



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:05 PM GMT

PDB ID : 4V9L  
Title : 70S Ribosome translocation intermediate FA-3.6A containing elongation factor EFG/FUSIDIC ACID/GDP, mRNA, and tRNA bound in the pe<sup>\*</sup>/E state.  
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.  
Deposited on : 2013-04-24  
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

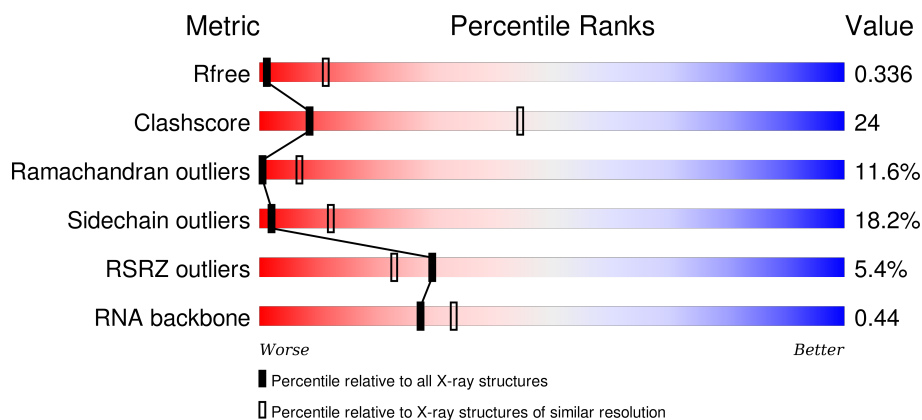
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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  $\geq 3$ , 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	<div> <div>3%</div> <div> <div></div> <div>34%</div> <div>45%</div> <div>18%</div> <div>.</div> </div> </div>
1	CB	235	<div> <div>9%</div> <div> <div></div> <div>40%</div> <div>45%</div> <div>15%</div> </div> </div>
2	AC	207	<div> <div>5%</div> <div> <div></div> <div>42%</div> <div>46%</div> <div>12%</div> </div> </div>
2	CC	207	<div> <div>5%</div> <div> <div></div> <div>49%</div> <div>43%</div> <div>8%</div> </div> </div>

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

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Mol	Chain	Length	Quality of chain
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AA	1511	
20	CA	1511	
21	AW	77	
21	CW	77	
22	AV	23	
22	CV	23	
23	AY	687	
23	CY	687	
24	AU	6	
24	CU	6	
25	BC	228	
25	DC	228	
26	BD	275	
26	DD	275	
27	BE	205	
27	DE	205	

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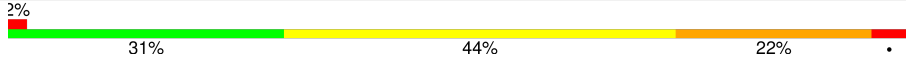
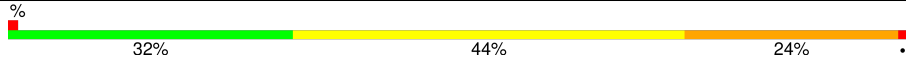
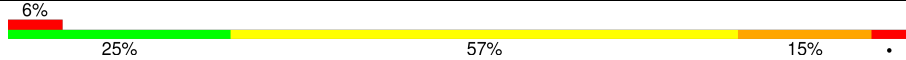
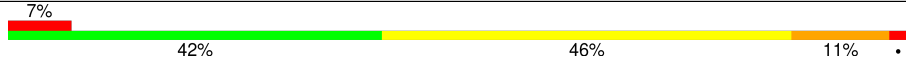
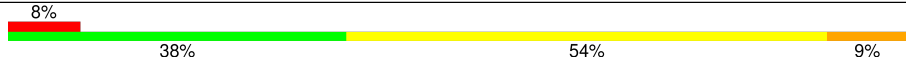
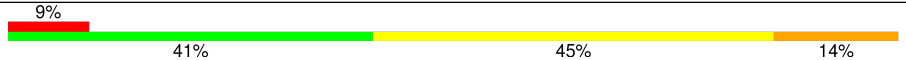
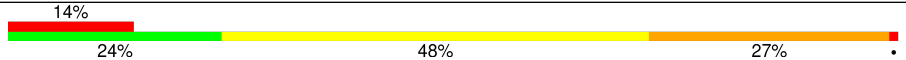
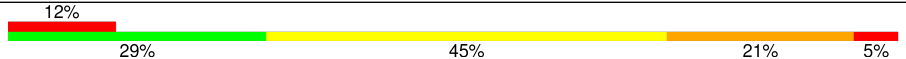
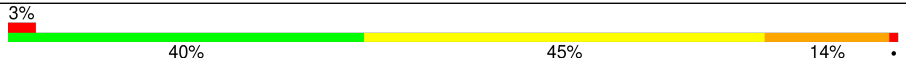
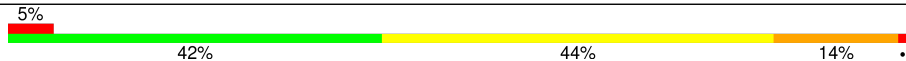
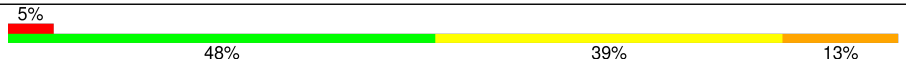
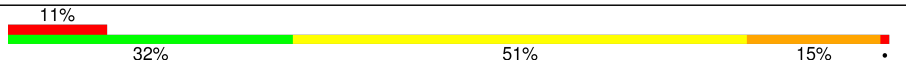
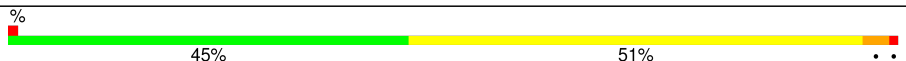
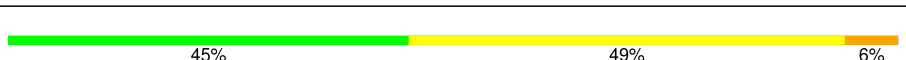
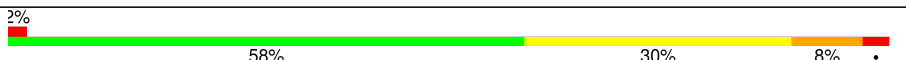

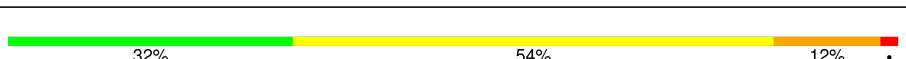
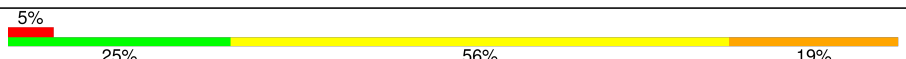
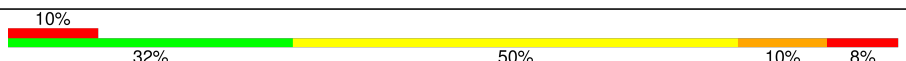
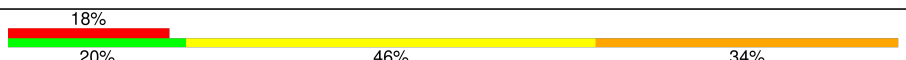
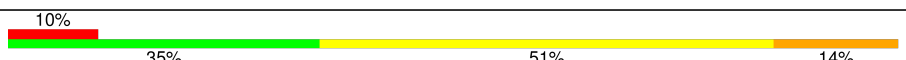
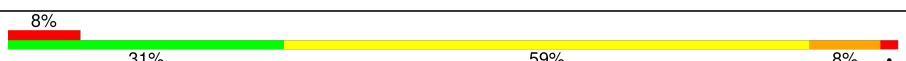
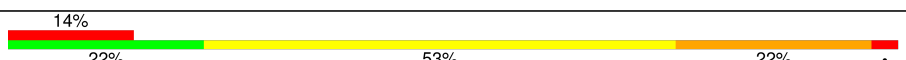
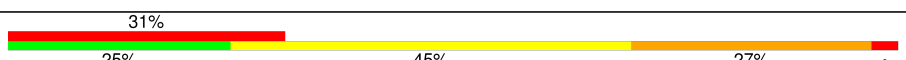


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Mol	Chain	Length	Quality of chain
28	BF	208	
28	DF	208	
29	BG	181	
29	DG	181	
30	BH	167	
30	DH	167	
31	BJ	170	
31	DJ	170	
32	BK	140	
32	DK	140	
33	BN	138	
33	DN	138	
34	BO	122	
34	DO	122	
35	BP	146	
35	DP	146	
36	BQ	141	
36	DQ	141	
37	BR	117	
37	DR	117	
38	BS	99	
38	DS	99	
39	BT	138	
39	DT	138	
40	BU	117	




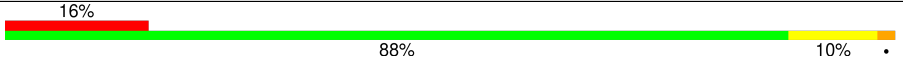
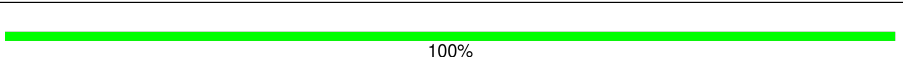
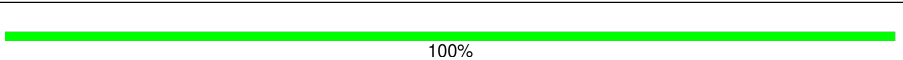
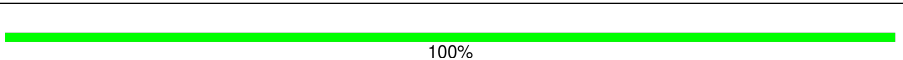
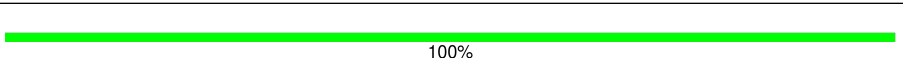
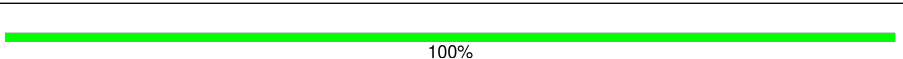
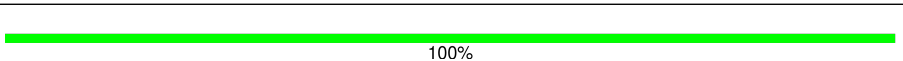
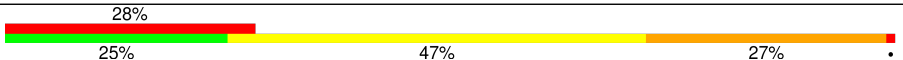
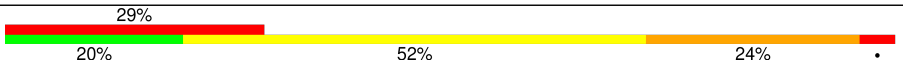
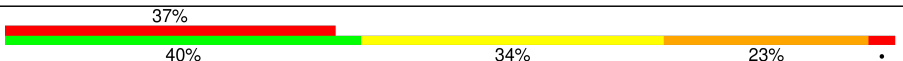
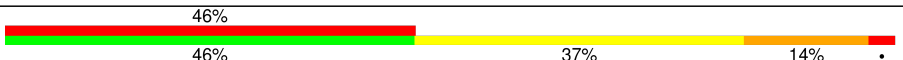
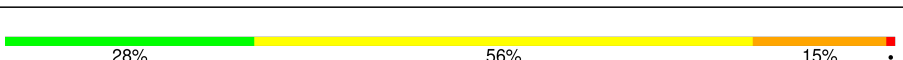
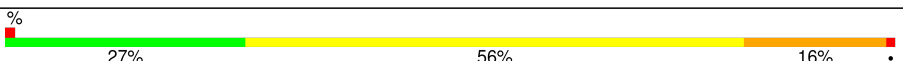
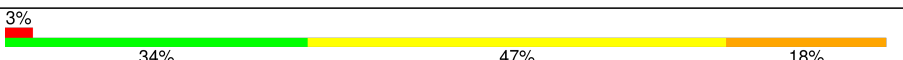
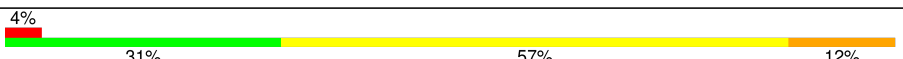
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Mol	Chain	Length	Quality of chain
40	DU	117	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	93	
43	DX	93	
44	BY	107	
44	DY	107	
45	BZ	185	
45	DZ	185	
46	B0	84	
46	D0	84	
47	B2	71	
47	D2	71	
48	B3	60	
48	D3	60	
49	B5	59	
49	D5	59	
50	B6	50	
50	D6	50	
51	B7	49	
51	D7	49	
52	B8	64	
52	D8	64	

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Mol	Chain	Length	Quality of chain
53	B9	37	
53	D9	37	
54	Be	102	
54	De	102	
55	Bf	31	
55	Bg	31	
55	Df	31	
55	Dg	31	
56	Bh	30	
56	Dh	30	
57	B1	93	
57	D1	93	
58	B4	35	
58	D4	35	
59	BA	2879	
59	DA	2879	
60	BB	119	
60	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
61	FUA	AY	701	-	-	-	X
61	FUA	CY	701	-	-	-	X
62	GDP	AY	702	-	-	X	X
62	GDP	CY	702	-	-	X	X

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 308166 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 21 is a RNA chain called transfer RNA.

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

- Molecule 22 is a RNA chain called messenger RNA.

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

- Molecule 23 is a protein called Elongation factor G.

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

- Molecule 24 is a protein called VIOMYCIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	6	Total	C	N	O	0	0	0
			48	25	13	10			
24	CU	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			
25	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 26 is a protein called 50S ribosomal protein L2.

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			
28	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 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
29	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 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L10.

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

- Molecule 32 is a protein called 50S ribosomal protein L11.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
34	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 35 is a protein called 50S ribosomal protein L15.

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

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	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 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			
39	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 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
46	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 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

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 50 is a protein called 50S ribosomal protein L33.

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

- Molecule 51 is a protein called 50S ribosomal protein L34.

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

- Molecule 52 is a protein called 50S ribosomal protein L35.

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

- Molecule 53 is a protein called 50S ribosomal protein L36.

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

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

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

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

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L7/L12.

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

- Molecule 57 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	B1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			
57	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 58 is a protein called 50S ribosomal protein L31.



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

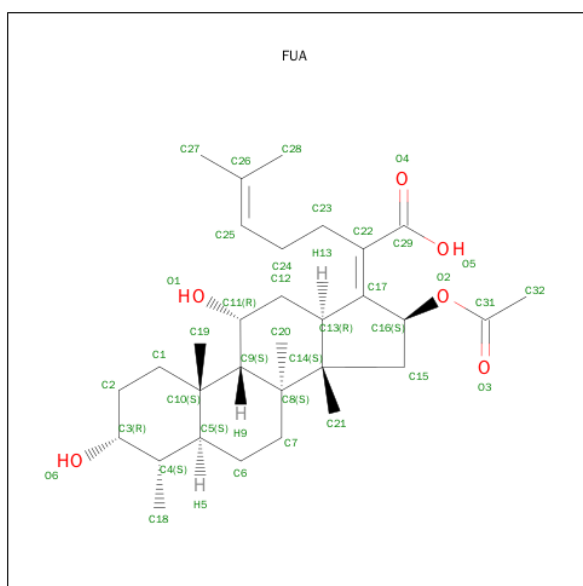
- Molecule 59 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 60 is a RNA chain called 5S ribosomal RNA.

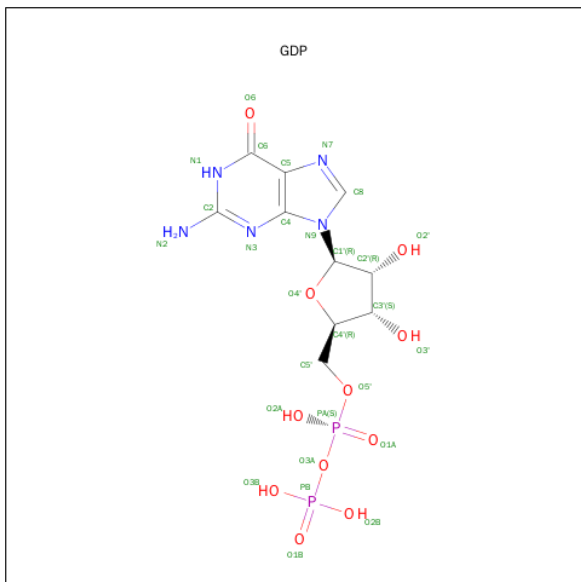
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
60	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 61 is FUSIDIC ACID (three-letter code: FUA) (formula:  $C_{31}H_{48}O_6$ ).



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

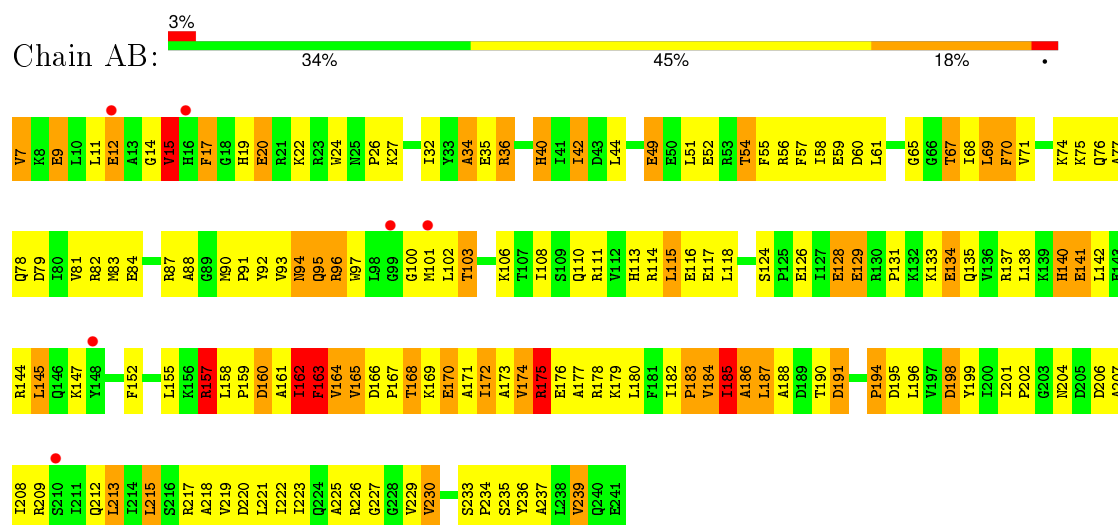
- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



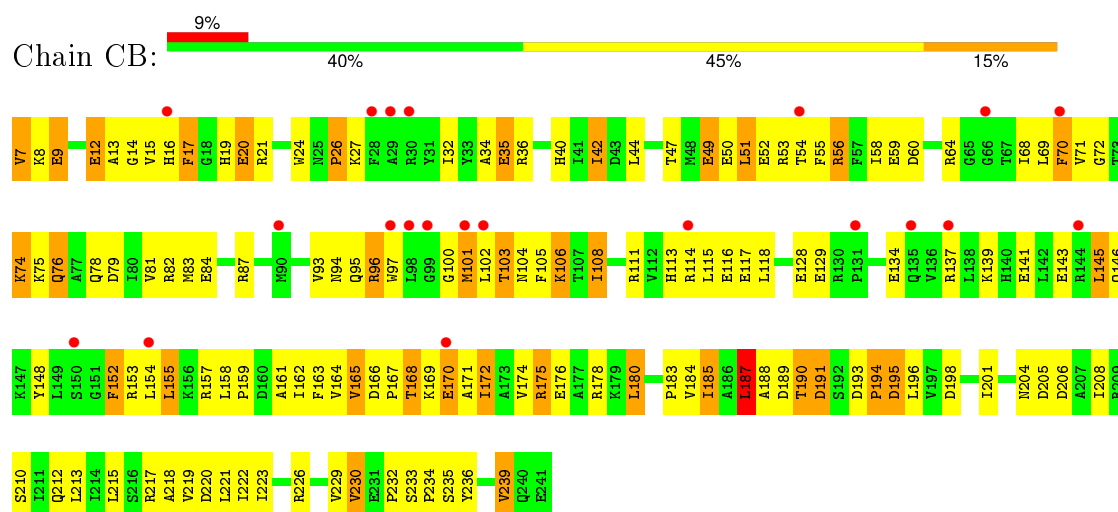
### 3 Residue-property plots

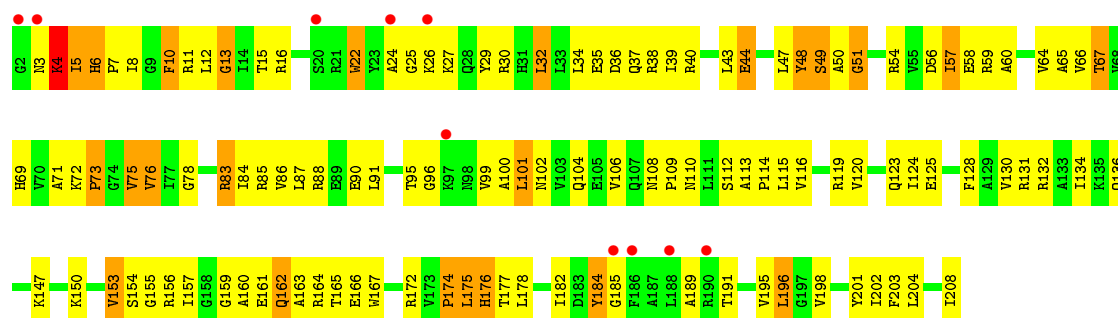
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

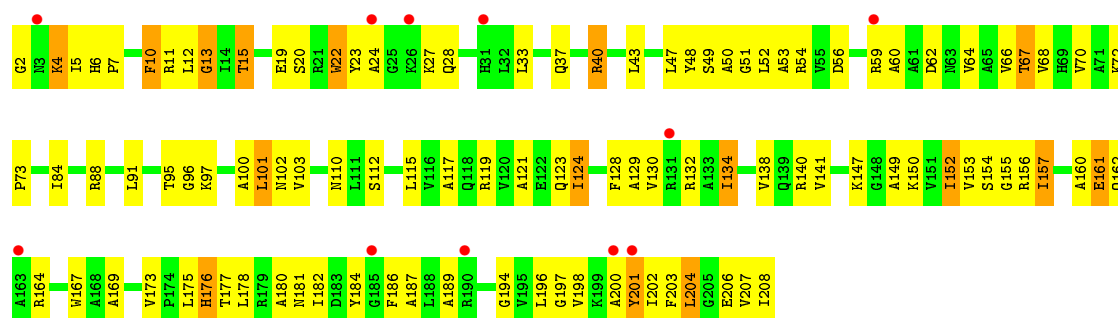


- Molecule 1: 30S ribosomal protein S2

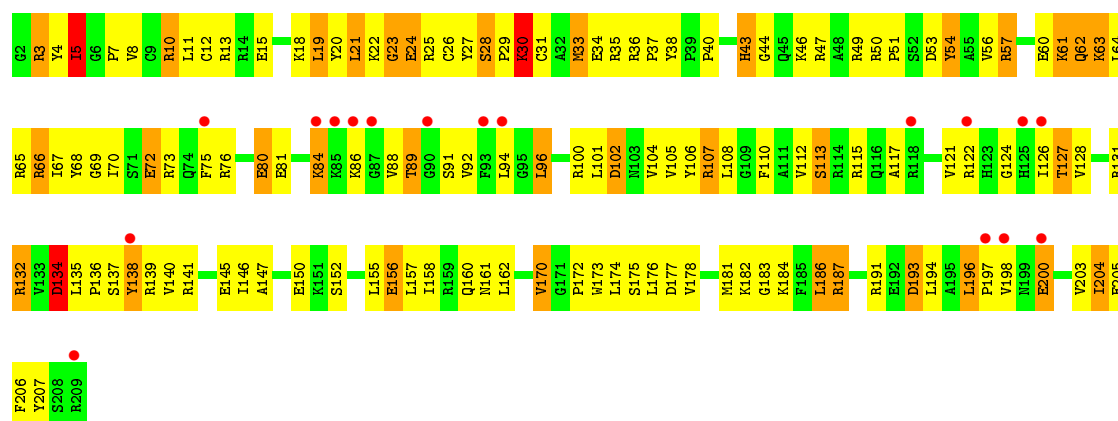




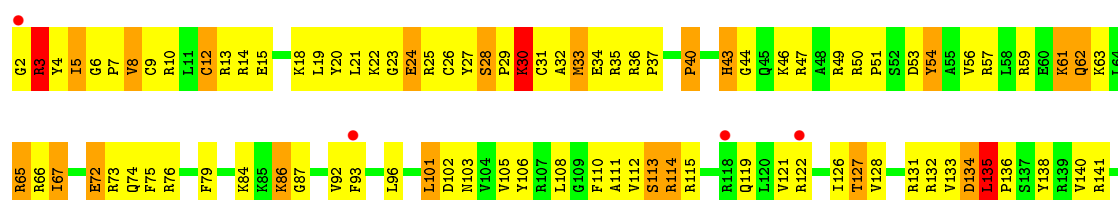
• Molecule 2: 30S ribosomal protein S3

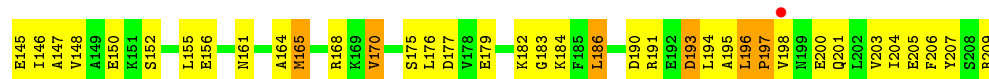


• Molecule 3: 30S ribosomal protein S4

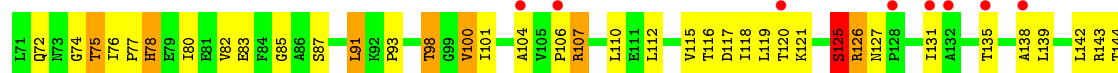
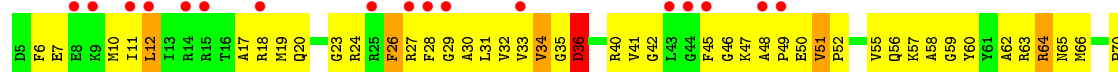
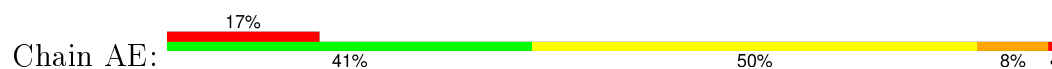


• Molecule 3: 30S ribosomal protein S4

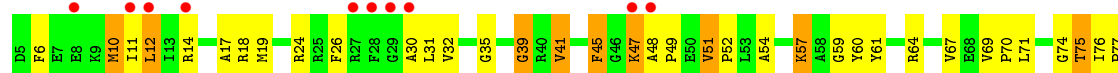




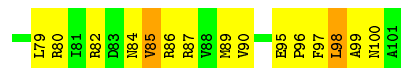
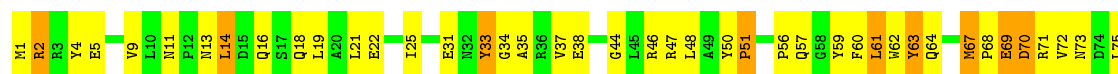
• Molecule 4: 30S ribosomal protein S5



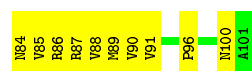
• Molecule 4: 30S ribosomal protein S5



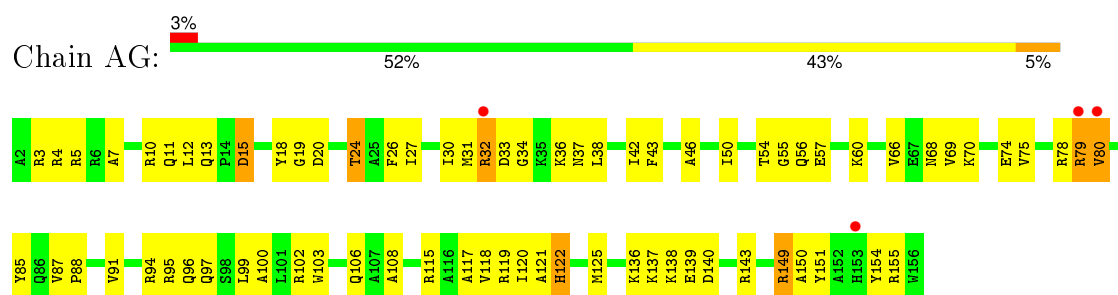
• Molecule 5: 30S ribosomal protein S6



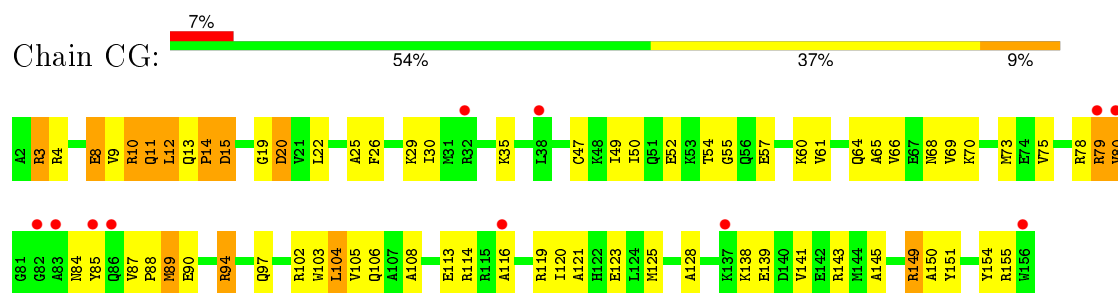
• Molecule 5: 30S ribosomal protein S6



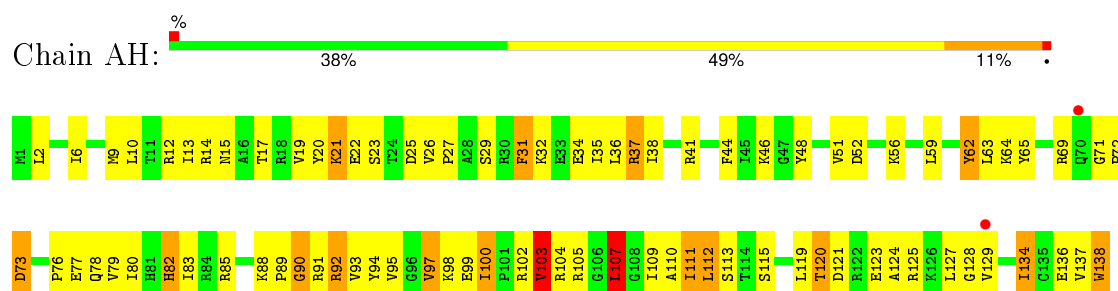
• Molecule 6: 30S ribosomal protein S7



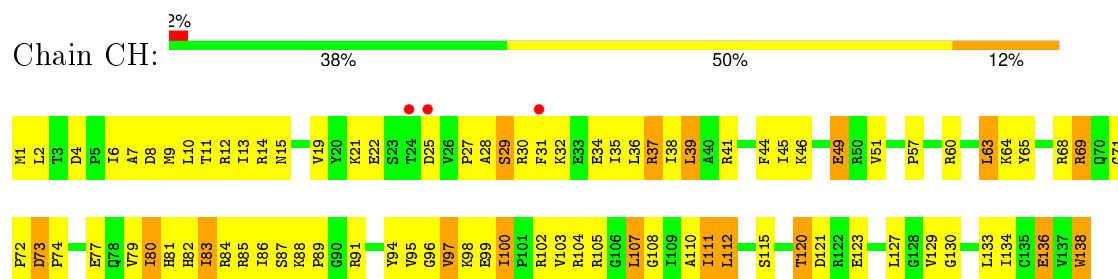
• Molecule 6: 30S ribosomal protein S7



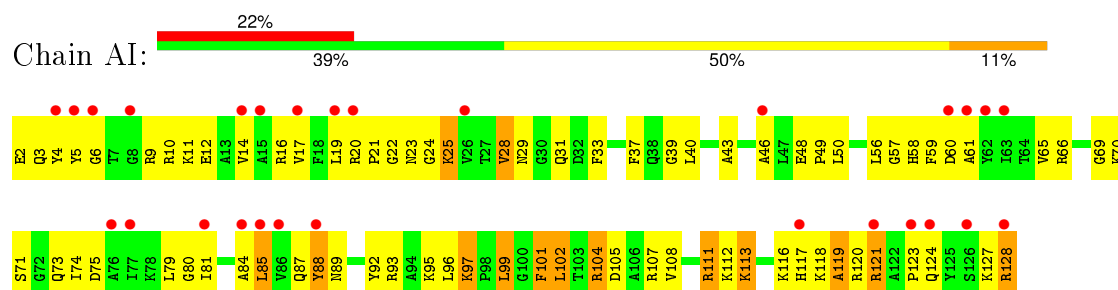
• Molecule 7: 30S ribosomal protein S8



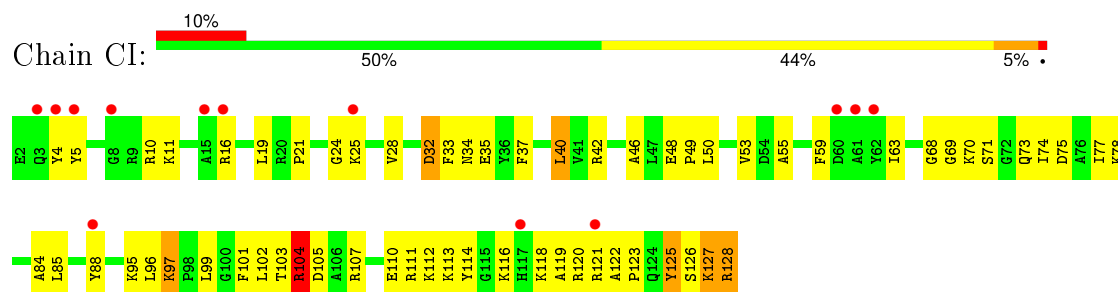
• Molecule 7: 30S ribosomal protein S8



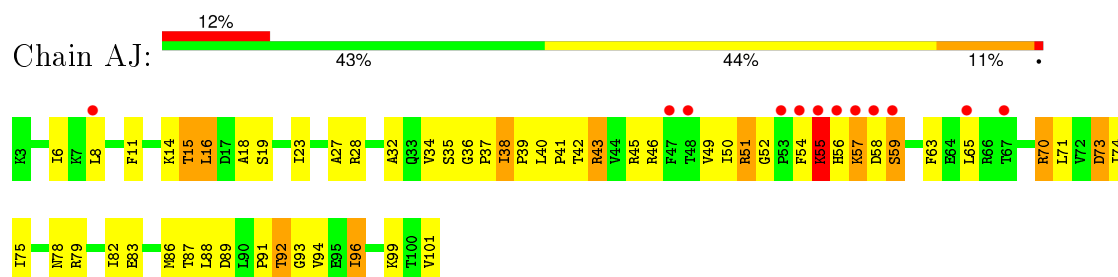
• Molecule 8: 30S ribosomal protein S9



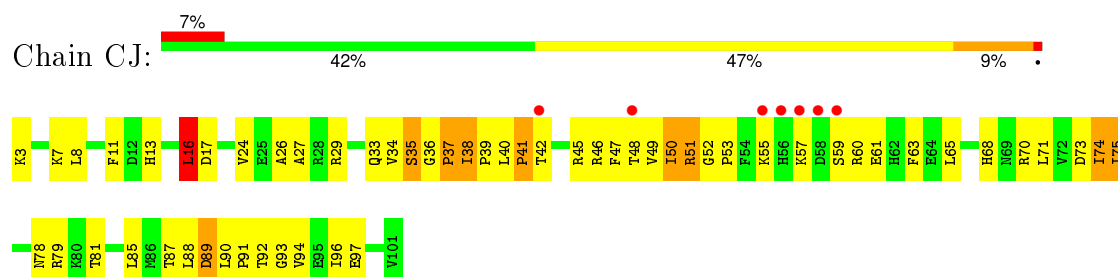
- Molecule 8: 30S ribosomal protein S9



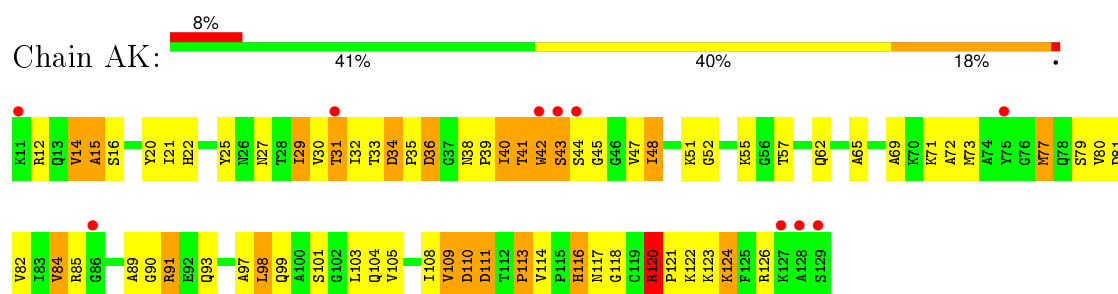
- Molecule 9: 30S ribosomal protein S10



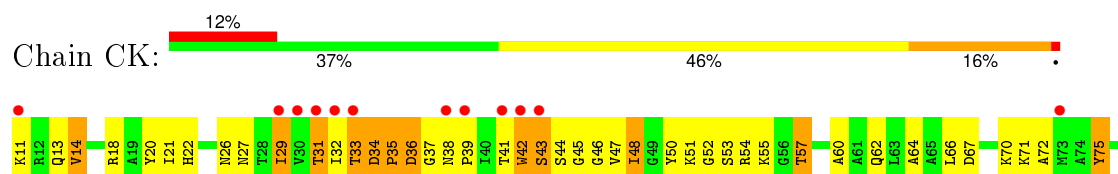
- Molecule 9: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S11

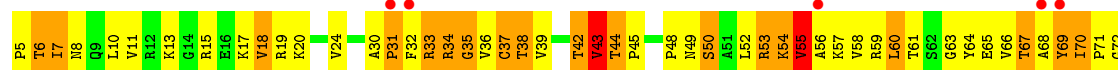


- Molecule 10: 30S ribosomal protein S11

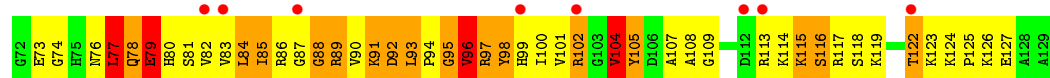
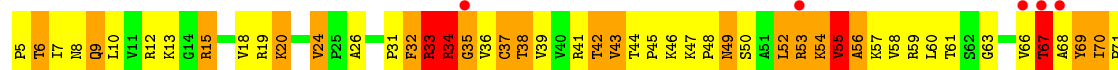
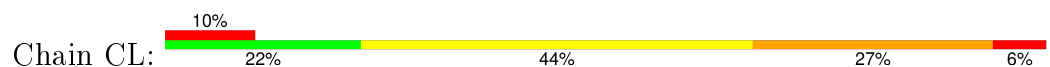




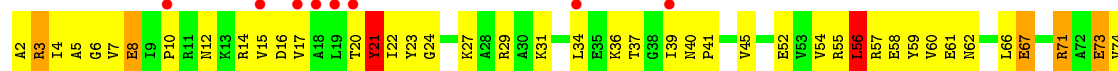
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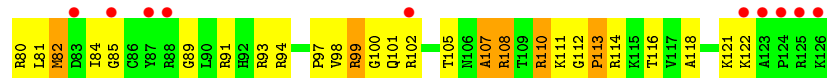
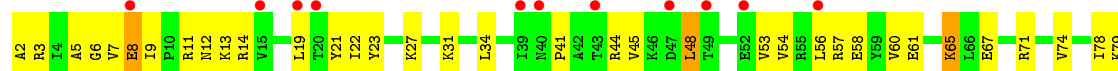
- Molecule 11: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S13



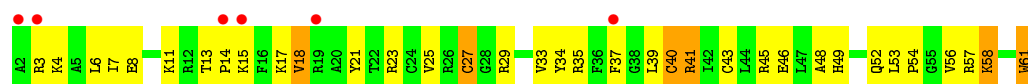
- Molecule 12: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S14 type Z



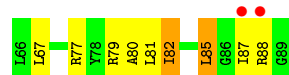
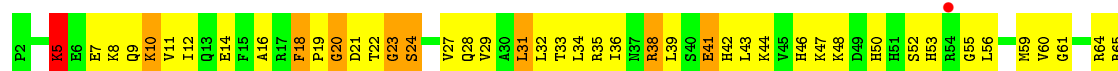




- Molecule 13: 30S ribosomal protein S14 type Z



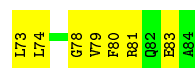
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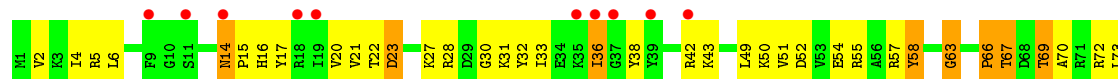
- Molecule 14: 30S ribosomal protein S15



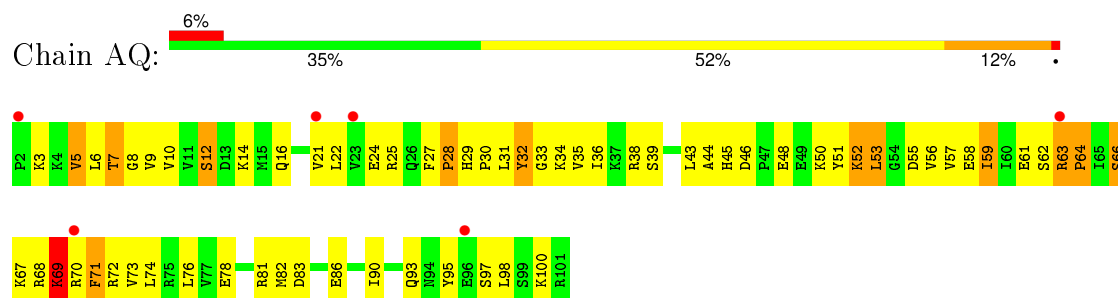
- Molecule 15: 30S ribosomal protein S16



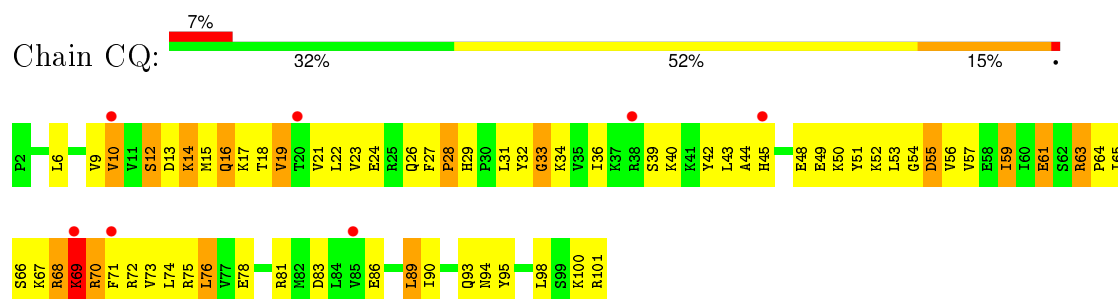
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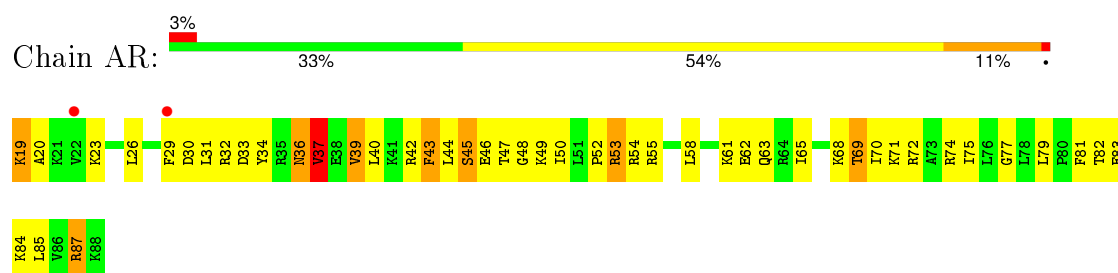
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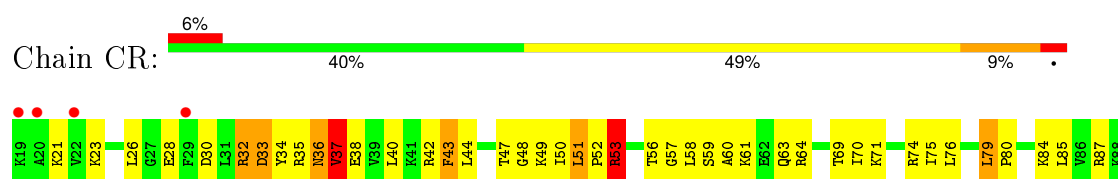
- Molecule 16: 30S ribosomal protein S17



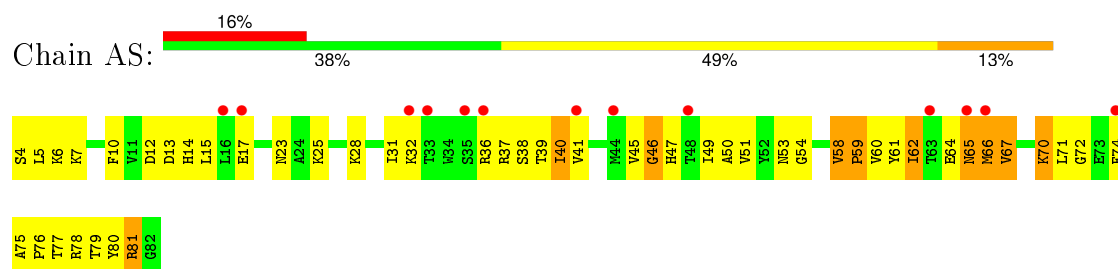
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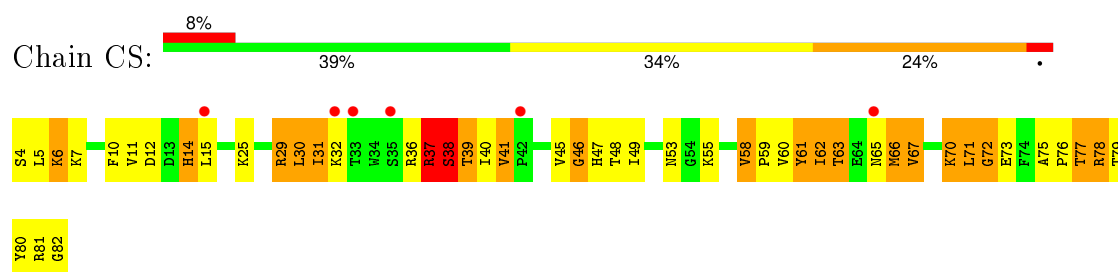
- Molecule 17: 30S ribosomal protein S18



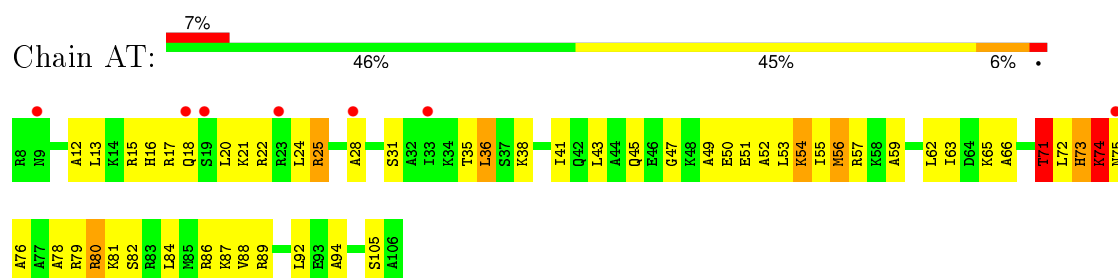
- Molecule 18: 30S ribosomal protein S19



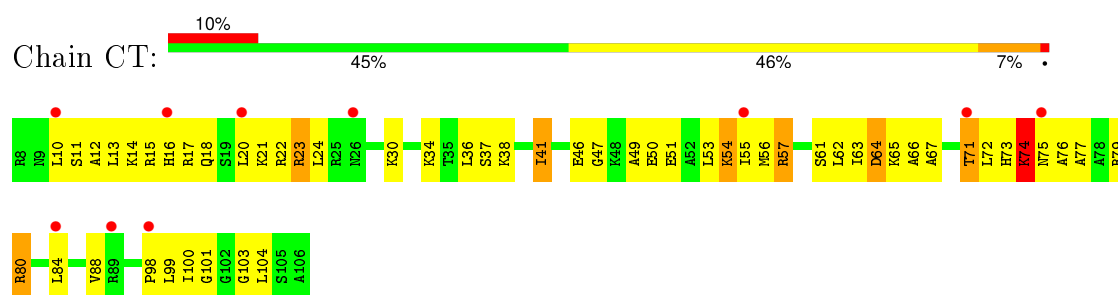
- Molecule 18: 30S ribosomal protein S19



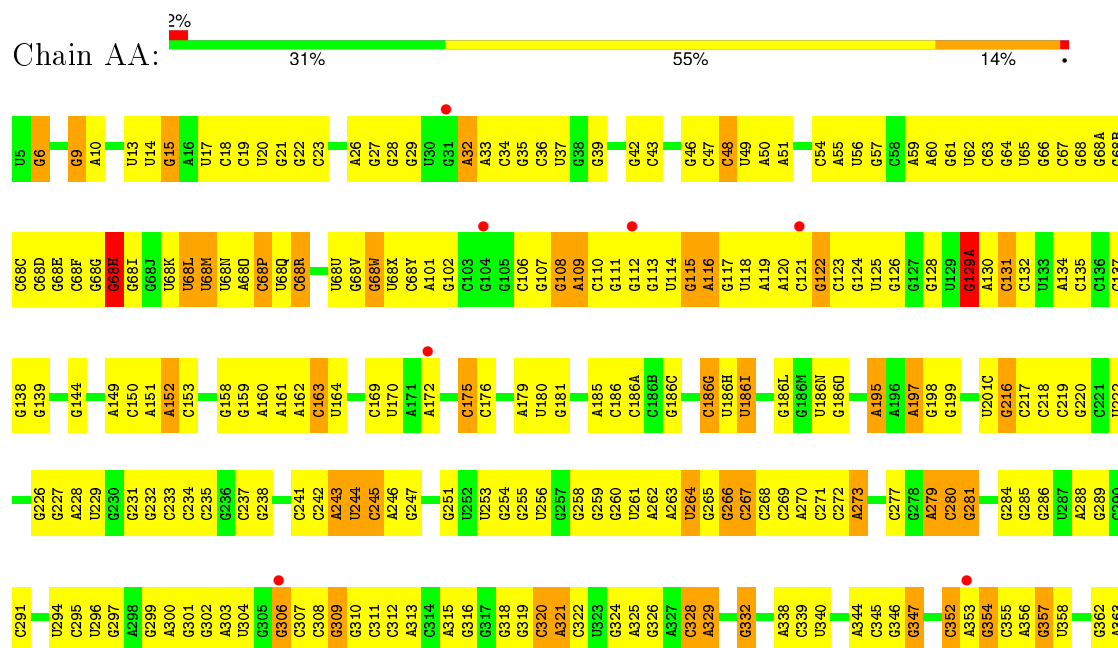
- Molecule 19: 30S ribosomal protein S20



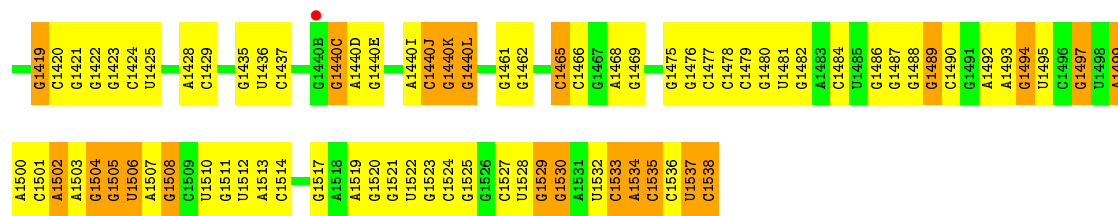
- Molecule 19: 30S ribosomal protein S20



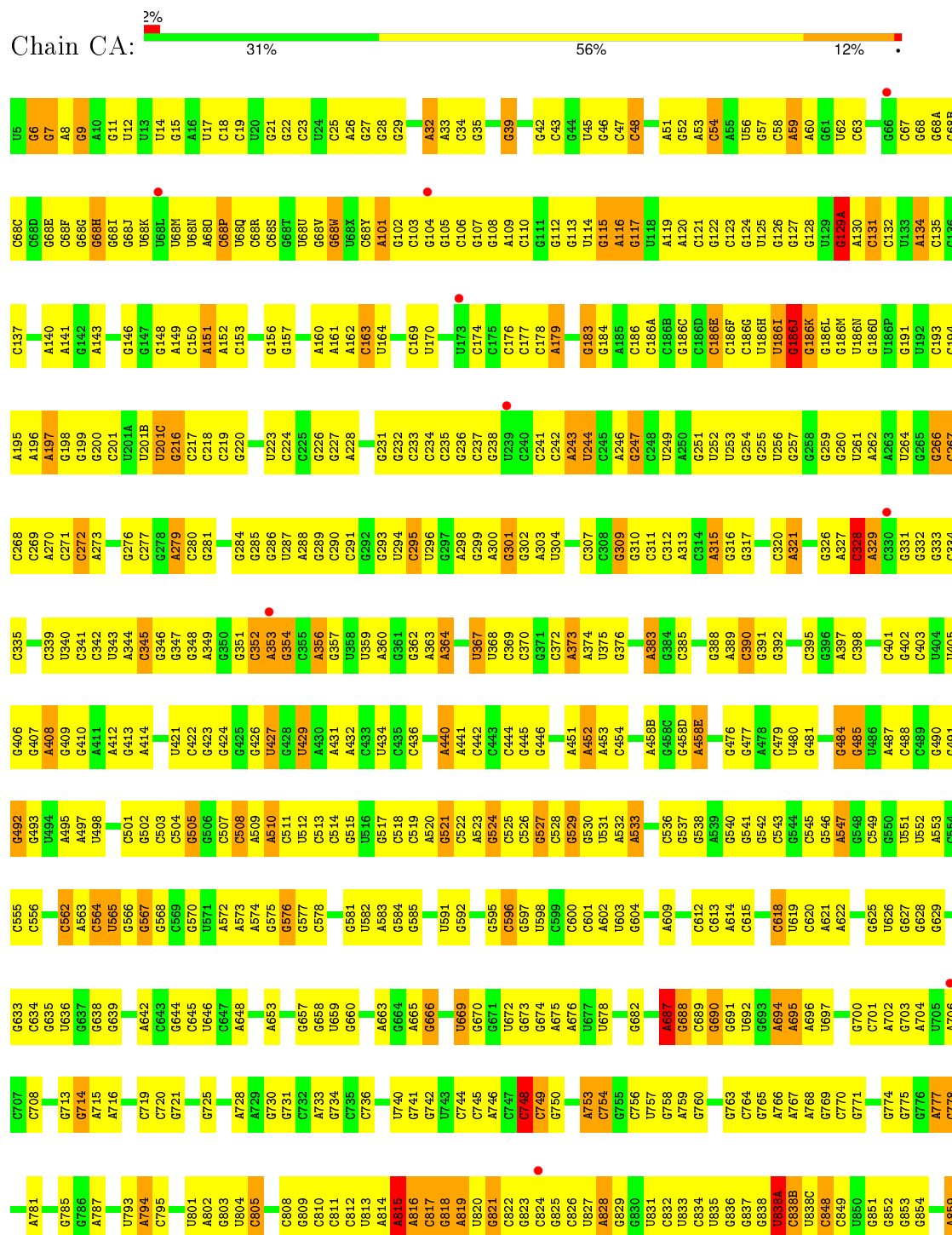
- Molecule 20: ribosomal RNA 16S

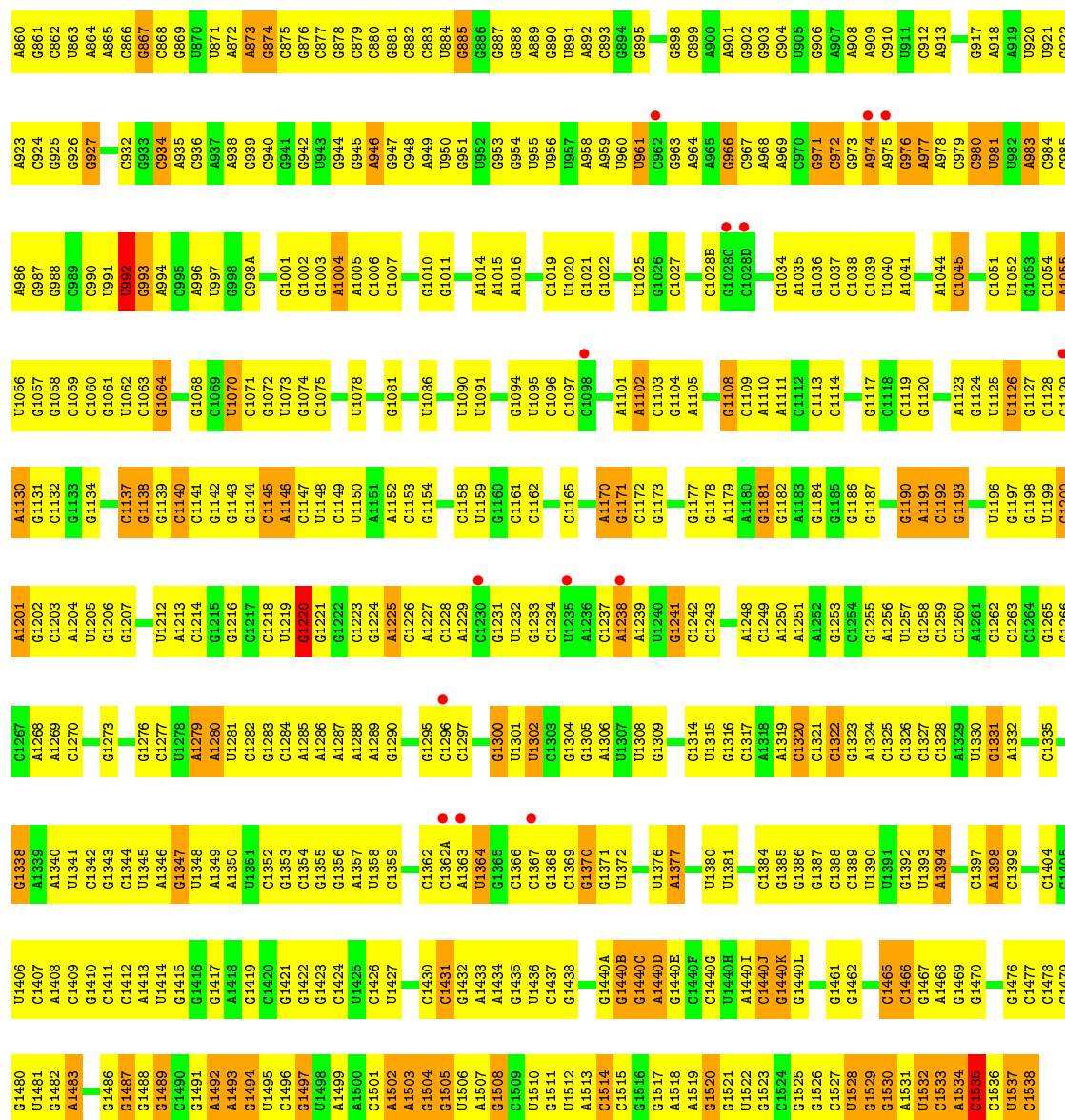


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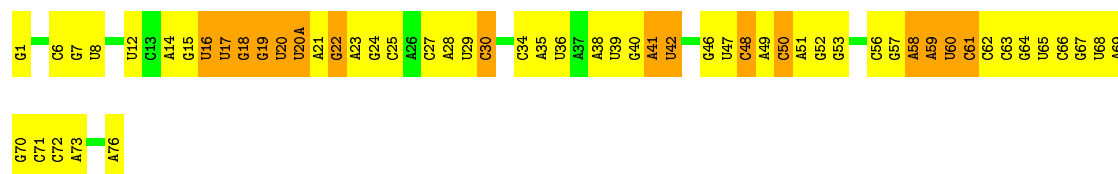
• Molecule 20: ribosomal RNA 16S





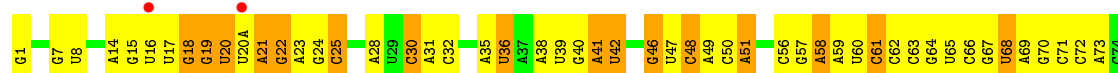
• Molecule 21: transfer RNA

Chain AW: 26% 53% 21%



• Molecule 21: transfer RNA

Chain CW: 3% 31% 48% 21%



C75  
A76

- Molecule 22: messenger RNA



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- Molecule 22: messenger RNA

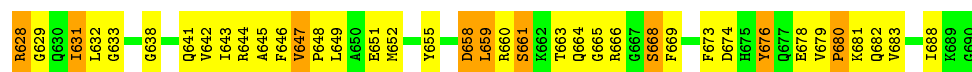


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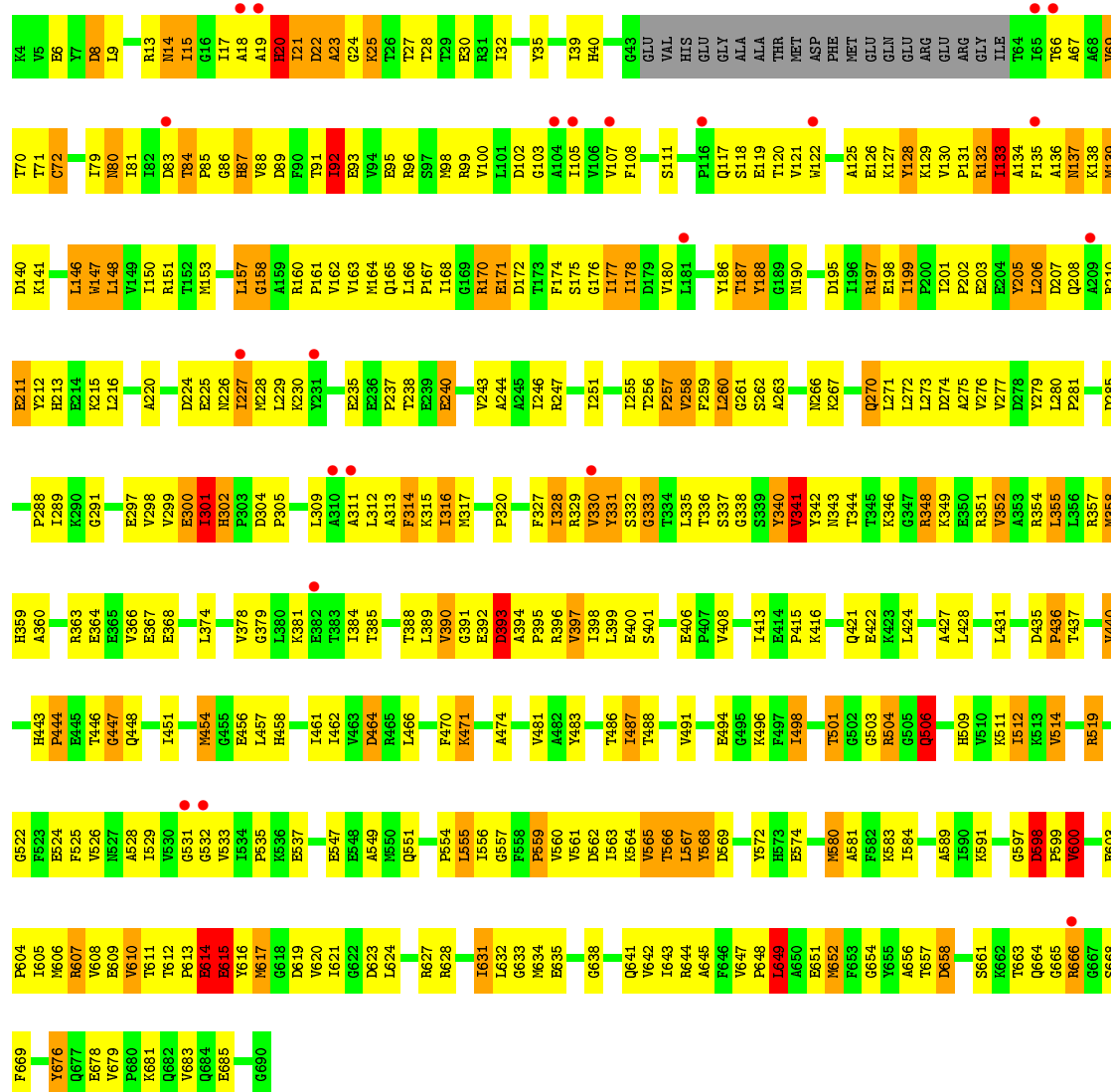
- Molecule 23: Elongation factor G



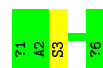
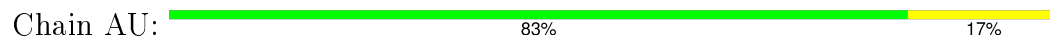
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• Molecule 23: Elongation factor G



• Molecule 24: VIOMYCIN



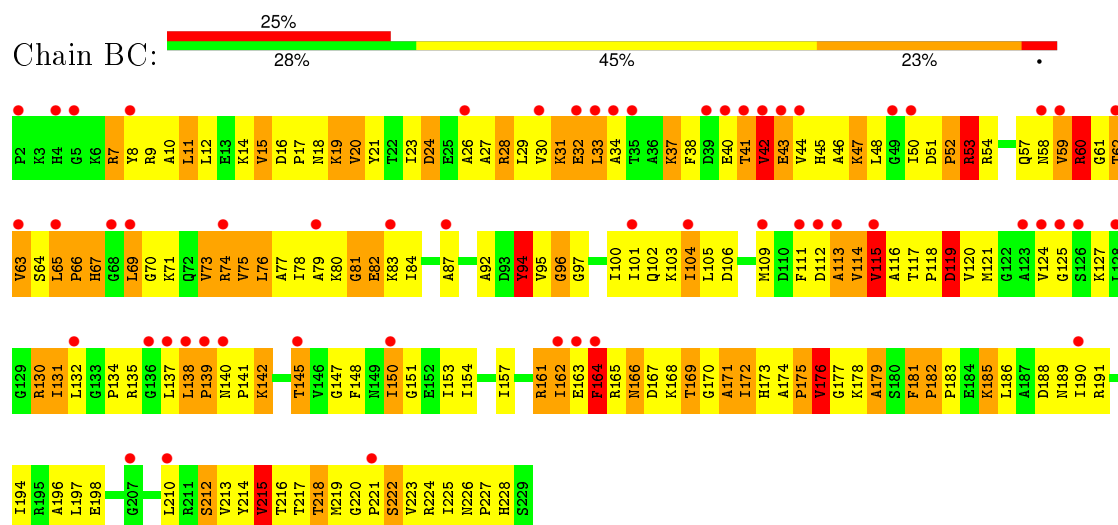
• Molecule 24: VIOMYCIN



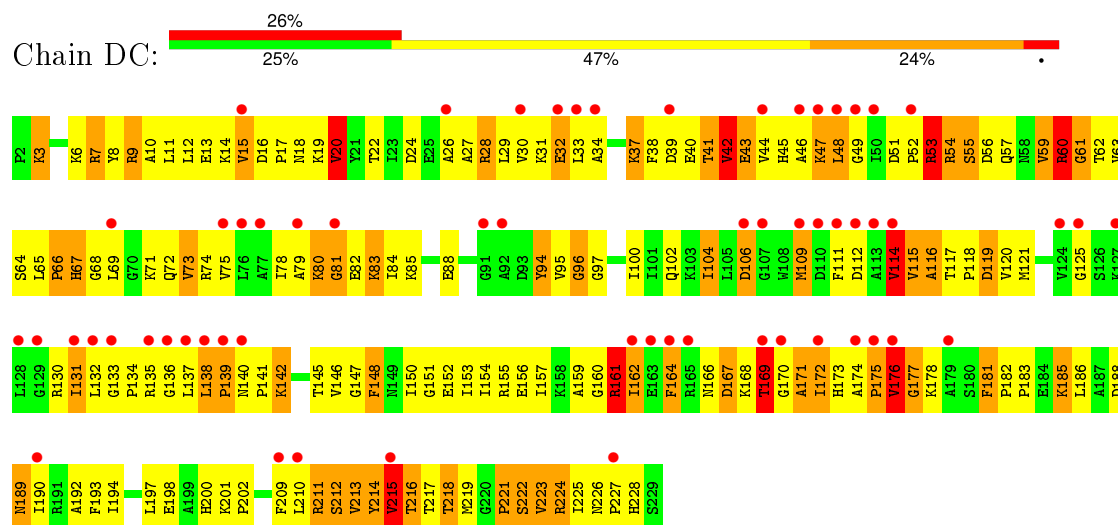




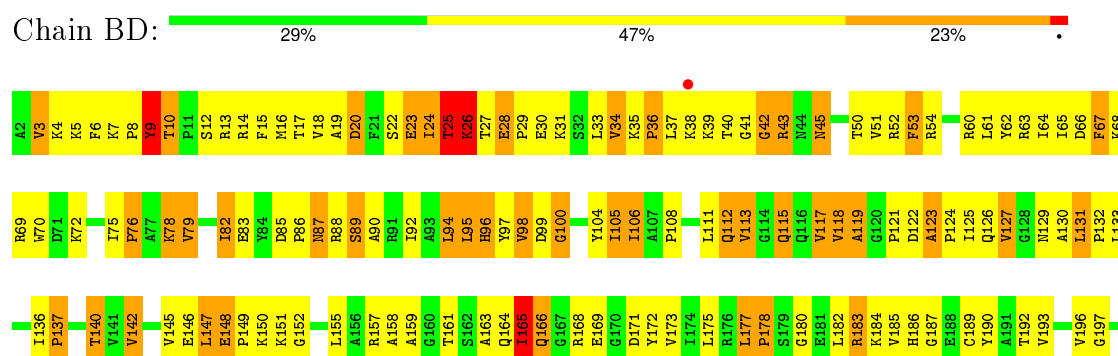
• Molecule 25: 50S ribosomal protein L1

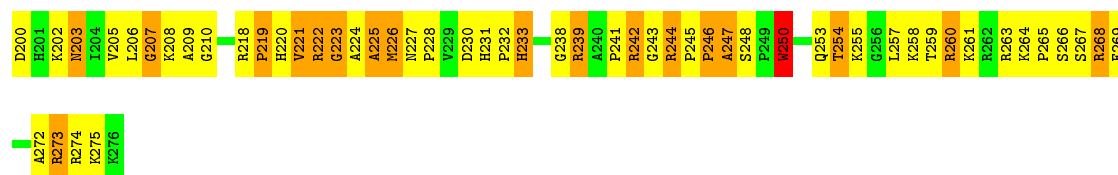


• Molecule 25: 50S ribosomal protein L1

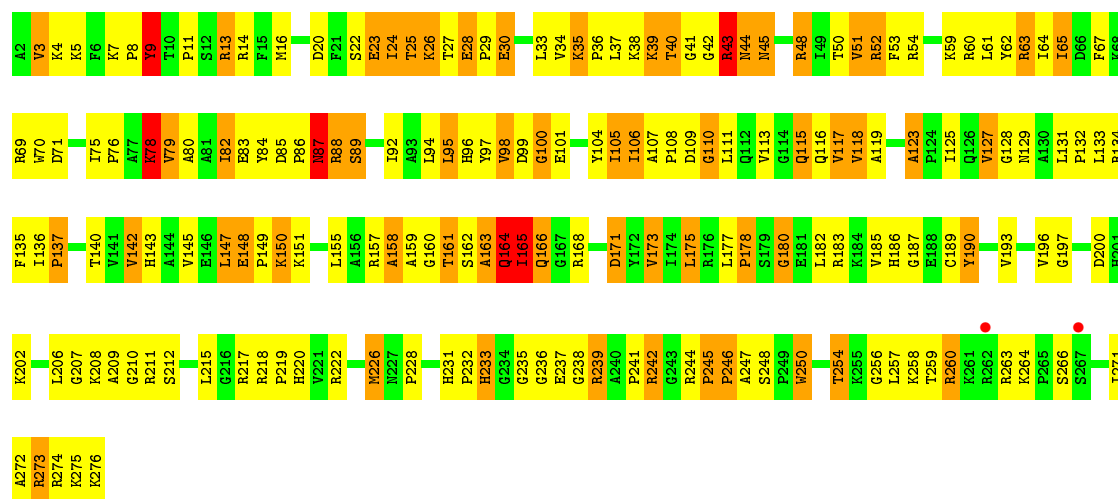


• Molecule 26: 50S ribosomal protein L2

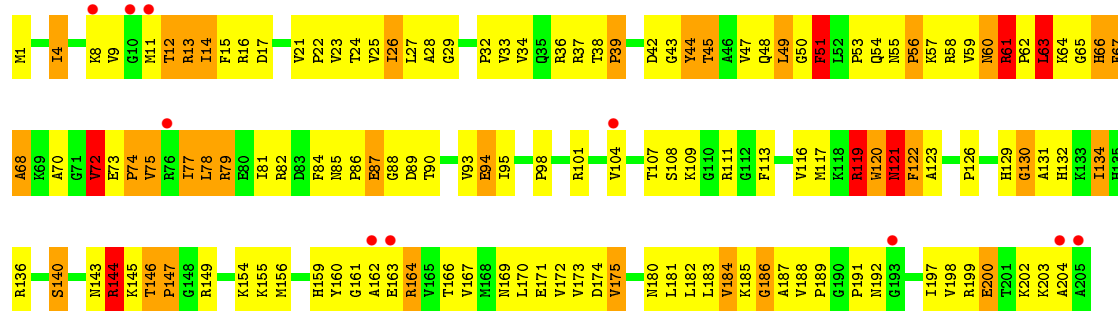




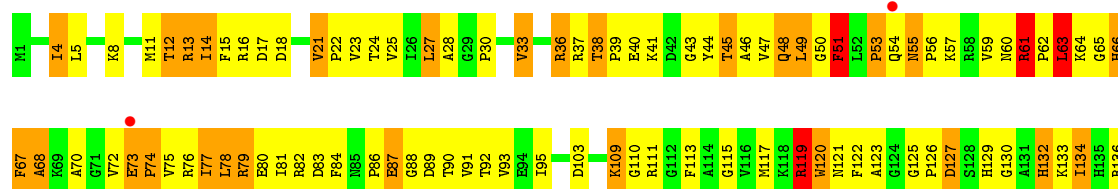
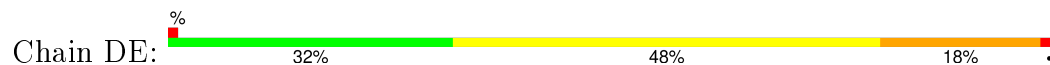
• Molecule 26: 50S ribosomal protein L2

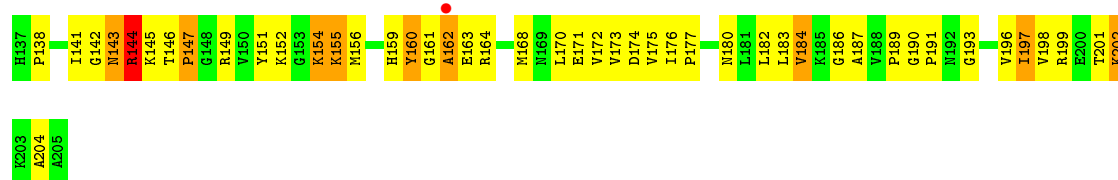


• Molecule 27: 50S ribosomal protein L3

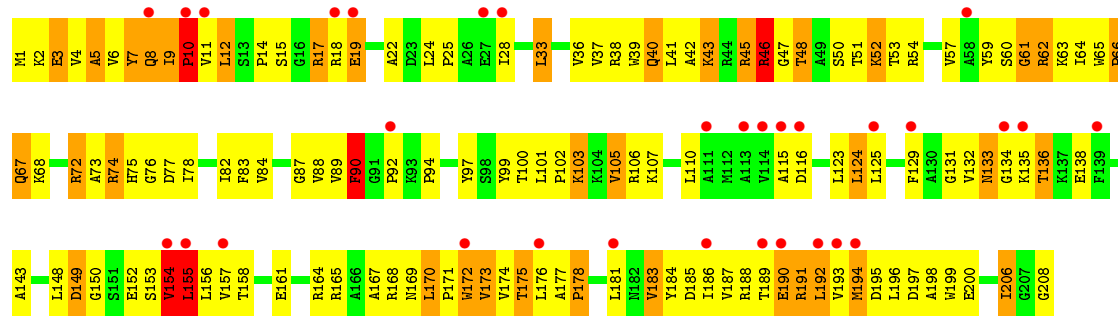


• Molecule 27: 50S ribosomal protein L3

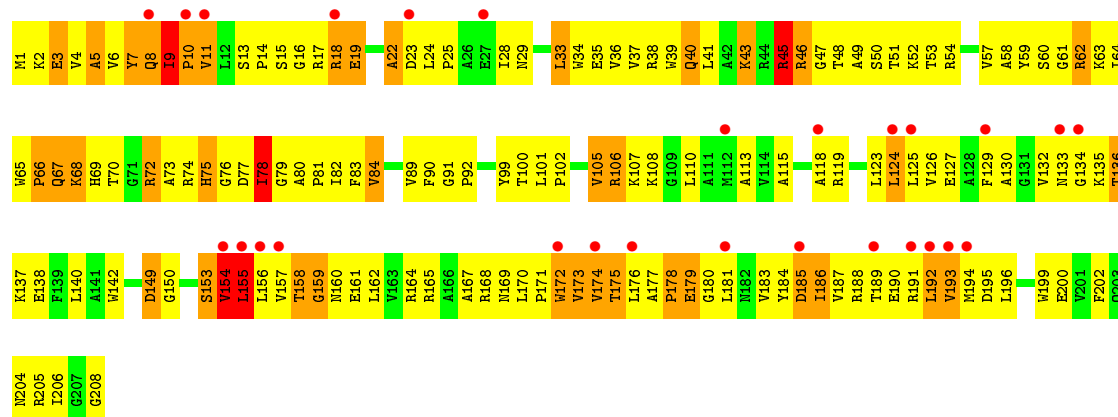




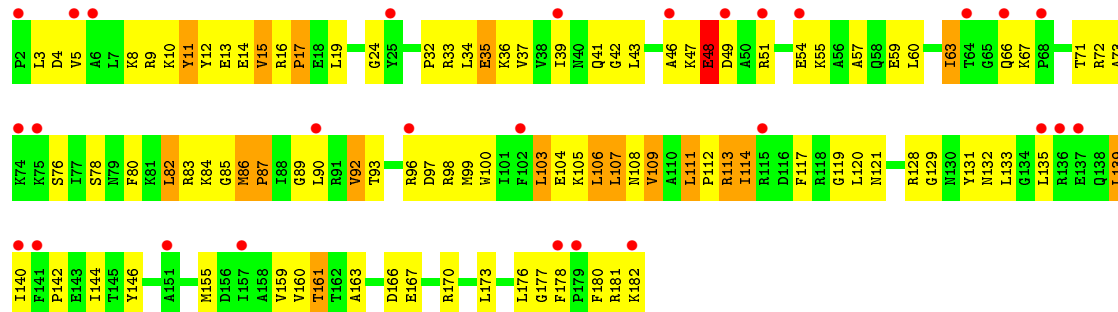
• Molecule 28: 50S ribosomal protein L4



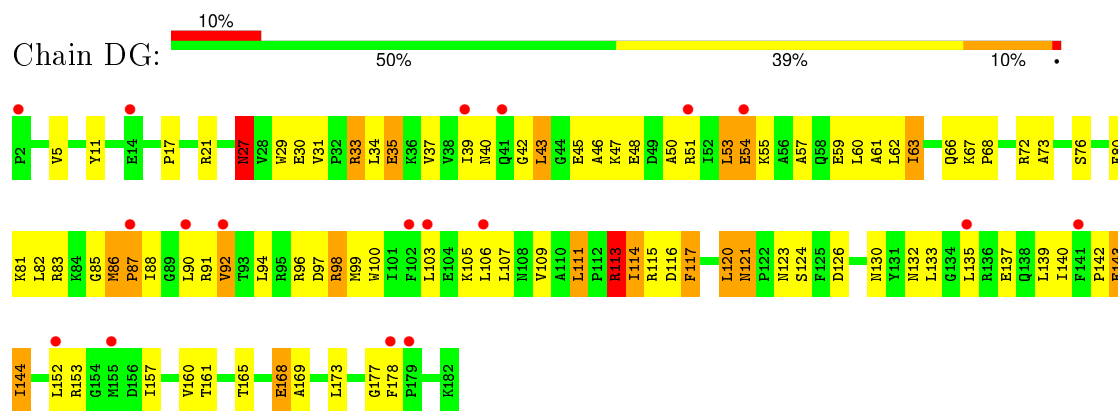
• Molecule 28: 50S ribosomal protein L4



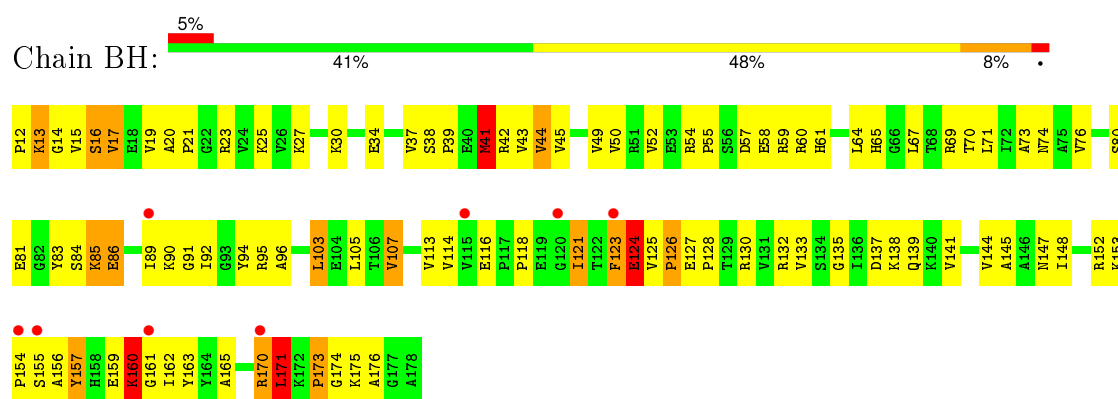
• Molecule 29: 50S ribosomal protein L5



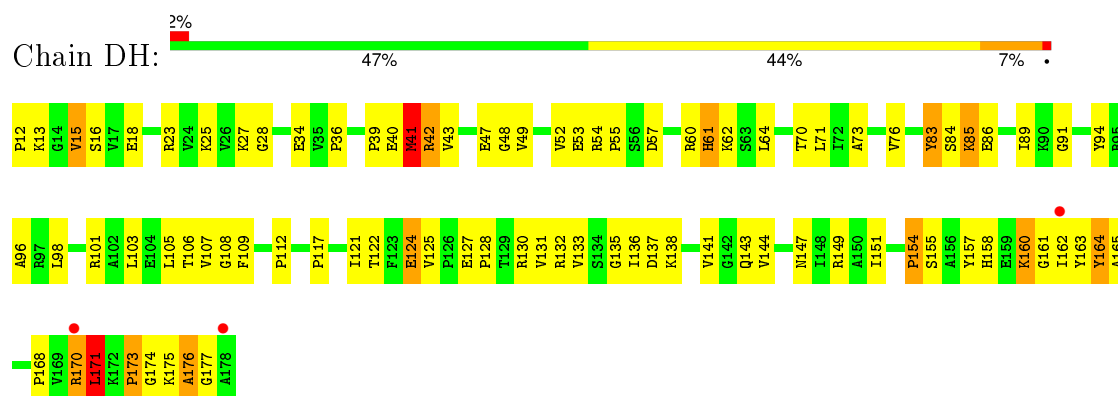
- Molecule 29: 50S ribosomal protein L5



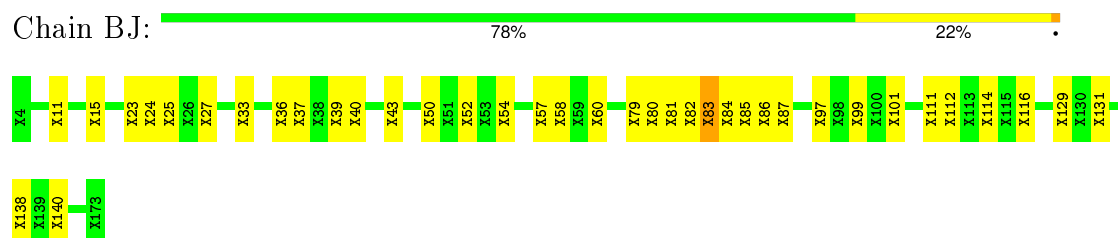
- Molecule 30: 50S ribosomal protein L6



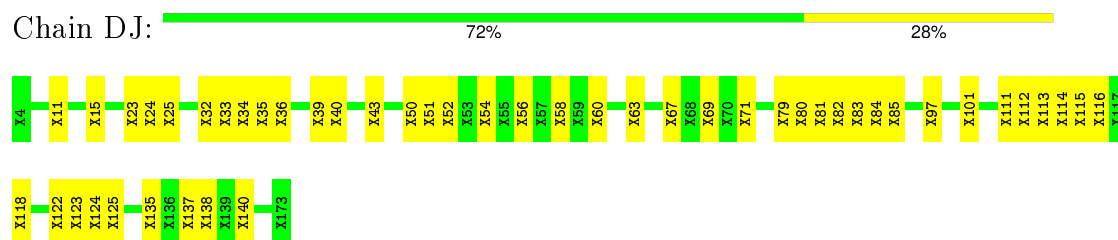
- Molecule 30: 50S ribosomal protein L6



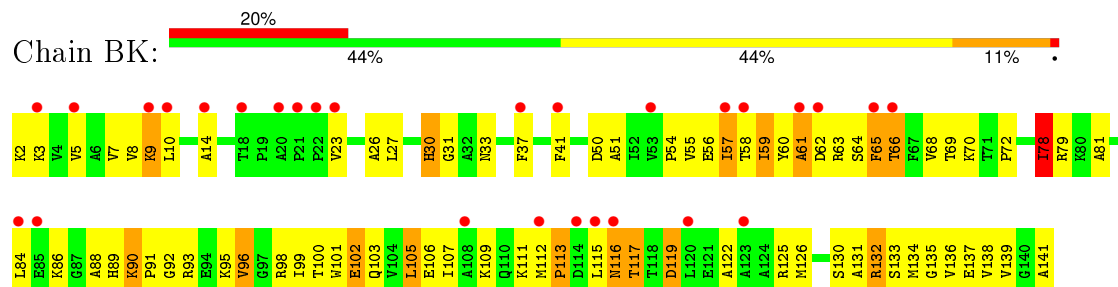
- Molecule 31: 50S RIBOSOMAL PROTEIN L10



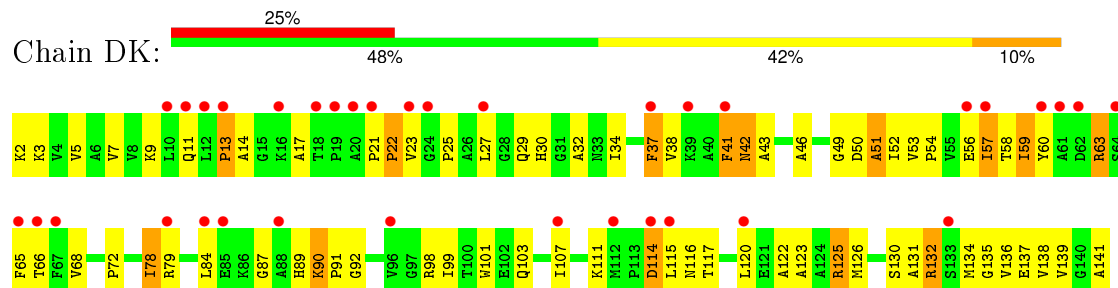
- Molecule 31: 50S RIBOSOMAL PROTEIN L10



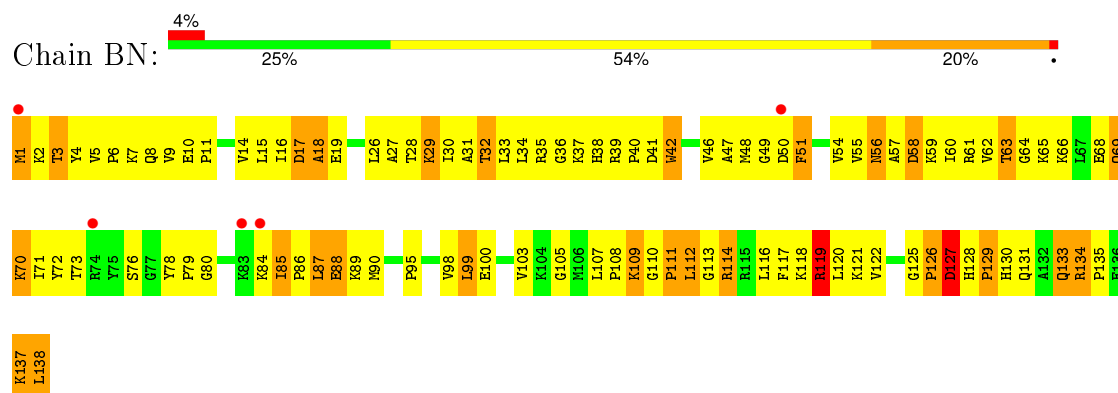
- Molecule 32: 50S ribosomal protein L11



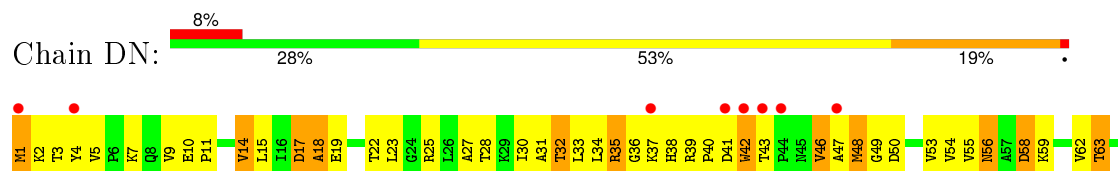
- Molecule 32: 50S ribosomal protein L11

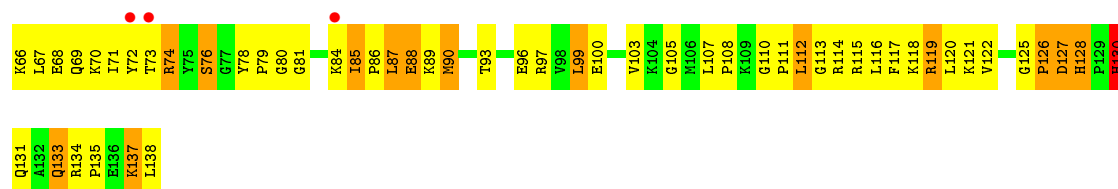


- Molecule 33: 50S ribosomal protein L13

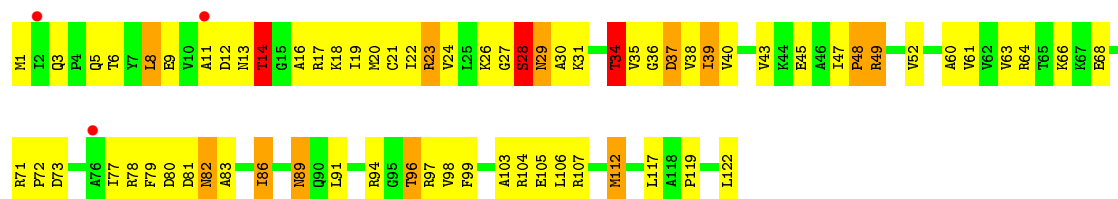
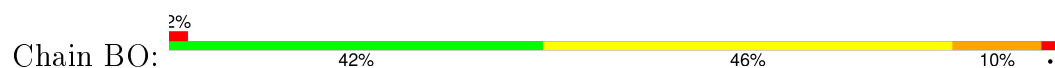


- Molecule 33: 50S ribosomal protein L13

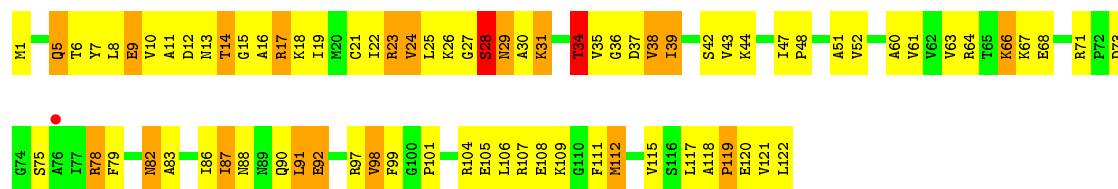
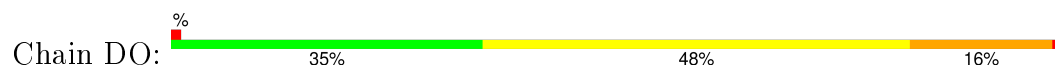




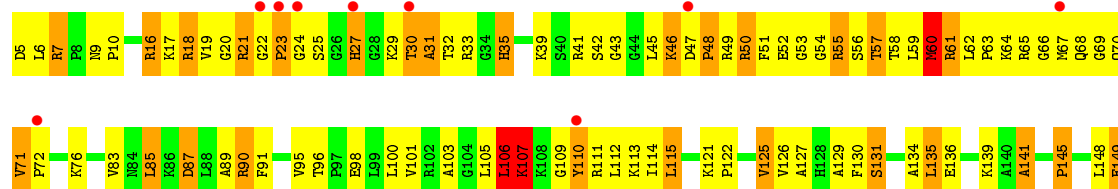
- Molecule 34: 50S ribosomal protein L14



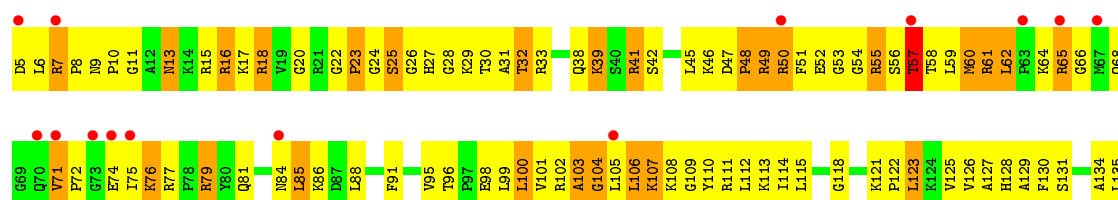
- Molecule 34: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L15

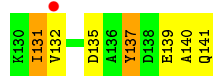
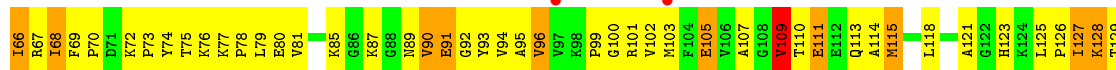
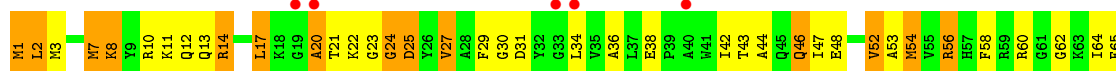


- Molecule 35: 50S ribosomal protein L15

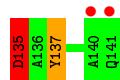
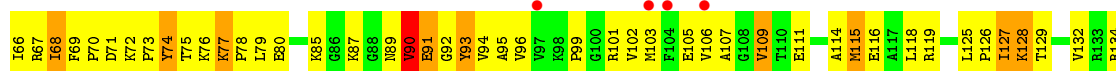
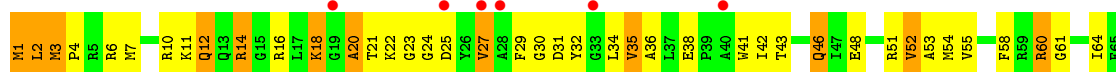




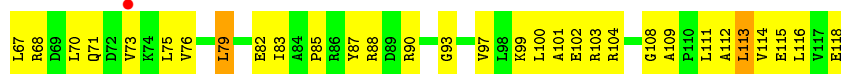
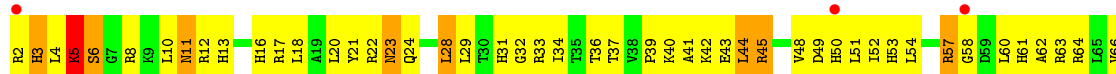
- Molecule 36: 50S ribosomal protein L16



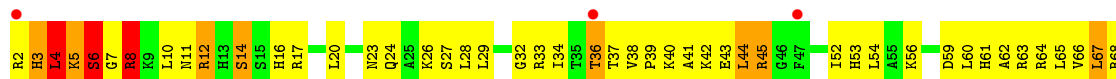
- Molecule 36: 50S ribosomal protein L16

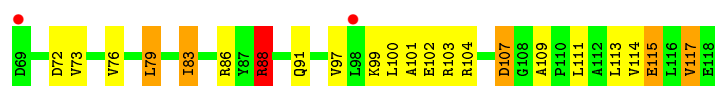


- Molecule 37: 50S ribosomal protein L17

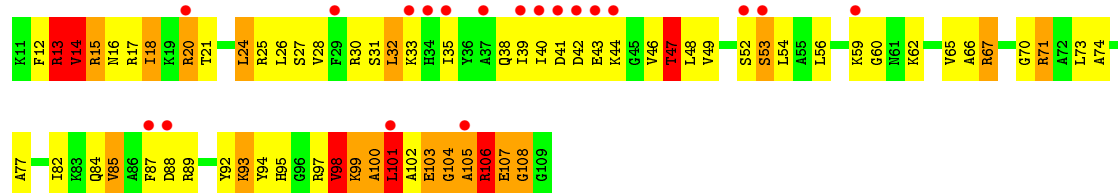


- Molecule 37: 50S ribosomal protein L17

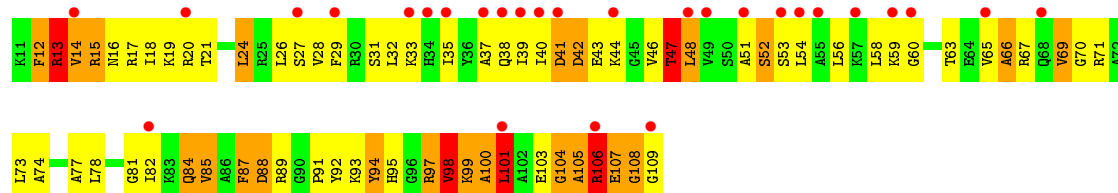




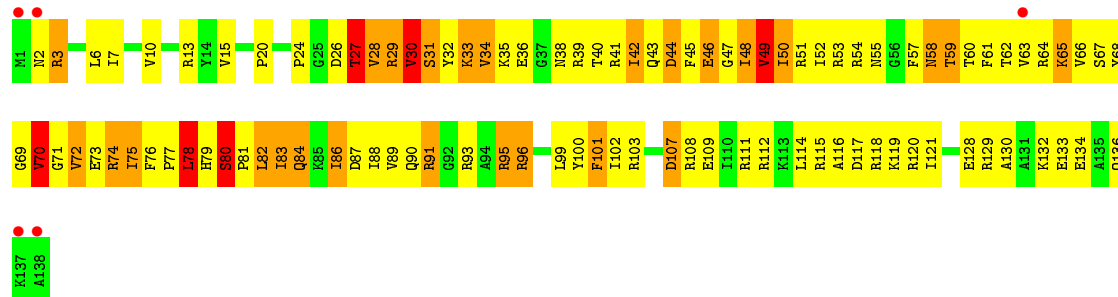
- Molecule 38: 50S ribosomal protein L18



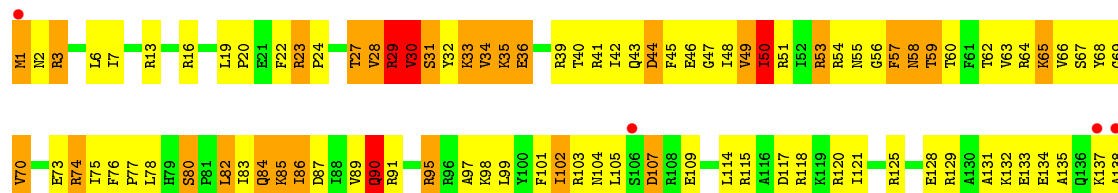
- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19

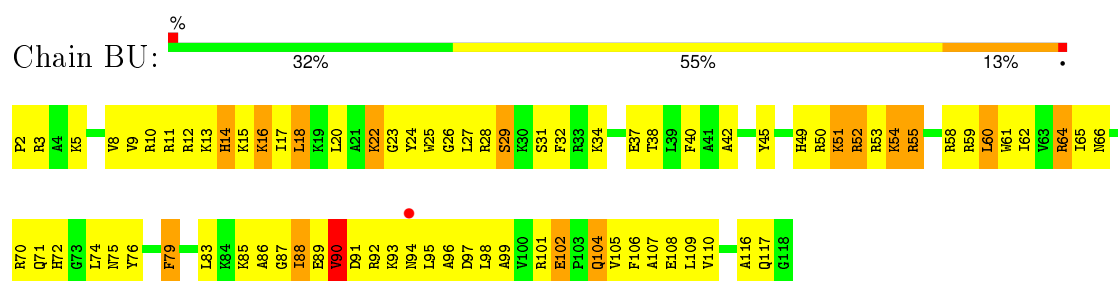


- Molecule 39: 50S ribosomal protein L19

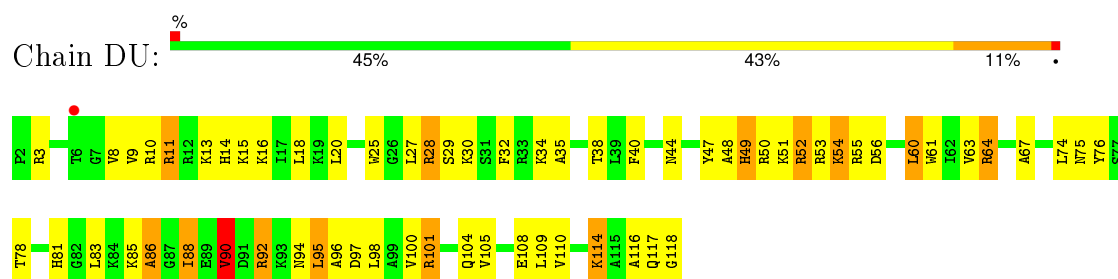


- Molecule 40: 50S ribosomal protein L20

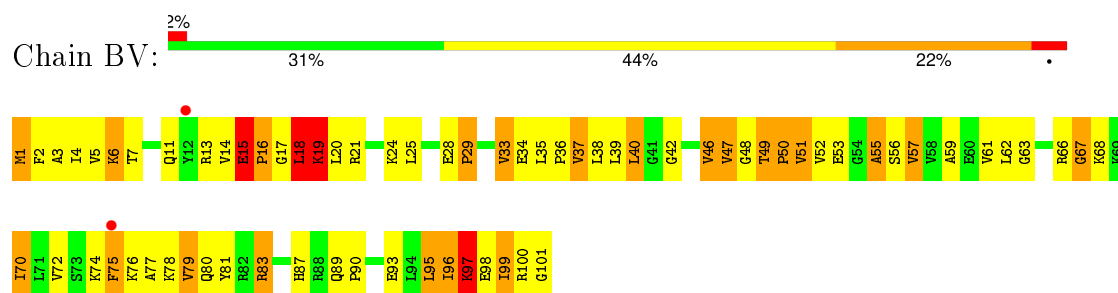




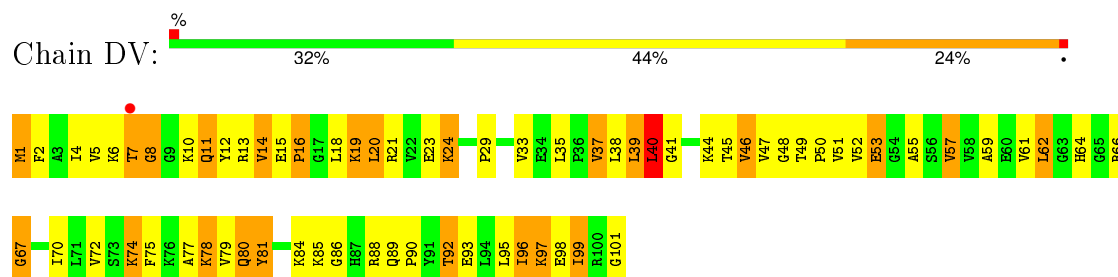
- Molecule 40: 50S ribosomal protein L20



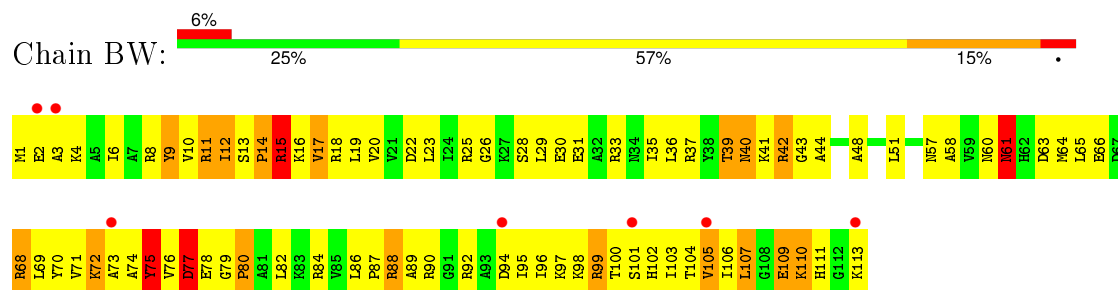
- Molecule 41: 50S ribosomal protein L21



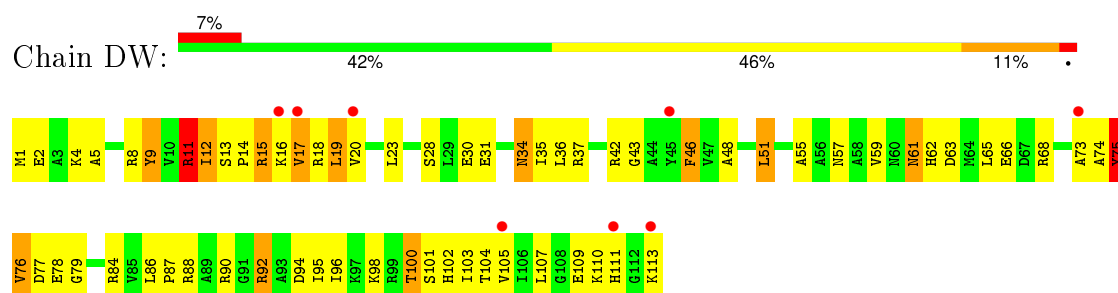
- Molecule 41: 50S ribosomal protein L21



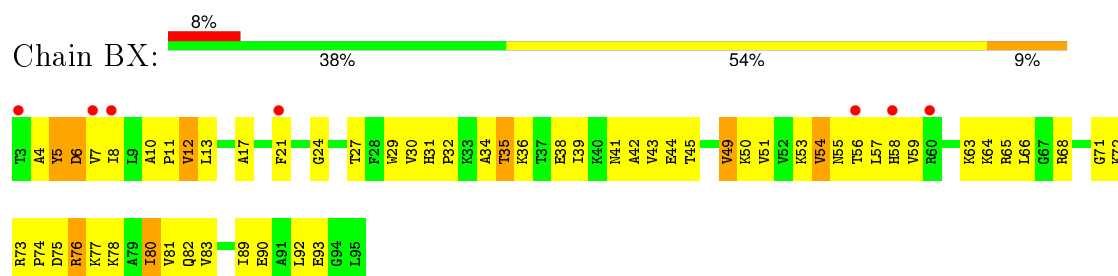
- Molecule 42: 50S ribosomal protein L22



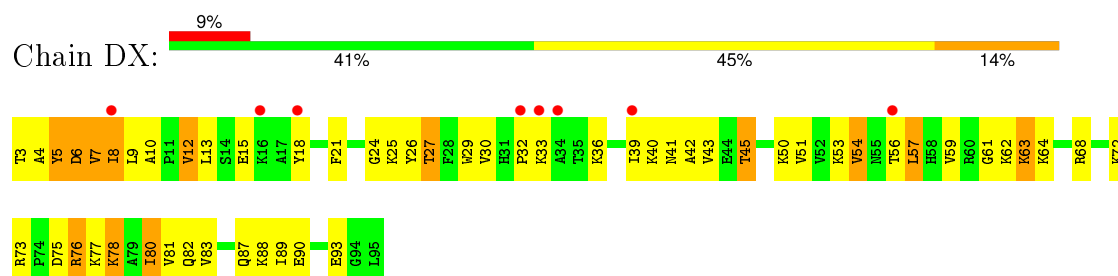
- Molecule 42: 50S ribosomal protein L22



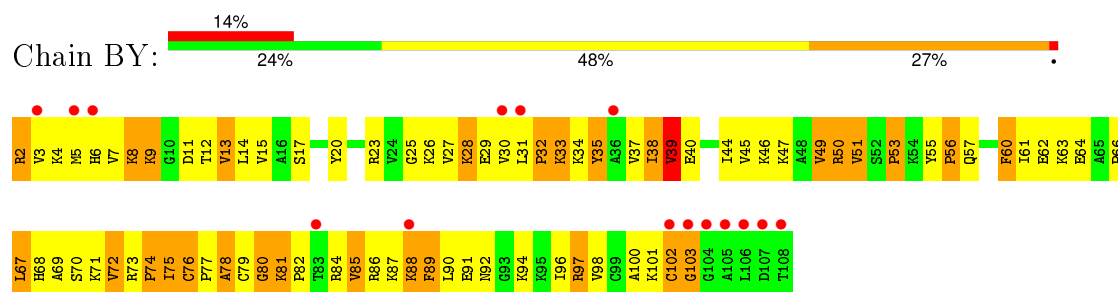
- Molecule 43: 50S ribosomal protein L23



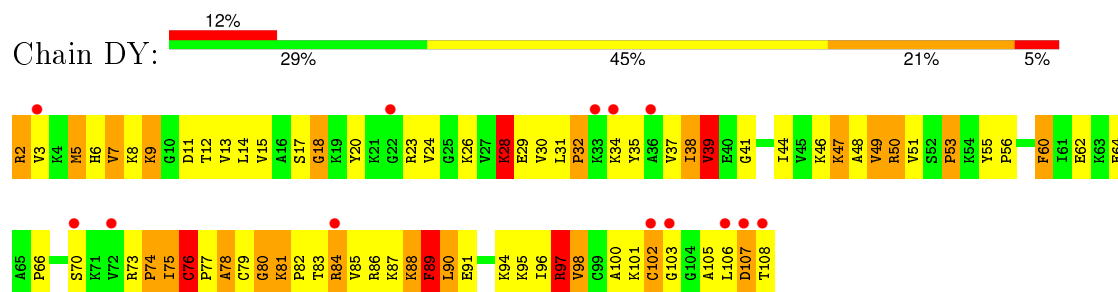
- Molecule 43: 50S ribosomal protein L23



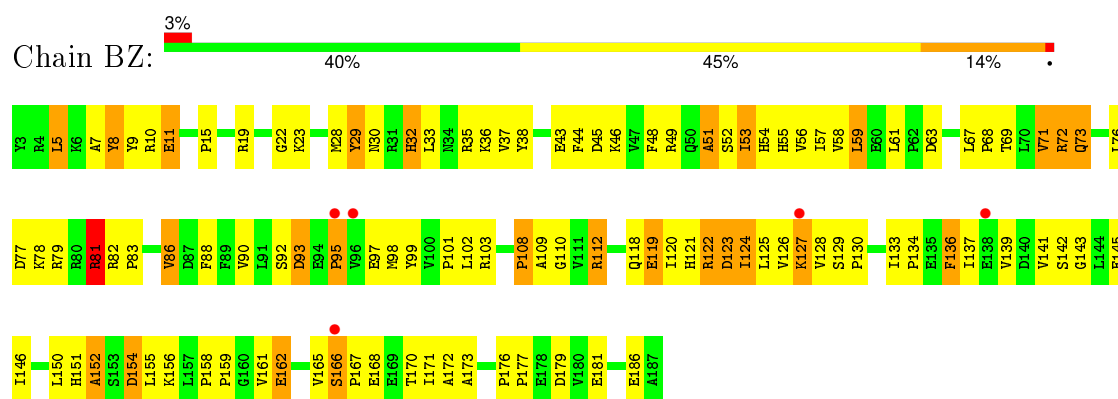
- Molecule 44: 50S ribosomal protein L24



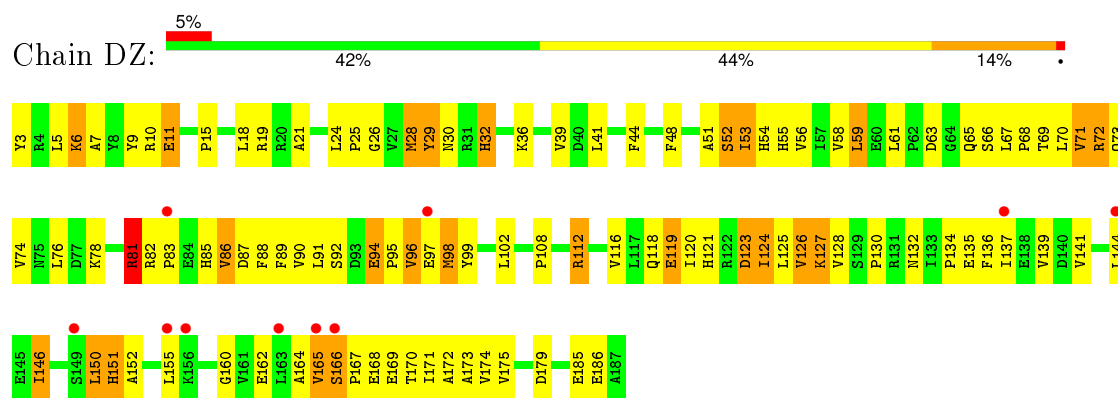
- Molecule 44: 50S ribosomal protein L24



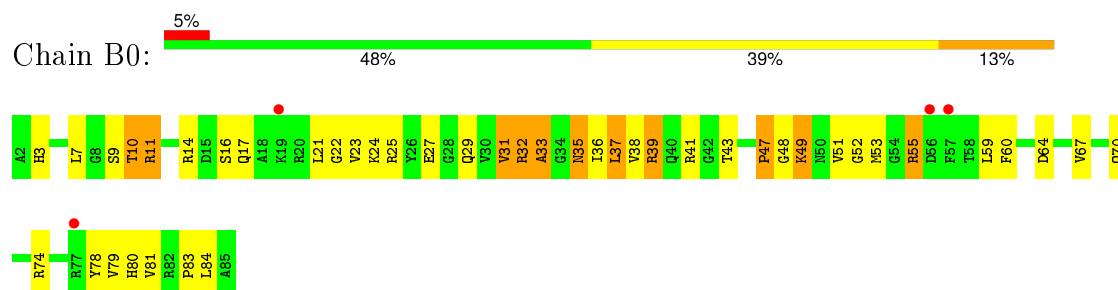
- Molecule 45: 50S ribosomal protein L25



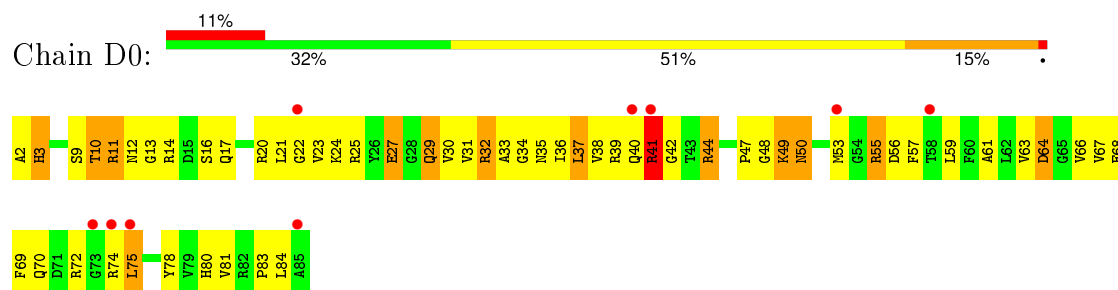
• Molecule 45: 50S ribosomal protein L25



• Molecule 46: 50S ribosomal protein L27

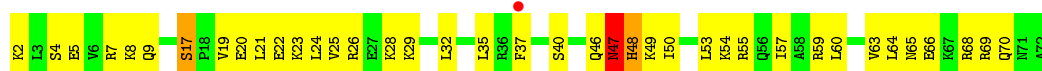


• Molecule 46: 50S ribosomal protein L27

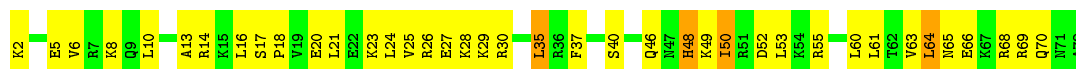


• Molecule 47: 50S ribosomal protein L29

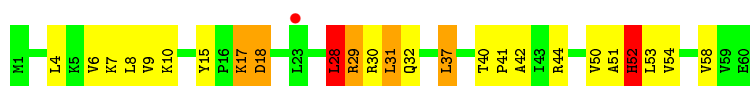




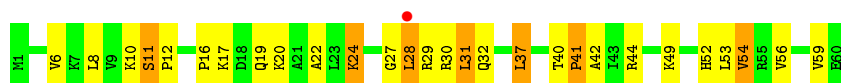
- Molecule 47: 50S ribosomal protein L29



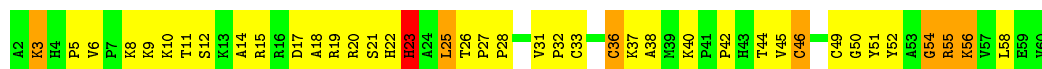
- Molecule 48: 50S ribosomal protein L30



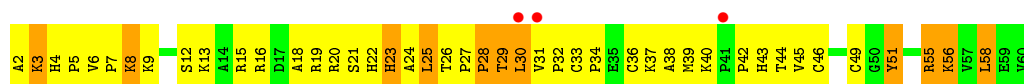
- Molecule 48: 50S ribosomal protein L30



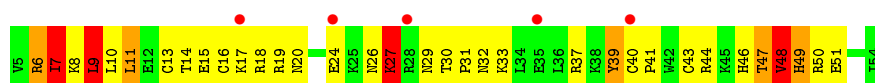
- Molecule 49: 50S ribosomal protein L32



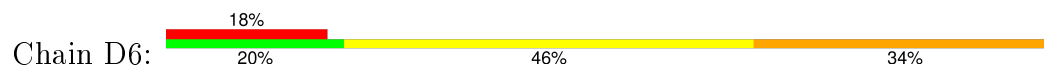
- Molecule 49: 50S ribosomal protein L32

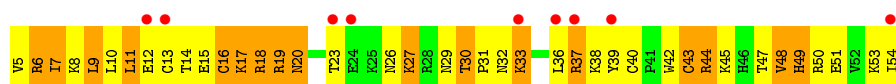


- Molecule 50: 50S ribosomal protein L33



- Molecule 50: 50S ribosomal protein L33





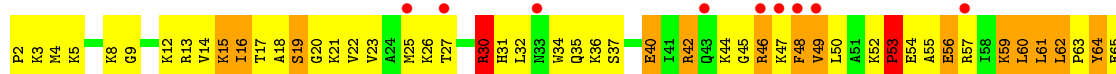
- Molecule 51: 50S ribosomal protein L34



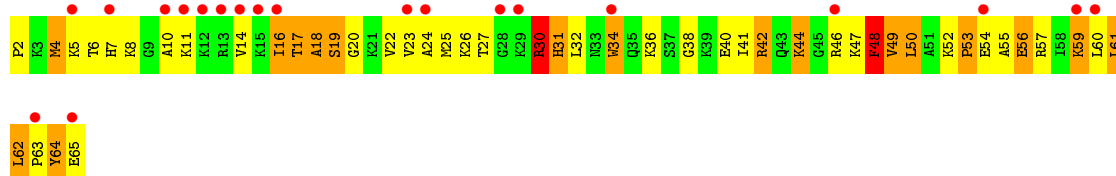
- Molecule 51: 50S ribosomal protein L34



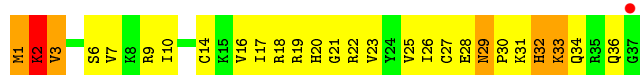
- Molecule 52: 50S ribosomal protein L35



- Molecule 52: 50S ribosomal protein L35



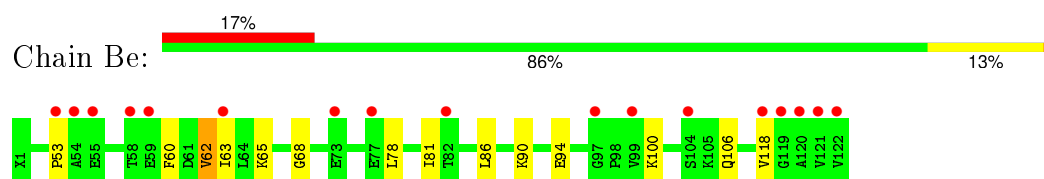
- Molecule 53: 50S ribosomal protein L36



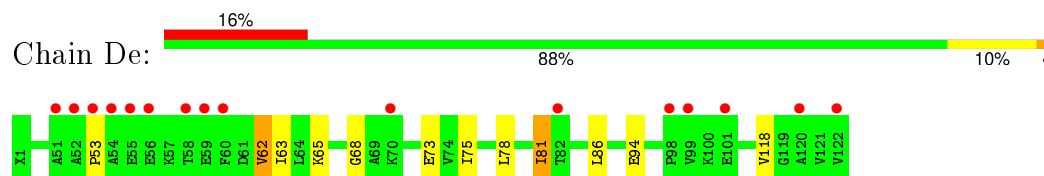
- Molecule 53: 50S ribosomal protein L36



- Molecule 54: 50S ribosomal protein L7/L12



- Molecule 54: 50S ribosomal protein L7/L12



- 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 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 L7/L12



There are no outlier residues recorded for this chain.

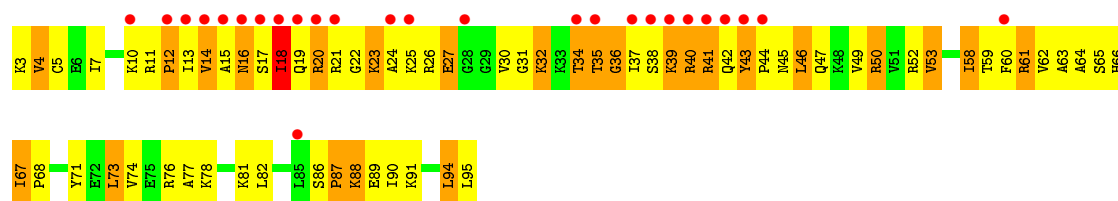
- Molecule 56: 50S RIBOSOMAL PROTEIN L7/L12



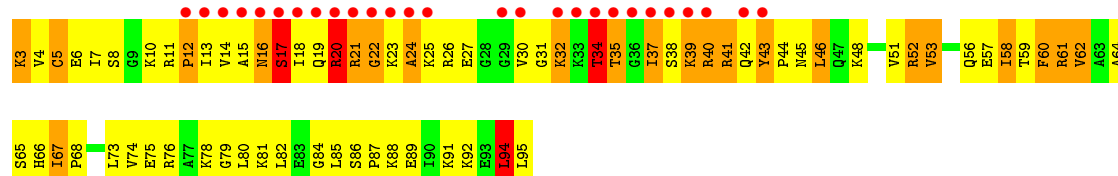
There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L28

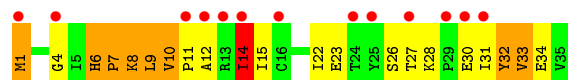
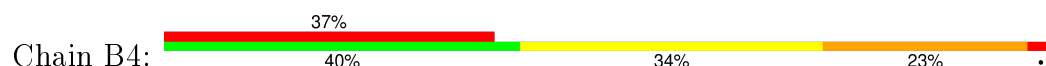




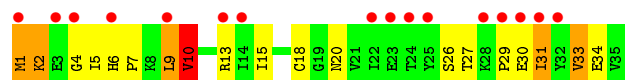
- Molecule 57: 50S ribosomal protein L28



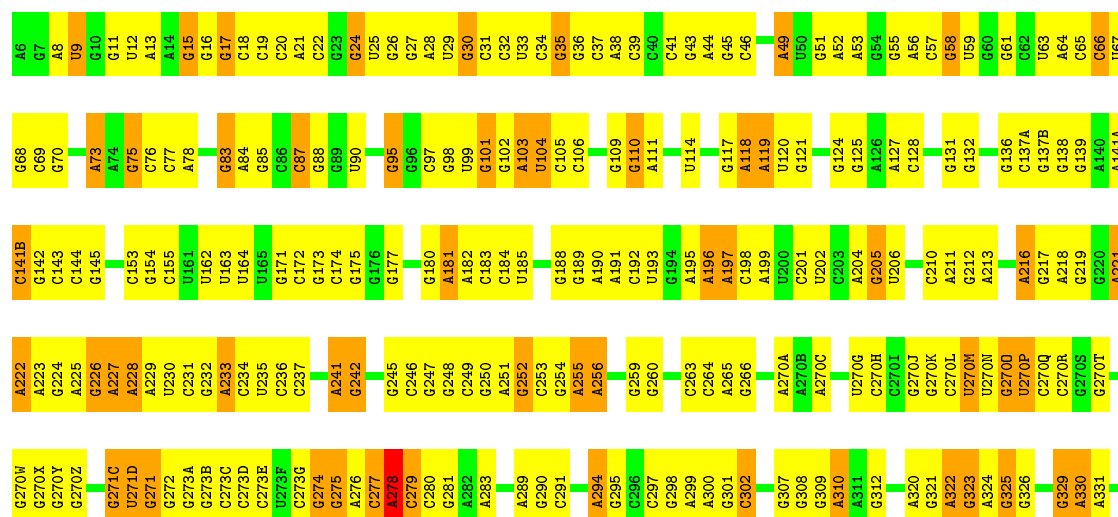
- Molecule 58: 50S ribosomal protein L31



- Molecule 58: 50S ribosomal protein L31



- Molecule 59: 23S ribosomal RNA



U1357	C1289	C1145	C1076	C1006	G945	U871	G809	U747	C679	U613	C543	A472	C404	C334
G1368	C1290	G1148	A1077	C1007	G946	A872	U810	G748	G680	U614	C544	G473	U405	C335
A1359	C1291	G1149	U1078	C1008	G947		U811	G749	G681	U615		G474	G406	C336
U1292	C1292	C1150	C1079	A1009	G948	G875	C812	C749	G682	G616	A547	U475	G407	
C1293	C1293	C1151	U1081	A1010	C949	C876	U814	A751	C683	G617	A548	G476	C408	U339
C1294	U1294	C1152	U1082	U1012	G950	U877	C815	A752	G684	G618A			C410	A340
C1295	C1295	C1153	U1083	U1013	C951	A878	C816	C753	A885	U618B			C341	
C1296	C1296	C1154	U1084	C1014		G879	C817	C754	G686	G619			G411	C342
		G1155	A1085	U1015	G955					G620			A412	
G1299	C1299	A1156	A1086	G1016	C956	G883	G818	U757	U888	A482			C413	A346
U1300	U1300	A1157	A1087	G1017	C957	C884	A819	C758	A889	C560			C414	
A1301	A1301	G1157	A1088	G1018	U957	C885	A820	G759	G690	C484			A415	A347
A1302	A1302		U1089	U1019	U958		A821	G760	C691	U562			C416	C348
		G1162	G1089	U1019	A959	A890	U822	A761	C692	U563			G349	
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		G1164	G1091	A1021	C961		A824	G763	U694	C565			G353	
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		C1166	U1097	U1023	U963	C897	G826	G765	G696	A627			A423	G355
		U1167	A1098	G1024	C964	C898	U827	C766	C697	G629			G356	
			A1099	G1025	C965	A898	U828	U767	C698				A429	
		G1171	C1100	U1026	G966	A900	A829	G768		C634			A432	
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		A1174	C1102	U1028	G968	C902	G831	G770	A705	G636			C433	
		U1175	A1103	A1029				G771	A706	A637			U434	
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		A1177	U1105		C971	U907	A835	U773	C708	U639			A501	A363G
			G1106	U1034	G972	C908	G836	G780	A718	A502			G438	C364
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		G1187	G1112	C1040	G977	C915	G846	C786	U724	U653			G448	G372
			U1113	C1041	G978	G916	G847	U787		U654			A449	G373
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		C1196	C1121	G1044	A981	G919	U847		G727	C593			C453	
		G1197	G1122	A1045	G982	G920	U847		G728	G593			A454	G386
		U1198	C1123	A1046	A983	G921	G848		C730	U594			C455	U387
		U1199	G1124	G1047	A984	U922	A849		C731	C595			C456	G388
		C1200	G1125	A1048	C985	C923	C850		C732	G596			A457	G389
			A1126	C1049	G986	C924	U851		A734	C597			G458	C391
		G1203	A1127		G987	C925	G852		G735	A528			U459	C392
		A1204	A1128	A1054	A988	A926	G853		C736	G600			A460	C393
		G1206	U1130	G1055	G989	G928	G854			C601			G463	A394
		G1207	G1131	A1057	A990	G929	C857		G737	G531			U464	U395
		A1274	A1132	G1058	C991	U930	U858		G738	A603			G465	G396
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		U1211	G1135	U1061	C993	G932	U860		G735	G599			C467	G398
		A1212	C1137	G1062	A996	G934	A861		C736	G600			G468	G400
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		G1216	C1141	A1000	A1001	G940	C865		G742	U606			G468	
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			A1143	C1072			U868		G745	A677			A470	
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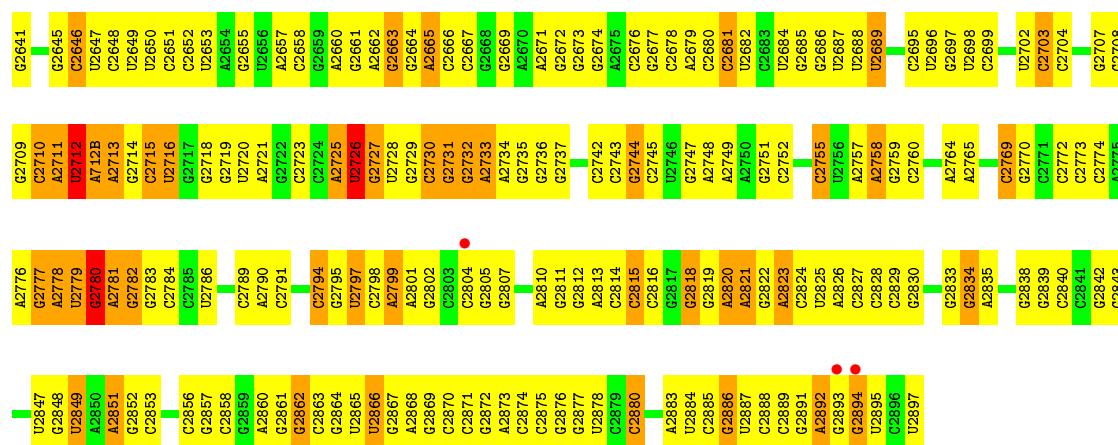


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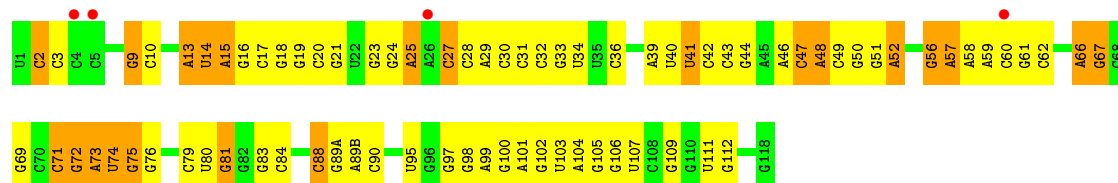


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A1486	U1419	U1420	U1352	A1284	A1210	G1143	C1076	A1010	G948	G882	A819	C754	G689	U626	C565
G1487	U1420	A1421	A1353	G1285	U1211	G1144	A1077	G1011	G949	G883	A820		G690	G627	
	G1422	G1422	G1355	A1286	G1212	C1145	U1078	U1012	G950	G884	A821	U757	C691	G628	G570
A1490	G1423	G1423	G1356	U1287	A1213	G1149	C1080	C1013	G952		U822	C758	C692	A631	A571
G1491	G1424	G1424	G1357	C1289	G1215	C1150	U1081	G1017	G955	G888	G823	G759	U694	A632	G573
G1492	G1425	G1425	G1358	C1290	G1216	G1151	U1082	C958	G956	C889	A824	G760	G695	A633	C574
G1493	A1494	G1426	A1359	C1291	C1217	C1152	U1083	C959	U958	C890	U826	U762	G696	G634	A575
A1494	A1495	A1427	G1360	U1292	C1221	G1153	A1084	A1021	A957	C892	U827	A764	C697	G635	U576
A1495	A1496	C1428	G1361	C1293	C1222	G1154	A1085	A1020	A959	C893	U828	A765	C698	G636	G577
C1496	C1497	C1429	A1365	U1294	C1223		G1086	U1023	A960	C894	A829	G765	A699	G637	A578
A1566	C1498	C1430	A1366	G1299	G1224	G1157	G1087	U1024	G961	U895	G832	C766	U639	U639	C580
A1567	G1500	U1431	A1367	U1300	G1225	C1158	G1088	G1025	G962	A896	U833	U767	A705	C640	C581
G1568	C1501	A1434	G1368	A1301	A1226	U1159	G1089	G1024	U963		U834	G768	A706	C641	G582
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C1570	U1503	C1437	C1370			G1163	C1092	A1027	G965	A901	A835	G770	C708	A643	C584
A1572		U1438	U1371	C1305	C1230	U1164	U1094	A1028	C966	G902	G836	G771	U709	A644	G585
	A1508		U1372	C1306	G1231	U1165	U1095	A1029	C967	C903	C837	C772	G710	C645	A586
A1509	A1510		G1373	A1307	G1232	C1166	A1095	G1030	G968	C904	C838	U773	G711	A646	C587
U1576		G1441	G1374	A1308	G1239	U1167	U1096	U1033	U969		U839	A774	G712	G647	U588
C1577	A1511		C1375	G1309	G1239	G1168	U1097		C970	U905	C840	G775		G648	C589
U1578	G1512	A144B	C1376	G1310	U1240	G1169		G1036	C971	G906	A841	G776	G715	G649	A590
A1579	C1513	C1445	G1377	A1311	A1241	U1101	U1101	U1101	G972	A909	G842		A716	C650	C591
A1580	U1514	C1446	A1378	U1312	A1242	G1173	A1103	C1037	A973	A910	G843	U779	A717	G651	G592
G1581	C1515	G1447	A1379	U1313	G1243	A1174	C1104	C1038	G974A	A911	C844	G780	G718	U652	G593
C1582	U1516	G1448	G1380	C1314	G1244	U1175	C1104	G1039	C974B	C912	G845	A781	C719	G653	G594
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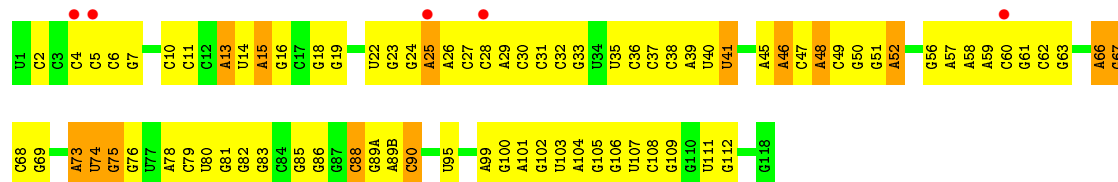
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U2620	G2358	C2293	G2218	C2143	U2079	U2016	G1954	A1873	C1797	A1637	C1637
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G2625	A2360	C2295	G2226	G2145	C2081	G2018	U1956	G1879	U1798	U1639	C1639
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G2627	G2362	G2297	G2228	G2147	G2083	A2020	C1958	G1881	C1800	A1641	G1641
C2628	C2363	C2300	C2229	G2148	C2084	U2022	C1959	G1882	G1801	G1642	G1642
U2629	G2364	G2301	G2230	G2149	C2085	U2023	U1963	G1883	A1802	G1643	G1643
G2630	G2365	C2302	C2231	U2150	G2086	G2024	G1964	G1884	A1803	C1644	C1644
U2631	A2366	G2303	U2232	G2151	G2087	G2025	C1965	G1885	U1804	G1645	C1645
C2632	G2367	G2304	U2233	G2152	U2089	C2026	C1966	G1886	U1805	G1646	C1646
G2633	G2368	A2305	G2234	G2153	G2090	A2030	C1967	G1887	G1718	C1647	C1647
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A2636	G2371	C2308	G2237	G2156	G2093	A2033	A1970	G1890	A1729	G1650	G1650
U2637	G2372	A2309	G2238	G2157	G2094	U2034	A1971	G1891	U1730	A1651	A1652
G2638	G2373	A2310	G2239	A2158	C2095	G2035	A1972	G1892	G1731	G1653	G1653
U2639	C2374	A2311	C2240	G2159	U2096	G2036	G1973	G1893	A1732	A1654	A1654
A2640	G2375	U2312	A2241	G2160	C2097	G2037	C1974	G1894	G1733	C1655	C1655
C2641	C2376	C2313	G2242	C2161		G2038		G1896			



● Molecule 60: 5S ribosomal RNA



● Molecule 60: 5S ribosomal RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	308.96Å 670.66Å 347.77Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 140.20 – 3.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 80.3 (140.20-3.57)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 3.58Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.284 , 0.328 0.298 , 0.336	Depositor DCC
$R_{free}$ test set	33469 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.8	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.14 , 34.2	EDS
Estimated twinning fraction	0.258 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.25$ , $\langle L^2 \rangle = 0.10$	Xtriage
Outliers	0 of 670940 reflections	Xtriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	308166	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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, MG, DPP, KBE, UAL, FUA, 5OH

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	0.38	0/1945	0.72	1/2621 (0.0%)
1	CB	0.37	0/1945	0.67	1/2621 (0.0%)
2	AC	0.28	0/1645	0.53	0/2216
2	CC	0.28	0/1645	0.52	0/2216
3	AD	0.30	0/1733	0.58	0/2318
3	CD	0.30	0/1733	0.58	1/2318 (0.0%)
4	AE	0.32	0/1172	0.58	1/1576 (0.1%)
4	CE	0.31	0/1172	0.58	1/1576 (0.1%)
5	AF	0.31	0/856	0.59	0/1154
5	CF	0.31	0/856	0.56	1/1154 (0.1%)
6	AG	0.29	0/1276	0.51	0/1709
6	CG	0.28	0/1276	0.52	0/1709
7	AH	0.30	0/1136	0.57	0/1527
7	CH	0.28	0/1136	0.55	0/1527
8	AI	0.29	0/1029	0.53	0/1379
8	CI	0.27	0/1029	0.49	0/1379
9	AJ	0.27	0/815	0.54	0/1095
9	CJ	0.28	0/815	0.57	1/1095 (0.1%)
10	AK	0.33	0/900	0.61	0/1213
10	CK	0.36	0/900	0.65	0/1213
11	AL	0.40	0/992	0.83	2/1327 (0.2%)
11	CL	0.40	0/992	0.82	1/1327 (0.1%)
12	AM	0.29	0/1008	0.59	1/1347 (0.1%)
12	CM	0.28	0/1008	0.54	0/1347
13	AN	0.30	0/501	0.52	0/664
13	CN	0.26	0/501	0.46	0/664
14	AO	0.31	0/745	0.52	0/992
14	CO	0.31	0/745	0.53	0/992
15	AP	0.28	0/722	0.50	0/970
15	CP	0.27	0/722	0.52	0/970
16	AQ	0.36	0/848	0.65	0/1131
16	CQ	0.37	0/848	0.71	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AR	0.31	0/579	0.59	0/768
17	CR	0.30	0/579	0.55	0/768
18	AS	0.31	0/647	0.60	0/870
18	CS	0.31	0/647	0.61	0/870
19	AT	0.33	0/765	0.56	0/1007
19	CT	0.32	0/765	0.55	0/1007
20	AA	0.37	0/36351	1.02	61/56736 (0.1%)
20	CA	0.36	0/36351	0.99	53/56736 (0.1%)
21	AW	0.33	0/1827	1.03	0/2845
21	CW	0.33	0/1827	1.01	5/2845 (0.2%)
22	AV	0.27	0/568	0.81	0/886
22	CV	0.29	0/568	0.92	0/886
23	AY	0.34	1/5317 (0.0%)	0.66	7/7198 (0.1%)
23	CY	0.37	2/5317 (0.0%)	0.61	1/7198 (0.0%)
24	AU	0.95	0/11	1.28	0/13
24	CU	0.92	0/11	1.04	0/13
25	BC	0.41	0/1774	0.74	1/2391 (0.0%)
25	DC	0.43	0/1774	0.72	1/2391 (0.0%)
26	BD	0.33	0/2195	0.65	1/2955 (0.0%)
26	DD	0.35	0/2195	0.65	0/2955
27	BE	0.32	0/1602	0.66	0/2160
27	DE	0.31	0/1602	0.66	0/2160
28	BF	0.35	0/1663	0.73	2/2249 (0.1%)
28	DF	0.37	0/1663	0.76	3/2249 (0.1%)
29	BG	0.40	1/1499 (0.1%)	0.59	0/2016
29	DG	0.38	1/1499 (0.1%)	0.61	0/2016
30	BH	0.30	0/1298	0.60	0/1751
30	DH	0.29	0/1298	0.57	0/1751
32	BK	0.27	0/1054	0.51	0/1427
32	DK	0.27	0/1054	0.50	0/1427
33	BN	0.45	0/1131	0.77	0/1525
33	DN	0.48	0/1131	0.74	0/1525
34	BO	0.30	0/943	0.57	0/1269
34	DO	0.29	0/943	0.55	0/1269
35	BP	0.30	0/1131	0.62	0/1504
35	DP	0.29	0/1131	0.62	0/1504
36	BQ	0.35	0/1143	0.63	0/1527
36	DQ	0.34	0/1143	0.60	0/1527
37	BR	0.30	0/974	0.60	0/1302
37	DR	0.31	0/974	0.61	0/1302
38	BS	0.34	0/783	0.69	0/1041
38	DS	0.33	0/783	0.70	0/1041
39	BT	0.34	0/1161	0.67	0/1549



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	DT	0.36	0/1161	0.66	0/1549
40	BU	0.36	0/982	0.57	0/1306
40	DU	0.40	0/982	0.60	0/1306
41	BV	0.38	0/790	0.70	1/1057 (0.1%)
41	DV	0.38	0/790	0.67	0/1057
42	BW	0.31	0/911	0.59	0/1220
42	DW	0.31	0/911	0.61	1/1220 (0.1%)
43	BX	0.30	0/748	0.55	0/1004
43	DX	0.29	0/748	0.54	1/1004 (0.1%)
44	BY	0.32	0/831	0.62	0/1108
44	DY	0.33	0/831	0.66	0/1108
45	BZ	0.29	0/1505	0.58	0/2042
45	DZ	0.28	0/1505	0.58	0/2042
46	B0	0.28	0/671	0.49	0/892
46	D0	0.28	0/671	0.54	0/892
47	B2	0.31	0/600	0.55	0/793
47	D2	0.32	0/600	0.55	0/793
48	B3	0.27	0/482	0.53	0/646
48	D3	0.27	0/482	0.55	0/646
49	B5	0.33	0/473	0.59	0/639
49	D5	0.31	0/473	0.57	0/639
50	B6	0.29	0/440	0.70	1/586 (0.2%)
50	D6	0.30	0/440	0.66	0/586
51	B7	0.33	0/438	0.64	0/575
51	D7	0.31	0/438	0.59	0/575
52	B8	0.34	0/525	0.68	0/691
52	D8	0.30	0/525	0.64	0/691
53	B9	0.30	0/310	0.55	0/407
53	D9	0.32	0/310	0.52	0/407
54	Be	0.28	0/538	0.50	0/715
54	De	0.26	0/538	0.49	0/715
57	B1	0.46	0/739	0.82	0/981
57	D1	0.47	0/739	0.84	1/981 (0.1%)
58	B4	0.32	0/276	0.58	0/372
58	D4	0.35	0/276	0.62	0/372
59	BA	0.40	0/69437	1.04	158/108401 (0.1%)
59	DA	0.40	3/69437 (0.0%)	1.03	149/108401 (0.1%)
60	BB	0.37	0/2853	1.08	11/4451 (0.2%)
60	DB	0.35	0/2853	1.03	5/4451 (0.1%)
All	All	0.37	8/330576 (0.0%)	0.92	474/492228 (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	3
1	CB	0	1
11	CL	0	2
23	AY	0	3
23	CY	0	2
25	BC	0	1
25	DC	0	3
26	BD	0	1
26	DD	0	2
28	BF	0	2
28	DF	0	2
29	BG	0	2
29	DG	0	2
31	BJ	0	1
31	DJ	0	1
35	DP	0	1
38	BS	0	3
38	DS	0	3
42	BW	0	1
42	DW	0	1
57	B1	0	2
57	D1	0	2
All	All	0	41

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CY	506	GLN	C-N	8.35	1.53	1.34
29	BG	114	ILE	N-CA	-7.50	1.31	1.46
29	DG	114	ILE	N-CA	-7.47	1.31	1.46
23	CY	25	LYS	C-N	6.18	1.48	1.34
23	AY	506	GLN	C-N	-5.48	1.21	1.34

The worst 5 of 474 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	DA	1006	C	C6-N1-C2	-13.61	114.86	120.30
59	DA	459	U	N1-C2-N3	12.63	122.48	114.90
59	BA	1006	C	C6-N1-C2	-12.54	115.28	120.30
23	AY	506	GLN	O-C-N	-12.49	102.72	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AA	815	A	C5-C6-N6	11.75	133.10	123.70

There are no chirality outliers.

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	162	ILE	Peptide
1	AB	170	GLU	Peptide
1	AB	185	ILE	Peptide
23	AY	133	ILE	Peptide
23	AY	503	GLY	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	135	0
1	CB	1910	0	1957	107	0
2	AC	1621	0	1688	87	0
2	CC	1621	0	1688	64	0
3	AD	1703	0	1763	104	0
3	CD	1703	0	1763	104	0
4	AE	1156	0	1213	70	0
4	CE	1156	0	1213	57	0
5	AF	843	0	857	42	0
5	CF	843	0	857	32	0
6	AG	1257	0	1296	54	0
6	CG	1257	0	1296	53	0
7	AH	1116	0	1177	67	0
7	CH	1116	0	1177	73	0
8	AI	1010	0	1037	78	0
8	CI	1010	0	1037	57	0
9	AJ	802	0	849	44	0
9	CJ	802	0	849	48	0
10	AK	885	0	904	54	0
10	CK	885	0	904	60	0
11	AL	976	0	1062	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CL	976	0	1062	103	0
12	AM	997	0	1072	67	0
12	CM	997	0	1072	49	0
13	AN	492	0	529	37	0
13	CN	492	0	529	26	0
14	AO	734	0	771	47	0
14	CO	734	0	771	43	0
15	AP	706	0	725	45	0
15	CP	706	0	725	28	0
16	AQ	835	0	904	64	0
16	CQ	835	0	904	57	0
17	AR	574	0	644	36	0
17	CR	574	0	644	37	0
18	AS	634	0	655	34	0
18	CS	634	0	655	45	0
19	AT	763	0	861	38	0
19	CT	763	0	861	37	0
20	AA	32474	0	16393	1002	0
20	CA	32474	0	16393	1036	0
21	AW	1635	0	831	63	0
21	CW	1635	0	831	53	0
22	AV	503	0	252	12	0
22	CV	503	0	252	15	0
23	AY	5219	0	5290	315	0
23	CY	5219	0	5291	323	0
24	AU	48	0	39	1	0
24	CU	48	0	39	3	0
25	BC	1742	0	1798	168	0
25	DC	1742	0	1798	180	0
26	BD	2145	0	2234	202	0
26	DD	2145	0	2234	199	0
27	BE	1569	0	1634	124	0
27	DE	1569	0	1634	121	0
28	BF	1628	0	1680	132	0
28	DF	1628	0	1680	153	0
29	BG	1474	0	1535	72	0
29	DG	1474	0	1535	71	0
30	BH	1274	0	1342	57	0
30	DH	1274	0	1342	49	0
31	BJ	851	0	197	31	0
31	DJ	851	0	193	39	0
32	BK	1035	0	1082	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	DK	1035	0	1082	53	0
33	BN	1104	0	1180	84	0
33	DN	1104	0	1180	97	0
34	BO	933	0	996	64	0
34	DO	933	0	996	77	0
35	BP	1114	0	1187	87	0
35	DP	1114	0	1187	87	0
36	BQ	1122	0	1179	74	0
36	DQ	1122	0	1179	71	0
37	BR	960	0	1021	70	0
37	DR	960	0	1021	61	0
38	BS	775	0	835	68	0
38	DS	775	0	835	62	0
39	BT	1147	0	1207	101	0
39	DT	1147	0	1207	100	0
40	BU	964	0	1022	84	0
40	DU	964	0	1022	60	1
41	BV	779	0	852	66	0
41	DV	779	0	852	69	0
42	BW	900	0	964	69	0
42	DW	900	0	964	49	0
43	BX	734	0	789	44	0
43	DX	734	0	789	42	0
44	BY	818	0	908	58	0
44	DY	818	0	908	59	0
45	BZ	1473	0	1497	80	0
45	DZ	1473	0	1497	69	0
46	B0	662	0	688	33	0
46	D0	662	0	688	46	0
47	B2	598	0	653	28	0
47	D2	598	0	653	31	0
48	B3	477	0	529	23	0
48	D3	477	0	529	19	0
49	B5	459	0	477	46	0
49	D5	459	0	477	47	0
50	B6	433	0	461	26	0
50	D6	433	0	461	38	0
51	B7	430	0	480	38	0
51	D7	430	0	480	37	0
52	B8	517	0	582	52	0
52	D8	517	0	582	47	0
53	B9	307	0	338	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	D9	307	0	335	17	0
54	Be	686	0	615	0	0
54	De	686	0	616	0	0
55	Bf	156	0	40	0	0
55	Bg	156	0	41	0	0
55	Df	156	0	40	0	0
55	Dg	156	0	37	0	0
56	Bh	151	0	39	0	0
56	Dh	151	0	40	0	0
57	B1	732	0	808	72	0
57	D1	732	0	808	81	0
58	B4	271	0	284	19	0
58	D4	271	0	284	18	0
59	BA	61997	0	31250	2039	1
59	DA	61997	0	31250	2203	0
60	BB	2551	0	1295	85	0
60	DB	2551	0	1295	85	0
61	AY	37	0	47	6	0
61	CY	37	0	47	7	0
62	AY	28	0	12	12	0
62	CY	28	0	12	13	0
63	BA	1	0	0	0	0
63	CY	1	0	0	0	0
All	All	308166	0	213086	12302	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 24.

The worst 5 of 12302 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)
23:CY:19:ALA:H	23:CY:25:LYS:CE	1.38	1.34
59:DA:2405:G:H21	59:DA:2412:A:N6	1.28	1.26
23:CY:19:ALA:N	23:CY:25:LYS:HE3	1.49	1.26
59:DA:2405:G:N2	59:DA:2412:A:H62	1.29	1.25
21:AW:15:G:N2	21:AW:48:C:H42	1.36	1.24

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)
59:BA:1015:G:O2'	40:DU:118:GLY:O[3_545]	2.09	0.11

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	154 (66%)	51 (22%)	28 (12%)	0	6
1	CB	233/235 (99%)	159 (68%)	50 (22%)	24 (10%)	1	9
2	AC	205/207 (99%)	154 (75%)	32 (16%)	19 (9%)	1	11
2	CC	205/207 (99%)	156 (76%)	36 (18%)	13 (6%)	2	21
3	AD	206/208 (99%)	149 (72%)	31 (15%)	26 (13%)	0	6
3	CD	206/208 (99%)	153 (74%)	32 (16%)	21 (10%)	1	9
4	AE	149/151 (99%)	117 (78%)	22 (15%)	10 (7%)	1	19
4	CE	149/151 (99%)	117 (78%)	25 (17%)	7 (5%)	3	29
5	AF	99/101 (98%)	75 (76%)	15 (15%)	9 (9%)	1	11
5	CF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	1	11
6	AG	153/155 (99%)	121 (79%)	25 (16%)	7 (5%)	3	29
6	CG	153/155 (99%)	124 (81%)	22 (14%)	7 (5%)	3	29
7	AH	136/138 (99%)	97 (71%)	27 (20%)	12 (9%)	1	12
7	CH	136/138 (99%)	97 (71%)	28 (21%)	11 (8%)	1	13
8	AI	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	4	33
8	CI	125/127 (98%)	99 (79%)	22 (18%)	4 (3%)	5	40
9	AJ	97/99 (98%)	75 (77%)	13 (13%)	9 (9%)	1	11
9	CJ	97/99 (98%)	75 (77%)	17 (18%)	5 (5%)	2	25
10	AK	117/119 (98%)	82 (70%)	21 (18%)	14 (12%)	0	6
10	CK	117/119 (98%)	82 (70%)	22 (19%)	13 (11%)	0	7
11	AL	123/125 (98%)	38 (31%)	52 (42%)	33 (27%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	CL	123/125 (98%)	47 (38%)	43 (35%)	33 (27%)	0	0
12	AM	123/125 (98%)	93 (76%)	20 (16%)	10 (8%)	1	13
12	CM	123/125 (98%)	91 (74%)	25 (20%)	7 (6%)	2	23
13	AN	58/60 (97%)	44 (76%)	7 (12%)	7 (12%)	0	6
13	CN	58/60 (97%)	44 (76%)	10 (17%)	4 (7%)	1	18
14	AO	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	13
14	CO	86/88 (98%)	60 (70%)	21 (24%)	5 (6%)	2	23
15	AP	82/84 (98%)	66 (80%)	15 (18%)	1 (1%)	16	61
15	CP	82/84 (98%)	64 (78%)	14 (17%)	4 (5%)	3	27
16	AQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	1	9
16	CQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	1	9
17	AR	68/70 (97%)	51 (75%)	10 (15%)	7 (10%)	1	9
17	CR	68/70 (97%)	48 (71%)	13 (19%)	7 (10%)	1	9
18	AS	77/79 (98%)	41 (53%)	23 (30%)	13 (17%)	0	3
18	CS	77/79 (98%)	46 (60%)	17 (22%)	14 (18%)	0	2
19	AT	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	3	33
19	CT	97/99 (98%)	79 (81%)	12 (12%)	6 (6%)	2	21
23	AY	663/687 (96%)	451 (68%)	138 (21%)	74 (11%)	0	7
23	CY	663/687 (96%)	461 (70%)	134 (20%)	68 (10%)	1	9
24	AU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
24	CU	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
25	BC	226/228 (99%)	110 (49%)	66 (29%)	50 (22%)	0	1
25	DC	226/228 (99%)	123 (54%)	59 (26%)	44 (20%)	0	2
26	BD	273/275 (99%)	174 (64%)	47 (17%)	52 (19%)	0	2
26	DD	273/275 (99%)	165 (60%)	61 (22%)	47 (17%)	0	2
27	BE	203/205 (99%)	128 (63%)	40 (20%)	35 (17%)	0	2
27	DE	203/205 (99%)	122 (60%)	45 (22%)	36 (18%)	0	2
28	BF	206/208 (99%)	130 (63%)	46 (22%)	30 (15%)	0	4
28	DF	206/208 (99%)	128 (62%)	44 (21%)	34 (16%)	0	3
29	BG	179/181 (99%)	122 (68%)	48 (27%)	9 (5%)	3	27
29	DG	179/181 (99%)	134 (75%)	36 (20%)	9 (5%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BH	165/167 (99%)	118 (72%)	27 (16%)	20 (12%)	0	6
30	DH	165/167 (99%)	111 (67%)	33 (20%)	21 (13%)	0	6
32	BK	138/140 (99%)	96 (70%)	30 (22%)	12 (9%)	1	12
32	DK	138/140 (99%)	97 (70%)	34 (25%)	7 (5%)	2	26
33	BN	136/138 (99%)	86 (63%)	28 (21%)	22 (16%)	0	3
33	DN	136/138 (99%)	88 (65%)	35 (26%)	13 (10%)	1	10
34	BO	120/122 (98%)	86 (72%)	24 (20%)	10 (8%)	1	13
34	DO	120/122 (98%)	87 (72%)	25 (21%)	8 (7%)	1	19
35	BP	144/146 (99%)	85 (59%)	39 (27%)	20 (14%)	0	4
35	DP	144/146 (99%)	81 (56%)	38 (26%)	25 (17%)	0	2
36	BQ	139/141 (99%)	96 (69%)	27 (19%)	16 (12%)	0	7
36	DQ	139/141 (99%)	97 (70%)	29 (21%)	13 (9%)	1	10
37	BR	115/117 (98%)	80 (70%)	27 (24%)	8 (7%)	1	18
37	DR	115/117 (98%)	83 (72%)	20 (17%)	12 (10%)	1	8
38	BS	97/99 (98%)	56 (58%)	21 (22%)	20 (21%)	0	1
38	DS	97/99 (98%)	56 (58%)	21 (22%)	20 (21%)	0	1
39	BT	136/138 (99%)	80 (59%)	31 (23%)	25 (18%)	0	2
39	DT	136/138 (99%)	85 (62%)	29 (21%)	22 (16%)	0	3
40	BU	115/117 (98%)	84 (73%)	25 (22%)	6 (5%)	2	25
40	DU	115/117 (98%)	90 (78%)	16 (14%)	9 (8%)	1	14
41	BV	99/101 (98%)	66 (67%)	16 (16%)	17 (17%)	0	2
41	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	4
42	BW	111/113 (98%)	85 (77%)	11 (10%)	15 (14%)	0	4
42	DW	111/113 (98%)	85 (77%)	15 (14%)	11 (10%)	1	10
43	BX	91/93 (98%)	72 (79%)	15 (16%)	4 (4%)	3	30
43	DX	91/93 (98%)	72 (79%)	14 (15%)	5 (6%)	2	24
44	BY	105/107 (98%)	51 (49%)	30 (29%)	24 (23%)	0	1
44	DY	105/107 (98%)	46 (44%)	26 (25%)	33 (31%)	0	0
45	BZ	183/185 (99%)	132 (72%)	33 (18%)	18 (10%)	1	10
45	DZ	183/185 (99%)	132 (72%)	32 (18%)	19 (10%)	1	8
46	B0	82/84 (98%)	59 (72%)	16 (20%)	7 (8%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	D0	82/84 (98%)	57 (70%)	15 (18%)	10 (12%)	0	6
47	B2	69/71 (97%)	51 (74%)	14 (20%)	4 (6%)	2	23
47	D2	69/71 (97%)	56 (81%)	10 (14%)	3 (4%)	3	31
48	B3	58/60 (97%)	48 (83%)	6 (10%)	4 (7%)	1	18
48	D3	58/60 (97%)	42 (72%)	10 (17%)	6 (10%)	1	9
49	B5	57/59 (97%)	43 (75%)	11 (19%)	3 (5%)	2	25
49	D5	57/59 (97%)	41 (72%)	12 (21%)	4 (7%)	1	18
50	B6	48/50 (96%)	28 (58%)	13 (27%)	7 (15%)	0	4
50	D6	48/50 (96%)	29 (60%)	8 (17%)	11 (23%)	0	1
51	B7	47/49 (96%)	35 (74%)	8 (17%)	4 (8%)	1	13
51	D7	47/49 (96%)	32 (68%)	9 (19%)	6 (13%)	0	5
52	B8	62/64 (97%)	35 (56%)	17 (27%)	10 (16%)	0	3
52	D8	62/64 (97%)	36 (58%)	18 (29%)	8 (13%)	0	5
53	B9	35/37 (95%)	18 (51%)	12 (34%)	5 (14%)	0	4
53	D9	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	1	12
54	Be	70/102 (69%)	38 (54%)	24 (34%)	8 (11%)	0	7
54	De	70/102 (69%)	41 (59%)	23 (33%)	6 (9%)	1	12
57	B1	91/93 (98%)	60 (66%)	19 (21%)	12 (13%)	0	5
57	D1	91/93 (98%)	56 (62%)	18 (20%)	17 (19%)	0	2
58	B4	33/35 (94%)	15 (46%)	13 (39%)	5 (15%)	0	3
58	D4	33/35 (94%)	17 (52%)	9 (27%)	7 (21%)	0	1
All	All	13260/13576 (98%)	9009 (68%)	2708 (20%)	1543 (12%)	0	7

5 of 1543 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	9	GLU
1	AB	76	GLN
1	AB	165	VAL
1	AB	194	PRO
2	AC	4	LYS

### 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%)	164 (81%)	39 (19%)	2	10
1	CB	203/203 (100%)	167 (82%)	36 (18%)	2	13
2	AC	161/161 (100%)	132 (82%)	29 (18%)	2	12
2	CC	161/161 (100%)	136 (84%)	25 (16%)	3	20
3	AD	180/180 (100%)	145 (81%)	35 (19%)	2	10
3	CD	180/180 (100%)	150 (83%)	30 (17%)	3	16
4	AE	116/116 (100%)	93 (80%)	23 (20%)	1	9
4	CE	116/116 (100%)	98 (84%)	18 (16%)	3	20
5	AF	90/90 (100%)	78 (87%)	12 (13%)	5	26
5	CF	90/90 (100%)	82 (91%)	8 (9%)	12	47
6	AG	126/126 (100%)	113 (90%)	13 (10%)	9	40
6	CG	126/126 (100%)	115 (91%)	11 (9%)	13	48
7	AH	119/119 (100%)	98 (82%)	21 (18%)	2	13
7	CH	119/119 (100%)	105 (88%)	14 (12%)	6	31
8	AI	98/98 (100%)	82 (84%)	16 (16%)	3	17
8	CI	98/98 (100%)	84 (86%)	14 (14%)	4	24
9	AJ	89/89 (100%)	75 (84%)	14 (16%)	3	19
9	CJ	89/89 (100%)	72 (81%)	17 (19%)	2	10
10	AK	90/90 (100%)	71 (79%)	19 (21%)	1	8
10	CK	90/90 (100%)	73 (81%)	17 (19%)	2	10
11	AL	104/104 (100%)	77 (74%)	27 (26%)	0	4
11	CL	104/104 (100%)	72 (69%)	32 (31%)	0	3
12	AM	100/100 (100%)	83 (83%)	17 (17%)	2	15
12	CM	100/100 (100%)	89 (89%)	11 (11%)	8	36
13	AN	49/49 (100%)	43 (88%)	6 (12%)	6	29
13	CN	49/49 (100%)	43 (88%)	6 (12%)	6	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	79/79 (100%)	71 (90%)	8 (10%)	9	40
14	CO	79/79 (100%)	65 (82%)	14 (18%)	2	13
15	AP	72/72 (100%)	66 (92%)	6 (8%)	14	50
15	CP	72/72 (100%)	62 (86%)	10 (14%)	4	25
16	AQ	95/95 (100%)	81 (85%)	14 (15%)	4	22
16	CQ	95/95 (100%)	79 (83%)	16 (17%)	2	15
17	AR	61/61 (100%)	51 (84%)	10 (16%)	3	17
17	CR	61/61 (100%)	53 (87%)	8 (13%)	5	27
18	AS	69/69 (100%)	55 (80%)	14 (20%)	1	9
18	CS	69/69 (100%)	54 (78%)	15 (22%)	1	7
19	AT	76/76 (100%)	64 (84%)	12 (16%)	3	19
19	CT	76/76 (100%)	67 (88%)	9 (12%)	6	31
23	AY	563/579 (97%)	470 (84%)	93 (16%)	3	16
23	CY	563/579 (97%)	463 (82%)	100 (18%)	2	13
24	AU	2/2 (100%)	2 (100%)	0	100	100
24	CU	2/2 (100%)	2 (100%)	0	100	100
25	BC	180/180 (100%)	140 (78%)	40 (22%)	1	6
25	DC	180/180 (100%)	138 (77%)	42 (23%)	1	5
26	BD	217/217 (100%)	169 (78%)	48 (22%)	1	6
26	DD	217/217 (100%)	164 (76%)	53 (24%)	1	5
27	BE	165/165 (100%)	134 (81%)	31 (19%)	2	11
27	DE	165/165 (100%)	127 (77%)	38 (23%)	1	5
28	BF	165/165 (100%)	133 (81%)	32 (19%)	2	10
28	DF	165/165 (100%)	135 (82%)	30 (18%)	2	12
29	BG	155/155 (100%)	130 (84%)	25 (16%)	3	18
29	DG	155/155 (100%)	127 (82%)	28 (18%)	2	12
30	BH	136/136 (100%)	116 (85%)	20 (15%)	4	22
30	DH	136/136 (100%)	125 (92%)	11 (8%)	15	52
32	BK	105/105 (100%)	90 (86%)	15 (14%)	4	24
32	DK	105/105 (100%)	89 (85%)	16 (15%)	3	21
33	BN	117/117 (100%)	95 (81%)	22 (19%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DN	117/117 (100%)	94 (80%)	23 (20%)	1	9
34	BO	100/100 (100%)	80 (80%)	20 (20%)	1	9
34	DO	100/100 (100%)	81 (81%)	19 (19%)	2	10
35	BP	112/112 (100%)	87 (78%)	25 (22%)	1	6
35	DP	112/112 (100%)	94 (84%)	18 (16%)	3	18
36	BQ	111/111 (100%)	82 (74%)	29 (26%)	0	4
36	DQ	111/111 (100%)	86 (78%)	25 (22%)	1	6
37	BR	100/100 (100%)	87 (87%)	13 (13%)	5	27
37	DR	100/100 (100%)	82 (82%)	18 (18%)	2	12
38	BS	77/77 (100%)	62 (80%)	15 (20%)	2	10
38	DS	77/77 (100%)	58 (75%)	19 (25%)	1	5
39	BT	120/120 (100%)	94 (78%)	26 (22%)	1	7
39	DT	120/120 (100%)	92 (77%)	28 (23%)	1	5
40	BU	93/93 (100%)	72 (77%)	21 (23%)	1	6
40	DU	93/93 (100%)	73 (78%)	20 (22%)	1	7
41	BV	82/82 (100%)	60 (73%)	22 (27%)	0	4
41	DV	82/82 (100%)	59 (72%)	23 (28%)	0	3
42	BW	92/92 (100%)	68 (74%)	24 (26%)	0	4
42	DW	92/92 (100%)	72 (78%)	20 (22%)	1	7
43	BX	75/75 (100%)	64 (85%)	11 (15%)	4	22
43	DX	75/75 (100%)	60 (80%)	15 (20%)	1	9
44	BY	88/88 (100%)	69 (78%)	19 (22%)	1	7
44	DY	88/88 (100%)	72 (82%)	16 (18%)	2	12
45	BZ	162/162 (100%)	133 (82%)	29 (18%)	2	13
45	DZ	162/162 (100%)	134 (83%)	28 (17%)	2	14
46	B0	66/66 (100%)	54 (82%)	12 (18%)	2	12
46	D0	66/66 (100%)	51 (77%)	15 (23%)	1	6
47	B2	66/66 (100%)	62 (94%)	4 (6%)	23	64
47	D2	66/66 (100%)	60 (91%)	6 (9%)	12	46
48	B3	52/52 (100%)	45 (86%)	7 (14%)	5	26
48	D3	52/52 (100%)	45 (86%)	7 (14%)	5	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B5	51/51 (100%)	44 (86%)	7 (14%)	4	25
49	D5	51/51 (100%)	41 (80%)	10 (20%)	1	9
50	B6	49/49 (100%)	38 (78%)	11 (22%)	1	6
50	D6	49/49 (100%)	37 (76%)	12 (24%)	1	5
51	B7	42/42 (100%)	35 (83%)	7 (17%)	3	16
51	D7	42/42 (100%)	38 (90%)	4 (10%)	11	43
52	B8	54/54 (100%)	39 (72%)	15 (28%)	0	3
52	D8	54/54 (100%)	37 (68%)	17 (32%)	0	3
53	B9	34/34 (100%)	28 (82%)	6 (18%)	2	13
53	D9	34/34 (100%)	32 (94%)	2 (6%)	24	65
54	Be	54/54 (100%)	47 (87%)	7 (13%)	5	27
54	De	54/54 (100%)	46 (85%)	8 (15%)	4	22
57	B1	78/78 (100%)	59 (76%)	19 (24%)	1	5
57	D1	78/78 (100%)	58 (74%)	20 (26%)	0	4
58	B4	31/31 (100%)	23 (74%)	8 (26%)	0	4
58	D4	31/31 (100%)	26 (84%)	5 (16%)	3	18
All	All	11142/11174 (100%)	9117 (82%)	2025 (18%)	2	12

5 of 2025 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	B0	27	GLU
5	CF	67	MET
43	DX	76	ARG
49	B5	46	CYS
1	CB	68	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
39	BT	58	ASN
10	CK	93	GLN
40	DU	71	GLN
39	BT	84	GLN
3	CD	119	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	AA	1510/1511 (99%)	305 (20%)	17 (1%)
20	CA	1510/1511 (99%)	285 (18%)	16 (1%)
21	AW	76/77 (98%)	23 (30%)	1 (1%)
21	CW	76/77 (98%)	22 (28%)	1 (1%)
22	AV	22/23 (95%)	8 (36%)	1 (4%)
22	CV	22/23 (95%)	8 (36%)	2 (9%)
59	BA	2878/2879 (99%)	665 (23%)	27 (0%)
59	DA	2878/2879 (99%)	666 (23%)	21 (0%)
60	BB	118/119 (99%)	21 (17%)	1 (0%)
60	DB	118/119 (99%)	17 (14%)	1 (0%)
All	All	9208/9218 (99%)	2020 (21%)	88 (0%)

5 of 2020 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	AA	6	G
20	AA	9	G
20	AA	13	U
20	AA	15	G
20	AA	29	G

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
59	BA	2171	A
20	CA	243	A
59	DA	2092	U
59	BA	2447	G
59	BA	2781	A

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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
24	KBE	AU	1	24	8,8,9	0.55	0	7,8,10	1.48	2 (28%)
24	DPP	AU	2	24	3,5,6	0.35	0	1,5,7	0.16	0
24	UAL	AU	5	24	7,8,9	2.52	2 (28%)	4,9,11	1.37	1 (25%)
24	5OH	AU	6	24	7,12,13	0.60	0	7,16,18	2.65	3 (42%)
24	KBE	CU	1	24	8,8,9	0.59	0	7,8,10	1.80	1 (14%)
24	DPP	CU	2	24	3,5,6	0.32	0	1,5,7	0.16	0
24	UAL	CU	5	24	7,8,9	2.58	2 (28%)	4,9,11	1.63	1 (25%)
24	5OH	CU	6	24	7,12,13	0.66	0	7,16,18	2.84	4 (57%)

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
24	KBE	AU	1	24	-	0/7/7/8	0/0/0/0
24	DPP	AU	2	24	-	0/1/4/6	0/0/0/0
24	UAL	AU	5	24	-	0/3/7/9	0/0/0/0
24	5OH	AU	6	24	-	0/1/18/20	0/1/1/1
24	KBE	CU	1	24	-	0/7/7/8	0/0/0/0
24	DPP	CU	2	24	-	0/1/4/6	0/0/0/0
24	UAL	CU	5	24	-	0/3/7/9	0/0/0/0
24	5OH	CU	6	24	-	0/1/18/20	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CU	5	UAL	C1-N1	-2.97	1.35	1.40
24	AU	5	UAL	C1-N1	-2.61	1.35	1.40
24	AU	5	UAL	C-CA	5.70	1.53	1.45
24	CU	5	UAL	C-CA	5.71	1.53	1.45

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CU	5	UAL	O-C-CA	-3.14	120.78	125.40
24	CU	6	5OH	O-C-CA	-2.48	118.88	125.44
24	AU	5	UAL	O-C-CA	-2.38	121.90	125.40
24	AU	1	KBE	CD-CG-CB	-2.11	108.27	115.16
24	AU	6	5OH	O-C-CA	-2.11	119.88	125.44



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CU	1	KBE	2	0
24	CU	2	DPP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
61	FUA	AY	701	-	37,40,40	1.71	6 (16%)	45,64,64	1.98	11 (24%)
62	GDP	AY	702	-	23,30,30	1.36	3 (13%)	30,47,47	1.81	7 (23%)
61	FUA	CY	701	-	37,40,40	1.65	6 (16%)	45,64,64	2.17	12 (26%)
62	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
61	FUA	AY	701	-	-	0/10/92/92	0/4/4/4
62	GDP	AY	702	-	-	0/12/32/32	0/3/3/3
61	FUA	CY	701	-	-	0/10/92/92	0/4/4/4
62	GDP	CY	702	-	-	0/12/32/32	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	FUA	C23-C22	-5.87	1.40	1.51
61	CY	701	FUA	C23-C22	-5.43	1.41	1.51
61	AY	701	FUA	C23-C24	-4.21	1.39	1.53
61	CY	701	FUA	C23-C24	-4.03	1.39	1.53
61	AY	701	FUA	C24-C25	-3.84	1.39	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	CY	701	FUA	C13-C12-C11	-6.65	102.94	111.95
61	AY	701	FUA	C13-C12-C11	-6.07	103.73	111.95
62	AY	702	GDP	N3-C2-N1	-4.75	120.21	127.44
62	CY	702	GDP	N3-C2-N1	-4.72	120.26	127.44
62	CY	702	GDP	PA-O3A-PB	-3.98	119.33	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AY	701	FUA	6	0
62	AY	702	GDP	12	0
61	CY	701	FUA	7	0
62	CY	702	GDP	13	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
54	Be	1
54	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	37.69
1	Be	30:UNK	C	51:ALA	N	36.65

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AB	235/235 (100%)	0.07	6 (2%) 59 49	4, 59, 144, 223	0
1	CB	235/235 (100%)	0.28	21 (8%) 12 10	5, 60, 155, 214	0
2	AC	207/207 (100%)	0.05	10 (4%) 34 27	4, 63, 136, 190	0
2	CC	207/207 (100%)	0.08	11 (5%) 30 23	3, 57, 130, 186	0
3	AD	208/208 (100%)	0.11	17 (8%) 14 12	4, 57, 142, 206	0
3	CD	208/208 (100%)	-0.03	5 (2%) 62 52	14, 72, 144, 196	0
4	AE	151/151 (100%)	0.61	25 (16%) 2 2	5, 34, 122, 151	0
4	CE	151/151 (100%)	0.40	18 (11%) 6 6	4, 35, 133, 165	0
5	AF	101/101 (100%)	-0.58	0 100 100	4, 27, 93, 145	0
5	CF	101/101 (100%)	-0.41	0 100 100	5, 37, 115, 163	0
6	AG	155/155 (100%)	-0.09	4 (2%) 59 49	10, 78, 153, 229	0
6	CG	155/155 (100%)	0.07	11 (7%) 19 15	3, 84, 172, 210	0
7	AH	138/138 (100%)	-0.25	2 (1%) 78 68	3, 31, 89, 166	0
7	CH	138/138 (100%)	-0.09	3 (2%) 65 55	1, 37, 130, 199	0
8	AI	127/127 (100%)	0.95	28 (22%) 1 1	6, 72, 140, 199	0
8	CI	127/127 (100%)	0.49	13 (10%) 9 8	14, 84, 152, 237	0
9	AJ	99/99 (100%)	0.35	12 (12%) 6 6	9, 68, 136, 163	0
9	CJ	99/99 (100%)	0.22	7 (7%) 19 15	13, 65, 154, 217	0
10	AK	119/119 (100%)	0.17	10 (8%) 14 12	7, 56, 137, 180	0
10	CK	119/119 (100%)	0.27	14 (11%) 6 6	8, 55, 145, 175	0
11	AL	125/125 (100%)	0.24	13 (10%) 8 8	5, 39, 105, 171	0
11	CL	125/125 (100%)	0.51	13 (10%) 8 8	8, 52, 134, 176	0
12	AM	125/125 (100%)	0.68	18 (14%) 3 4	23, 90, 167, 199	0
12	CM	125/125 (100%)	0.60	21 (16%) 2 2	14, 90, 166, 190	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	AN	60/60 (100%)	0.62	6 (10%)	9 9	8, 38, 114, 139	0
13	CN	60/60 (100%)	0.51	3 (5%)	32 25	8, 42, 131, 166	0
14	AO	88/88 (100%)	-0.14	3 (3%)	49 40	5, 37, 108, 158	0
14	CO	88/88 (100%)	0.00	1 (1%)	82 73	8, 49, 130, 197	0
15	AP	84/84 (100%)	0.77	16 (19%)	2 2	18, 68, 131, 171	0
15	CP	84/84 (100%)	0.60	10 (11%)	6 6	8, 79, 159, 224	0
16	AQ	100/100 (100%)	0.27	6 (6%)	25 19	9, 43, 120, 169	0
16	CQ	100/100 (100%)	0.35	7 (7%)	19 15	5, 43, 118, 142	0
17	AR	70/70 (100%)	-0.16	2 (2%)	55 45	7, 30, 134, 185	0
17	CR	70/70 (100%)	-0.10	4 (5%)	27 21	7, 28, 130, 193	0
18	AS	79/79 (100%)	0.82	13 (16%)	2 3	15, 78, 159, 206	0
18	CS	79/79 (100%)	0.32	6 (7%)	17 14	10, 80, 154, 204	0
19	AT	99/99 (100%)	0.28	7 (7%)	19 15	4, 64, 120, 187	0
19	CT	99/99 (100%)	0.60	10 (10%)	9 9	16, 71, 155, 187	0
20	AA	1511/1511 (100%)	-0.18	24 (1%)	74 65	3, 62, 163, 289	0
20	CA	1511/1511 (100%)	-0.16	23 (1%)	76 67	5, 63, 173, 323	0
21	AW	77/77 (100%)	-0.25	0	100 100	21, 91, 179, 234	0
21	CW	77/77 (100%)	0.00	2 (2%)	59 49	44, 97, 221, 273	0
22	AV	23/23 (100%)	0.66	1 (4%)	39 30	56, 136, 187, 205	0
22	CV	23/23 (100%)	0.77	2 (8%)	13 12	66, 119, 215, 230	0
23	AY	667/687 (97%)	-0.11	23 (3%)	49 40	5, 64, 147, 208	0
23	CY	667/687 (97%)	-0.03	22 (3%)	50 41	4, 68, 150, 203	0
24	AU	2/6 (33%)	0.84	0	100 100	155, 155, 155, 155	0
24	CU	2/6 (33%)	0.54	0	100 100	81, 81, 81, 88	0
25	BC	228/228 (100%)	1.15	56 (24%)	1 1	45, 128, 217, 259	0
25	DC	228/228 (100%)	1.23	60 (26%)	1 1	33, 153, 230, 287	0
26	BD	275/275 (100%)	-0.21	1 (0%)	93 90	4, 26, 103, 166	0
26	DD	275/275 (100%)	-0.17	2 (0%)	89 82	4, 25, 107, 210	0
27	BE	205/205 (100%)	-0.08	10 (4%)	33 25	1, 31, 135, 229	0
27	DE	205/205 (100%)	-0.19	3 (1%)	76 67	6, 41, 144, 221	0
28	BF	208/208 (100%)	0.75	31 (14%)	3 3	6, 49, 162, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DF	208/208 (100%)	0.64	27 (12%) 5 5	10, 62, 162, 266	0
29	BG	181/181 (100%)	0.75	28 (15%) 3 3	11, 91, 152, 197	0
29	DG	181/181 (100%)	0.58	18 (9%) 9 9	33, 105, 176, 209	0
30	BH	167/167 (100%)	-0.11	8 (4%) 34 27	3, 47, 130, 224	0
30	DH	167/167 (100%)	-0.22	3 (1%) 71 62	6, 56, 141, 187	0
31	BJ	0/170	-	-	-	-
31	DJ	0/170	-	-	-	-
32	BK	140/140 (100%)	1.14	28 (20%) 1 2	17, 104, 194, 230	0
32	DK	140/140 (100%)	1.07	35 (25%) 1 1	37, 124, 205, 244	0
33	BN	138/138 (100%)	0.23	5 (3%) 46 37	59, 83, 108, 111	0
33	DN	138/138 (100%)	0.47	11 (7%) 15 12	59, 81, 104, 111	0
34	BO	122/122 (100%)	-0.07	3 (2%) 61 50	5, 33, 94, 148	0
34	DO	122/122 (100%)	-0.11	1 (0%) 87 80	4, 30, 131, 183	0
35	BP	146/146 (100%)	0.20	9 (6%) 24 19	7, 55, 131, 173	0
35	DP	146/146 (100%)	0.27	15 (10%) 9 8	1, 60, 152, 204	0
36	BQ	141/141 (100%)	-0.10	8 (5%) 27 21	20, 43, 113, 170	0
36	DQ	141/141 (100%)	0.07	12 (8%) 13 12	8, 32, 107, 219	0
37	BR	117/117 (100%)	0.10	4 (3%) 49 40	7, 38, 125, 156	0
37	DR	117/117 (100%)	0.02	5 (4%) 39 30	2, 38, 126, 213	0
38	BS	99/99 (100%)	0.88	19 (19%) 2 2	27, 104, 191, 225	0
38	DS	99/99 (100%)	1.31	28 (28%) 1 1	11, 106, 194, 248	0
39	BT	138/138 (100%)	-0.15	5 (3%) 46 37	6, 53, 139, 225	0
39	DT	138/138 (100%)	-0.09	4 (2%) 55 45	3, 68, 141, 201	0
40	BU	117/117 (100%)	-0.12	1 (0%) 85 78	11, 22, 80, 175	0
40	DU	117/117 (100%)	-0.24	1 (0%) 85 78	6, 20, 94, 136	0
41	BV	101/101 (100%)	-0.16	2 (1%) 68 59	0, 32, 104, 143	0
41	DV	101/101 (100%)	-0.18	1 (0%) 84 76	2, 32, 117, 147	0
42	BW	113/113 (100%)	0.35	7 (6%) 24 19	8, 32, 103, 140	0
42	DW	113/113 (100%)	0.48	8 (7%) 19 15	2, 31, 116, 157	0
43	BX	93/93 (100%)	0.33	7 (7%) 17 14	5, 51, 118, 172	0
43	DX	93/93 (100%)	0.36	8 (8%) 13 12	7, 50, 136, 198	0
44	BY	107/107 (100%)	0.62	15 (14%) 4 4	12, 69, 151, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	DY	107/107 (100%)	0.59	13 (12%) 6 6	6, 70, 150, 196	0
45	BZ	185/185 (100%)	-0.24	5 (2%) 58 47	13, 52, 123, 175	0
45	DZ	185/185 (100%)	-0.00	10 (5%) 29 23	10, 61, 135, 194	0
46	B0	84/84 (100%)	0.08	4 (4%) 34 27	6, 53, 127, 163	0
46	D0	84/84 (100%)	0.42	9 (10%) 8 7	7, 58, 132, 217	0
47	B2	71/71 (100%)	-0.20	1 (1%) 78 68	12, 61, 137, 175	0
47	D2	71/71 (100%)	-0.40	0 100 100	9, 60, 127, 145	0
48	B3	60/60 (100%)	-0.29	1 (1%) 73 64	8, 31, 96, 111	0
48	D3	60/60 (100%)	-0.07	1 (1%) 73 64	13, 29, 101, 126	0
49	B5	59/59 (100%)	-0.06	0 100 100	8, 37, 148, 208	0
49	D5	59/59 (100%)	0.29	3 (5%) 32 24	6, 44, 156, 223	0
50	B6	50/50 (100%)	0.39	5 (10%) 9 9	12, 92, 147, 163	0
50	D6	50/50 (100%)	0.78	9 (18%) 2 2	31, 89, 175, 242	0
51	B7	49/49 (100%)	0.46	5 (10%) 9 8	9, 16, 135, 218	0
51	D7	49/49 (100%)	0.32	4 (8%) 14 12	11, 32, 107, 180	0
52	B8	64/64 (100%)	0.81	9 (14%) 4 4	5, 46, 98, 130	0
52	D8	64/64 (100%)	1.39	20 (31%) 1 1	7, 56, 123, 178	0
53	B9	37/37 (100%)	0.23	1 (2%) 58 47	10, 26, 148, 246	0
53	D9	37/37 (100%)	0.19	1 (2%) 58 47	8, 19, 104, 158	0
54	Be	72/102 (70%)	1.30	17 (23%) 1 1	24, 113, 183, 201	0
54	De	72/102 (70%)	1.32	16 (22%) 1 1	18, 114, 206, 259	0
55	Bf	0/31	-	-	-	-
55	Bg	0/31	-	-	-	-
55	Df	0/31	-	-	-	-
55	Dg	0/31	-	-	-	-
56	Bh	0/30	-	-	-	-
56	Dh	0/30	-	-	-	-
57	B1	93/93 (100%)	1.07	26 (27%) 1 1	1, 79, 187, 243	0
57	D1	93/93 (100%)	1.00	27 (29%) 1 1	8, 72, 174, 241	0
58	B4	35/35 (100%)	1.60	13 (37%) 0 0	74, 144, 233, 266	0
58	D4	35/35 (100%)	2.23	16 (45%) 0 0	64, 158, 226, 275	0
59	BA	2879/2879 (100%)	-0.18	14 (0%) 91 88	3, 43, 145, 276	0
59	DA	2879/2879 (100%)	-0.12	20 (0%) 89 82	0, 47, 163, 315	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
60	BB	119/119 (100%)	0.01	4 (3%) 49 40	21, 108, 175, 210	0
60	DB	119/119 (100%)	0.11	5 (4%) 40 31	23, 97, 186, 258	0
All	All	22686/23318 (97%)	0.09	1221 (5%) 29 23	0, 57, 160, 323	0

The worst 5 of 1221 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	DC	113	ALA	11.6
54	De	122	VAL	10.4
58	D4	4	GLY	10.1
44	DY	107	ASP	9.3
38	BS	44	LYS	8.2

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

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
24	UAL	AU	5	9/10	0.65	0.51	-	149,151,153,154	0
24	DPP	AU	2	6/7	0.64	0.32	-	153,153,154,154	0
24	KBE	AU	1	9/10	0.81	0.34	-	154,155,156,156	0
24	KBE	CU	1	9/10	0.86	0.34	-	69,74,77,77	0
24	DPP	CU	2	6/7	0.83	0.21	-	77,79,80,82	0
24	5OH	AU	6	12/13	0.81	0.50	-	151,153,154,154	0
24	5OH	CU	6	12/13	0.75	0.42	-	84,88,89,89	0
24	UAL	CU	5	9/10	0.88	0.39	-	89,90,91,91	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
61	FUA	AY	701	37/37	0.82	0.47	4.41	154,155,156,156	0
62	GDP	AY	702	28/28	0.80	0.27	2.86	78,82,83,84	0
62	GDP	CY	702	28/28	0.74	0.36	2.18	78,82,83,84	0
61	FUA	CY	701	37/37	0.52	0.62	1.23	199,200,202,202	0
63	MG	BA	2901	1/1	0.89	0.14	-0.38	5,5,5,5	0
63	MG	CY	703	1/1	0.98	0.08	-	1,1,1,1	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.