C1150	A1086	G1025	U963	A900
C1675	G1542	C1474	G1347	G1347	G1280	G1215	G1151	C1087	U1026	C964	A901
A1676	A1543	U1415	G1348	U1348	G1281	G1216	C1152	A1088	A1027	C965	C902
A1677	C1544	G1416	A1349	A1349	A1286	G1217	G1153	C1089	A1028	G966	C903
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U1679	A1546	G1418	C1351	U1351	U1288	G1219	A1155	G1091	G1030	G968	U905
U1680	C1617	U1419	U1352	C1352	C1289	A1220	A1156	C1092	G1031	U969	U906
G1681	A1618	G1483	A1353	C1353	C1290	C1221	G1157	G1093	A1032	C970	G906
C1683	C1547	G1484	A1354	A1354	C1291	C1222	C1158	U1094	U1033	C971	U907
G1684	C1548	G1485	G1421	G1421	U1292	C1223	U1159	A1095	G1034	G972	C908
C1685	C1550	G1486	G1422	G1355	C1293	G1224	C1160	A1096	U1035	A973	A909
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U1693	G1563	A1496	C1432	U1372	A1302	G1232	C1169	G1107	A1045	C982	A917
C1694	A1563	U1497	U1433	C1375	A1303	C1233	G1170	A1046	A1046	A983	A918
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A1701	U1639	U1503	A1439	G1379	G1309	G1239	A1177	G1052	A990	A990	A926
G1702	C1640	C1504	G1440	G1378	G1310	U1240	C1177	C1053	C991	G991	G928
G1703	A1641	C1505	G1441	A1379	G1311	A1241	C1179	A1054	C992	C992	G929
C1704	G1642	U1506	G1442	G1380	U1312	A1242	C1180	G1116	A1048	G993	U930
A1791	G1645	A1509	G1443	G1381	U1313	G1243	G1183	G1120	G1049	C994	G931
G1792	A1510	A1510	G1444	G1382	C1314	G1244	G1184	C1121	A1049	C995	A932
U1796	C1646	A1444	A1444	C1383	C1314	G1244	C1185	G1122	G1050	A996	A933
		A1512	C1445	A1384	U1316	A1246	C1185	C1123	G1059	G997	G934

C1797	U1864	G1954	U2022	C2084	G2151	G2228	G2300	G2362	A2435	G2489	U2554	C2622	C2690	
U1796	A1871	U1955	G2023	C2085	G2154	C2229	C2301	C2363	A2426	G2490	G2557	G2625	C2695	
C1800	A1872	U1956	G2024	U2086	G2155	C2230	G2302	C2364	C2427	U2493	G2558	C2626	U2696	
G1801	G1878	C1957	C2025	G2087	G2156	C2231	G2303	G2365	G2428	G2494	C2559	G2627	G2697	
A1802	C1879	C1958	G2026	G2088	G2157	U2232	G2304	A2366	A2429	G2495	A2564	A2628	C2698	
A1803	C1879	C1958	G2027	U2089	G2158	G2233	C2305	C2368	U2431	C2496	A2564	A2629	C2699	
C1806	A1884	U1963	A2030	G2090	G2159	G2234	C2306	C2369	U2432	A2497	A2565	G2630	C2700	
G1807	A1885	U1964	A2031	U2091	G2160	C2235	G2307	A2369	A2432	A2497	A2566	G2631	C2701	
U1808	A1886	U1965	A2032	G2092	G2161	C2236	G2308	C2370	C2433	C2498	A2567	G2632	U2702	
C1809	C1887	C1966	A2033	G2093	G2162	G2237	A2309	C2371	A2434	C2499	C2568	A2633	C2703	
A1810	A1888	U1967	G2034	G2094	U2166	U2238	A2310	G2372	A2435	U2500	G2569	G2634	C2704	
G1811	A1889	U1968	U2035	C2095	U2167	G2239	U2311	C2373	G2436	G2501	G2570	U2636	A2705	
A1812	A1890	U1969	C2036	U2096	G2168	C2240	U2312	G2374	G2437	G2502	C2571	U2637	G2706	
G1813	G1891	A1970	G2037	G2097	G2169	A2241	C2313	G2375	A2438	A2503	C2572	U2638	G2707	
A1814	G1892	A1971	G2038	G2101	A2170	C2242	G2314	A2376	C2440	U2504	A2573	G2639	G2708	
A1815	G1893	A1972	C2039	U2102	A2171	U2243	G2315	A2377	C2441	G2505	C2574	A2639	C2709	
G1816	C1900	G1973	C2040	U2103	A2172	U2244	C2316	A2378	C2442	U2506	G2575	G2640	C2710	
G1817	A1900	G1974	U2041	G2104	A2173	G2245	G2318	C2380	G2445	G2508	G2576	G2642	A2711	
U1818	A1901	U1975	U2042	G2106	C2174	G2246	G2319	C2381	G2446	G2509	A2577	G2643	U2712	
A1819	A1902	U1976	A2043	G2107	C2175	C2247	G2320	G2382	G2447	C2510	G2578	C2646	A1712B	
U1820	G1903	A1977	C2044	U2107	A2176	C2248	G2321	G2383	A2448	U2511	C2579	U2647	A2713	
A1821	G1904	U1978	C2045	C2108	A2177	U2249	G2322	G2384	U2449	C2512	U2580	U2648	G2714	
G1822	C1905	U1979	G2046	C2109	C2178	G2250	G2323	C2385	U2450	G2513	G2581	C2648	C2715	
G1823	G1906	U1980	U2047	G2110	C2179	C2251	G2324	C2386	A2451	U2514	G2582	U2649	U2716	
A1824	C1907	A1881	G2048	C2111	U2180	G2252	G2325	U2387	C2452	C2515	G2583	U2650	G2717	
A1825	A1911	C1982	G2049	G2112	G2181	U2253	C2326	U2388	A2453	G2516	U2584	C2651	G2718	
G1826	A1912	U1983	C2050	U2113	G2182	G2254	G2327	U2389	G2454	G2517	U2585	C2652	G2719	
C1827	A1913	C1984	G2051	A2114	G2183	U2255	A2328	G2391	G2455	A2518	C2586	U2653	U2720	
G1828	A1914	U1985	A2052	G2115	G2184	G2256	G2329	A2392	G2456	U2519	A2587	U2654	A2721	
A1829	U1915	C1986	G2053	G2116	C2185	U2257	G2330	G2393	U2457	C2520	A2590	U2655	G2722	
C1830	A1916	U1987	A2054	U2117	G2186	U2258	G2331	G2394	G2458	C2521	U2591	U2656	C2723	
A1831	A1918	C1988	C2055	U2118	G2187	U2259	U2332	C2395	A2459	U2522	C2592	A2657	C2724	
U1834	C1924	U1989	A2056	G2119	U2189	A2260	G2333	C2396	U2462	G2525	G2593	G2658	A2725	
C1924	C1924	C1989	A2057	U2120	G2190	A2261	G2334	G2397	U2463	G2526	U2594	G2659	U2726	
A1927	A1928	G2000	A2058	G2121	G2191	A2262	A2335	U2398	C2464	C2527	C2595	G2660	G2727	
G1842	G1929	A2001	A2059	C2122	G2192	A2263	G2336	G2399	C2465	U2528	G2596	G2661	U2728	
C1843	G1930	G2002	G2060	U2122	G2193	A2264	G2337	G2400	C2466	G2529	A2598	A2662	G2729	
G1844	U1931	G2003	C2061	G2125	C2196	U2271	U2338	U2401	C2467	A2530	G2599	G2663	C2730	
G1845	A1932	A2004	A2062	A2126	U2197	A2272	G2340	C2403	C2468	A2531	A2600	A2664	G2731	
G1846	A1932	A2005	C2066	C2128	U2198	A2273	G2341	C2404	A2469	G2532	C2601	A2665	A2732	
A1847	G1933	G2006	G2067	U2130	A2199	A2274	C2342	G2405	G2470	G2533	A2602	C2666	G2733	
A1848	G1934	C2007	G2068	G2131	G2207	U2275	C2343	U2408	G2471	G2534	G2603	C2667	G2736	
G1849	G1935	G2008	U2068	U2132	U2208	A2276	U2344	U2409	G2472	G2535	U2604	G2668	G2737	
G1850	A1936	C2009	G2069	G2133	C2209	G2282	A2346	G2409	U2473	G2536	U2605	A2669	C2742	
U1851	A1937	G2010	G2070	A2134	G2210	C2283	C2347	G2410	G2476	U2537	G2606	G2670	C2743	
C1852	A1938	G2011	A2071	A2135	G2211	C2284	U2348	A2411	C2477	C2538	G2607	G2671	G2744	
A1853	U1939	G2012	G2072	C2136	A2212	C2285	G2349	A2412	A2478	C2539	U2608	A2679	C2745	
G1854	U1940	G2013	G2073	C2137	U2213	A2286	C2350	G2415	G2479	U2540	U2609	C2680	U2746	
G1855	U1940	A2013	U2074	U2138	G2215	A2287	G2351	C2416	C2480	A2541	G2610	C2681	G2747	
G1856	C1947	A2014	U2075	C2139	G2216	A2288	A2352	C2417	C2481	G2542	U2611	U2682	A2748	
G1857	G1948	A2015	G2078	U2144	G2217	G2290	G2353	A2418	G2482	G2543	C2612	C2683	A2749	
A1858	G1949	A2016	U2079	U2145	G2218	U2291	G2354	U2419	C2483	G2544	U2613	G2684	C2744	
A1859	G1950	U2017	G2080	C2146	G2219	C2292	U2355	C2420	G2484	U2545	C2614	G2685	G2745	
G1860	U1951	G2018	G2081	G2147	G2224	C2293	C2356	G2421	G2485	U2547	G2615	G2686	U2746	
A1952	A2020	A2019	A2082	G2148	A2225	C2294	G2358	A2422	G2486	U2548	U2616	U2687	G2747	
G1863	A1953	C2021	G2083	G2149	A2227	G2299	A2361	C2424	A2488	G2549	C2617	U2688	U2756	
													U2755	A2757



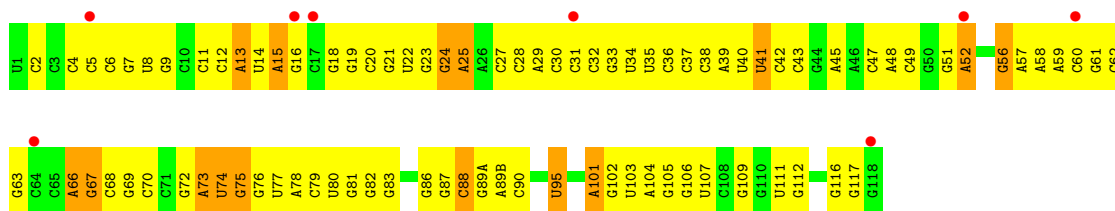
• Molecule 59: 5S ribosomal RNA

Chain BB:



• Molecule 59: 5S ribosomal RNA

Chain DB:



4 Data and refinement statistics i

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 – 4.00 145.84 – 3.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-4.00) 77.8 (145.84-3.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 4.01Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.281 , 0.329 0.285 , 0.324	Depositor DCC
R_{free} test set	25982 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	74.5	Xtrriage
Anisotropy	0.337	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 14.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.24$, $\langle L^2 \rangle = 0.09$	Xtrriage
Estimated twinning fraction	0.249 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	308068	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtrriage'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	0.37	0/1945	0.70	1/2621 (0.0%)
1	CB	0.37	0/1945	0.70	1/2621 (0.0%)
2	AC	0.27	0/1645	0.53	0/2216
2	CC	0.27	0/1645	0.55	0/2216
3	AD	0.29	0/1733	0.61	1/2318 (0.0%)
3	CD	0.29	0/1733	0.57	0/2318
4	AE	0.28	0/1172	0.58	1/1576 (0.1%)
4	CE	0.30	0/1172	0.57	1/1576 (0.1%)
5	AF	0.28	0/856	0.59	1/1154 (0.1%)
5	CF	0.29	0/856	0.57	1/1154 (0.1%)
6	AG	0.27	0/1276	0.52	0/1709
6	CG	0.28	0/1276	0.53	0/1709
7	AH	0.29	0/1136	0.61	0/1527
7	CH	0.28	0/1136	0.58	0/1527
8	AI	0.28	0/1029	0.51	0/1379
8	CI	0.26	0/1029	0.52	0/1379
9	AJ	0.25	0/815	0.56	1/1095 (0.1%)
9	CJ	0.27	0/815	0.58	1/1095 (0.1%)
10	AK	0.33	0/900	0.66	1/1213 (0.1%)
10	CK	0.35	0/900	0.63	0/1213
11	AL	0.39	0/992	0.86	1/1327 (0.1%)
11	CL	0.38	0/992	0.83	1/1327 (0.1%)
12	AM	0.28	0/1008	0.62	1/1347 (0.1%)
12	CM	0.25	0/1008	0.55	0/1347
13	AN	0.28	0/501	0.49	0/664
13	CN	0.28	0/501	0.47	0/664
14	AO	0.31	0/745	0.56	0/992
14	CO	0.28	0/745	0.56	0/992
15	AP	0.28	0/722	0.51	0/970
15	CP	0.26	0/722	0.50	0/970
16	AQ	0.37	0/848	0.71	0/1131
16	CQ	0.36	0/848	0.72	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.29	0/579	0.60	0/768
17	CR	0.27	0/579	0.62	0/768
18	AS	0.28	0/647	0.60	1/870 (0.1%)
18	CS	0.28	0/647	0.64	0/870
19	AT	0.32	0/765	0.57	0/1007
19	CT	0.31	0/765	0.57	0/1007
20	AA	0.35	0/36351	1.03	78/56736 (0.1%)
20	CA	0.34	0/36351	1.01	66/56736 (0.1%)
21	AW	0.35	0/1827	1.09	6/2845 (0.2%)
21	CW	0.36	0/1827	1.10	8/2845 (0.3%)
22	AV	0.26	0/568	0.83	0/886
22	CV	0.28	0/568	0.90	0/886
23	AY	0.33	1/5317 (0.0%)	0.70	10/7198 (0.1%)
23	CY	0.34	1/5317 (0.0%)	0.71	6/7198 (0.1%)
24	BC	0.39	0/1774	0.75	0/2391
24	DC	0.41	0/1774	0.75	1/2391 (0.0%)
25	BD	0.33	0/2195	0.68	2/2955 (0.1%)
25	DD	0.34	0/2195	0.67	1/2955 (0.0%)
26	BE	0.31	0/1602	0.66	0/2160
26	DE	0.31	0/1602	0.67	0/2160
27	BF	0.34	0/1663	0.74	2/2249 (0.1%)
27	DF	0.35	0/1663	0.76	2/2249 (0.1%)
28	BG	0.27	0/1499	0.56	0/2016
28	DG	0.33	1/1499 (0.1%)	0.63	3/2016 (0.1%)
29	BH	0.29	0/1298	0.61	0/1751
29	DH	0.31	0/1298	0.59	0/1751
31	BK	0.26	0/1054	0.50	0/1427
31	DK	0.26	0/1054	0.49	0/1427
32	BN	0.34	0/1131	0.66	0/1525
32	DN	0.34	0/1131	0.66	0/1525
33	BO	0.29	0/943	0.57	0/1269
33	DO	0.27	0/943	0.55	0/1269
34	BP	0.29	0/1131	0.61	0/1504
34	DP	0.29	0/1131	0.66	0/1504
35	BQ	0.32	0/1143	0.64	0/1527
35	DQ	0.32	0/1143	0.61	0/1527
36	BR	0.30	0/974	0.63	0/1302
36	DR	0.31	0/974	0.65	0/1302
37	BS	0.33	0/783	0.69	0/1041
37	DS	0.34	0/783	0.73	0/1041
38	BT	0.34	0/1161	0.70	1/1549 (0.1%)
38	DT	0.33	0/1161	0.66	0/1549
39	BU	0.37	0/982	0.62	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DU	0.37	0/982	0.62	1/1306 (0.1%)
40	BV	0.34	0/790	0.71	0/1057
40	DV	0.36	0/790	0.70	0/1057
41	BW	0.30	0/911	0.60	0/1220
41	DW	0.31	0/911	0.65	2/1220 (0.2%)
42	BX	0.27	0/748	0.55	0/1004
42	DX	0.29	0/748	0.58	0/1004
43	BY	0.31	0/831	0.60	0/1108
43	DY	0.30	0/831	0.65	0/1108
44	BZ	0.27	0/1505	0.60	0/2042
44	DZ	0.28	0/1505	0.60	0/2042
45	B0	0.25	0/671	0.51	0/892
45	D0	0.26	0/671	0.56	0/892
46	B2	0.32	0/600	0.59	0/793
46	D2	0.31	0/600	0.61	0/793
47	B3	0.26	0/482	0.54	0/646
47	D3	0.24	0/482	0.54	0/646
48	B5	0.27	0/473	0.55	0/639
48	D5	0.26	0/473	0.58	0/639
49	B6	0.31	0/440	0.72	1/586 (0.2%)
49	D6	0.31	0/440	0.68	1/586 (0.2%)
50	B7	0.32	0/438	0.64	0/575
50	D7	0.30	0/438	0.59	0/575
51	B8	0.31	0/525	0.67	0/691
51	D8	0.29	0/525	0.63	2/691 (0.3%)
52	B9	0.27	0/310	0.55	0/407
52	D9	0.27	0/310	0.50	0/407
53	Be	0.45	1/538 (0.2%)	0.55	0/715
53	De	0.26	0/538	0.51	0/715
56	B1	0.46	0/739	0.84	0/981
56	D1	0.46	0/739	0.86	0/981
57	B4	0.33	0/276	0.62	0/372
57	D4	0.34	0/276	0.58	0/372
58	BA	0.37	3/69437 (0.0%)	1.06	184/108401 (0.2%)
58	DA	0.37	1/69437 (0.0%)	1.05	153/108401 (0.1%)
59	BB	0.35	0/2853	1.07	9/4451 (0.2%)
59	DB	0.34	0/2853	1.03	11/4451 (0.2%)
All	All	0.35	8/330554 (0.0%)	0.94	564/492202 (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 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BA	1914	C	O3'-P	-10.49	1.48	1.61
53	Be	87	LYS	C-N	8.65	1.53	1.34
58	BA	1911	U	O3'-P	-6.43	1.53	1.61
58	BA	1006	C	N1-C2	5.82	1.46	1.40
58	DA	1911	U	O3'-P	-5.77	1.54	1.61

The worst 5 of 564 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CY	500	GLN	CA-C-N	17.19	155.01	117.20
58	BA	1006	C	C6-N1-C2	-16.88	113.55	120.30
58	BA	1006	C	N3-C2-O2	-14.80	111.54	121.90
23	CY	500	GLN	C-N-CA	14.70	158.44	121.70
58	BA	1006	C	N1-C2-O2	13.47	126.98	118.90

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1910	0	1957	137	0
1	CB	1910	0	1957	134	0
2	AC	1621	0	1688	88	0
2	CC	1621	0	1688	70	0
3	AD	1703	0	1763	134	0
3	CD	1703	0	1763	105	0
4	AE	1156	0	1213	66	0
4	CE	1156	0	1213	71	0
5	AF	843	0	857	45	0
5	CF	843	0	857	43	0
6	AG	1257	0	1296	49	0
6	CG	1257	0	1296	49	0
7	AH	1116	0	1177	71	0
7	CH	1116	0	1177	73	0
8	AI	1010	0	1037	56	0
8	CI	1010	0	1037	60	0
9	AJ	802	0	849	52	0
9	CJ	802	0	849	48	0
10	AK	885	0	904	56	0
10	CK	885	0	904	55	0
11	AL	976	0	1062	97	0
11	CL	976	0	1062	110	0
12	AM	997	0	1072	55	0
12	CM	997	0	1072	56	0
13	AN	492	0	529	37	0
13	CN	492	0	529	29	0
14	AO	734	0	771	51	0
14	CO	734	0	771	41	0
15	AP	706	0	725	42	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	60	0
16	CQ	835	0	904	65	0
17	AR	574	0	644	35	0
17	CR	574	0	644	43	0
18	AS	634	0	655	38	0
18	CS	634	0	655	43	0
19	AT	763	0	861	43	0
19	CT	763	0	861	45	0
20	AA	32474	0	16393	1058	0
20	CA	32474	0	16393	1056	0
21	AW	1635	0	831	68	0
21	CW	1635	0	831	51	0
22	AV	503	0	252	13	0
22	CV	503	0	252	16	0
23	AY	5219	0	5290	335	0
23	CY	5219	0	5290	319	0
24	BC	1742	0	1798	162	0
24	DC	1742	0	1798	172	0
25	BD	2145	0	2234	214	0
25	DD	2145	0	2234	202	0
26	BE	1569	0	1634	132	0
26	DE	1569	0	1634	142	0
27	BF	1628	0	1680	141	0
27	DF	1628	0	1680	141	0
28	BG	1474	0	1535	96	0
28	DG	1474	0	1535	80	0
29	BH	1274	0	1342	79	0
29	DH	1274	0	1342	66	0
30	BJ	851	0	196	31	0
30	DJ	851	0	196	41	0
31	BK	1035	0	1082	53	0
31	DK	1035	0	1082	51	0
32	BN	1104	0	1179	205	0
32	DN	1104	0	1180	217	0
33	BO	933	0	996	62	0
33	DO	933	0	996	69	0
34	BP	1114	0	1187	96	0
34	DP	1114	0	1187	97	0
35	BQ	1122	0	1179	68	0
35	DQ	1122	0	1179	69	0
36	BR	960	0	1021	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DR	960	0	1021	79	0
37	BS	775	0	835	77	0
37	DS	775	0	835	68	0
38	BT	1147	0	1207	107	0
38	DT	1147	0	1207	90	0
39	BU	964	0	1020	95	0
39	DU	964	0	1022	103	1
40	BV	779	0	852	70	0
40	DV	779	0	852	72	0
41	BW	900	0	964	53	0
41	DW	900	0	964	56	0
42	BX	734	0	789	42	0
42	DX	734	0	789	50	0
43	BY	818	0	908	59	0
43	DY	818	0	908	53	0
44	BZ	1473	0	1497	83	0
44	DZ	1473	0	1497	76	0
45	B0	662	0	688	41	0
45	D0	662	0	688	42	0
46	B2	598	0	653	30	0
46	D2	598	0	653	38	0
47	B3	477	0	529	19	0
47	D3	477	0	529	30	0
48	B5	459	0	477	27	0
48	D5	459	0	477	45	0
49	B6	433	0	461	27	0
49	D6	433	0	461	29	0
50	B7	430	0	480	37	0
50	D7	430	0	480	30	0
51	B8	517	0	582	49	0
51	D8	517	0	582	43	0
52	B9	307	0	338	22	0
52	D9	307	0	335	14	0
53	Be	686	0	617	0	0
53	De	686	0	615	0	0
54	Bf	156	0	41	0	0
54	Bg	156	0	38	0	0
54	Df	156	0	42	0	0
54	Dg	156	0	40	0	0
55	Bh	151	0	41	0	0
55	Dh	151	0	40	0	0
56	B1	732	0	808	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	D1	732	0	808	78	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	2317	0
59	BB	2551	0	1295	93	0
59	DB	2551	0	1295	94	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	6	0
All	All	308068	0	213012	12886	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 25.

The worst 5 of 12886 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
23:AY:580:MET:HE2	58:BA:1913:A:N1	1.37	1.35
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

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	7
1	CB	233/235 (99%)	152 (65%)	55 (24%)	26 (11%)	0	7
2	AC	205/207 (99%)	156 (76%)	33 (16%)	16 (8%)	1	14
2	CC	205/207 (99%)	148 (72%)	41 (20%)	16 (8%)	1	14
3	AD	206/208 (99%)	145 (70%)	37 (18%)	24 (12%)	0	6
3	CD	206/208 (99%)	150 (73%)	32 (16%)	24 (12%)	0	6
4	AE	149/151 (99%)	124 (83%)	17 (11%)	8 (5%)	2	21
4	CE	149/151 (99%)	116 (78%)	25 (17%)	8 (5%)	2	21
5	AF	99/101 (98%)	73 (74%)	20 (20%)	6 (6%)	1	19
5	CF	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	1	19
6	AG	153/155 (99%)	122 (80%)	23 (15%)	8 (5%)	2	21
6	CG	153/155 (99%)	116 (76%)	28 (18%)	9 (6%)	1	19
7	AH	136/138 (99%)	93 (68%)	29 (21%)	14 (10%)	0	8
7	CH	136/138 (99%)	101 (74%)	22 (16%)	13 (10%)	0	10
8	AI	125/127 (98%)	93 (74%)	28 (22%)	4 (3%)	4	31
8	CI	125/127 (98%)	97 (78%)	22 (18%)	6 (5%)	2	23
9	AJ	97/99 (98%)	73 (75%)	14 (14%)	10 (10%)	0	8
9	CJ	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	1	18
10	AK	117/119 (98%)	85 (73%)	16 (14%)	16 (14%)	0	4
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%)	1	12
12	CM	123/125 (98%)	90 (73%)	24 (20%)	9 (7%)	1	15
13	AN	58/60 (97%)	43 (74%)	8 (14%)	7 (12%)	0	5
13	CN	58/60 (97%)	44 (76%)	8 (14%)	6 (10%)	0	8
14	AO	86/88 (98%)	62 (72%)	15 (17%)	9 (10%)	0	8
14	CO	86/88 (98%)	62 (72%)	20 (23%)	4 (5%)	2	23
15	AP	82/84 (98%)	64 (78%)	14 (17%)	4 (5%)	2	22
15	CP	82/84 (98%)	62 (76%)	16 (20%)	4 (5%)	2	22
16	AQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	CQ	98/100 (98%)	68 (69%)	21 (21%)	9 (9%)	1	11
17	AR	68/70 (97%)	52 (76%)	11 (16%)	5 (7%)	1	15
17	CR	68/70 (97%)	47 (69%)	19 (28%)	2 (3%)	4	32
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	18
19	CT	97/99 (98%)	76 (78%)	17 (18%)	4 (4%)	3	25
23	AY	663/687 (96%)	436 (66%)	147 (22%)	80 (12%)	0	5
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	3
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	3
27	BF	206/208 (99%)	132 (64%)	53 (26%)	21 (10%)	0	9
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	15
28	DG	179/181 (99%)	131 (73%)	35 (20%)	13 (7%)	1	15
29	BH	165/167 (99%)	113 (68%)	32 (19%)	20 (12%)	0	5
29	DH	165/167 (99%)	102 (62%)	42 (26%)	21 (13%)	0	5
31	BK	138/140 (99%)	98 (71%)	30 (22%)	10 (7%)	1	16
31	DK	138/140 (99%)	100 (72%)	31 (22%)	7 (5%)	2	22
32	BN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	0	6
32	DN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	0	6
33	BO	120/122 (98%)	84 (70%)	20 (17%)	16 (13%)	0	4
33	DO	120/122 (98%)	86 (72%)	24 (20%)	10 (8%)	1	13
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%)	1	12
35	DQ	139/141 (99%)	99 (71%)	30 (22%)	10 (7%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BR	115/117 (98%)	80 (70%)	21 (18%)	14 (12%)	0	5
36	DR	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	0	8
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%)	2	21
39	DU	115/117 (98%)	90 (78%)	21 (18%)	4 (4%)	3	29
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%)	1	12
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	17
42	DX	91/93 (98%)	70 (77%)	15 (16%)	6 (7%)	1	17
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	10
45	B0	82/84 (98%)	58 (71%)	17 (21%)	7 (8%)	1	12
45	D0	82/84 (98%)	51 (62%)	24 (29%)	7 (8%)	1	12
46	B2	69/71 (97%)	50 (72%)	13 (19%)	6 (9%)	1	12
46	D2	69/71 (97%)	50 (72%)	16 (23%)	3 (4%)	2	25
47	B3	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	2	21
47	D3	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	2	21
48	B5	57/59 (97%)	41 (72%)	12 (21%)	4 (7%)	1	16
48	D5	57/59 (97%)	36 (63%)	18 (32%)	3 (5%)	2	21
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	25
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%)	4	32
53	Be	70/102 (69%)	35 (50%)	28 (40%)	7 (10%)	0	9
53	De	70/102 (69%)	39 (56%)	24 (34%)	7 (10%)	0	9
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	6

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 [i](#)

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%)	161 (79%)	42 (21%)	1	6
1	CB	203/203 (100%)	158 (78%)	45 (22%)	1	6
2	AC	161/161 (100%)	136 (84%)	25 (16%)	2	16
2	CC	161/161 (100%)	136 (84%)	25 (16%)	2	16
3	AD	180/180 (100%)	142 (79%)	38 (21%)	1	6
3	CD	180/180 (100%)	150 (83%)	30 (17%)	2	14
4	AE	116/116 (100%)	95 (82%)	21 (18%)	1	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CE	116/116 (100%)	92 (79%)	24 (21%)	1	6
5	AF	90/90 (100%)	80 (89%)	10 (11%)	6	26
5	CF	90/90 (100%)	85 (94%)	5 (6%)	21	49
6	AG	126/126 (100%)	112 (89%)	14 (11%)	6	26
6	CG	126/126 (100%)	114 (90%)	12 (10%)	8	31
7	AH	119/119 (100%)	97 (82%)	22 (18%)	1	10
7	CH	119/119 (100%)	104 (87%)	15 (13%)	4	22
8	AI	98/98 (100%)	83 (85%)	15 (15%)	2	16
8	CI	98/98 (100%)	82 (84%)	16 (16%)	2	15
9	AJ	89/89 (100%)	73 (82%)	16 (18%)	1	11
9	CJ	89/89 (100%)	70 (79%)	19 (21%)	1	6
10	AK	90/90 (100%)	76 (84%)	14 (16%)	2	16
10	CK	90/90 (100%)	71 (79%)	19 (21%)	1	6
11	AL	104/104 (100%)	82 (79%)	22 (21%)	1	6
11	CL	104/104 (100%)	74 (71%)	30 (29%)	0	2
12	AM	100/100 (100%)	81 (81%)	19 (19%)	1	9
12	CM	100/100 (100%)	88 (88%)	12 (12%)	5	23
13	AN	49/49 (100%)	40 (82%)	9 (18%)	1	10
13	CN	49/49 (100%)	42 (86%)	7 (14%)	3	19
14	AO	79/79 (100%)	70 (89%)	9 (11%)	5	25
14	CO	79/79 (100%)	68 (86%)	11 (14%)	3	20
15	AP	72/72 (100%)	65 (90%)	7 (10%)	8	30
15	CP	72/72 (100%)	69 (96%)	3 (4%)	30	56
16	AQ	95/95 (100%)	78 (82%)	17 (18%)	2	11
16	CQ	95/95 (100%)	82 (86%)	13 (14%)	3	20
17	AR	61/61 (100%)	53 (87%)	8 (13%)	4	21
17	CR	61/61 (100%)	51 (84%)	10 (16%)	2	14
18	AS	69/69 (100%)	53 (77%)	16 (23%)	1	5
18	CS	69/69 (100%)	53 (77%)	16 (23%)	1	5
19	AT	76/76 (100%)	64 (84%)	12 (16%)	2	16
19	CT	76/76 (100%)	69 (91%)	7 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	AY	563/579 (97%)	466 (83%)	97 (17%)	2	13
23	CY	563/579 (97%)	460 (82%)	103 (18%)	1	11
24	BC	180/180 (100%)	135 (75%)	45 (25%)	0	4
24	DC	180/180 (100%)	139 (77%)	41 (23%)	1	5
25	BD	217/217 (100%)	173 (80%)	44 (20%)	1	7
25	DD	217/217 (100%)	171 (79%)	46 (21%)	1	6
26	BE	165/165 (100%)	134 (81%)	31 (19%)	1	10
26	DE	165/165 (100%)	133 (81%)	32 (19%)	1	9
27	BF	165/165 (100%)	127 (77%)	38 (23%)	1	5
27	DF	165/165 (100%)	133 (81%)	32 (19%)	1	9
28	BG	155/155 (100%)	126 (81%)	29 (19%)	1	10
28	DG	155/155 (100%)	127 (82%)	28 (18%)	1	11
29	BH	136/136 (100%)	111 (82%)	25 (18%)	1	10
29	DH	136/136 (100%)	120 (88%)	16 (12%)	5	24
31	BK	105/105 (100%)	85 (81%)	20 (19%)	1	9
31	DK	105/105 (100%)	88 (84%)	17 (16%)	2	15
32	BN	117/117 (100%)	100 (86%)	17 (14%)	3	18
32	DN	117/117 (100%)	100 (86%)	17 (14%)	3	18
33	BO	100/100 (100%)	84 (84%)	16 (16%)	2	15
33	DO	100/100 (100%)	87 (87%)	13 (13%)	4	22
34	BP	112/112 (100%)	92 (82%)	20 (18%)	2	11
34	DP	112/112 (100%)	88 (79%)	24 (21%)	1	6
35	BQ	111/111 (100%)	88 (79%)	23 (21%)	1	6
35	DQ	111/111 (100%)	87 (78%)	24 (22%)	1	6
36	BR	100/100 (100%)	83 (83%)	17 (17%)	2	13
36	DR	100/100 (100%)	83 (83%)	17 (17%)	2	13
37	BS	77/77 (100%)	63 (82%)	14 (18%)	1	11
37	DS	77/77 (100%)	59 (77%)	18 (23%)	1	4
38	BT	120/120 (100%)	95 (79%)	25 (21%)	1	6
38	DT	120/120 (100%)	91 (76%)	29 (24%)	0	4
39	BU	93/93 (100%)	71 (76%)	22 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DU	93/93 (100%)	75 (81%)	18 (19%)	1	9
40	BV	82/82 (100%)	65 (79%)	17 (21%)	1	6
40	DV	82/82 (100%)	62 (76%)	20 (24%)	0	4
41	BW	92/92 (100%)	71 (77%)	21 (23%)	1	5
41	DW	92/92 (100%)	76 (83%)	16 (17%)	2	12
42	BX	75/75 (100%)	61 (81%)	14 (19%)	1	10
42	DX	75/75 (100%)	60 (80%)	15 (20%)	1	8
43	BY	88/88 (100%)	65 (74%)	23 (26%)	0	3
43	DY	88/88 (100%)	71 (81%)	17 (19%)	1	9
44	BZ	162/162 (100%)	132 (82%)	30 (18%)	1	10
44	DZ	162/162 (100%)	134 (83%)	28 (17%)	2	13
45	B0	66/66 (100%)	52 (79%)	14 (21%)	1	6
45	D0	66/66 (100%)	53 (80%)	13 (20%)	1	8
46	B2	66/66 (100%)	59 (89%)	7 (11%)	6	27
46	D2	66/66 (100%)	60 (91%)	6 (9%)	9	33
47	B3	52/52 (100%)	42 (81%)	10 (19%)	1	9
47	D3	52/52 (100%)	48 (92%)	4 (8%)	13	40
48	B5	51/51 (100%)	41 (80%)	10 (20%)	1	8
48	D5	51/51 (100%)	40 (78%)	11 (22%)	1	6
49	B6	49/49 (100%)	43 (88%)	6 (12%)	5	23
49	D6	49/49 (100%)	38 (78%)	11 (22%)	1	6
50	B7	42/42 (100%)	36 (86%)	6 (14%)	3	19
50	D7	42/42 (100%)	36 (86%)	6 (14%)	3	19
51	B8	54/54 (100%)	37 (68%)	17 (32%)	0	2
51	D8	54/54 (100%)	40 (74%)	14 (26%)	0	4
52	B9	34/34 (100%)	30 (88%)	4 (12%)	5	24
52	D9	34/34 (100%)	32 (94%)	2 (6%)	19	48
53	Be	54/54 (100%)	47 (87%)	7 (13%)	4	22
53	De	54/54 (100%)	46 (85%)	8 (15%)	3	17
56	B1	78/78 (100%)	64 (82%)	14 (18%)	2	11
56	D1	78/78 (100%)	59 (76%)	19 (24%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	B4	31/31 (100%)	26 (84%)	5 (16%)	2	15
57	D4	31/31 (100%)	25 (81%)	6 (19%)	1	9
All	All	11138/11170 (100%)	9124 (82%)	2014 (18%)	1	11

5 of 2014 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	B0	15	ASP
38	DT	11	GLU
4	CE	144	THR
37	DS	13	ARG
44	DZ	70	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
23	CY	625	ASN
32	DN	131	GLN
25	DD	143	HIS
29	DH	111	HIS
36	DR	23	ASN

5.3.3 RNA [i](#)

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%)	665 (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%)	2003 (21%)	88 (0%)

5 of 2003 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 monosaccharides 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	CY	702	-	24,30,30	1.28	2 (8%)	30,47,47	1.56	7 (23%)
60	FUA	AY	701	-	39,40,40	1.64	7 (17%)	49,64,64	2.07	11 (22%)
60	FUA	CY	701	-	39,40,40	1.67	5 (12%)	49,64,64	2.38	13 (26%)
61	GDP	AY	702	-	24,30,30	1.28	2 (8%)	30,47,47	1.56	6 (20%)

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	CY	702	-	-	3/12/32/32	0/3/3/3
60	FUA	AY	701	-	-	8/15/92/92	0/4/4/4
60	FUA	CY	701	-	-	9/15/92/92	0/4/4/4
61	GDP	AY	702	-	-	3/12/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	CY	701	FUA	C23-C22	-4.41	1.39	1.51
60	CY	701	FUA	C23-C24	-4.36	1.39	1.53
60	AY	701	FUA	C23-C22	-4.31	1.40	1.51
60	AY	701	FUA	C23-C24	-4.30	1.39	1.53
60	CY	701	FUA	C29-C22	4.24	1.53	1.47

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CY	701	FUA	C13-C12-C11	-7.76	101.03	111.90
60	AY	701	FUA	C13-C12-C11	-7.72	101.09	111.90
60	CY	701	FUA	C5-C4-C3	-6.75	98.38	110.60
60	CY	701	FUA	C16-O2-C31	-4.91	109.60	117.06
60	CY	701	FUA	C1-C10-C5	4.71	114.44	107.76

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

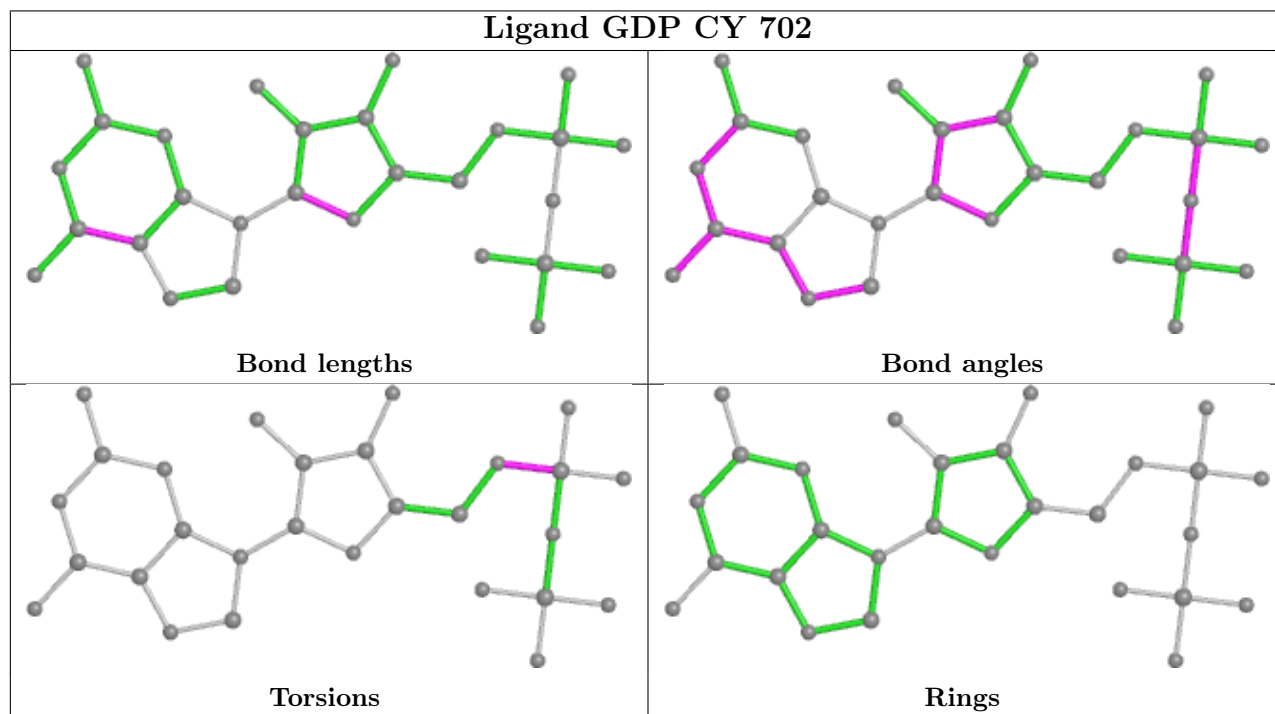
Mol	Chain	Res	Type	Atoms
60	AY	701	FUA	C13-C17-C22-C29
60	AY	701	FUA	C17-C22-C23-C24
60	AY	701	FUA	C29-C22-C23-C24
60	CY	701	FUA	C13-C17-C22-C29
60	CY	701	FUA	C17-C22-C23-C24

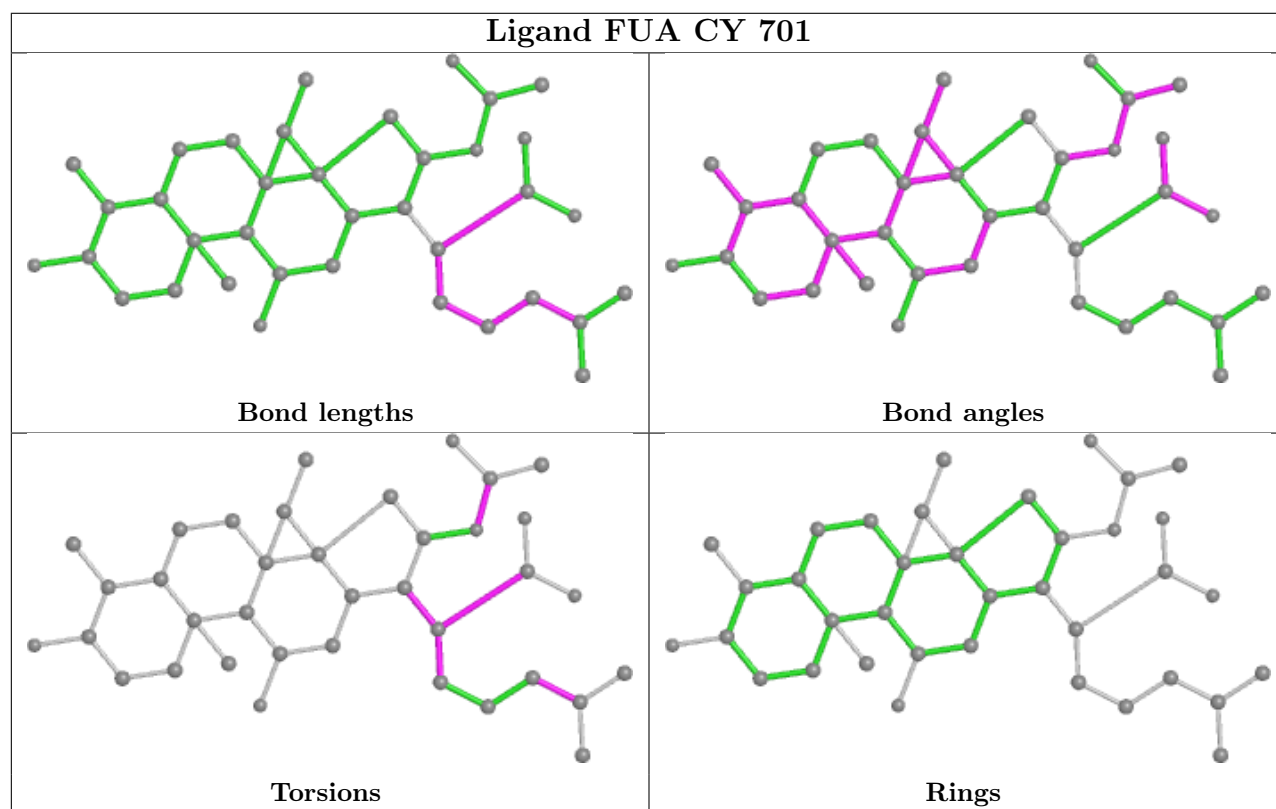
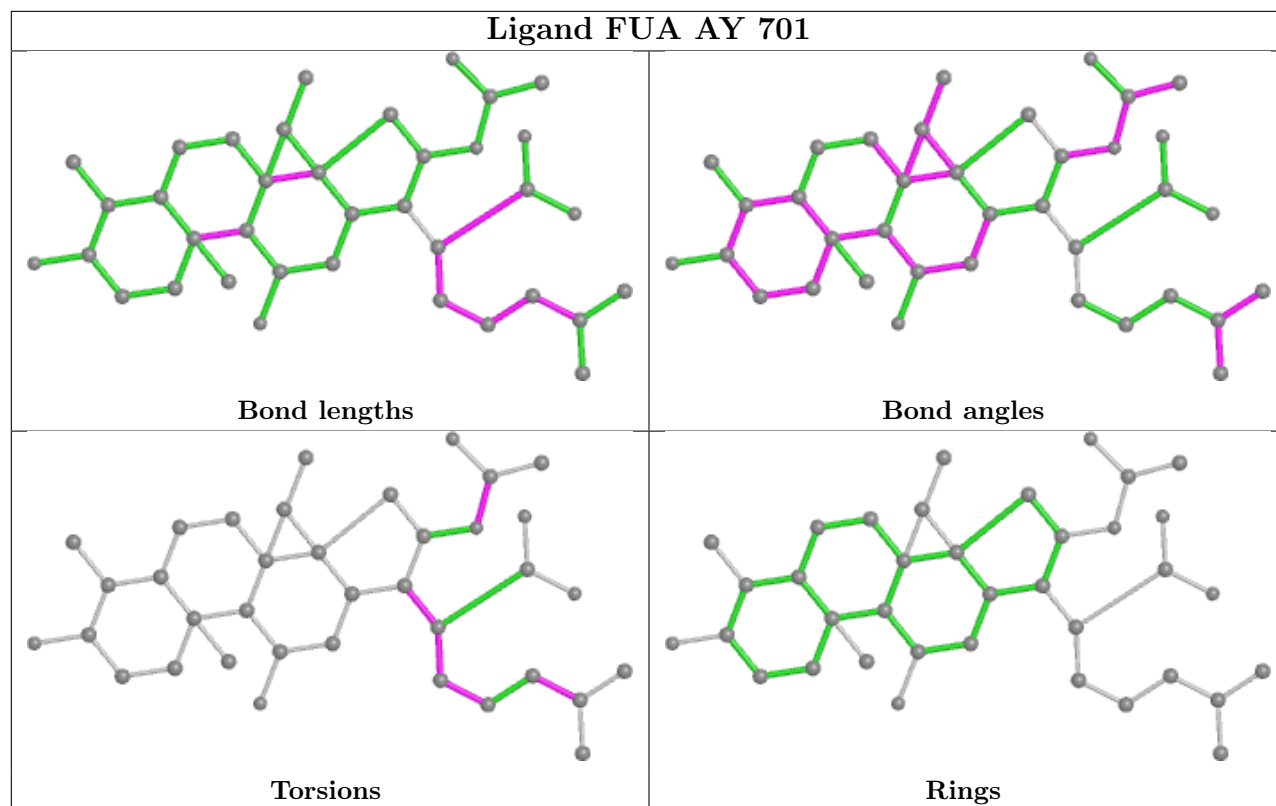
There are no ring outliers.

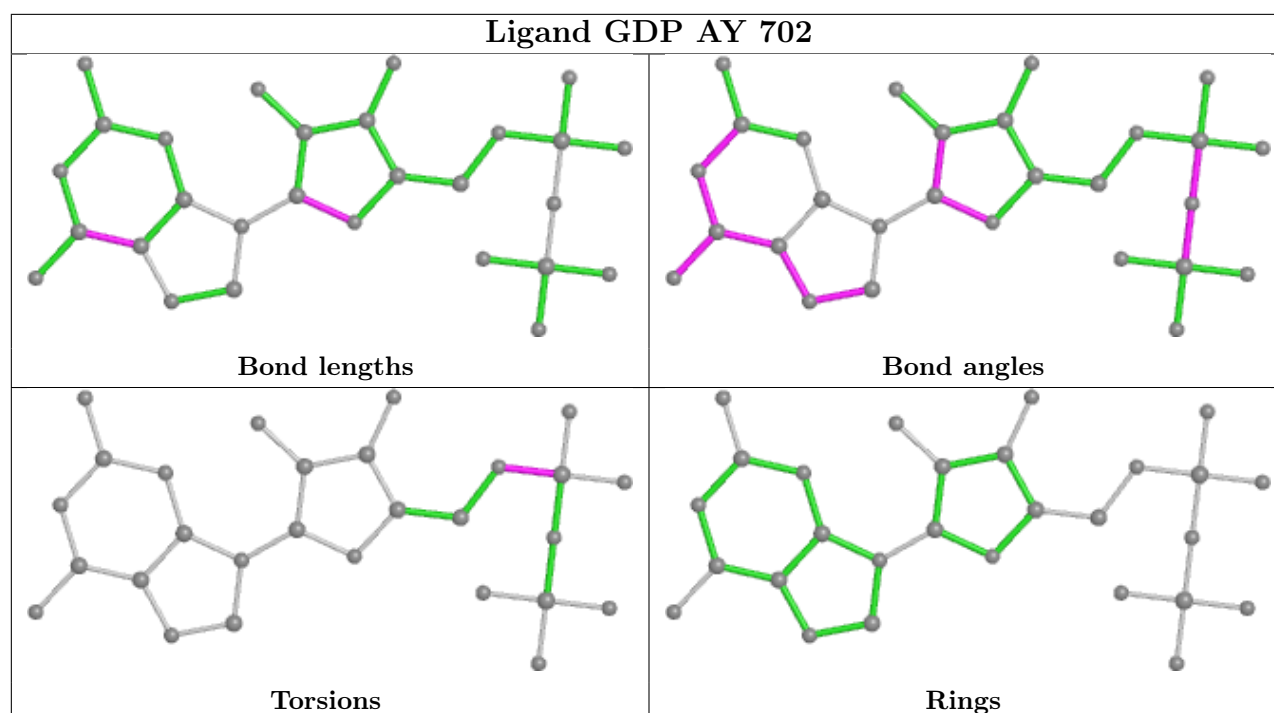
4 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	CY	702	GDP	6	0
60	AY	701	FUA	13	0
60	CY	701	FUA	10	0
61	AY	702	GDP	6	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	235/235 (100%)	-0.59	0 100 100	41, 81, 119, 159	0
1	CB	235/235 (100%)	-0.50	2 (0%) 84 77	38, 80, 117, 178	0
2	AC	207/207 (100%)	0.23	24 (11%) 4 5	34, 76, 116, 152	0
2	CC	207/207 (100%)	0.25	27 (13%) 3 4	44, 78, 121, 158	0
3	AD	208/208 (100%)	-0.57	3 (1%) 75 65	37, 71, 125, 178	0
3	CD	208/208 (100%)	-0.47	4 (1%) 66 58	51, 83, 120, 165	0
4	AE	151/151 (100%)	0.68	29 (19%) 1 1	30, 57, 93, 133	0
4	CE	151/151 (100%)	0.62	33 (21%) 0 1	31, 61, 99, 185	0
5	AF	101/101 (100%)	-0.74	0 100 100	31, 52, 87, 115	0
5	CF	101/101 (100%)	-0.81	0 100 100	25, 52, 78, 129	0
6	AG	155/155 (100%)	0.23	13 (8%) 11 10	54, 100, 147, 204	0
6	CG	155/155 (100%)	0.62	20 (12%) 3 4	57, 99, 155, 218	0
7	AH	138/138 (100%)	-0.09	2 (1%) 75 65	28, 49, 83, 117	0
7	CH	138/138 (100%)	0.24	9 (6%) 18 15	29, 57, 101, 142	0
8	AI	127/127 (100%)	0.37	3 (2%) 59 49	48, 87, 128, 163	0
8	CI	127/127 (100%)	0.25	10 (7%) 12 11	51, 91, 136, 195	0
9	AJ	99/99 (100%)	0.05	8 (8%) 12 11	46, 74, 108, 114	0
9	CJ	99/99 (100%)	-0.09	11 (11%) 5 5	37, 82, 121, 145	0
10	AK	119/119 (100%)	0.07	5 (4%) 36 29	41, 71, 114, 157	0
10	CK	119/119 (100%)	-0.14	5 (4%) 36 29	22, 59, 106, 135	0
11	AL	125/125 (100%)	0.39	14 (11%) 5 5	31, 63, 97, 178	0
11	CL	125/125 (100%)	0.28	12 (9%) 8 7	29, 68, 109, 136	0
12	AM	125/125 (100%)	0.25	11 (8%) 10 9	61, 101, 139, 150	0
12	CM	125/125 (100%)	0.80	21 (16%) 1 2	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%)	0.78	7 (11%) 4 5	42, 64, 97, 106	0
13	CN	60/60 (100%)	0.19	1 (1%) 70 60	47, 67, 112, 156	0
14	AO	88/88 (100%)	-0.52	1 (1%) 80 72	32, 61, 102, 172	0
14	CO	88/88 (100%)	-0.51	0 100 100	29, 61, 108, 215	0
15	AP	84/84 (100%)	1.77	32 (38%) 0 0	47, 80, 118, 187	0
15	CP	84/84 (100%)	1.38	27 (32%) 0 0	53, 81, 118, 174	0
16	AQ	100/100 (100%)	0.40	15 (15%) 2 3	33, 56, 100, 124	0
16	CQ	100/100 (100%)	0.10	4 (4%) 38 30	30, 58, 89, 139	0
17	AR	70/70 (100%)	-0.13	2 (2%) 51 41	30, 55, 101, 156	0
17	CR	70/70 (100%)	-0.17	5 (7%) 16 13	32, 46, 123, 186	0
18	AS	79/79 (100%)	0.32	7 (8%) 9 8	68, 90, 148, 159	0
18	CS	79/79 (100%)	0.59	10 (12%) 3 4	59, 92, 146, 215	0
19	AT	99/99 (100%)	-0.13	4 (4%) 38 30	58, 86, 116, 146	0
19	CT	99/99 (100%)	0.13	3 (3%) 50 39	42, 81, 114, 147	0
20	AA	1511/1511 (100%)	0.05	79 (5%) 27 24	25, 78, 180, 324	0
20	CA	1511/1511 (100%)	0.01	64 (4%) 36 29	19, 82, 182, 332	0
21	AW	77/77 (100%)	-0.32	1 (1%) 77 68	55, 121, 189, 218	0
21	CW	77/77 (100%)	-0.48	0 100 100	58, 118, 230, 278	0
22	AV	23/23 (100%)	1.57	9 (39%) 0 0	70, 138, 188, 222	0
22	CV	23/23 (100%)	2.77	11 (47%) 0 0	88, 142, 211, 231	0
23	AY	667/687 (97%)	-0.26	25 (3%) 41 32	29, 79, 132, 191	0
23	CY	667/687 (97%)	-0.31	20 (2%) 50 39	32, 84, 131, 188	0
24	BC	228/228 (100%)	0.41	22 (9%) 8 7	91, 147, 211, 238	0
24	DC	228/228 (100%)	0.18	15 (6%) 18 14	89, 175, 227, 263	0
25	BD	275/275 (100%)	0.25	26 (9%) 8 7	24, 52, 90, 160	0
25	DD	275/275 (100%)	0.08	17 (6%) 20 17	23, 50, 94, 155	0
26	BE	205/205 (100%)	-0.15	2 (0%) 82 74	25, 52, 97, 202	0
26	DE	205/205 (100%)	-0.11	5 (2%) 59 49	28, 60, 135, 173	0
27	BF	208/208 (100%)	0.17	21 (10%) 7 7	32, 67, 126, 195	0
27	DF	208/208 (100%)	0.42	26 (12%) 3 5	34, 86, 165, 230	0
28	BG	181/181 (100%)	0.78	26 (14%) 2 3	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%)	0.70	26 (14%) 2 3	73, 110, 158, 205	0
29	BH	167/167 (100%)	-0.04	5 (2%) 50 39	38, 64, 111, 161	0
29	DH	167/167 (100%)	-0.09	11 (6%) 18 14	40, 74, 130, 167	0
30	BJ	0/170	-	-	-	-
30	DJ	0/170	-	-	-	-
31	BK	140/140 (100%)	0.04	13 (9%) 8 8	67, 118, 175, 206	0
31	DK	140/140 (100%)	0.01	9 (6%) 19 15	66, 132, 200, 220	0
32	BN	138/138 (100%)	0.21	12 (8%) 10 9	58, 85, 106, 118	0
32	DN	138/138 (100%)	0.10	6 (4%) 35 29	63, 87, 111, 121	0
33	BO	122/122 (100%)	-0.10	2 (1%) 72 62	24, 49, 67, 114	0
33	DO	122/122 (100%)	-0.02	4 (3%) 46 37	30, 56, 88, 124	0
34	BP	146/146 (100%)	-0.18	6 (4%) 37 30	28, 73, 113, 171	0
34	DP	146/146 (100%)	-0.34	4 (2%) 54 44	31, 84, 130, 202	0
35	BQ	141/141 (100%)	-0.56	2 (1%) 75 65	40, 66, 100, 164	0
35	DQ	141/141 (100%)	-0.42	5 (3%) 44 35	36, 64, 104, 161	0
36	BR	117/117 (100%)	-0.67	0 100 100	29, 53, 85, 105	0
36	DR	117/117 (100%)	-0.64	0 100 100	21, 53, 88, 156	0
37	BS	99/99 (100%)	0.07	6 (6%) 21 17	60, 111, 172, 189	0
37	DS	99/99 (100%)	0.90	21 (21%) 0 1	38, 128, 194, 220	0
38	BT	138/138 (100%)	-0.39	3 (2%) 62 52	36, 64, 106, 201	0
38	DT	138/138 (100%)	-0.28	3 (2%) 62 52	32, 71, 115, 216	0
39	BU	117/117 (100%)	-0.30	3 (2%) 56 46	26, 44, 83, 132	0
39	DU	117/117 (100%)	-0.26	3 (2%) 56 46	6, 45, 90, 155	0
40	BV	101/101 (100%)	0.35	11 (10%) 5 5	31, 51, 79, 104	0
40	DV	101/101 (100%)	-0.18	0 100 100	38, 70, 111, 124	0
41	BW	113/113 (100%)	0.15	8 (7%) 16 13	22, 51, 104, 120	0
41	DW	113/113 (100%)	0.41	7 (6%) 20 17	30, 49, 105, 202	0
42	BX	93/93 (100%)	0.13	1 (1%) 80 72	31, 59, 93, 113	0
42	DX	93/93 (100%)	-0.05	1 (1%) 80 72	29, 63, 111, 175	0
43	BY	107/107 (100%)	-0.50	3 (2%) 53 42	35, 71, 133, 156	0
43	DY	107/107 (100%)	-0.50	4 (3%) 41 32	55, 87, 133, 209	0
44	BZ	185/185 (100%)	-0.49	2 (1%) 80 72	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%)	-0.36	4 (2%) 62 52	36, 75, 123, 161	0
45	B0	84/84 (100%)	-0.11	2 (2%) 59 49	38, 70, 99, 162	0
45	D0	84/84 (100%)	0.15	2 (2%) 59 49	33, 67, 139, 212	0
46	B2	71/71 (100%)	-0.48	1 (1%) 75 65	44, 71, 114, 167	0
46	D2	71/71 (100%)	-0.53	0 100 100	53, 76, 129, 183	0
47	B3	60/60 (100%)	-0.61	0 100 100	26, 43, 74, 113	0
47	D3	60/60 (100%)	-0.23	1 (1%) 70 60	27, 57, 99, 111	0
48	B5	59/59 (100%)	-0.39	0 100 100	22, 56, 142, 156	0
48	D5	59/59 (100%)	-0.22	1 (1%) 70 60	18, 67, 175, 198	0
49	B6	50/50 (100%)	-0.20	0 100 100	65, 91, 124, 176	0
49	D6	50/50 (100%)	0.48	8 (16%) 1 2	66, 106, 136, 139	0
50	B7	49/49 (100%)	1.55	12 (24%) 0 0	30, 48, 107, 132	0
50	D7	49/49 (100%)	2.05	17 (34%) 0 0	38, 51, 125, 168	0
51	B8	64/64 (100%)	0.26	1 (1%) 72 62	30, 62, 80, 89	0
51	D8	64/64 (100%)	0.52	3 (4%) 31 26	38, 70, 114, 148	0
52	B9	37/37 (100%)	1.35	14 (37%) 0 0	41, 63, 116, 166	0
52	D9	37/37 (100%)	0.28	1 (2%) 54 44	36, 55, 111, 148	0
53	Be	72/102 (70%)	1.44	23 (31%) 0 0	69, 117, 170, 201	0
53	De	72/102 (70%)	1.21	16 (22%) 0 1	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%)	1.16	26 (27%) 0 0	40, 87, 151, 208	0
56	D1	93/93 (100%)	1.43	26 (27%) 0 0	42, 84, 174, 216	0
57	B4	35/35 (100%)	0.93	7 (20%) 1 1	96, 160, 227, 248	0
57	D4	35/35 (100%)	1.88	16 (45%) 0 0	116, 170, 265, 282	0
58	BA	2879/2879 (100%)	-0.24	21 (0%) 87 82	17, 60, 166, 304	0
58	DA	2879/2879 (100%)	-0.27	18 (0%) 89 84	17, 62, 182, 341	0
59	BB	119/119 (100%)	-0.24	0 100 100	32, 114, 187, 214	0
59	DB	119/119 (100%)	0.20	8 (6%) 17 14	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%)	-0.03	1162 (5%) 28 24	6, 73, 161, 341	0

The worst 5 of 1162 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
50	D7	48	LYS	10.1
56	D1	42	GLN	10.0
6	CG	82	GLY	9.2
53	Be	122	VAL	9.2
24	DC	227	PRO	9.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

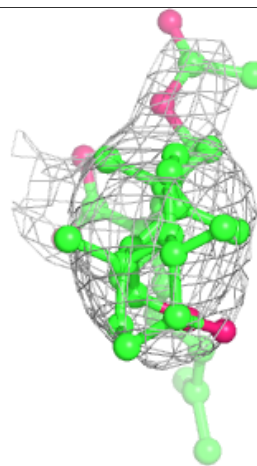
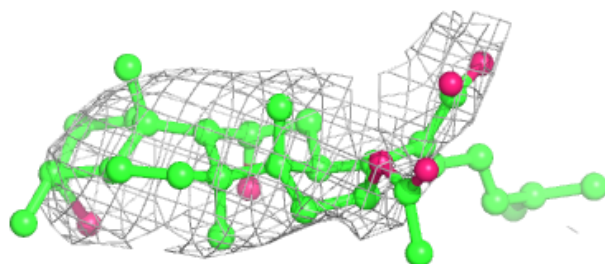
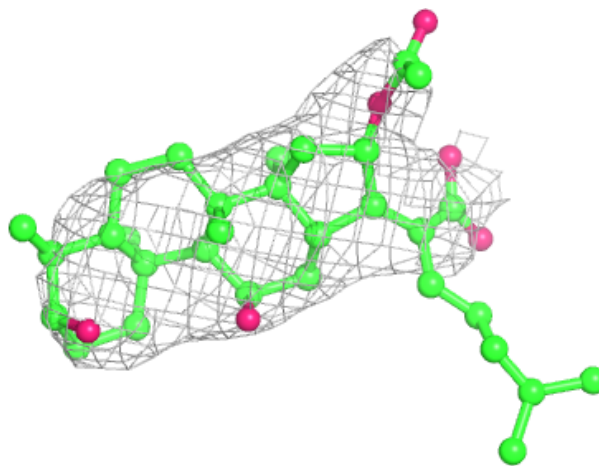
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.85	0.62	119,146,161,162	0
60	FUA	CY	701	37/37	0.92	0.22	125,150,161,166	0
61	GDP	AY	702	28/28	0.93	0.23	58,89,106,121	0
61	GDP	CY	702	28/28	0.96	0.15	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.

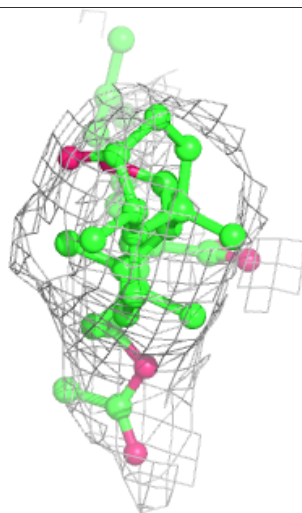
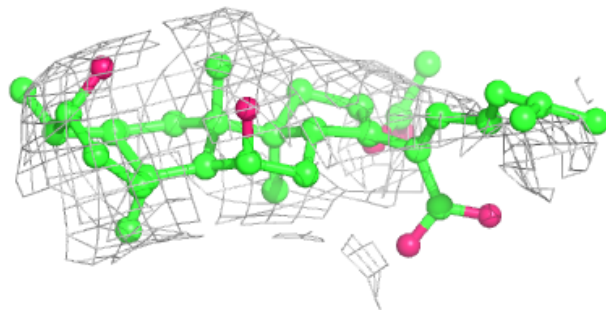
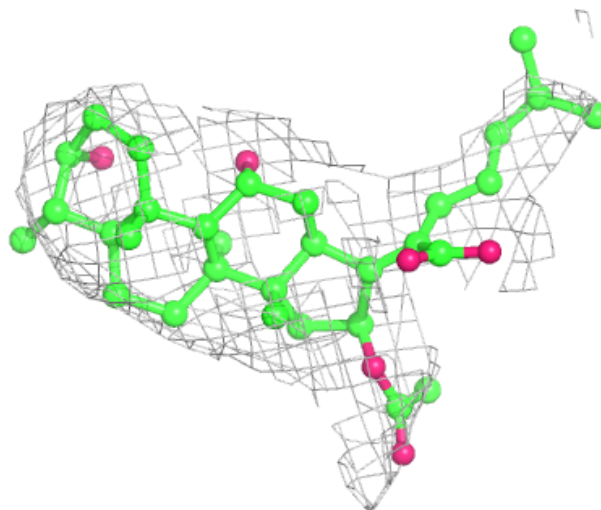
Electron density around FUA AY 701:

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



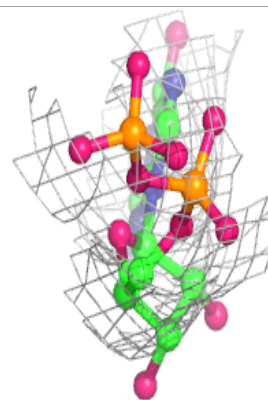
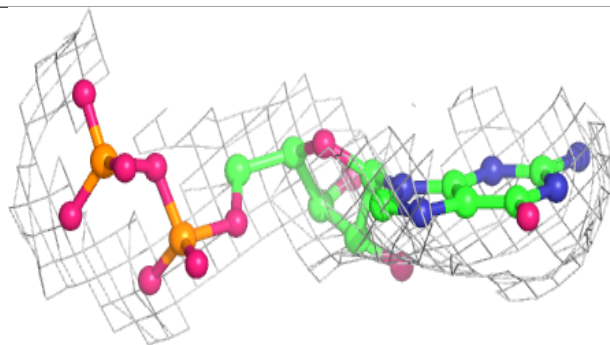
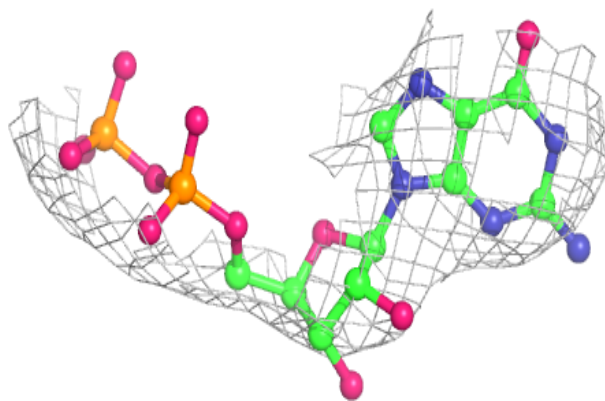
Electron density around FUA CY 701:

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

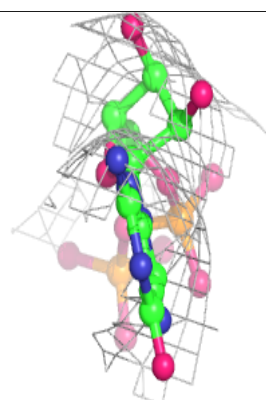
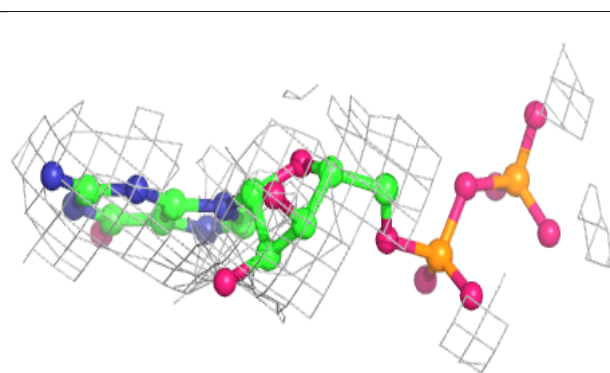
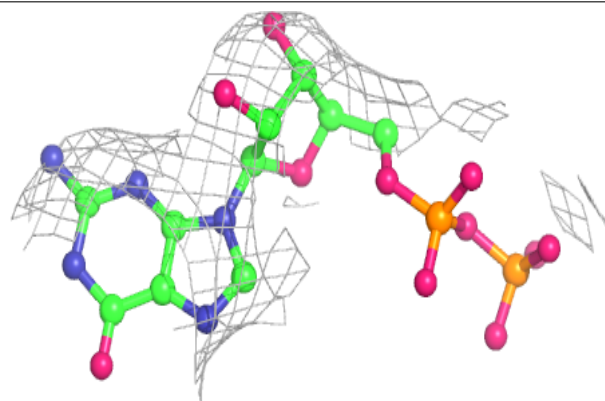


Electron density around GDP AY 702:

$2mF_o-DF_c$ (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.