



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:04 am GMT

PDB ID : 4V9J
Title : 70S ribosome translocation intermediate GDPNP-II containing elongation factor EFG/GDPNP, mRNA, and tRNA bound in the pe^*/E state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-23
Resolution : 3.86 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28972

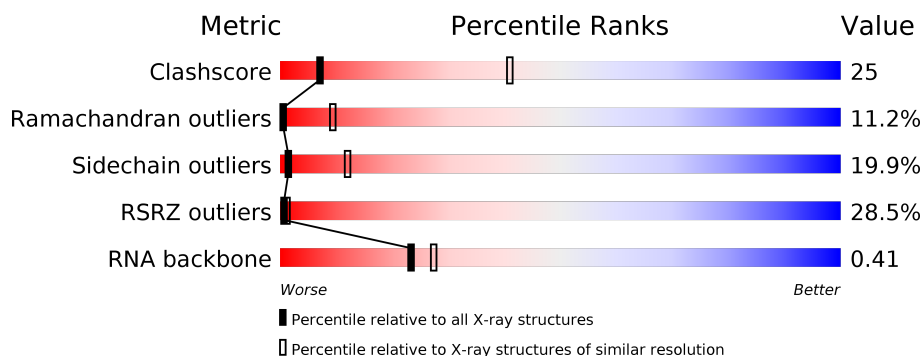
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.86 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))
Clashscore	112137	1029 (4.12-3.60)
Ramachandran outliers	110173	1017 (4.14-3.58)
Sidechain outliers	110143	1010 (4.14-3.58)
RSRZ outliers	101464	1023 (4.16-3.56)
RNA backbone	2435	1017 (4.76-2.90)

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

Mol	Chain	Length	Quality of chain
1	AB	235	<div> <div>24%</div> <div>36%</div> <div>46%</div> <div>15%</div> <div>•</div> </div>
1	CB	235	<div> <div>23%</div> <div>36%</div> <div>48%</div> <div>14%</div> <div>•</div> </div>
2	AC	207	<div> <div>26%</div> <div>40%</div> <div>46%</div> <div>14%</div> </div>
2	CC	207	<div> <div>33%</div> <div>40%</div> <div>44%</div> <div>15%</div> <div>•</div> </div>
3	AD	208	<div> <div>61%</div> <div>36%</div> <div>49%</div> <div>15%</div> <div>•</div> </div>
3	CD	208	<div> <div>61%</div> <div>36%</div> <div>50%</div> <div>12%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
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	
15	CP	84	
16	AQ	100	

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Mol	Chain	Length	Quality of chain
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	AV	18	
21	CV	18	
22	AW	77	
22	CW	77	
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	
28	BF	208	
28	DF	208	

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Mol	Chain	Length	Quality of chain
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	BO	122	
33	DO	122	
34	BP	146	
34	DP	146	
35	BQ	141	
35	DQ	141	
36	BR	117	
36	DR	117	
37	BS	99	
37	DS	99	
38	BT	138	
38	DT	138	
39	BU	117	
39	DU	117	
40	BV	101	
40	DV	101	
41	BW	113	

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Mol	Chain	Length	Quality of chain
41	DW	113	
42	BX	93	
42	DX	93	
43	BY	107	
43	DY	107	
44	BZ	185	
44	DZ	185	
45	B0	84	
45	D0	84	
46	B1	93	
46	D1	93	
47	B4	35	
47	D4	35	
48	BN	138	
48	DN	138	
49	B2	71	
49	D2	71	
50	B3	60	
50	D3	60	
51	B5	59	
51	D5	59	
52	B6	50	
52	D6	50	
53	B7	49	
53	D7	49	

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Mol	Chain	Length	Quality of chain
54	B8	64	
54	D8	64	
55	B9	37	
55	D9	37	
56	Be	103	
56	De	103	
57	Bf	31	
57	Bg	31	
57	Df	31	
57	Dg	31	
58	Bh	30	
58	Dh	30	
59	BB	119	
59	DB	119	
60	BA	2879	
60	DA	2879	

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
24	DPP	AU	2	-	-	X	-
24	5OH	AU	6	-	-	X	-
24	5OH	CU	6	-	-	X	-
61	GNP	CY	702	-	-	X	-

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 308202 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
			1011	639	198	174			
8	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	156	143	2			
16	CQ	100	Total	C	N	O	S	0	0	0
			835	534	156	143	2			

- 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
			762	469	162	129	2			
19	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

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

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 messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	18	Total	C	N	O	P	0	0	0
			393	177	81	118	17			
21	CV	18	Total	C	N	O	P	0	0	0
			393	177	81	118	17			

- Molecule 22 is a RNA chain called tRNA-Met.

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

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AY	687	Total	C	N	O	S	0	0	0
			5380	3414	922	1024	20			
23	CY	687	Total	C	N	O	S	0	0	0
			5380	3414	922	1024	20			

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
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 L14.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			
46	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 47 is a protein called 50S ribosomal protein L31.

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

- Molecule 48 is a protein called 50S ribosomal protein L13.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

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

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

- Molecule 57 is a protein called 50S ribosomal protein L7/L12.

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

- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

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

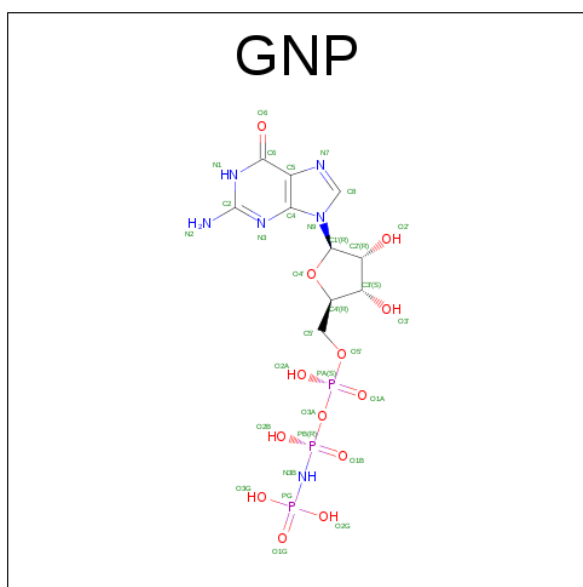
- Molecule 59 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 60 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 61 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



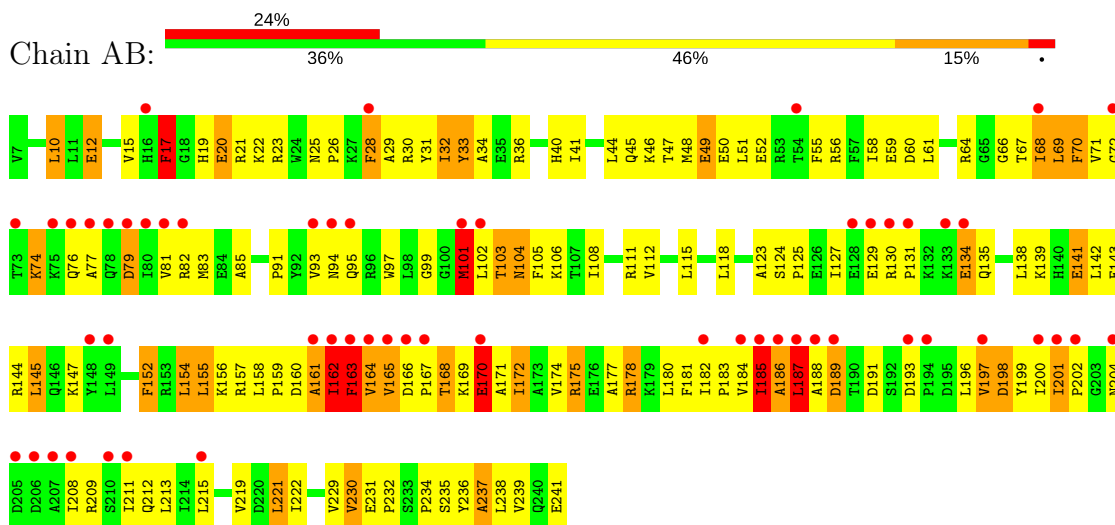
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CY	1	Total	Mg	0	0
			1	1		

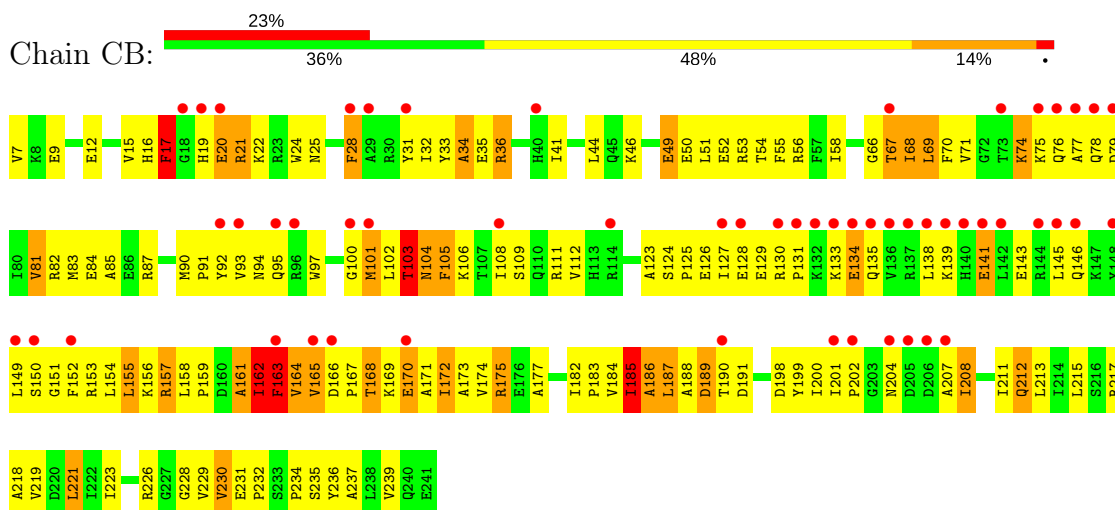
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 30S ribosomal protein S2

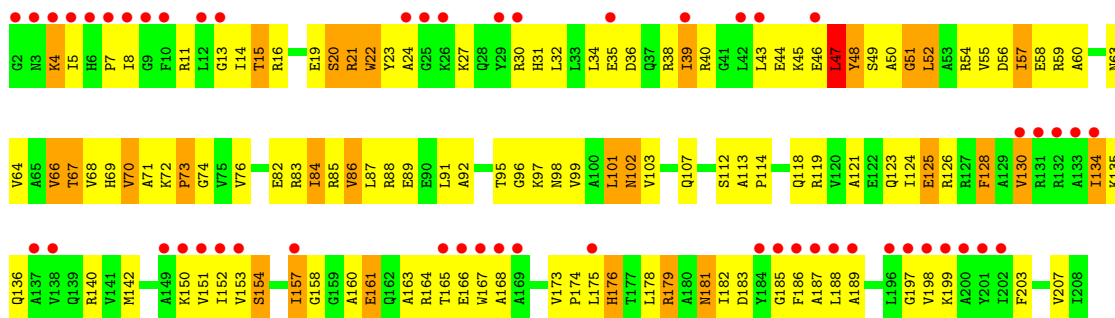


• Molecule 1: 30S ribosomal protein S2

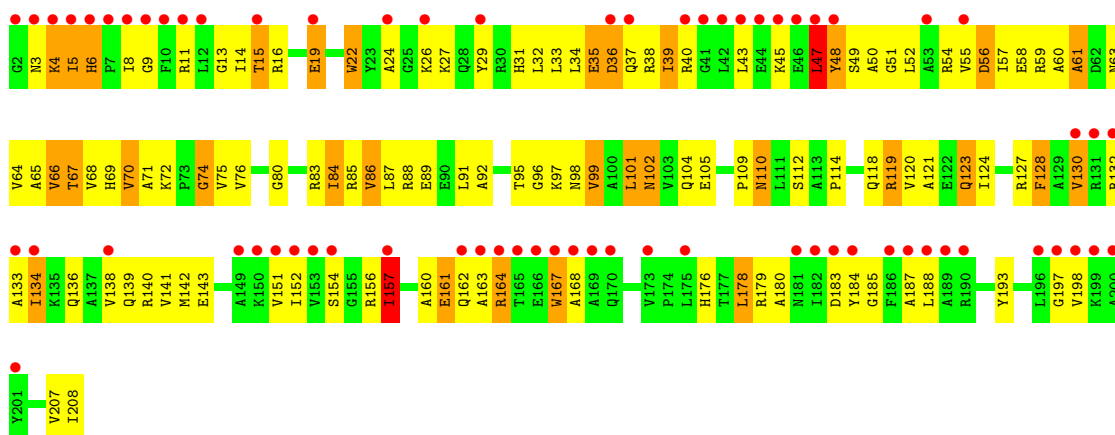


• Molecule 2: 30S ribosomal protein S3

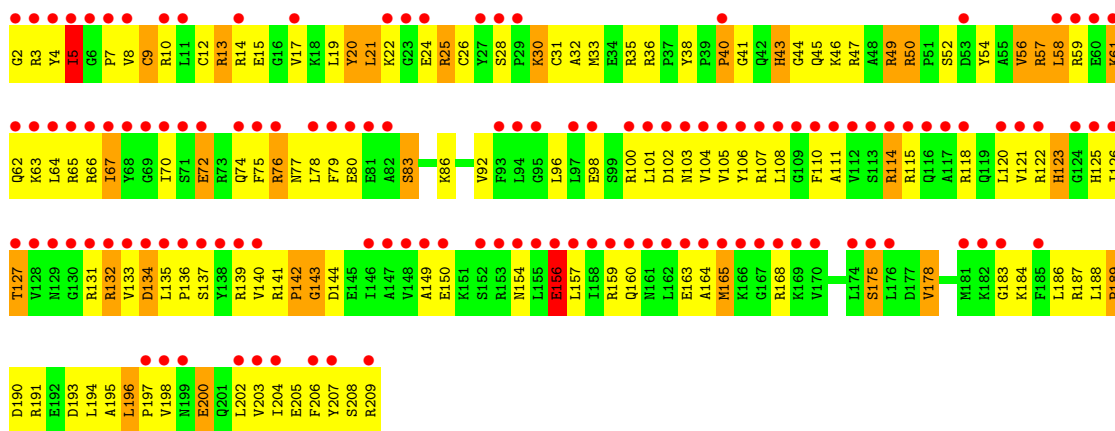




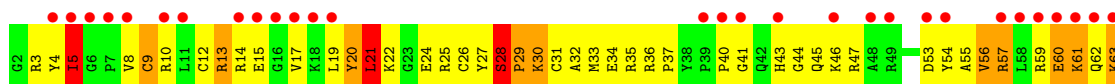
• Molecule 2: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S4

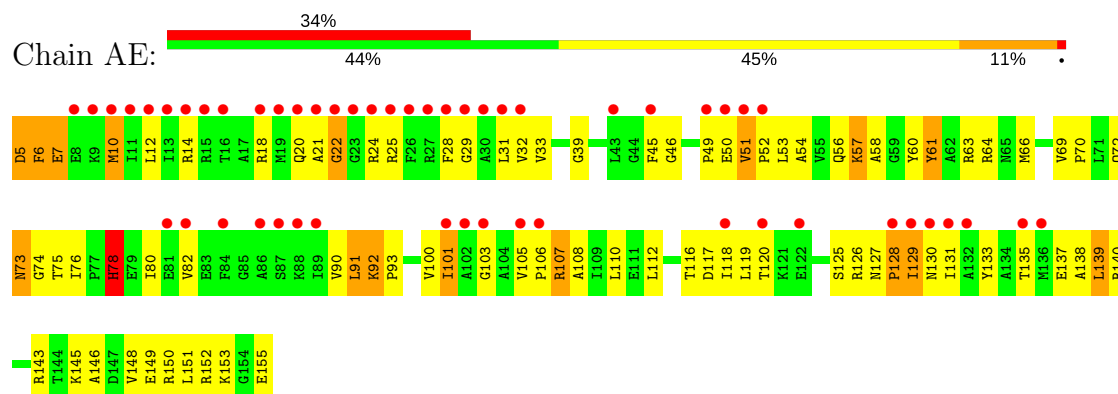


• Molecule 3: 30S ribosomal protein S4

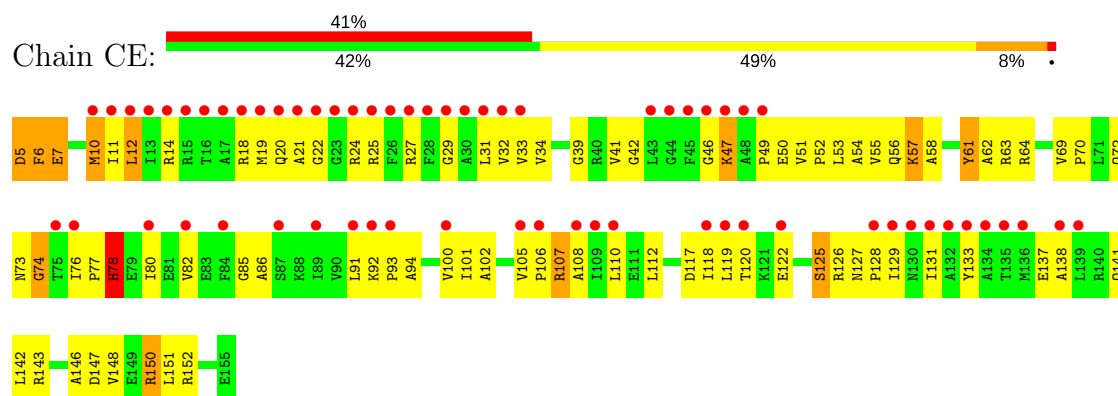




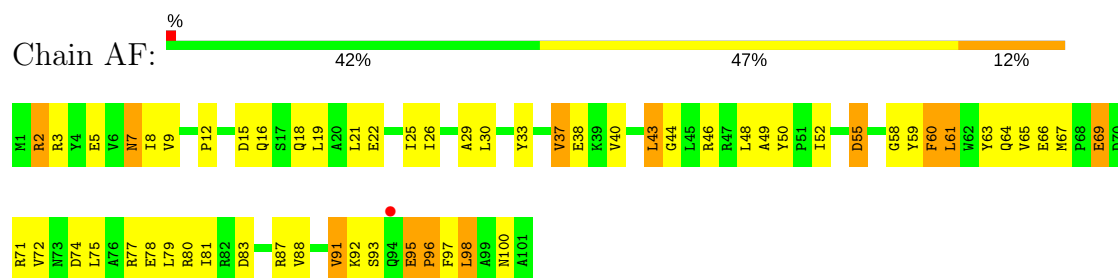
• Molecule 4: 30S ribosomal protein S5



• Molecule 4: 30S ribosomal protein S5

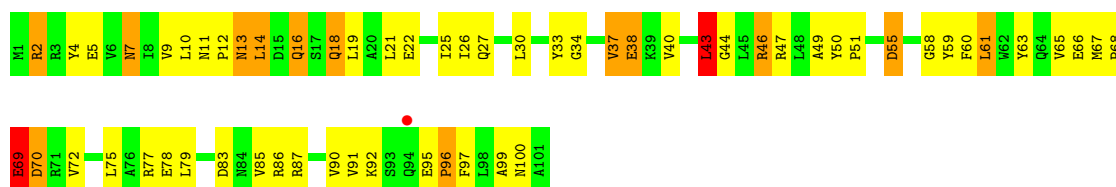


• Molecule 5: 30S ribosomal protein S6

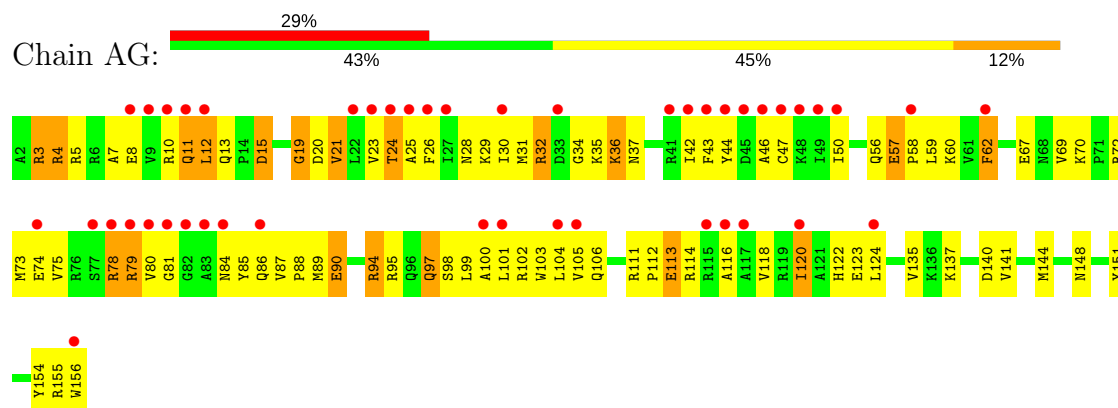


• Molecule 5: 30S ribosomal protein S6

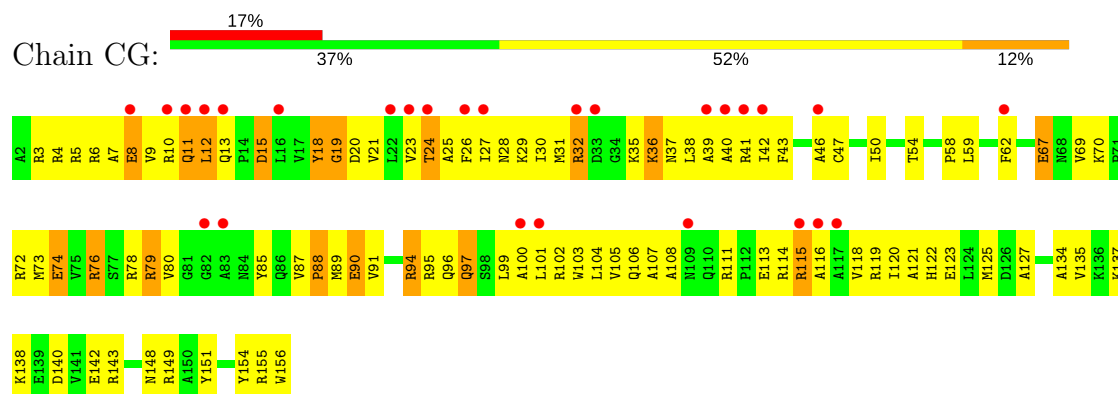




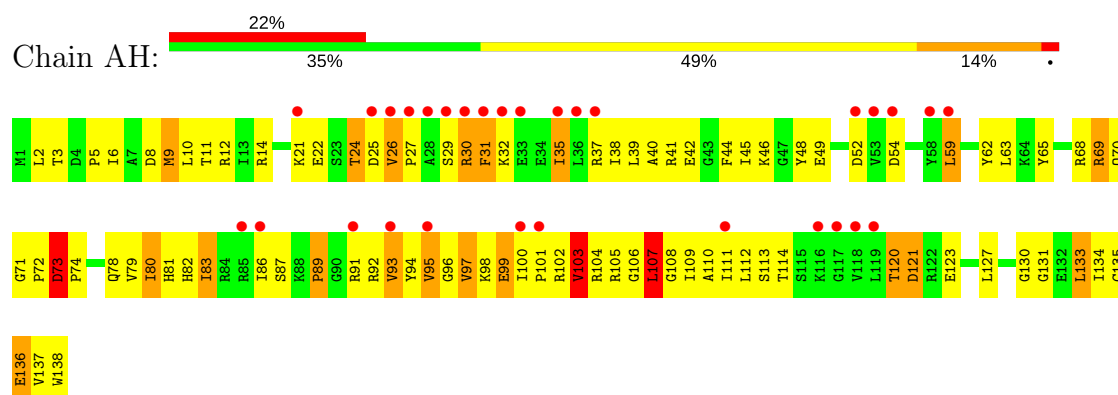
• Molecule 6: 30S ribosomal protein S7



• Molecule 6: 30S ribosomal protein S7

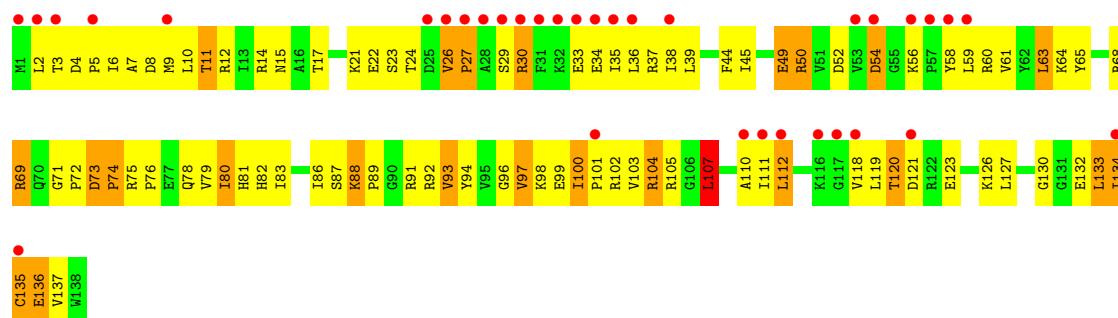


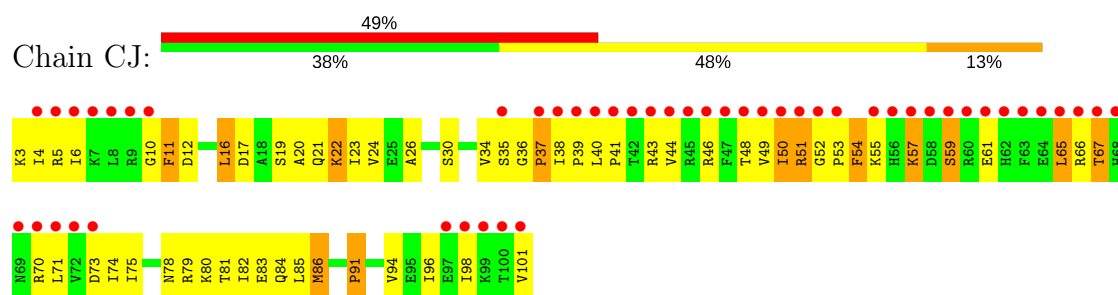
• Molecule 7: 30S ribosomal protein S8



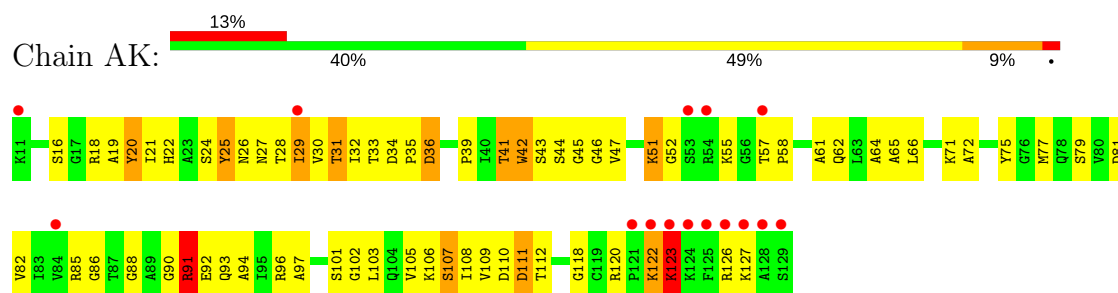
• Molecule 7: 30S ribosomal protein S8



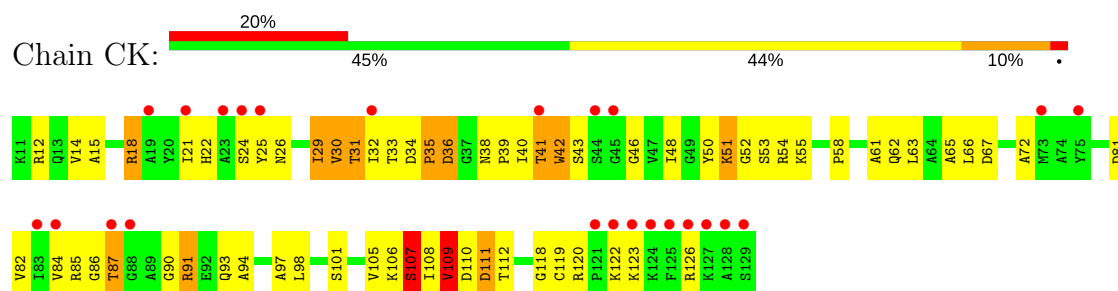




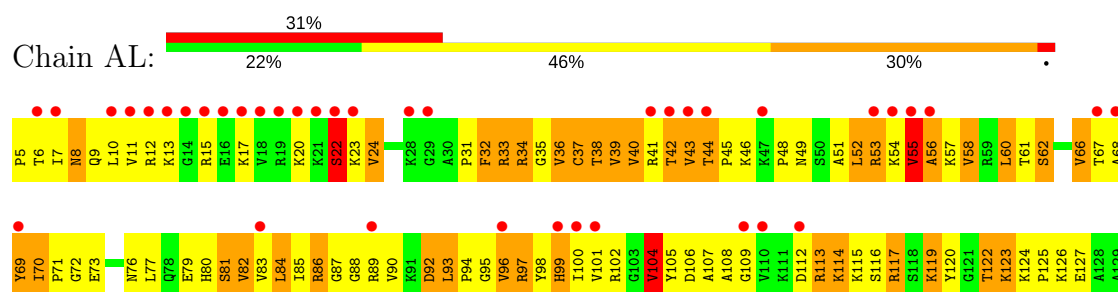
- Molecule 10: 30S ribosomal protein S11



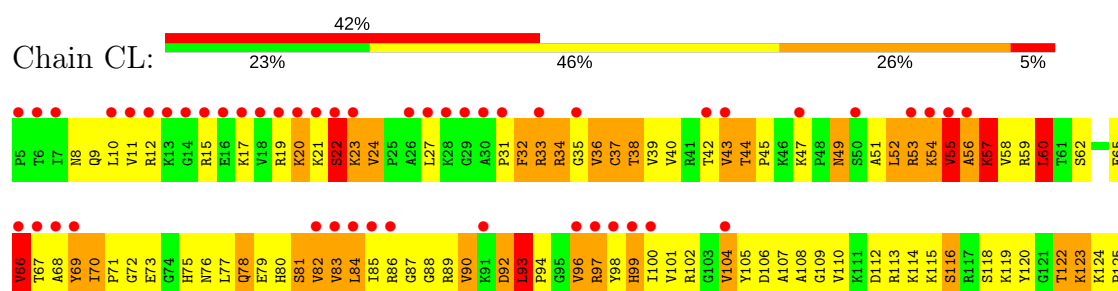
- Molecule 10: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S12

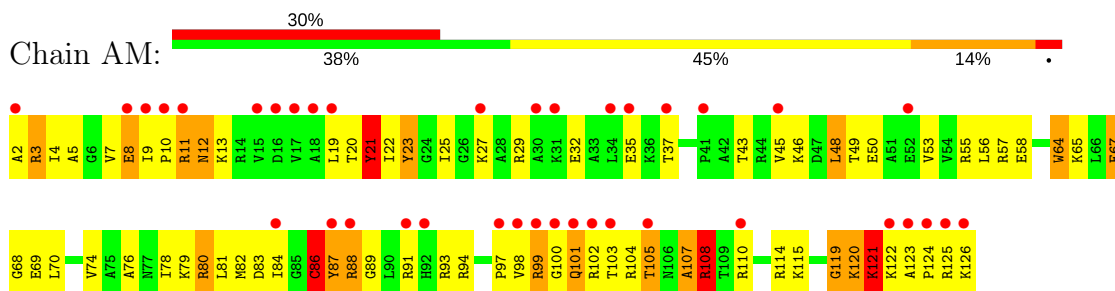


- Molecule 11: 30S ribosomal protein S12

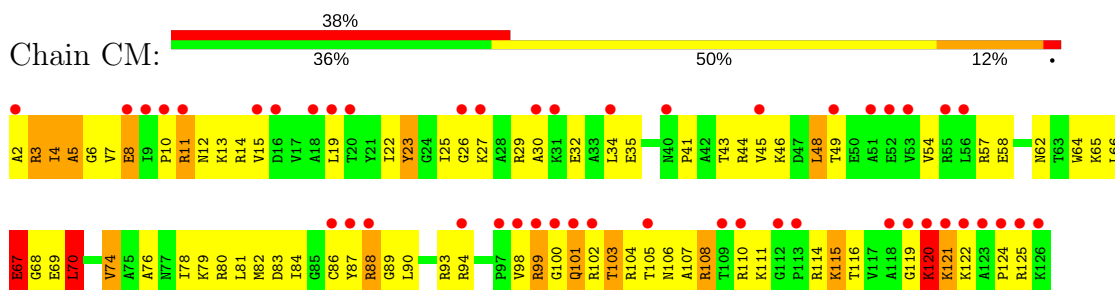




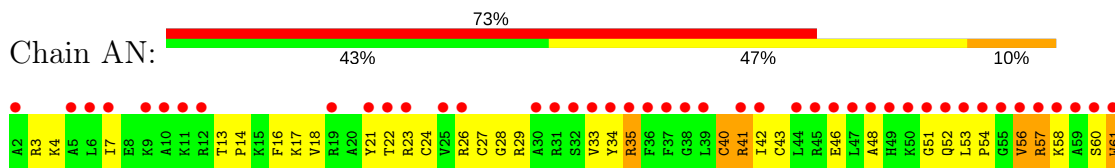
- Molecule 12: 30S ribosomal protein S13



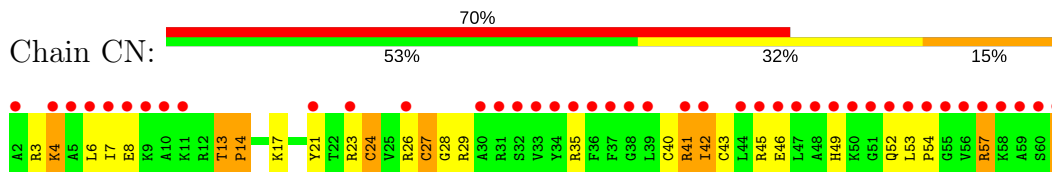
- Molecule 12: 30S ribosomal protein S13



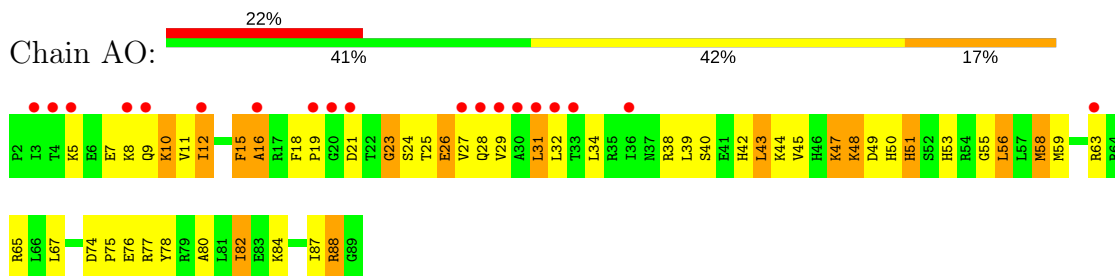
- Molecule 13: 30S ribosomal protein S14 type Z



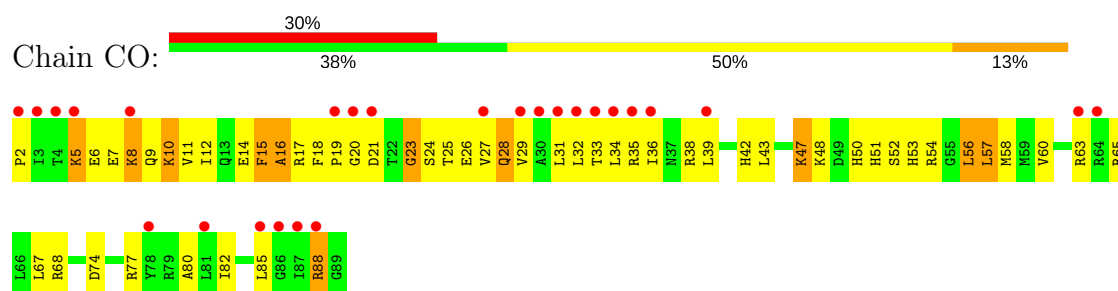
- Molecule 13: 30S ribosomal protein S14 type Z



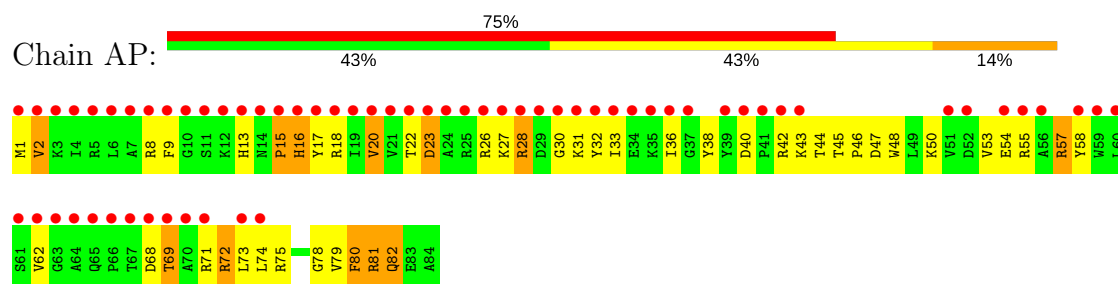
- Molecule 14: 30S ribosomal protein S15



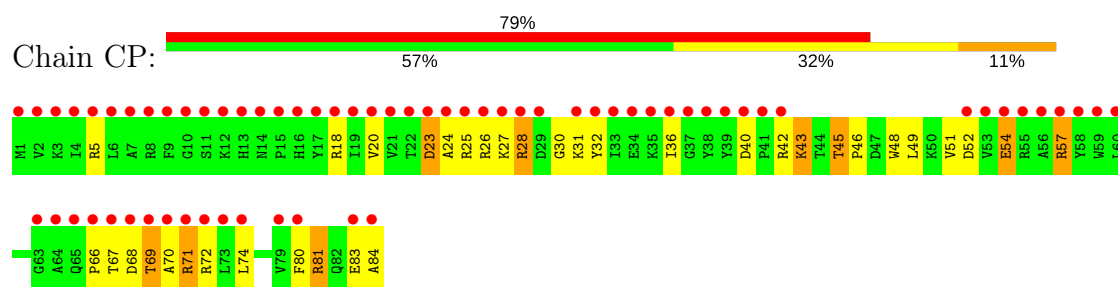
- Molecule 14: 30S ribosomal protein S15



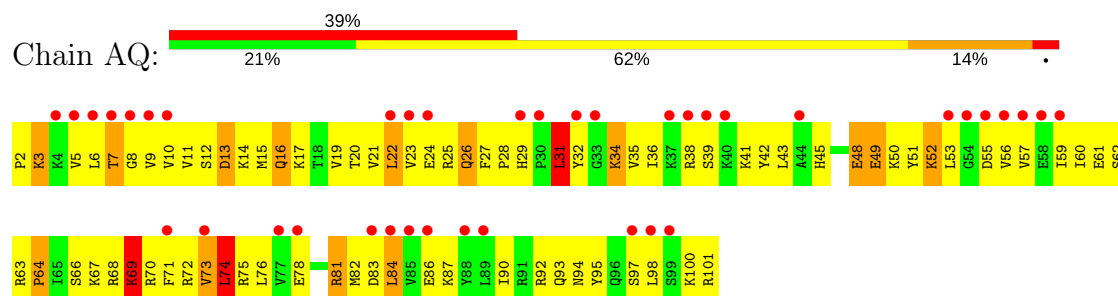
• Molecule 15: 30S ribosomal protein S16



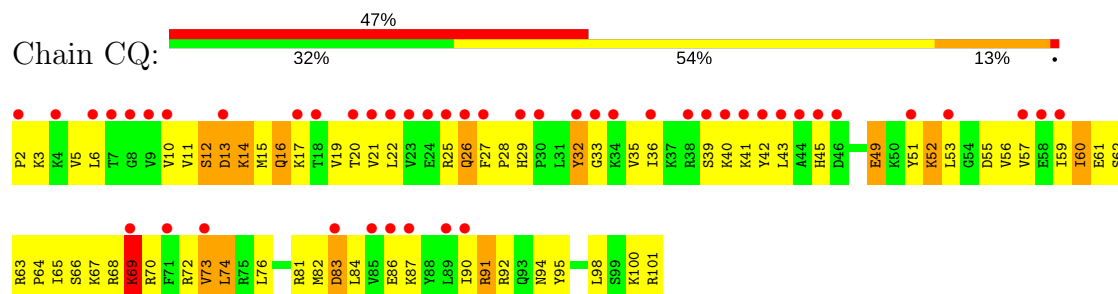
• Molecule 15: 30S ribosomal protein S16



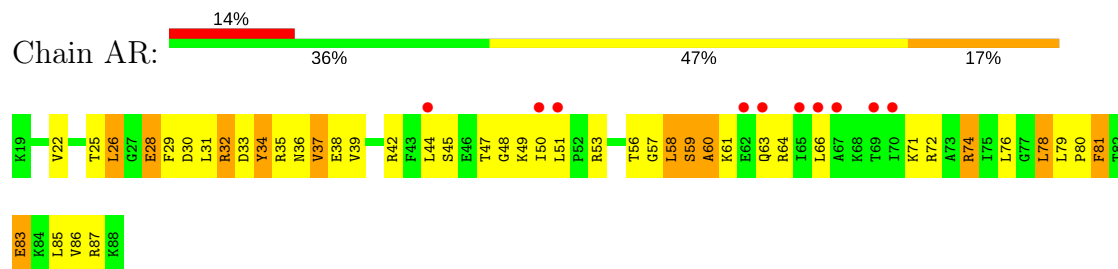
• Molecule 16: 30S ribosomal protein S17



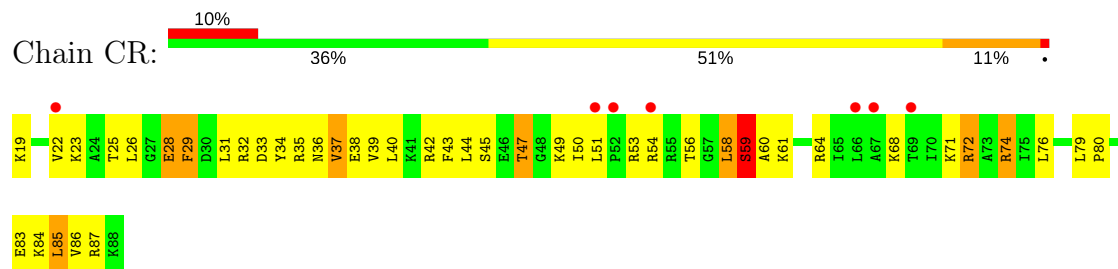
• Molecule 16: 30S ribosomal protein S17



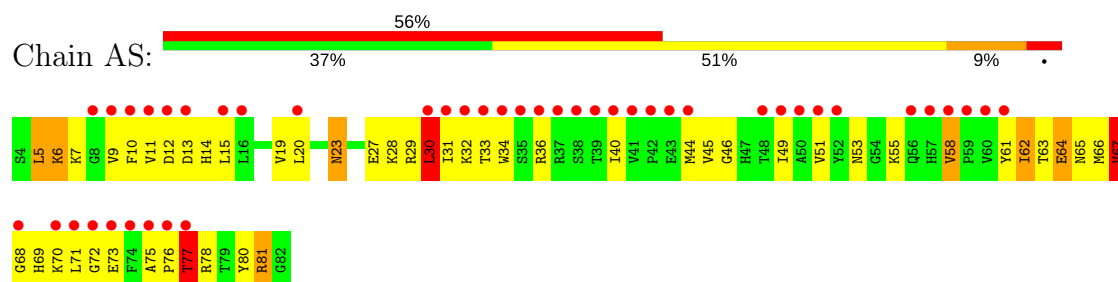
- Molecule 17: 30S ribosomal protein S18



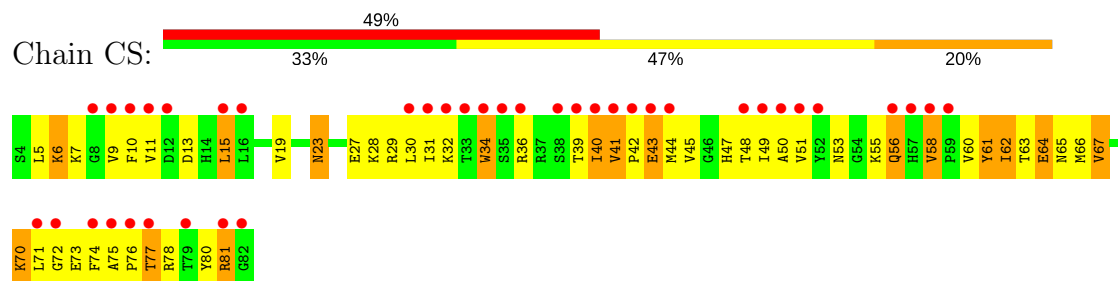
- Molecule 17: 30S ribosomal protein S18



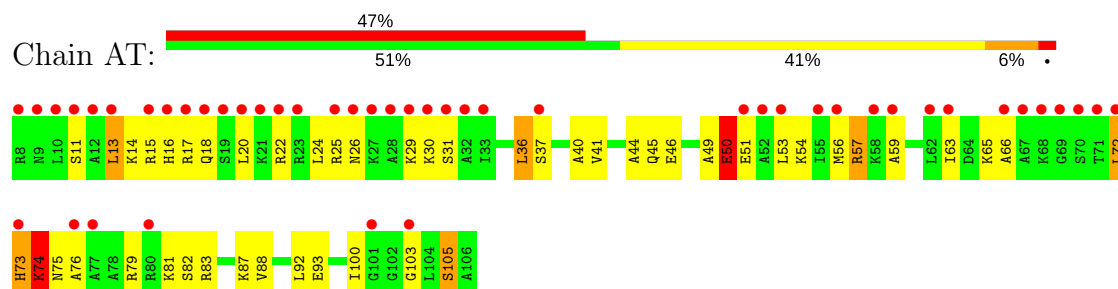
- Molecule 18: 30S ribosomal protein S19



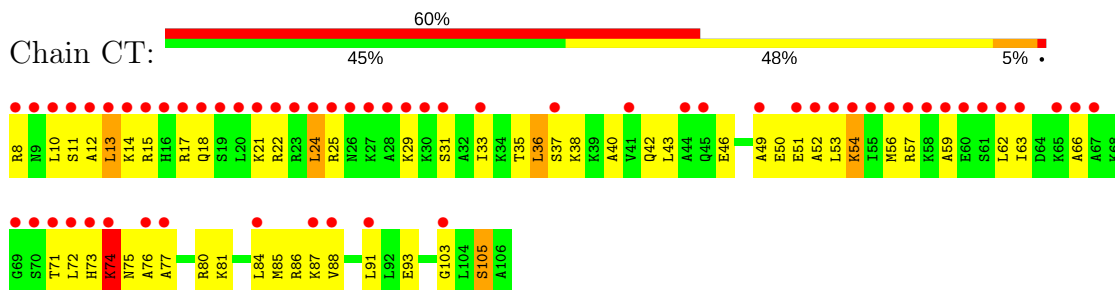
- Molecule 18: 30S ribosomal protein S19



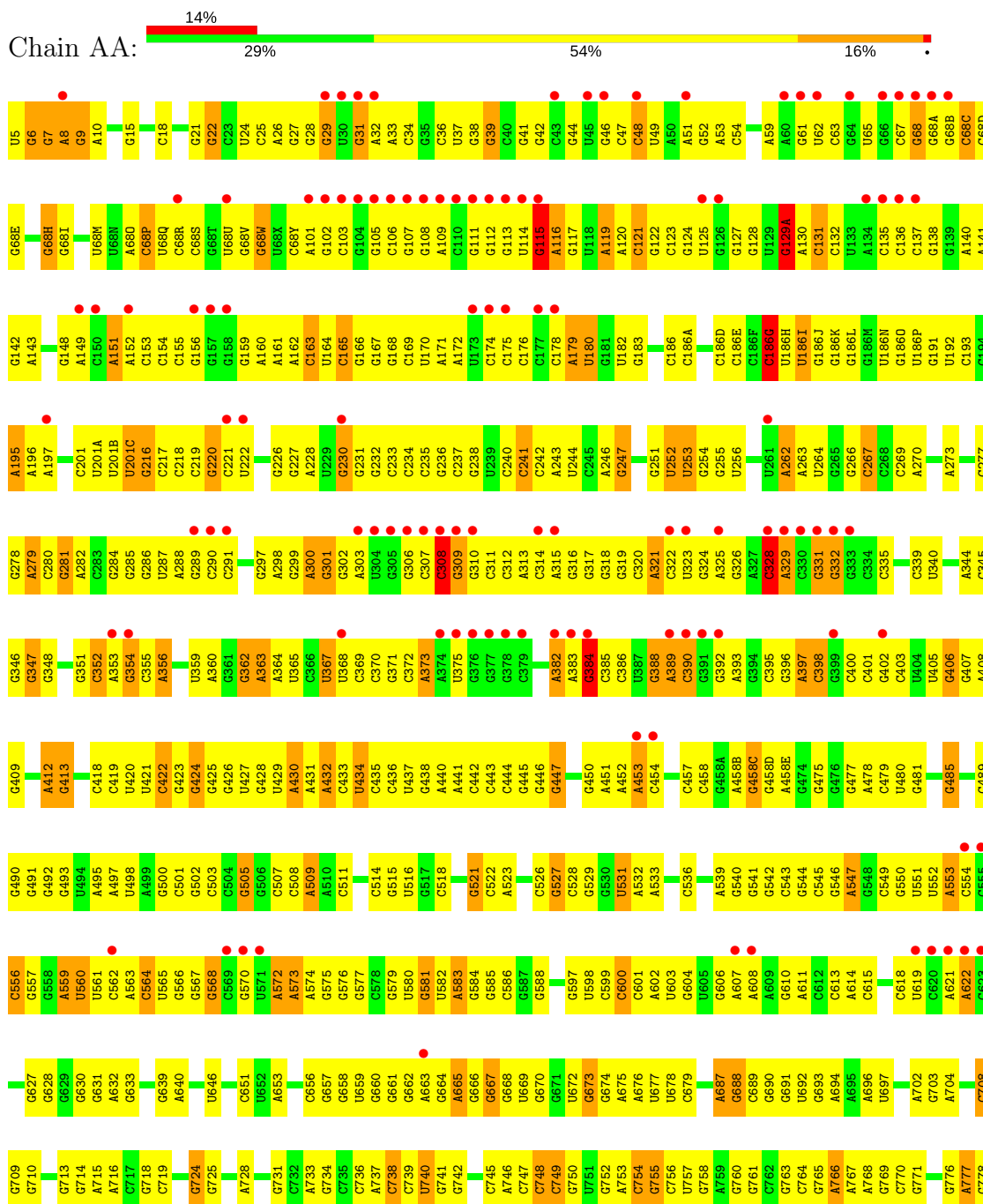
- Molecule 19: 30S ribosomal protein S20

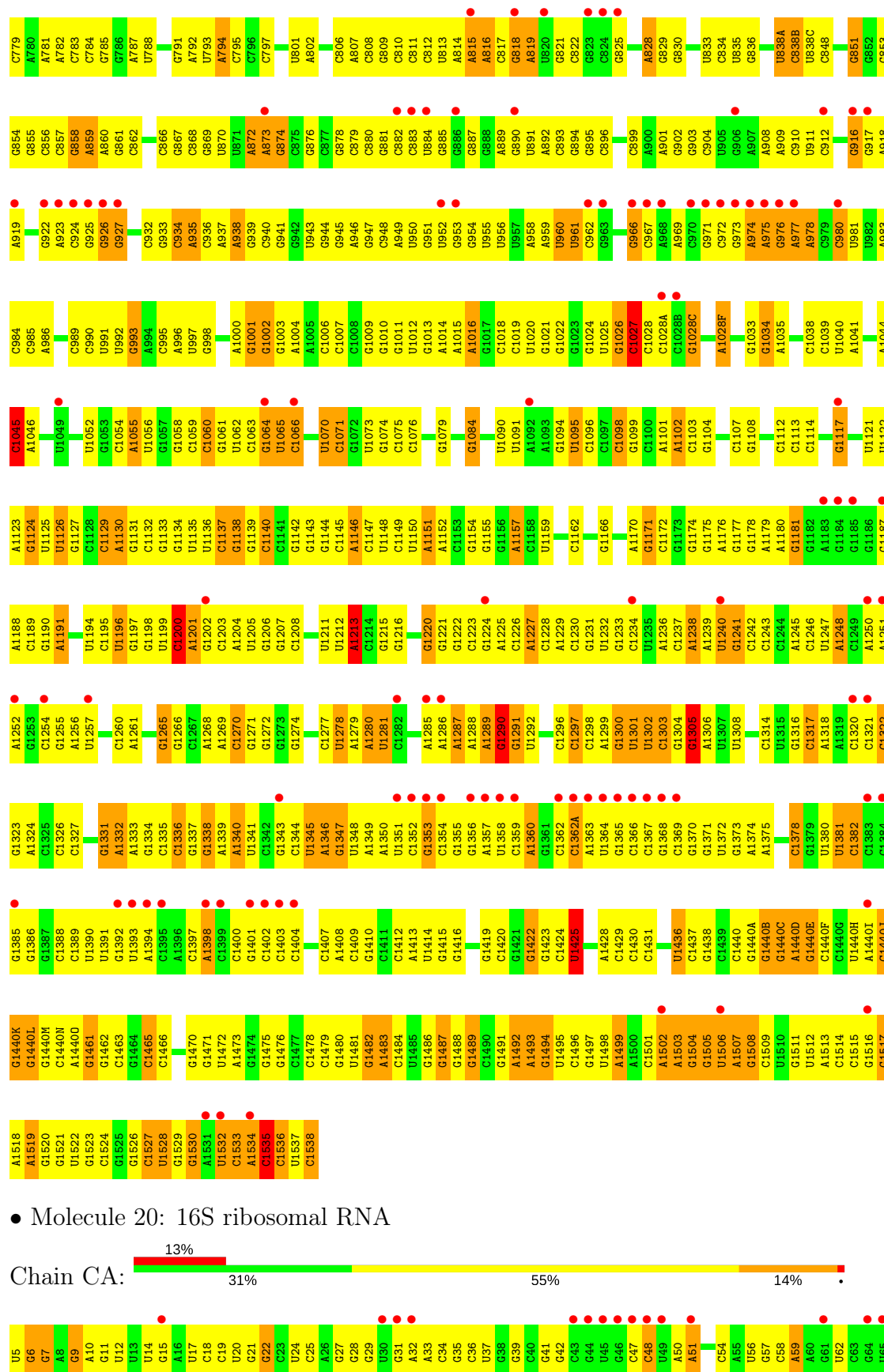


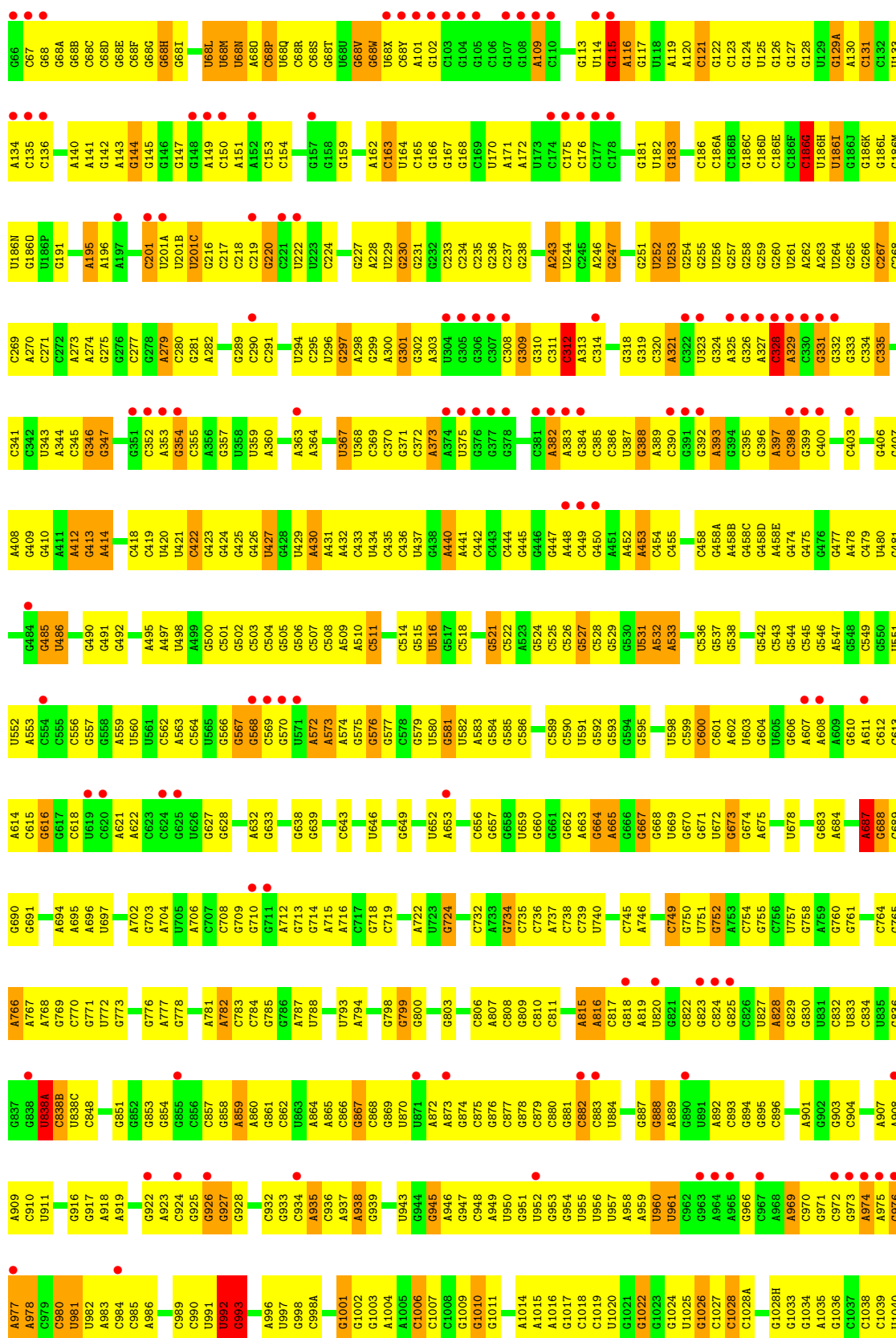
• Molecule 19: 30S ribosomal protein S20



• Molecule 20: 16S ribosomal RNA







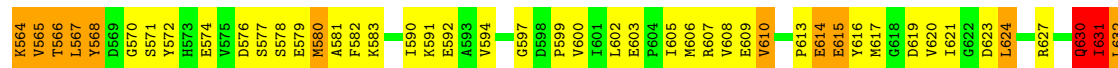
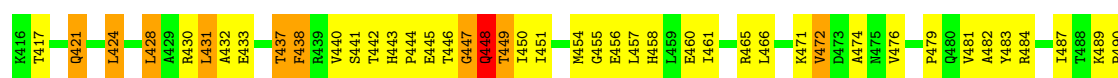
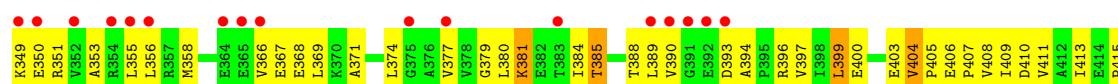
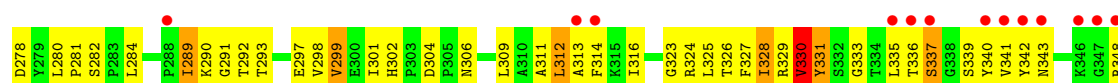
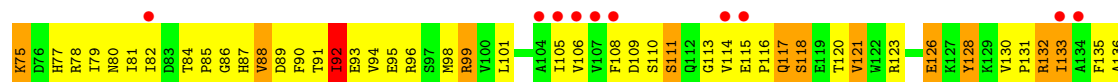
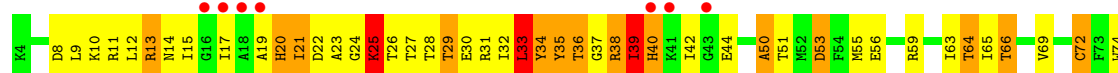




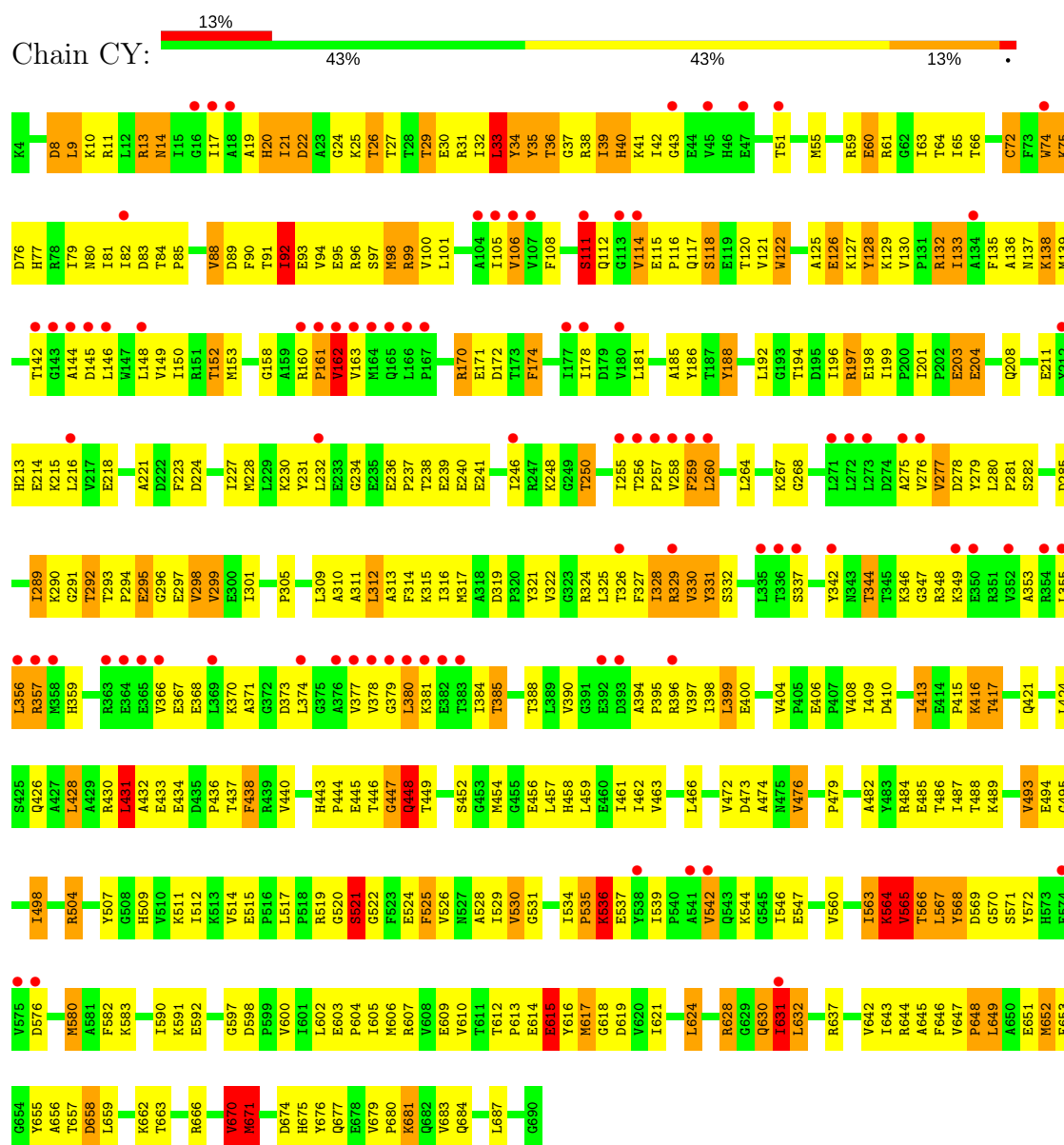
• Molecule 22: tRNA-Met



• Molecule 23: Elongation factor G



• Molecule 23: Elongation factor G



• Molecule 24: Viomycin

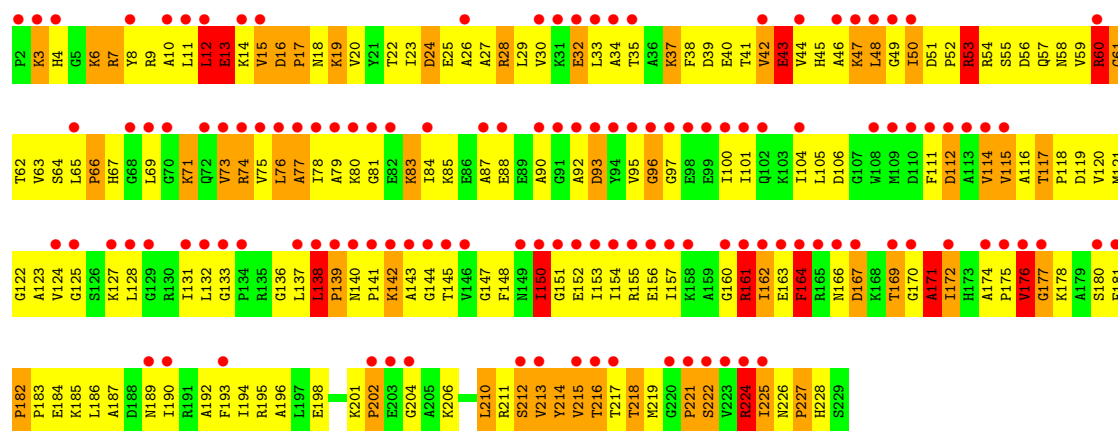


• Molecule 24: Viomycin

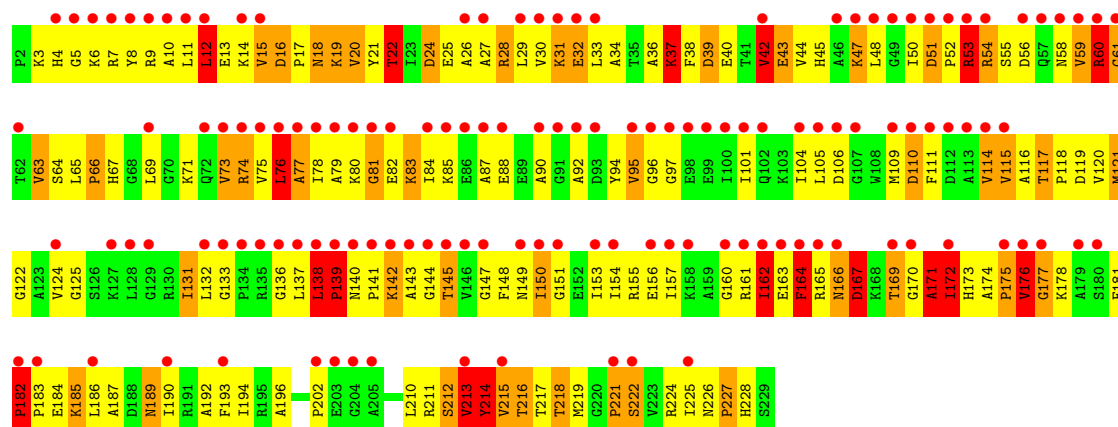


• Molecule 25: 50S ribosomal protein L1

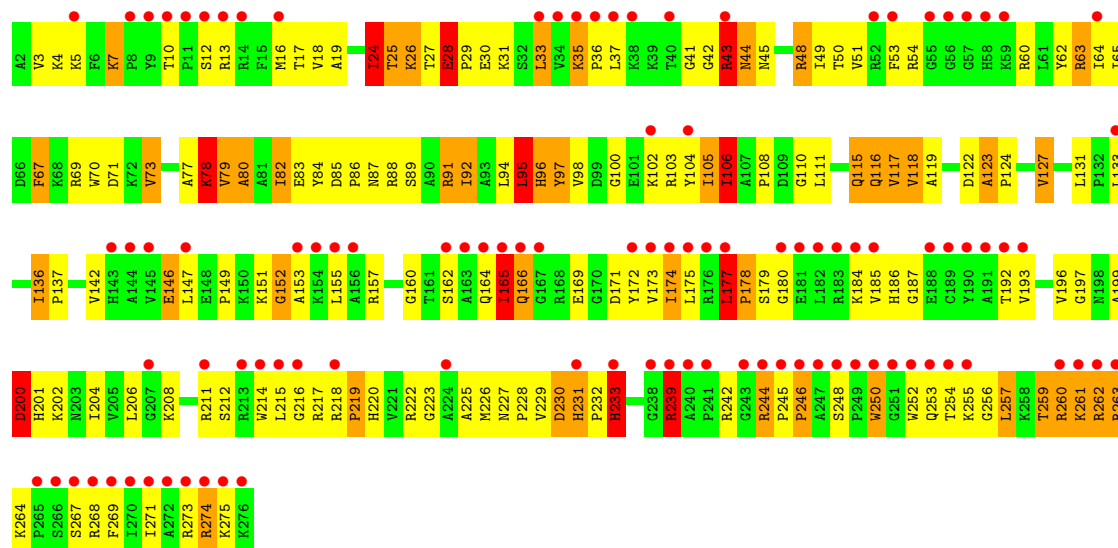
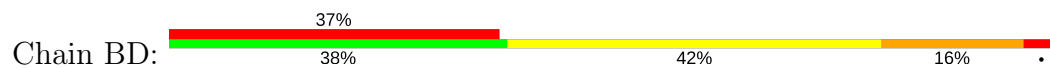


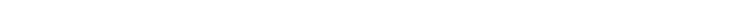


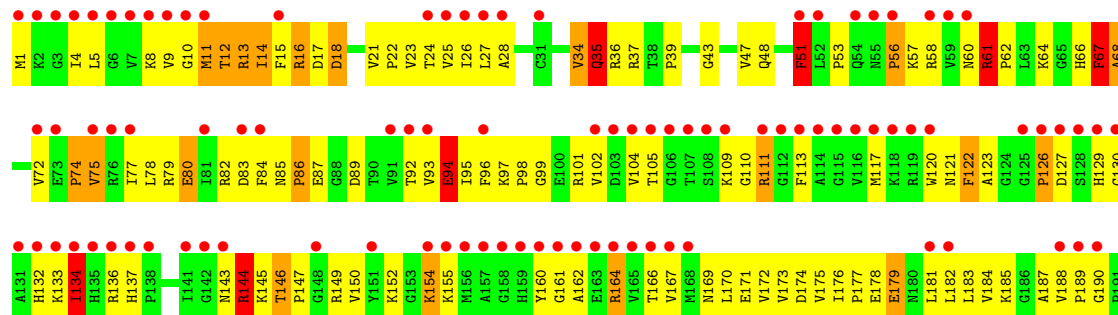
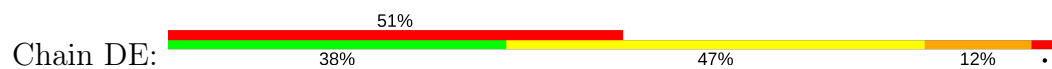
• Molecule 25: 50S ribosomal protein L1

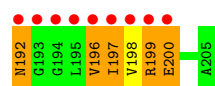


• Molecule 26: 50S ribosomal protein L2

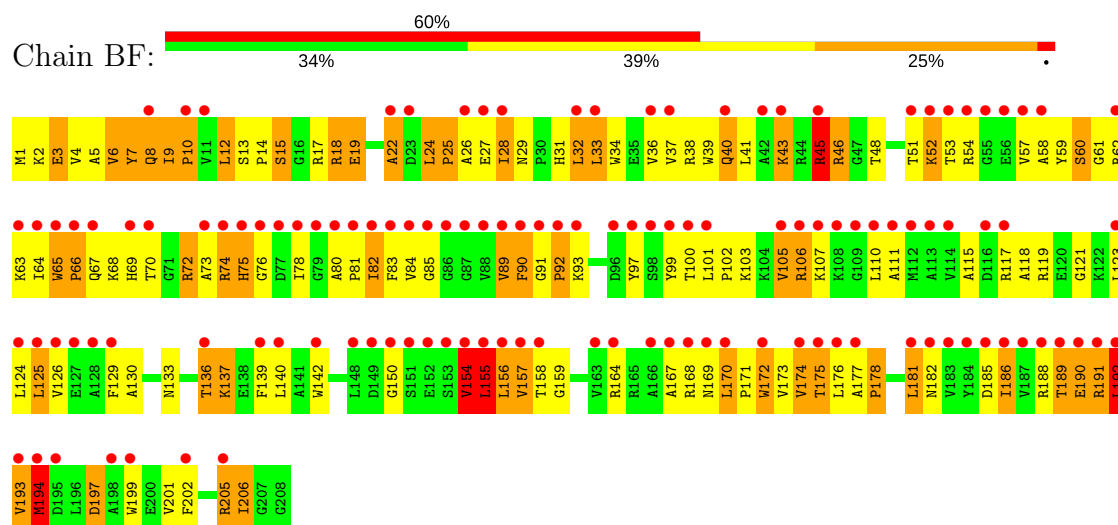


Chain DD: 

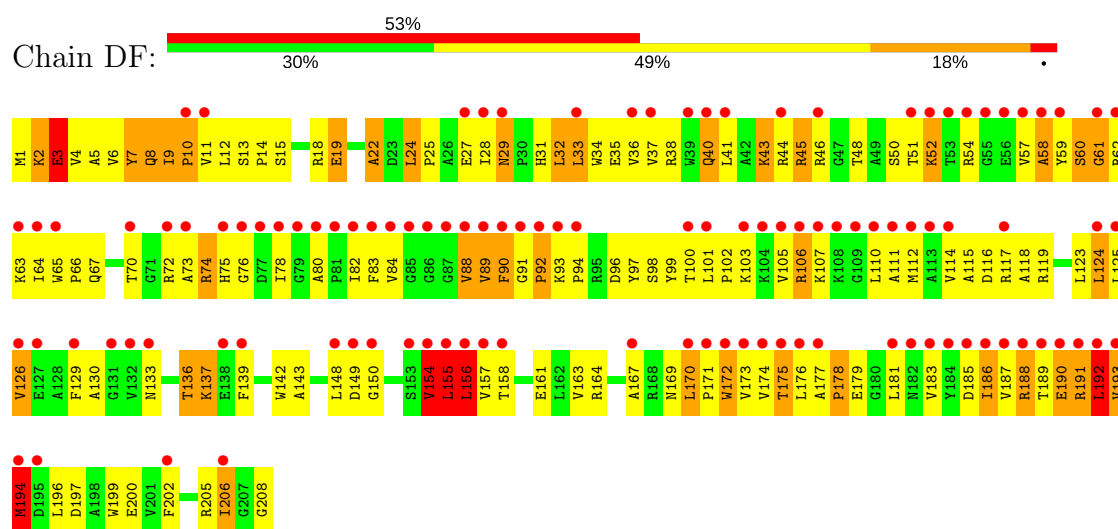




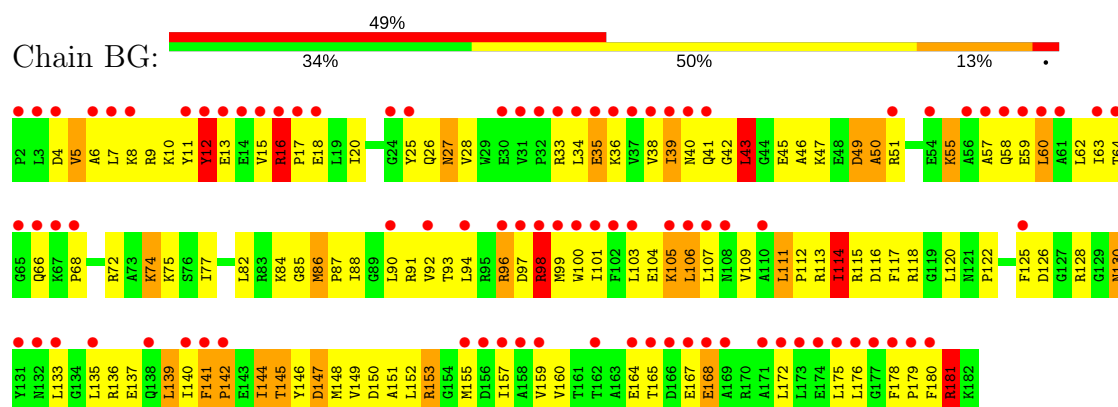
• Molecule 28: 50S ribosomal protein L4



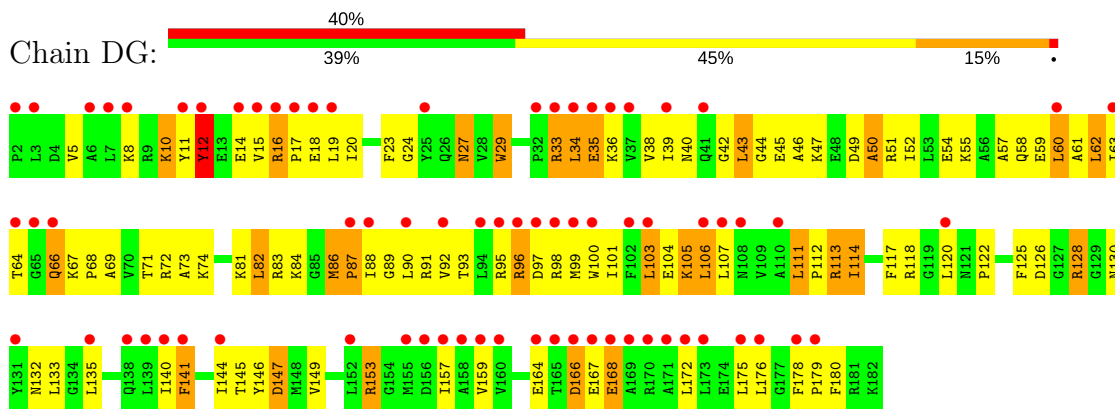
• Molecule 28: 50S ribosomal protein L4



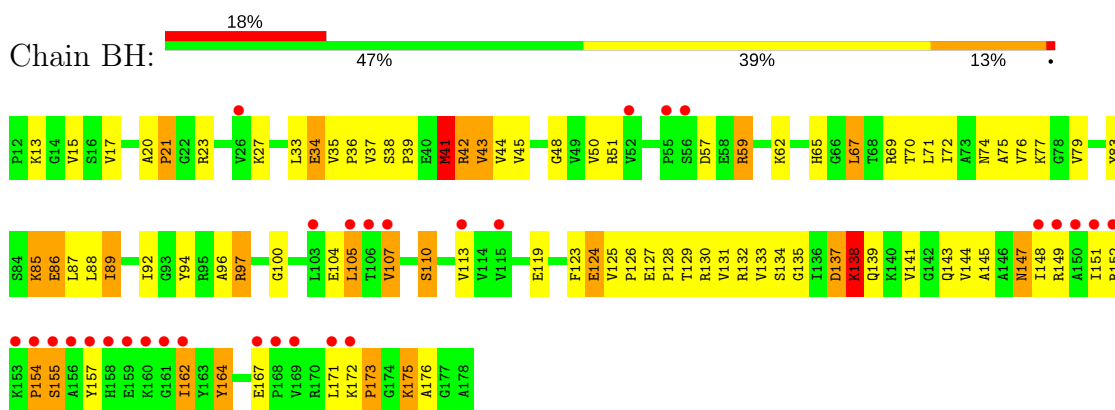
• Molecule 29: 50S ribosomal protein L5



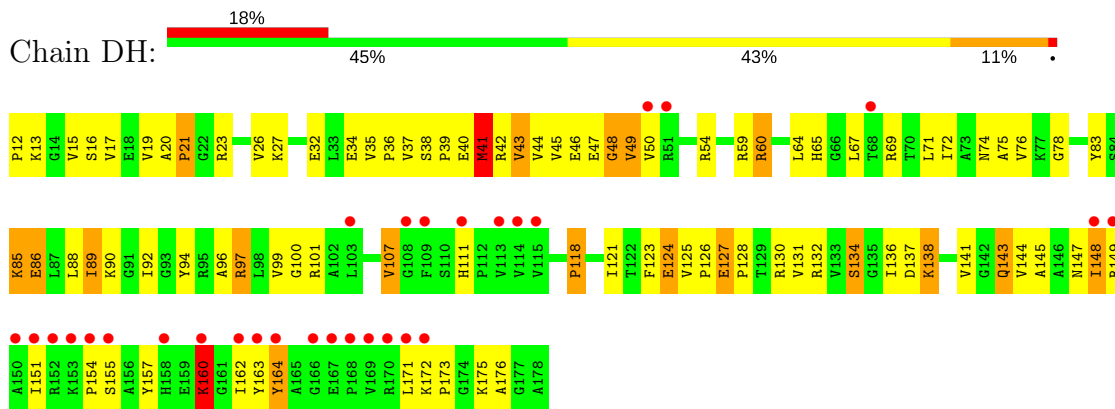
- Molecule 29: 50S ribosomal protein L5



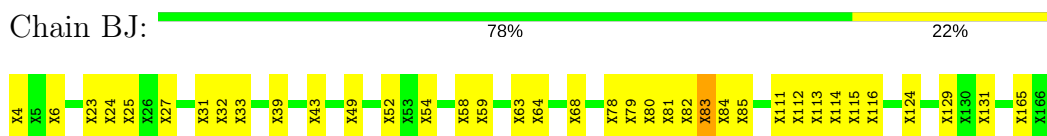
- Molecule 30: 50S ribosomal protein L6



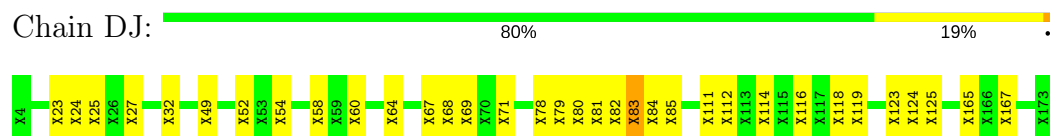
- Molecule 30: 50S ribosomal protein L6



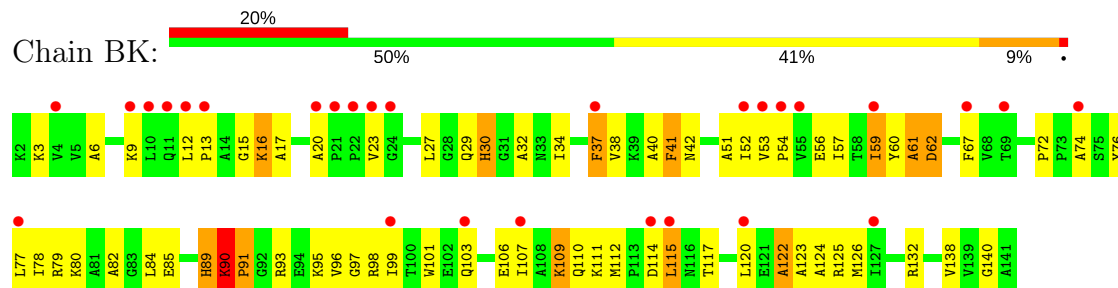
- Molecule 31: 50S ribosomal protein L10



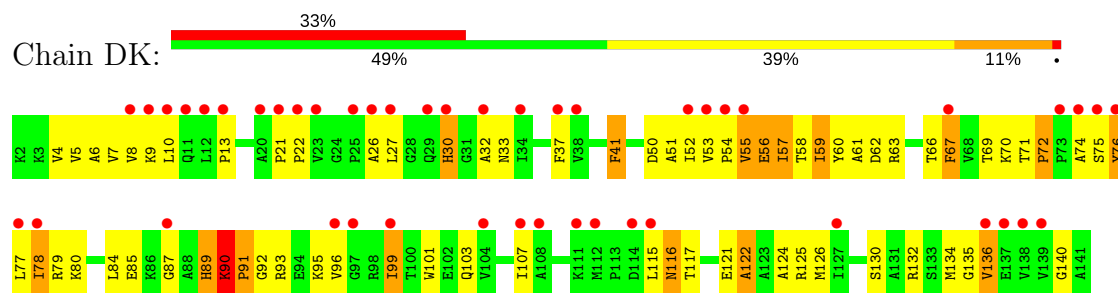
- Molecule 31: 50S ribosomal protein L10



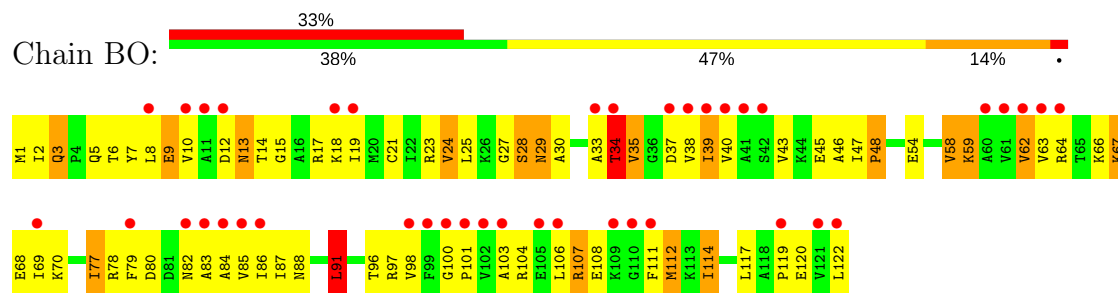
- Molecule 32: 50S ribosomal protein L11



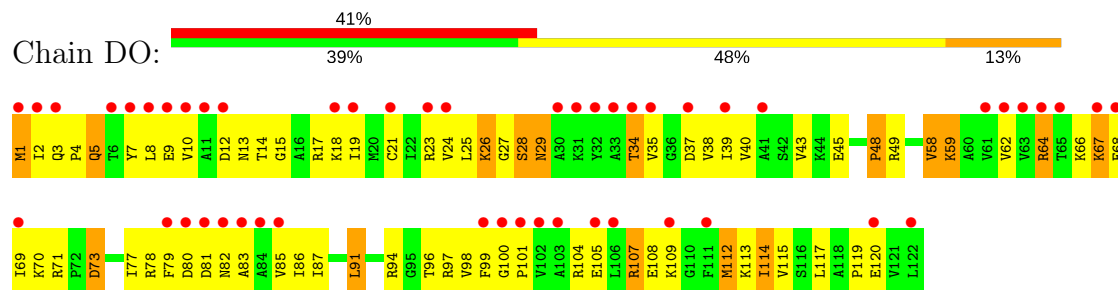
- Molecule 32: 50S ribosomal protein L11



- Molecule 33: 50S ribosomal protein L14

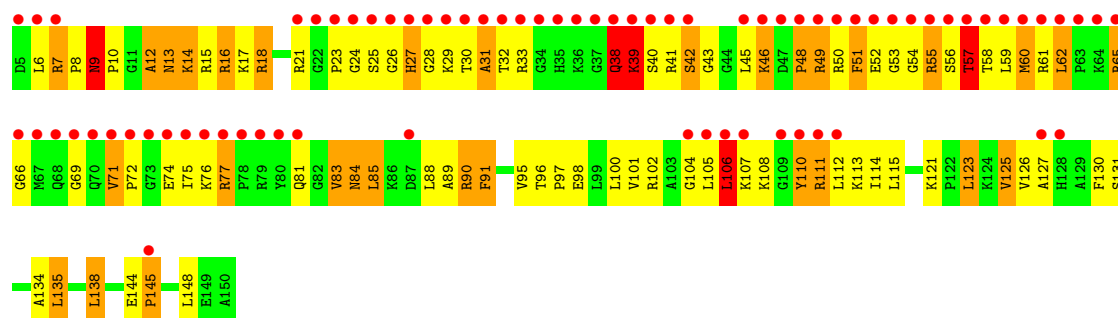


- Molecule 33: 50S ribosomal protein L14

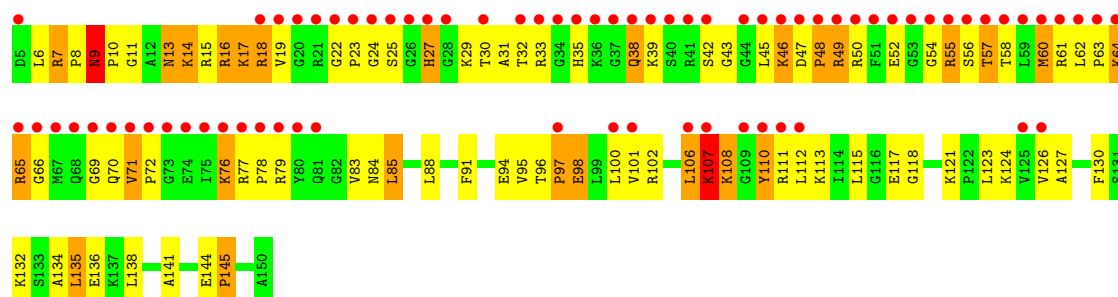


- Molecule 34: 50S ribosomal protein L15

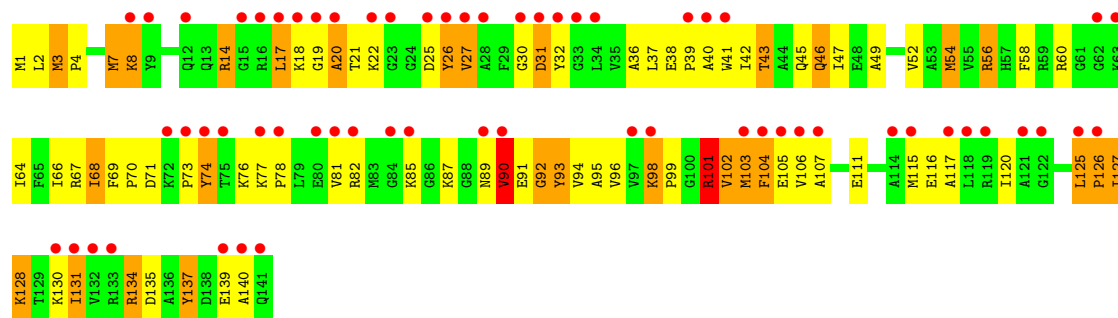
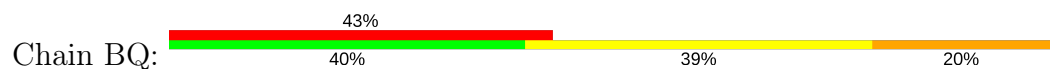




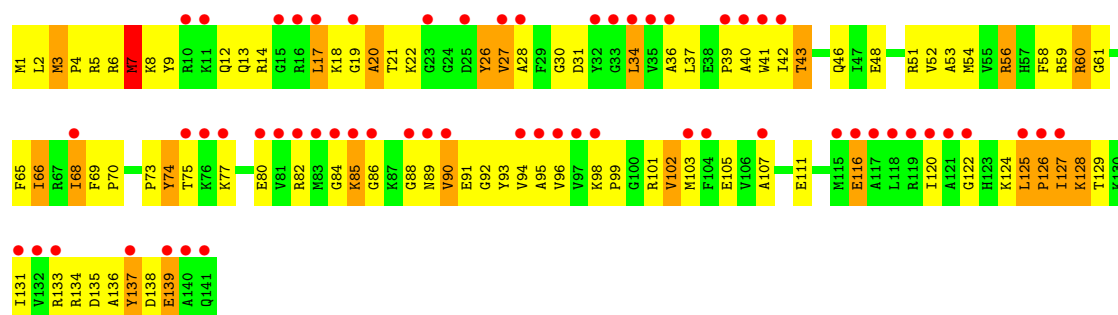
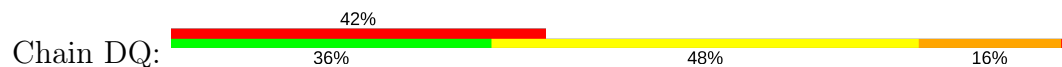
• Molecule 34: 50S ribosomal protein L15



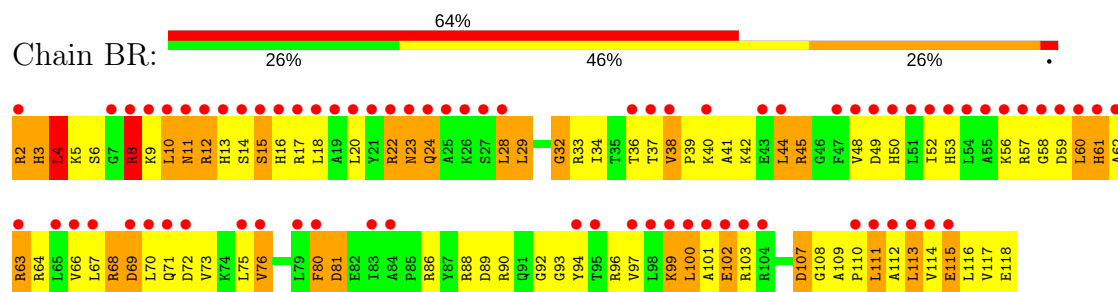
• Molecule 35: 50S ribosomal protein L16



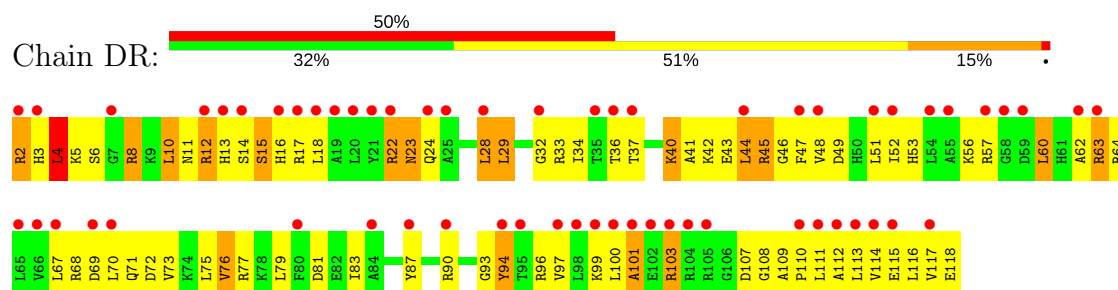
• Molecule 35: 50S ribosomal protein L16



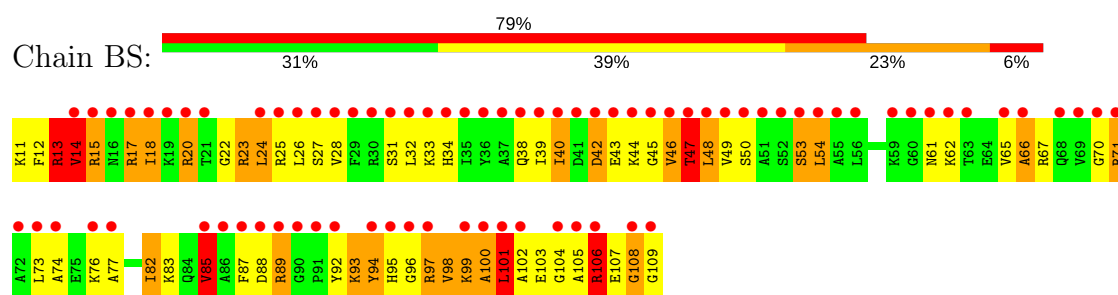
- Molecule 36: 50S ribosomal protein L17



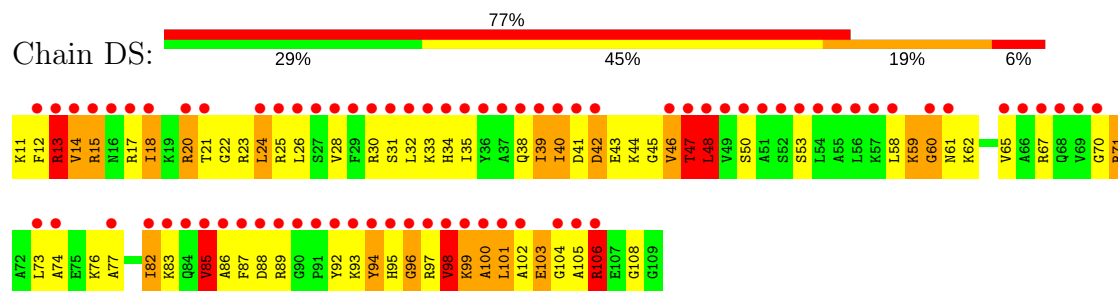
- Molecule 36: 50S ribosomal protein L17

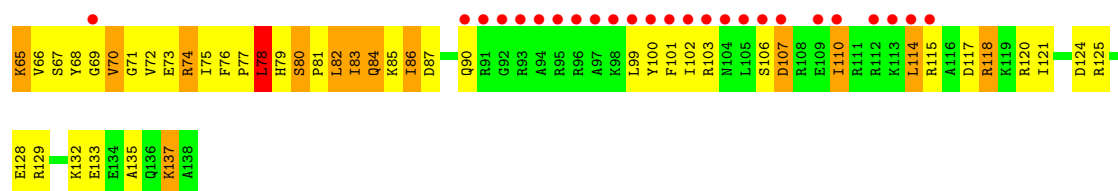


- Molecule 37: 50S ribosomal protein L18

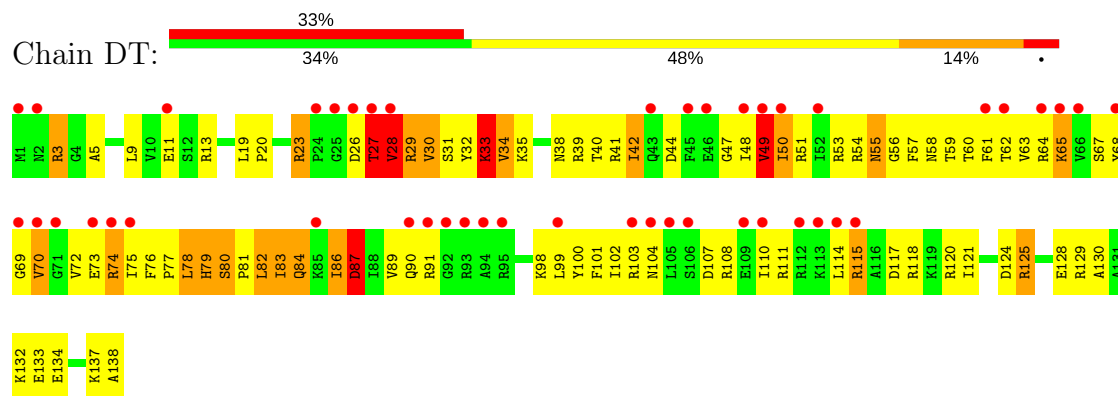


- Molecule 37: 50S ribosomal protein L18

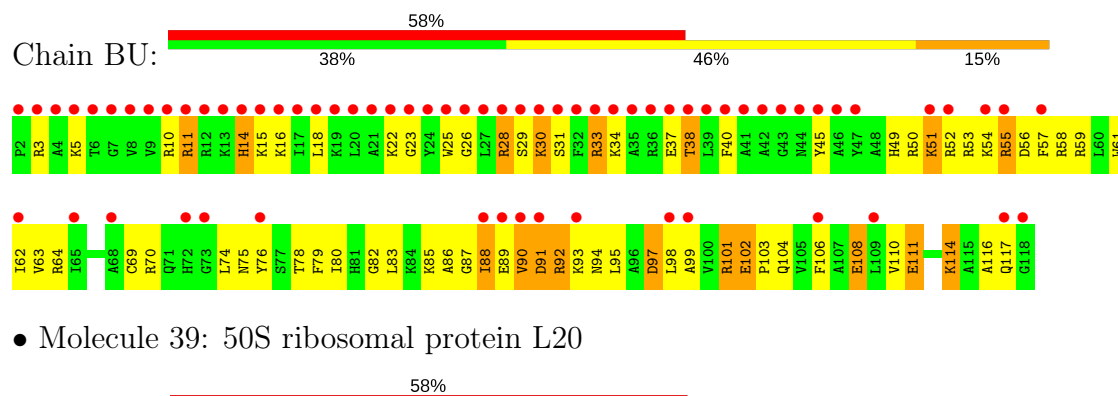




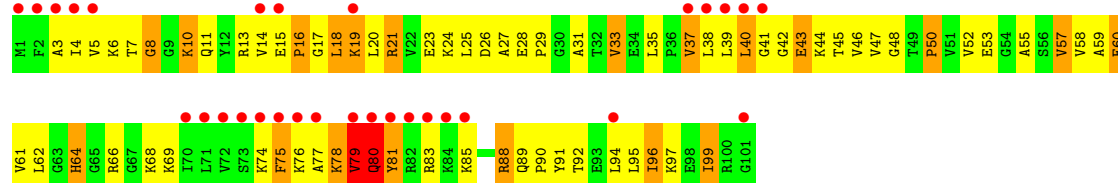
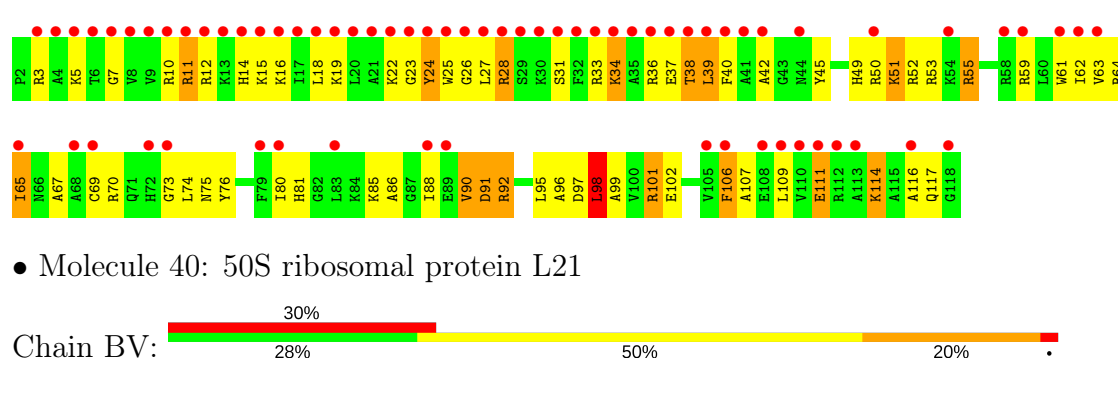
• Molecule 38: 50S ribosomal protein L19



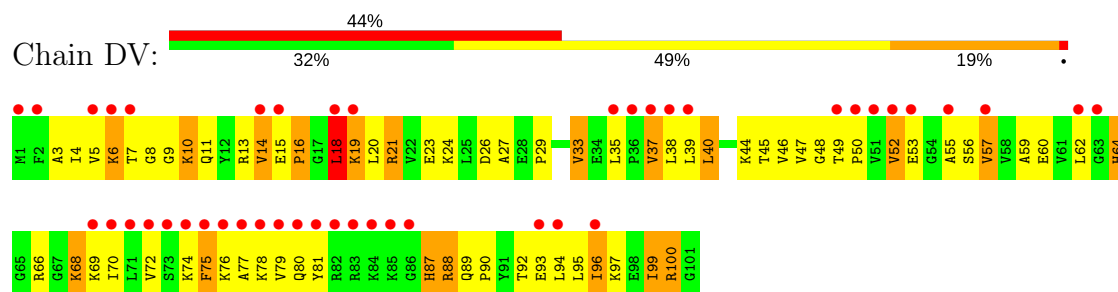
• Molecule 39: 50S ribosomal protein L20



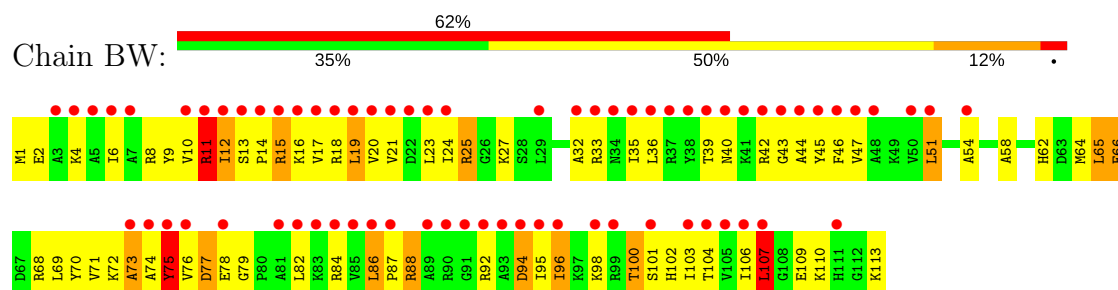
• Molecule 40: 50S ribosomal protein L21



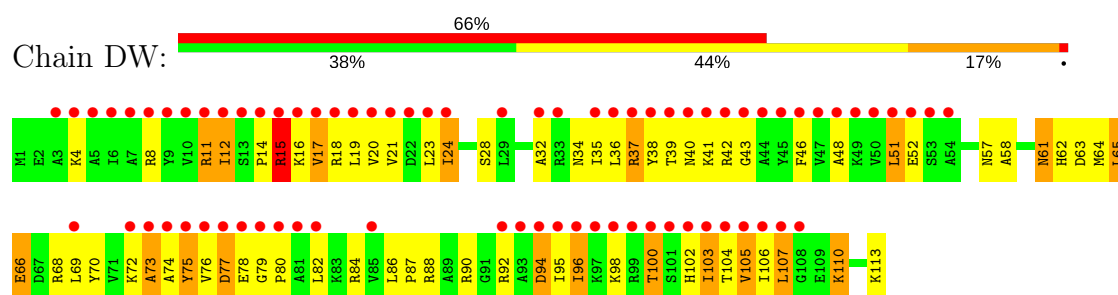
- Molecule 40: 50S ribosomal protein L21



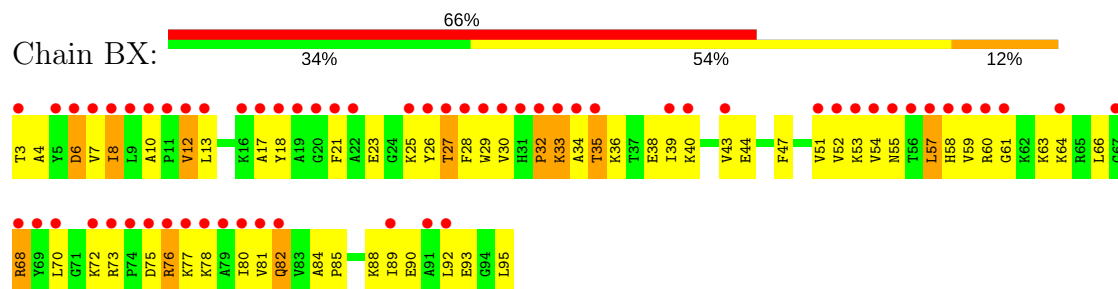
- Molecule 41: 50S ribosomal protein L22



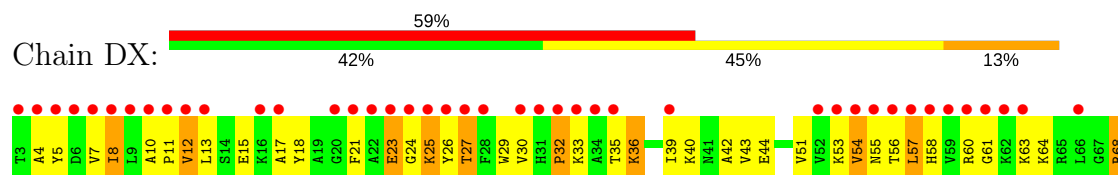
- Molecule 41: 50S ribosomal protein L22

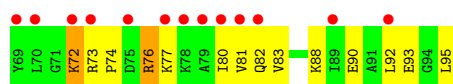


- Molecule 42: 50S ribosomal protein L23

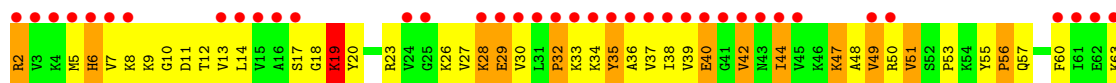
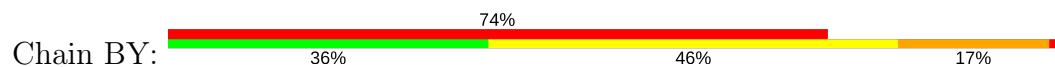


- Molecule 42: 50S ribosomal protein L23

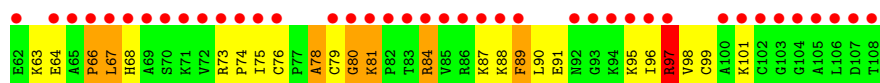
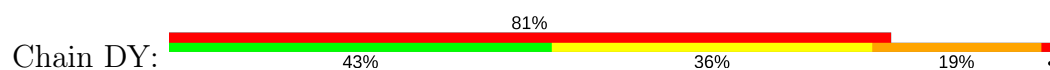




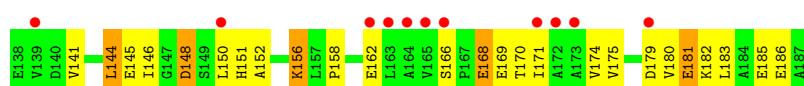
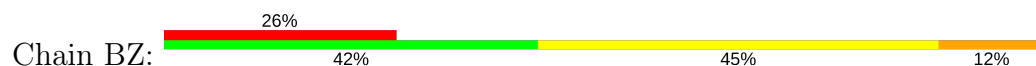
- Molecule 43: 50S ribosomal protein L24



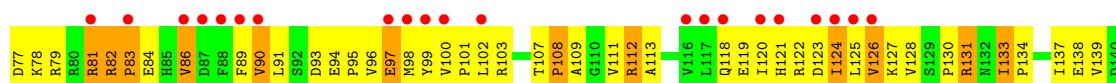
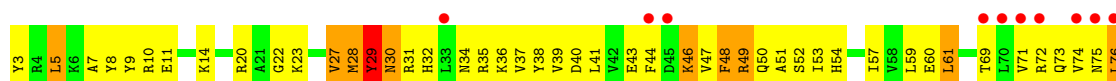
- Molecule 43: 50S ribosomal protein L24

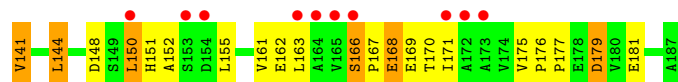


- Molecule 44: 50S ribosomal protein L25

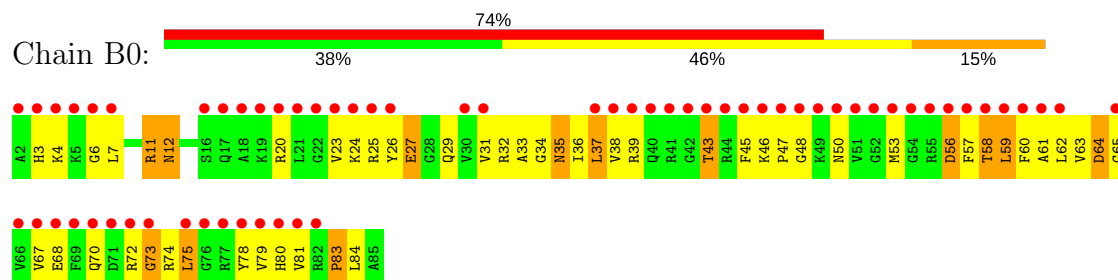


- Molecule 44: 50S ribosomal protein L25

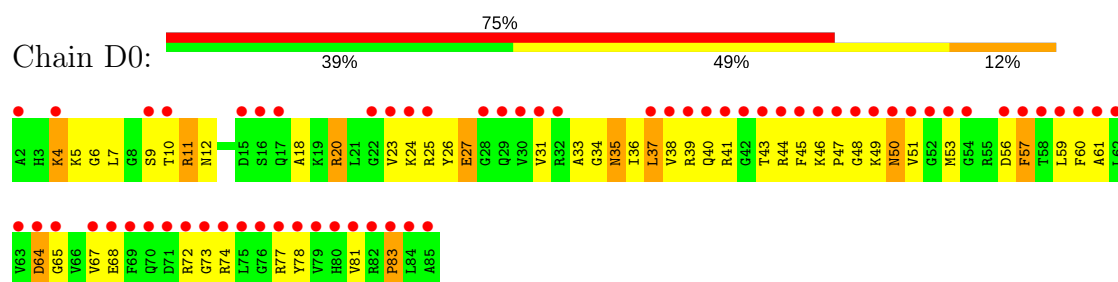




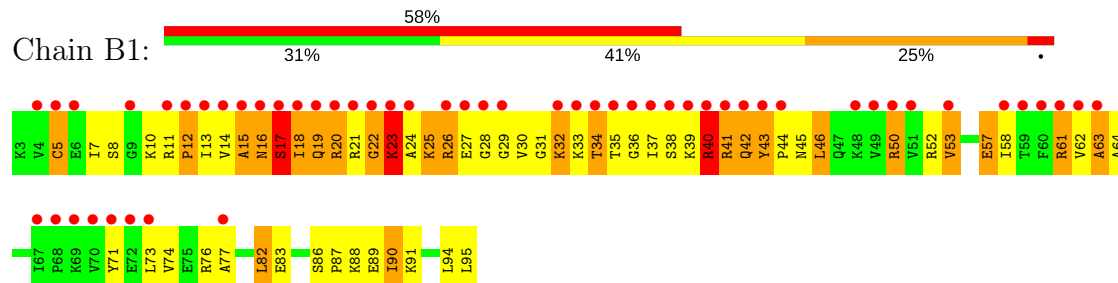
• Molecule 45: 50S ribosomal protein L27



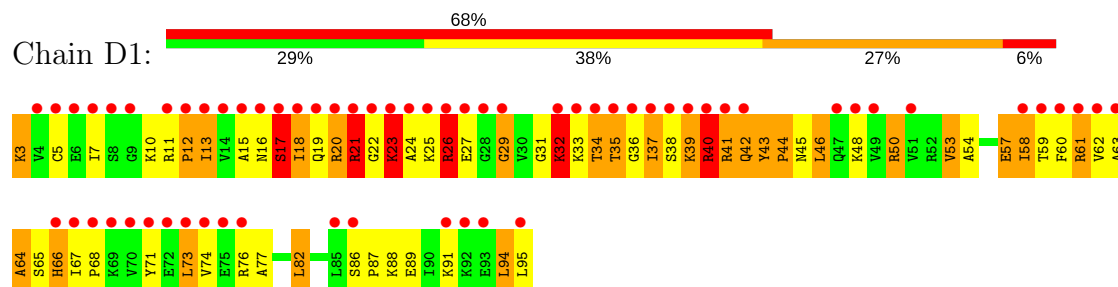
• Molecule 45: 50S ribosomal protein L27



• Molecule 46: 50S ribosomal protein L28

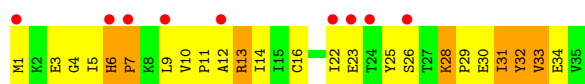


• Molecule 46: 50S ribosomal protein L28

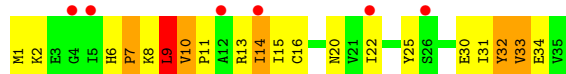


• Molecule 47: 50S ribosomal protein L31

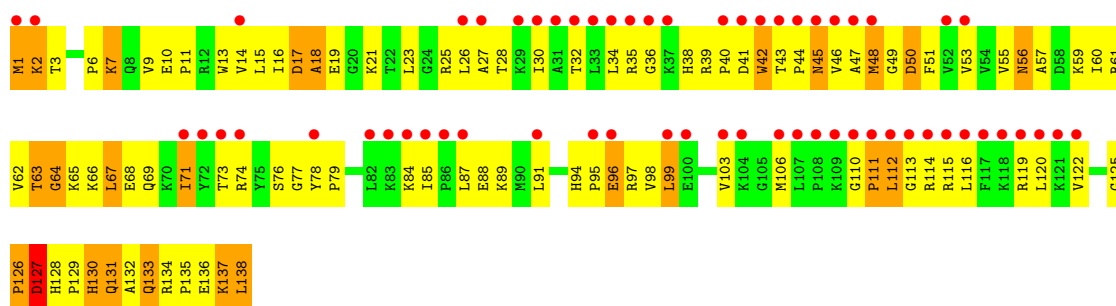




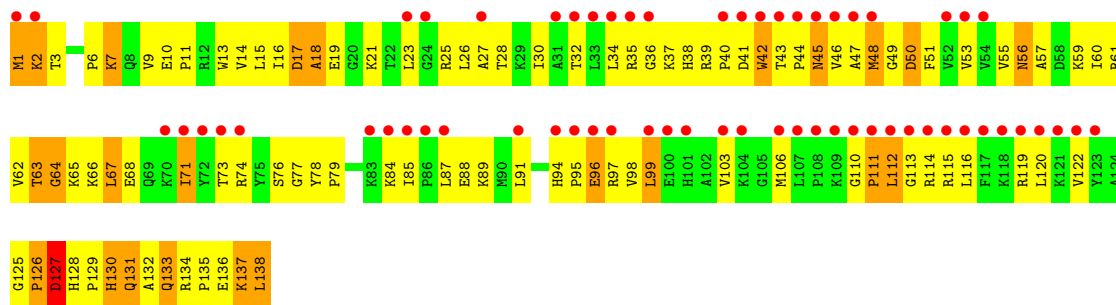
- Molecule 47: 50S ribosomal protein L31



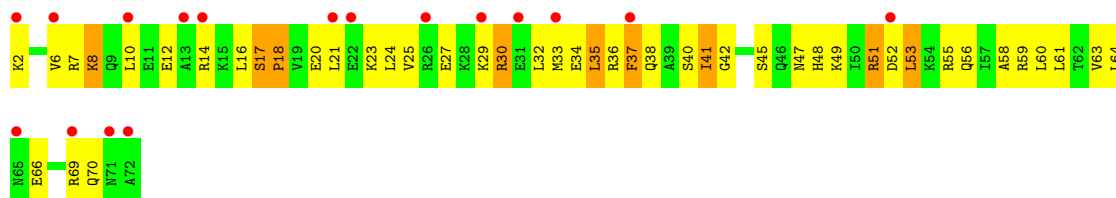
- Molecule 48: 50S ribosomal protein L13



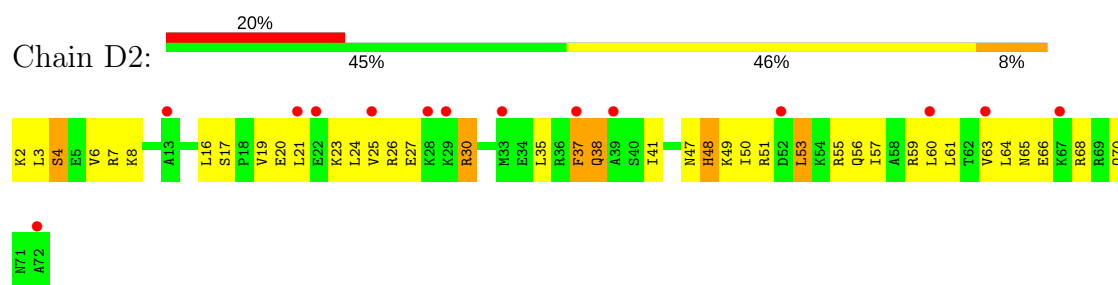
- Molecule 48: 50S ribosomal protein L13



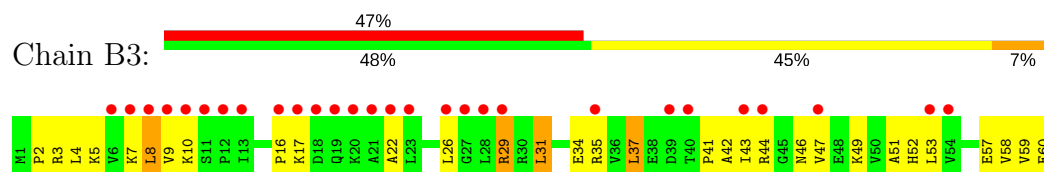
- Molecule 49: 50S ribosomal protein L29



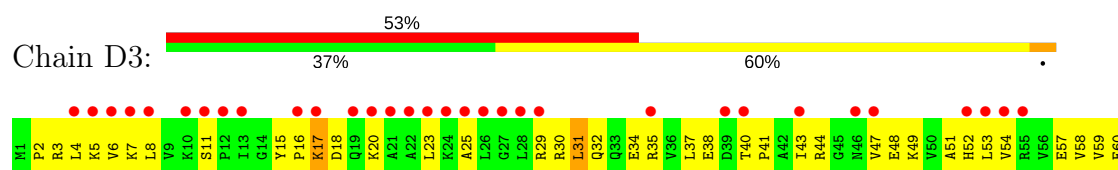
- Molecule 49: 50S ribosomal protein L29



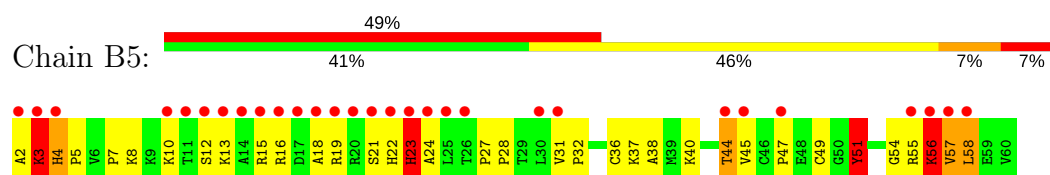
- Molecule 50: 50S ribosomal protein L30



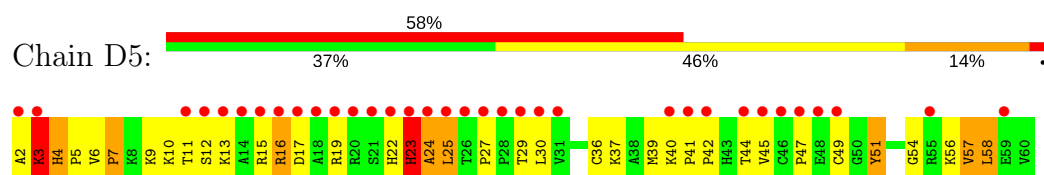
- Molecule 50: 50S ribosomal protein L30



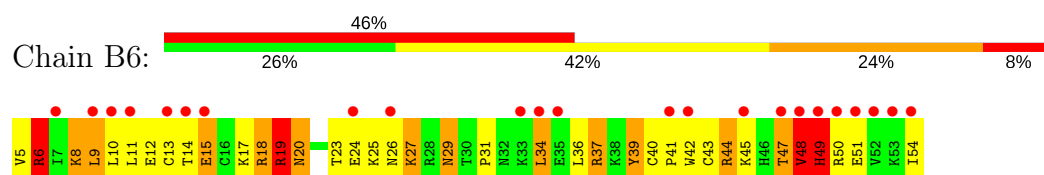
- Molecule 51: 50S ribosomal protein L32



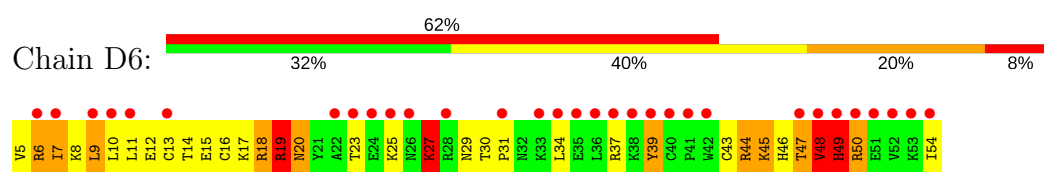
- Molecule 51: 50S ribosomal protein L32



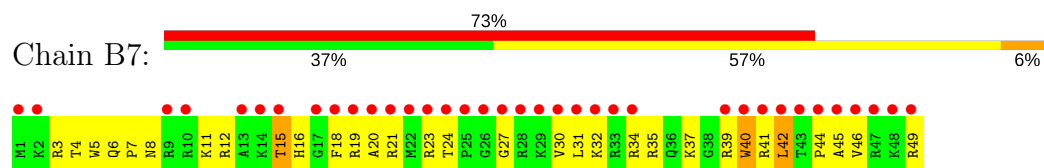
- Molecule 52: 50S ribosomal protein L33



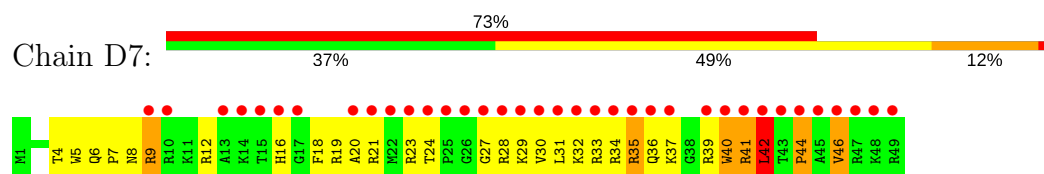
- Molecule 52: 50S ribosomal protein L33



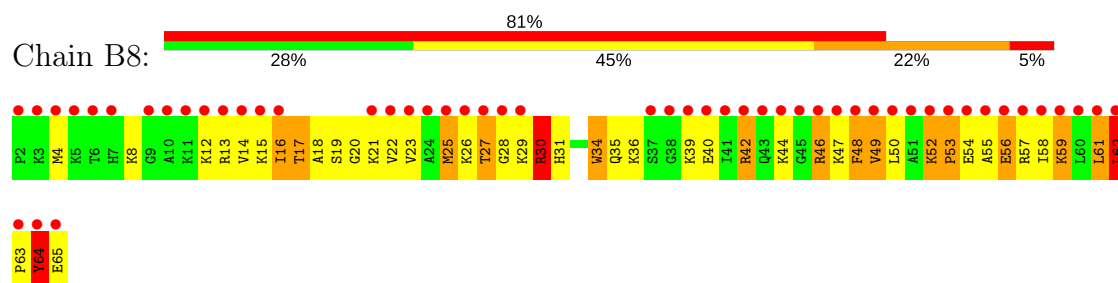
- Molecule 53: 50S ribosomal protein L34



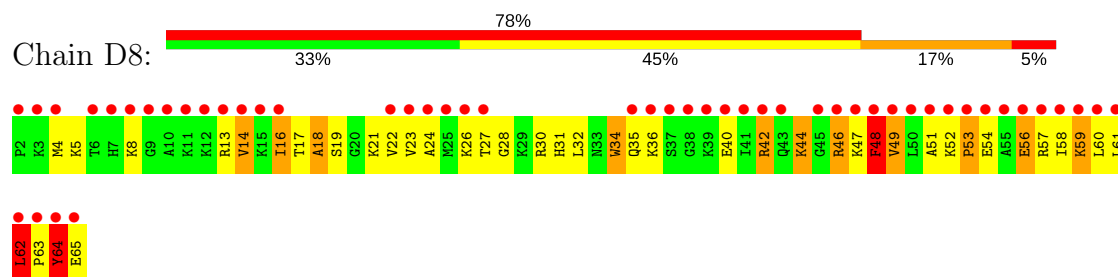
- Molecule 53: 50S ribosomal protein L34



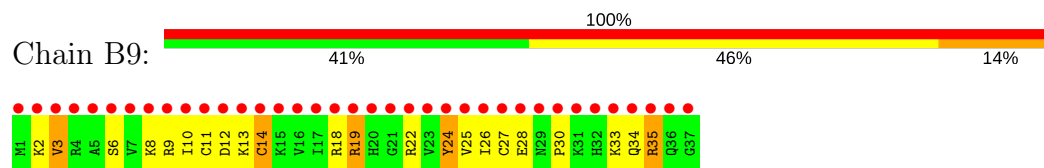
- Molecule 54: 50S ribosomal protein L35



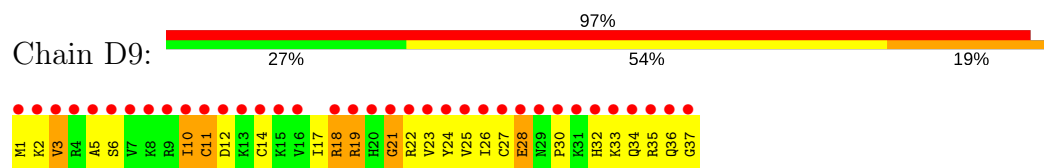
- Molecule 54: 50S ribosomal protein L35



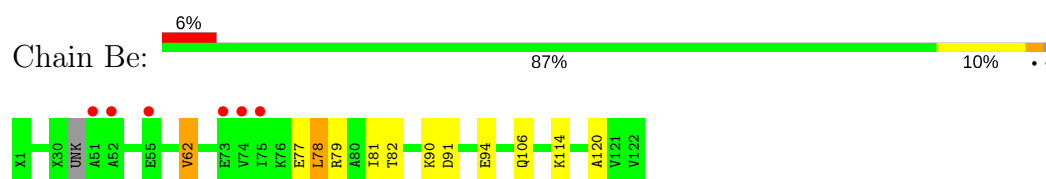
- Molecule 55: 50S ribosomal protein L36



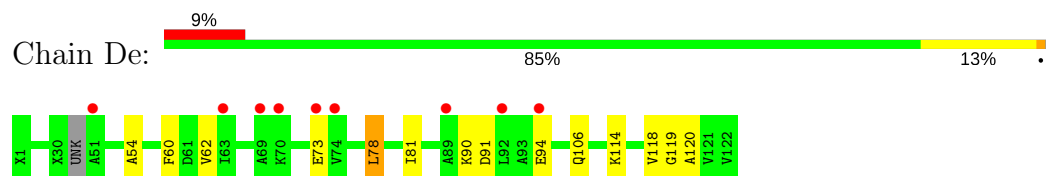
- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L7/L12



- Molecule 56: 50S ribosomal protein L7/L12



- Molecule 57: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 58: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

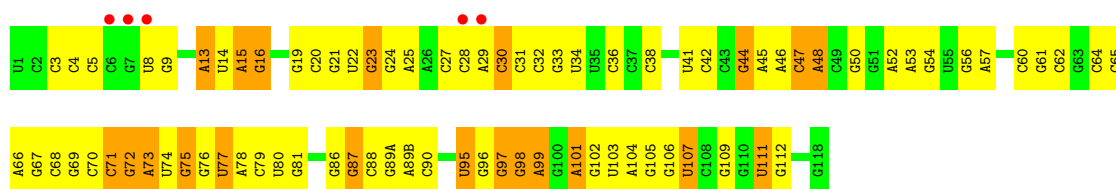
- Molecule 58: 50S ribosomal protein L7/L12



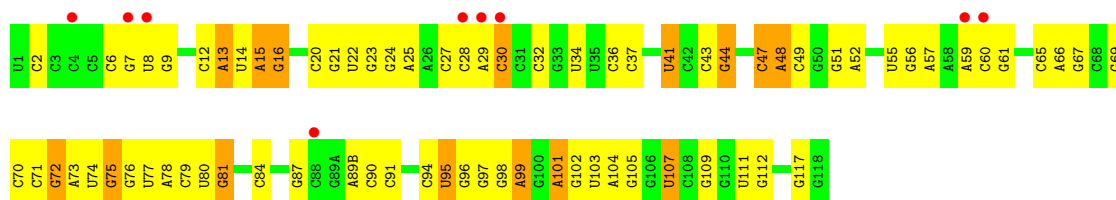
There are no outlier residues recorded for this chain.

- Molecule 59: 5S ribosomal RNA

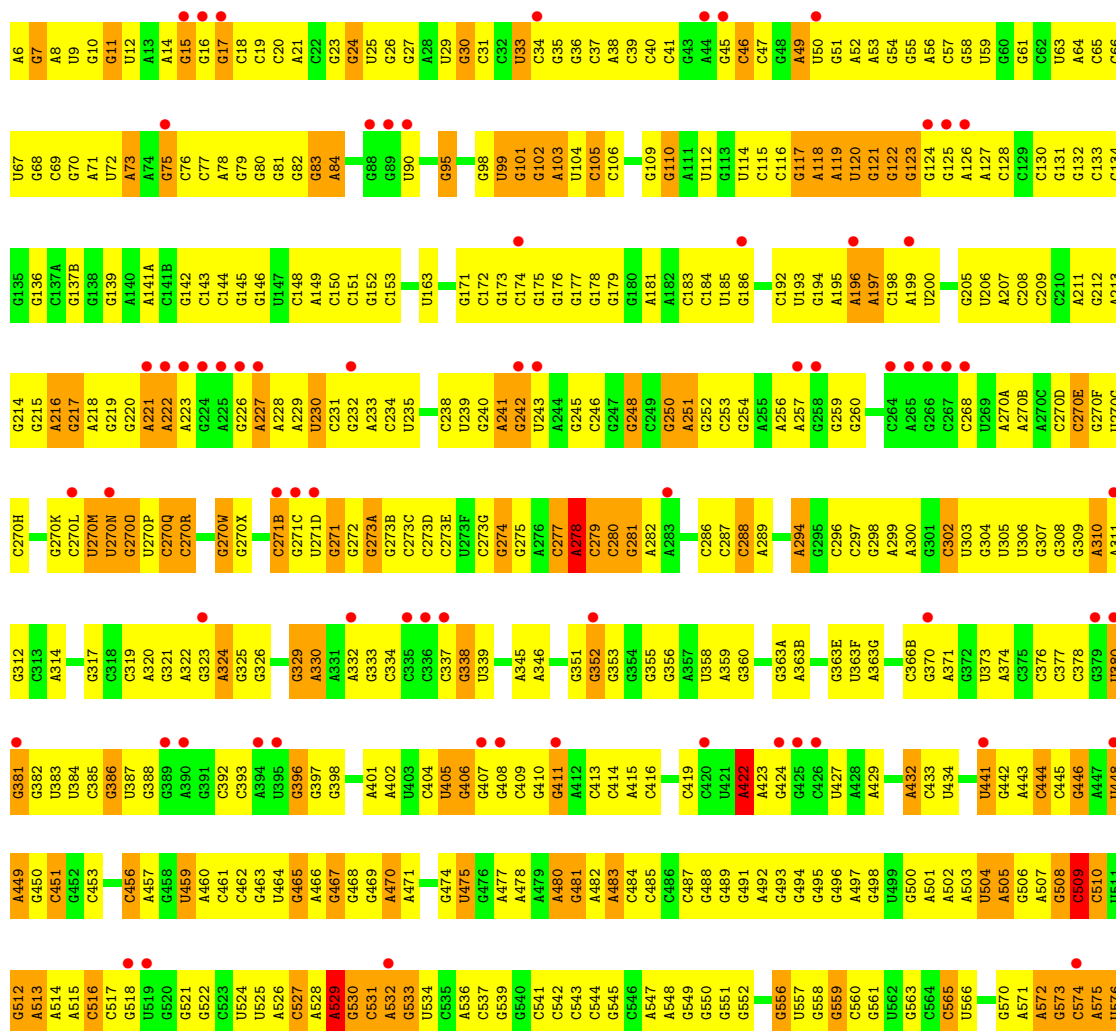


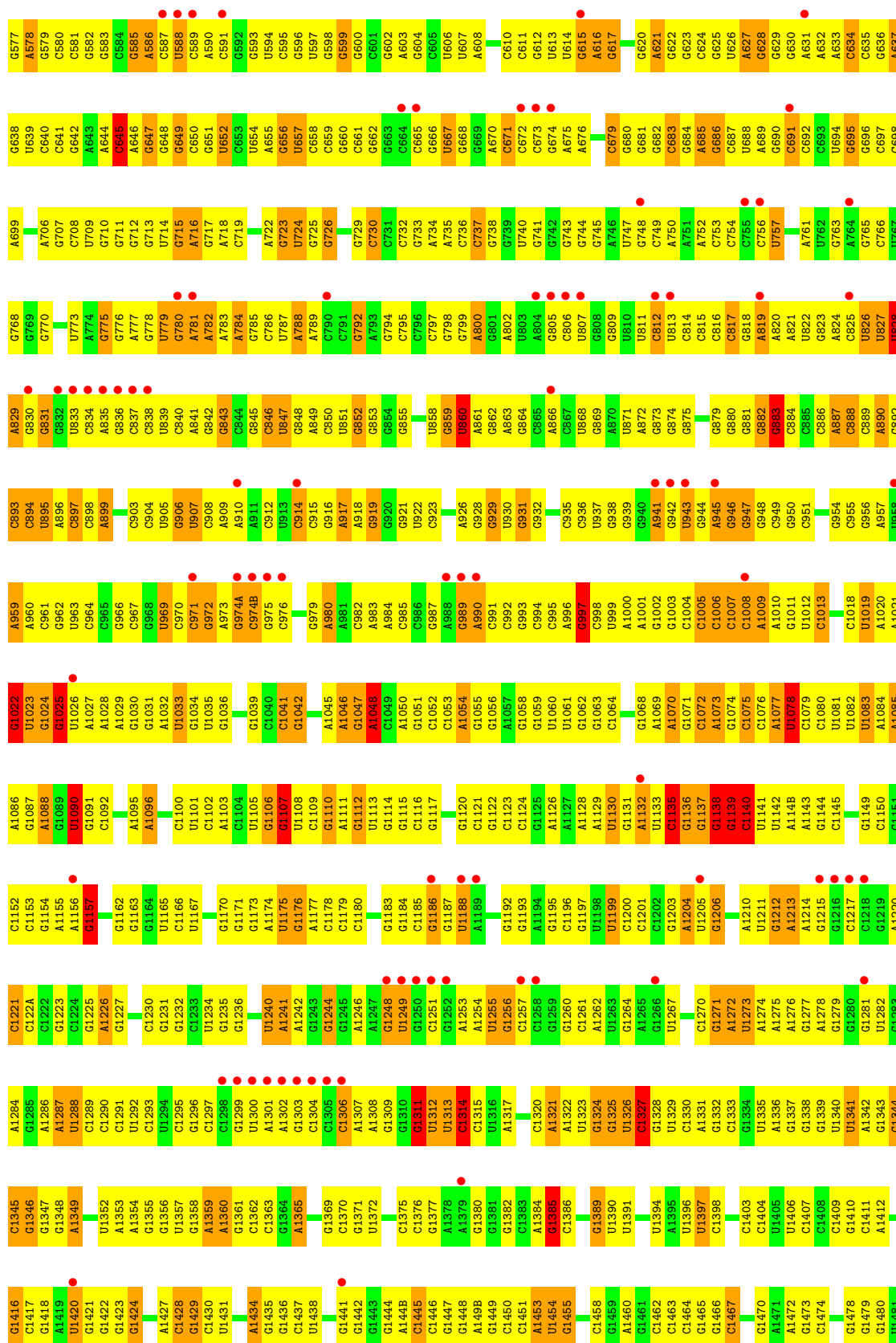


● Molecule 59: 5S ribosomal RNA

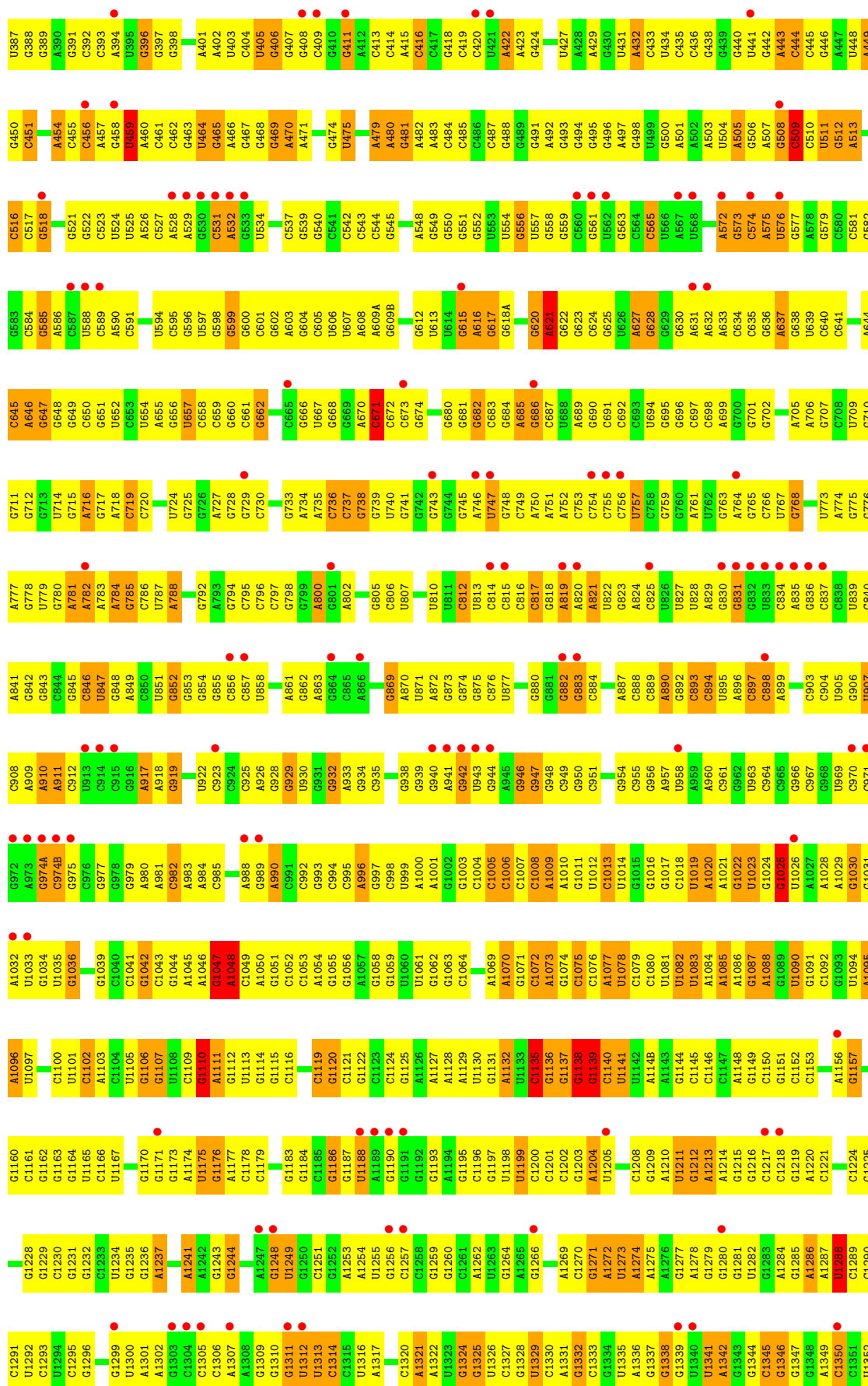


● Molecule 60: 23S ribosomal RNA





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C2258	G2259	C2260	C2261	U2262	C2263	C2264	U2265	U2266	U2267	A2268	A2269	A2270	C2271	U2272	U2273	U2274	A2275	U2276	G2277	A2278	G2279	G2282	G2283	C2284	G2285	A2286	U2287	A2288	G2289	C2290	U2291	C2292	C2293	C2294	C2295	G2302	G2303	C2304	A2305	C2306	C2307	C2308	A2309	A2310	A2311	U2312	C2313	C2314	C2315	C2316	C2317	C2318	C2319	A2320	G2321	A2322	G2325				
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C2258	G2259	C2260	C2261	U2262	C2263	C2264	U2265	U2266	U2267	A2268	A2269	A2270	C2271	U2272	U2273	U2274	A2275	U2276	G2277	A2278	G2279	G2282	G2283	C2284	G2285	A2286	U2287	A2288	G2289	C2290	U2291	C2292	C2293	C2294	C2295	G2302	G2303	C2304	A2305	C2306	C2307	C2308	A2309	A2310	A2311	U2312	C2313	C2314	C2315	C2316	C2317	C2318	C2319	A2320	G2321	A2322	G2325				
A2328	A2329	A2330	A2331	A2334	A2335	A2336	A2337	A2338	A2339	A2340	A2341	A2342	A2343	A2344	A2345	A2346	A2347	A2348	A2349	A2350	A2351	A2352	A2353	A2354	A2355	A2358	A2359	A2360	A2361	A2362	C2363	C2364	C2365	A2366	C2367	C2368	C2369	A2370	A2371	A2372	A2373	A2374	A2375	A2376	A2377	A2378	A2379	A2380	A2381	A2382	A2383	A2384	A2385	A2386	A2387	A2388	A2389	A2390	A2391	A2392	A2393
C1547	C1548	C1549	A1554	G1555	A1490	A1491	A1492	C1493	A1494	A1495	A1496	U1497	C1498	G1499	G1500	G1501	C1502	U1503	C1504	C1505	A1510	A1511	G1512	C1513	U1514	C1515	U1516	G1517	C1518	G1521	U1522	U1523	G1524	G1525	G1526	G1527	A1528	A1529	G1530	C1531	C1532	C1533	U1534	U1535	A1536	C1537	G1538	C1539	C1540	U1541	C1542	A1543	C1544	A1545	C1546	C1547					
C1685	C1686	C1687	U1688	A1689	A1690	C1691	U1692	U1693	C1694	G1695	G1696	G1697	A1698	G1699	C1700	A1701	G1702	G1703	G1704	U1709	A1802	A1803	C1804	G1726	U1727	G1728	A1729	C1648	G1649	G1731	G1732	G1733	C1734	U1735	C1741	C1655	C1656	C1657	C1658	U1757	C1661	A1664	A1665	G1666	G1667	A1668	A1669	C1670	U1671	G1672	C1673	G1674	C1675	A1676	A1677	G1678	G1681	C1682	C1683	C1684	
C1781	C1782	A1783	A1784	U1785	A1786	A1787	C1788	A1789	C1790	A1791	G1792	C1793	U1794	C1795	C1796	C1797	A1798	G1799	C1800	A1802	A1803	C1804	G1726	U1727	G1728	A1729	C1648	G1649	G1731	G1732	G1733	C1734	U1735	C1741	C1655	C1656	C1657	C1658	U1757	C1661	A1664	A1665	G1666	G1667	A1668	A1669	C1670	U1671	G1672	C1673	G1674	C1675	A1676	A1677	G1678	G1681	C1682	C1683	C1684		
A1847	A1848	G1849	U1851	G1856	G1857	A1858	A1859	G1861	G1862	G1863	U1864	A1869	C1870	A1871	A1872	G1873	C1874	C1875	C1880	C1881	A1884	G1888	A1889	A1890	A1891	A1892	C1893	C1894	C1895	G1896	G1897	U1898	G1899	A1900	C1901	G1902	G1903	G1904	C1905	G1906	G1907	C1908	A1912	A1913	C1914	U1915	G1916	U1917	A1918	A1919	C1920	G1921	C1924								
A1927	A1928	G1929	U1931	A1932	G1933	A1936	A1937	A1938	U1939	U1940	C1941	C1942	U1943	U1944	G1945	U1946	U1947	G1948	U1951	A1952	A1953	G1954	U1955	U1956	C1957	C1958	C1961	C1962	U1963	G1964	C1965	A1966	C1967	G1968	A1969	A1970	A1971	A1972	G1975	U1976	U1977	C1978	A1979	G1980	U1981	C1982	C1983	G1984	A1985	A1986	U1987	U1991									
G1992	U1993	C1996	G1997	G1998	U1999	G2000	A2001	G2002	G2003	G2004	C2007	C2008	G2009	G2010	U2011	G2012	A2013	A2014	A2015	U2016	U2017	G2018	A2019	A2020	C2021	U2022	C2023	G2024	C2025	C2026	G2027	U2028	G2029	A2030	C2031	G2032	A2033	U2034	G2035	C2036	G2037	G2038	C2039	C2040	C2041	A2042	C2043	C2044	C2045	C2046	U2047	G2048	G2049	C2050	A2051	C2052	C2053				
A2054	C2055	G2056	A2057	A2058	A2059	A2060	G2061	A2062	C2063	C2064	C2065	C2066	G2067	U2068	G2069	G2070	A2071	G2072	C2073	U2074	A2077	G2078	U2079	G2080	C2081	A2082	C2083	G2084	C2085	U2086	G2087	G2088	U2089	G2090	U2091	U2092	G2093	G2094	C2095	U2096	C2097	U2098	G2101	U2102	C2103	G2104	C2105	G2106	C2107	C2108	U2109	G2110	A2114	G2115	G2116	A2117					
U2118	A2119	G2120	G2121	U2122	G2123	G2124	G2125	A2126	G2127	G2128	C2129	U2130	G2131	U2132	G2133	A2134	A2135	C2136	C2137	C2138	C2139	C2140	G2141	C2142	C2143	U2144	C2145	C2146	G2147	G2148	C2149	U2150	G2151	C2152	G2153	G2154	C2155	G2156	G2157	A2158	C2159	G2162	C2163	U2167	C2168	U2169	A2170	A2171	U2172	A2173	C2174	C2175	G2176	C2177	C2178	C2179	U2180				
G2181	G2182	C2185	C2186	G2189	G2190	G2191	G2192	G2193	G2194	A2198	A2199	C2205	C2206	C2207	C2208	C2209	C2210	C2211	C2212	C2213	C2215	C2216	C2217	C2218	C2219	C2220	C2221	C2222	C2223	C2224	C2225	C2226	C2227	C2228	C2229	C2230	C2231	C2232	C2233	C2234	C2235	C2236	C2237	C2238	C2239	C2240	A2241	C2242	U2243	U2244	U2245	U2246	U2247	U2248	U2249	U2250	U2251	G2252	U2257		
C2258	G2259	C2260	C2261	U2262	C2263	C2264	U2265	U2266	U2267	A2268	A2269	A2270	C2271	U2272	U2273	U2274	A2275	U2276	G2277	A2278	G2279	G2282	G2283	C2284	G2285	A2286	U2287	A2288	G2289	C2290	U2291	C2292	C2293	C2294	C2295	G2302	G2303	C2304	A2305	C2306	C2307	C2308	A2309	A2310	A2311	U2312	C2313	C2314	C2315	C2316	C2317	C2318	C2319	A2320	G2321	A2322	G2325				
A2328	A2329	A2330	A2331	A2334	A2335	A2336	A2337	A2338	A2339	A2340	A2341	A2342	A2343	A2344	A2345	A2346	A2347	A2348	A2349	A2350	A2351	A2352	A2353	A2354	A2355	A2358	A2359	A2360	A2361	A2362	C2363	C2364	C2365	A2366	C2367	C2368	C2369	A2370	A2371	A2372	A2373	A2374	A2375	A2376	A2377	A2378	A2379	A2380	A2381	A2382	A2383	A2384	A2385	A2386	A2387	A2388	A2389	A2390	A2391	A2392	A2393
C1547	C1548	C1549	A1554	G1555	A1490	A1491	A1492	C1493	A1494	A1495	A1496	U1497	C1498	G1499	G1500	G1501	C1502	U1503	C1504	C1505	A1510	A1511	G1512	C1513	U1514	C1515	U1516	G1517	C1518	G1521	U1522	U1523	G1524	G1525	G1526	G1527	A1528	A1529	G1530	C1531	C1532	C1533	U1534	U1535	A1536	C1537	G1538	C1539	C1540	U1541	C1542	A1543	C1544	A1545	C1546	C1547					
C1685	C1686	C1687	U1688	A1689	A1690	C1691	U1692	U1693	C1694	G1695	G1696	G1697	A1698	G1699	C1700	A1701	G1702	G1703	G1704	U1709	A1802	A1803	C1804	G1726	U1727	G1728	A1729	C1648	G1649	G1731	G1732	G1733	C1734	U1735	C1741	C1655	C1656	C1657	C1658	U1757	C1661	A1664	A1665	G1666	G1667	A1668	A1669	C1670	U1671	G1672	C1673	G1674	C1675	A1676	A1677	G1678	G1681	C1682	C1683	C1684	
C1781	C1782	A1783	A1784	U1785	A1786	A1787	C1788	A1789	C1790	A1791	G1792	C1793	U1794	C1795	C1796	C1797	A1798	G1799	C1800	A1802	A1803	C1804	G1726	U1727	G1728	A1729	C1648	G1649	G1731	G1732	G1733	C1734	U1735	C1741	C1655	C1656	C1657	C1658	U1757	C1661	A1664	A1665	G1666	G1667	A1668	A1669	C1670	U1671	G1672	C1673	G1674	C1675	A1676	A1677	G1678	G1681	C1682	C1683	C1684		
A1847	A1848	G1849	U1851	G1856	G1857	A1858	A1859	G1861	G1862	G1863	U1864	A1869	C1870	A1871	A1872	G1873	C1874	C1875	C1880	C1881	A1884	G1888	A1889	A1890	A1891	A1892	C1893	C1894	C1895	G1896	G1897	U1898	G1899	A1900	C1901	G1902	G1903	G1904	C1905	G1906	G1907	C1908	A1912	A1913	C1914	U1915	G1916	U1917	A1918	A1919	C1920	G1921	C1924								
A1927	A1928	G1929	U1931	A1932	G1933	A1936	A1937	A1938	U1939	U1940	C1941	C1942	U1943	U1944	G1945	U1946	U1947	G1948	U1951	A1952	A1953	G1954	U1955	U1956	C1957	C1958	C1961	C1962	U1963	G1964	C1965	A1966	C1967	G1968	A1969	A1970	A1971	A1972	G1975	U1976	U1977	C1978	A1979	G1980	U1981	C1982	C1983	G1984	A1985	A1986	U1987	U1991									
G1992	U1993	C1996	G1997	G1998	U1999																																																								





G2867	G2868	A2799	G2729	G2668	G2603	A2533	A2469	G2405	G2338
A2868	A2869	A2801	G2730	G2669	U2604	G2536	G2470	U2406	G2339
G2870	G2871	G2802	G2731	A2670	U2605	U2537	G2471	G2407	G2340
G2872	G2873	G2803	G2732	A2671	G2606	G2538	G2472	U2408	G2341
A2874	A2875	G2804	A2733	G2672	G2607	C2538	A2476	G2409	C2342
A2876	G2877	G2805	A2734	G2673	G2608	A2542	C2477	G2410	C2343
G2878	G2879	G2806	G2735	G2674	U2609	A2543	A2478	A2411	U2344
G2880	G2881	G2807	G2736	A2675	G2610	G2544	A2479	A2412	A2345
C2882	G2883	A2808	G2737	C2678	U2611	G2545	C2480	G2413	A2346
A2884	G2885	A2809	A2738	A2679	G2612	U2552	G2481	G2414	C2347
G2886	G2887	A2810	U2739	C2680	U2613	U2553	C2482	G2415	C2350
G2888	G2889	G2811	A2740	C2681	A2614	U2554	C2483	C2416	C2353
G2891	G2892	A2812	A2741	U2682	C2615	U2555	C2484	C2417	G2354
G2893	G2894	A2813	G2742	C2683	C2616	C2556	G2485	A2418	G2355
G2895	G2896	C2816	G2743	U2684	G2617	C2557	G2486	U2419	C2356
G2897	G2898	G2817	G2744	G2685	G2618	G2558	G2487	G2421	U2357
G2899	G2900	G2818	U2745	G2686	C2619	C2559	A2488	A2422	G2358
G2901	G2902	G2819	G2746	G2687	C2620	C2560	G2489	U2423	C2359
G2903	G2904	A2820	G2747	U2688	A2621	U2561	G2490	G2424	
G2905	G2906	A2821	A2748	U2689	G2625	U2562		A2425	
G2907	G2908	A2822	A2749	C2690	G2626	U2563	U2493	A2426	G2364
G2909	G2910	G2823	A2750	C2691	G2627	A2564	G2494	C2427	G2365
G2911	G2912	U2825	A2753	C2692	C2628	A2565	G2495	G2428	A2366
G2913	G2914	A2826	U2754	A2693	A2629	A2566	C2496	G2429	G2367
G2915	G2916	G2827	G2755	G2694	G2630	G2567	U2497	A2430	C2368
G2917	G2918	C2828	U2756	U2695	G2631	C2568	C2498	U2431	A2369
G2919	G2920	G2829	A2757	U2696	A2632	C2569	U2500	A2432	G2370
G2921	G2922	G2830		G2697			U2501	A2433	G2371
G2923	G2924	U2831	G2762	U2698	C2635	A2572	C2502	A2434	G2372
G2925	G2926	A2832	G2763	C2699	U2636	C2573	A2503	A2435	G2373
G2927	G2928	G2833	A2764	C2700	U2637	C2574	U2504	G2436	G2374
G2929	G2930	G2834	A2765	C2701	G2638	C2575	G2505	U2437	G2375
G2931	G2932	A2835	G2766	U2702	A2639	G2576	U2506	U2438	A2376
G2933	G2934	U2836	G2767	C2703	G2640	A2577	A2439	A2440	A2377
G2935	G2936	G2837		G2704	G2641	G2578	C2507	C2441	A2378
G2937	G2938	U2838	G2772	A2705	G2642	C2579	G2508		
G2939	G2940	G2839	G2773	G2706	G2643	U2580	G2509	C2381	
G2941	G2942	C2840	G2774	G2707	G2644	G2581	C2510	G2382	
G2943	G2944	U2841		G2708	G2645	G2582	U2511	G2383	
G2945	G2946	G2842	G2777	G2709	U2646	C2583	C2512	G2384	
G2947	G2948		A2778	G2710	C2647	U2584	G2513	U2448	
G2949	G2950		U2779	A2711	G2648	U2585	U2514	U2449	
G2951	G2952		G2780	U2712	U2649	C2586	A2451	C2385	
G2953	G2954		A2781	A712B	U2650	A2587	C2515	U2387	
G2955	G2956		G2782	A2713	C2651	G2588			
G2957	G2958		G2783	G2714	G2652	A2589	U2518	U2390	
G2959	G2960		C2784	G2715	U2653	A2590	U2519	G2391	
G2961	G2962		G2785	U2716	A2654	C2591	C2520	A2392	
G2963	G2964		U2786		G2655	G2592	U2521	A2393	
G2965	G2966		G2787	G2719	U2656	U2593	U2522	C2394	
G2967	G2968		C2788	U2720	U2657	G2594	G2523	C2395	
G2969	G2970		G2789	A2721	C2658	G2595	G2524	G2396	
G2971	G2972		A2790	G2722		U2596	U2460	G2397	
G2973	G2974		G2791	C2723	A2662	U2597	G2526	U2398	
G2975	G2976		G2792	G2724	G2663	G2598	C2527	G2399	
G2977	G2978		G2793	A2725	G2664	U2599	U2528	G2400	
G2979	G2980		G2794	U2726	A2665	G2600	G2529	U2401	
G2981	G2982		G2795	G2727	C2666	C2601	A2530	C2402	
G2983	G2984		U2797	U2728	C2667	A2602	G2532	C2403	
G2985	G2986							C2404	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	302.39Å 683.92Å 356.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.86 182.04 – 3.87	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.86) 64.4 (182.04-3.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.34	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.89Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.264 , 0.317 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	76.3	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 478.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.24$, $\langle L^2 \rangle = 0.09$	Xtriage
Estimated twinning fraction	0.320 for h,-k,-l	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	308202	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, DPP, MG, KBE, UAL, 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	0.46	0/1945	0.80	9/2621 (0.3%)
1	CB	0.43	0/1945	0.80	6/2621 (0.2%)
2	AC	0.30	0/1645	0.60	0/2216
2	CC	0.30	0/1645	0.58	0/2216
3	AD	0.31	0/1733	0.61	0/2318
3	CD	0.30	0/1733	0.59	0/2318
4	AE	0.30	0/1172	0.57	0/1576
4	CE	0.30	0/1172	0.58	0/1576
5	AF	0.29	0/856	0.54	0/1154
5	CF	0.28	0/856	0.56	0/1154
6	AG	0.29	0/1276	0.54	0/1709
6	CG	0.29	0/1276	0.53	0/1709
7	AH	0.31	0/1136	0.61	0/1527
7	CH	0.31	0/1136	0.61	0/1527
8	AI	0.33	0/1029	0.56	1/1378 (0.1%)
8	CI	0.32	0/1029	0.56	1/1378 (0.1%)
9	AJ	0.29	0/815	0.56	0/1095
9	CJ	0.30	0/815	0.55	0/1095
10	AK	0.37	0/900	0.71	0/1213
10	CK	0.39	0/900	0.67	0/1213
11	AL	0.49	0/992	0.91	2/1327 (0.2%)
11	CL	0.47	0/992	0.88	2/1327 (0.2%)
12	AM	0.30	0/1008	0.61	0/1347
12	CM	0.27	0/1008	0.59	0/1347
13	AN	0.30	0/501	0.46	0/664
13	CN	0.30	0/501	0.49	0/664
14	AO	0.31	0/745	0.56	0/992
14	CO	0.32	0/745	0.62	0/992
15	AP	0.28	0/722	0.54	0/970
15	CP	0.27	0/722	0.52	0/970
16	AQ	0.40	0/848	0.71	0/1131
16	CQ	0.41	0/848	0.73	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.31	0/579	0.64	0/768
17	CR	0.29	0/579	0.61	0/768
18	AS	0.30	0/647	0.60	0/870
18	CS	0.30	0/647	0.61	0/870
19	AT	0.34	0/764	0.62	0/1006
19	CT	0.33	0/764	0.61	0/1006
20	AA	0.39	0/36351	1.06	104/56736 (0.2%)
20	CA	0.38	2/36351 (0.0%)	1.06	96/56736 (0.2%)
21	AV	0.47	0/443	1.09	5/691 (0.7%)
21	CV	0.29	0/443	0.86	0/691
22	AW	0.42	0/1827	1.14	7/2845 (0.2%)
22	CW	0.37	0/1827	1.06	7/2845 (0.2%)
23	AY	0.37	0/5481	0.68	8/7418 (0.1%)
23	CY	0.41	0/5481	0.69	3/7418 (0.0%)
24	AU	1.08	0/11	1.84	0/13
24	CU	1.09	0/11	1.84	0/13
25	BC	0.52	0/1774	0.84	3/2391 (0.1%)
25	DC	0.55	1/1774 (0.1%)	0.93	7/2391 (0.3%)
26	BD	0.34	0/2195	0.65	2/2955 (0.1%)
26	DD	0.34	0/2195	0.64	2/2955 (0.1%)
27	BE	0.37	0/1602	0.68	2/2160 (0.1%)
27	DE	0.34	0/1602	0.65	1/2160 (0.0%)
28	BF	0.47	1/1663 (0.1%)	0.87	6/2249 (0.3%)
28	DF	0.43	0/1663	0.87	6/2249 (0.3%)
29	BG	0.42	1/1499 (0.1%)	1.33	5/2016 (0.2%)
29	DG	0.39	1/1499 (0.1%)	0.63	0/2016
30	BH	0.30	0/1298	0.56	0/1751
30	DH	0.30	0/1298	0.56	0/1751
32	BK	0.28	0/1054	0.55	0/1427
32	DK	0.27	0/1054	0.52	0/1427
33	BO	0.29	0/943	0.58	0/1269
33	DO	0.29	0/943	0.55	0/1269
34	BP	0.32	0/1131	0.68	0/1504
34	DP	0.30	0/1131	0.62	0/1504
35	BQ	0.33	0/1143	0.60	0/1527
35	DQ	0.32	0/1143	0.63	0/1527
36	BR	0.31	0/974	0.63	0/1302
36	DR	0.32	0/974	0.63	0/1302
37	BS	0.36	0/783	0.69	0/1041
37	DS	0.36	0/783	0.68	0/1041
38	BT	0.34	0/1161	0.67	0/1549
38	DT	0.32	0/1161	0.65	0/1549
39	BU	0.38	0/982	0.59	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DU	0.38	0/982	0.61	0/1306
40	BV	0.38	0/790	0.73	0/1057
40	DV	0.34	0/790	0.66	1/1057 (0.1%)
41	BW	0.35	0/911	0.66	2/1220 (0.2%)
41	DW	0.34	0/911	0.63	0/1220
42	BX	0.31	0/748	0.57	0/1004
42	DX	0.29	0/748	0.55	1/1004 (0.1%)
43	BY	0.32	0/831	0.61	0/1108
43	DY	0.31	0/831	0.58	0/1108
44	BZ	0.30	0/1505	0.60	0/2042
44	DZ	0.31	0/1505	0.60	0/2042
45	B0	0.27	0/671	0.54	0/892
45	D0	0.27	0/671	0.53	0/892
46	B1	0.48	0/739	0.77	2/981 (0.2%)
46	D1	0.50	0/739	0.82	3/981 (0.3%)
47	B4	0.40	0/276	0.62	0/372
47	D4	0.36	0/276	0.59	0/372
48	BN	0.34	0/1131	0.66	0/1525
48	DN	0.34	0/1131	0.66	0/1525
49	B2	0.36	0/600	0.62	0/793
49	D2	0.34	0/600	0.58	0/793
50	B3	0.29	0/482	0.53	0/646
50	D3	0.29	0/482	0.53	0/646
51	B5	0.33	0/473	0.65	0/639
51	D5	0.31	0/473	0.58	0/639
52	B6	0.32	0/440	0.67	0/586
52	D6	0.34	0/440	0.66	0/586
53	B7	0.31	0/438	0.56	0/575
53	D7	0.32	0/438	0.55	0/575
54	B8	0.33	0/525	0.66	0/691
54	D8	0.32	0/525	0.63	0/691
55	B9	0.43	0/310	0.69	0/407
55	D9	0.30	0/310	0.63	0/407
56	Be	0.33	0/538	0.56	0/715
56	De	0.31	0/538	0.56	0/715
59	BB	0.39	0/2853	1.12	15/4451 (0.3%)
59	DB	0.38	0/2853	1.07	10/4451 (0.2%)
60	BA	0.39	0/69437	1.09	229/108401 (0.2%)
60	DA	0.38	3/69437 (0.0%)	1.06	187/108401 (0.2%)
All	All	0.38	9/330652 (0.0%)	0.97	735/492274 (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	3
11	AL	0	1
11	CL	0	2
23	AY	0	4
23	CY	0	4
25	BC	0	5
25	DC	0	3
26	BD	0	2
26	DD	0	2
28	BF	0	1
28	DF	0	1
29	BG	0	2
29	DG	0	2
31	BJ	0	1
31	DJ	0	1
37	BS	0	3
37	DS	0	3
38	DT	0	1
41	BW	0	1
41	DW	0	2
46	B1	0	2
46	D1	0	2
All	All	0	51

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BG	114	ILE	C-N	10.70	1.58	1.34
20	CA	1393	U	N1-C2	9.25	1.46	1.38
29	DG	114	ILE	N-CA	-7.54	1.31	1.46
25	DC	214	TYR	CD1-CE1	6.83	1.49	1.39
28	BF	157	VAL	CB-CG1	-5.60	1.41	1.52

The worst 5 of 735 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BG	114	ILE	O-C-N	-51.93	39.62	122.70
60	BA	1006	C	C6-N1-C2	-15.70	114.02	120.30
60	BA	1006	C	N3-C2-O2	-13.26	112.62	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AA	1535	C	P-O3'-C3'	12.55	134.76	119.70
60	BA	2505	G	N1-C6-O6	12.54	127.43	119.90

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	170	GLU	Peptide
1	AB	185	ILE	Peptide
1	AB	68	ILE	Peptide
11	AL	32	PHE	Peptide
23	AY	34	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1910	0	1957	119	0
1	CB	1910	0	1957	120	0
2	AC	1621	0	1688	78	0
2	CC	1621	0	1688	86	0
3	AD	1703	0	1763	112	0
3	CD	1703	0	1763	116	0
4	AE	1156	0	1213	57	0
4	CE	1156	0	1213	62	0
5	AF	843	0	857	46	0
5	CF	843	0	857	47	0
6	AG	1257	0	1296	70	0
6	CG	1257	0	1296	82	0
7	AH	1116	0	1177	77	0
7	CH	1116	0	1177	83	0
8	AI	1011	0	1043	60	0
8	CI	1011	0	1043	58	0
9	AJ	802	0	849	54	0
9	CJ	802	0	849	59	0
10	AK	885	0	904	50	0
10	CK	885	0	904	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AL	976	0	1062	128	0
11	CL	976	0	1062	108	0
12	AM	997	0	1072	68	0
12	CM	997	0	1072	67	0
13	AN	492	0	529	30	0
13	CN	492	0	529	24	0
14	AO	734	0	771	41	0
14	CO	734	0	771	41	0
15	AP	706	0	725	36	0
15	CP	706	0	725	29	0
16	AQ	835	0	906	81	0
16	CQ	835	0	906	71	0
17	AR	574	0	644	42	0
17	CR	574	0	644	42	0
18	AS	634	0	655	37	0
18	CS	634	0	655	43	0
19	AT	762	0	859	44	0
19	CT	762	0	859	44	0
20	AA	32474	0	16393	1073	0
20	CA	32474	0	16393	1050	0
21	AV	393	0	197	18	0
21	CV	393	0	197	14	0
22	AW	1635	0	831	72	0
22	CW	1635	0	831	72	0
23	AY	5380	0	5435	322	0
23	CY	5380	0	5436	310	0
24	AU	48	0	40	42	0
24	CU	48	0	41	16	0
25	BC	1742	0	1798	177	0
25	DC	1742	0	1798	182	0
26	BD	2145	0	2234	170	0
26	DD	2145	0	2234	162	0
27	BE	1569	0	1634	145	0
27	DE	1569	0	1634	129	0
28	BF	1628	0	1680	174	0
28	DF	1628	0	1680	164	0
29	BG	1474	0	1535	88	0
29	DG	1474	0	1535	80	0
30	BH	1274	0	1342	64	0
30	DH	1274	0	1342	52	0
31	BJ	851	0	199	35	0
31	DJ	851	0	203	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BK	1035	0	1082	49	0
32	DK	1035	0	1082	62	0
33	BO	933	0	996	65	0
33	DO	933	0	996	59	0
34	BP	1114	0	1187	85	0
34	DP	1114	0	1187	76	0
35	BQ	1122	0	1179	67	0
35	DQ	1122	0	1179	71	0
36	BR	960	0	1021	84	0
36	DR	960	0	1021	71	0
37	BS	775	0	835	66	0
37	DS	775	0	835	67	0
38	BT	1147	0	1207	102	0
38	DT	1147	0	1207	83	0
39	BU	964	0	1022	86	0
39	DU	964	0	1022	83	0
40	BV	779	0	852	63	0
40	DV	779	0	852	63	0
41	BW	900	0	964	57	0
41	DW	900	0	964	60	0
42	BX	734	0	789	41	0
42	DX	734	0	789	48	0
43	BY	818	0	908	45	0
43	DY	818	0	908	42	0
44	BZ	1473	0	1497	66	0
44	DZ	1473	0	1497	70	0
45	B0	662	0	688	44	0
45	D0	662	0	688	44	0
46	B1	732	0	808	78	0
46	D1	732	0	808	77	0
47	B4	271	0	284	17	0
47	D4	271	0	284	16	0
48	BN	1104	0	1180	201	0
48	DN	1104	0	1180	211	0
49	B2	598	0	653	34	0
49	D2	598	0	653	29	0
50	B3	477	0	529	20	0
50	D3	477	0	529	25	0
51	B5	459	0	477	32	0
51	D5	459	0	477	40	0
52	B6	433	0	461	37	0
52	D6	433	0	461	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	B7	430	0	480	38	0
53	D7	430	0	480	37	0
54	B8	517	0	582	46	0
54	D8	517	0	582	38	0
55	B9	307	0	336	21	0
55	D9	307	0	338	29	0
56	Be	686	0	620	0	0
56	De	686	0	620	0	0
57	Bf	156	0	37	0	0
57	Bg	156	0	39	0	0
57	Df	156	0	38	0	0
57	Dg	156	0	40	0	0
58	Bh	151	0	39	0	0
58	Dh	151	0	40	0	0
59	BB	2551	0	1295	93	0
59	DB	2551	0	1295	84	0
60	BA	61997	0	31250	2252	0
60	DA	61997	0	31250	2185	0
61	AY	32	0	13	8	0
61	CY	32	0	13	18	0
62	AY	1	0	0	0	0
62	CY	1	0	0	0	0
All	All	308202	0	213207	12967	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 12967 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)
48:DN:78:TYR:CD2	60:DA:2642:G:C5'	1.74	1.62
39:DU:64:ARG:CD	48:DN:41:ASP:HA	1.14	1.60
39:BU:64:ARG:CD	48:BN:41:ASP:HA	1.32	1.57
39:DU:64:ARG:HD2	48:DN:41:ASP:CA	1.06	1.52
39:BU:64:ARG:HD2	48:BN:41:ASP:CA	1.37	1.49

There are no symmetry-related clashes.

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%)	60 (26%)	19 (8%)	1	17
1	CB	233/235 (99%)	164 (70%)	49 (21%)	20 (9%)	1	16
2	AC	205/207 (99%)	140 (68%)	43 (21%)	22 (11%)	0	10
2	CC	205/207 (99%)	136 (66%)	47 (23%)	22 (11%)	0	10
3	AD	206/208 (99%)	146 (71%)	46 (22%)	14 (7%)	1	23
3	CD	206/208 (99%)	140 (68%)	49 (24%)	17 (8%)	1	17
4	AE	149/151 (99%)	118 (79%)	22 (15%)	9 (6%)	2	25
4	CE	149/151 (99%)	125 (84%)	16 (11%)	8 (5%)	2	28
5	AF	99/101 (98%)	82 (83%)	14 (14%)	3 (3%)	5	41
5	CF	99/101 (98%)	81 (82%)	10 (10%)	8 (8%)	1	17
6	AG	153/155 (99%)	113 (74%)	27 (18%)	13 (8%)	1	16
6	CG	153/155 (99%)	116 (76%)	24 (16%)	13 (8%)	1	16
7	AH	136/138 (99%)	98 (72%)	21 (15%)	17 (12%)	0	7
7	CH	136/138 (99%)	90 (66%)	29 (21%)	17 (12%)	0	7
8	AI	125/127 (98%)	98 (78%)	16 (13%)	11 (9%)	1	15
8	CI	125/127 (98%)	100 (80%)	16 (13%)	9 (7%)	1	21
9	AJ	97/99 (98%)	69 (71%)	22 (23%)	6 (6%)	2	25
9	CJ	97/99 (98%)	71 (73%)	20 (21%)	6 (6%)	2	25
10	AK	117/119 (98%)	81 (69%)	23 (20%)	13 (11%)	0	9
10	CK	117/119 (98%)	82 (70%)	22 (19%)	13 (11%)	0	9
11	AL	123/125 (98%)	55 (45%)	38 (31%)	30 (24%)	0	1
11	CL	123/125 (98%)	54 (44%)	41 (33%)	28 (23%)	0	1
12	AM	123/125 (98%)	85 (69%)	21 (17%)	17 (14%)	0	5
12	CM	123/125 (98%)	85 (69%)	22 (18%)	16 (13%)	0	6
13	AN	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	CN	58/60 (97%)	45 (78%)	8 (14%)	5 (9%)	1	16
14	AO	86/88 (98%)	59 (69%)	20 (23%)	7 (8%)	1	17
14	CO	86/88 (98%)	60 (70%)	20 (23%)	6 (7%)	1	22
15	AP	82/84 (98%)	61 (74%)	14 (17%)	7 (8%)	1	16
15	CP	82/84 (98%)	59 (72%)	20 (24%)	3 (4%)	4	37
16	AQ	98/100 (98%)	71 (72%)	14 (14%)	13 (13%)	0	6
16	CQ	98/100 (98%)	72 (74%)	17 (17%)	9 (9%)	1	15
17	AR	68/70 (97%)	43 (63%)	17 (25%)	8 (12%)	0	8
17	CR	68/70 (97%)	49 (72%)	16 (24%)	3 (4%)	3	32
18	AS	77/79 (98%)	45 (58%)	21 (27%)	11 (14%)	0	5
18	CS	77/79 (98%)	38 (49%)	29 (38%)	10 (13%)	0	6
19	AT	97/99 (98%)	77 (79%)	16 (16%)	4 (4%)	3	34
19	CT	97/99 (98%)	79 (81%)	14 (14%)	4 (4%)	3	34
23	AY	685/687 (100%)	474 (69%)	144 (21%)	67 (10%)	1	13
23	CY	685/687 (100%)	476 (70%)	143 (21%)	66 (10%)	1	13
24	AU	2/6 (33%)	2 (100%)	0	0	100	100
24	CU	2/6 (33%)	2 (100%)	0	0	100	100
25	BC	226/228 (99%)	109 (48%)	65 (29%)	52 (23%)	0	1
25	DC	226/228 (99%)	108 (48%)	66 (29%)	52 (23%)	0	1
26	BD	273/275 (99%)	177 (65%)	66 (24%)	30 (11%)	0	10
26	DD	273/275 (99%)	179 (66%)	57 (21%)	37 (14%)	0	5
27	BE	203/205 (99%)	123 (61%)	50 (25%)	30 (15%)	0	5
27	DE	203/205 (99%)	133 (66%)	41 (20%)	29 (14%)	0	5
28	BF	206/208 (99%)	130 (63%)	47 (23%)	29 (14%)	0	5
28	DF	206/208 (99%)	126 (61%)	55 (27%)	25 (12%)	0	7
29	BG	179/181 (99%)	116 (65%)	45 (25%)	18 (10%)	1	12
29	DG	179/181 (99%)	121 (68%)	43 (24%)	15 (8%)	1	16
30	BH	165/167 (99%)	115 (70%)	35 (21%)	15 (9%)	1	15
30	DH	165/167 (99%)	121 (73%)	26 (16%)	18 (11%)	0	10
32	BK	138/140 (99%)	97 (70%)	28 (20%)	13 (9%)	1	14
32	DK	138/140 (99%)	91 (66%)	35 (25%)	12 (9%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	BO	120/122 (98%)	88 (73%)	25 (21%)	7 (6%)	2	26
33	DO	120/122 (98%)	90 (75%)	22 (18%)	8 (7%)	1	23
34	BP	144/146 (99%)	82 (57%)	41 (28%)	21 (15%)	0	5
34	DP	144/146 (99%)	88 (61%)	35 (24%)	21 (15%)	0	5
35	BQ	139/141 (99%)	93 (67%)	32 (23%)	14 (10%)	1	12
35	DQ	139/141 (99%)	99 (71%)	26 (19%)	14 (10%)	1	12
36	BR	115/117 (98%)	72 (63%)	28 (24%)	15 (13%)	0	6
36	DR	115/117 (98%)	78 (68%)	26 (23%)	11 (10%)	1	13
37	BS	97/99 (98%)	54 (56%)	22 (23%)	21 (22%)	0	1
37	DS	97/99 (98%)	52 (54%)	24 (25%)	21 (22%)	0	1
38	BT	136/138 (99%)	84 (62%)	33 (24%)	19 (14%)	0	5
38	DT	136/138 (99%)	89 (65%)	28 (21%)	19 (14%)	0	5
39	BU	115/117 (98%)	89 (77%)	21 (18%)	5 (4%)	3	32
39	DU	115/117 (98%)	84 (73%)	20 (17%)	11 (10%)	1	13
40	BV	99/101 (98%)	59 (60%)	22 (22%)	18 (18%)	0	3
40	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	5
41	BW	111/113 (98%)	88 (79%)	16 (14%)	7 (6%)	1	25
41	DW	111/113 (98%)	90 (81%)	10 (9%)	11 (10%)	1	12
42	BX	91/93 (98%)	71 (78%)	12 (13%)	8 (9%)	1	15
42	DX	91/93 (98%)	69 (76%)	17 (19%)	5 (6%)	2	28
43	BY	105/107 (98%)	48 (46%)	33 (31%)	24 (23%)	0	1
43	DY	105/107 (98%)	50 (48%)	34 (32%)	21 (20%)	0	2
44	BZ	183/185 (99%)	126 (69%)	42 (23%)	15 (8%)	1	17
44	DZ	183/185 (99%)	120 (66%)	45 (25%)	18 (10%)	1	13
45	B0	82/84 (98%)	59 (72%)	15 (18%)	8 (10%)	1	13
45	D0	82/84 (98%)	55 (67%)	20 (24%)	7 (8%)	1	16
46	B1	91/93 (98%)	55 (60%)	19 (21%)	17 (19%)	0	3
46	D1	91/93 (98%)	55 (60%)	17 (19%)	19 (21%)	0	2
47	B4	33/35 (94%)	17 (52%)	13 (39%)	3 (9%)	1	15
47	D4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	4
48	BN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	DN	136/138 (99%)	94 (69%)	26 (19%)	16 (12%)	0	8
49	B2	69/71 (97%)	52 (75%)	13 (19%)	4 (6%)	2	26
49	D2	69/71 (97%)	51 (74%)	14 (20%)	4 (6%)	2	26
50	B3	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	2	29
50	D3	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	2	29
51	B5	57/59 (97%)	37 (65%)	10 (18%)	10 (18%)	0	3
51	D5	57/59 (97%)	37 (65%)	13 (23%)	7 (12%)	0	7
52	B6	48/50 (96%)	26 (54%)	11 (23%)	11 (23%)	0	1
52	D6	48/50 (96%)	26 (54%)	11 (23%)	11 (23%)	0	1
53	B7	47/49 (96%)	32 (68%)	11 (23%)	4 (8%)	1	16
53	D7	47/49 (96%)	34 (72%)	9 (19%)	4 (8%)	1	16
54	B8	62/64 (97%)	38 (61%)	18 (29%)	6 (10%)	1	13
54	D8	62/64 (97%)	37 (60%)	17 (27%)	8 (13%)	0	6
55	B9	35/37 (95%)	16 (46%)	14 (40%)	5 (14%)	0	5
55	D9	35/37 (95%)	19 (54%)	12 (34%)	4 (11%)	0	9
56	Be	70/103 (68%)	38 (54%)	25 (36%)	7 (10%)	1	12
56	De	70/103 (68%)	40 (57%)	23 (33%)	7 (10%)	1	12
All	All	13304/13578 (98%)	8936 (67%)	2877 (22%)	1491 (11%)	0	9

5 of 1491 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	20	GLU
1	AB	67	THR
1	AB	76	GLN
1	AB	103	THR
1	AB	157	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	203/203 (100%)	161 (79%)	42 (21%)	1	10
1	CB	203/203 (100%)	165 (81%)	38 (19%)	2	14
2	AC	161/161 (100%)	124 (77%)	37 (23%)	1	8
2	CC	161/161 (100%)	121 (75%)	40 (25%)	1	6
3	AD	180/180 (100%)	138 (77%)	42 (23%)	1	7
3	CD	180/180 (100%)	149 (83%)	31 (17%)	2	18
4	AE	116/116 (100%)	91 (78%)	25 (22%)	1	9
4	CE	116/116 (100%)	93 (80%)	23 (20%)	1	12
5	AF	90/90 (100%)	72 (80%)	18 (20%)	1	12
5	CF	90/90 (100%)	74 (82%)	16 (18%)	2	16
6	AG	126/126 (100%)	109 (86%)	17 (14%)	4	28
6	CG	126/126 (100%)	106 (84%)	20 (16%)	3	21
7	AH	119/119 (100%)	92 (77%)	27 (23%)	1	8
7	CH	119/119 (100%)	99 (83%)	20 (17%)	2	19
8	AI	98/98 (100%)	79 (81%)	19 (19%)	1	13
8	CI	98/98 (100%)	82 (84%)	16 (16%)	3	20
9	AJ	89/89 (100%)	72 (81%)	17 (19%)	2	13
9	CJ	89/89 (100%)	74 (83%)	15 (17%)	2	19
10	AK	90/90 (100%)	76 (84%)	14 (16%)	3	22
10	CK	90/90 (100%)	78 (87%)	12 (13%)	4	28
11	AL	104/104 (100%)	83 (80%)	21 (20%)	1	11
11	CL	104/104 (100%)	77 (74%)	27 (26%)	0	5
12	AM	100/100 (100%)	83 (83%)	17 (17%)	2	18
12	CM	100/100 (100%)	82 (82%)	18 (18%)	2	15
13	AN	49/49 (100%)	37 (76%)	12 (24%)	1	6
13	CN	49/49 (100%)	40 (82%)	9 (18%)	2	14
14	AO	79/79 (100%)	63 (80%)	16 (20%)	1	11
14	CO	79/79 (100%)	62 (78%)	17 (22%)	1	10
15	AP	72/72 (100%)	56 (78%)	16 (22%)	1	9
15	CP	72/72 (100%)	60 (83%)	12 (17%)	2	19
16	AQ	95/95 (100%)	77 (81%)	18 (19%)	2	13
16	CQ	95/95 (100%)	82 (86%)	13 (14%)	4	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AR	61/61 (100%)	51 (84%)	10 (16%)	2	20
17	CR	61/61 (100%)	48 (79%)	13 (21%)	1	10
18	AS	69/69 (100%)	51 (74%)	18 (26%)	0	5
18	CS	69/69 (100%)	54 (78%)	15 (22%)	1	9
19	AT	76/76 (100%)	66 (87%)	10 (13%)	5	28
19	CT	76/76 (100%)	69 (91%)	7 (9%)	11	43
23	AY	579/579 (100%)	475 (82%)	104 (18%)	2	15
23	CY	579/579 (100%)	472 (82%)	107 (18%)	2	14
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%)	138 (77%)	42 (23%)	1	7
25	DC	180/180 (100%)	130 (72%)	50 (28%)	0	4
26	BD	217/217 (100%)	164 (76%)	53 (24%)	1	6
26	DD	217/217 (100%)	173 (80%)	44 (20%)	1	11
27	BE	165/165 (100%)	131 (79%)	34 (21%)	1	11
27	DE	165/165 (100%)	134 (81%)	31 (19%)	2	14
28	BF	165/165 (100%)	127 (77%)	38 (23%)	1	8
28	DF	165/165 (100%)	126 (76%)	39 (24%)	1	7
29	BG	155/155 (100%)	118 (76%)	37 (24%)	1	7
29	DG	155/155 (100%)	121 (78%)	34 (22%)	1	9
30	BH	136/136 (100%)	109 (80%)	27 (20%)	1	12
30	DH	136/136 (100%)	115 (85%)	21 (15%)	3	22
32	BK	105/105 (100%)	94 (90%)	11 (10%)	8	37
32	DK	105/105 (100%)	88 (84%)	17 (16%)	3	20
33	BO	100/100 (100%)	80 (80%)	20 (20%)	1	12
33	DO	100/100 (100%)	84 (84%)	16 (16%)	3	21
34	BP	112/112 (100%)	80 (71%)	32 (29%)	0	3
34	DP	112/112 (100%)	91 (81%)	21 (19%)	2	14
35	BQ	111/111 (100%)	81 (73%)	30 (27%)	0	4
35	DQ	111/111 (100%)	85 (77%)	26 (23%)	1	7
36	BR	100/100 (100%)	72 (72%)	28 (28%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DR	100/100 (100%)	81 (81%)	19 (19%)	2	13
37	BS	77/77 (100%)	55 (71%)	22 (29%)	0	3
37	DS	77/77 (100%)	60 (78%)	17 (22%)	1	9
38	BT	120/120 (100%)	99 (82%)	21 (18%)	2	17
38	DT	120/120 (100%)	99 (82%)	21 (18%)	2	17
39	BU	93/93 (100%)	77 (83%)	16 (17%)	2	18
39	DU	93/93 (100%)	76 (82%)	17 (18%)	2	14
40	BV	82/82 (100%)	61 (74%)	21 (26%)	0	6
40	DV	82/82 (100%)	60 (73%)	22 (27%)	0	4
41	BW	92/92 (100%)	73 (79%)	19 (21%)	1	10
41	DW	92/92 (100%)	74 (80%)	18 (20%)	1	12
42	BX	75/75 (100%)	59 (79%)	16 (21%)	1	10
42	DX	75/75 (100%)	60 (80%)	15 (20%)	1	12
43	BY	88/88 (100%)	69 (78%)	19 (22%)	1	9
43	DY	88/88 (100%)	72 (82%)	16 (18%)	2	15
44	BZ	162/162 (100%)	129 (80%)	33 (20%)	1	11
44	DZ	162/162 (100%)	128 (79%)	34 (21%)	1	10
45	B0	66/66 (100%)	55 (83%)	11 (17%)	2	19
45	D0	66/66 (100%)	56 (85%)	10 (15%)	3	23
46	B1	78/78 (100%)	61 (78%)	17 (22%)	1	9
46	D1	78/78 (100%)	53 (68%)	25 (32%)	0	2
47	B4	31/31 (100%)	23 (74%)	8 (26%)	0	5
47	D4	31/31 (100%)	25 (81%)	6 (19%)	1	13
48	BN	117/117 (100%)	100 (86%)	17 (14%)	4	25
48	DN	117/117 (100%)	100 (86%)	17 (14%)	4	25
49	B2	66/66 (100%)	55 (83%)	11 (17%)	2	19
49	D2	66/66 (100%)	58 (88%)	8 (12%)	6	31
50	B3	52/52 (100%)	45 (86%)	7 (14%)	4	28
50	D3	52/52 (100%)	45 (86%)	7 (14%)	4	28
51	B5	51/51 (100%)	42 (82%)	9 (18%)	2	17
51	D5	51/51 (100%)	42 (82%)	9 (18%)	2	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	B6	49/49 (100%)	36 (74%)	13 (26%)	0	5
52	D6	49/49 (100%)	37 (76%)	12 (24%)	1	6
53	B7	42/42 (100%)	39 (93%)	3 (7%)	17	54
53	D7	42/42 (100%)	36 (86%)	6 (14%)	4	26
54	B8	54/54 (100%)	35 (65%)	19 (35%)	0	1
54	D8	54/54 (100%)	40 (74%)	14 (26%)	0	5
55	B9	34/34 (100%)	29 (85%)	5 (15%)	3	24
55	D9	34/34 (100%)	29 (85%)	5 (15%)	3	24
56	Be	54/54 (100%)	47 (87%)	7 (13%)	5	29
56	De	54/54 (100%)	46 (85%)	8 (15%)	3	24
All	All	11174/11174 (100%)	8954 (80%)	2220 (20%)	1	12

5 of 2220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	BZ	123	ASP
3	CD	107	ARG
43	DY	44	ILE
46	B1	26	ARG
54	B8	48	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
2	CC	123	GLN
7	CH	78	GLN
46	D1	45	ASN
2	CC	136	GLN
3	CD	125	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	AA	1510/1511 (99%)	330 (21%)	0
20	CA	1510/1511 (99%)	304 (20%)	0
21	AV	17/18 (94%)	8 (47%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	CV	17/18 (94%)	8 (47%)	0
22	AW	76/77 (98%)	27 (35%)	0
22	CW	76/77 (98%)	22 (28%)	0
59	BB	118/119 (99%)	26 (22%)	0
59	DB	118/119 (99%)	19 (16%)	0
60	BA	2878/2879 (99%)	729 (25%)	0
60	DA	2878/2879 (99%)	692 (24%)	0
All	All	9198/9208 (99%)	2165 (23%)	0

5 of 2165 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	AA	6	G
20	AA	7	G
20	AA	8	A
20	AA	9	G
20	AA	22	G

There are no RNA pucker outliers to report.

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	1.02	0	7,8,10	2.12	1 (14%)
24	DPP	AU	2	24	4,5,6	0.77	0	1,5,7	0.67	0
24	UAL	AU	5	24	8,8,9	2.52	3 (37%)	4,9,11	2.17	1 (25%)
24	5OH	AU	6	24	8,12,13	0.65	0	5,16,18	0.99	1 (20%)
24	KBE	CU	1	24	8,8,9	1.02	0	7,8,10	2.12	1 (14%)
24	DPP	CU	2	24	4,5,6	0.77	0	1,5,7	0.67	0
24	UAL	CU	5	24	8,8,9	2.51	3 (37%)	4,9,11	2.18	1 (25%)
24	5OH	CU	6	24	8,12,13	0.65	0	5,16,18	0.99	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	KBE	AU	1	24	-	0/7/7/8	0/0/0/0
24	DPP	AU	2	24	-	0/2/4/6	0/0/0/0
24	UAL	AU	5	24	-	0/3/7/9	0/0/0/0
24	5OH	AU	6	24	-	0/2/18/20	0/1/1/1
24	KBE	CU	1	24	-	0/7/7/8	0/0/0/0
24	DPP	CU	2	24	-	0/2/4/6	0/0/0/0
24	UAL	CU	5	24	-	0/3/7/9	0/0/0/0
24	5OH	CU	6	24	-	0/2/18/20	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AU	5	UAL	C1-N1	-3.18	1.34	1.40
24	CU	5	UAL	C1-N1	-3.15	1.35	1.40
24	CU	5	UAL	CB-CA	2.17	1.41	1.35
24	AU	5	UAL	CB-CA	2.17	1.41	1.35
24	CU	5	UAL	C-CA	5.36	1.54	1.45

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CU	5	UAL	O-C-CA	-4.26	120.03	125.47
24	AU	5	UAL	O-C-CA	-4.23	120.06	125.47
24	AU	6	5OH	O-C-CA	-2.14	120.16	125.15
24	CU	6	5OH	O-C-CA	-2.14	120.17	125.15
24	AU	1	KBE	CB-CA-C	5.21	120.14	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AU	2	DPP	12	0
24	AU	5	UAL	1	0
24	AU	6	5OH	27	0
24	CU	2	DPP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CU	5	UAL	1	0
24	CU	6	5OH	12	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	GNP	AY	701	62	27,34,34	2.89	6 (22%)	26,54,54	1.90	8 (30%)
61	GNP	CY	702	62	27,34,34	2.90	6 (22%)	26,54,54	1.90	8 (30%)

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	GNP	AY	701	62	-	0/16/38/38	0/3/3/3
61	GNP	CY	702	62	-	0/16/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CY	702	GNP	C4-N9	-8.13	1.36	1.47
61	AY	701	GNP	C4-N9	-8.10	1.37	1.47
61	AY	701	GNP	C5-C6	-7.98	1.38	1.53
61	CY	702	GNP	C5-C6	-7.98	1.38	1.53
61	AY	701	GNP	C8-N9	-3.09	1.37	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
61	AY	701	GNP	PA-O3A-PB	-4.62	116.08	132.38
61	CY	702	GNP	PA-O3A-PB	-4.61	116.10	132.38
61	CY	702	GNP	O3G-PG-O1G	-2.94	105.95	113.41
61	AY	701	GNP	O3G-PG-O1G	-2.92	105.98	113.41
61	CY	702	GNP	C5'-C4'-C3'	-2.22	106.82	115.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AY	701	GNP	8	0
61	CY	702	GNP	18	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9	
1	AB	235/235 (100%)	0.81	56 (23%)	1 1	13, 75, 147, 218	0
1	CB	235/235 (100%)	0.71	55 (23%)	1 1	26, 78, 150, 182	0
2	AC	207/207 (100%)	1.30	53 (25%)	1 1	21, 64, 129, 194	0
2	CC	207/207 (100%)	1.20	68 (32%)	0 1	33, 66, 122, 164	0
3	AD	208/208 (100%)	2.77	126 (60%)	0 1	24, 71, 131, 187	0
3	CD	208/208 (100%)	3.03	127 (61%)	0 1	16, 79, 141, 186	0
4	AE	151/151 (100%)	1.12	52 (34%)	0 1	10, 57, 124, 176	0
4	CE	151/151 (100%)	2.07	62 (41%)	0 1	23, 71, 126, 185	0
5	AF	101/101 (100%)	-0.63	1 (0%)	82 74	36, 69, 131, 173	0
5	CF	101/101 (100%)	-0.57	1 (0%)	82 74	29, 64, 127, 176	0
6	AG	155/155 (100%)	0.89	45 (29%)	1 1	20, 84, 135, 192	0
6	CG	155/155 (100%)	0.39	27 (17%)	2 2	39, 86, 144, 209	0
7	AH	138/138 (100%)	0.80	30 (21%)	1 1	21, 64, 118, 145	0
7	CH	138/138 (100%)	0.76	34 (24%)	1 1	33, 67, 126, 179	0
8	AI	127/127 (100%)	4.12	98 (77%)	0 0	13, 74, 122, 146	0
8	CI	127/127 (100%)	4.55	99 (77%)	0 0	16, 69, 128, 177	0
9	AJ	99/99 (100%)	1.80	39 (39%)	0 1	34, 74, 129, 147	0
9	CJ	99/99 (100%)	2.34	49 (49%)	0 1	24, 81, 132, 167	0
10	AK	119/119 (100%)	0.19	15 (12%)	4 5	17, 68, 129, 145	0
10	CK	119/119 (100%)	0.85	24 (20%)	1 2	37, 83, 128, 165	0
11	AL	125/125 (100%)	1.33	39 (31%)	0 1	22, 64, 128, 177	0
11	CL	125/125 (100%)	1.93	53 (42%)	0 1	21, 72, 139, 179	0
12	AM	125/125 (100%)	1.38	38 (30%)	0 1	54, 96, 167, 207	0
12	CM	125/125 (100%)	1.60	47 (37%)	0 1	58, 97, 159, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	3.82	44 (73%)	0	0	3, 48, 113, 131	0
13	CN	60/60 (100%)	3.60	42 (70%)	0	0	30, 54, 113, 147	0
14	AO	88/88 (100%)	0.85	19 (21%)	1	1	24, 64, 113, 158	0
14	CO	88/88 (100%)	1.15	26 (29%)	1	1	32, 73, 127, 165	0
15	AP	84/84 (100%)	6.13	63 (75%)	0	0	35, 82, 143, 179	0
15	CP	84/84 (100%)	5.62	66 (78%)	0	0	29, 73, 132, 175	0
16	AQ	100/100 (100%)	1.70	39 (39%)	0	1	25, 66, 120, 137	0
16	CQ	100/100 (100%)	2.14	47 (47%)	0	1	42, 74, 130, 159	0
17	AR	70/70 (100%)	0.26	10 (14%)	3	3	29, 54, 107, 143	0
17	CR	70/70 (100%)	0.38	7 (10%)	8	7	26, 69, 132, 198	0
18	AS	79/79 (100%)	3.21	44 (55%)	0	1	25, 95, 172, 193	0
18	CS	79/79 (100%)	2.40	39 (49%)	0	1	26, 89, 165, 199	0
19	AT	99/99 (100%)	2.19	47 (47%)	0	1	16, 66, 130, 188	0
19	CT	99/99 (100%)	2.69	59 (59%)	0	1	27, 80, 144, 169	0
20	AA	1511/1511 (100%)	0.43	216 (14%)	3	3	11, 79, 165, 273	0
20	CA	1511/1511 (100%)	0.44	194 (12%)	4	5	6, 84, 166, 265	0
21	AV	18/18 (100%)	2.58	12 (66%)	0	1	41, 113, 170, 197	0
21	CV	18/18 (100%)	2.94	12 (66%)	0	1	33, 135, 179, 181	0
22	AW	77/77 (100%)	-0.21	3 (3%)	40	32	24, 109, 168, 243	0
22	CW	77/77 (100%)	-0.01	3 (3%)	40	32	43, 116, 183, 208	0
23	AY	687/687 (100%)	-0.02	61 (8%)	10	9	26, 80, 149, 224	0
23	CY	687/687 (100%)	0.10	87 (12%)	4	5	25, 86, 158, 217	0
24	AU	2/6 (33%)	-0.70	0	100	100	66, 66, 66, 66	0
24	CU	2/6 (33%)	-1.14	0	100	100	66, 66, 66, 66	0
25	BC	228/228 (100%)	2.67	127 (55%)	0	1	77, 137, 202, 235	0
25	DC	228/228 (100%)	2.93	132 (57%)	0	1	73, 140, 196, 228	0
26	BD	275/275 (100%)	1.65	103 (37%)	0	1	12, 58, 126, 156	0
26	DD	275/275 (100%)	1.60	106 (38%)	0	1	18, 59, 122, 191	0
27	BE	205/205 (100%)	2.22	90 (43%)	0	1	16, 58, 123, 159	0
27	DE	205/205 (100%)	2.48	104 (50%)	0	1	20, 74, 138, 209	0
28	BF	208/208 (100%)	2.80	124 (59%)	0	1	41, 78, 145, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	DF	208/208 (100%)	2.78	110 (52%)	0	1	26, 76, 155, 199	0
29	BG	181/181 (100%)	2.10	89 (49%)	0	1	24, 87, 153, 191	0
29	DG	181/181 (100%)	1.69	73 (40%)	0	1	40, 94, 165, 199	0
30	BH	167/167 (100%)	0.49	30 (17%)	2	2	7, 68, 133, 171	0
30	DH	167/167 (100%)	0.50	30 (17%)	2	2	11, 67, 139, 168	0
31	BJ	0/170	-	-	-	-	-	-
31	DJ	0/170	-	-	-	-	-	-
32	BK	140/140 (100%)	0.85	28 (20%)	1	2	24, 91, 182, 225	0
32	DK	140/140 (100%)	1.29	46 (32%)	0	1	30, 110, 178, 234	0
33	BO	122/122 (100%)	1.43	40 (32%)	0	1	24, 45, 123, 162	0
33	DO	122/122 (100%)	1.75	50 (40%)	0	1	20, 58, 106, 159	0
34	BP	146/146 (100%)	2.88	74 (50%)	0	1	22, 76, 132, 175	0
34	DP	146/146 (100%)	2.59	73 (50%)	0	1	28, 78, 141, 189	0
35	BQ	141/141 (100%)	1.83	61 (43%)	0	1	17, 63, 130, 200	0
35	DQ	141/141 (100%)	2.09	59 (41%)	0	1	22, 68, 140, 174	0
36	BR	117/117 (100%)	2.73	75 (64%)	0	1	15, 57, 119, 178	0
36	DR	117/117 (100%)	2.13	59 (50%)	0	1	18, 69, 143, 195	0
37	BS	99/99 (100%)	5.89	78 (78%)	0	0	22, 104, 172, 208	0
37	DS	99/99 (100%)	4.96	76 (76%)	0	0	18, 106, 167, 216	0
38	BT	138/138 (100%)	1.13	39 (28%)	1	1	22, 71, 133, 179	0
38	DT	138/138 (100%)	1.27	45 (32%)	0	1	19, 75, 153, 238	0
39	BU	117/117 (100%)	3.44	68 (58%)	0	1	40, 57, 131, 184	0
39	DU	117/117 (100%)	3.07	68 (58%)	0	1	24, 61, 118, 158	0
40	BV	101/101 (100%)	1.70	30 (29%)	1	1	13, 54, 114, 146	0
40	DV	101/101 (100%)	2.41	44 (43%)	0	1	20, 72, 127, 200	0
41	BW	113/113 (100%)	2.88	70 (61%)	0	1	16, 55, 121, 147	0
41	DW	113/113 (100%)	3.79	75 (66%)	0	1	5, 65, 136, 178	0
42	BX	93/93 (100%)	3.08	61 (65%)	0	1	18, 60, 114, 149	0
42	DX	93/93 (100%)	2.97	55 (59%)	0	1	34, 63, 128, 170	0
43	BY	107/107 (100%)	4.27	79 (73%)	0	0	8, 86, 151, 180	0
43	DY	107/107 (100%)	4.05	87 (81%)	0	0	35, 76, 151, 176	0
44	BZ	185/185 (100%)	0.87	48 (25%)	1	1	30, 76, 142, 176	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
44	DZ	185/185 (100%)	0.56	41 (22%)	1	1	36, 82, 147, 226	0
45	B0	84/84 (100%)	5.18	62 (73%)	0	0	18, 92, 159, 181	0
45	D0	84/84 (100%)	5.01	63 (75%)	0	0	19, 85, 145, 160	0
46	B1	93/93 (100%)	3.52	54 (58%)	0	1	26, 91, 161, 204	0
46	D1	93/93 (100%)	4.57	63 (67%)	0	1	38, 92, 166, 194	0
47	B4	35/35 (100%)	0.80	9 (25%)	1	1	49, 106, 171, 203	0
47	D4	35/35 (100%)	0.45	6 (17%)	2	2	82, 115, 164, 187	0
48	BN	138/138 (100%)	2.11	60 (43%)	0	1	59, 83, 108, 111	0
48	DN	138/138 (100%)	2.04	61 (44%)	0	1	58, 84, 107, 116	0
49	B2	71/71 (100%)	1.12	17 (23%)	1	1	38, 79, 143, 185	0
49	D2	71/71 (100%)	0.92	14 (19%)	1	2	42, 70, 130, 187	0
50	B3	60/60 (100%)	1.69	28 (46%)	0	1	34, 62, 117, 150	0
50	D3	60/60 (100%)	2.58	32 (53%)	0	1	53, 68, 130, 149	0
51	B5	59/59 (100%)	2.54	29 (49%)	0	1	26, 56, 131, 149	0
51	D5	59/59 (100%)	2.50	34 (57%)	0	1	16, 83, 166, 185	0
52	B6	50/50 (100%)	1.98	23 (46%)	0	1	63, 99, 159, 175	0
52	D6	50/50 (100%)	3.07	31 (62%)	0	1	61, 118, 161, 188	0
53	B7	49/49 (100%)	3.44	36 (73%)	0	0	18, 47, 122, 156	0
53	D7	49/49 (100%)	3.54	36 (73%)	0	0	33, 61, 140, 186	0
54	B8	64/64 (100%)	4.20	52 (81%)	0	0	29, 63, 152, 160	0
54	D8	64/64 (100%)	5.09	50 (78%)	0	0	28, 75, 142, 191	0
55	B9	37/37 (100%)	10.16	37 (100%)	0	0	71, 109, 177, 183	0
55	D9	37/37 (100%)	12.55	36 (97%)	0	0	102, 132, 185, 210	0
56	Be	72/103 (69%)	-0.04	6 (8%)	12	10	40, 109, 188, 239	0
56	De	72/103 (69%)	0.14	9 (12%)	4	5	46, 118, 183, 199	0
57	Bf	0/31	-	-	-	-	-	-
57	Bg	0/31	-	-	-	-	-	-
57	Df	0/31	-	-	-	-	-	-
57	Dg	0/31	-	-	-	-	-	-
58	Bh	0/30	-	-	-	-	-	-
58	Dh	0/30	-	-	-	-	-	-
59	BB	119/119 (100%)	-0.32	5 (4%)	37	29	27, 111, 173, 187	0
59	DB	119/119 (100%)	-0.18	9 (7%)	15	11	35, 118, 182, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	BA	2879/2879 (100%)	0.22	290 (10%) 8 7	7, 78, 171, 308	0
60	DA	2879/2879 (100%)	0.23	286 (9%) 8 7	5, 79, 177, 310	0
All	All	22716/23310 (97%)	1.26	6463 (28%) 1 1	3, 79, 161, 310	0

The worst 5 of 6463 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	D9	11	CYS	26.6
55	D9	27	CYS	26.1
60	DA	2250	G	24.1
55	D9	34	GLN	24.1
55	B9	14	CYS	23.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	DPP	CU	2	6/7	0.92	0.10	-	65,65,65,65	0
24	5OH	AU	6	12/13	0.96	0.25	-	99,101,102,102	0
24	KBE	CU	1	9/10	0.92	0.30	-	65,65,65,65	0
24	UAL	CU	5	9/10	0.94	0.10	-	65,65,65,65	0
24	5OH	CU	6	12/13	0.97	0.09	-	99,101,102,102	0
24	DPP	AU	2	6/7	0.96	0.12	-	65,65,65,65	0
24	UAL	AU	5	9/10	0.89	0.18	-	65,65,65,65	0
24	KBE	AU	1	9/10	0.93	1.01	-	65,65,65,65	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
61	GNP	AY	701	32/32	0.95	0.20	0.16	58,71,81,83	0
61	GNP	CY	702	32/32	0.94	0.13	-0.53	58,71,81,83	0
62	MG	CY	701	1/1	0.97	0.11	-	104,104,104,104	0
62	MG	AY	702	1/1	0.96	0.20	-	124,124,124,124	0

6.5 Other polymers

There are no such residues in this entry.