



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:11 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

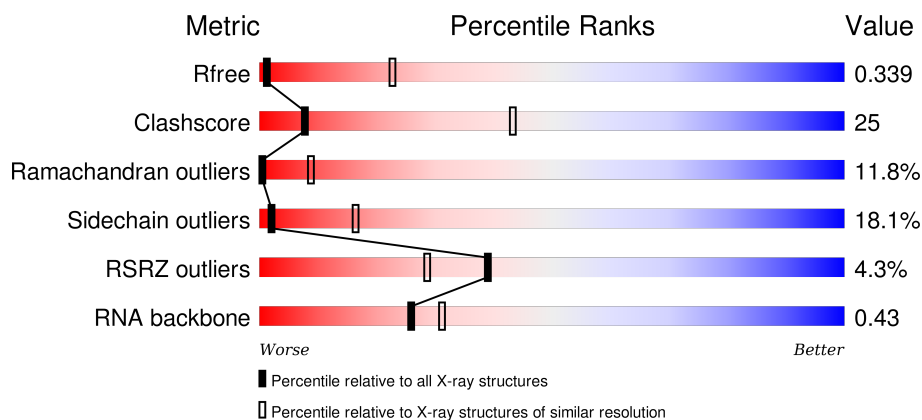
1 Overall quality at a glance

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}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)
RNA backbone	2183	1079 (5.04-2.80)

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

Mol	Chain	Length	Quality of chain
1	AB	235	
1	CB	235	
2	AC	207	
2	CC	207	

Continued on next page...

Continued from previous page...

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	

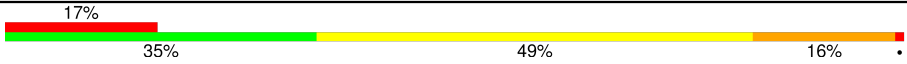

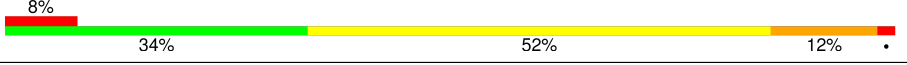
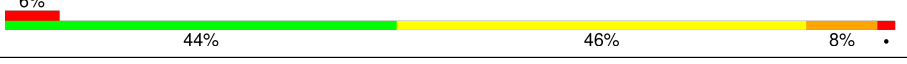
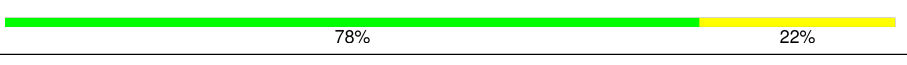
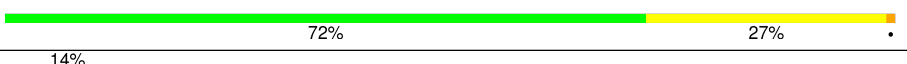


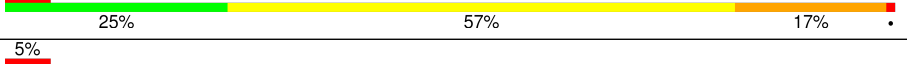
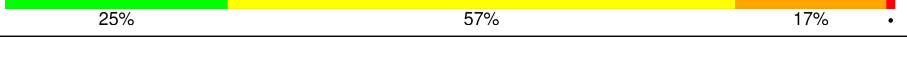

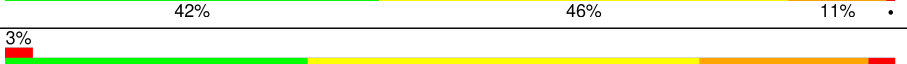
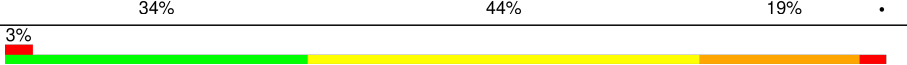
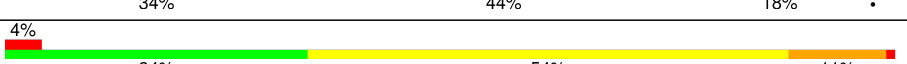
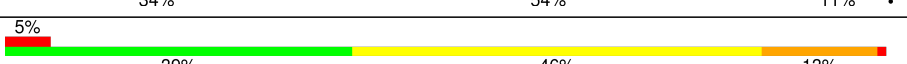
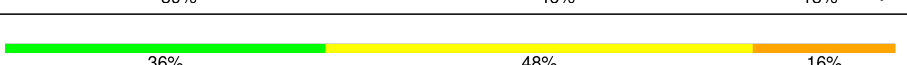
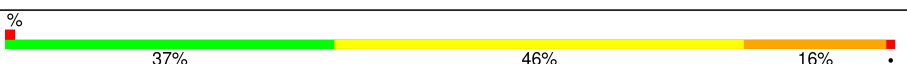
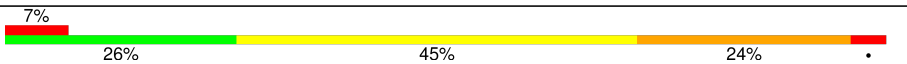
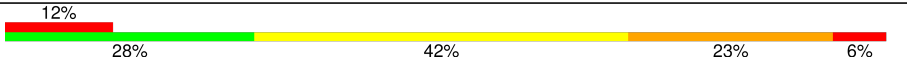
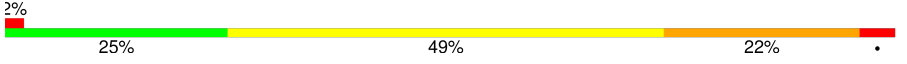
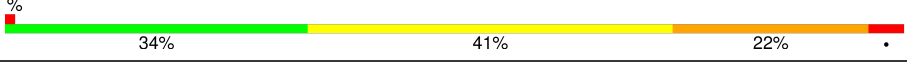
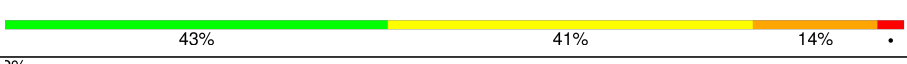

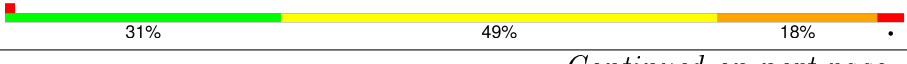

Continued on next page...

Continued from previous page...

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	

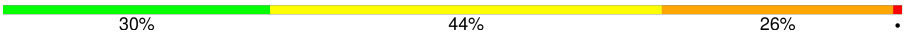

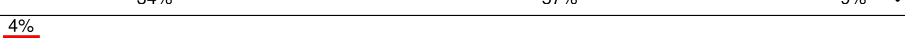
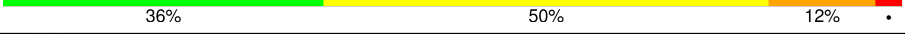
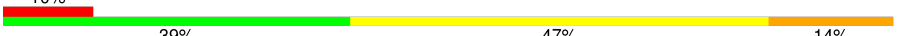
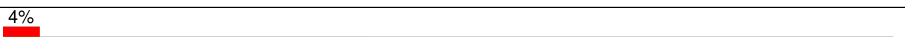
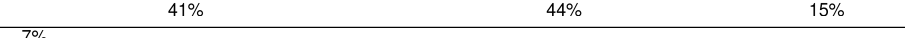
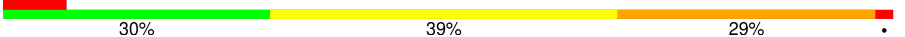

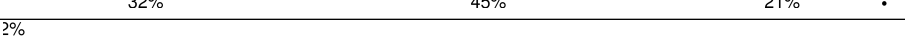
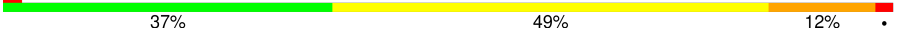
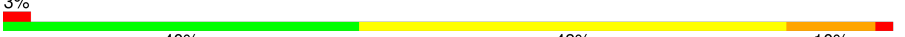
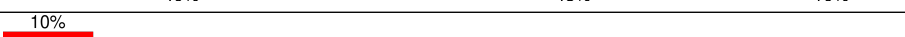


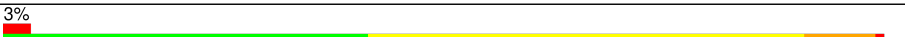
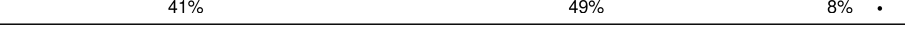
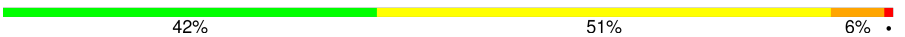

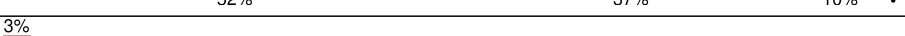


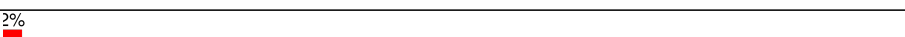


Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	Be	102	
53	De	102	
54	Bf	31	
54	Bg	31	
54	Df	31	
54	Dg	31	
55	Bh	30	
55	Dh	30	
56	B1	93	
56	D1	93	
57	B4	35	
57	D4	35	
58	BA	2879	
58	DA	2879	
59	BB	119	
59	DB	119	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	FUA	AY	701	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 308068 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 30S ribosomal protein S2.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 21 is a RNA chain called transfer RNA.

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

- Molecule 22 is a RNA chain called messenger RNA.

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

- Molecule 23 is a protein called Elongation factor G.

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

There are 4 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 10 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

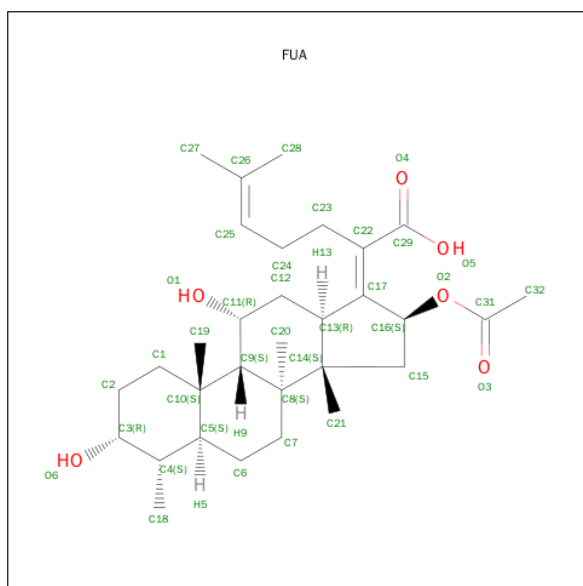
- Molecule 58 is a RNA chain called 23S ribosomal RNA.

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

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

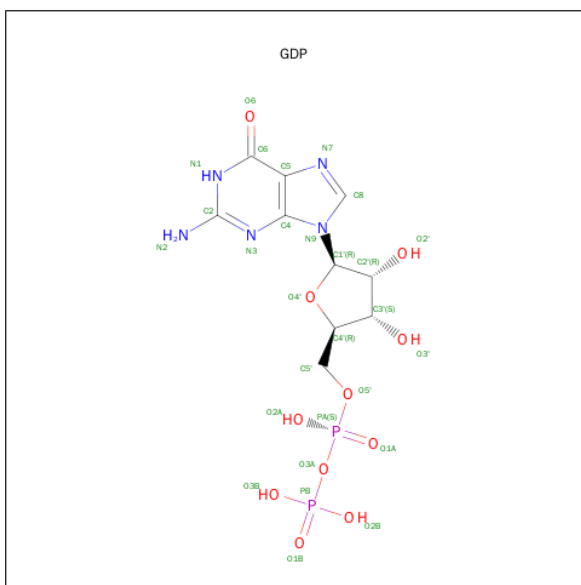
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
59	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

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



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

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

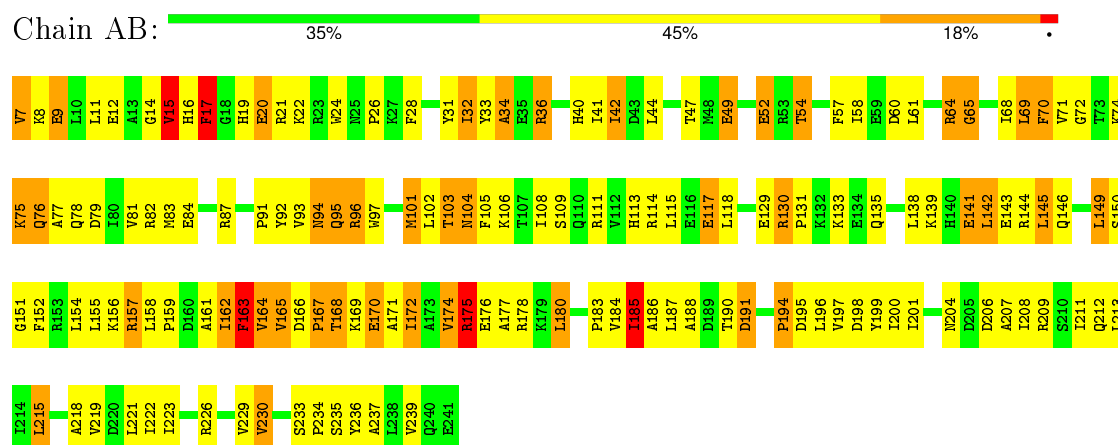


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AY	1	Total 28	C 10	N 5	O 11	P 2	0	0
61	CY	1	Total 28	C 10	N 5	O 11	P 2	0	0

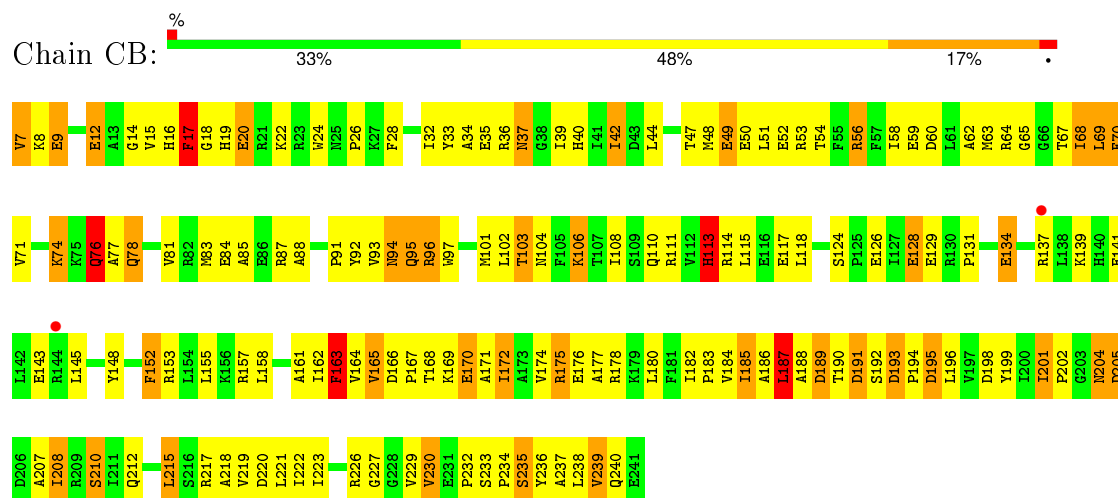
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

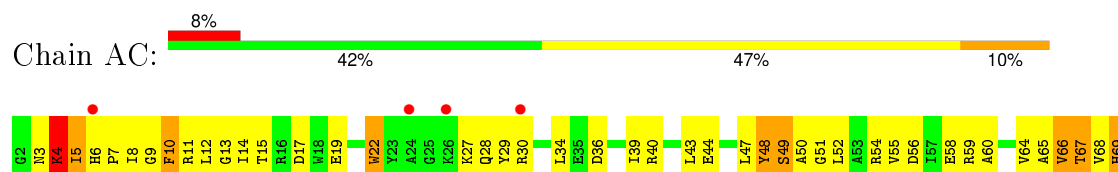
• Molecule 1: 30S ribosomal protein S2

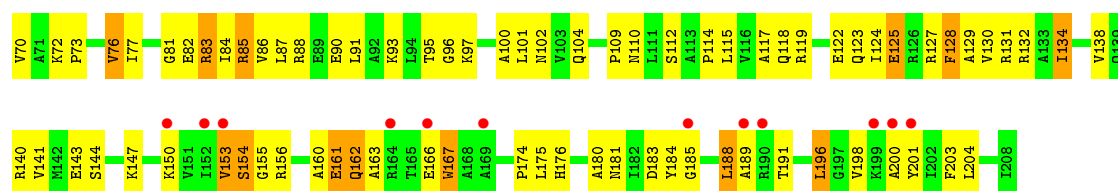


• Molecule 1: 30S ribosomal protein S2

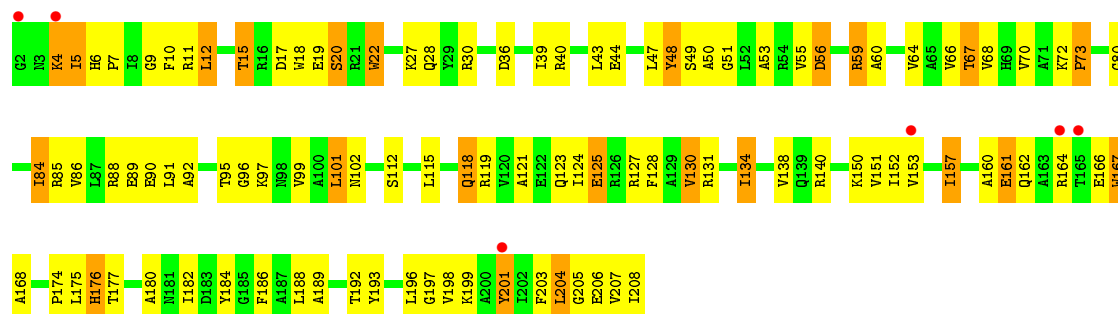


• Molecule 2: 30S ribosomal protein S3

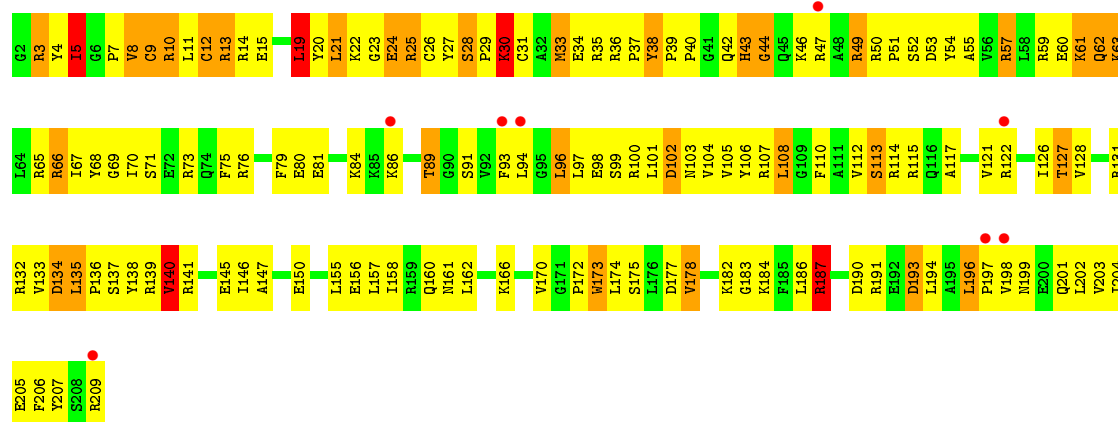




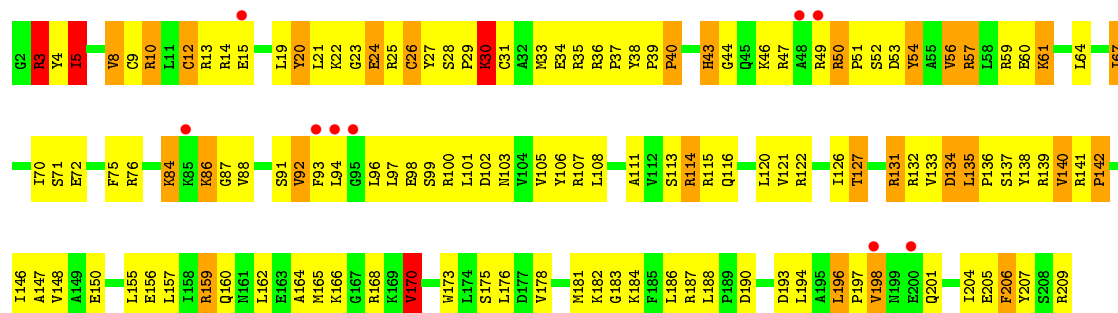
• Molecule 2: 30S ribosomal protein S3



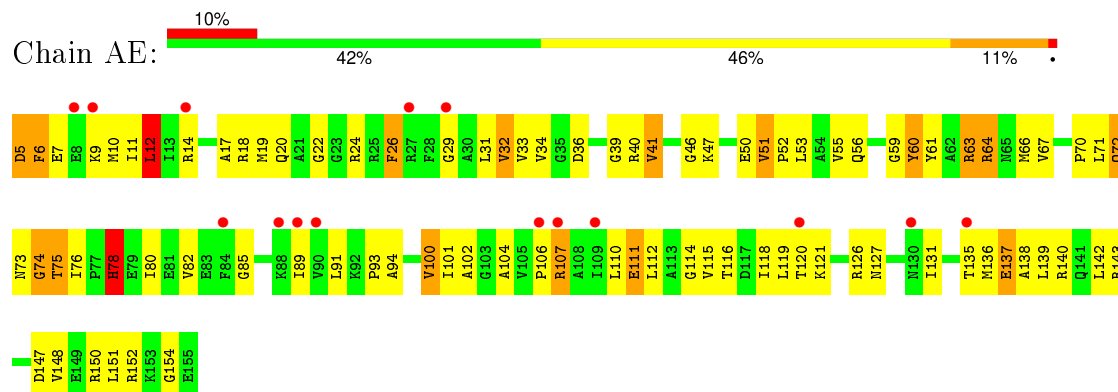
• Molecule 3: 30S ribosomal protein S4



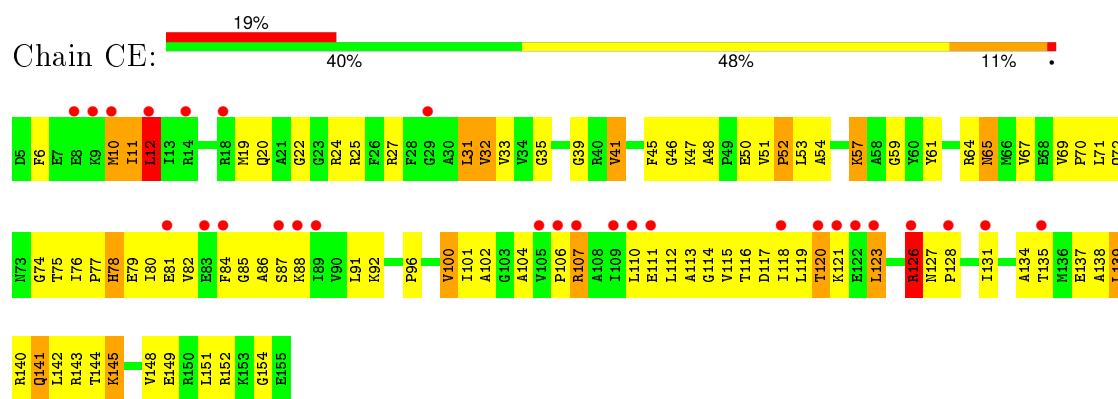
• Molecule 3: 30S ribosomal protein S4



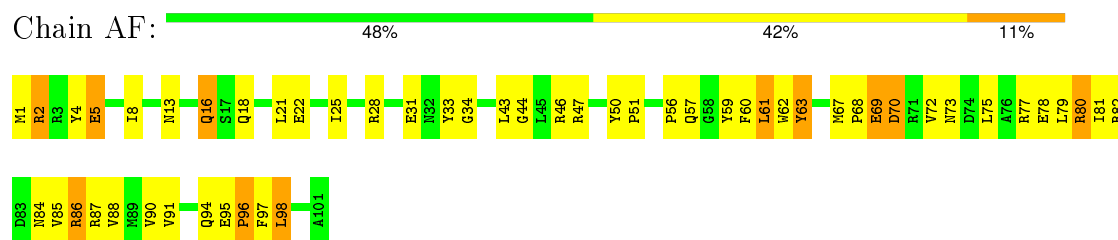
- Molecule 4: 30S ribosomal protein S5



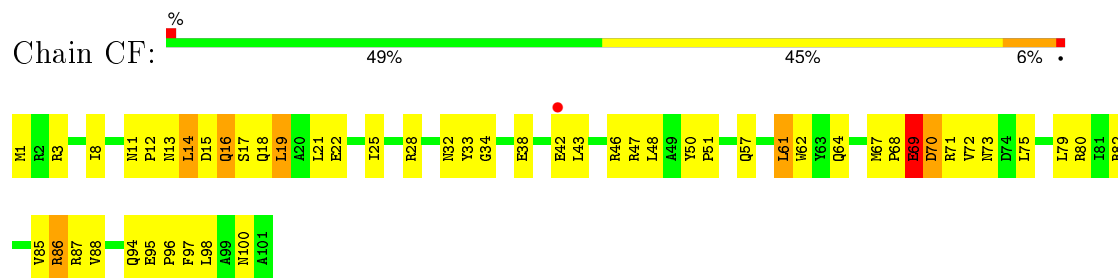
- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6

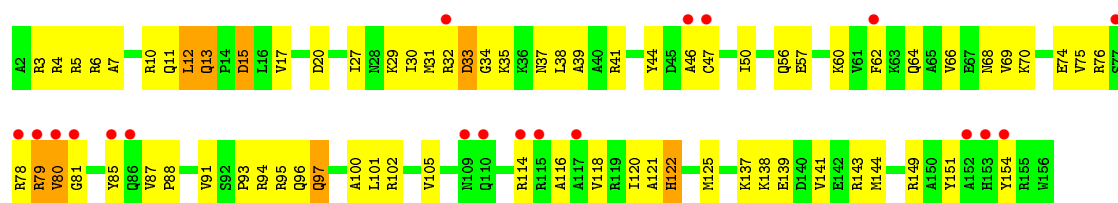


- Molecule 5: 30S ribosomal protein S6

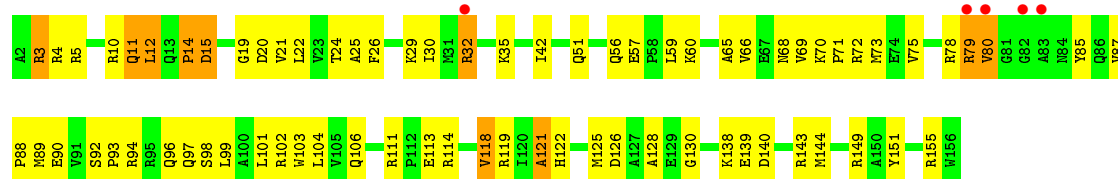


- Molecule 6: 30S ribosomal protein S7

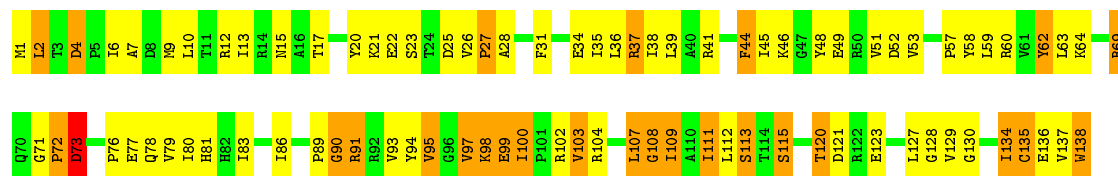




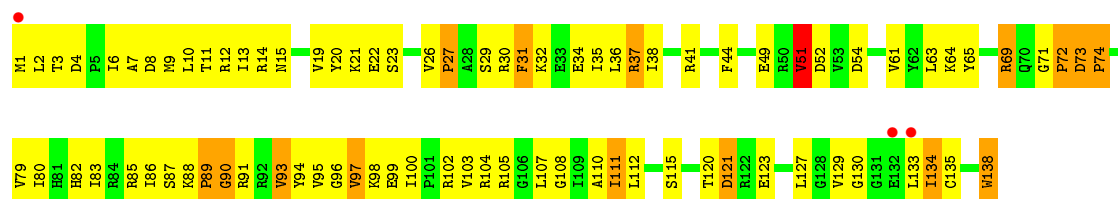
• Molecule 6: 30S ribosomal protein S7



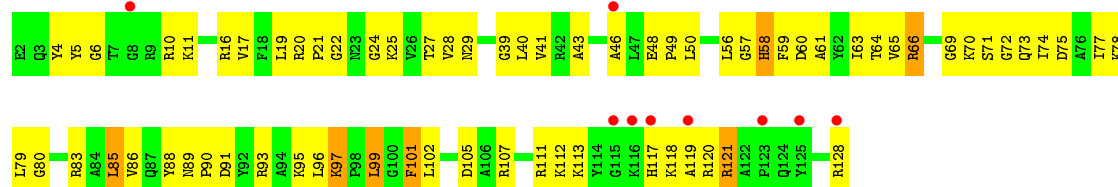
• Molecule 7: 30S ribosomal protein S8



• Molecule 7: 30S ribosomal protein S8

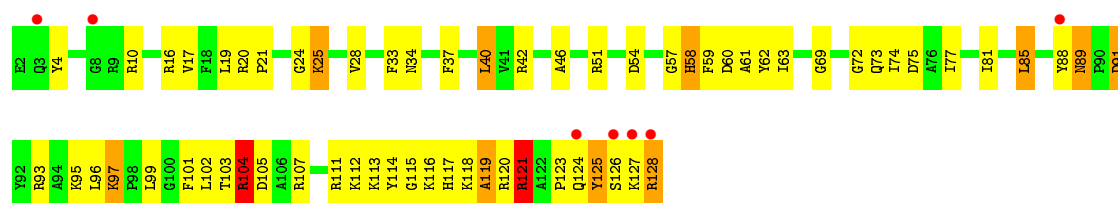


• Molecule 8: 30S ribosomal protein S9

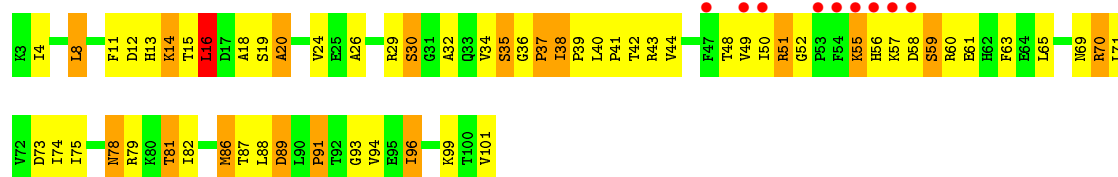


• Molecule 8: 30S ribosomal protein S9

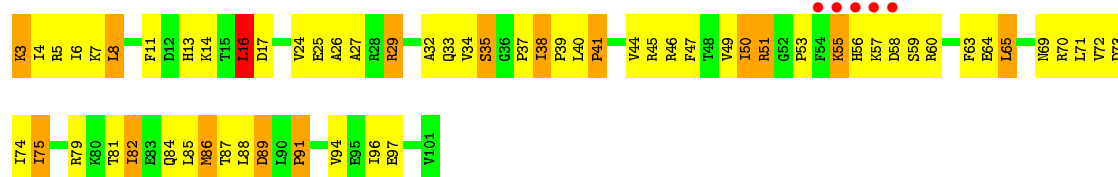




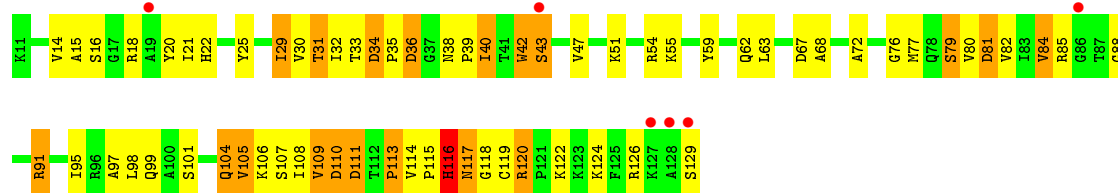
• Molecule 9: 30S ribosomal protein S10



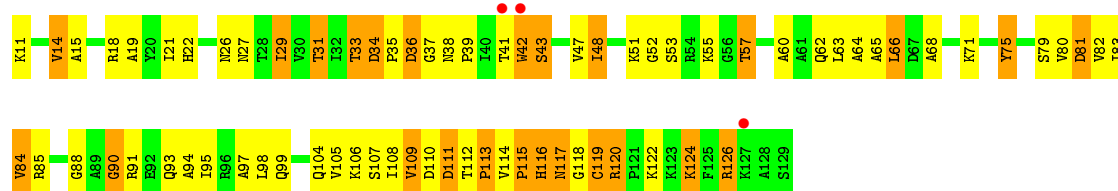
• Molecule 9: 30S ribosomal protein S10



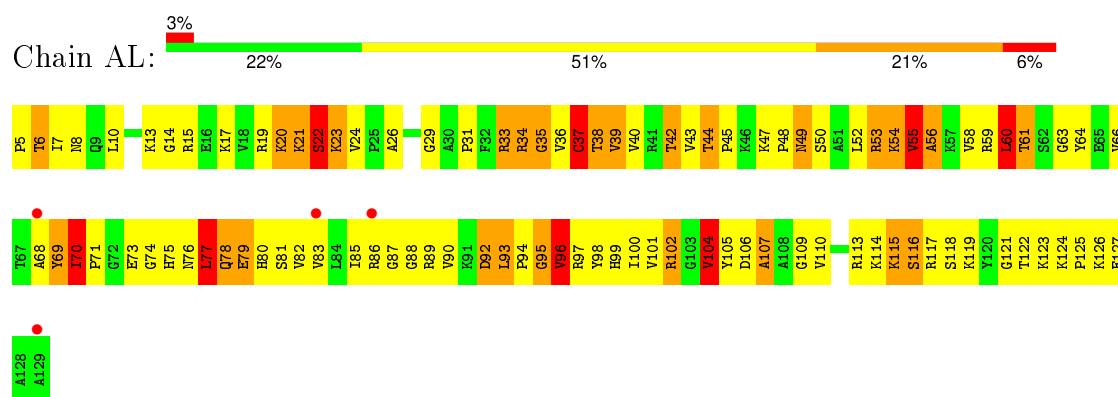
• Molecule 10: 30S ribosomal protein S11



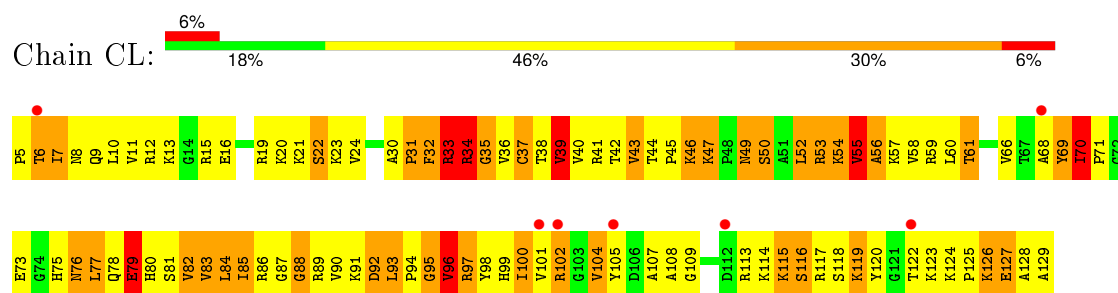
• Molecule 10: 30S ribosomal protein S11



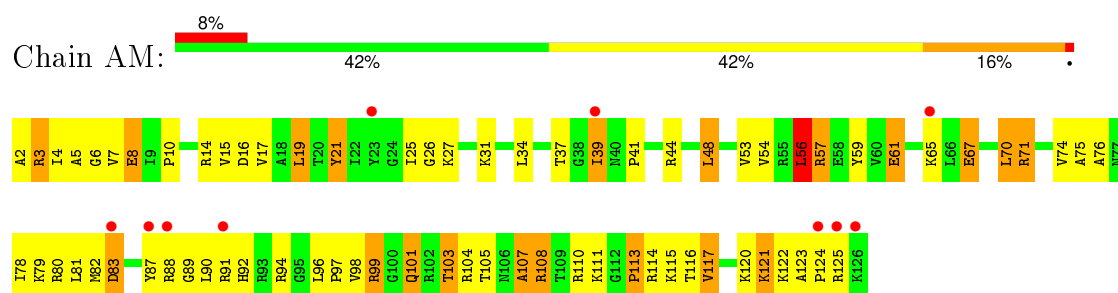
• Molecule 11: 30S ribosomal protein S12



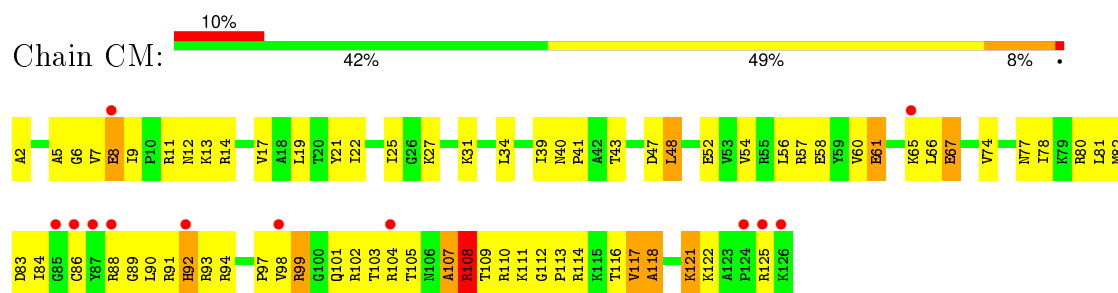
• Molecule 11: 30S ribosomal protein S12



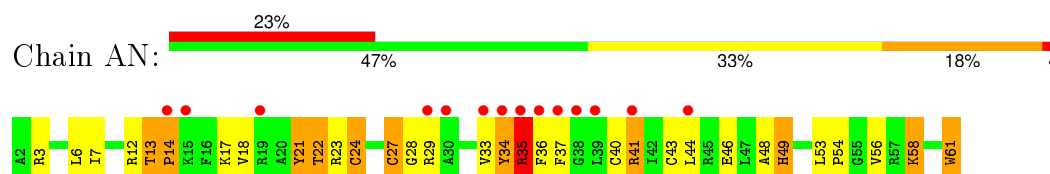
• Molecule 12: 30S ribosomal protein S13



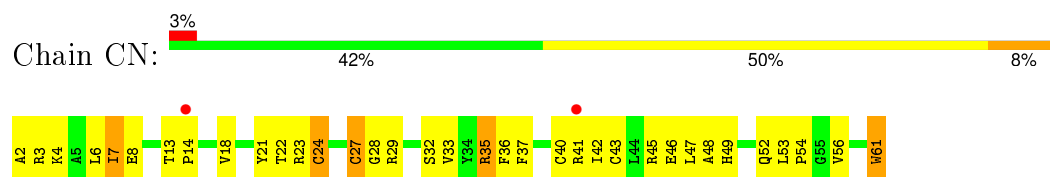
• Molecule 12: 30S ribosomal protein S13



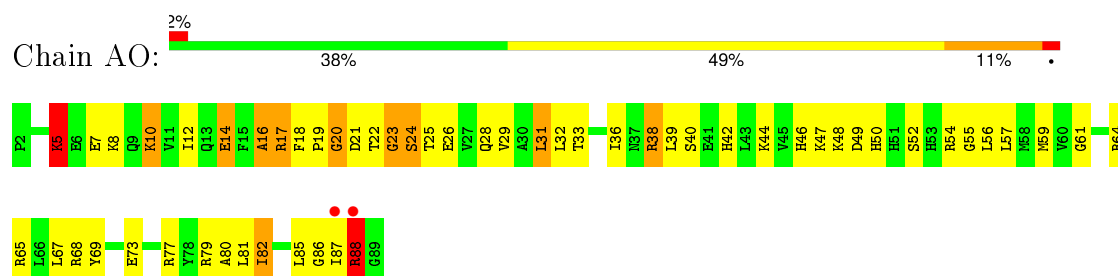
• Molecule 13: 30S ribosomal protein S14 type Z



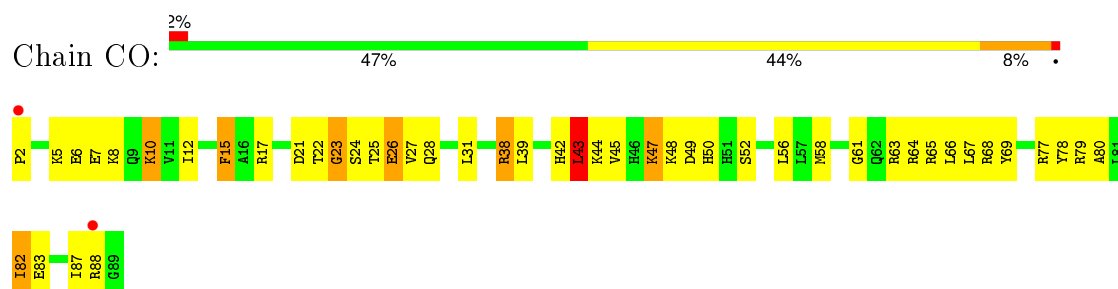
- Molecule 13: 30S ribosomal protein S14 type Z



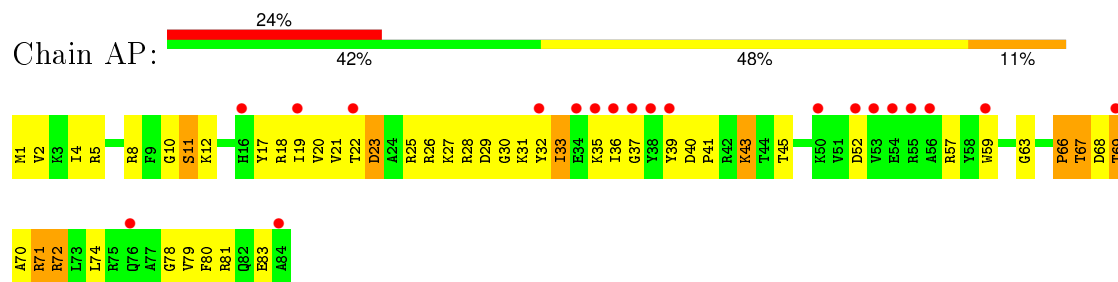
- Molecule 14: 30S ribosomal protein S15



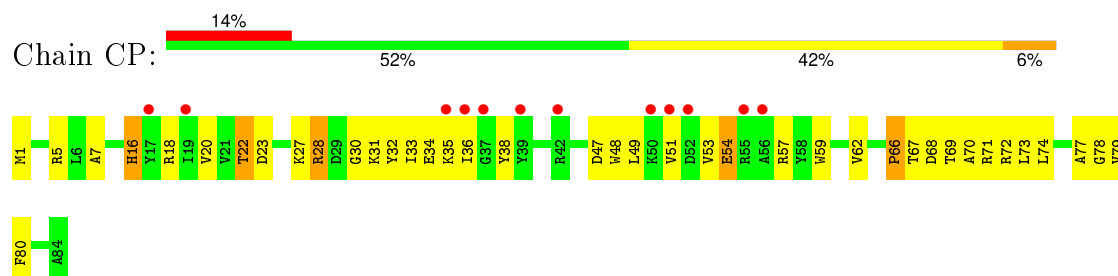
- Molecule 14: 30S ribosomal protein S15



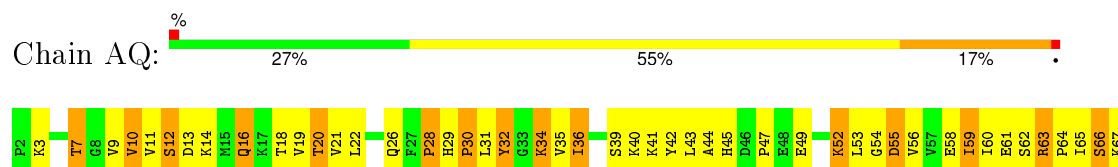
- Molecule 15: 30S ribosomal protein S16



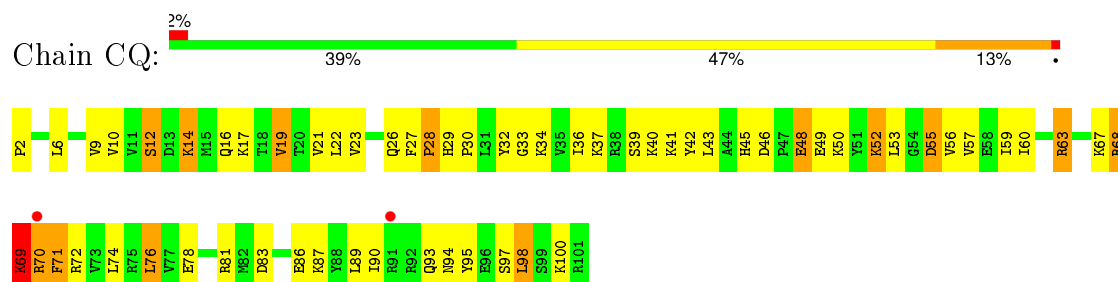
- Molecule 15: 30S ribosomal protein S16



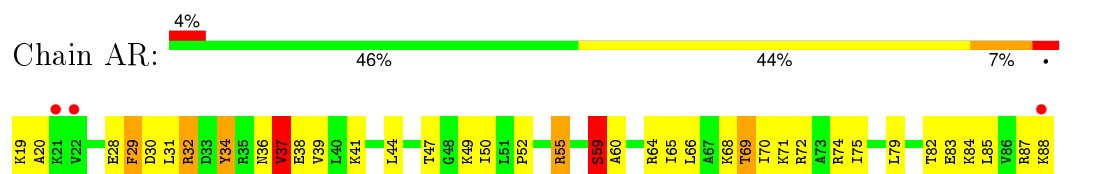
- Molecule 16: 30S ribosomal protein S17



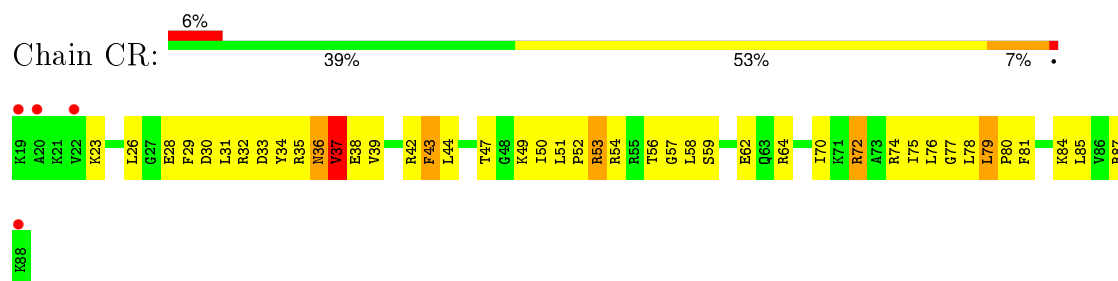
- Molecule 16: 30S ribosomal protein S17



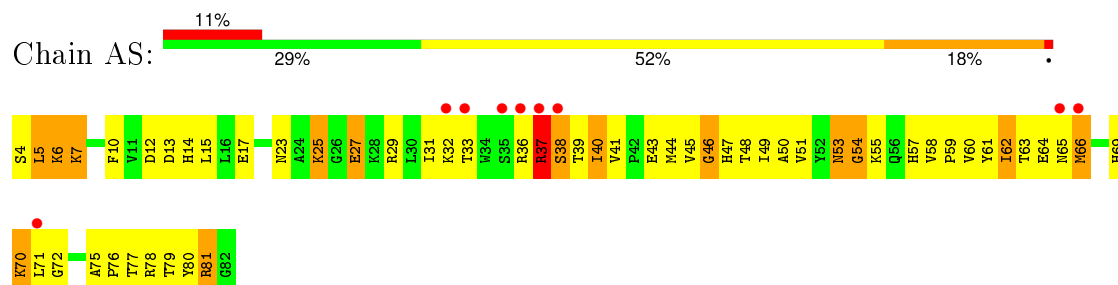
- Molecule 17: 30S ribosomal protein S18



- Molecule 17: 30S ribosomal protein S18

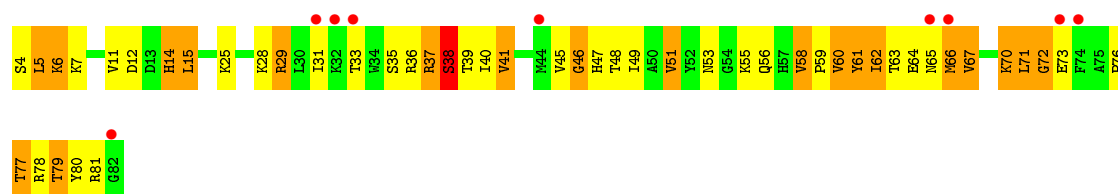


- Molecule 18: 30S ribosomal protein S19

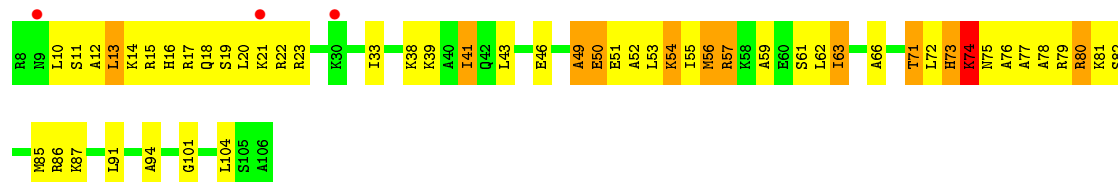


- Molecule 18: 30S ribosomal protein S19

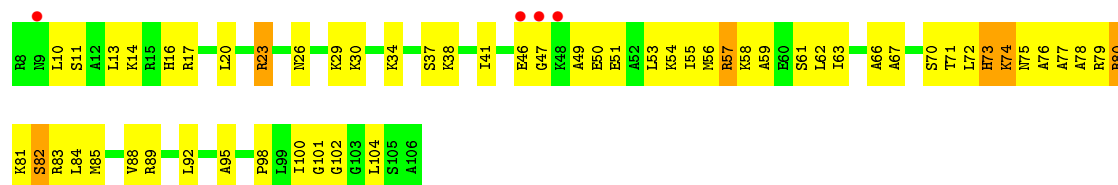
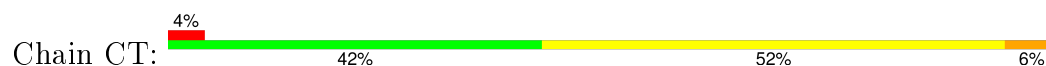




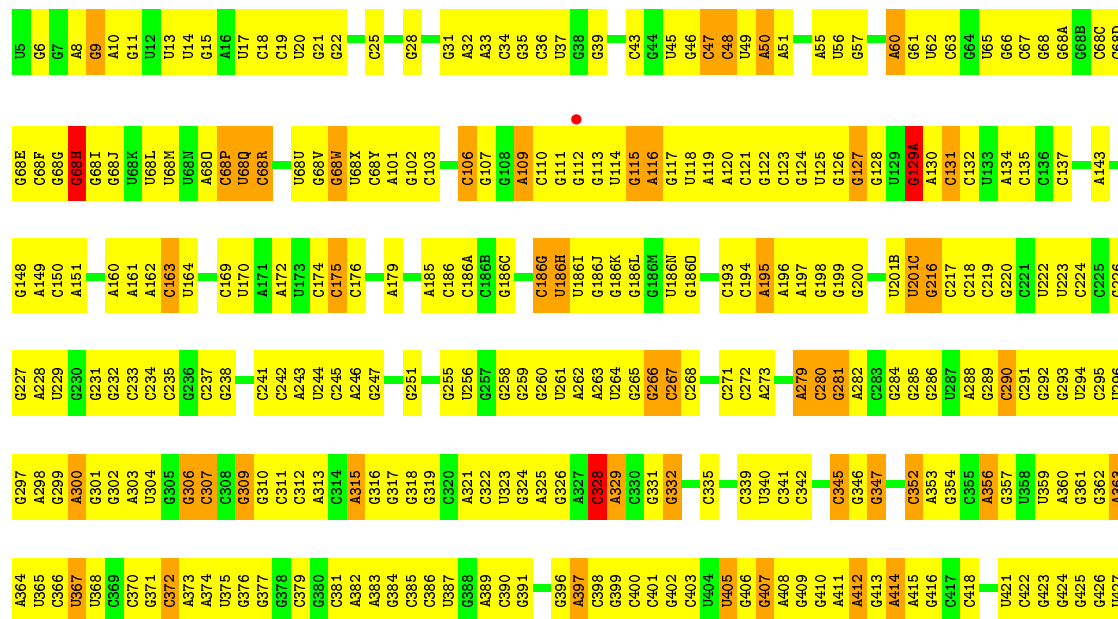
- Molecule 19: 30S ribosomal protein S20



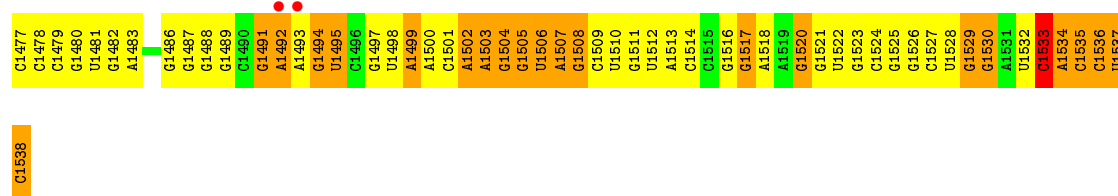
- Molecule 19: 30S ribosomal protein S20



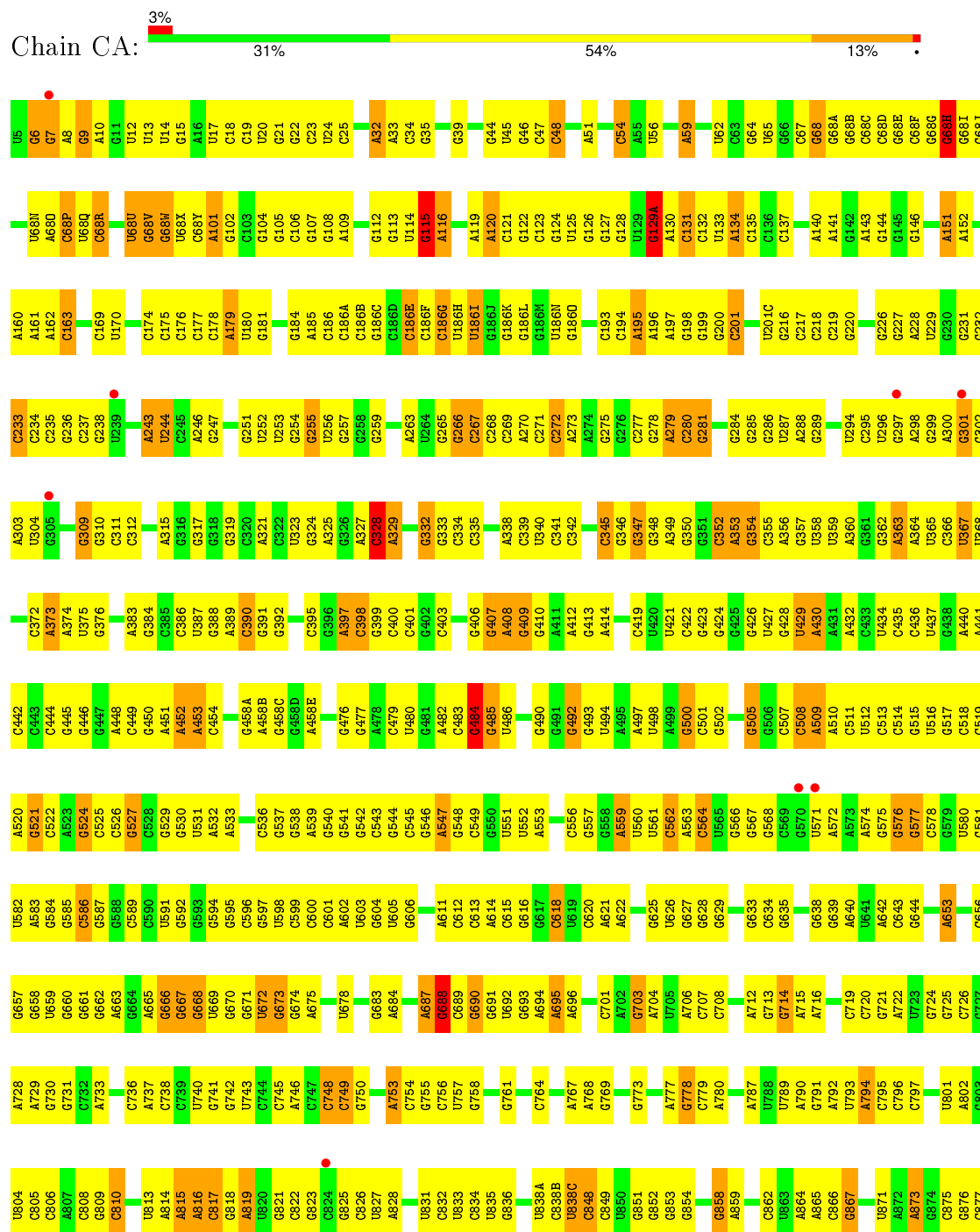
- Molecule 20: ribosomal RNA 16S

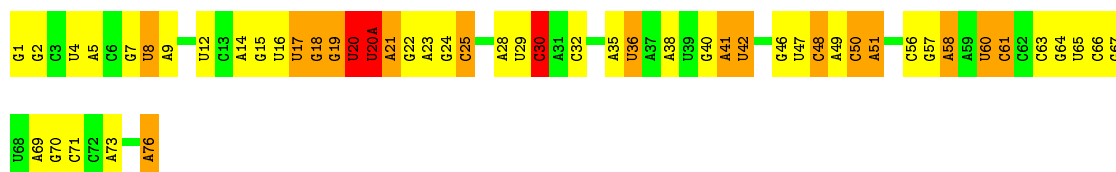


C1397	C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1407	C1408	C1409	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426	C1427	C1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438	C1439	C1440	C1441	C1442	C1443	C1444	C1445	C1446	C1447	C1448	C1449	C1450	C1451	C1452	C1453	C1454	C1455	C1456	C1457	C1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	C1476	
G1331	A1332	A1333	G1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	G1353	G1354	G1355	G1356	G1357	G1358	G1359	A1360	G1361	G1362	C1362A	A1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	A1374	A1375	A1376	A1377	C1378	G1379	A1380	A1381	C1384	G1385	G1386	G1387	C1388	C1389	A1390	A1391	C1392	C1393	A1394									
C1260	A1261	C1262	C1263	G1266	A1269	C1270	G1271	G1274	A1275	A1279	A1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	A1288	A1289	G1290	G1291	C1296	C1297	C1298	A1299	G1300	U1301	A1227	C1228	A1229	C1303	G1304	G1305	A1306	U1307	U1308	G1309	U1313	C1314	U1315	U1316	C1317	A1318	C1319	C1320	C1321	C1322	G1323	A1324	C1325	A1329	U1330												
A1191	C1192	G1193	U1194	C1195	C1196	C1197	G1198	G1199	C1200	A1201	G1202	C1203	A1204	U1205	G1206	G1207	C1208	U1212	C1213	C1214	G1215	C1216	G1217	C1218	U1219	G1220	G1221	G1222	C1223	G1224	A1225	C1226	A1227	C1228	A1229	C1230	G1231	U1232	U1235	U1236	A1237	A1238	A1239	U1240	G1241	U1247	A1248	C1249	C1250	A1251	G1252	G1253	C1254	G1255	A1256	U1257									
U1122	A1123	G1124	C1125	U1126	G1127	C1128	C1129	A1130	G1131	C1132	G1133	U1134	U1135	U1136	C1137	G1138	C1139	C1140	G1143	G1144	G1145	A1146	C1147	U1148	A1151	A1152	C1153	G1154	C1155	G1156	A1157	C1158	U1159	G1160	C1161	C1162	A1170	G1171	C1172	G1173	A1176	G1177	G1178	A1179	A1180	G1181	C1182	A1183	G1184	C1185	G1186	G1187	A1188	C1189	G1190										
U1056	G1057	G1058	C1059	C1060	G1061	U1062	C1063	G1064	C1065	U1066	C1067	U1070	C1071	G1072	U1073	G1074	C1075	C1076	G1077	U1078	G1079	C1080	G1081	G1082	U1083	G1084	U1085	U1086	G1087	C1088	G1089	U1090	U1091	G1094	U1095	C1096	C1097	C1098	G1099	C1100	A1101	A1102	C1103	G1104	C1107	G1108	C1109	A1110	A1111	C1112	C1113	C1118	C1119	G1120	U1121										
A996	U997	G998	C998A	U999	A999	A1000	G1001	G1002	G1003	A1004	A1005	C1006	C1007	G1010	G1011	U1012	G1013	A1014	A1015	A1016	G1017	C1018	C1019	U1020	G1021	U1025	U1026	C1027	C1028	C1029	C1028B	A1028F	G1028G	G1033	G1034	A1035	C1036	C1037	C1038	C1039	U1040	A1041	C1042	C1043	A1044	C1045	A1046	G1047	G1048	U1049	G1050	C1051	U1052	G1053	C1054	A1055									
C934	A935	C936	C937	A938	A939	A940	C940	G941	G942	U943	A944	A945	A946	G947	C948	A949	U950	G951	U952	G953	U954	U955	U956	U957	A958	A959	U960	U961	C962	G963	U964	C965	C966	C967	A968	A969	C970	G971	C972	G973	A974	A975	G976	A977	A978	C979	U980	U981	U982	A983	C984	C985	A986	G987	G988	C989	C990	U991	U992	A993	A994	C995			
G858	A859	A860	G861	A864	A865	A866	G867	C868	G869	U870	U871	A872	A873	G874	C877	G878	C879	C880	G881	C882	C883	U884	G885	A889	A890	U891	A892	C893	G894	G895	C896	A901	G902	G906	A907	A908	A909	C910	A914	A919	U920	A923	C924	G925	G926	G927	C931	C932	G933																
C783	C784	G785	U789	A790	C791	A792	U793	A794	C795	G796	C797	G798	G799	A800	C801	C802	G803	U804	C805	C806	A807	C808	G809	C810	C811	C812	C813	C814	A815	A816	C817	G818	C819	U820	C821	C822	G823	C824	G825	C826	U827	A828	G829	U830	U831	C832	U833	C834	U835	G836	G837	G838	U838A	C838B	U838C	C848	G851								
C717	G718	C719	C720	G721	A722	U723	C726	G727	G728	C729	G730	A733	G734	U735	C736	A737	G738	C739	G741	C744	C745	A746	C747	C748	C749	U750	U751	G752	A753	C754	C755	C756	U757	G758	A759	C762	G763	C764	G765	A766	A767	A768	G769	C770	U771	C775	G776	G777	U778	C779	A780	A781	A782												
G633	G634	G635	A640	U641	A642	A643	G644	G645	U646	A653	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	G671	U672	G673	G674	A675	A676	U677	A684	G685	U686	A687	A688	G689	C689	G821	C822	G823	C824	G825	C826	U827	A828	G829	U830	U831	C832	U833	C834	U835	G836	G837	G838	U838A	C838B	U838C	C848	G851						
G567	G568	C569	G570	U571	A572	A573	A574	G575	G576	G577	C578	G579	U580	G581	U582	A583	A584	G585	C586	C587	G588	U591	G592	G593	G594	G595	C596	U597	A598	U599	C600	C601	G604	U605	G606	A607	A608	A609	G610	A547	A611	C612	C613	A614	C615	U552	G616	A553	C617	C618	U619	C620	G558	A559	A621	U560	A622	C623	C624	G562	U498	A499	G500	C501	G502
C503	C504	G505	A509	C511	G514	G515	U516	G517	C518	C519	G520	G521	G522	A523	G524	C525	C526	G527	A528	G529	C530	U531	A532	A533	U534	C535	C536	U537	A538	U539	C540	G542	C543	G544	C545	A546	A547	C548	C549	G550	C551	A552	G553	C556	G557	C558	A559	A562	U560	A563	C562	U564	A565	C566	G567										
G428	U429	A430	A431	U434	C435	C436	G437	G438	A440	A441	C442	C443	C444	G445	G446	G447	A448	C449	G450	A451	A452	A453	C454	C455	C456	C457	C458	G459	A458A	A458B	G458C	G458D	A458E	G476	G477	A478	C479	U480	G481	A482	C483	G484	G485	C488	C489	G490	G491	G492	G493	U494	A495	A496	U497	U498	A499	G500	C501	G502							



• Molecule 20: ribosomal RNA 16S

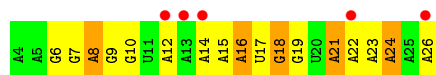




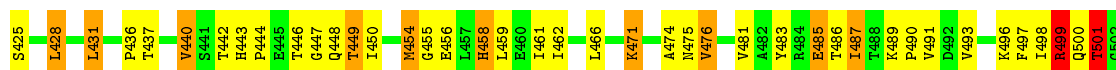
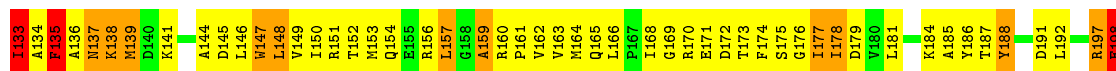
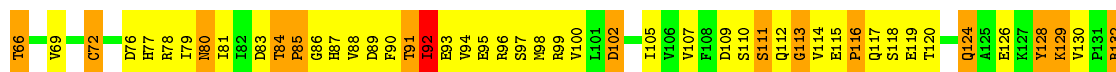
- Molecule 22: messenger RNA

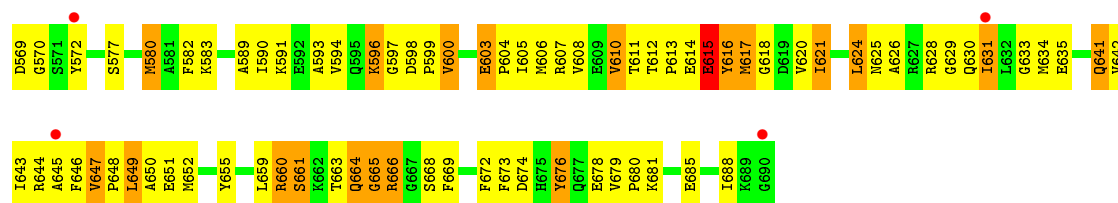


- Molecule 22: messenger RNA

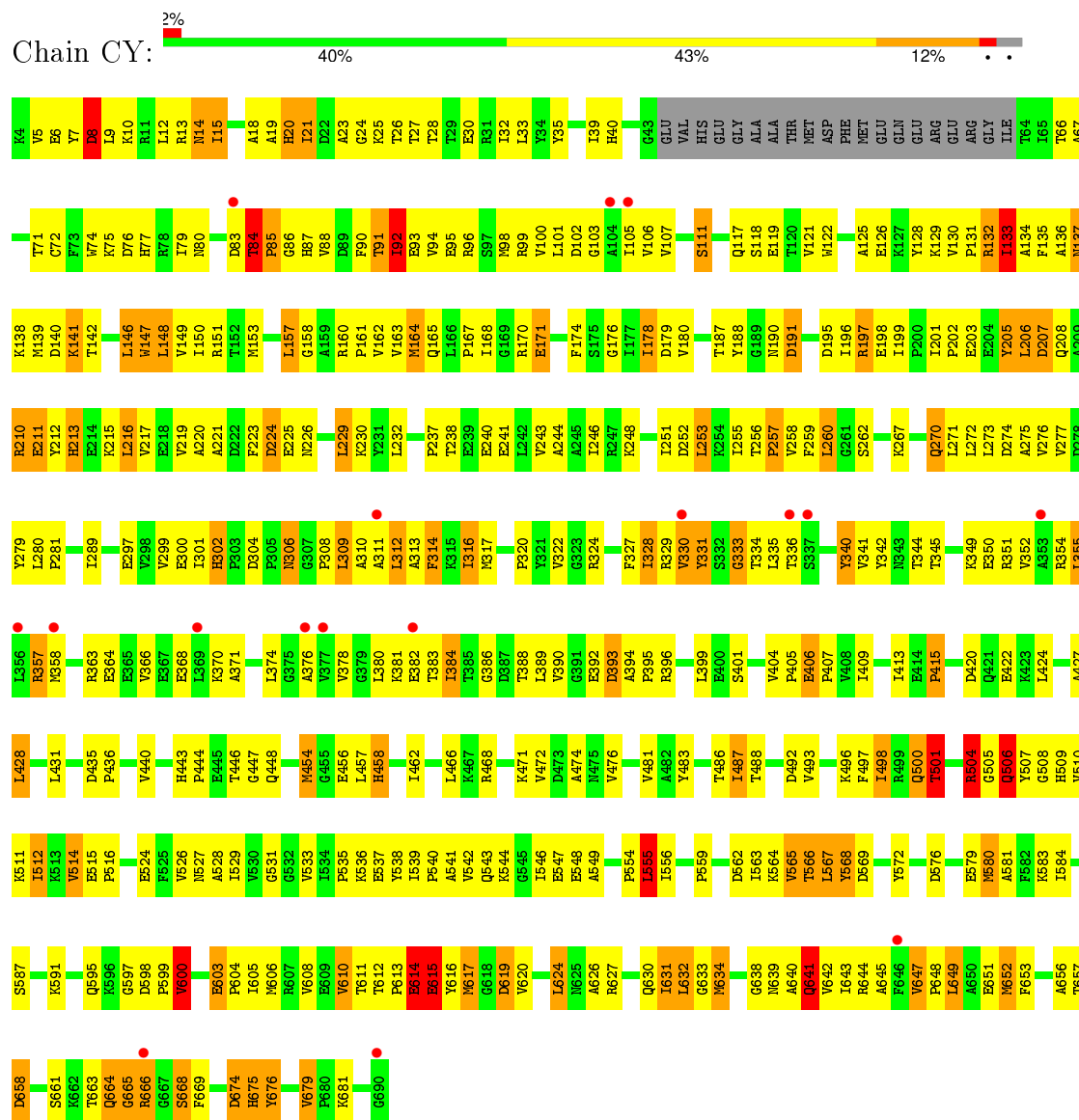


- Molecule 23: Elongation factor G

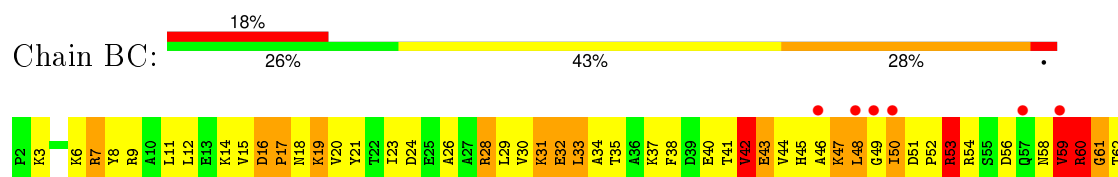


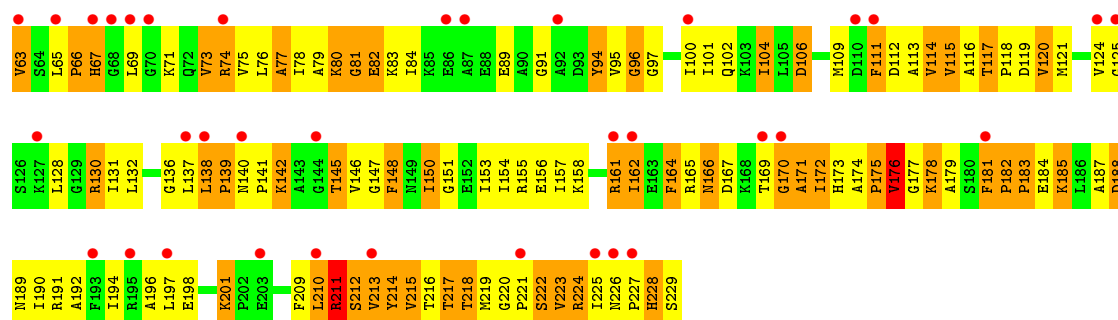


• Molecule 23: Elongation factor G

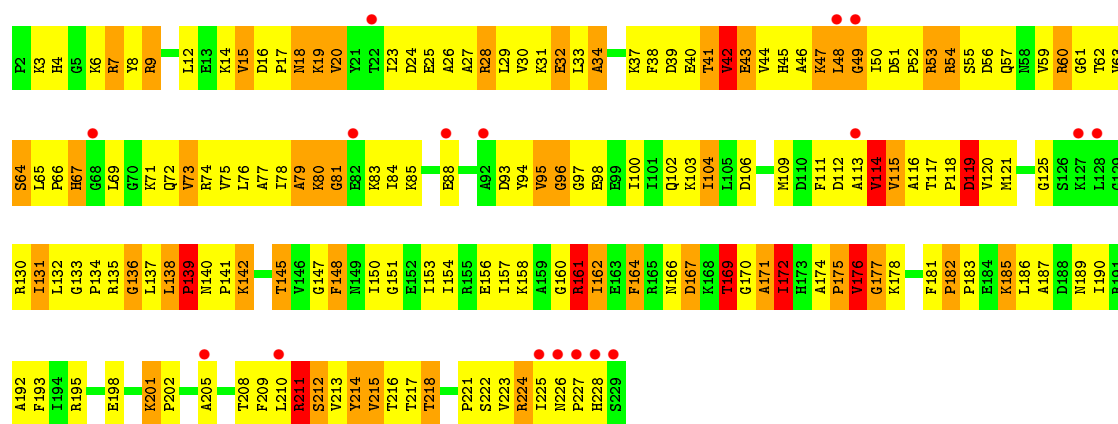


• Molecule 24: 50S ribosomal protein L1

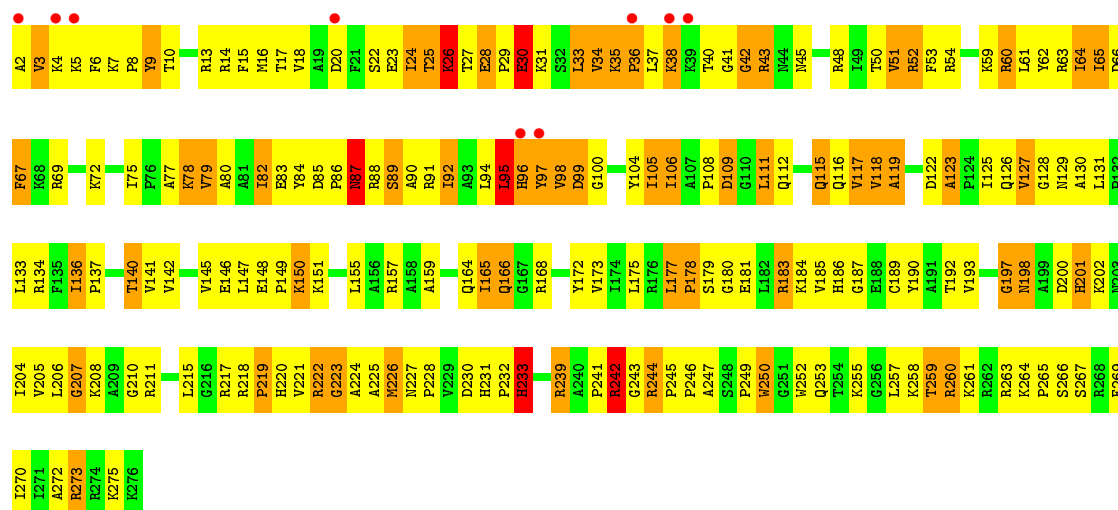




• Molecule 24: 50S ribosomal protein L1

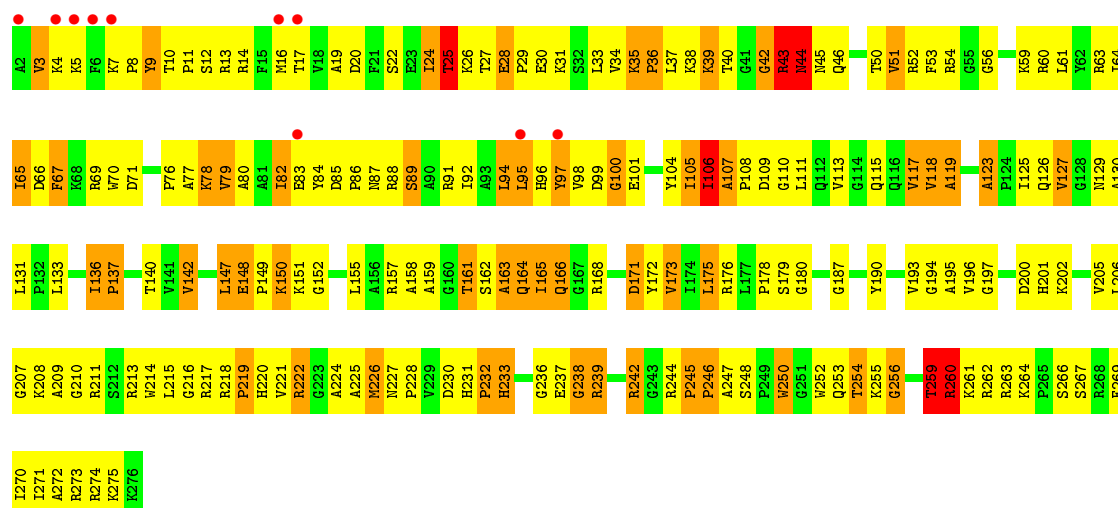


• Molecule 25: 50S ribosomal protein L2

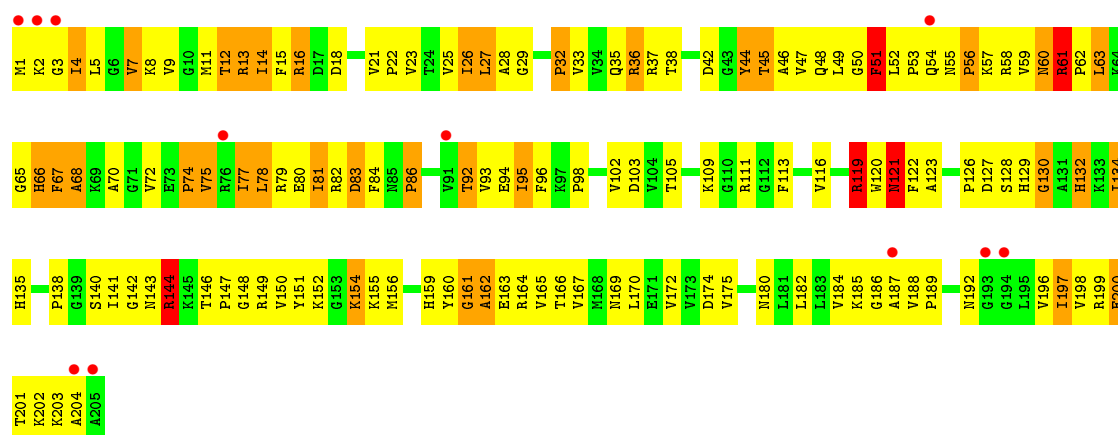


• Molecule 25: 50S ribosomal protein L2

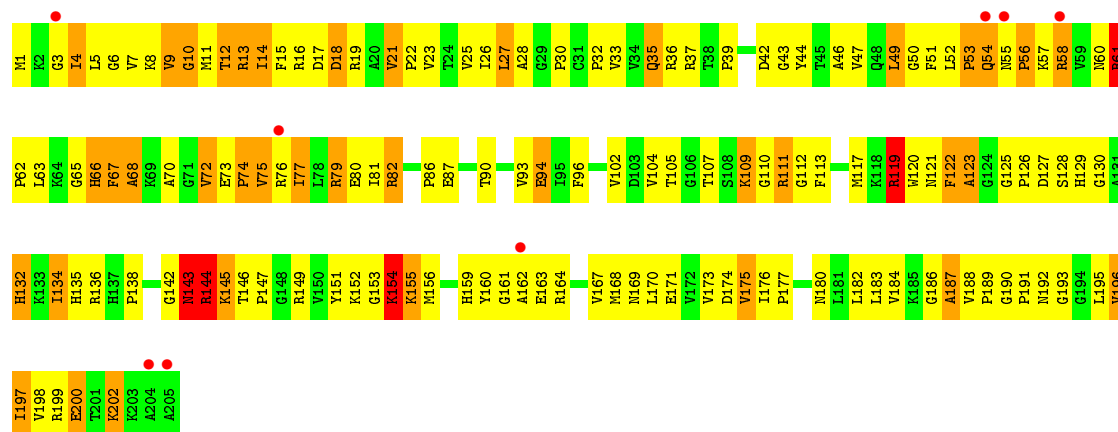




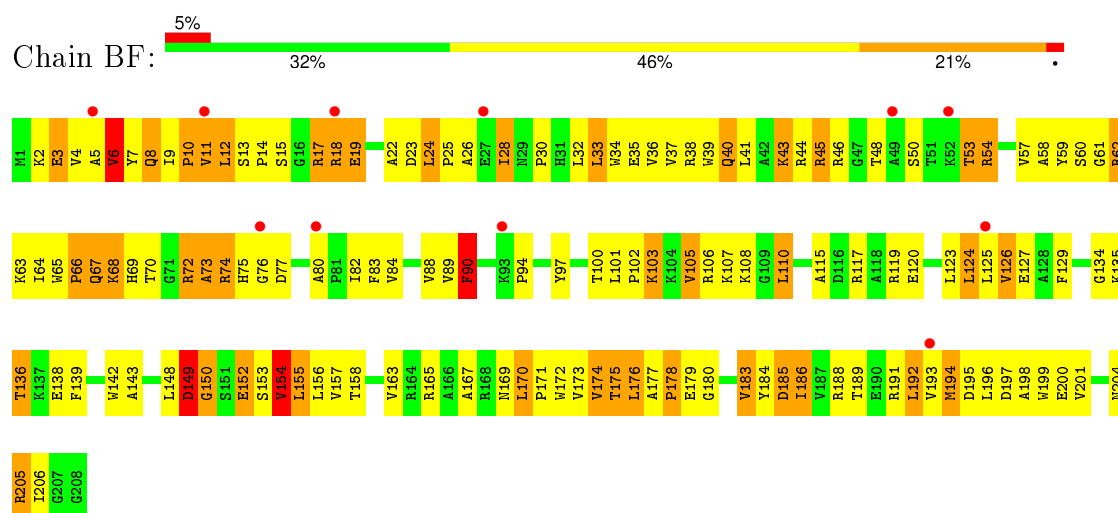
• Molecule 26: 50S ribosomal protein L3



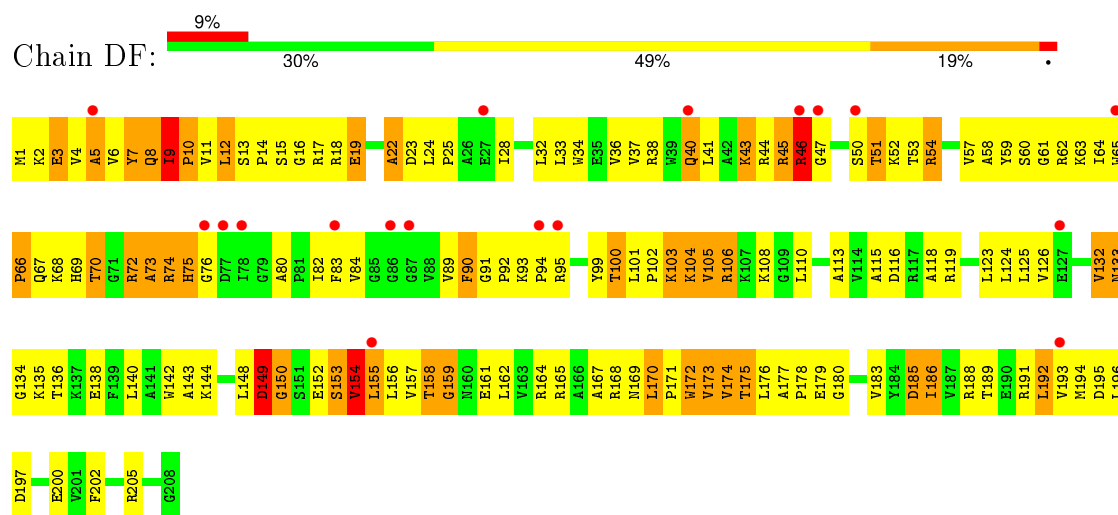
• Molecule 26: 50S ribosomal protein L3



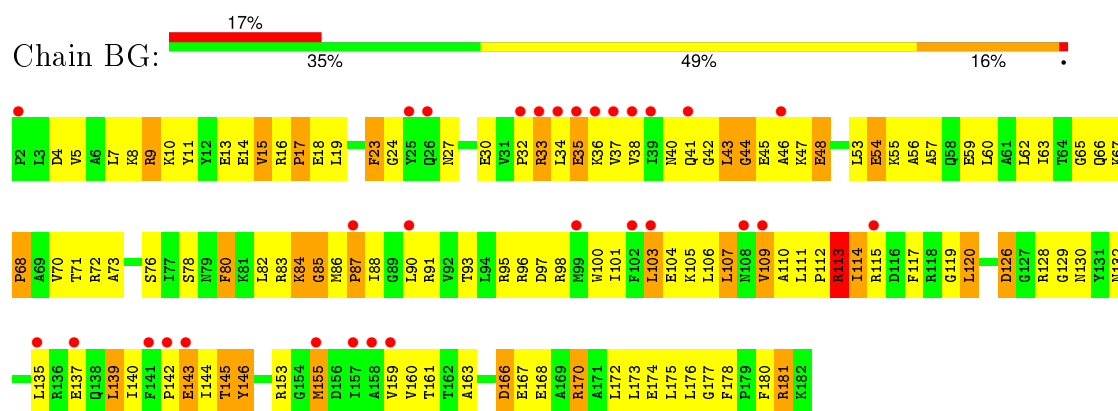
• Molecule 27: 50S ribosomal protein L4



- Molecule 27: 50S ribosomal protein L4

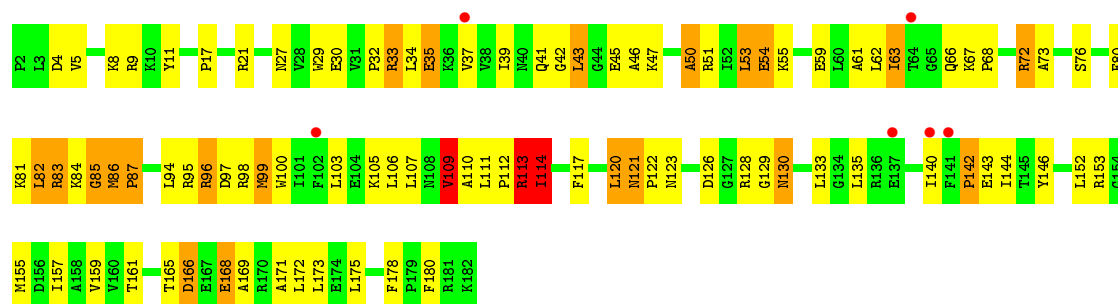


- Molecule 28: 50S ribosomal protein L5

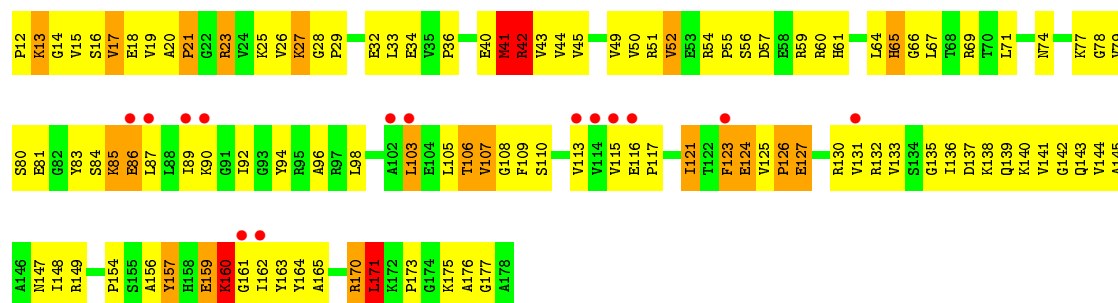


- Molecule 28: 50S ribosomal protein L5

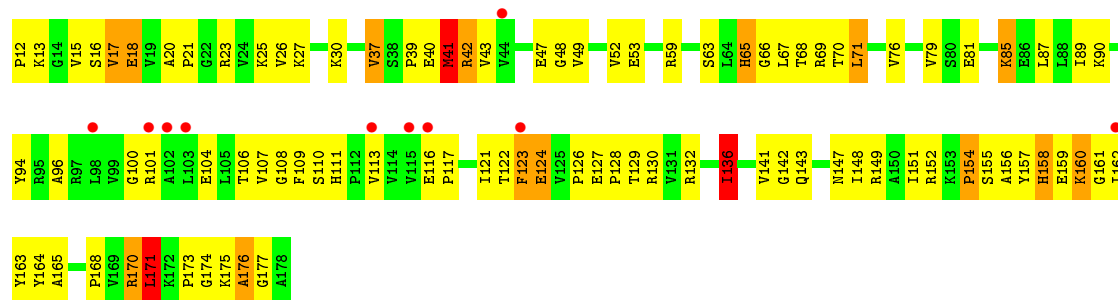




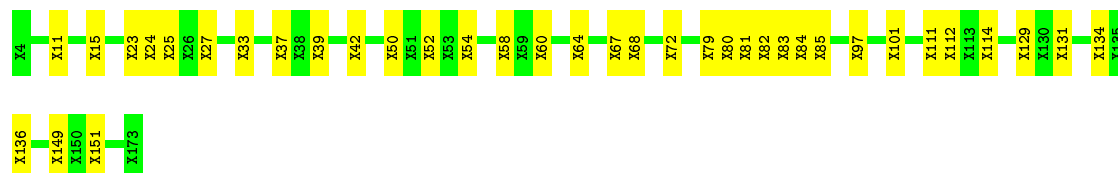
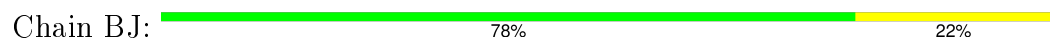
- Molecule 29: 50S ribosomal protein L6



- Molecule 29: 50S ribosomal protein L6

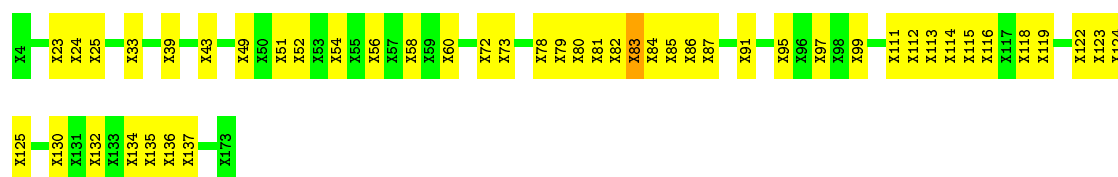


- Molecule 30: 50S ribosomal protein L10

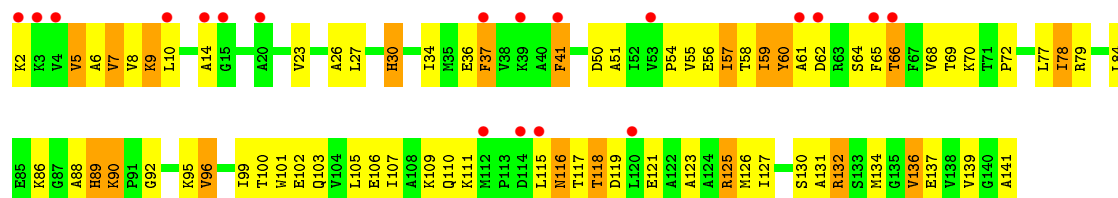


- Molecule 30: 50S ribosomal protein L10

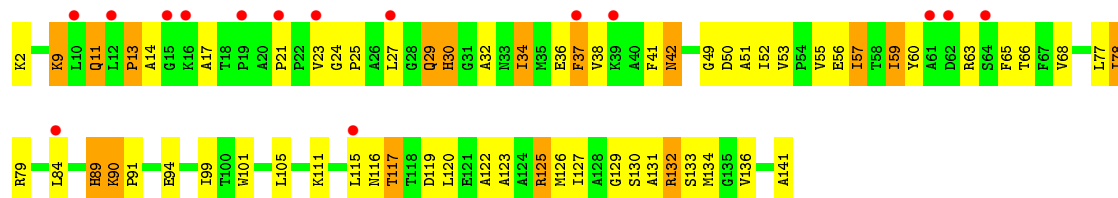




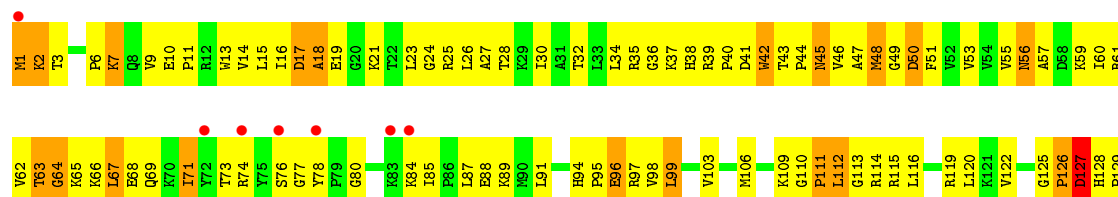
- Molecule 31: 50S ribosomal protein L11



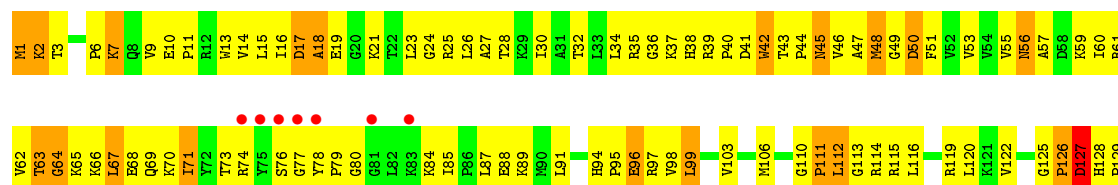
- Molecule 31: 50S ribosomal protein L11



- Molecule 32: 50S ribosomal protein L13



- Molecule 32: 50S ribosomal protein L13



H130
Q131
A132
Q133
R134
P135
E136
K137
L138

• Molecule 33: 50S ribosomal protein L14

Chain BO: 37% 48% 13% .

H1 T6 T7 L3 E9 V10 A11 A12 A13 G15 T14 G16 A16 R17 K18 N19 N20 C21 T22 T23 T24 L25 L26 K26 G27 S28 N29 A30 F31 T34 T35 T36 T37 T38 T39 V40 V41 S42 V43 K44 E45 E46 T47 P48 R49 V52 K53 E54 V57 V58 K59 V63 R64 T65 R66 K67 E68

I69 R70 R71 P72 D73 G74 I77 R78 F79 D80 D81 N82 A83 N88 L91 E92 T96 R97 V98 F99 A103 R104 E105 S106 L107 E108 M112 K113 I114 V115 S116 L117 A118 P119 E120 E121 L122

• Molecule 33: 50S ribosomal protein L14

Chain DO: 42% 46% 11% .

M1 I2 Q3 P4 Q5 T6 T7 L8 E9 A10 A11 A12 A13 T14 G15 A16 R17 K18 L19 I19 M20 C21 I22 R23 L24 V25 K26 G27 S28 N29 A30 F31 T34 T35 T36 T37 T38 T39 V40 V41 S42 V43 K44 E45 E46 T47 P48 R49 V52 K53 E54 V57 V58 K59 V63 R64 T65 R66 K67 E68

G74 S75 A76 I77 R78 F79 N82 A83 I87 N88 L91 E92 T96 R97 V98 F99 G100 G101 V102 A103 R104 E105 L106 L107 E108 F111 M112 K113 I114 L117 E120 V121 L122

• Molecule 34: 50S ribosomal protein L15

Chain BP: 3% 34% 44% 19% .

D5 L6 R7 P8 N9 P10 G11 A12 N13 K14 R15 R16 R17 R18 V19 G20 G21 G22 P23 G24 S25 G26 H27 G28 K29 T30 A31 T32 T33 R33 Q38 K39 S40 R41 S42 G43 G44 L45 K46 P47 P48 R49 R50 E51 E52 G53 G54 R55 S56 T57 T58 L59 M60 R61 K62 K63 K64 R65 G66 M67

Q70 V71 P72 K76 Q81 L85 R86 D87 L88 A89 V95 T96 L100 V101 R102 A103 G104 G105 L106 K107 R108 T109 Y110 R111 L112 L113 I114 L115 G116 E117 G118 K121 P122 L123 P124 V125 V126 A127 H128 A129 F130 S131 A134 L135 E136 K137 L138 K139 K64 R65 G66

A150

• Molecule 34: 50S ribosomal protein L15

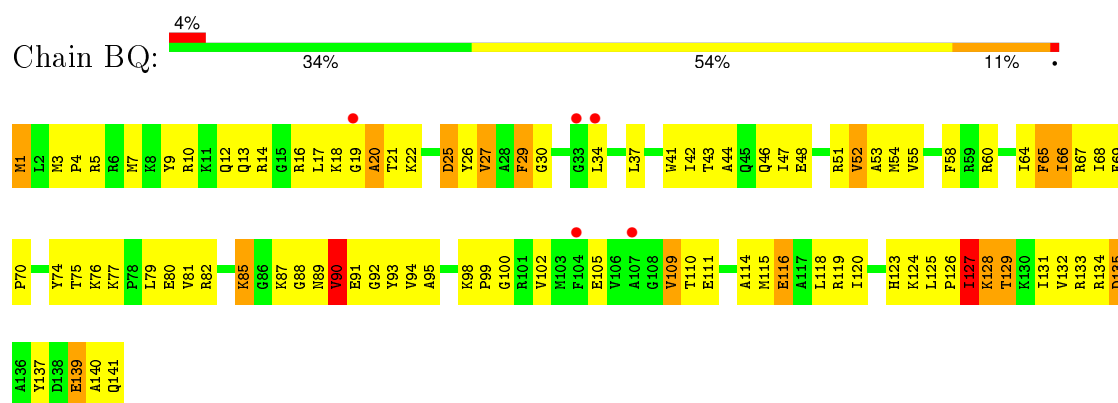
Chain DP: 3% 34% 44% 18% .

D5 L6 R7 P8 N9 P10 G11 A12 N13 K14 R15 R16 R17 R18 V19 G20 G21 G22 P23 G24 S25 G26 H27 G28 K29 T30 A31 T32 T33 R33 Q38 K39 S40 R41 S42 L45 K46 P47 P48 R49 R50 E51 E52 G53 G54 R55 S56 T57 T58 L59 M60 R61 K62 K63 K64 R65 G66

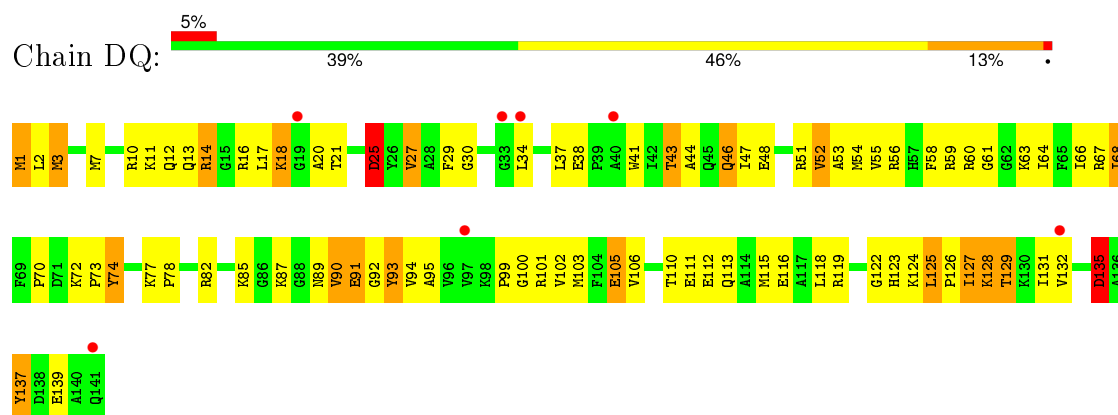
G69 Q70 V71 P72 K76 Q81 L85 R86 D87 L88 A89 V95 T96 L100 V101 R102 A103 G104 G105 L106 K107 R108 T109 Y110 R111 L112 L113 I114 L115 G116 E117 G118 K121 P122 L123 P124 V125 V126 A127 H128 A129 F130 S131 A134 L135 E136 K137 L138 K139 K64 R65 G66

K139 A140 A141 E144 P145 E149 A150

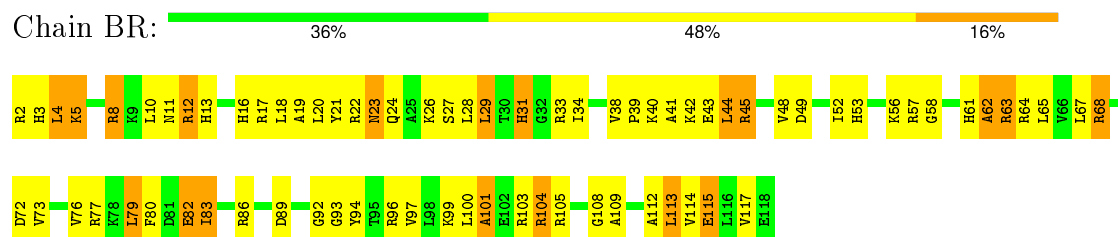
• Molecule 35: 50S ribosomal protein L16



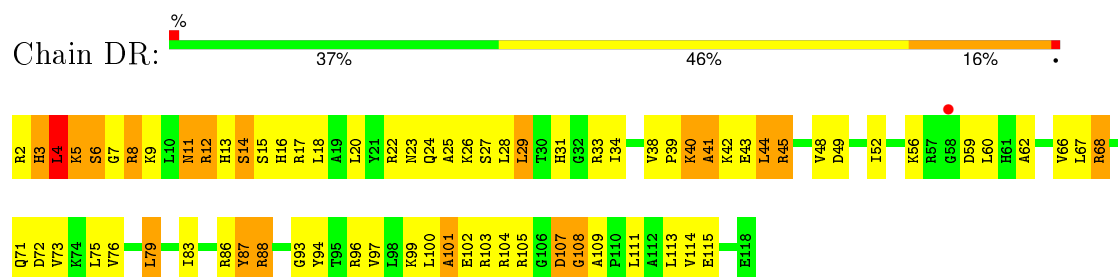
- Molecule 35: 50S ribosomal protein L16



- Molecule 36: 50S ribosomal protein L17

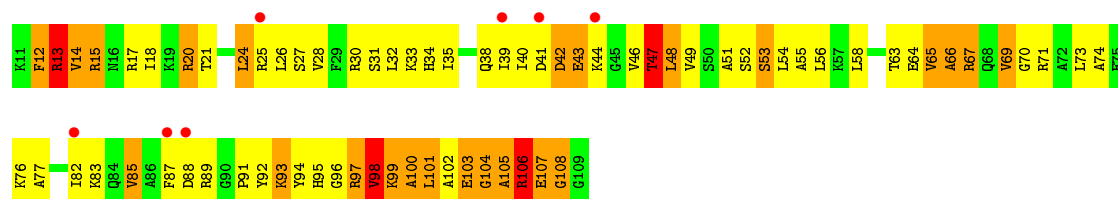


- Molecule 36: 50S ribosomal protein L17

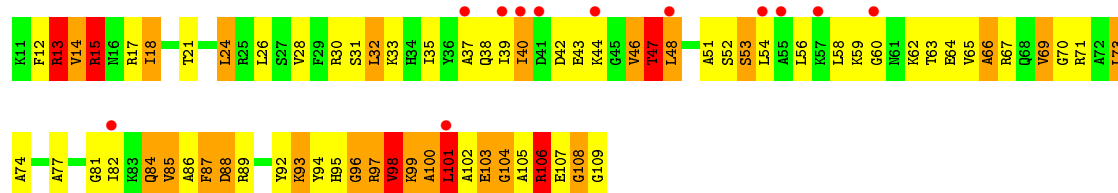


- Molecule 37: 50S ribosomal protein L18

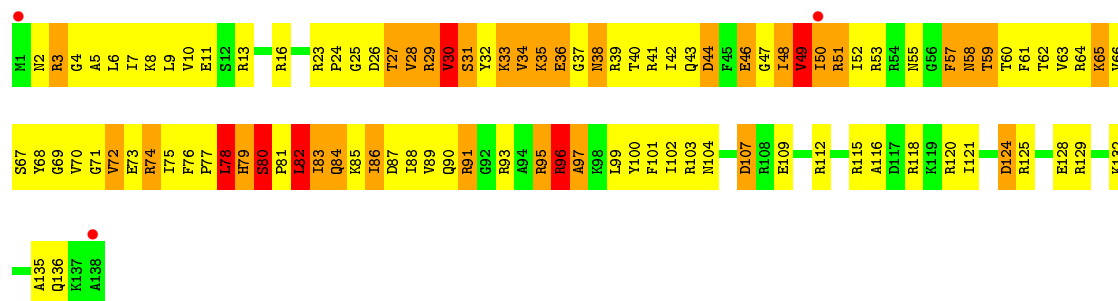




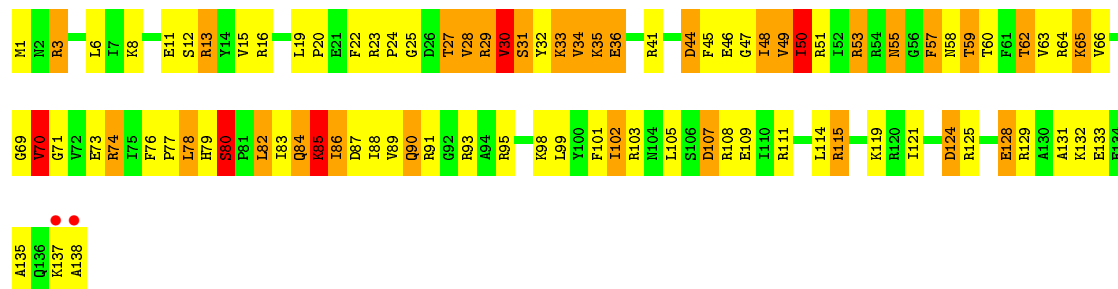
• Molecule 37: 50S ribosomal protein L18



• Molecule 38: 50S ribosomal protein L19

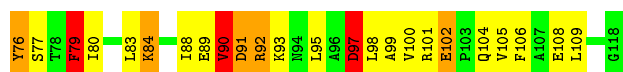


• Molecule 38: 50S ribosomal protein L19

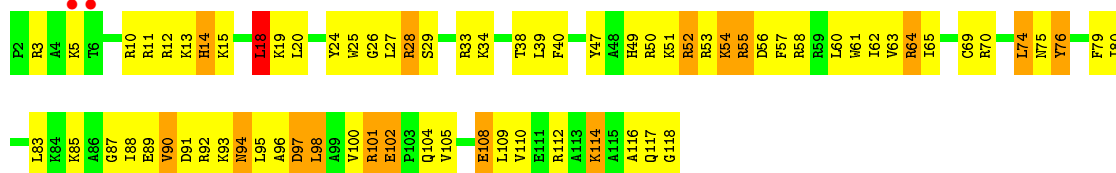


• Molecule 39: 50S ribosomal protein L20

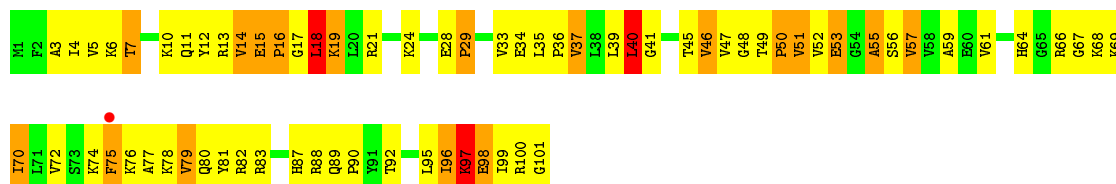




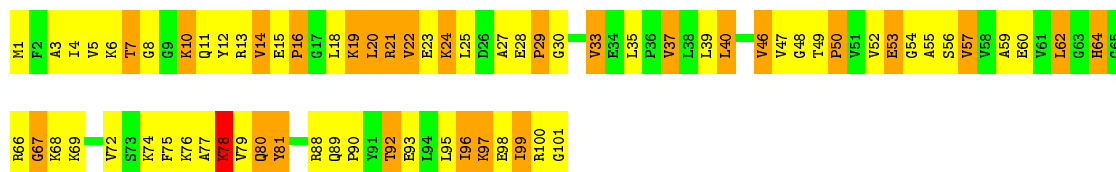
- Molecule 39: 50S ribosomal protein L20



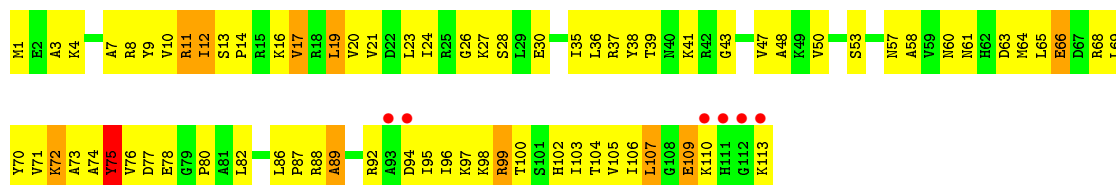
- Molecule 40: 50S ribosomal protein L21



- Molecule 40: 50S ribosomal protein L21

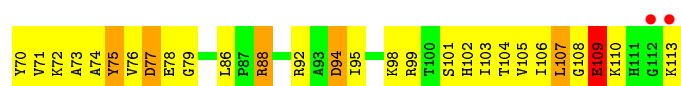


- Molecule 41: 50S ribosomal protein L22

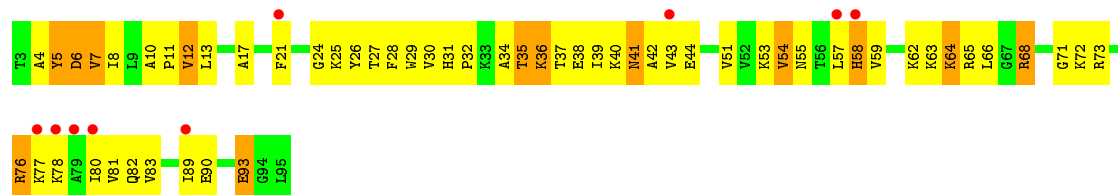
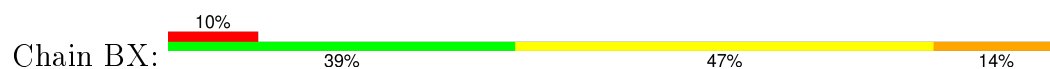


- Molecule 41: 50S ribosomal protein L22

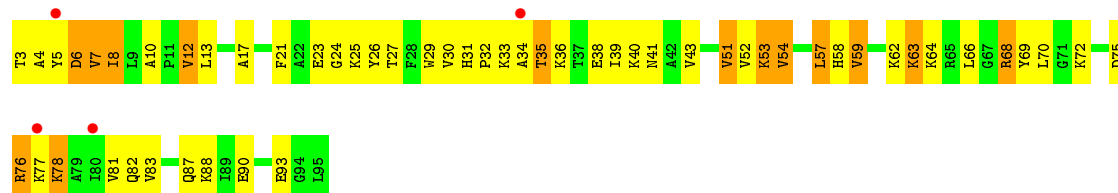
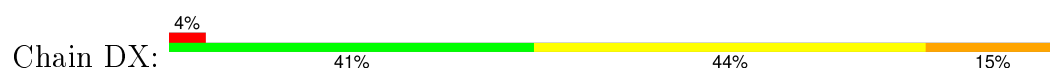




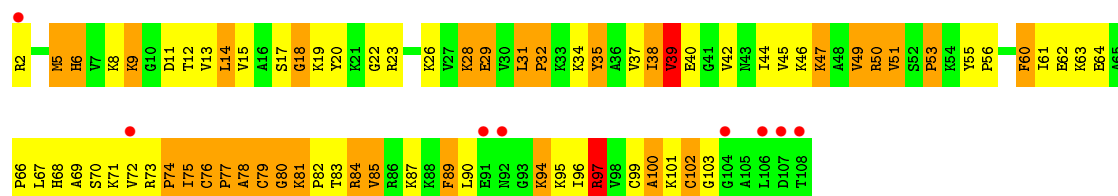
• Molecule 42: 50S ribosomal protein L23



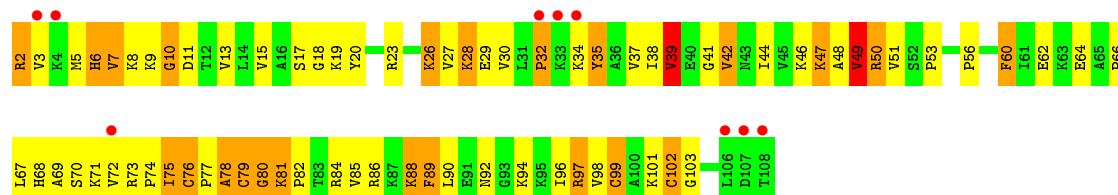
• Molecule 42: 50S ribosomal protein L23



• Molecule 43: 50S ribosomal protein L24

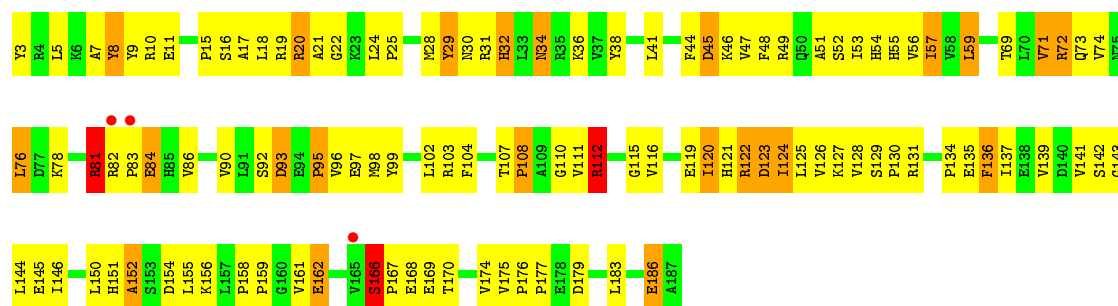


• Molecule 43: 50S ribosomal protein L24

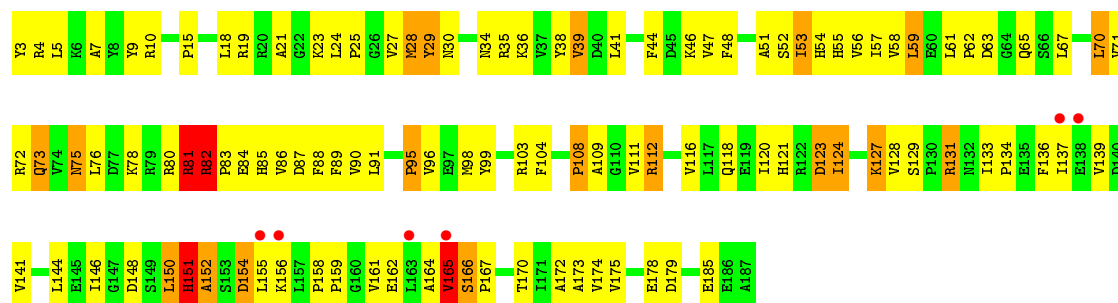
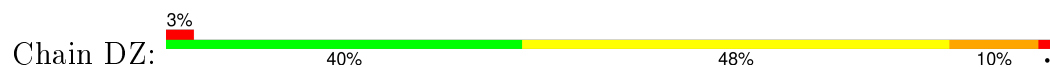


• Molecule 44: 50S ribosomal protein L25

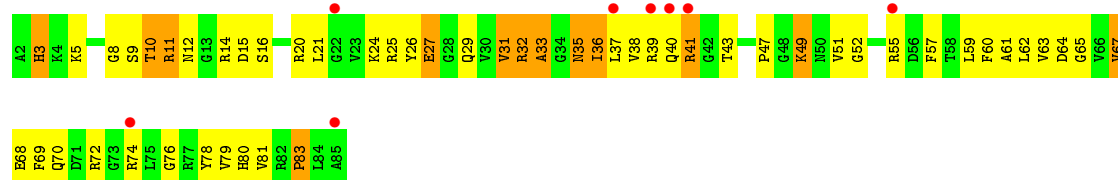




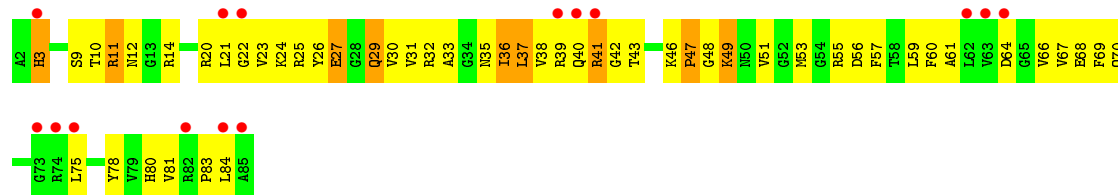
• Molecule 44: 50S ribosomal protein L25



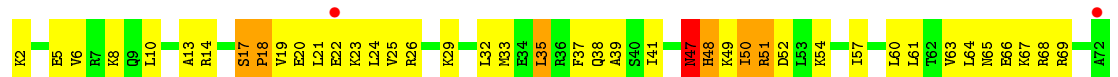
• Molecule 45: 50S ribosomal protein L27



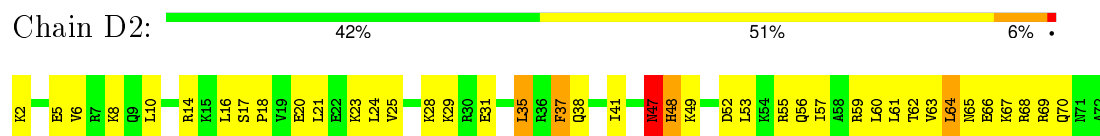
• Molecule 45: 50S ribosomal protein L27



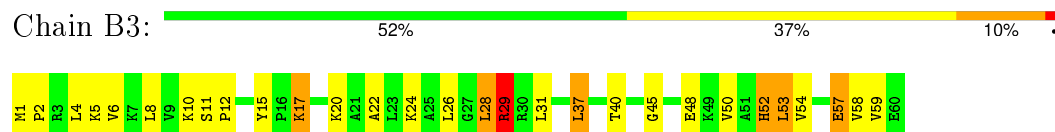
• Molecule 46: 50S ribosomal protein L29



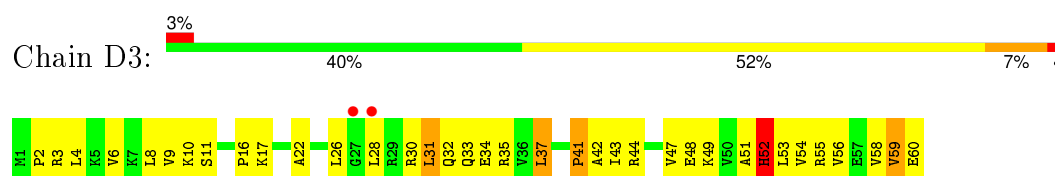
- Molecule 46: 50S ribosomal protein L29



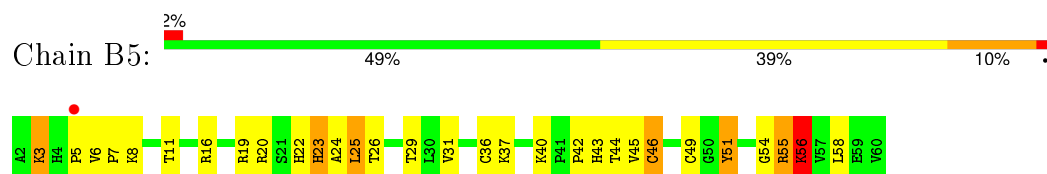
- Molecule 47: 50S ribosomal protein L30



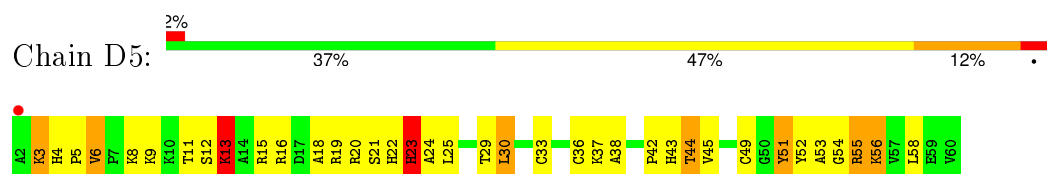
- Molecule 47: 50S ribosomal protein L30



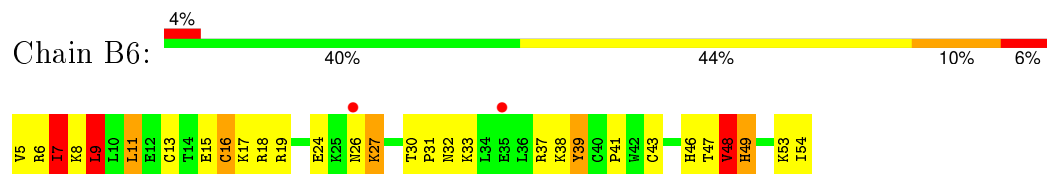
- Molecule 48: 50S ribosomal protein L32



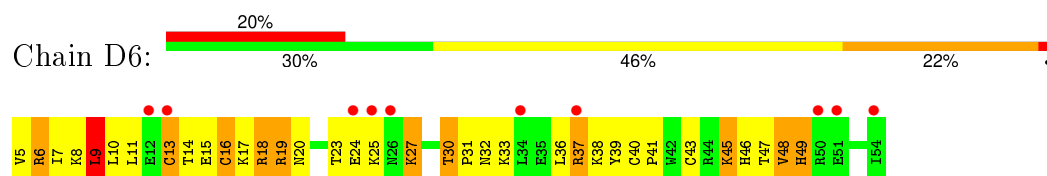
- Molecule 48: 50S ribosomal protein L32



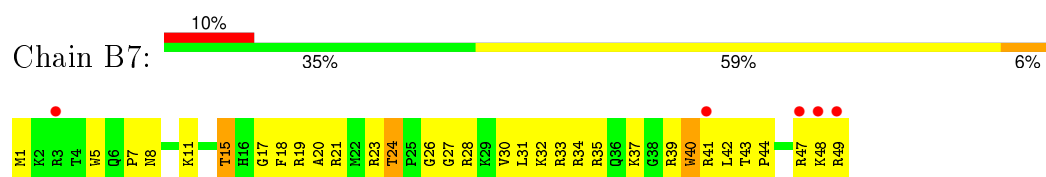
- Molecule 49: 50S ribosomal protein L33



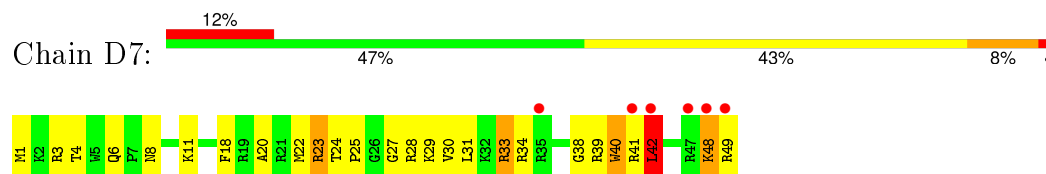
- Molecule 49: 50S ribosomal protein L33



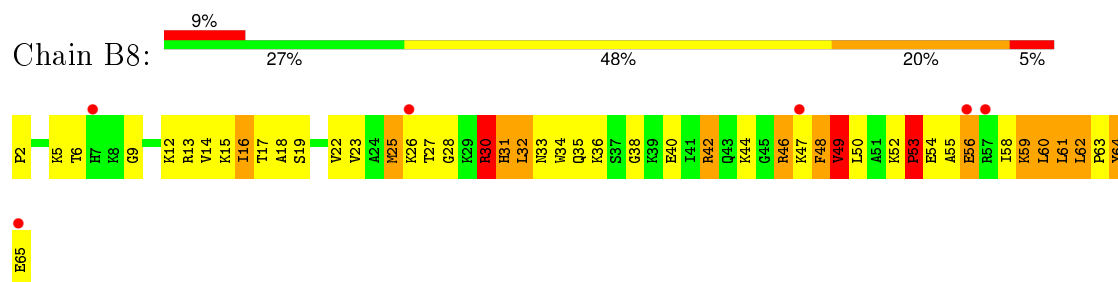
- Molecule 50: 50S ribosomal protein L34



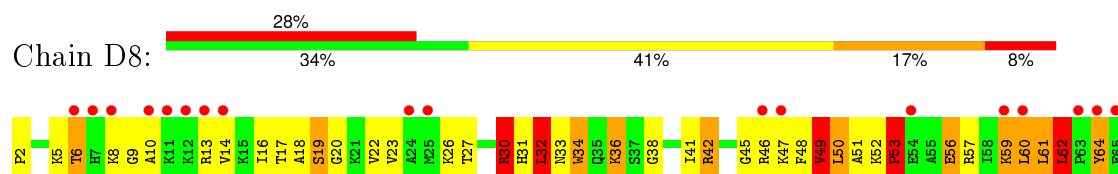
- Molecule 50: 50S ribosomal protein L34



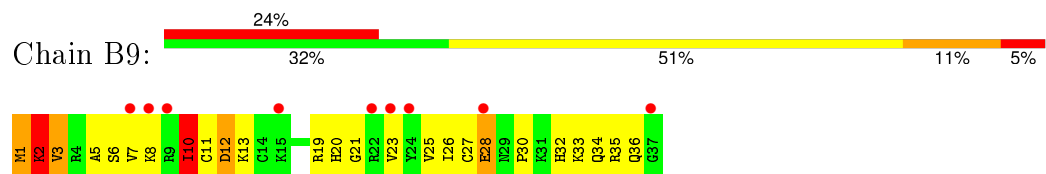
- Molecule 51: 50S ribosomal protein L35



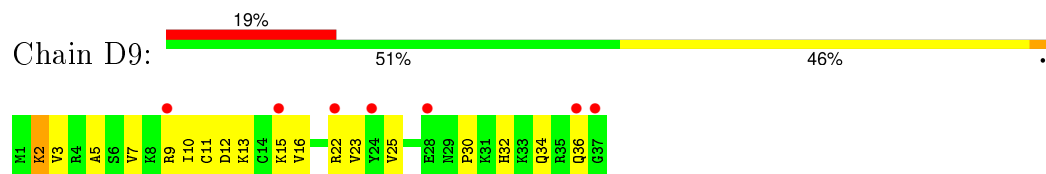
- Molecule 51: 50S ribosomal protein L35



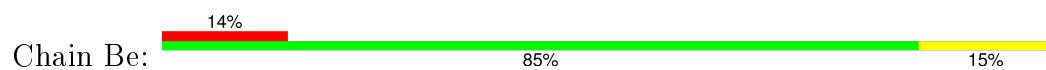
- Molecule 52: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L36

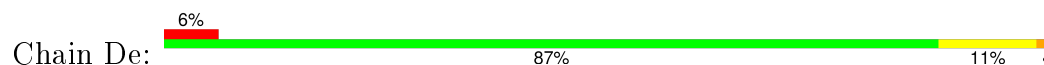


- Molecule 53: 50S ribosomal protein L7/L12





- 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



There are no outlier residues recorded for this chain.

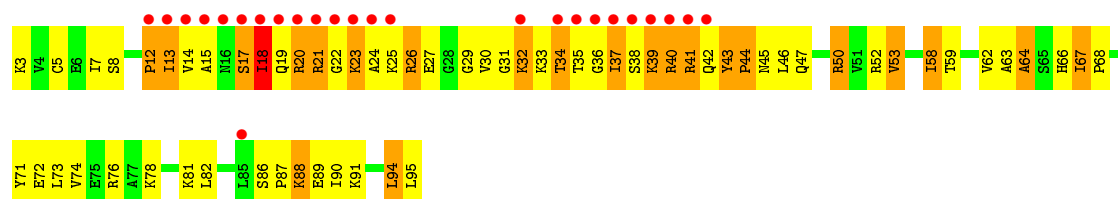
- Molecule 55: 50S ribosomal protein L7/L12



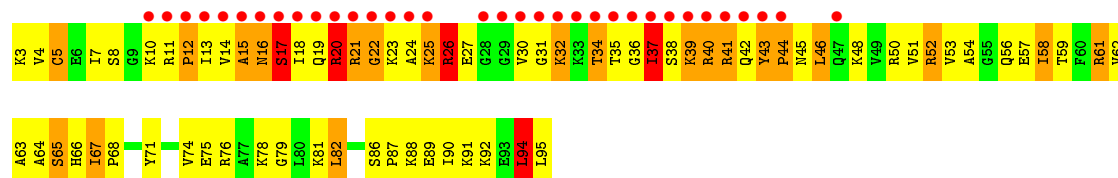
There are no outlier residues recorded for this chain.

- Molecule 56: 50S ribosomal protein L28

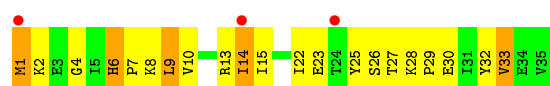
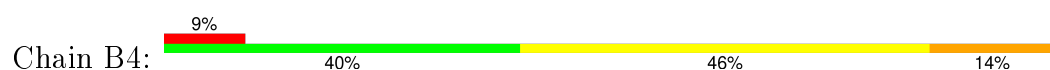




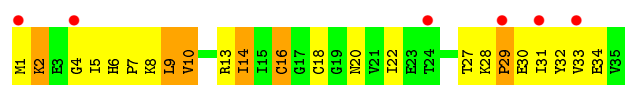
- Molecule 56: 50S ribosomal protein L28



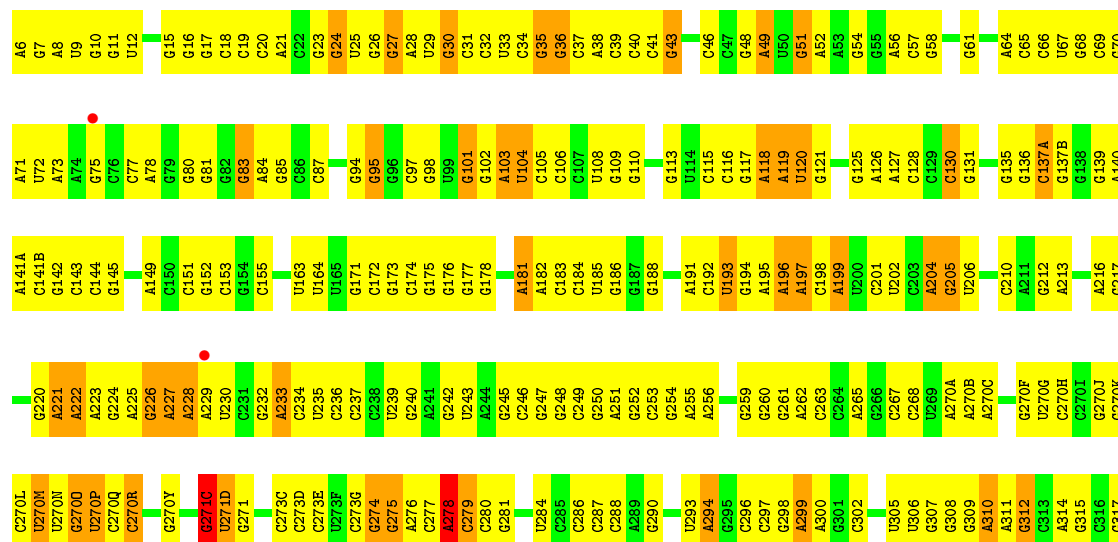
- Molecule 57: 50S ribosomal protein L31



- Molecule 57: 50S ribosomal protein L31

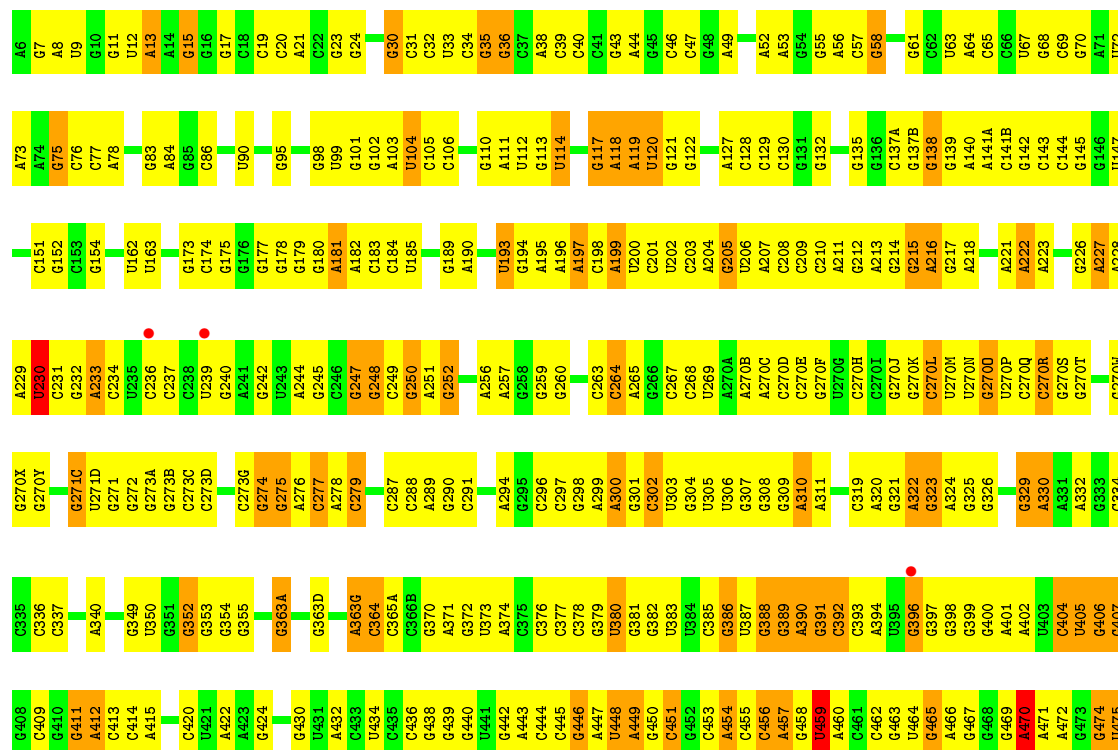


- Molecule 58: 23S ribosomal RNA



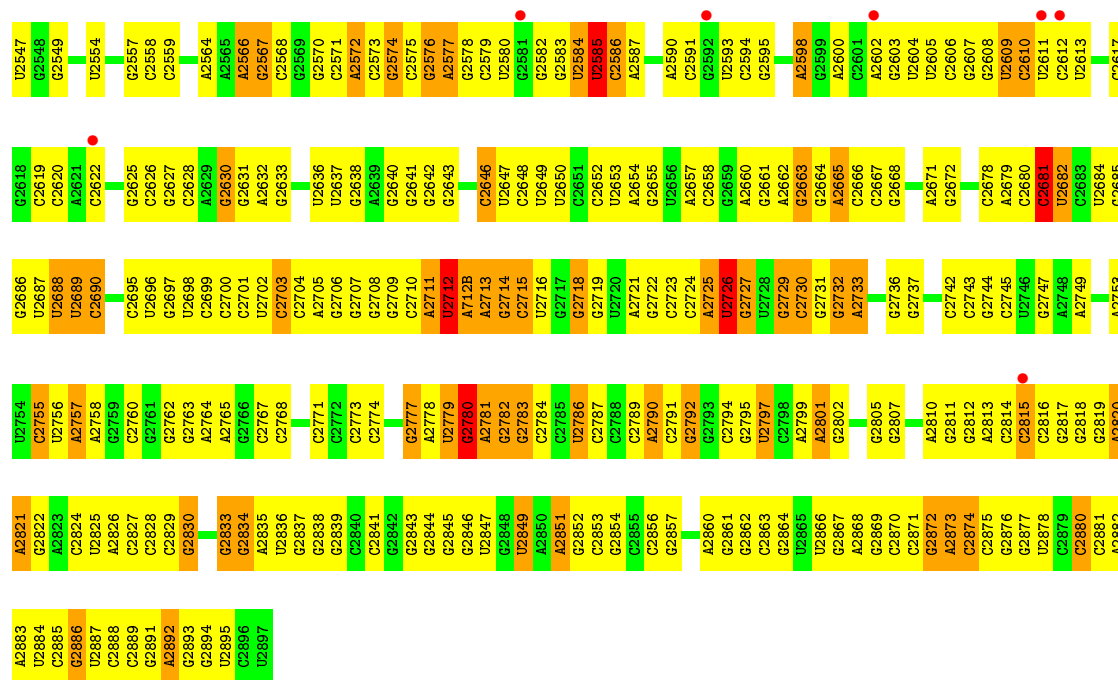
C1333	U1267	G1206	G1139	C1072	G1002	A941	G862	C795	G728	C658	C595	C523	A454	A390	C318
G1334	A1268	G1207	C1140	A1073	G1003	G942	A863	C796	G729	C659	G596	C524	G455	G391	C319
U1335	A1269	C1208	U1141	G1074	C1004	U943	G864	C797	C730	C660	U957	U524	G456	C392	A320
A1336	G1270	U1142	U1142	C1075	G1005	G944	G865	C798	C731	C661	G598	C527	A457	C393	G321
G1337	A1271	A1143	A1143	A1076	G1006	A945	A866	G799	G732	C662	G599	A528	G458	A322	A322
U1341	A1272	U1111	A1143	A1077	C1007	G946	A867	A800	G733	C663	G600	A529	U459	G323	G323
U1273	U1273	G1212	G1144	U1078	C1008	G947	A870	G803	C737	C664	C801	G530	A460	A324	A324
A1342	A1274	A1213	C1145	C1079	A1009	G948	U871	A802	G738	C665	G602	C531	C461	G325	G325
G1343	A1275	A1214	C1146	C1080	A1010	G949	A872	A802	G739	C666	A603	A532	G462	G396	G396
G1344	A1276	G1215	U1081	U1081	G1011	G950	A873	G805	U740	C667	C804	G533	G463	G400	G400
C1345	G1277	G1216	A1148	U1082	U1012	C951	G879	U807	G741	C668	C805	U534	U464	A401	A401
U1349	A1278	C1217	G1149	U1083	C1013	G952	G880	U807	G742	C669	U806	C535	G465	A402	A402
U1279	G1280	A1220	G1150	A1084	U1014	A953	G880	C871	G743	C670	U807	A536	G466	U403	A331
G1352	G1281	C1221	G1151	A1085	G1015	G954	C881	U811	G744	C671	A608	C537	G467	C404	C404
A1353	G1282	G1222	C1152	A1086	G1016	C955	A873	C812	G745	C672	A609A	G539	G468	U405	C335
A1354	G1285	G1223	C1153	G1087	U1017	G956	C885	U813	A746	C673	G612	A547	G469	G406	G406
G1355	A1286	G1224	G1154	A1088	C1018	A957	A874	C814	U747	C674	U613	A548	A470	G407	G407
G1356	A1287	G1225	A1155	U1089	U1019	U958	A890	C815	A747	C675	U614	G549	A471	U339	U339
U1357	U1288	A1226	A1156	U1090	A1020	A959	G892	C816	A750	C676	G615	G550	A472	A340	A340
C1358	C1289	G1227	G1157	G1091	A1021	A960	A896	C817	A751	C679	G616	G551	A473	G410	G410
A1359	G1290	G1228	C1161	U1092	U1023	G962	C897	A819	A752	C680	G617	G552	A474	G411	G411
A1360	C1291	G1229	G1162	G1093	G1024	U963	A897	A820	C753	C681	G618A	U553	U475	A412	A412
G1361	G1361	C1230	G1163	A1096	U1025	C964	A901	A821	C754	C682	G618B	U554	A476	C413	C413
C1362	U1294	G1231	G1164	U1096	G1026	C965	C902	U822	C755	C683	G619	U554	A477	C414	C414
C1295	C1295	G1232	U1165	U1101	A1027	G966	U905	G823	C756	C684	G620	U557	A478	C415	A415
G1296	G1296	G1233	C1166	A1102	A1028	C967	U906	A824	C757	C685	G621	G558	A479	C416	C416
C1297	U1234	C1234	U1167	A1103	G1036	G968	C906	A824	C758	C686	G622	G559	A480	G417	G417
C1298	C1298	G1235	U1168	C1104	U1033	U969	U907	U827	G759	C687	G623	G560	A481	C419	C419
G1299	U1300	G1236	G1171	U1105	A1032	C971	A909	A829	A761	C688	G625	G563	A482	U421	U421
U1301	A1301	A1237	A1174	G1107	G1034	C972	A910	G830	U762	C689	A627	C564	A488	A422	A422
A1302	U1302	U1239	U1175	U1108	U1035	C973	A911	G831	C763	C690	G628	C565	A489	A399	U358
C1305	C1305	U1240	A1176	G1110	G1036	G974A	C912	G832	C764	C691	G629	C566	A491	A422	A422
G1306	G1306	A1242	C1178	A1111	U1037	G975	C914	U833	C765	C692	A631	U568	A492	U427	G363A
A1307	A1307	G1243	C1179	U1112	C1041	C976	C915	A835	C766	C693	A632	U569	G493	A428	A428
A1308	G1244	G1245	C1180	U1113	G1042	C977	C916	G836	C767	C694	A633	G570	G494	A429	A429
G1309	G1245	G1246	G1183	G1114	C1043	G978	A917	C837	C768	C695	C634	A571	U499	G430	G430
G1310	G1310	U1246	G1184	C1118	U1044	G979	A918	C838	C769	C696	G635	A572	G500	U431	U363F
G1311	G1311	A1247	C1185	C1119	A1045	A980	G920	U839	A774	C704	A637	C574	A503	A432	A363G
G1312	U1312	G1248	G1186	G1120	A1046	A981	A926	C840	G775	A705	G638	U576	U504	C433	C364
U1313	U1249	C1249	G1187	C1121	G1047	C982	G921	A841	G776	A706	U639	U577	A505	C435	A371
G1314	C1250	C1251	C1188	G1122	A1048	A983	U922	G842	C776	A706	C641	G577	G506	C436	G372
G1315	C1251	C1252	C1189	C1123	C1049	A984	C923	G845	C779	U709	C642	G578	A507	G438	U373
U1316	C1252	G1253	G1190	C1124	C1053	G987	C924	C846	C779	U709	G642	G579	G508	G439	A374
A1317	A1317	A1254	G1191	C1125	A1054	A988	A926	U847	A781	C710	C645	C580	C509	G440	C377
U1321	A1321	U1256	G1192	A1126	A1054	G989	G928	G848	A782	C711	A646	G581	C510	U441	G378
U1322	U1322	U1257	G1193	A1127	A1057	A990	G929	G849	A783	C712	G647	G582	U511	G442	G379
U1323	U1323	C1257	C1196	A1128	A1058	A991	U930	G852	A784	C713	G648	G583	G512	A443	U380
G1324	G1324	G1258	G1197	A1129	G1059	G993	G931	G853	A785	C714	G649	A586	A513	C444	G381
G1325	G1325	U1259	U1198	U1130	U1060	C994	A932	G854	C788	C720	C850	C587	A515	C445	G382
U1326	U1326	G1260	U1199	G1131	U1061	C995	A933	G854	A789	C721	G851	C588	C516	A446	U383
C1327	C1327	C1261	G1200	A1132	G1062	A996	G934	G855	C790	A722	C852	C589	C517	U448	U384
G1328	G1328	A1262	C1201	U1133	G1063	G997	C935	C856	C791	C723	C853	A590	G518	A449	C385
U1329	U1329	U1263	C1202	C1135	G1063	C998	C936	C857	C792	C724	U854	C591	U519	G450	C386
C1330	C1330	G1264	G1203	U1136	A1069	U999	U937	U858	A793	C725	A855	G592	G520	G451	U387
G1410	G1410	A1265	A1204	G1137	A1070	U999	U937	U858	A793	C725	A855	G592	G520	G451	G388
C1411	G1332	G1266	U1205	G1138	G1071	A1001	G940	A861	G794	A727	U857	U594	G522	G453	G389

WORLDWIDE
PDB
PROTEIN DATA BANK

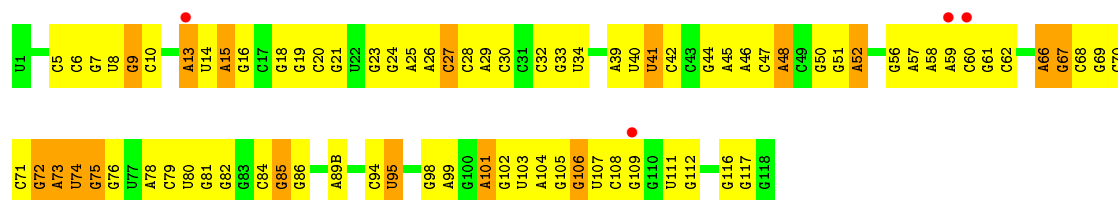


G1448	C1387	A1321	G1248	G1187	G1125	U1061	U999	G936	G869	G805	G738	U667	U607	C541	G476
A1495B	G1388	A1322	U1249	U1188	A1126	G1062	A1000	U937	A870	C806	G739	G668	A608	C542	A477
G1449	G1389	U1323	A1283	A1189	A1127	G1063	A1001	G940	A871	U807	U740	C871	A609A	C543	A478
G1450	G1390	A1284	A1254	G1190	A1128	C1064	G1002	G941	A872	G808	G741	C872	G609B	G545	A479
C1451	G1325	U1325	U1255	G1193	U1130	U1065	G1003	G942	G873	G809	G742	C873	C610	C546	A480
A1453	U1326	G1326	G1256	G1194	U1131	U1066	G1004	G943	G874	U810	G743	C874	C611	A547	A481
U1454	C1327	A1327	G1256	A1194	G1131	A1067	G1005	U944	G875	U811	G744	C875	C612	A548	A482
G1455	G1328	U1328	A1262	G1195	A1132	G1068	C1006	G944	C876	C812	G745	A675	A616	G549	A483
A1395	U1329	G1329	A1262	G1196	U1133	A1069	C1007	A945	U877	U813	A746	A676	G617	G556	A484
G1459	G1397	A1397	G1263	G1197	C1135	G1070	C1008	G946	A878	C814	U747	A677	G618	U557	C485
G1460	G1398	A1331	G1264	U1198	G1136	G1071	A1009	G947	G879	C815	G748	C878	G618B	G558	C486
A1461	G1399	G1332	A1265	U1199	G1137	A1072	G1010	G948	G880	C816	G749	C879	G619	G559	C487
G1462	G1400	U1335	A1268	C1200	G1138	A1073	G1011	G949	G881	G817	G750	C880	G620	G560	C488
C1463	G1401	U1336	A1269	C1201	G1139	G1074	U1012	G950	G882	G818	G751	C883	G621	G561	C489
C1464	C1402	A1336	A1269	G1202	C1140	C1075	C1013	C951	C884	A819	C754	G884	G622	G562	A492
G1465	G1337	G1337	C1270	G1203	U1141	C1076	G1016	G954	C889	A820	C755	G885	G623	G563	G493
G1466	G1338	A1204	A1271	G1204	U1142	U1077	G1017	C955	A890	G830	C756	C886	G624	G564	G494
U1465	G1338	U1205	A1272	U1205	A1148	A1078	G1017	C956	A891	G831	C757	C887	G625	G565	G495
C1467	G1405	G1339	A1273	G1206	A1143	C1079	U1018	A957	G892	G832	C758	U688	G626	U566	G496
C1468	U1406	U1340	A1273	G1207	G1144	C1080	U1019	U958	A893	G833	C759	U689	G627	A567	A497
C1469	G1407	U1341	A1274	U1207	G1145	U1081	U1020	U959	G894	G834	C760	C890	G628	U568	
A1469	C1408	A1342	A1275	U1210	G1146	U1082	A1021	A960	C894	U828	C761	C891	G629	U569	
G1470	G1343	G1343	A1276	G1211	C1147	U1083	G1022	A961	U895	G835	C762	C892	G630	G570	A501
A1471	G1344	A1344	G1277	G1212	G1147	U1084	U1023	C961	A896	G836	C763	C893	G631	A571	A502
A1472	G1345	G1148	A1278	G1213	A1148	A1085	G1024	G962	C897	G837	C764	C894	G632	A572	A503
G1473	G1346	C1346	G1279	A1214	G1149	A1086	G1025	U963	A900	G838	C765	U694	G633	A573	U504
C1474	G1347	G1347	G1280	A1214	C1150	U1087	U1026	C964	A901	G839	C766	C895	G634	C574	A505
	U1415	G1348	A1286	G1215	G1151	G1088	U1027	C965	A902	C834	C767	C896	G635	C580	U511
G1478	G1416	A1349	A1287	G1216	G1152	A1089	U1028	C971	A903	C840	C768	C897	G636	C581	G512
G1479	G1417	G1350	A1288	C1217	C1153	G1089	A1029	G972	C908	A841	C769	A705	G637	G582	A513
G1480	G1418	C1351	U1288	G1218	G1154	U1090	G1030	G973	C909	G842	C770	A706	G640	C583	
U1481	U1419	U1352	C1289	G1219	A1155	G1091	G1031	G974A	C904	G843	C771	U709	G641	C584	C516
G1483	U1420	U1353	C1290	A1220	A1156	C1092	G1031	C975	U905	G844	C772	C710	G642	C585	C517
	G1421	A1354	C1291	C1221	G1157	G1093	A1032	C976	C906	U846	C773	C711	G643	C586	G518
A1486	G1422	G1355	U1292	C1222	C1158	U1094	U1033	G979	A901	U847	C774	C712	G644	C587	
G1487	G1423	G1355	C1293	C1223	U1159	A1095	G1034	A980	C915	G848	C775	C713	G645	C588	G521
G1488	G1424	A1358	U1294	G1224	G1160	A1096	U1035	A981	C916	A849	C776	C714	G646	C589	G522
U1489	G1425	G1359	C1295	G1225	C1161	U1097	G1036	A982	C917	C850	C777	C715	G647	C590	G523
A1490	G1426	A1360	G1296	G1226	G1162	U1097	G1036	C982	C918	U851	C778	C716	G648	C591	U524
G1491	A1427	U1367	C1297	A1226	G1163	U1101	G1039	A983	A918	G852	C779	C717	G649	C592	G525
G1492	G1428	C1363	C1298	G1227	G1164	C1102	C1040	A984	C919	G853	C780	C718	G650	C593	A526
C1493	G1429	G1364	G1299	G1228	U1165	A1103	G1041	A985	C920	G854	C781	C719	G651	U594	G527
A1494	C1430	A1365	U1300	G1229	C1166	G1104	G1042	C986	C921	C855	C782	C720	G652	C595	A528
A1495	U1431	A1366	A1301	C1230	U1167	U1105	G1043	A987	U922	C856	C783	C721	G653	C596	A529
A1496	C1432	U1367	A1302	G1231	U1168	G1106	G1044	C988	C923	C857	C784	C722	G654	U597	G530
U1497	U1433	G1368	G1303	G1232	G1169	G1107	U1045	A989	C924	U858	C785	C723	G655	C598	G531
C1498	A1434	U1372	C1304	G1233	G1170	U1108	A1046	G989	A926	G859	C786	C724	G656	C599	A532
C1499	G1435	U1373	C1305	U1234	G1171	C1109	G1047	C985	C928	G862	C787	C725	G657	C600	G533
G1500	G1436	A1374	G1306	G1235	G1172	C1110	G1048	C986	C929	C863	C788	C726	G658	G601	G534
C1501	C1437	G1375	A1307	G1236	A1174	A1111	G1049	G987	U922	C864	C789	C727	G659	C602	C535
C1502	U1438	C1376	U1308	U1237	U1175	G1112	A1050	A988	C923	C865	C790	C728	G660	C603	A536
U1503	A1439	G1377	G1309	G1238	G1176	U1113	G1051	G989	A926	C866	C791	C729	G661	C604	C537
C1504	G1440	A1378	G1310	G1239	A1177	G1114	C1052	A990	C928	G867	C792	C730	G662	G605	G539
C1505	G1441	G1379	U1311	G1240	C1178	G1115	A1054	C991	C929	C868	C793	C731	G663	C606	
	G1442	A1380	A1312	A1241	C1179	C1116	G1055	C992	C930	C869	C794	C732	G664	C607	
A1509	G1443	G1381	U1313	A1242	C1180	G1120	G1056	C993	U930	C870	C795	C733	G665	C608	
A1510	G1444	G1382	C1314	G1243	C1181	C1121	A1057	C994	C931	C871	C796	C734	G666	C609	
A1511	A1445	C1383	C1315	G1244	G1183	C1122	A1058	C995	C932	C872	C797	C735	G667	C610	
A1512	G1446	A1384	U1316	G1245	G1184	G1123	G1059	A996	C933	C873	C798	C736	G668	C611	
C1513	G1447	C1385	A1317	A1246	G1185	C1124	C1060	C997	C934	C874	C799	C737	G669	C612	
U1514		C1386		A1247	G1186	C1124	U1060	C998	C935	U968	A804		G670	U606	

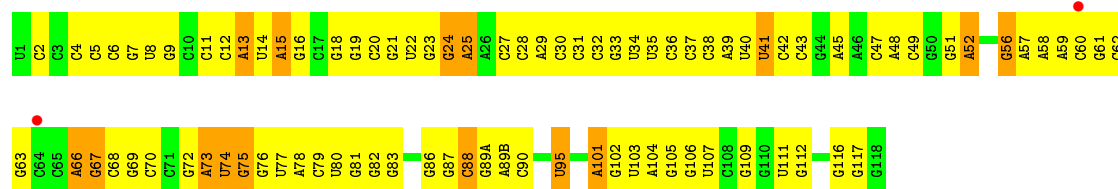




● Molecule 59: 5S ribosomal RNA



● Molecule 59: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	307.21Å 670.44Å 350.40Å 90.00° 92.37° 90.00°	Depositor
Resolution (Å)	40.00 – 4.00 145.85 – 3.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-4.00) 86.3 (145.85-3.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 4.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.281 , 0.329 0.302 , 0.339	Depositor DCC
R_{free} test set	25911 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	74.5	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , -10.0	EDS
Estimated twinning fraction	0.249 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.24$, $\langle L^2 \rangle = 0.09$	Xtriage
Outliers	0 of 517738 reflections	Xtriage
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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
58:BA:2681:C:N4	58:BA:2725:A:H62	1.22	1.35
23:AY:580:MET:HE2	58:BA:1913:A:N1	1.37	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	10
1	CB	233/235 (99%)	152 (65%)	55 (24%)	26 (11%)	0	10
2	AC	205/207 (99%)	156 (76%)	33 (16%)	16 (8%)	1	20
2	CC	205/207 (99%)	148 (72%)	41 (20%)	16 (8%)	1	20
3	AD	206/208 (99%)	145 (70%)	37 (18%)	24 (12%)	0	9
3	CD	206/208 (99%)	150 (73%)	32 (16%)	24 (12%)	0	9
4	AE	149/151 (99%)	124 (83%)	17 (11%)	8 (5%)	2	30
4	CE	149/151 (99%)	116 (78%)	25 (17%)	8 (5%)	2	30
5	AF	99/101 (98%)	73 (74%)	20 (20%)	6 (6%)	2	27
5	CF	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	2	27
6	AG	153/155 (99%)	122 (80%)	23 (15%)	8 (5%)	2	31
6	CG	153/155 (99%)	116 (76%)	28 (18%)	9 (6%)	2	28
7	AH	136/138 (99%)	93 (68%)	29 (21%)	14 (10%)	1	12
7	CH	136/138 (99%)	101 (74%)	22 (16%)	13 (10%)	1	14
8	AI	125/127 (98%)	93 (74%)	28 (22%)	4 (3%)	5	44
8	CI	125/127 (98%)	97 (78%)	22 (18%)	6 (5%)	3	32
9	AJ	97/99 (98%)	73 (75%)	14 (14%)	10 (10%)	1	12
9	CJ	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	2	27
10	AK	117/119 (98%)	85 (73%)	16 (14%)	16 (14%)	0	6
10	CK	117/119 (98%)	79 (68%)	21 (18%)	17 (14%)	0	5
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	17
12	CM	123/125 (98%)	90 (73%)	24 (20%)	9 (7%)	1	22
13	AN	58/60 (97%)	43 (74%)	8 (14%)	7 (12%)	0	8
13	CN	58/60 (97%)	44 (76%)	8 (14%)	6 (10%)	1	12
14	AO	86/88 (98%)	62 (72%)	15 (17%)	9 (10%)	1	11
14	CO	86/88 (98%)	62 (72%)	20 (23%)	4 (5%)	3	33
15	AP	82/84 (98%)	64 (78%)	14 (17%)	4 (5%)	3	32
15	CP	82/84 (98%)	62 (76%)	16 (20%)	4 (5%)	3	32
16	AQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	1	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	CQ	98/100 (98%)	68 (69%)	21 (21%)	9 (9%)	1	16
17	AR	68/70 (97%)	52 (76%)	11 (16%)	5 (7%)	1	21
17	CR	68/70 (97%)	47 (69%)	19 (28%)	2 (3%)	6	46
18	AS	77/79 (98%)	41 (53%)	24 (31%)	12 (16%)	0	5
18	CS	77/79 (98%)	50 (65%)	11 (14%)	16 (21%)	0	2
19	AT	97/99 (98%)	81 (84%)	10 (10%)	6 (6%)	2	27
19	CT	97/99 (98%)	76 (78%)	17 (18%)	4 (4%)	3	37
23	AY	663/687 (96%)	436 (66%)	147 (22%)	80 (12%)	0	8
23	CY	663/687 (96%)	454 (68%)	139 (21%)	70 (11%)	0	11
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	3
25	BD	273/275 (99%)	177 (65%)	52 (19%)	44 (16%)	0	5
25	DD	273/275 (99%)	171 (63%)	56 (20%)	46 (17%)	0	4
26	BE	203/205 (99%)	127 (63%)	45 (22%)	31 (15%)	0	5
26	DE	203/205 (99%)	128 (63%)	40 (20%)	35 (17%)	0	4
27	BF	206/208 (99%)	132 (64%)	53 (26%)	21 (10%)	1	13
27	DF	206/208 (99%)	131 (64%)	42 (20%)	33 (16%)	0	5
28	BG	179/181 (99%)	126 (70%)	40 (22%)	13 (7%)	1	22
28	DG	179/181 (99%)	131 (73%)	35 (20%)	13 (7%)	1	22
29	BH	165/167 (99%)	113 (68%)	32 (19%)	20 (12%)	0	8
29	DH	165/167 (99%)	102 (62%)	42 (26%)	21 (13%)	0	8
31	BK	138/140 (99%)	98 (71%)	30 (22%)	10 (7%)	1	23
31	DK	138/140 (99%)	100 (72%)	31 (22%)	7 (5%)	2	31
32	BN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	0	9
32	DN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	0	9
33	BO	120/122 (98%)	84 (70%)	20 (17%)	16 (13%)	0	6
33	DO	120/122 (98%)	86 (72%)	24 (20%)	10 (8%)	1	18
34	BP	144/146 (99%)	82 (57%)	36 (25%)	26 (18%)	0	3
34	DP	144/146 (99%)	81 (56%)	35 (24%)	28 (19%)	0	3
35	BQ	139/141 (99%)	94 (68%)	33 (24%)	12 (9%)	1	17
35	DQ	139/141 (99%)	99 (71%)	30 (22%)	10 (7%)	1	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BR	115/117 (98%)	80 (70%)	21 (18%)	14 (12%)	0	8
36	DR	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	1	12
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	2
38	DT	136/138 (99%)	90 (66%)	22 (16%)	24 (18%)	0	3
39	BU	115/117 (98%)	91 (79%)	18 (16%)	6 (5%)	2	31
39	DU	115/117 (98%)	90 (78%)	21 (18%)	4 (4%)	4	42
40	BV	99/101 (98%)	65 (66%)	16 (16%)	18 (18%)	0	3
40	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	6
41	BW	111/113 (98%)	84 (76%)	17 (15%)	10 (9%)	1	17
41	DW	111/113 (98%)	85 (77%)	14 (13%)	12 (11%)	0	11
42	BX	91/93 (98%)	66 (72%)	19 (21%)	6 (7%)	1	25
42	DX	91/93 (98%)	70 (77%)	15 (16%)	6 (7%)	1	25
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	11
44	DZ	183/185 (99%)	121 (66%)	44 (24%)	18 (10%)	1	14
45	B0	82/84 (98%)	58 (71%)	17 (21%)	7 (8%)	1	17
45	D0	82/84 (98%)	51 (62%)	24 (29%)	7 (8%)	1	17
46	B2	69/71 (97%)	50 (72%)	13 (19%)	6 (9%)	1	17
46	D2	69/71 (97%)	50 (72%)	16 (23%)	3 (4%)	3	35
47	B3	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	2	31
47	D3	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	2	31
48	B5	57/59 (97%)	41 (72%)	12 (21%)	4 (7%)	1	23
48	D5	57/59 (97%)	36 (63%)	18 (32%)	3 (5%)	2	31
49	B6	48/50 (96%)	27 (56%)	13 (27%)	8 (17%)	0	4
49	D6	48/50 (96%)	28 (58%)	11 (23%)	9 (19%)	0	3
50	B7	47/49 (96%)	31 (66%)	14 (30%)	2 (4%)	3	35
50	D7	47/49 (96%)	36 (77%)	6 (13%)	5 (11%)	0	11
51	B8	62/64 (97%)	32 (52%)	22 (36%)	8 (13%)	0	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	D8	62/64 (97%)	38 (61%)	14 (23%)	10 (16%)	0	5
52	B9	35/37 (95%)	23 (66%)	7 (20%)	5 (14%)	0	6
52	D9	35/37 (95%)	26 (74%)	8 (23%)	1 (3%)	6	46
53	Be	70/102 (69%)	35 (50%)	28 (40%)	7 (10%)	1	13
53	De	70/102 (69%)	39 (56%)	24 (34%)	7 (10%)	1	13
56	B1	91/93 (98%)	53 (58%)	19 (21%)	19 (21%)	0	2
56	D1	91/93 (98%)	57 (63%)	15 (16%)	19 (21%)	0	2
57	B4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	5
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	9

5 of 1569 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	203/203 (100%)	161 (79%)	42 (21%)	1	11
1	CB	203/203 (100%)	158 (78%)	45 (22%)	1	10
2	AC	161/161 (100%)	136 (84%)	25 (16%)	3	24
2	CC	161/161 (100%)	136 (84%)	25 (16%)	3	24
3	AD	180/180 (100%)	142 (79%)	38 (21%)	1	11
3	CD	180/180 (100%)	150 (83%)	30 (17%)	3	21
4	AE	116/116 (100%)	95 (82%)	21 (18%)	2	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CE	116/116 (100%)	92 (79%)	24 (21%)	1	11
5	AF	90/90 (100%)	80 (89%)	10 (11%)	8	38
5	CF	90/90 (100%)	85 (94%)	5 (6%)	26	65
6	AG	126/126 (100%)	112 (89%)	14 (11%)	8	38
6	CG	126/126 (100%)	114 (90%)	12 (10%)	11	45
7	AH	119/119 (100%)	97 (82%)	22 (18%)	2	15
7	CH	119/119 (100%)	104 (87%)	15 (13%)	5	31
8	AI	98/98 (100%)	83 (85%)	15 (15%)	3	24
8	CI	98/98 (100%)	82 (84%)	16 (16%)	3	22
9	AJ	89/89 (100%)	73 (82%)	16 (18%)	2	17
9	CJ	89/89 (100%)	70 (79%)	19 (21%)	1	11
10	AK	90/90 (100%)	76 (84%)	14 (16%)	3	24
10	CK	90/90 (100%)	71 (79%)	19 (21%)	1	11
11	AL	104/104 (100%)	82 (79%)	22 (21%)	1	11
11	CL	104/104 (100%)	74 (71%)	30 (29%)	0	4
12	AM	100/100 (100%)	81 (81%)	19 (19%)	2	14
12	CM	100/100 (100%)	88 (88%)	12 (12%)	6	33
13	AN	49/49 (100%)	40 (82%)	9 (18%)	2	15
13	CN	49/49 (100%)	42 (86%)	7 (14%)	4	28
14	AO	79/79 (100%)	70 (89%)	9 (11%)	7	36
14	CO	79/79 (100%)	68 (86%)	11 (14%)	4	29
15	AP	72/72 (100%)	65 (90%)	7 (10%)	10	43
15	CP	72/72 (100%)	69 (96%)	3 (4%)	36	72
16	AQ	95/95 (100%)	78 (82%)	17 (18%)	2	17
16	CQ	95/95 (100%)	82 (86%)	13 (14%)	4	29
17	AR	61/61 (100%)	53 (87%)	8 (13%)	5	30
17	CR	61/61 (100%)	51 (84%)	10 (16%)	3	21
18	AS	69/69 (100%)	53 (77%)	16 (23%)	1	8
18	CS	69/69 (100%)	53 (77%)	16 (23%)	1	8
19	AT	76/76 (100%)	64 (84%)	12 (16%)	3	23
19	CT	76/76 (100%)	69 (91%)	7 (9%)	11	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	AY	563/579 (97%)	466 (83%)	97 (17%)	2	19
23	CY	563/579 (97%)	460 (82%)	103 (18%)	2	16
24	BC	180/180 (100%)	135 (75%)	45 (25%)	1	7
24	DC	180/180 (100%)	139 (77%)	41 (23%)	1	9
25	BD	217/217 (100%)	173 (80%)	44 (20%)	1	12
25	DD	217/217 (100%)	171 (79%)	46 (21%)	1	11
26	BE	165/165 (100%)	134 (81%)	31 (19%)	2	15
26	DE	165/165 (100%)	133 (81%)	32 (19%)	2	14
27	BF	165/165 (100%)	127 (77%)	38 (23%)	1	9
27	DF	165/165 (100%)	133 (81%)	32 (19%)	2	14
28	BG	155/155 (100%)	126 (81%)	29 (19%)	2	15
28	DG	155/155 (100%)	127 (82%)	28 (18%)	2	16
29	BH	136/136 (100%)	111 (82%)	25 (18%)	2	15
29	DH	136/136 (100%)	120 (88%)	16 (12%)	6	35
31	BK	105/105 (100%)	85 (81%)	20 (19%)	2	14
31	DK	105/105 (100%)	88 (84%)	17 (16%)	3	22
32	BN	117/117 (100%)	100 (86%)	17 (14%)	4	27
32	DN	117/117 (100%)	100 (86%)	17 (14%)	4	27
33	BO	100/100 (100%)	84 (84%)	16 (16%)	3	23
33	DO	100/100 (100%)	87 (87%)	13 (13%)	5	31
34	BP	112/112 (100%)	92 (82%)	20 (18%)	2	17
34	DP	112/112 (100%)	88 (79%)	24 (21%)	1	11
35	BQ	111/111 (100%)	88 (79%)	23 (21%)	1	11
35	DQ	111/111 (100%)	87 (78%)	24 (22%)	1	10
36	BR	100/100 (100%)	83 (83%)	17 (17%)	2	20
36	DR	100/100 (100%)	83 (83%)	17 (17%)	2	20
37	BS	77/77 (100%)	63 (82%)	14 (18%)	2	16
37	DS	77/77 (100%)	59 (77%)	18 (23%)	1	8
38	BT	120/120 (100%)	95 (79%)	25 (21%)	1	11
38	DT	120/120 (100%)	91 (76%)	29 (24%)	1	7
39	BU	93/93 (100%)	71 (76%)	22 (24%)	1	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DU	93/93 (100%)	75 (81%)	18 (19%)	2	14
40	BV	82/82 (100%)	65 (79%)	17 (21%)	1	11
40	DV	82/82 (100%)	62 (76%)	20 (24%)	1	7
41	BW	92/92 (100%)	71 (77%)	21 (23%)	1	9
41	DW	92/92 (100%)	76 (83%)	16 (17%)	2	18
42	BX	75/75 (100%)	61 (81%)	14 (19%)	2	15
42	DX	75/75 (100%)	60 (80%)	15 (20%)	1	13
43	BY	88/88 (100%)	65 (74%)	23 (26%)	0	6
43	DY	88/88 (100%)	71 (81%)	17 (19%)	2	14
44	BZ	162/162 (100%)	132 (82%)	30 (18%)	2	15
44	DZ	162/162 (100%)	134 (83%)	28 (17%)	2	19
45	B0	66/66 (100%)	52 (79%)	14 (21%)	1	11
45	D0	66/66 (100%)	53 (80%)	13 (20%)	1	13
46	B2	66/66 (100%)	59 (89%)	7 (11%)	8	39
46	D2	66/66 (100%)	60 (91%)	6 (9%)	12	47
47	B3	52/52 (100%)	42 (81%)	10 (19%)	2	14
47	D3	52/52 (100%)	48 (92%)	4 (8%)	16	55
48	B5	51/51 (100%)	41 (80%)	10 (20%)	1	14
48	D5	51/51 (100%)	40 (78%)	11 (22%)	1	10
49	B6	49/49 (100%)	43 (88%)	6 (12%)	6	33
49	D6	49/49 (100%)	38 (78%)	11 (22%)	1	10
50	B7	42/42 (100%)	36 (86%)	6 (14%)	4	28
50	D7	42/42 (100%)	36 (86%)	6 (14%)	4	28
51	B8	54/54 (100%)	37 (68%)	17 (32%)	0	3
51	D8	54/54 (100%)	40 (74%)	14 (26%)	0	6
52	B9	34/34 (100%)	30 (88%)	4 (12%)	6	35
52	D9	34/34 (100%)	32 (94%)	2 (6%)	24	64
53	Be	54/54 (100%)	47 (87%)	7 (13%)	5	31
53	De	54/54 (100%)	46 (85%)	8 (15%)	4	26
56	B1	78/78 (100%)	64 (82%)	14 (18%)	2	17
56	D1	78/78 (100%)	59 (76%)	19 (24%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	B4	31/31 (100%)	26 (84%)	5 (16%)	3	22
57	D4	31/31 (100%)	25 (81%)	6 (19%)	2	14
All	All	11138/11170 (100%)	9124 (82%)	2014 (18%)	2	16

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

Mol	Chain	Res	Type
44	BZ	112	ARG
4	CE	31	LEU
42	DX	57	LEU
45	B0	67	VAL
57	B4	23	GLU

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

Mol	Chain	Res	Type
42	BX	58	HIS
11	CL	8	ASN
40	DV	64	HIS
44	BZ	30	ASN
3	CD	116	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	AA	1510/1511 (99%)	291 (19%)	17 (1%)
20	CA	1510/1511 (99%)	294 (19%)	16 (1%)
21	AW	76/77 (98%)	21 (27%)	2 (2%)
21	CW	76/77 (98%)	24 (31%)	2 (2%)
22	AV	22/23 (95%)	11 (50%)	1 (4%)
22	CV	22/23 (95%)	8 (36%)	2 (9%)
58	BA	2878/2879 (99%)	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
58	BA	2750	A
20	CA	484	G
58	DA	2212	A
58	BA	2780	G
20	CA	115	G

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 carbohydrates 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
60	FUA	AY	701	-	37,40,40	1.67	7 (18%)	45,64,64	2.23	10 (22%)
61	GDP	AY	702	-	23,30,30	1.35	3 (13%)	30,47,47	1.81	7 (23%)
60	FUA	CY	701	-	37,40,40	1.69	4 (10%)	45,64,64	2.50	15 (33%)
61	GDP	CY	702	-	23,30,30	1.36	3 (13%)	30,47,47	1.81	7 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	FUA	AY	701	-	-	0/10/92/92	0/4/4/4
61	GDP	AY	702	-	-	0/12/32/32	0/3/3/3
60	FUA	CY	701	-	-	0/10/92/92	0/4/4/4
61	GDP	CY	702	-	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	CY	701	FUA	C23-C22	-6.02	1.39	1.51
60	AY	701	FUA	C23-C22	-5.88	1.40	1.51
60	CY	701	FUA	C23-C24	-4.27	1.39	1.53
60	AY	701	FUA	C23-C24	-4.21	1.39	1.53
60	AY	701	FUA	C24-C25	-3.77	1.39	1.50

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CY	701	FUA	C13-C12-C11	-8.06	101.03	111.95
60	AY	701	FUA	C13-C12-C11	-8.02	101.09	111.95
60	CY	701	FUA	C5-C4-C3	-6.50	98.38	110.53
61	CY	702	GDP	N3-C2-N1	-4.76	120.19	127.44
61	AY	702	GDP	N3-C2-N1	-4.76	120.20	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 35 short contacts:

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

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	Be	1
53	De	1

All chain breaks are listed below:

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

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	235/235 (100%)	-0.18	0 100 100	41, 81, 119, 159	0
1	CB	235/235 (100%)	0.00	2 (0%) 85 80	38, 80, 117, 178	0
2	AC	207/207 (100%)	0.17	16 (7%) 16 11	34, 76, 116, 152	0
2	CC	207/207 (100%)	-0.18	6 (2%) 55 42	44, 78, 121, 158	0
3	AD	208/208 (100%)	-0.09	8 (3%) 44 34	37, 71, 125, 178	0
3	CD	208/208 (100%)	-0.02	9 (4%) 39 29	51, 83, 120, 165	0
4	AE	151/151 (100%)	0.43	15 (9%) 9 7	30, 57, 93, 133	0
4	CE	151/151 (100%)	0.73	28 (18%) 2 2	31, 61, 99, 185	0
5	AF	101/101 (100%)	-0.59	0 100 100	31, 52, 87, 115	0
5	CF	101/101 (100%)	-0.40	1 (0%) 84 77	25, 52, 78, 129	0
6	AG	155/155 (100%)	0.66	19 (12%) 5 5	54, 100, 147, 205	0
6	CG	155/155 (100%)	-0.07	5 (3%) 51 38	57, 99, 155, 218	0
7	AH	138/138 (100%)	-0.50	0 100 100	28, 49, 83, 117	0
7	CH	138/138 (100%)	-0.15	3 (2%) 65 54	29, 57, 101, 142	0
8	AI	127/127 (100%)	0.27	9 (7%) 19 13	48, 87, 128, 163	0
8	CI	127/127 (100%)	0.04	7 (5%) 29 21	51, 91, 136, 195	0
9	AJ	99/99 (100%)	0.29	9 (9%) 11 8	46, 74, 108, 114	0
9	CJ	99/99 (100%)	0.12	5 (5%) 32 23	37, 82, 121, 145	0
10	AK	119/119 (100%)	0.08	6 (5%) 32 24	41, 71, 114, 157	0
10	CK	119/119 (100%)	-0.16	3 (2%) 61 49	22, 59, 106, 135	0
11	AL	125/125 (100%)	0.06	4 (3%) 51 38	31, 63, 97, 178	0
11	CL	125/125 (100%)	0.33	7 (5%) 28 20	29, 68, 109, 136	0
12	AM	125/125 (100%)	0.30	10 (8%) 15 11	61, 101, 139, 150	0
12	CM	125/125 (100%)	0.53	12 (9%) 10 8	52, 106, 160, 199	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	1.13	14 (23%) 1 2	42, 64, 97, 106	0
13	CN	60/60 (100%)	0.27	2 (3%) 50 38	47, 67, 112, 156	0
14	AO	88/88 (100%)	-0.18	2 (2%) 64 52	32, 61, 102, 172	0
14	CO	88/88 (100%)	-0.14	2 (2%) 64 52	29, 61, 108, 215	0
15	AP	84/84 (100%)	1.06	20 (23%) 1 1	47, 80, 118, 187	0
15	CP	84/84 (100%)	0.65	12 (14%) 4 4	53, 81, 118, 174	0
16	AQ	100/100 (100%)	0.22	1 (1%) 84 77	33, 56, 100, 124	0
16	CQ	100/100 (100%)	0.23	2 (2%) 68 57	30, 58, 89, 139	0
17	AR	70/70 (100%)	0.12	3 (4%) 39 29	30, 55, 101, 156	0
17	CR	70/70 (100%)	0.05	4 (5%) 27 19	32, 46, 123, 186	0
18	AS	79/79 (100%)	0.49	9 (11%) 7 6	68, 90, 148, 159	0
18	CS	79/79 (100%)	0.43	9 (11%) 7 6	59, 92, 146, 215	0
19	AT	99/99 (100%)	0.30	3 (3%) 54 41	58, 86, 116, 146	0
19	CT	99/99 (100%)	0.45	4 (4%) 42 31	42, 81, 114, 147	0
20	AA	1511/1511 (100%)	-0.02	22 (1%) 76 66	25, 78, 180, 324	0
20	CA	1511/1511 (100%)	0.01	40 (2%) 59 47	19, 82, 182, 332	0
21	AW	77/77 (100%)	-0.17	0 100 100	55, 121, 189, 218	0
21	CW	77/77 (100%)	-0.03	0 100 100	58, 118, 230, 278	0
22	AV	23/23 (100%)	1.32	6 (26%) 1 1	70, 138, 188, 222	0
22	CV	23/23 (100%)	1.53	5 (21%) 1 2	88, 142, 211, 231	0
23	AY	667/687 (97%)	-0.33	14 (2%) 67 56	29, 79, 132, 191	0
23	CY	667/687 (97%)	-0.20	17 (2%) 61 49	32, 84, 131, 188	0
24	BC	228/228 (100%)	0.91	41 (17%) 2 2	91, 147, 211, 238	0
24	DC	228/228 (100%)	0.25	17 (7%) 17 12	89, 175, 227, 263	0
25	BD	275/275 (100%)	-0.03	9 (3%) 50 38	24, 52, 90, 160	0
25	DD	275/275 (100%)	-0.00	10 (3%) 46 36	23, 50, 94, 155	0
26	BE	205/205 (100%)	0.17	11 (5%) 29 21	25, 52, 97, 202	0
26	DE	205/205 (100%)	0.19	8 (3%) 43 32	28, 60, 135, 173	0
27	BF	208/208 (100%)	0.22	11 (5%) 30 22	32, 67, 126, 195	0
27	DF	208/208 (100%)	0.40	18 (8%) 13 10	34, 86, 165, 230	0
28	BG	181/181 (100%)	0.73	30 (16%) 2 3	52, 103, 150, 206	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	DG	181/181 (100%)	0.27	6 (3%)	50	38	73, 110, 158, 205	0
29	BH	167/167 (100%)	0.29	14 (8%)	14	10	38, 64, 111, 161	0
29	DH	167/167 (100%)	0.09	10 (5%)	25	17	40, 74, 130, 167	0
30	BJ	0/170	-	-	-	-	-	-
30	DJ	0/170	-	-	-	-	-	-
31	BK	140/140 (100%)	0.52	19 (13%)	4	4	67, 118, 175, 206	0
31	DK	140/140 (100%)	0.33	15 (10%)	8	6	66, 132, 200, 220	0
32	BN	138/138 (100%)	0.04	7 (5%)	32	23	58, 85, 106, 118	0
32	DN	138/138 (100%)	0.22	7 (5%)	32	23	63, 87, 111, 121	0
33	BO	122/122 (100%)	-0.31	0	100	100	24, 49, 67, 114	0
33	DO	122/122 (100%)	-0.02	1 (0%)	87	82	30, 56, 88, 125	0
34	BP	146/146 (100%)	-0.15	4 (2%)	58	46	28, 73, 113, 171	0
34	DP	146/146 (100%)	-0.20	5 (3%)	49	37	31, 84, 130, 202	0
35	BQ	141/141 (100%)	-0.15	5 (3%)	48	37	40, 66, 100, 164	0
35	DQ	141/141 (100%)	-0.02	7 (4%)	32	24	36, 64, 104, 161	0
36	BR	117/117 (100%)	-0.26	0	100	100	29, 53, 85, 105	0
36	DR	117/117 (100%)	-0.20	1 (0%)	85	80	21, 53, 88, 156	0
37	BS	99/99 (100%)	0.28	7 (7%)	19	13	60, 111, 172, 189	0
37	DS	99/99 (100%)	0.52	12 (12%)	6	6	38, 128, 194, 220	0
38	BT	138/138 (100%)	-0.33	3 (2%)	65	54	36, 64, 106, 201	0
38	DT	138/138 (100%)	-0.30	2 (1%)	78	68	32, 71, 115, 216	0
39	BU	117/117 (100%)	-0.37	0	100	100	26, 44, 83, 132	0
39	DU	117/117 (100%)	-0.30	2 (1%)	73	62	6, 45, 90, 155	0
40	BV	101/101 (100%)	0.17	1 (0%)	84	77	31, 51, 79, 104	0
40	DV	101/101 (100%)	-0.11	0	100	100	38, 70, 111, 124	0
41	BW	113/113 (100%)	0.35	6 (5%)	30	22	22, 51, 104, 120	0
41	DW	113/113 (100%)	0.48	5 (4%)	38	28	30, 49, 105, 202	0
42	BX	93/93 (100%)	0.80	9 (9%)	10	7	31, 59, 93, 113	0
42	DX	93/93 (100%)	0.47	4 (4%)	39	29	29, 63, 111, 175	0
43	BY	107/107 (100%)	0.01	8 (7%)	17	12	35, 71, 133, 156	0
43	DY	107/107 (100%)	0.07	9 (8%)	14	10	55, 87, 133, 209	0
44	BZ	185/185 (100%)	-0.37	3 (1%)	74	64	42, 78, 126, 158	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DZ	185/185 (100%)	-0.26	6 (3%) 51 38	36, 75, 123, 161	0
45	B0	84/84 (100%)	0.73	8 (9%) 10 8	38, 70, 99, 162	0
45	D0	84/84 (100%)	0.85	15 (17%) 2 2	33, 67, 139, 212	0
46	B2	71/71 (100%)	-0.23	2 (2%) 56 44	44, 71, 114, 167	0
46	D2	71/71 (100%)	-0.30	0 100 100	53, 76, 129, 183	0
47	B3	60/60 (100%)	-0.43	0 100 100	26, 43, 74, 113	0
47	D3	60/60 (100%)	-0.12	2 (3%) 50 38	27, 57, 99, 111	0
48	B5	59/59 (100%)	0.21	1 (1%) 73 62	22, 56, 142, 156	0
48	D5	59/59 (100%)	0.29	1 (1%) 73 62	18, 67, 175, 198	0
49	B6	50/50 (100%)	0.14	2 (4%) 42 31	65, 91, 124, 176	0
49	D6	50/50 (100%)	0.63	10 (20%) 1 2	66, 106, 136, 139	0
50	B7	49/49 (100%)	0.71	5 (10%) 9 7	30, 48, 107, 132	0
50	D7	49/49 (100%)	0.72	6 (12%) 5 5	38, 51, 125, 168	0
51	B8	64/64 (100%)	0.83	6 (9%) 11 8	30, 62, 80, 89	0
51	D8	64/64 (100%)	1.32	18 (28%) 1 1	38, 70, 114, 148	0
52	B9	37/37 (100%)	1.16	9 (24%) 1 1	41, 63, 116, 166	0
52	D9	37/37 (100%)	0.96	7 (18%) 2 2	36, 55, 111, 148	0
53	Be	72/102 (70%)	0.84	14 (19%) 1 2	69, 117, 170, 201	0
53	De	72/102 (70%)	0.35	6 (8%) 14 10	82, 121, 212, 249	0
54	Bf	0/31	-	-	-	-
54	Bg	0/31	-	-	-	-
54	Df	0/31	-	-	-	-
54	Dg	0/31	-	-	-	-
55	Bh	0/30	-	-	-	-
55	Dh	0/30	-	-	-	-
56	B1	93/93 (100%)	0.90	25 (26%) 1 1	40, 87, 151, 208	0
56	D1	93/93 (100%)	1.49	34 (36%) 0 1	42, 84, 174, 216	0
57	B4	35/35 (100%)	0.79	3 (8%) 13 10	96, 160, 227, 248	0
57	D4	35/35 (100%)	1.03	6 (17%) 2 3	116, 170, 265, 282	0
58	BA	2879/2879 (100%)	0.02	35 (1%) 81 72	17, 60, 166, 304	0
58	DA	2879/2879 (100%)	0.03	48 (1%) 73 62	17, 62, 182, 341	0
59	BB	119/119 (100%)	0.08	4 (3%) 49 37	32, 114, 187, 214	0
59	DB	119/119 (100%)	0.09	2 (1%) 73 62	53, 104, 162, 246	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	22682/23306 (97%)	0.09	977 (4%) 39 29	6, 73, 161, 341	0

The worst 5 of 977 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
56	D1	42	GLN	10.1
24	DC	227	PRO	9.0
43	DY	107	ASP	7.8
56	D1	34	THR	7.7
56	D1	17	SER	7.4

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	FUA	AY	701	37/37	0.83	0.42	3.16	119,146,161,162	0
60	FUA	CY	701	37/37	0.83	0.38	1.50	125,150,161,166	0
61	GDP	AY	702	28/28	0.84	0.25	1.34	58,89,106,121	0
61	GDP	CY	702	28/28	0.88	0.21	0.60	58,90,102,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.