



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 20, 2017 – 02:58 AM EDT

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
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) : rb-20029077

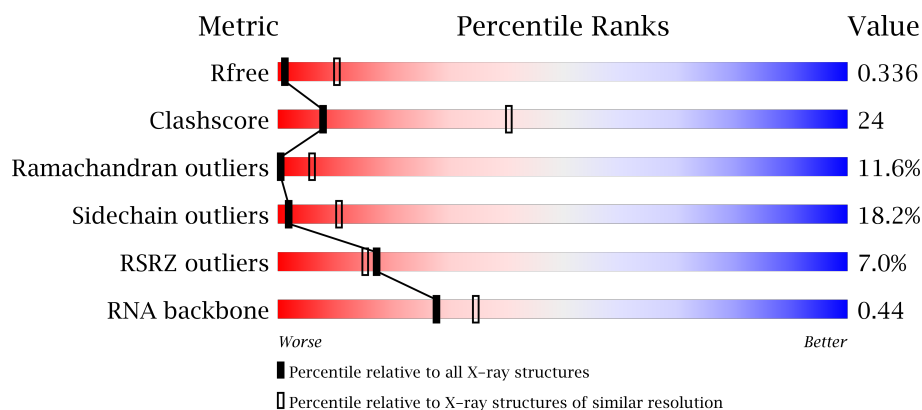
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)
RNA backbone	2435	1024 (4.10-2.86)

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

Mol	Chain	Length	Quality of chain
1	AB	235	<div> <div>14%</div> <div>34%</div> <div>45%</div> <div>18%</div> <div>.</div> </div>
1	CB	235	<div> <div>12%</div> <div>40%</div> <div>45%</div> <div>15%</div> </div>
2	AC	207	<div> <div>11%</div> <div>42%</div> <div>46%</div> <div>12%</div> </div>
2	CC	207	<div> <div>11%</div> <div>49%</div> <div>43%</div> <div>8%</div> </div>

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

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

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






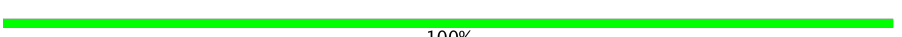
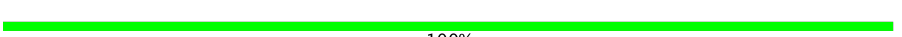



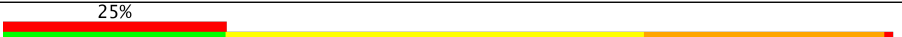
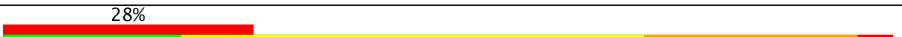


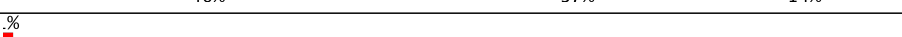
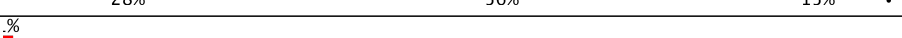

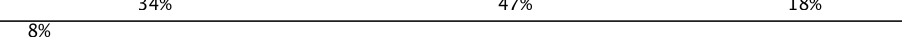
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Mol	Chain	Length	Quality of chain
40	DU	117	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	93	
43	DX	93	
44	BY	107	
44	DY	107	
45	BZ	185	
45	DZ	185	
46	B0	84	
46	D0	84	
47	B2	71	
47	D2	71	
48	B3	60	
48	D3	60	
49	B5	59	
49	D5	59	
50	B6	50	
50	D6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

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Mol	Chain	Length	Quality of chain
53	B9	37	
53	D9	37	
54	Be	102	
54	De	102	
55	Bf	31	
55	Bg	31	
55	Df	31	
55	Dg	31	
56	Bh	30	
56	Dh	30	
57	B1	93	
57	D1	93	
58	B4	35	
58	D4	35	
59	BA	2879	
59	DA	2879	
60	BB	119	
60	DB	119	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	FUA	AY	701	-	-	-	X
61	FUA	CY	701	-	-	-	X
62	GDP	AY	702	-	-	X	-
62	GDP	CY	702	-	-	X	-
63	MG	BA	2901	-	-	-	X

## 2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 21 is a RNA chain called transfer RNA.

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

- Molecule 22 is a RNA chain called messenger RNA.

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

- Molecule 23 is a protein called Elongation factor G.

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

- Molecule 24 is a protein called VIOMYCIN.

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

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

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

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

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

There are 10 discrepancies between the modelled and reference sequences:

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 58 is a protein called 50S ribosomal protein L31.



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

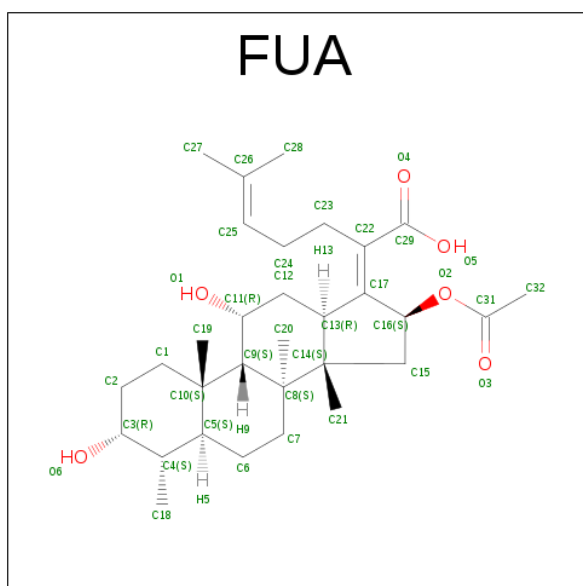
- Molecule 59 is a RNA chain called 23S ribosomal RNA.

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

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

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

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



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

- # GDP
- 
- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine ring system with an amino group at C2) linked to a ribose sugar via a glycosidic bond at the C1 position. The ribose sugar is further linked to two phosphate groups (P1 and P2) via phosphodiester bonds. The structure is labeled with atom names and numbers, including C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C799, C800, C801, C802, C803, C804, C805, C806, C807, C808, C809, C810, C811, C812, C813, C81

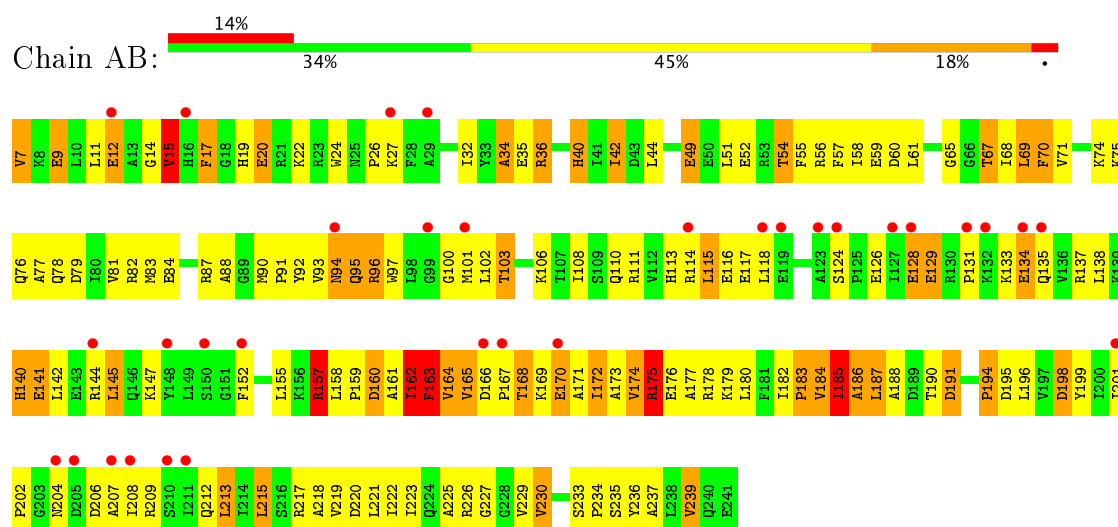
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
62	AY	1	Total 28	C 10	N 5	O 11	P 2	0	0
62	CY	1	Total 28	C 10	N 5	O 11	P 2	0	0

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 63  | BA    | 1        | Total Mg<br>1 1 | 0       | 0       |
| 63  | CY    | 1        | Total Mg<br>1 1 | 0       | 0       |

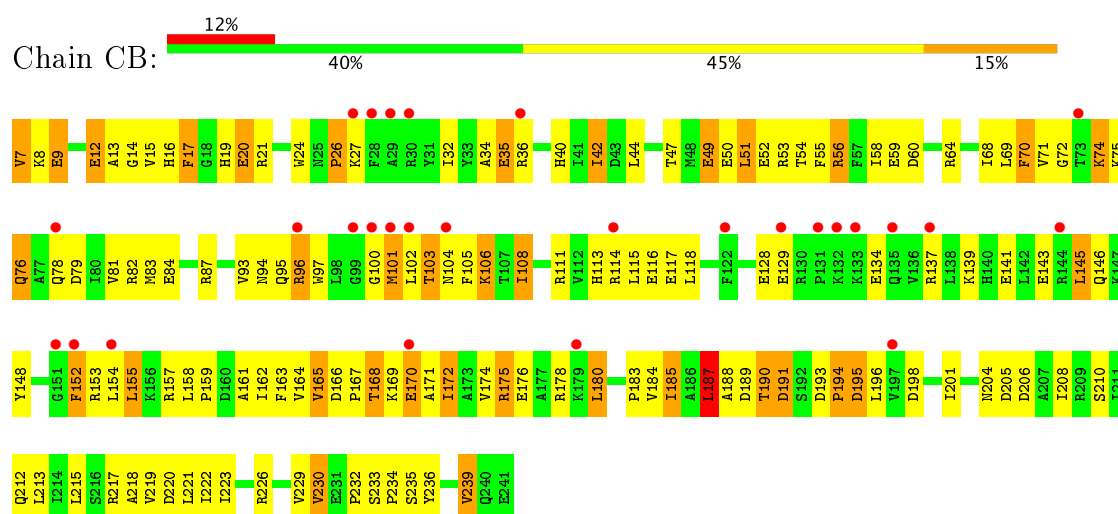
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

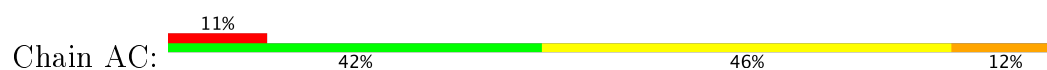
#### • Molecule 1: 30S ribosomal protein S2

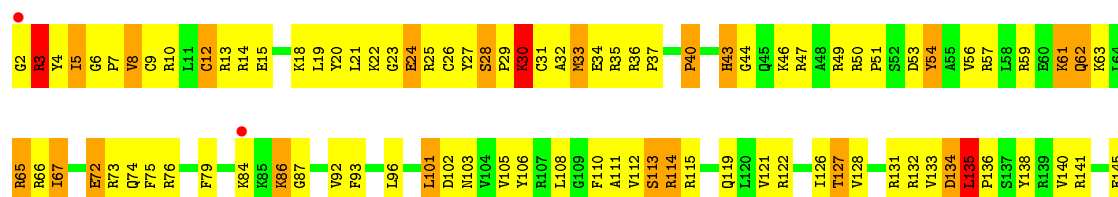


#### • Molecule 1: 30S ribosomal protein S2



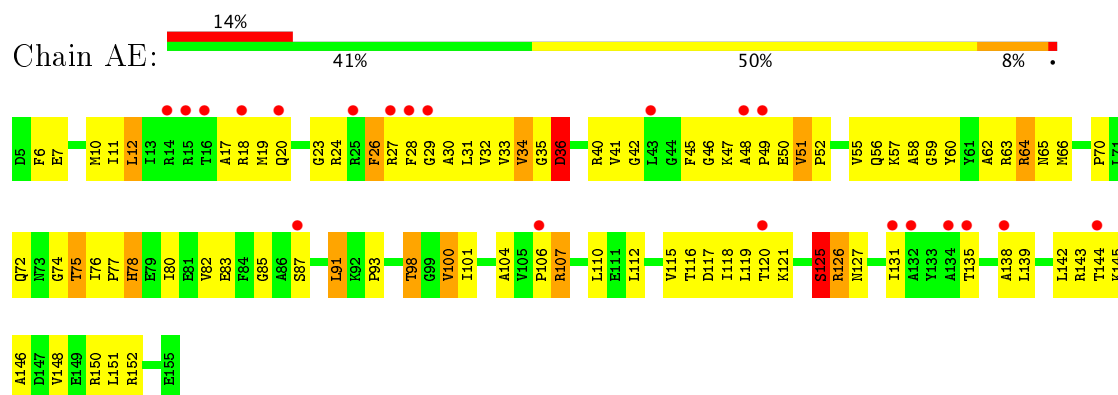
#### • Molecule 2: 30S ribosomal protein S3



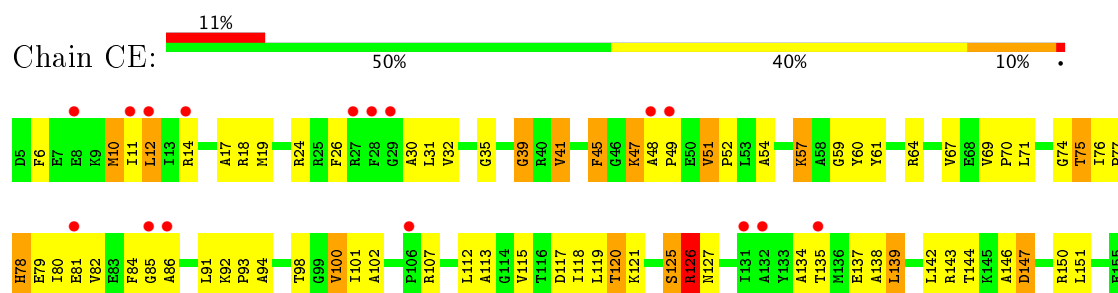




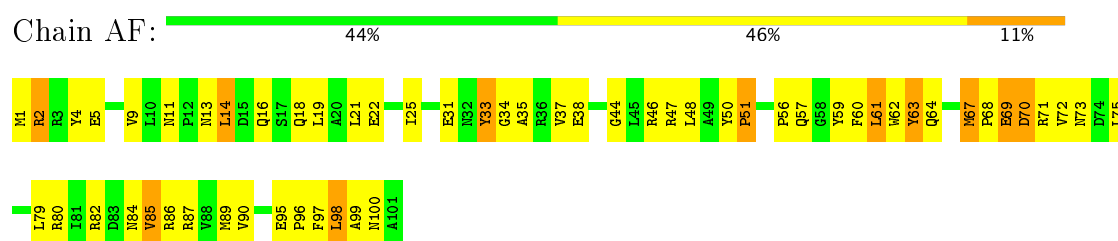
• Molecule 4: 30S ribosomal protein S5



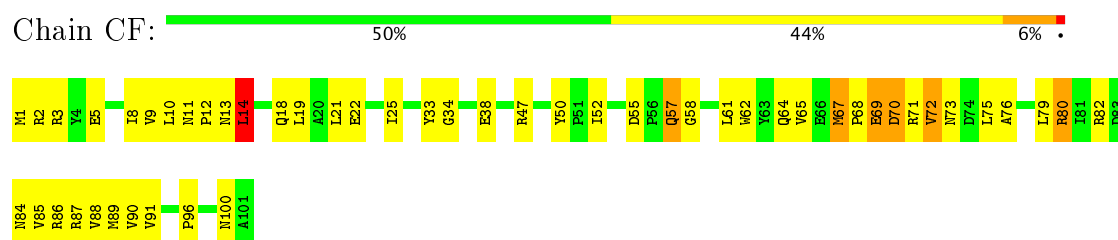
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6

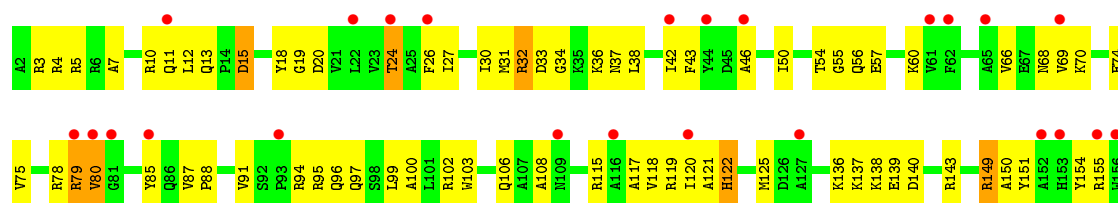


• Molecule 5: 30S ribosomal protein S6

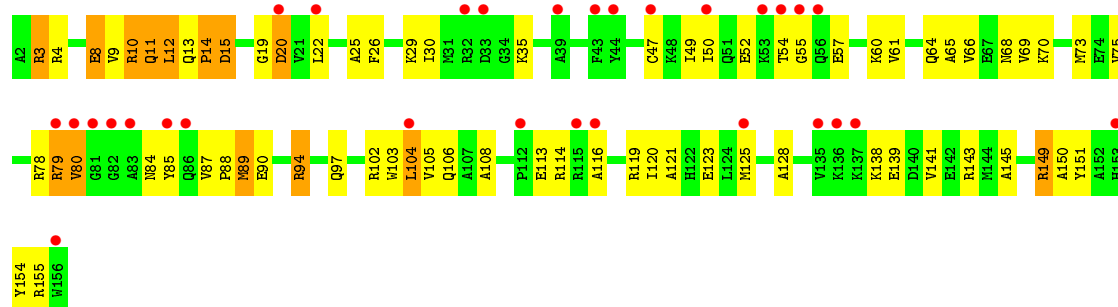


• Molecule 6: 30S ribosomal protein S7

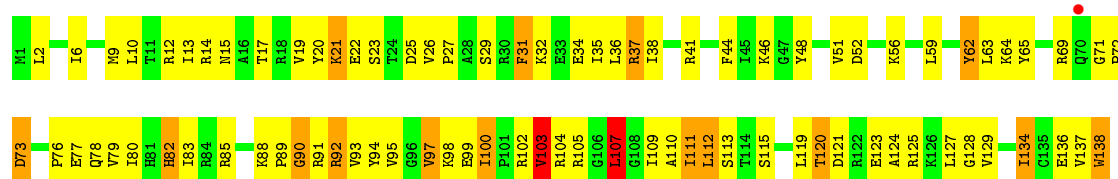
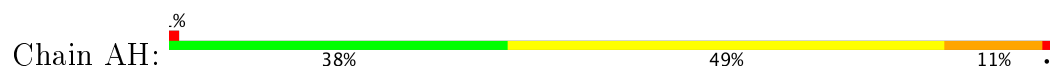




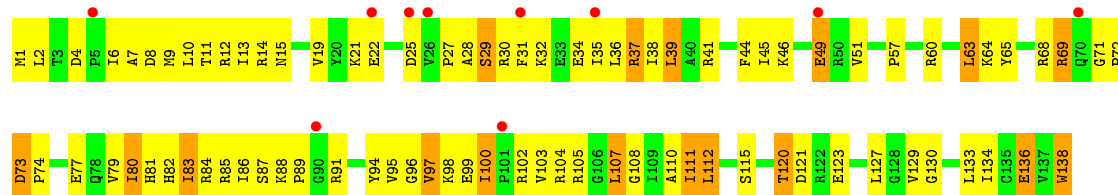
• Molecule 6: 30S ribosomal protein S7



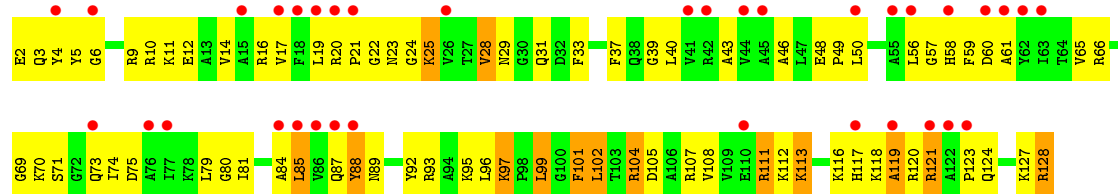
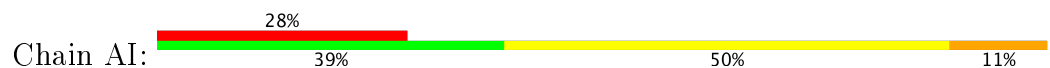
• Molecule 7: 30S ribosomal protein S8



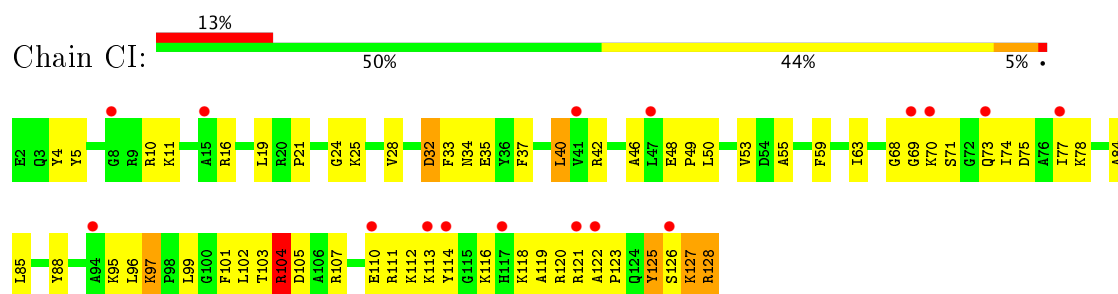
• Molecule 7: 30S ribosomal protein S8



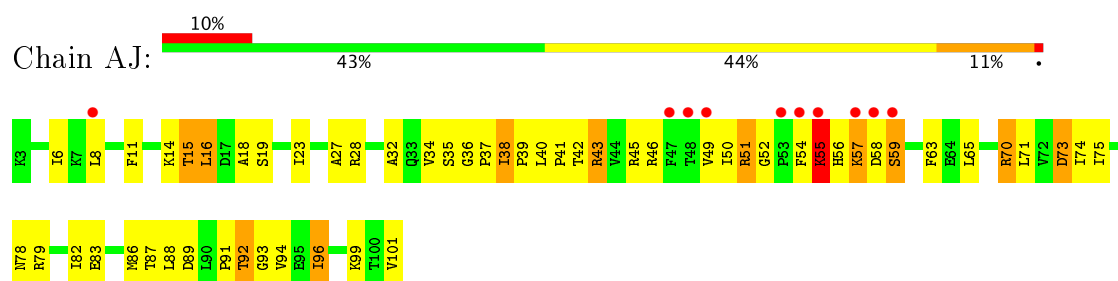
• Molecule 8: 30S ribosomal protein S9



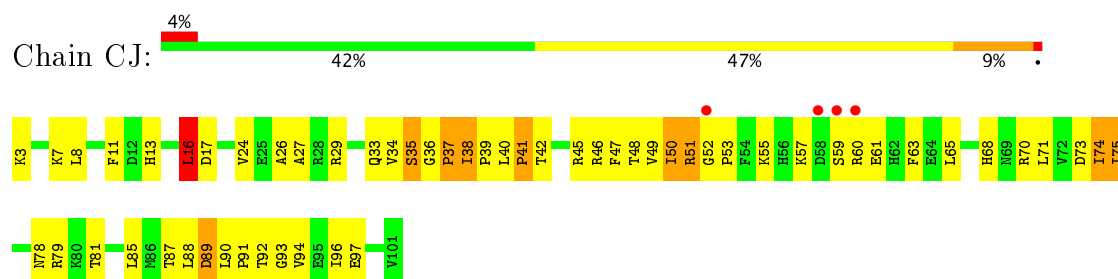
- Molecule 8: 30S ribosomal protein S9



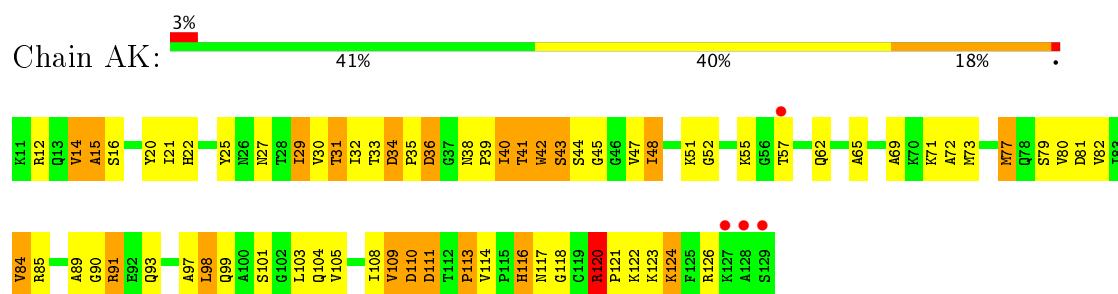
- Molecule 9: 30S ribosomal protein S10



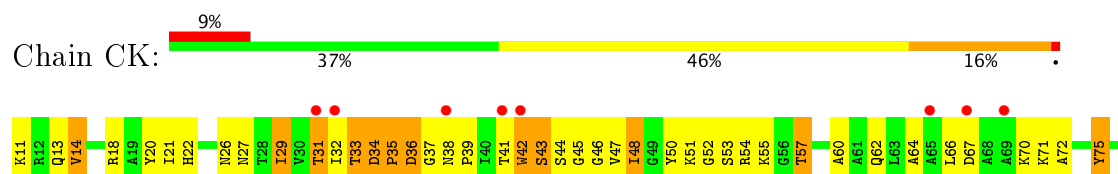
- Molecule 9: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S11

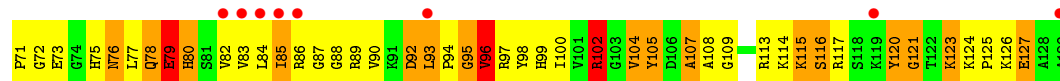
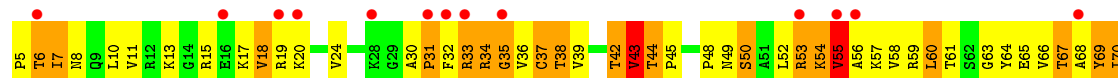


- Molecule 10: 30S ribosomal protein S11

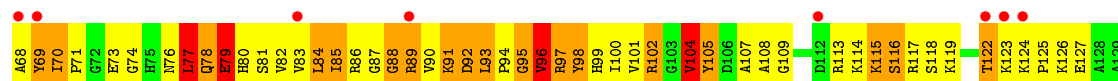
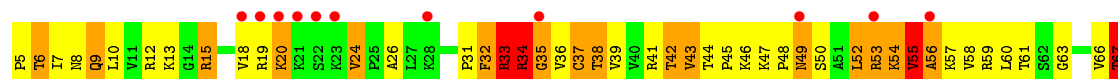
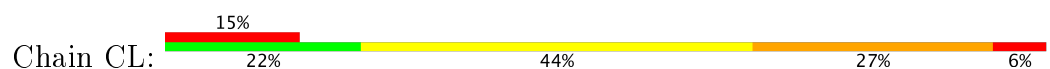




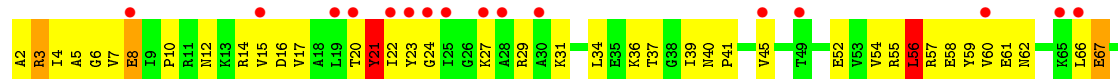
- Molecule 11: 30S ribosomal protein S12



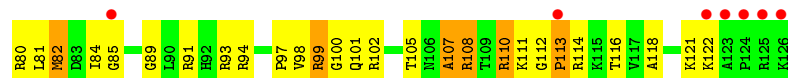
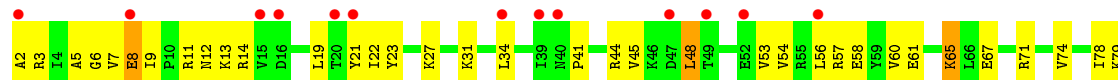
- Molecule 11: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S13



- Molecule 12: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S14 type Z



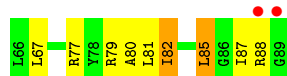
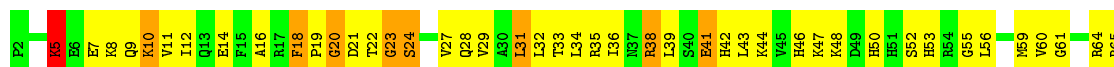




- Molecule 13: 30S ribosomal protein S14 type Z



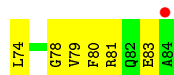
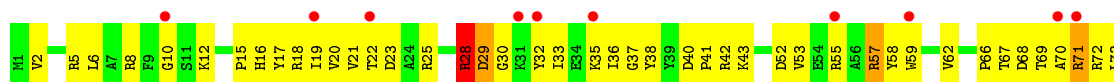
- Molecule 14: 30S ribosomal protein S15



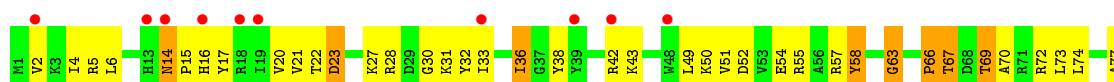
- Molecule 14: 30S ribosomal protein S15



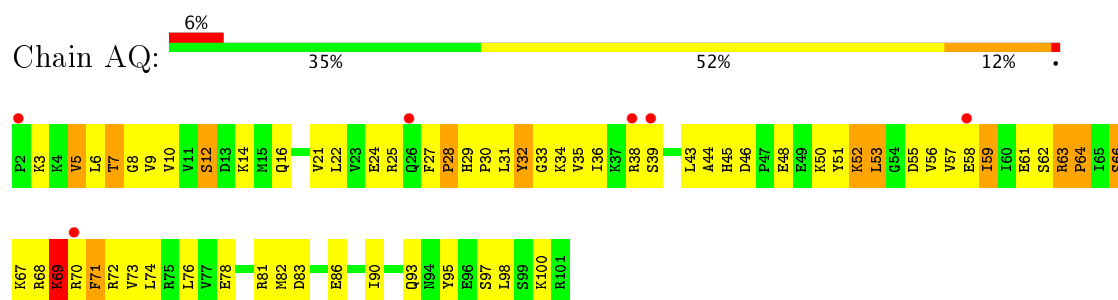
- Molecule 15: 30S ribosomal protein S16



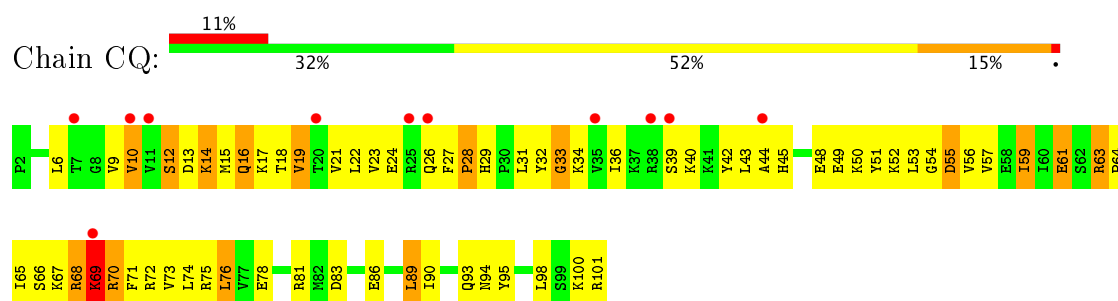
- Molecule 15: 30S ribosomal protein S16



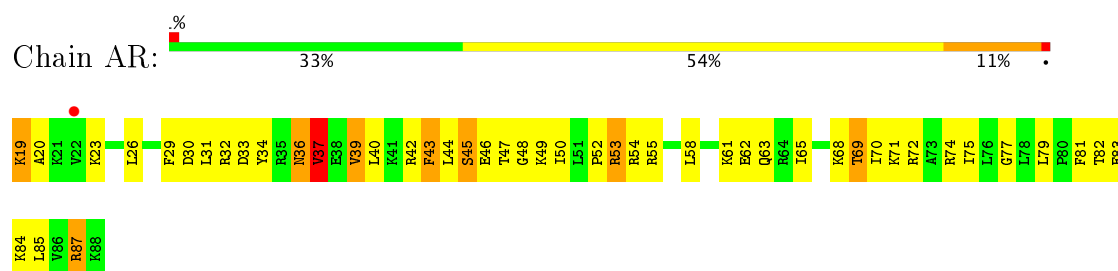
- Molecule 16: 30S ribosomal protein S17



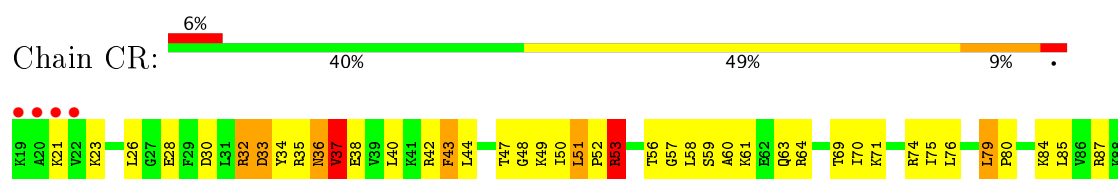
- Molecule 16: 30S ribosomal protein S17



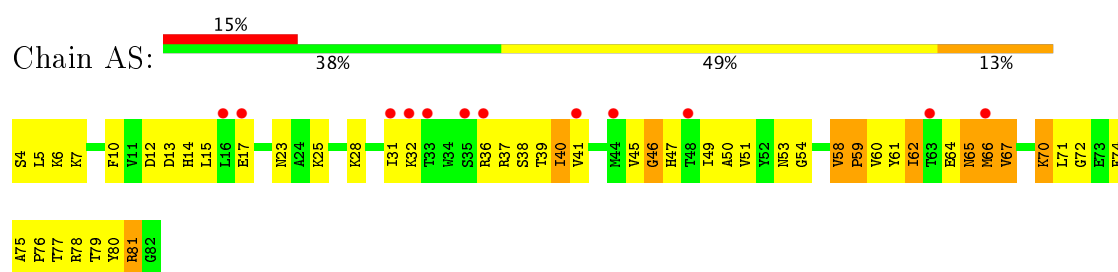
- Molecule 17: 30S ribosomal protein S18



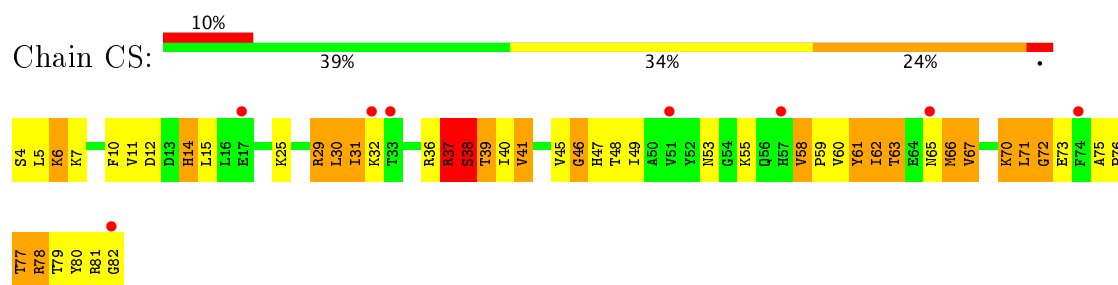
- Molecule 17: 30S ribosomal protein S18



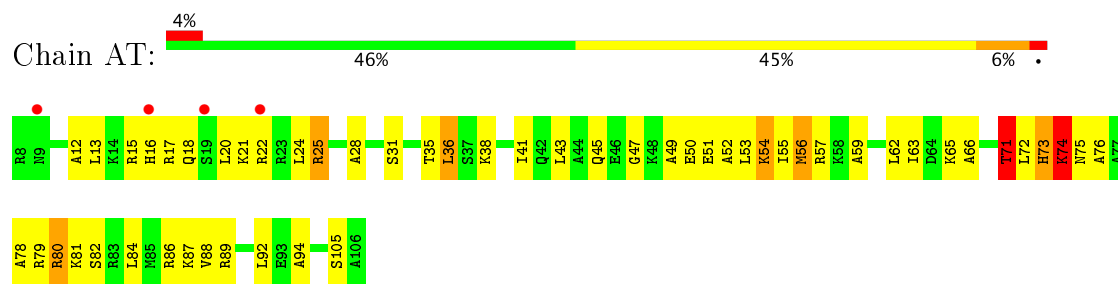
- Molecule 18: 30S ribosomal protein S19



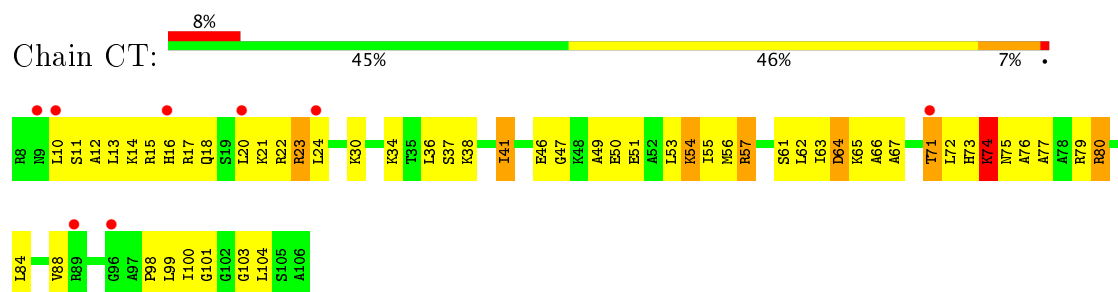
- Molecule 18: 30S ribosomal protein S19



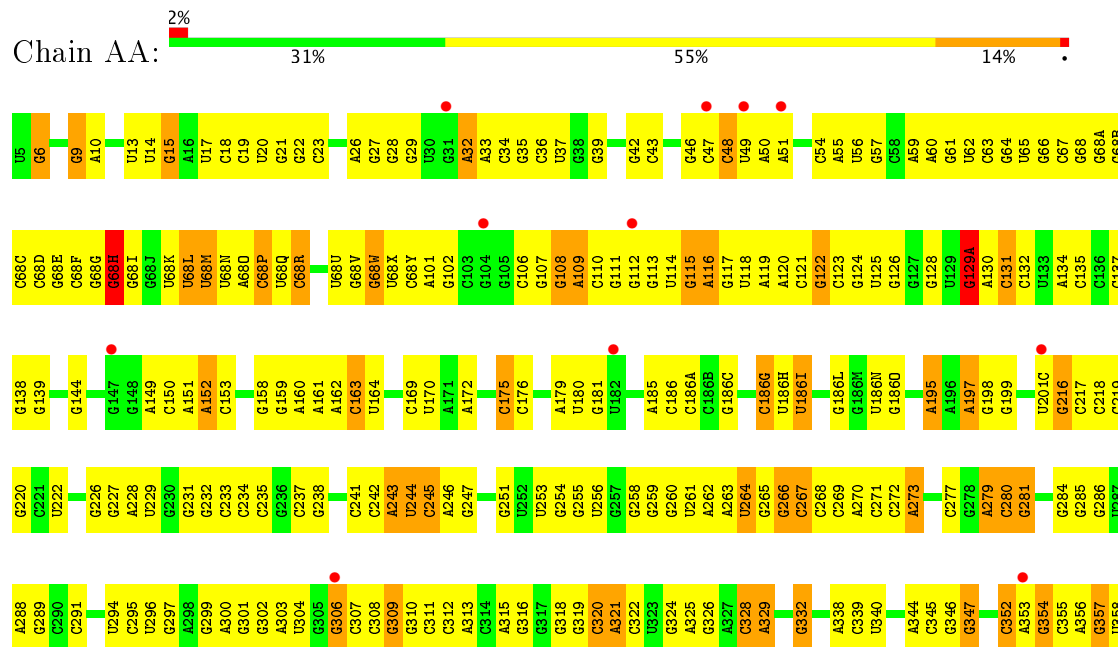
• Molecule 19: 30S ribosomal protein S20



• Molecule 19: 30S ribosomal protein S20

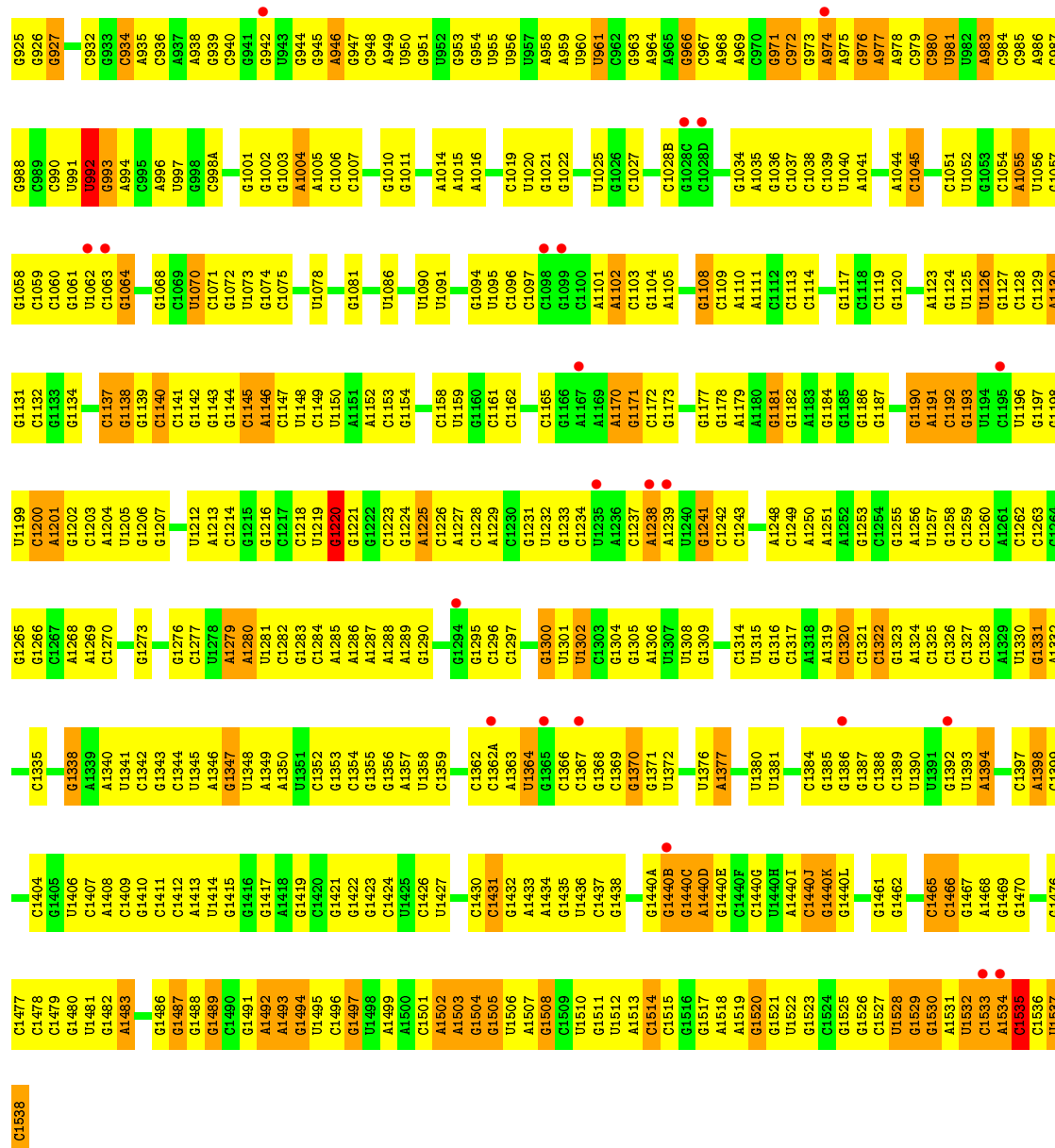


• Molecule 20: ribosomal RNA 16S



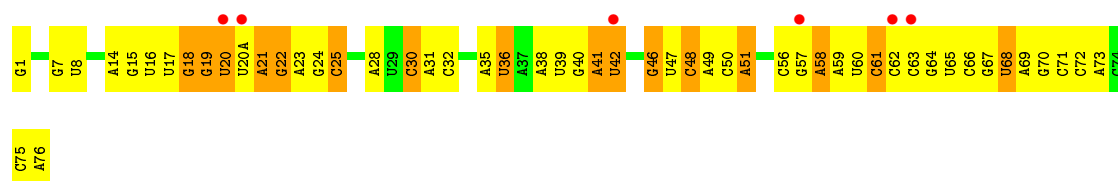
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U1345	U1278	G1134	G1066	A994	G933	A767	G629	G567	G505	A428	A363
A1346	A1279	U1135	A1067	C934	C934	A768	G630	G568	G506	U429	U364
G1347	U1280	U1136	G1068	U997	A935	G769	G631	G569	C507	A431	U365
U1348	U1281	G1137	G1069	G998	C936	A770	G632	C570	C508	A432	G366
A1349	U1282	G1138	U1070	C998A	A937	G771	G633	G571	A509	A433	U367
G1350	U1283	G1139	G1071	U999	A938	A772	G634	G572	A510	C433	U368
A1351	A1284	G1140	G1072	A1000	A939	G773	G635	A573	C511	U434	G369
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C1354	A1287	G1143	G1075	G1003	C942	A781	U641	G576	G514	U437	C372
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G1361	C1226	U1150	G1082	A1016	A949	U793	G653	U583	C522	G447	A383
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A1363	A1228	A1152	U1084	C1018	G951	C789	G655	G585	G524	C449	C385
U1364	A1229	C1153	U1085	U1019	U952	G795	U656	G586	C525	C450	C386
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G1365	G1231	G1154	U1085	G1021	G954	A801	G658	G588	C527	A453	G388
G1366	G1304	A1157	U1090	U1025	U955	A802	G659	C589	C528	C454	A389
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G1368	U1235	U1159	A1092	U1026	U957	A807	G664	G591	G530	A456	G391
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G1370	A1238	U1095	G1094	G1028E	U961	C811	G666	G593	U532	A458	A383
C1371	A1239	C1096	U1095	U1036	U962	C812	G667	C596	A532	C459	C395
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G1373	G1241	U1098	C1098	A1035	G964	C814	U669	U598	U534	A458B	A397
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A1381	G1252	G1182	G1108	A1044	C972	G821	U678	A607	G544	U480	G406
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A1394	C1262	G1192	C1116	U1052	G980	G830	U686	C615	U552	C489	A414
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G1400	A1270	G1197	G1057	C1057	G985	U835	G691	C620	G557	U494	C419
A1401	C1271	G1198	G1058	G1058	A986	G836	G692	A621	U558	A495	U420
C1402	U1271	U1199	C1059	C1060	G987	C924	U757	G622	A559	A497	U421
A1403	A1274	C1200	U1125	U1060	G988	G925	G693	C623	U560	U498	G422
C1404	U1341	A1201	U1126	G1061	G989	G926	A694	C624	U561	A499	G423
G1405	C1342	G1202	C1127	U1062	C990	G927	A695	G625	C562	C501	G424
		C1128	U1128	U1062	C990	G927	A696	G626	C563	G502	G425
		C1129	C1129	C1063	U991	C930	U697	U626	A563		



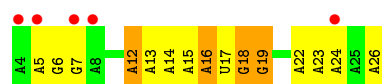


• Molecule 21: transfer RNA

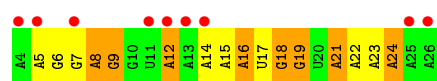
• Molecule 21: transfer RNA



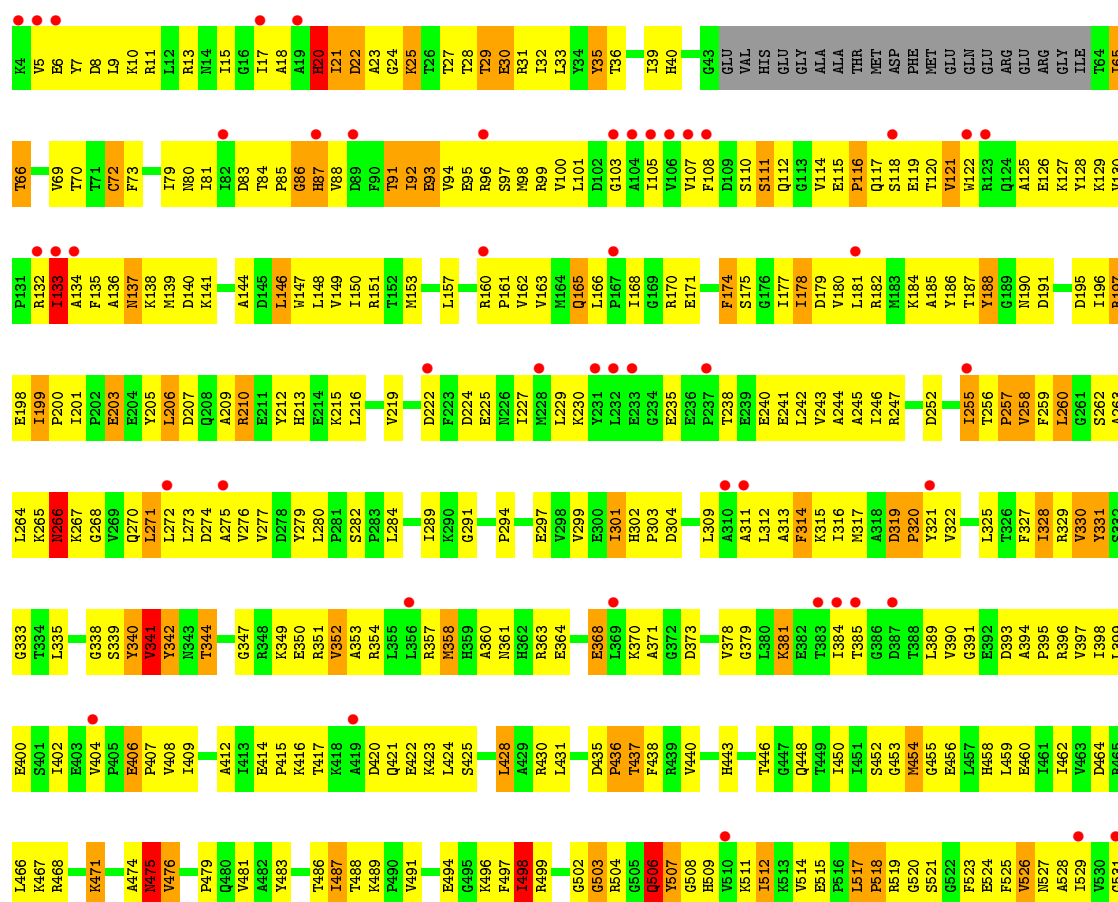
- Molecule 22: messenger RNA

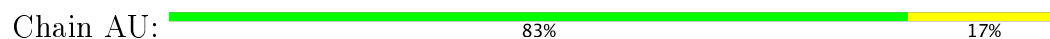


- Molecule 22: messenger RNA



- Molecule 23: Elongation factor G





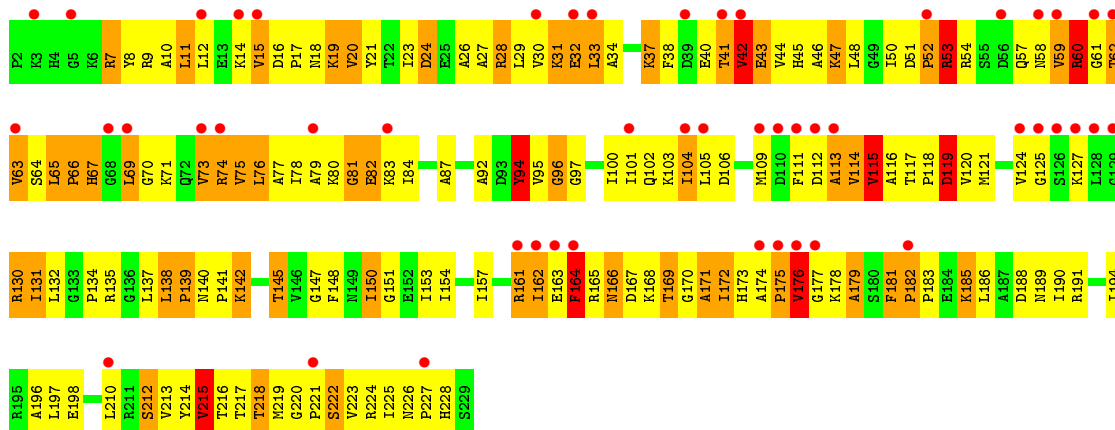




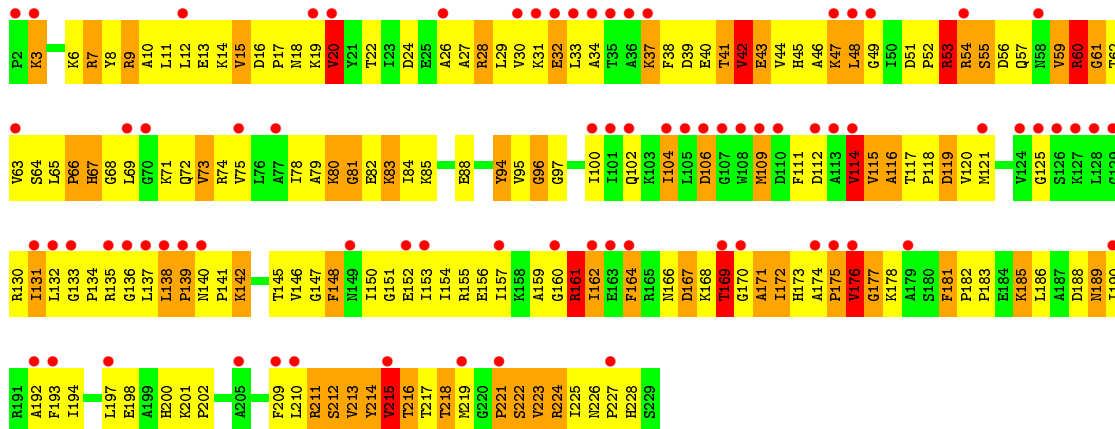
• Molecule 24: VIOMYCIN



• Molecule 25: 50S ribosomal protein L1

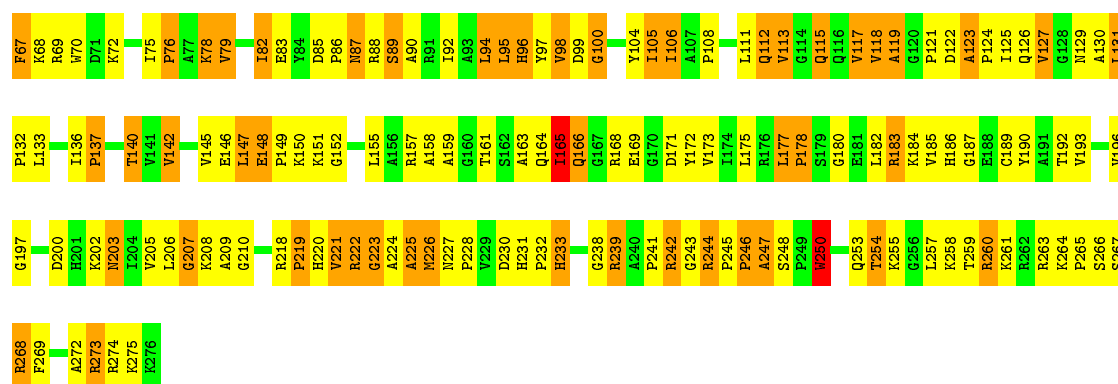


• Molecule 25: 50S ribosomal protein L1

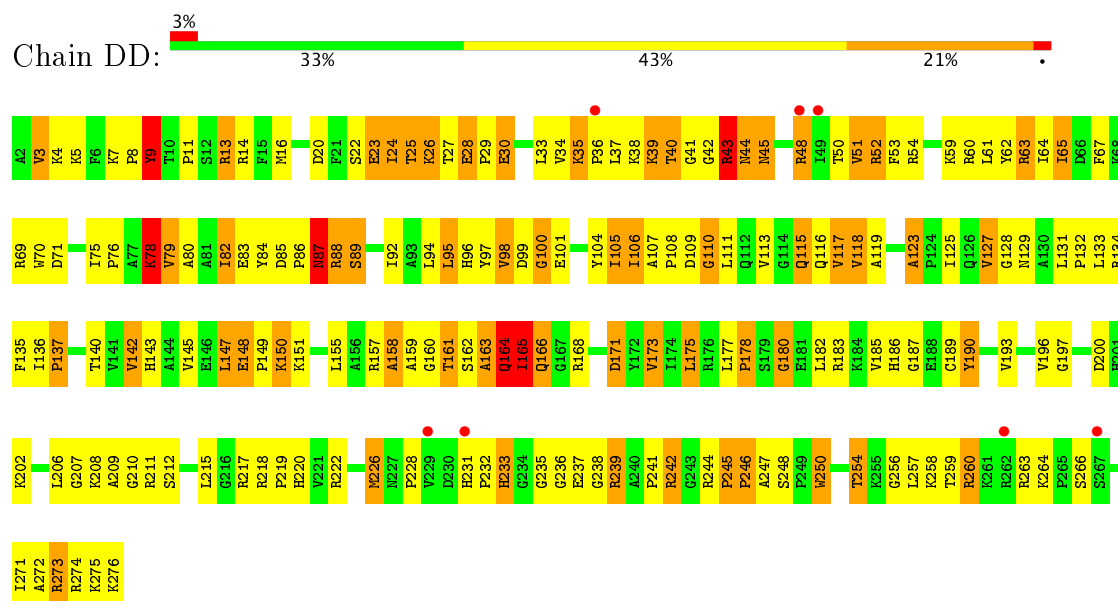


• Molecule 26: 50S ribosomal protein L2

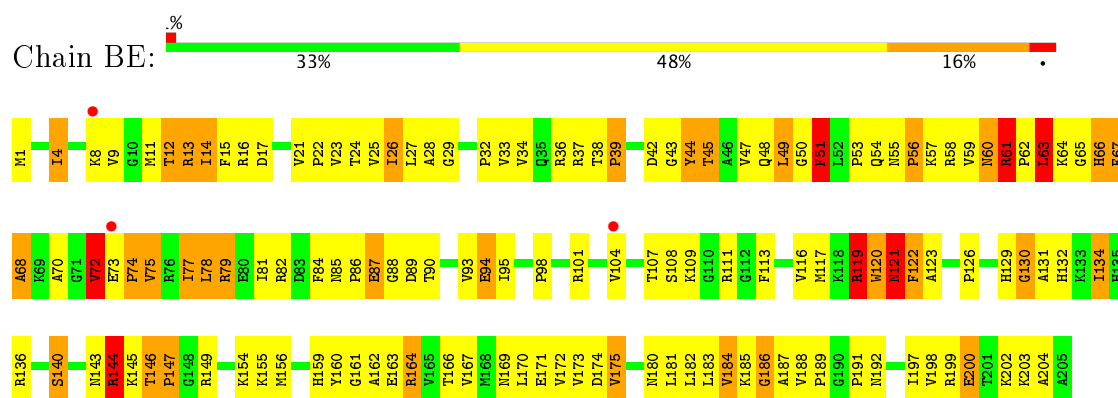




- Molecule 26: 50S ribosomal protein L2

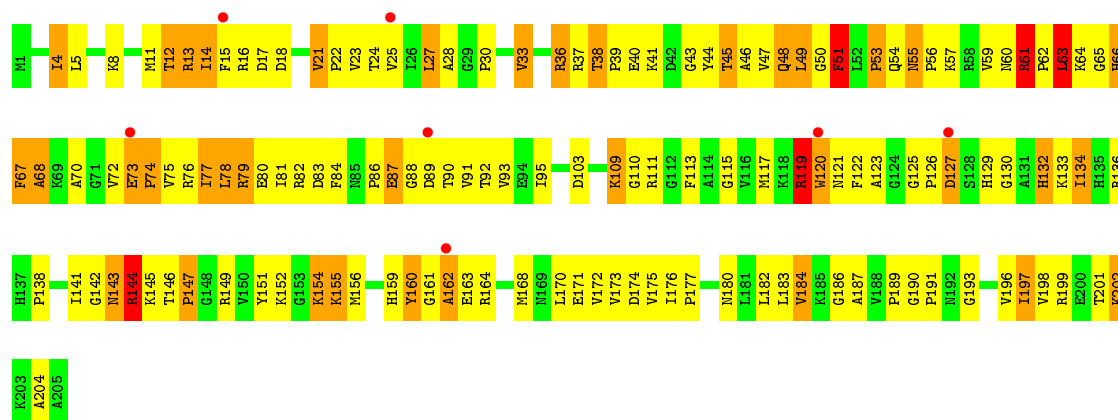


- Molecule 27: 50S ribosomal protein L3

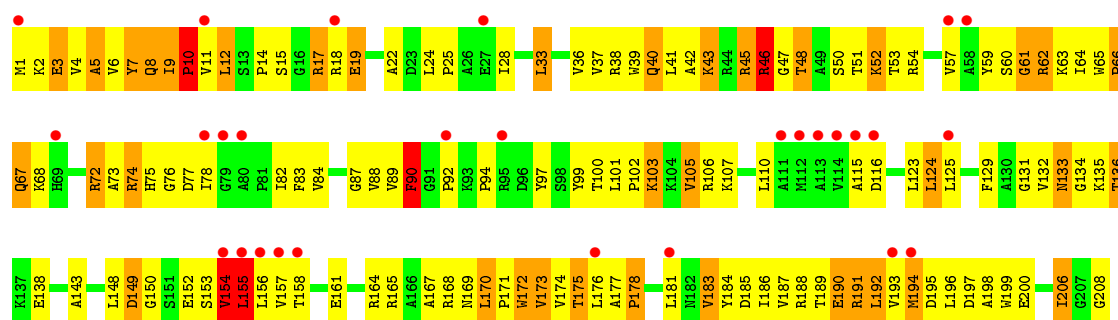


- Molecule 27: 50S ribosomal protein L3

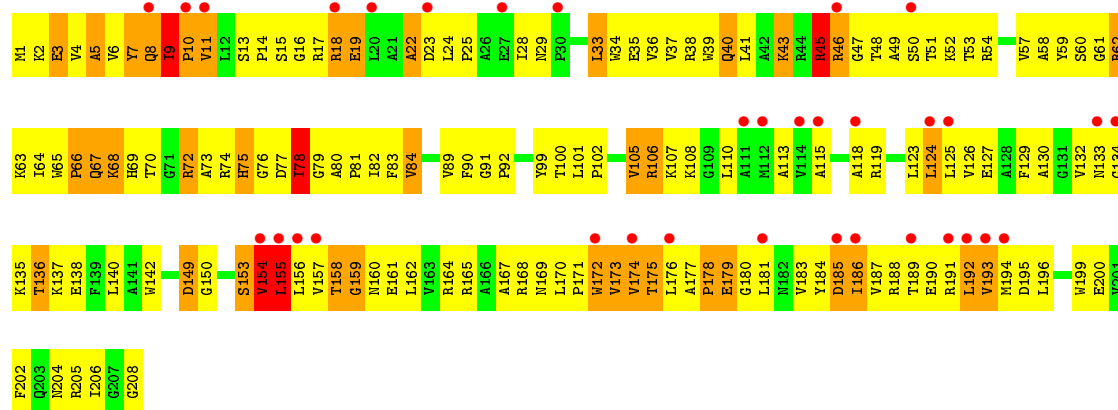




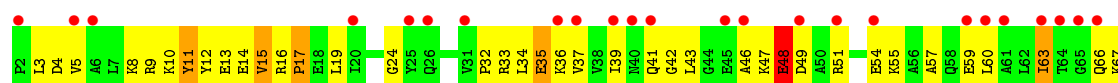
• Molecule 28: 50S ribosomal protein L4

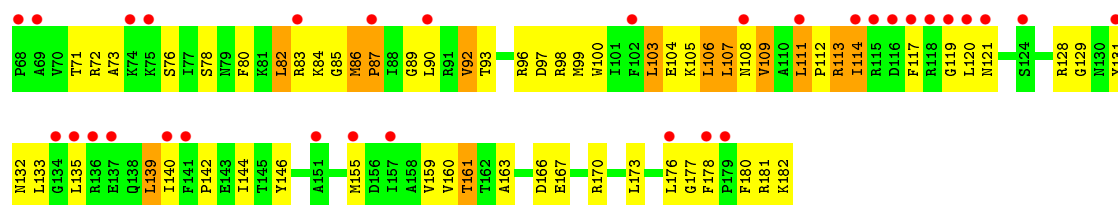


• Molecule 28: 50S ribosomal protein L4

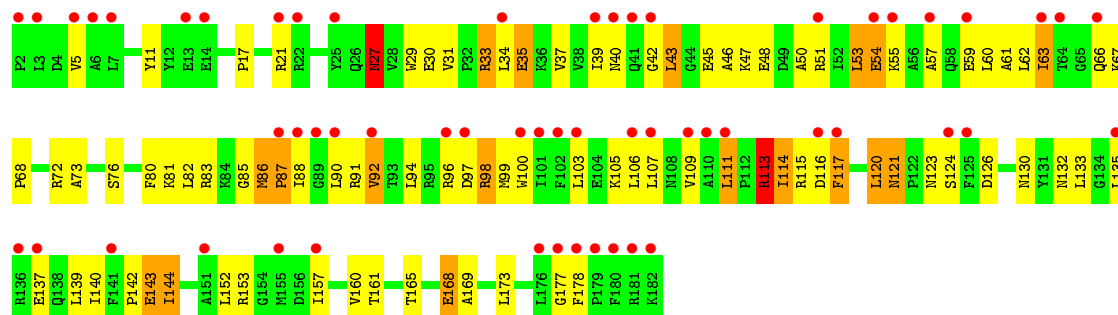


• Molecule 29: 50S ribosomal protein L5

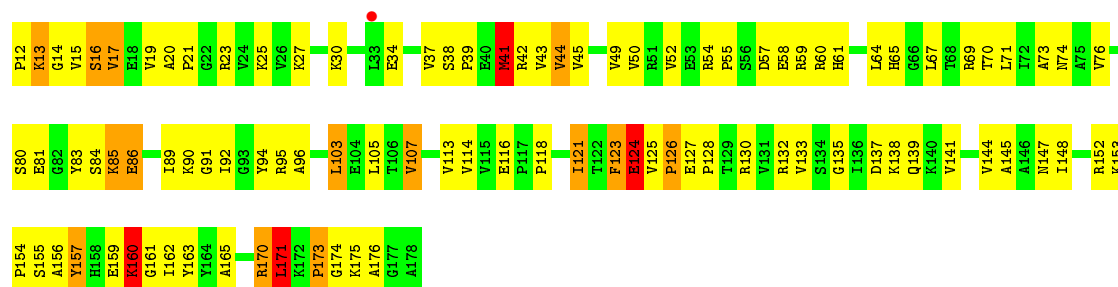




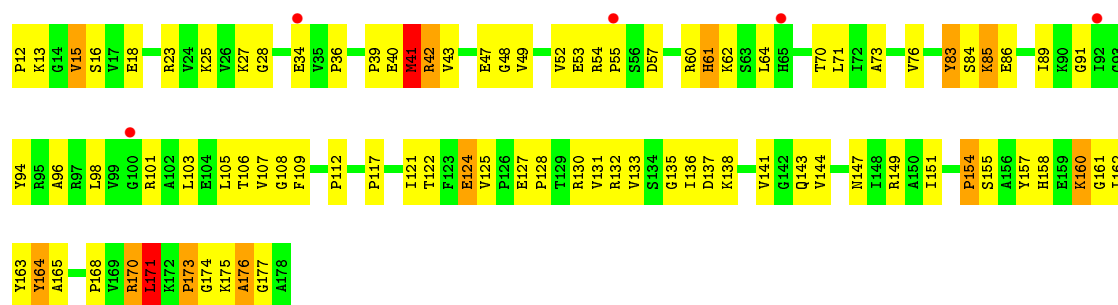
• Molecule 29: 50S ribosomal protein L5



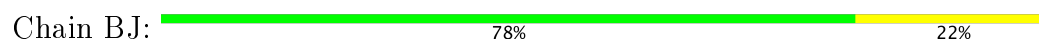
• Molecule 30: 50S ribosomal protein L6



• Molecule 30: 50S ribosomal protein L6



• Molecule 31: 50S RIBOSOMAL PROTEIN L10



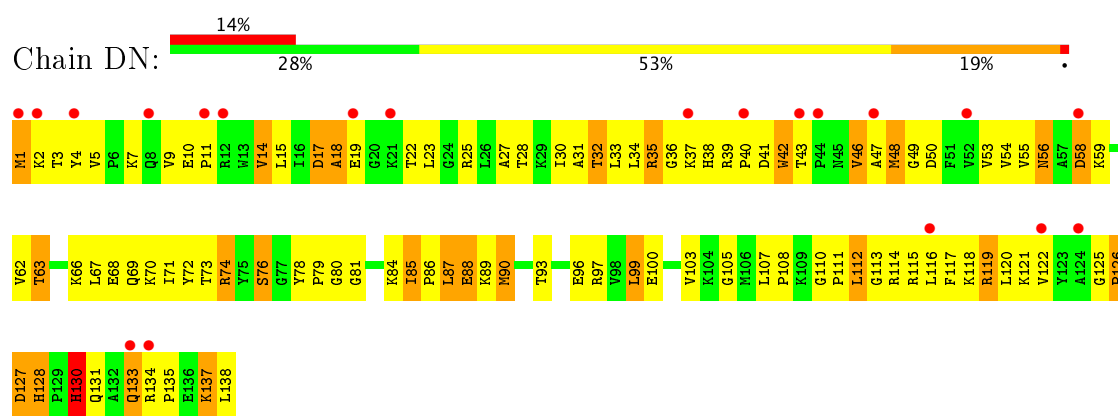
- Molecule 31: 50S RIBOSOMAL PROTEIN L10

- Molecule 32: 50S ribosomal protein L11

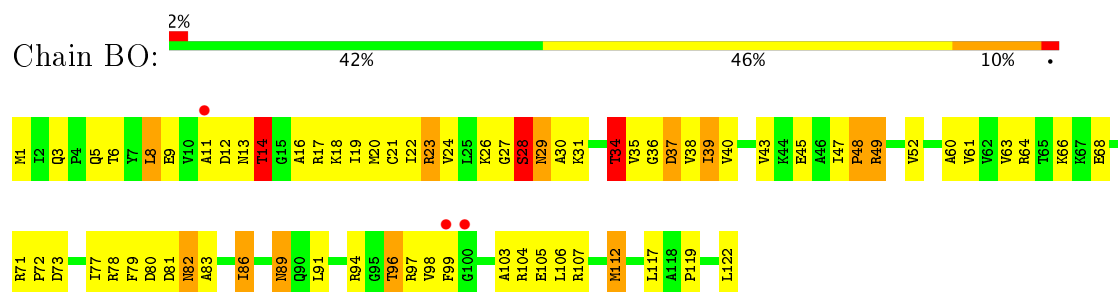
- Molecule 32: 50S ribosomal protein L11

- Molecule 33: 50S ribosomal protein L13

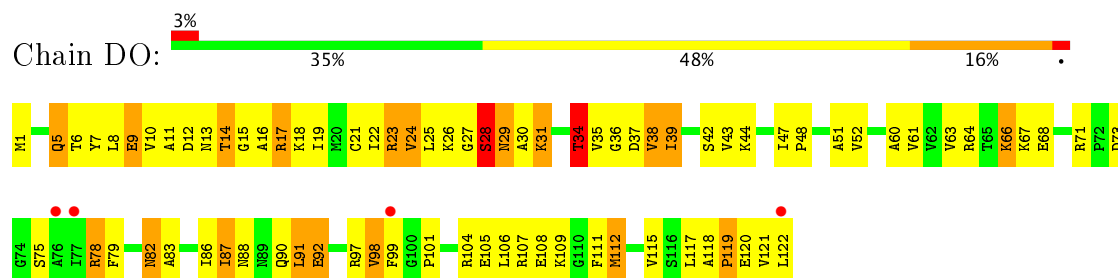
- Molecule 33: 50S ribosomal protein L13



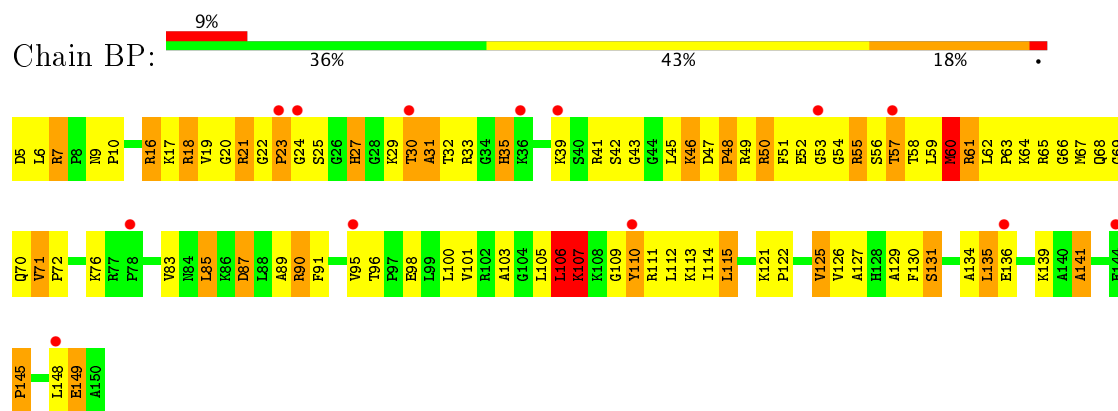
• Molecule 34: 50S ribosomal protein L14



• Molecule 34: 50S ribosomal protein L14

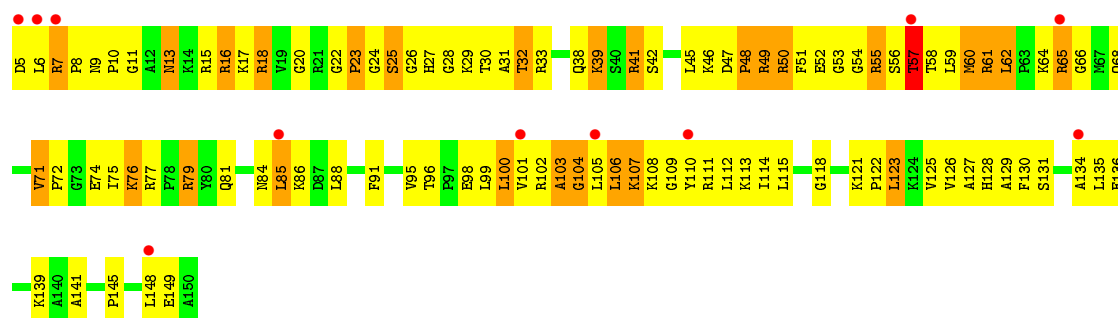


• Molecule 35: 50S ribosomal protein L15

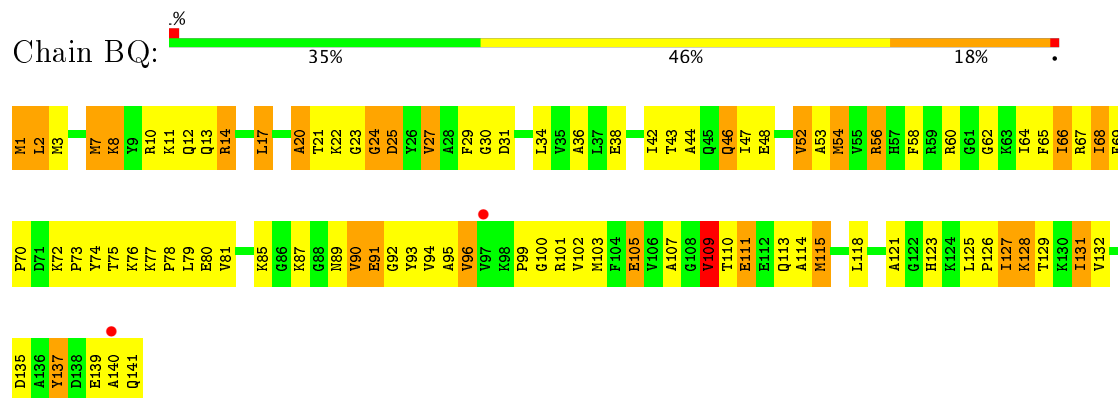


• Molecule 35: 50S ribosomal protein L15

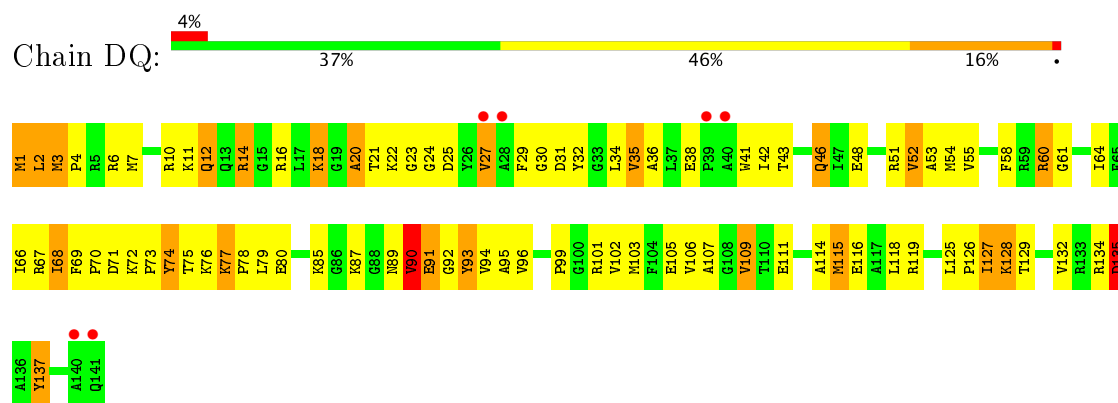




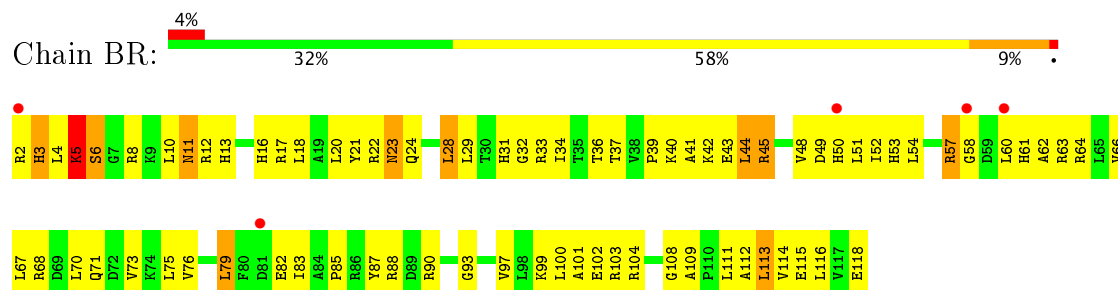
- Molecule 36: 50S ribosomal protein L16



- Molecule 36: 50S ribosomal protein L16

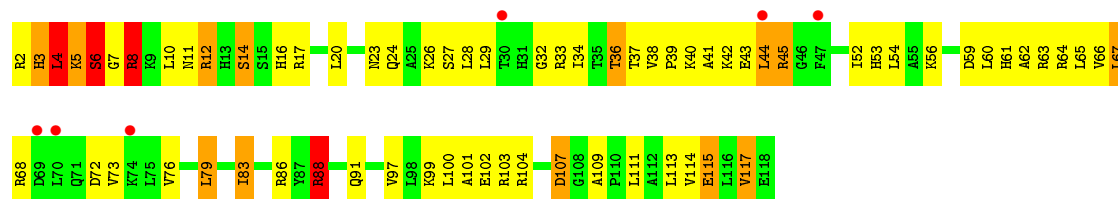


- Molecule 37: 50S ribosomal protein L17

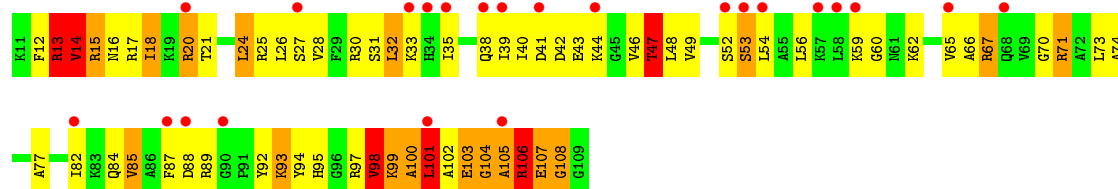


- Molecule 37: 50S ribosomal protein L17

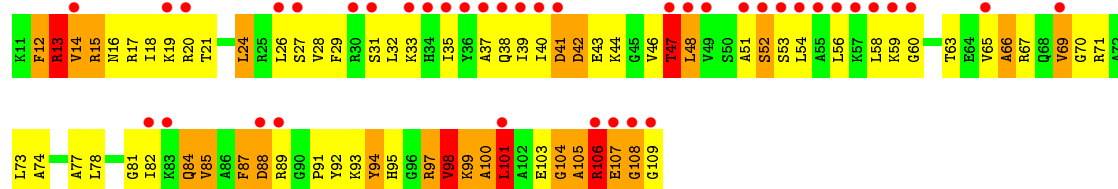




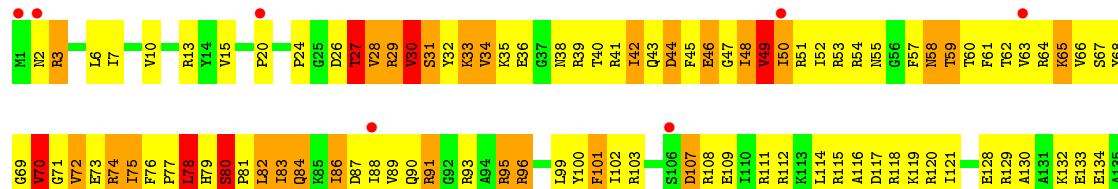
• Molecule 38: 50S ribosomal protein L18



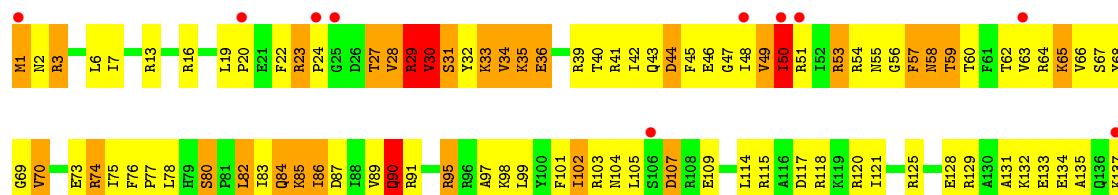
• Molecule 38: 50S ribosomal protein L18



• Molecule 39: 50S ribosomal protein L19



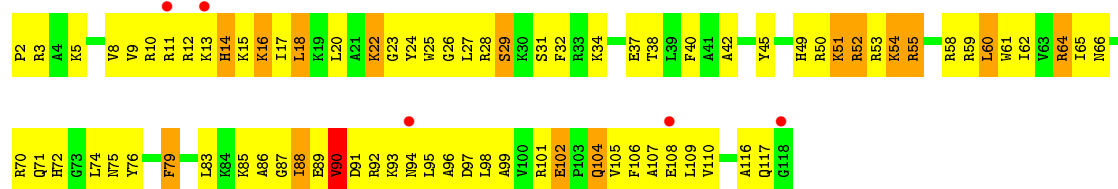
• Molecule 39: 50S ribosomal protein L19



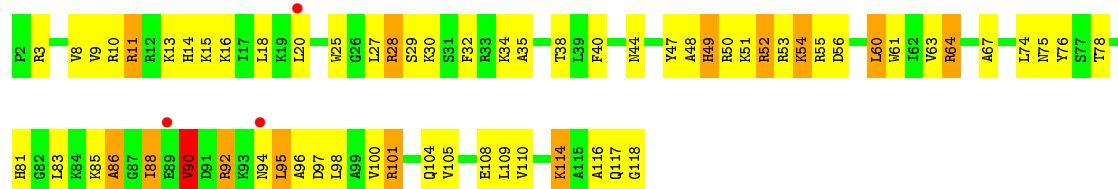




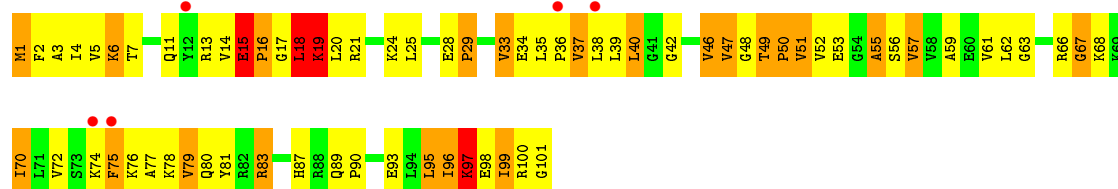
- Molecule 40: 50S ribosomal protein L20



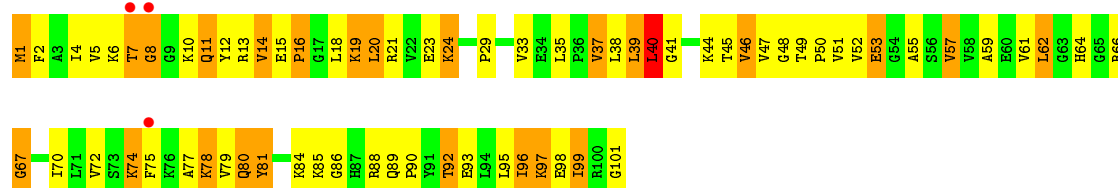
- Molecule 40: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L21

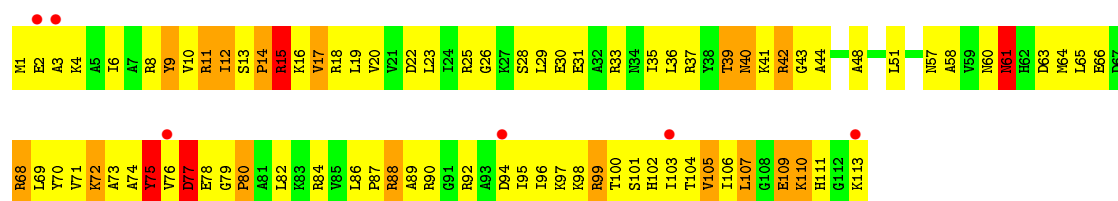


- Molecule 41: 50S ribosomal protein L21

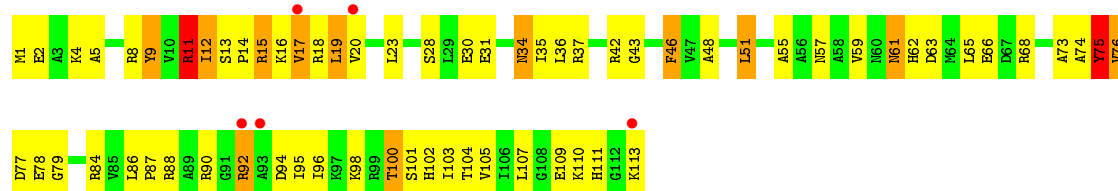


- Molecule 42: 50S ribosomal protein L22

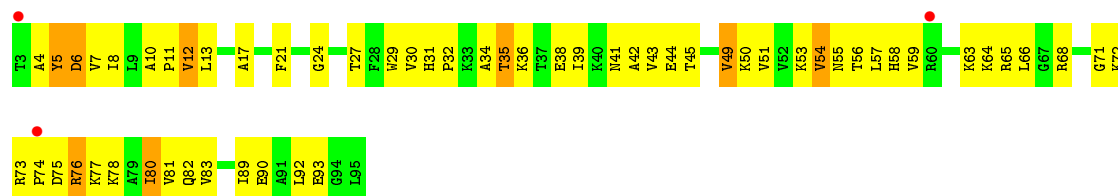




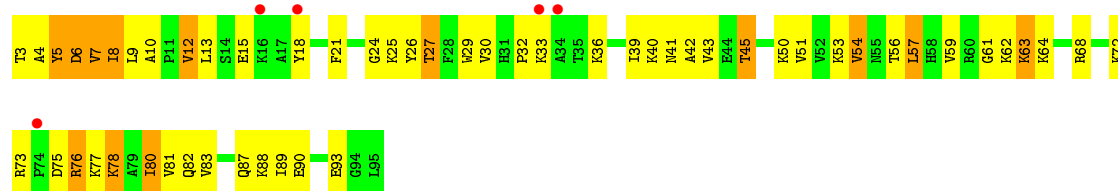
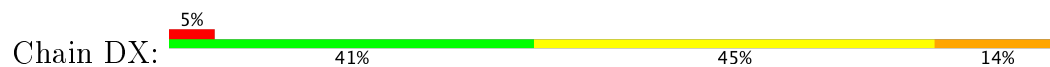
• Molecule 42: 50S ribosomal protein L22



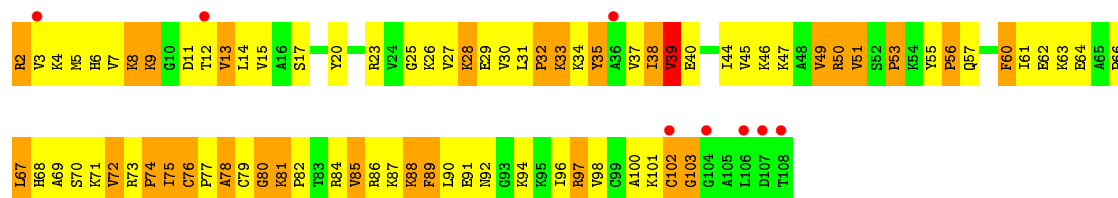
• Molecule 43: 50S ribosomal protein L23



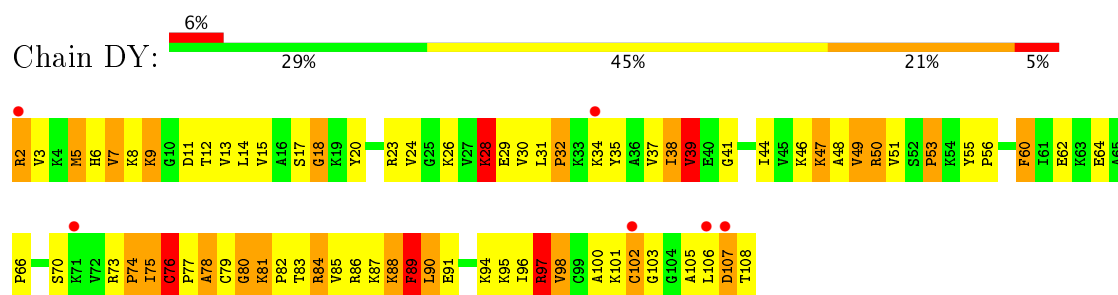
• Molecule 43: 50S ribosomal protein L23



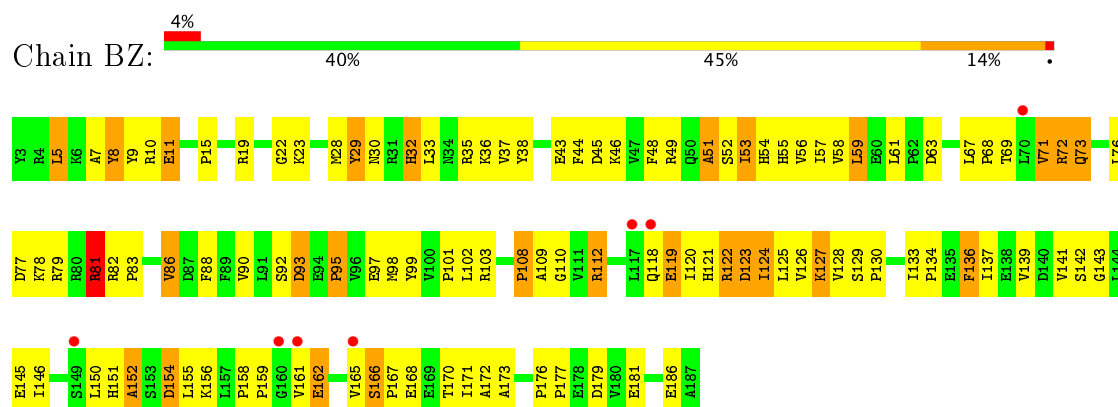
• Molecule 44: 50S ribosomal protein L24



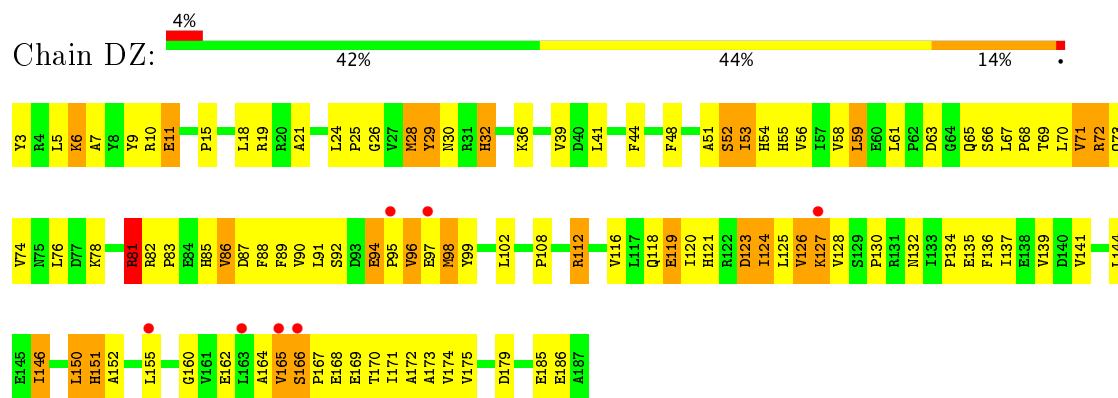
• Molecule 44: 50S ribosomal protein L24



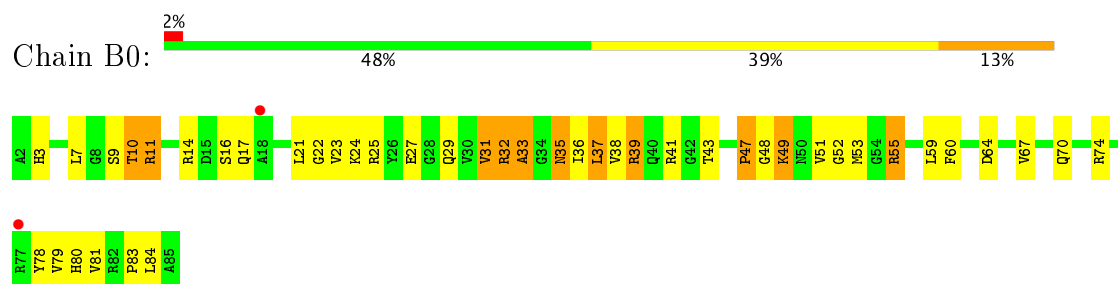
• Molecule 45: 50S ribosomal protein L25



• Molecule 45: 50S ribosomal protein L25

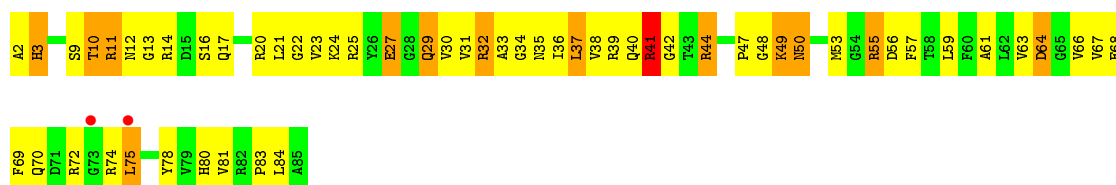


• Molecule 46: 50S ribosomal protein L27



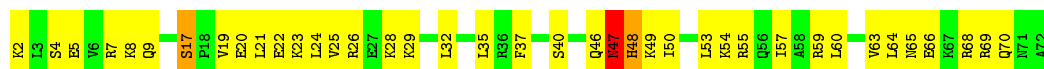
• Molecule 46: 50S ribosomal protein L27





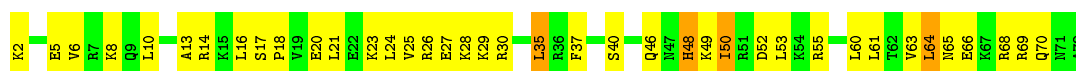
• Molecule 47: 50S ribosomal protein L29

Chain B2: 45% 51%



• Molecule 47: 50S ribosomal protein L29

Chain D2: 45% 49% 6%



• Molecule 48: 50S ribosomal protein L30

Chain B3: 58% 30% 8%



• Molecule 48: 50S ribosomal protein L30

Chain D3: 53% 35% 12%



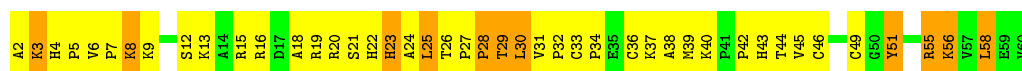
• Molecule 49: 50S ribosomal protein L32

Chain B5: 2% 32% 54% 12%



• Molecule 49: 50S ribosomal protein L32

Chain D5: 25% 56% 19%

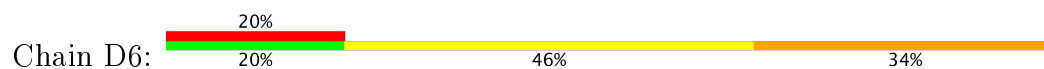


• Molecule 50: 50S ribosomal protein L33

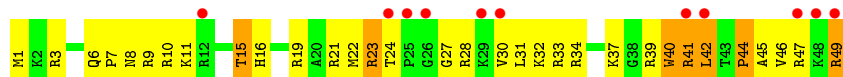
Chain B6: 8% 32% 50% 10% 8%



- Molecule 50: 50S ribosomal protein L33



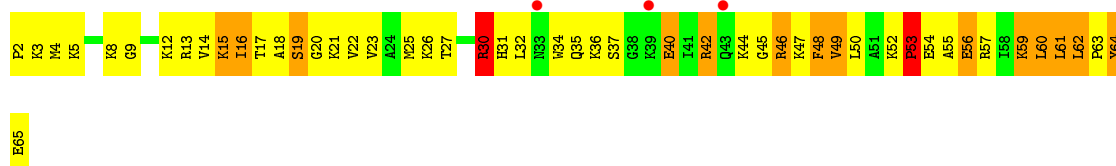
- Molecule 51: 50S ribosomal protein L34



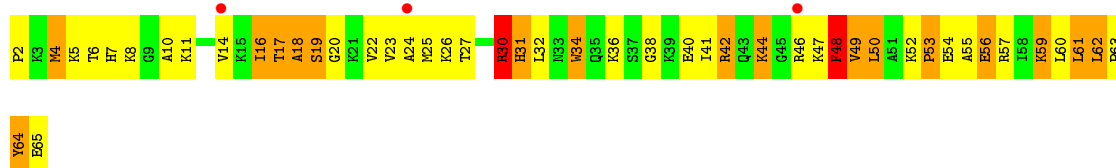
- Molecule 51: 50S ribosomal protein L34



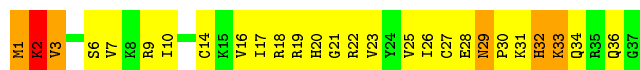
- Molecule 52: 50S ribosomal protein L35



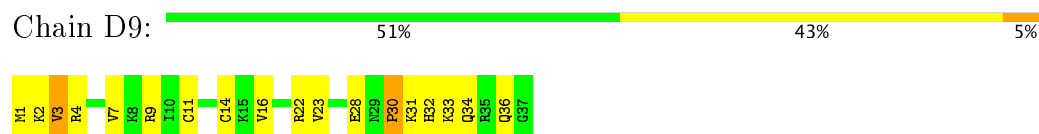
- Molecule 52: 50S ribosomal protein L35



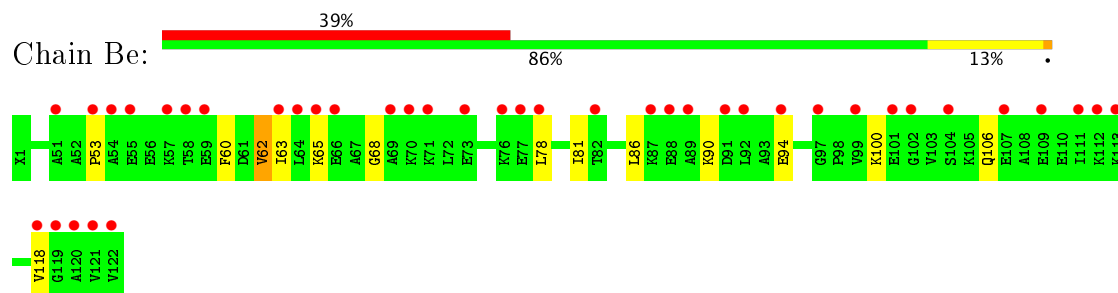
- Molecule 53: 50S ribosomal protein L36



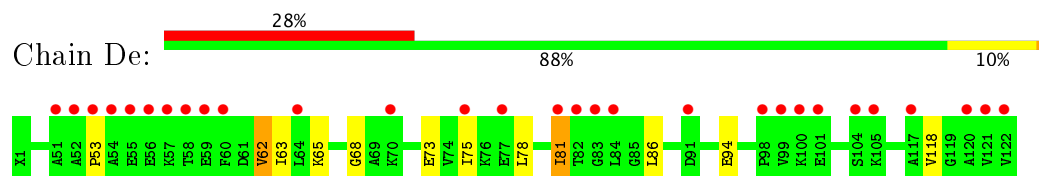
- Molecule 53: 50S ribosomal protein L36



- Molecule 54: 50S ribosomal protein L7/L12



- Molecule 54: 50S ribosomal protein L7/L12



- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12



There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12



There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12



There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12



There are no outlier residues recorded for this chain.

- Molecule 56: 50S RIBOSOMAL PROTEIN L7/L12



There are no outlier residues recorded for this chain.

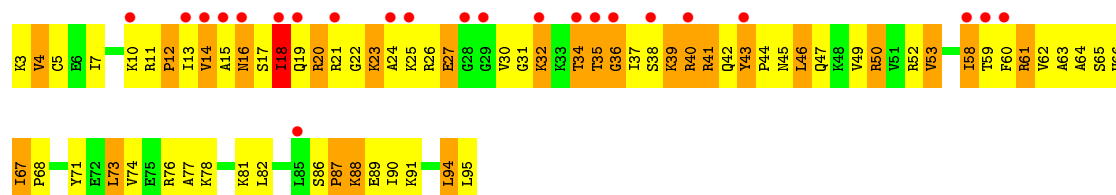
- Molecule 56: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dh:  100%

There are no outlier residues recorded for this chain.

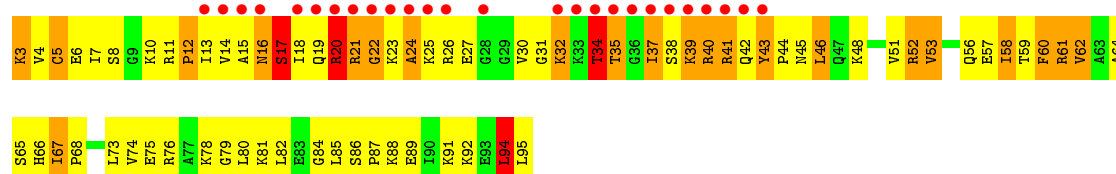
- Molecule 57: 50S ribosomal protein L28

Chain B1:  25% 47% 27% .



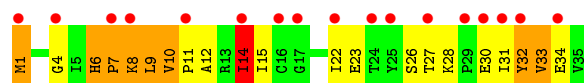
- Molecule 57: 50S ribosomal protein L28

Chain D1:  28% 52% 24% .



- Molecule 58: 50S ribosomal protein L31

Chain B4:  49% 40% 23% .



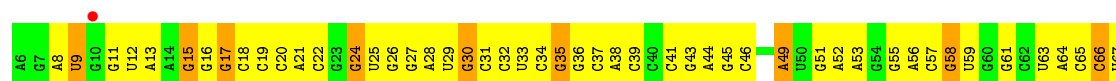
- Molecule 58: 50S ribosomal protein L31

Chain D4:  66% 46% 37% 14% .



- Molecule 59: 23S ribosomal RNA

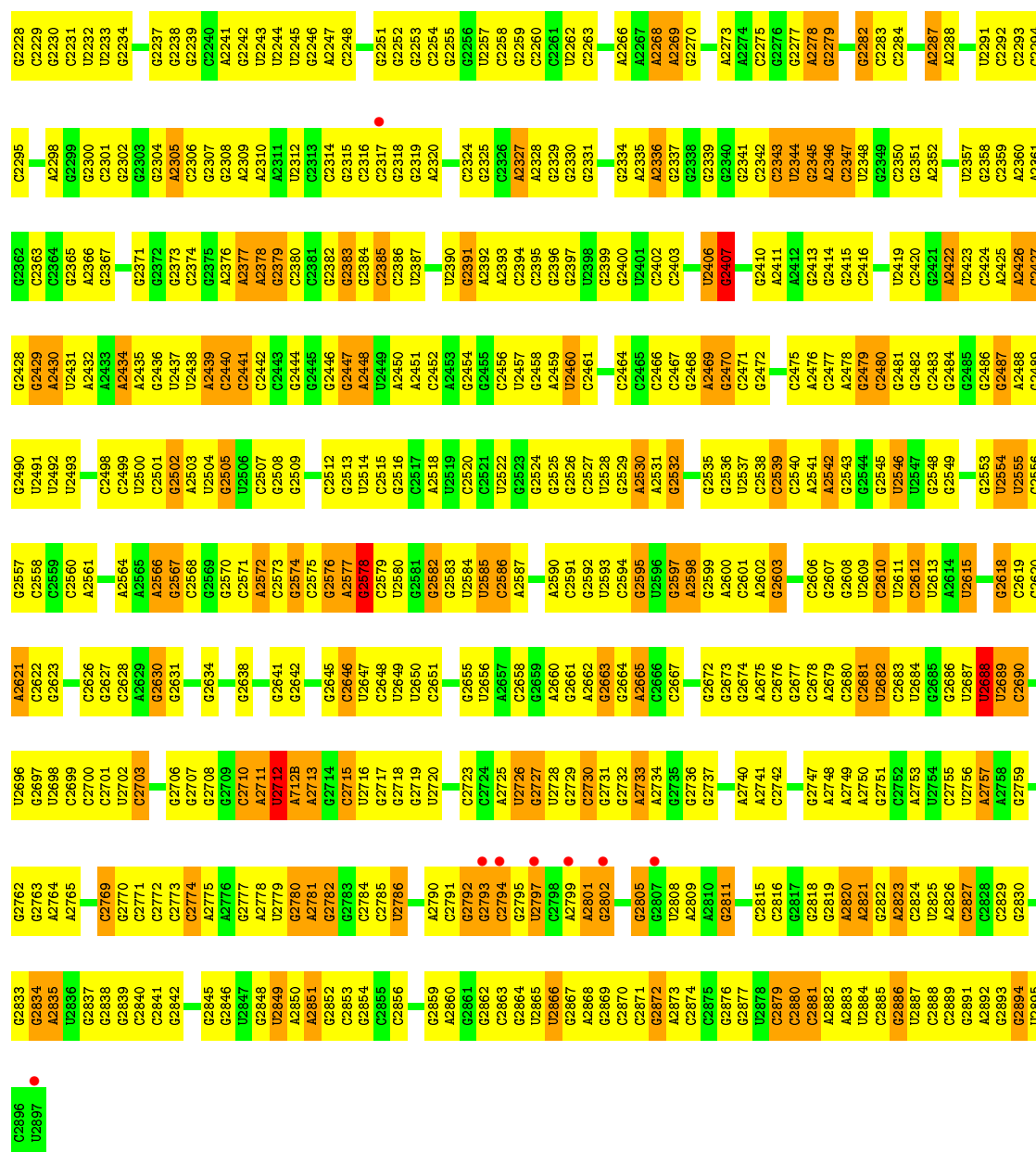
Chain BA:  28% 56% 15% .



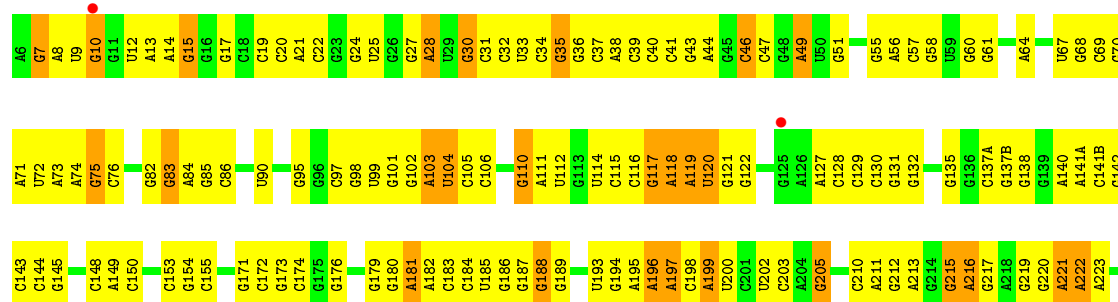






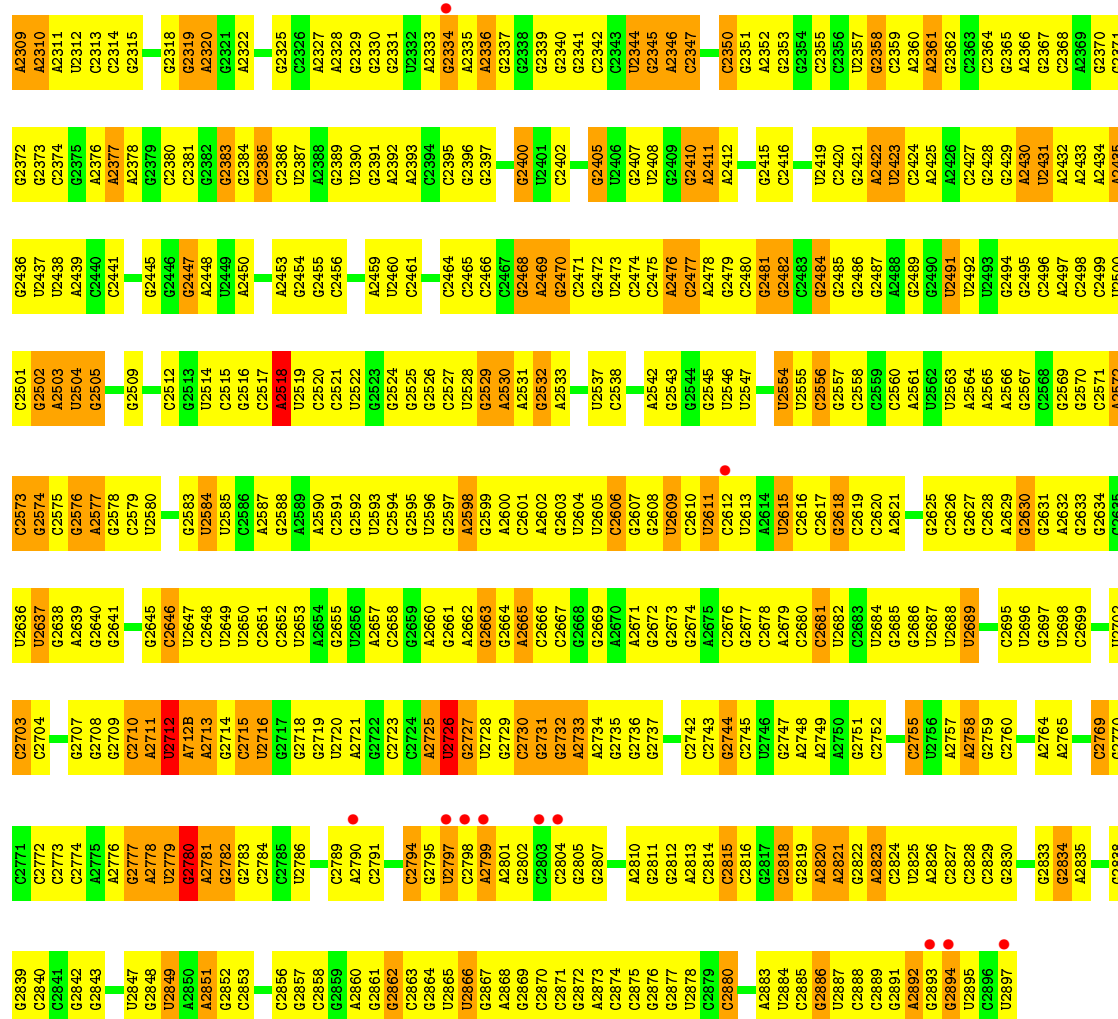


### ● Molecule 59: 23S ribosomal RNA

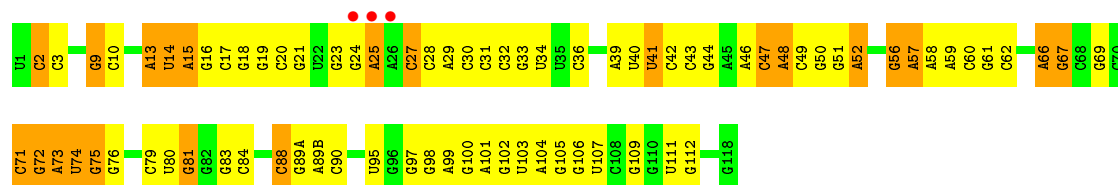


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C1177	G1106	G1043	G978	C915	U847	A783	A721	A655	G596	C527	G398	C461	A332	G271	A228
G1179	C1178	A1045	G979	C916	G848	A784	A722	G656	U597	A528	G399	G462	G333	G272	G229
C1180	U1113	G1046	A980	A917	C850	G785	U724	C658	G598	A529	G400	G463	C334	G273A	A229
C1181	U1113	G1047	A980	A918	U851	G786	G725	C659	G599	G530	A401	U464	C335	G273B	G229
A1182	G1114	A1048	A983	G919	G852	A788	G726	G660	G600	C531	A402	G465	C336	C273C	C231
C1183	G1115	C1049	A984	G920	G853	A789	G727	C661	C801	A532	U403	G466	C337	C273D	G232
C1184	G1116	A1050	C985	G921	G854	C790	G728	C662	G602	G533	G404	G467	C234	C273E	A233
C1185	G1117	G1051	C986	U922	G855	C791	G729	G663	G604	U534	U405	G468	G273F	G273G	U235
C1186	G1117	C1052	G987	C923	C856	G792	C730	C664	C805	A536	G407	A470	G342	G274	C236
G1187	G1120	C1053	A988	C924	C857	A793	C731	G667	U606	C537	G408	A471	G343	G275	C237
U1188	C1121	A1054	G989	C925	U858	G794	C732	U667	U607	G539	G409	A472	G344	A276	G242
U1189	G1122	G1055	A990	A926	G859	G795	G733	G668	A608	C541	G410	G473	G349	A277	U243
G1190	C1123	G1056	C991	G928	G860	C796	A734	G669	A609A	G542	G411	G474	U350	A244	A244
C1124	G1125	A1057	C992	U930	G862	G797	A735	A670	G609B	C543	A412	U475	G351	G279	G245
G1193	C1126	G1058	G993	G929	A863	G798	C736	G671	G610	C543	C413	G476	G352	C287	G246
A1194	A1126	G1059	C994	G931	G864	G799	C737	G672	C611	C544	C414	A477	G353	C288	G247
G1195	A1127	U1060	C995	G932	C865	A800	G738	G673	G612	G545	A415	A478	G354	C289	G248
C1196	C1128	U1061	A996	A933	A866	G801	G739	G674	U613	C546	A416	A479	G354	G290	G249
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U1198	U1130	G1063	C998	C935	U868	G741	G741	G676	G615	A548	A418	G481	U358	G291	G251
U1199	G1131	C1064	U999	G936	G869	G805	G742	C678	A616	G549	C419	A482	A359	G292	A251
C1200	U1065	A1000	A1000	G938	A870	C806	G743	C679	G617	G556	C420	A483	A359	G293	A252
C1201	G1135	U1066	A1001	G939	G871	U807	G744	G680	G618A	C557	U421	A485	G363A	G294	G256
C1202	G1136	G1002	G1002	G940	A872	G808	G745	G681	C618B	U557	A422	C485	A363B	C296	A257
G1203	G1137	A1069	G1003	G941	A873	G809	A746	G682	C619	G558	A423	C486	G363C	C297	G258
A1204	G1138	A1070	G1004	G942	G874	G809	U747	C683	G620	G559	G487	C487	G363D	G298	G259
U1205	C1139	A1071	C1005	U943	G875	C812	G748	G684	A621	C560	G425	C488	G363E	G299	G260
C1206	C1140	G1071	C1006	G944	G876	U813	G749	A685	G622	G561	G426	C489	U363F	A300	G261
C1207	U1141	C1072	C1007	A945	A878	C814	A750	G686	G623	U562	G491	C490	A363G	G301	G262
U1208	U1142	G1073	C1008	G946	G879	G817	G751	C687	C624	G563	A492	C492	C364	C302	A265
G1209	A1143	C1074	C1009	G947	G880	C817	A752	U688	G625	C564	G493	U431	C365A	G304	G266
C1210	A1143	C1075	A1009	G948	G881	G818	G753	G689	U626	C565	A494	A432	G366B	G305	G266
U1211	G1144	A1077	G882	C949	G882	A819	C754	G690	A627	G570	G371	U433	G370	U305	G266
C1212	C1145	U1078	U1012	G950	G883	A820	G754	C691	G628	G570	A371	U433	G370	U306	G266
A1213	G1149	C1079	C1013	G952	C894	A821	U757	C692	G693	A571	G372	G307	G372	G307	A270C
C1214	U1150	G1080	G1016	G952	G892	U822	G758	C693	A631	A572	C436	C270D	U373	G308	G270E
G1215	G1151	U1081	C1017	C955	A837	G823	G759	U694	G632	G573	G438	G309	A374	G309	C270F
C1216	C1152	U1082	C1018	G956	C888	A824	G760	G695	A633	C574	A501	G310	A310	A310	U270G
C1217	C1152	U1083	G1018	A957	C889	G825	A761	G696	G634	A575	A502	G311	G377	G312	C270H
C1221	C1163	A1084	U1019	A957	A890	U826	U762	C697	C635	U576	A503	G313	C378	G313	G270I
C1222	G1154	A1085	G892	U958	A892	U827	G763	C698	G636	G577	U504	G314	G379	C313	C270J
G1157	G1157	A1086	A1021	A959	C893	U828	A764	A699	A637	A578	G381	G315	U380	G315	G270K
U1158	C1158	G1087	G1022	A960	C894	A829	G765	G700	G638	G579	G506	G316	G382	G316	C270L
C1224	C1158	A1088	U1023	C961	A896	U895	G766	A705	C640	C581	A507	G317	G382	G317	U270M
G1225	U1159	G1089	G1024	G962	A896	U895	U767	A706	C581	C581	G508	G317	U383	G317	U270N
A1226	G1160	U1090	G1025	U963	C897	U833	G768	A707	C641	G582	G509	G318	U384	G318	G270O
C1227	G1162	G1091	U1026	C964	C897	U834	G769	A708	G642	G583	C510	G319	U384	G319	G270P
C1230	G1163	C1092	A1027	C965	A900	A835	G770	C708	A643	G584	A449	G320	U387	G320	U270Q
G1231	G1164	C1093	G1028	G966	A901	G836	G771	U709	A644	G585	A513	G321	G388	G321	C270R
C1232	U1165	U1094	A1029	C967	C902	C837	G772	G710	G645	A586	A514	G322	G388	G322	G270S
G1233	C1166	A1095	G1030	G968	C903	G838	U773	G711	A646	A587	A515	G323	G389	G323	G270T
U1167	U1167	A1096	C1030	U969	C904	U839	A774	G712	G647	U588	A516	A324	A390	A324	G270U
G1239	G1168	U1097	U1033	C970	G905	C940	G775	G715	G648	C589	G517	G325	A390	A325	G270V
C1241	G1169	G1098	A841	C971	U906	C941	G776	G715	G649	C590	G518	G326	A391	G326	G270W
A1242	G1173	U1101	G1036	G972	A909	G842	U779	A716	G650	C591	G519	G327	A392	G327	G270X
C1243	U1174	C1102	G1037	A973	A910	G843	G780	G717	G651	G592	C456	G328	A393	G328	C271B
U1244	U1175	A1103	C1038	G974B	A910	C844	G781	A718	U852	G593	A457	G329	A394	G329	G271C
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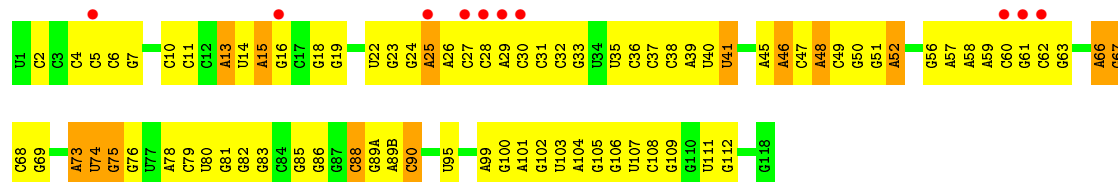
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G2240	G2159	U2096	C2036	A1972	C1894	G1816		C1657	A1586	C1519	G1450	C1383	C1451	G1248
A2241	G2160	C2097	G2037	C1973	C1895	G1817		C1658		U1520	C1451	A1384	G1384	U1249
G2242	C2161		G2038	C1974	G1896	U1818	G1748	U1659	C1589		A1453	G1385		
U2243		G2101	G2039	G1975	G1897	A1819	A1749		U1590	G1524	U1454	C1386	A1321	A1253
U2244	U2102	U2103	G2040	U1976	U1898	U1820		C1663	G1591	G1525	U1455	C1387	A1322	A1254
U2245	U2167	C2103	U2041	A1977	G1999	A1821	G1753	A1664	G1595	G1526	U1459	G1388	U1323	U1255
G2246	G2168	G2104	A2042	A1978	A1900	G1822		A1665			G1459	G1389	G1324	G1256
A2247	A2169	C2105	G2043	G1979	A1901	G1823	G1758	G1666	C1598	A1529	A1460	G1395	G1325	C1257
G2248	A2170	G2106	C2044	G1980	C1902	G1824	A1759	A1668	C1599	G1530	G1461	G1396	U1326	G1258
A2171	C2107	C2108	G2045	A1981	G1903	A1825				C1531	C1462	U1390	G1327	G1259
U2172	U2172	U2109	G2046	C1982	G1904	G1826	A1762	A1669	U1602	U1535	C1463	A1395	G1328	G1260
A2173	A2173	G2110	U2047	C1983	C1905	C1827	G1763	C1670	A1603	U1536	U1396	U1396	U1329	C1261
C2174	C2174	G2110	G2048	G1984	G1906	G1828	G1764	U1671	G1604	G1465	C1464	C1330	C1330	A1262
C2175	C2111	C2111	G2049	G1985		A1829	G1765	U1673	C1605	A1537	C1399	G1332	U1263	G1263
A2176	U2112	U2112	C2050	A1986	C1924	A1830	U1766	G1674	C1586	C1467	C1468	G1400	G1333	A1264
C2177	U2113	U2113	A2051		A1912	G1831				G1538	G1401	C1333	A1265	A1266
					A1913									
					C1914									



• Molecule 60: 5S ribosomal RNA



• Molecule 60: 5S ribosomal RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	308.96Å 670.66Å 347.77Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 140.20 – 3.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 74.7 (140.20-3.57)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 3.58Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.284 , 0.328 0.298 , 0.336	Depositor DCC
$R_{free}$ test set	33469 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.8	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.25$ , $\langle L^2 \rangle = 0.10$	Xtriage
Estimated twinning fraction	0.258 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	308166	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

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

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: GDP, MG, DPP, KBE, UAL, FUA, 5OH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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



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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	3
1	CB	0	1
11	CL	0	2
23	AY	0	3
23	CY	0	2
25	BC	0	1
25	DC	0	3
26	BD	0	1
26	DD	0	2
28	BF	0	2
28	DF	0	2
29	BG	0	2
29	DG	0	2
31	BJ	0	1
31	DJ	0	1
35	DP	0	1
38	BS	0	3
38	DS	0	3
42	BW	0	1
42	DW	0	1
57	B1	0	2
57	D1	0	2
All	All	0	41

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

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

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

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

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

There are no chirality outliers.

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	162	ILE	Peptide
1	AB	170	GLU	Peptide
1	AB	185	ILE	Peptide
23	AY	133	ILE	Peptide
23	AY	503	GLY	Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1910	0	1957	135	0
1	CB	1910	0	1957	107	0
2	AC	1621	0	1688	87	0
2	CC	1621	0	1688	64	0
3	AD	1703	0	1763	104	0
3	CD	1703	0	1763	104	0
4	AE	1156	0	1213	70	0
4	CE	1156	0	1213	57	0
5	AF	843	0	857	42	0
5	CF	843	0	857	32	0
6	AG	1257	0	1296	54	0
6	CG	1257	0	1296	53	0
7	AH	1116	0	1177	67	0
7	CH	1116	0	1177	73	0
8	AI	1010	0	1037	78	0
8	CI	1010	0	1037	57	0
9	AJ	802	0	849	44	0
9	CJ	802	0	849	48	0
10	AK	885	0	904	54	0
10	CK	885	0	904	60	0
11	AL	976	0	1062	113	0

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 12302 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CY:19:ALA:H	23:CY:25:LYS:CE	1.38	1.34
59:DA:2405:G:H21	59:DA:2412:A:N6	1.28	1.26
23:CY:19:ALA:N	23:CY:25:LYS:HE3	1.49	1.26
59:DA:2405:G:N2	59:DA:2412:A:H62	1.29	1.25
21:AW:15:G:N2	21:AW:48:C:H42	1.36	1.24

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BA:1015:G:O2'	40:DU:118:GLY:O[3_545]	2.09	0.11

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	233/235 (99%)	154 (66%)	51 (22%)	28 (12%)	0	6
1	CB	233/235 (99%)	159 (68%)	50 (22%)	24 (10%)	0	8
2	AC	205/207 (99%)	154 (75%)	32 (16%)	19 (9%)	1	9
2	CC	205/207 (99%)	156 (76%)	36 (18%)	13 (6%)	1	18
3	AD	206/208 (99%)	149 (72%)	31 (15%)	26 (13%)	0	5
3	CD	206/208 (99%)	153 (74%)	32 (16%)	21 (10%)	1	8
4	AE	149/151 (99%)	117 (78%)	22 (15%)	10 (7%)	1	17
4	CE	149/151 (99%)	117 (78%)	25 (17%)	7 (5%)	3	26
5	AF	99/101 (98%)	75 (76%)	15 (15%)	9 (9%)	1	9
5	CF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	1	9
6	AG	153/155 (99%)	121 (79%)	25 (16%)	7 (5%)	3	26
6	CG	153/155 (99%)	124 (81%)	22 (14%)	7 (5%)	3	26
7	AH	136/138 (99%)	97 (71%)	27 (20%)	12 (9%)	1	10
7	CH	136/138 (99%)	97 (71%)	28 (21%)	11 (8%)	1	12
8	AI	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	3	30
8	CI	125/127 (98%)	99 (79%)	22 (18%)	4 (3%)	5	36
9	AJ	97/99 (98%)	75 (77%)	13 (13%)	9 (9%)	1	9
9	CJ	97/99 (98%)	75 (77%)	17 (18%)	5 (5%)	2	23
10	AK	117/119 (98%)	82 (70%)	21 (18%)	14 (12%)	0	6
10	CK	117/119 (98%)	82 (70%)	22 (19%)	13 (11%)	0	6
11	AL	123/125 (98%)	38 (31%)	52 (42%)	33 (27%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	CL	123/125 (98%)	47 (38%)	43 (35%)	33 (27%)	0	0
12	AM	123/125 (98%)	93 (76%)	20 (16%)	10 (8%)	1	12
12	CM	123/125 (98%)	91 (74%)	25 (20%)	7 (6%)	2	21
13	AN	58/60 (97%)	44 (76%)	7 (12%)	7 (12%)	0	5
13	CN	58/60 (97%)	44 (76%)	10 (17%)	4 (7%)	1	16
14	AO	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	12
14	CO	86/88 (98%)	60 (70%)	21 (24%)	5 (6%)	2	20
15	AP	82/84 (98%)	66 (80%)	15 (18%)	1 (1%)	15	57
15	CP	82/84 (98%)	64 (78%)	14 (17%)	4 (5%)	2	24
16	AQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	1	8
16	CQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	1	8
17	AR	68/70 (97%)	51 (75%)	10 (15%)	7 (10%)	0	8
17	CR	68/70 (97%)	48 (71%)	13 (19%)	7 (10%)	0	8
18	AS	77/79 (98%)	41 (53%)	23 (30%)	13 (17%)	0	2
18	CS	77/79 (98%)	46 (60%)	17 (22%)	14 (18%)	0	2
19	AT	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	3	29
19	CT	97/99 (98%)	79 (81%)	12 (12%)	6 (6%)	2	19
23	AY	663/687 (96%)	451 (68%)	138 (21%)	74 (11%)	0	6
23	CY	663/687 (96%)	461 (70%)	134 (20%)	68 (10%)	0	8
24	AU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
24	CU	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
25	BC	226/228 (99%)	110 (49%)	66 (29%)	50 (22%)	0	1
25	DC	226/228 (99%)	123 (54%)	59 (26%)	44 (20%)	0	1
26	BD	273/275 (99%)	174 (64%)	47 (17%)	52 (19%)	0	2
26	DD	273/275 (99%)	165 (60%)	61 (22%)	47 (17%)	0	2
27	BE	203/205 (99%)	128 (63%)	40 (20%)	35 (17%)	0	2
27	DE	203/205 (99%)	122 (60%)	45 (22%)	36 (18%)	0	2
28	BF	206/208 (99%)	130 (63%)	46 (22%)	30 (15%)	0	3
28	DF	206/208 (99%)	128 (62%)	44 (21%)	34 (16%)	0	2
29	BG	179/181 (99%)	122 (68%)	48 (27%)	9 (5%)	2	24
29	DG	179/181 (99%)	134 (75%)	36 (20%)	9 (5%)	2	24

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	D0	82/84 (98%)	57 (70%)	15 (18%)	10 (12%)	0	5
47	B2	69/71 (97%)	51 (74%)	14 (20%)	4 (6%)	2	20
47	D2	69/71 (97%)	56 (81%)	10 (14%)	3 (4%)	3	28
48	B3	58/60 (97%)	48 (83%)	6 (10%)	4 (7%)	1	16
48	D3	58/60 (97%)	42 (72%)	10 (17%)	6 (10%)	0	8
49	B5	57/59 (97%)	43 (75%)	11 (19%)	3 (5%)	2	22
49	D5	57/59 (97%)	41 (72%)	12 (21%)	4 (7%)	1	15
50	B6	48/50 (96%)	28 (58%)	13 (27%)	7 (15%)	0	3
50	D6	48/50 (96%)	29 (60%)	8 (17%)	11 (23%)	0	1
51	B7	47/49 (96%)	35 (74%)	8 (17%)	4 (8%)	1	11
51	D7	47/49 (96%)	32 (68%)	9 (19%)	6 (13%)	0	5
52	B8	62/64 (97%)	35 (56%)	17 (27%)	10 (16%)	0	3
52	D8	62/64 (97%)	36 (58%)	18 (29%)	8 (13%)	0	5
53	B9	35/37 (95%)	18 (51%)	12 (34%)	5 (14%)	0	3
53	D9	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	1	11
54	Be	70/102 (69%)	38 (54%)	24 (34%)	8 (11%)	0	6
54	De	70/102 (69%)	41 (59%)	23 (33%)	6 (9%)	1	11
57	B1	91/93 (98%)	60 (66%)	19 (21%)	12 (13%)	0	4
57	D1	91/93 (98%)	56 (62%)	18 (20%)	17 (19%)	0	2
58	B4	33/35 (94%)	15 (46%)	13 (39%)	5 (15%)	0	3
58	D4	33/35 (94%)	17 (52%)	9 (27%)	7 (21%)	0	1
All	All	13260/13576 (98%)	9009 (68%)	2708 (20%)	1543 (12%)	0	6

5 of 1543 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	203/203 (100%)	164 (81%)	39 (19%)	1	9
1	CB	203/203 (100%)	167 (82%)	36 (18%)	2	12
2	AC	161/161 (100%)	132 (82%)	29 (18%)	2	11
2	CC	161/161 (100%)	136 (84%)	25 (16%)	3	18
3	AD	180/180 (100%)	145 (81%)	35 (19%)	1	8
3	CD	180/180 (100%)	150 (83%)	30 (17%)	2	14
4	AE	116/116 (100%)	93 (80%)	23 (20%)	1	8
4	CE	116/116 (100%)	98 (84%)	18 (16%)	3	18
5	AF	90/90 (100%)	78 (87%)	12 (13%)	4	24
5	CF	90/90 (100%)	82 (91%)	8 (9%)	11	43
6	AG	126/126 (100%)	113 (90%)	13 (10%)	8	36
6	CG	126/126 (100%)	115 (91%)	11 (9%)	12	44
7	AH	119/119 (100%)	98 (82%)	21 (18%)	2	12
7	CH	119/119 (100%)	105 (88%)	14 (12%)	6	29
8	AI	98/98 (100%)	82 (84%)	16 (16%)	3	15
8	CI	98/98 (100%)	84 (86%)	14 (14%)	4	22
9	AJ	89/89 (100%)	75 (84%)	14 (16%)	3	18
9	CJ	89/89 (100%)	72 (81%)	17 (19%)	2	9
10	AK	90/90 (100%)	71 (79%)	19 (21%)	1	7
10	CK	90/90 (100%)	73 (81%)	17 (19%)	2	9
11	AL	104/104 (100%)	77 (74%)	27 (26%)	0	3
11	CL	104/104 (100%)	72 (69%)	32 (31%)	0	2
12	AM	100/100 (100%)	83 (83%)	17 (17%)	2	14
12	CM	100/100 (100%)	89 (89%)	11 (11%)	7	33
13	AN	49/49 (100%)	43 (88%)	6 (12%)	6	27
13	CN	49/49 (100%)	43 (88%)	6 (12%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	79/79 (100%)	71 (90%)	8 (10%)	9	37
14	CO	79/79 (100%)	65 (82%)	14 (18%)	2	12
15	AP	72/72 (100%)	66 (92%)	6 (8%)	13	46
15	CP	72/72 (100%)	62 (86%)	10 (14%)	4	23
16	AQ	95/95 (100%)	81 (85%)	14 (15%)	3	20
16	CQ	95/95 (100%)	79 (83%)	16 (17%)	2	14
17	AR	61/61 (100%)	51 (84%)	10 (16%)	2	15
17	CR	61/61 (100%)	53 (87%)	8 (13%)	5	25
18	AS	69/69 (100%)	55 (80%)	14 (20%)	1	7
18	CS	69/69 (100%)	54 (78%)	15 (22%)	1	6
19	AT	76/76 (100%)	64 (84%)	12 (16%)	3	17
19	CT	76/76 (100%)	67 (88%)	9 (12%)	6	29
23	AY	563/579 (97%)	470 (84%)	93 (16%)	2	15
23	CY	563/579 (97%)	463 (82%)	100 (18%)	2	12
24	AU	2/2 (100%)	2 (100%)	0	100	100
24	CU	2/2 (100%)	2 (100%)	0	100	100
25	BC	180/180 (100%)	140 (78%)	40 (22%)	1	6
25	DC	180/180 (100%)	138 (77%)	42 (23%)	1	4
26	BD	217/217 (100%)	169 (78%)	48 (22%)	1	6
26	DD	217/217 (100%)	164 (76%)	53 (24%)	1	4
27	BE	165/165 (100%)	134 (81%)	31 (19%)	2	9
27	DE	165/165 (100%)	127 (77%)	38 (23%)	1	5
28	BF	165/165 (100%)	133 (81%)	32 (19%)	1	8
28	DF	165/165 (100%)	135 (82%)	30 (18%)	2	11
29	BG	155/155 (100%)	130 (84%)	25 (16%)	3	16
29	DG	155/155 (100%)	127 (82%)	28 (18%)	2	11
30	BH	136/136 (100%)	116 (85%)	20 (15%)	3	20
30	DH	136/136 (100%)	125 (92%)	11 (8%)	14	48
32	BK	105/105 (100%)	90 (86%)	15 (14%)	4	22
32	DK	105/105 (100%)	89 (85%)	16 (15%)	3	19
33	BN	117/117 (100%)	95 (81%)	22 (19%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DN	117/117 (100%)	94 (80%)	23 (20%)	1	8
34	BO	100/100 (100%)	80 (80%)	20 (20%)	1	8
34	DO	100/100 (100%)	81 (81%)	19 (19%)	2	9
35	BP	112/112 (100%)	87 (78%)	25 (22%)	1	5
35	DP	112/112 (100%)	94 (84%)	18 (16%)	3	16
36	BQ	111/111 (100%)	82 (74%)	29 (26%)	0	3
36	DQ	111/111 (100%)	86 (78%)	25 (22%)	1	5
37	BR	100/100 (100%)	87 (87%)	13 (13%)	5	25
37	DR	100/100 (100%)	82 (82%)	18 (18%)	2	11
38	BS	77/77 (100%)	62 (80%)	15 (20%)	1	8
38	DS	77/77 (100%)	58 (75%)	19 (25%)	1	4
39	BT	120/120 (100%)	94 (78%)	26 (22%)	1	6
39	DT	120/120 (100%)	92 (77%)	28 (23%)	1	4
40	BU	93/93 (100%)	72 (77%)	21 (23%)	1	5
40	DU	93/93 (100%)	73 (78%)	20 (22%)	1	6
41	BV	82/82 (100%)	60 (73%)	22 (27%)	0	3
41	DV	82/82 (100%)	59 (72%)	23 (28%)	0	3
42	BW	92/92 (100%)	68 (74%)	24 (26%)	0	3
42	DW	92/92 (100%)	72 (78%)	20 (22%)	1	6
43	BX	75/75 (100%)	64 (85%)	11 (15%)	3	20
43	DX	75/75 (100%)	60 (80%)	15 (20%)	1	8
44	BY	88/88 (100%)	69 (78%)	19 (22%)	1	6
44	DY	88/88 (100%)	72 (82%)	16 (18%)	2	11
45	BZ	162/162 (100%)	133 (82%)	29 (18%)	2	11
45	DZ	162/162 (100%)	134 (83%)	28 (17%)	2	13
46	B0	66/66 (100%)	54 (82%)	12 (18%)	2	11
46	D0	66/66 (100%)	51 (77%)	15 (23%)	1	5
47	B2	66/66 (100%)	62 (94%)	4 (6%)	22	60
47	D2	66/66 (100%)	60 (91%)	6 (9%)	11	42
48	B3	52/52 (100%)	45 (86%)	7 (14%)	4	24
48	D3	52/52 (100%)	45 (86%)	7 (14%)	4	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B5	51/51 (100%)	44 (86%)	7 (14%)	4	23
49	D5	51/51 (100%)	41 (80%)	10 (20%)	1	8
50	B6	49/49 (100%)	38 (78%)	11 (22%)	1	5
50	D6	49/49 (100%)	37 (76%)	12 (24%)	1	4
51	B7	42/42 (100%)	35 (83%)	7 (17%)	2	14
51	D7	42/42 (100%)	38 (90%)	4 (10%)	10	40
52	B8	54/54 (100%)	39 (72%)	15 (28%)	0	3
52	D8	54/54 (100%)	37 (68%)	17 (32%)	0	2
53	B9	34/34 (100%)	28 (82%)	6 (18%)	2	12
53	D9	34/34 (100%)	32 (94%)	2 (6%)	23	61
54	Be	54/54 (100%)	47 (87%)	7 (13%)	5	25
54	De	54/54 (100%)	46 (85%)	8 (15%)	3	20
57	B1	78/78 (100%)	59 (76%)	19 (24%)	1	4
57	D1	78/78 (100%)	58 (74%)	20 (26%)	0	4
58	B4	31/31 (100%)	23 (74%)	8 (26%)	0	4
58	D4	31/31 (100%)	26 (84%)	5 (16%)	3	16
All	All	11142/11174 (100%)	9117 (82%)	2025 (18%)	2	11

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

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

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

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

### 5.3.3 RNA ⓘ

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

5 of 2020 RNA backbone outliers are listed below:

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

5 of 88 RNA pucker outliers are listed below:

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

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	KBE	AU	1	24	8,8,9	0.59	0	7,8,10	1.52	1 (14%)
24	DPP	AU	2	24	4,5,6	0.34	0	1,5,7	0.33	0
24	UAL	AU	5	24	8,8,9	2.36	3 (37%)	4,9,11	1.53	1 (25%)
24	5OH	AU	6	24	8,12,13	1.49	1 (12%)	5,16,18	2.44	2 (40%)
24	KBE	CU	1	24	8,8,9	0.62	0	7,8,10	1.82	1 (14%)
24	DPP	CU	2	24	4,5,6	0.31	0	1,5,7	0.32	0
24	UAL	CU	5	24	8,8,9	2.40	3 (37%)	4,9,11	1.87	1 (25%)
24	5OH	CU	6	24	8,12,13	1.25	1 (12%)	5,16,18	2.88	3 (60%)

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 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CU	5	UAL	C1-N1	-3.01	1.35	1.40
24	AU	5	UAL	C1-N1	-2.64	1.35	1.40
24	CU	5	UAL	CB-CA	2.09	1.40	1.35
24	AU	5	UAL	CB-CA	2.33	1.41	1.35
24	CU	6	5OH	CA-C	3.08	1.54	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CU	5	UAL	O-C-CA	-3.67	120.78	125.47
24	AU	5	UAL	O-C-CA	-2.79	121.90	125.47
24	CU	6	5OH	O-C-CA	-2.69	118.88	125.15
24	AU	6	5OH	O-C-CA	-2.26	119.88	125.15
24	CU	6	5OH	CR-CB-CA	2.39	115.44	112.78



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
61	FUA	AY	701	-	37,40,40	1.72	6 (16%)	45,64,64	2.01	12 (26%)
62	GDP	AY	702	-	25,30,30	1.27	3 (12%)	26,47,47	2.03	6 (23%)
61	FUA	CY	701	-	37,40,40	1.66	6 (16%)	45,64,64	2.19	13 (28%)
62	GDP	CY	702	-	25,30,30	1.28	3 (12%)	26,47,47	2.02	6 (23%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	FUA	C23-C22	-6.28	1.40	1.51
61	CY	701	FUA	C23-C22	-5.82	1.41	1.51
61	AY	701	FUA	C23-C24	-4.18	1.39	1.53
61	CY	701	FUA	C23-C24	-3.99	1.39	1.53
61	CY	701	FUA	C14-C8	-3.15	1.53	1.58

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	CY	701	FUA	C13-C12-C11	-6.49	102.94	111.97
61	AY	701	FUA	C13-C12-C11	-5.92	103.73	111.97
62	AY	702	GDP	N3-C2-N1	-4.96	120.21	127.46
62	CY	702	GDP	N3-C2-N1	-4.93	120.26	127.46
61	AY	701	FUA	C16-O2-C31	-3.94	110.99	117.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AY	701	FUA	6	0
62	AY	702	GDP	12	0
61	CY	701	FUA	7	0
62	CY	702	GDP	13	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
54	Be	1
54	De	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	De	30:UNK	C	51:ALA	N	37.69
1	Be	30:UNK	C	51:ALA	N	36.65

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AB	235/235 (100%)	0.47	32 (13%) 3 4	4, 59, 144, 223	0
1	CB	235/235 (100%)	0.48	28 (11%) 5 6	5, 60, 155, 214	0
2	AC	207/207 (100%)	0.27	23 (11%) 6 7	4, 63, 136, 190	0
2	CC	207/207 (100%)	0.42	22 (10%) 7 8	3, 57, 130, 186	0
3	AD	208/208 (100%)	-0.54	4 (1%) 67 59	4, 57, 142, 206	0
3	CD	208/208 (100%)	-0.41	3 (1%) 75 67	14, 72, 144, 196	0
4	AE	151/151 (100%)	0.43	21 (13%) 3 4	5, 34, 122, 151	0
4	CE	151/151 (100%)	0.17	16 (10%) 7 8	4, 35, 133, 165	0
5	AF	101/101 (100%)	-0.86	0 100 100	4, 27, 93, 145	0
5	CF	101/101 (100%)	-0.87	0 100 100	5, 37, 115, 163	0
6	AG	155/155 (100%)	0.57	24 (15%) 2 3	10, 78, 153, 229	0
6	CG	155/155 (100%)	1.02	30 (19%) 1 1	3, 84, 172, 210	0
7	AH	138/138 (100%)	0.06	1 (0%) 87 82	3, 31, 89, 166	0
7	CH	138/138 (100%)	0.20	10 (7%) 16 14	1, 37, 130, 199	0
8	AI	127/127 (100%)	1.07	35 (27%) 1 1	6, 72, 140, 199	0
8	CI	127/127 (100%)	0.61	16 (12%) 4 5	14, 84, 152, 237	0
9	AJ	99/99 (100%)	-0.12	10 (10%) 8 8	9, 68, 136, 163	0
9	CJ	99/99 (100%)	-0.27	4 (4%) 39 32	13, 65, 154, 217	0
10	AK	119/119 (100%)	-0.12	4 (3%) 46 38	7, 56, 137, 180	0
10	CK	119/119 (100%)	0.10	11 (9%) 10 10	8, 55, 145, 175	0
11	AL	125/125 (100%)	0.49	21 (16%) 2 2	5, 39, 105, 171	0
11	CL	125/125 (100%)	0.64	19 (15%) 2 3	8, 52, 134, 176	0
12	AM	125/125 (100%)	0.93	26 (20%) 1 1	23, 90, 167, 199	0
12	CM	125/125 (100%)	0.59	20 (16%) 2 3	14, 90, 166, 190	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AN	60/60 (100%)	0.56	8 (13%) 4 5	8, 38, 114, 139	0
13	CN	60/60 (100%)	0.12	0 100 100	8, 42, 131, 166	0
14	AO	88/88 (100%)	-0.65	2 (2%) 61 51	5, 37, 108, 158	0
14	CO	88/88 (100%)	-0.50	0 100 100	8, 49, 130, 197	0
15	AP	84/84 (100%)	0.57	11 (13%) 4 5	18, 68, 131, 171	0
15	CP	84/84 (100%)	0.51	11 (13%) 4 5	8, 79, 159, 224	0
16	AQ	100/100 (100%)	0.12	6 (6%) 23 19	9, 43, 120, 169	0
16	CQ	100/100 (100%)	0.29	11 (11%) 6 7	5, 43, 118, 142	0
17	AR	70/70 (100%)	-0.52	1 (1%) 75 67	7, 30, 134, 185	0
17	CR	70/70 (100%)	-0.32	4 (5%) 24 20	7, 28, 130, 193	0
18	AS	79/79 (100%)	0.56	12 (15%) 2 3	15, 78, 159, 206	0
18	CS	79/79 (100%)	0.09	8 (10%) 8 8	10, 80, 154, 204	0
19	AT	99/99 (100%)	-0.10	4 (4%) 39 32	4, 64, 120, 187	0
19	CT	99/99 (100%)	0.10	8 (8%) 13 12	16, 71, 155, 187	0
20	AA	1511/1511 (100%)	-0.31	34 (2%) 61 51	3, 62, 163, 289	0
20	CA	1511/1511 (100%)	-0.34	27 (1%) 69 60	5, 63, 173, 323	0
21	AW	77/77 (100%)	-0.49	1 (1%) 77 69	21, 91, 179, 234	0
21	CW	77/77 (100%)	-0.10	6 (7%) 14 13	44, 97, 221, 273	0
22	AV	23/23 (100%)	0.89	5 (21%) 1 1	56, 136, 187, 205	0
22	CV	23/23 (100%)	2.09	9 (39%) 0 0	66, 119, 215, 230	0
23	AY	667/687 (97%)	-0.10	49 (7%) 16 14	5, 64, 147, 208	0
23	CY	667/687 (97%)	0.03	63 (9%) 9 9	4, 68, 150, 203	0
24	AU	2/6 (33%)	0.19	0 100 100	155, 155, 155, 155	0
24	CU	2/6 (33%)	-0.17	0 100 100	81, 81, 81, 88	0
25	BC	228/228 (100%)	0.85	50 (21%) 1 1	45, 128, 217, 259	0
25	DC	228/228 (100%)	1.69	78 (34%) 0 0	33, 153, 230, 287	0
26	BD	275/275 (100%)	-0.42	5 (1%) 69 60	4, 26, 103, 166	0
26	DD	275/275 (100%)	-0.53	7 (2%) 58 48	4, 25, 107, 210	0
27	BE	205/205 (100%)	-0.41	3 (1%) 74 66	1, 31, 135, 229	0
27	DE	205/205 (100%)	-0.28	7 (3%) 46 38	6, 41, 144, 221	0
28	BF	208/208 (100%)	0.50	28 (13%) 3 5	6, 49, 162, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DF	208/208 (100%)	0.61	34 (16%) 2 2	10, 62, 162, 266	0
29	BG	181/181 (100%)	1.38	56 (30%) 0 0	11, 91, 152, 197	0
29	DG	181/181 (100%)	1.34	57 (31%) 0 0	33, 105, 176, 209	0
30	BH	167/167 (100%)	-0.50	1 (0%) 89 84	3, 47, 130, 224	0
30	DH	167/167 (100%)	-0.32	5 (2%) 51 42	6, 56, 141, 187	0
31	BJ	0/170	-	-	-	-
31	DJ	0/170	-	-	-	-
32	BK	140/140 (100%)	1.15	39 (27%) 1 1	17, 104, 194, 230	0
32	DK	140/140 (100%)	1.57	44 (31%) 0 0	37, 124, 205, 244	0
33	BN	138/138 (100%)	0.59	23 (16%) 2 2	59, 83, 108, 111	0
33	DN	138/138 (100%)	0.49	20 (14%) 3 3	59, 81, 104, 111	0
34	BO	122/122 (100%)	-0.03	3 (2%) 58 48	5, 33, 94, 148	0
34	DO	122/122 (100%)	-0.16	4 (3%) 47 39	4, 30, 131, 183	0
35	BP	146/146 (100%)	0.21	13 (8%) 10 10	7, 55, 131, 173	0
35	DP	146/146 (100%)	0.02	11 (7%) 15 14	1, 60, 152, 204	0
36	BQ	141/141 (100%)	-0.65	2 (1%) 75 67	20, 43, 113, 170	0
36	DQ	141/141 (100%)	-0.49	6 (4%) 36 29	8, 32, 107, 219	0
37	BR	117/117 (100%)	-0.19	5 (4%) 36 29	7, 38, 125, 156	0
37	DR	117/117 (100%)	-0.25	6 (5%) 29 23	2, 38, 126, 213	0
38	BS	99/99 (100%)	1.01	23 (23%) 1 1	27, 104, 191, 225	0
38	DS	99/99 (100%)	2.03	40 (40%) 0 0	11, 106, 194, 248	0
39	BT	138/138 (100%)	-0.10	7 (5%) 29 23	6, 53, 139, 225	0
39	DT	138/138 (100%)	0.09	11 (7%) 13 12	3, 68, 141, 201	0
40	BU	117/117 (100%)	-0.06	5 (4%) 36 29	11, 22, 80, 175	0
40	DU	117/117 (100%)	-0.22	3 (2%) 56 47	6, 20, 94, 136	0
41	BV	101/101 (100%)	0.15	5 (4%) 30 24	0, 32, 104, 143	0
41	DV	101/101 (100%)	-0.21	3 (2%) 51 42	2, 32, 117, 147	0
42	BW	113/113 (100%)	-0.04	6 (5%) 27 22	8, 32, 103, 140	0
42	DW	113/113 (100%)	-0.04	5 (4%) 35 28	2, 31, 116, 157	0
43	BX	93/93 (100%)	-0.30	3 (3%) 48 40	5, 51, 118, 172	0
43	DX	93/93 (100%)	0.09	5 (5%) 26 22	7, 50, 136, 198	0
44	BY	107/107 (100%)	-0.27	8 (7%) 15 14	12, 69, 151, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	DY	107/107 (100%)	-0.13	6 (5%) 25 21	6, 70, 150, 196	0
45	BZ	185/185 (100%)	-0.41	7 (3%) 41 35	13, 52, 123, 175	0
45	DZ	185/185 (100%)	-0.18	7 (3%) 41 35	10, 61, 135, 194	0
46	B0	84/84 (100%)	-0.50	2 (2%) 59 50	6, 53, 127, 163	0
46	D0	84/84 (100%)	-0.30	2 (2%) 59 50	7, 58, 132, 217	0
47	B2	71/71 (100%)	-0.70	0 100 100	12, 61, 137, 175	0
47	D2	71/71 (100%)	-0.70	0 100 100	9, 60, 127, 145	0
48	B3	60/60 (100%)	-0.44	0 100 100	8, 31, 96, 111	0
48	D3	60/60 (100%)	-0.25	0 100 100	13, 29, 101, 126	0
49	B5	59/59 (100%)	-0.52	1 (1%) 70 62	8, 37, 148, 208	0
49	D5	59/59 (100%)	-0.39	0 100 100	6, 44, 156, 223	0
50	B6	50/50 (100%)	0.06	4 (8%) 13 12	12, 92, 147, 163	0
50	D6	50/50 (100%)	0.84	10 (20%) 1 1	31, 89, 175, 242	0
51	B7	49/49 (100%)	1.04	11 (22%) 1 1	9, 16, 135, 218	0
51	D7	49/49 (100%)	1.55	13 (26%) 1 1	11, 32, 107, 180	0
52	B8	64/64 (100%)	-0.01	3 (4%) 32 26	5, 46, 98, 130	0
52	D8	64/64 (100%)	0.09	3 (4%) 32 26	7, 56, 123, 178	0
53	B9	37/37 (100%)	-0.51	0 100 100	10, 26, 148, 246	0
53	D9	37/37 (100%)	-0.58	0 100 100	8, 19, 104, 158	0
54	Be	72/102 (70%)	2.72	40 (55%) 0 0	24, 113, 183, 201	0
54	De	72/102 (70%)	2.75	29 (40%) 0 0	18, 114, 206, 259	0
55	Bf	0/31	-	-	-	-
55	Bg	0/31	-	-	-	-
55	Df	0/31	-	-	-	-
55	Dg	0/31	-	-	-	-
56	Bh	0/30	-	-	-	-
56	Dh	0/30	-	-	-	-
57	B1	93/93 (100%)	0.95	23 (24%) 1 1	1, 79, 187, 243	0
57	D1	93/93 (100%)	1.06	26 (27%) 1 1	8, 72, 174, 241	0
58	B4	35/35 (100%)	2.44	17 (48%) 0 0	74, 144, 233, 266	0
58	D4	35/35 (100%)	3.00	23 (65%) 0 0	64, 158, 226, 275	0
59	BA	2879/2879 (100%)	-0.50	17 (0%) 89 84	3, 43, 145, 276	0
59	DA	2879/2879 (100%)	-0.46	30 (1%) 82 75	0, 47, 163, 315	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
60	BB	119/119 (100%)	-0.42	3 (2%) 58 48	21, 108, 175, 210	0
60	DB	119/119 (100%)	0.03	10 (8%) 12 12	23, 97, 186, 258	0
All	All	22686/23318 (97%)	-0.05	1578 (6%) 17 15	0, 57, 160, 323	0

The worst 5 of 1578 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
54	Be	58	THR	13.8
32	DK	67	PHE	12.3
54	De	99	VAL	12.2
54	De	59	GLU	12.2
32	DK	62	ASP	12.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
24	UAL	AU	5	9/10	0.52	0.37	-	149,151,153,154	0
24	DPP	AU	2	6/7	0.65	0.23	-	153,153,154,154	0
24	KBE	AU	1	9/10	0.84	0.21	-	154,155,156,156	0
24	KBE	CU	1	9/10	0.90	0.30	-	69,74,77,77	0
24	DPP	CU	2	6/7	0.90	0.17	-	77,79,80,82	0
24	5OH	AU	6	12/13	0.86	0.55	-	151,153,154,154	0
24	5OH	CU	6	12/13	0.82	0.34	-	84,88,89,89	0
24	UAL	CU	5	9/10	0.73	0.34	-	89,90,91,91	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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



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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
61	FUA	AY	701	37/37	0.81	0.43	3.09	154,155,156,156	0
63	MG	BA	2901	1/1	0.98	0.28	2.97	5,5,5,5	0
62	GDP	CY	702	28/28	0.84	0.29	1.97	78,82,83,84	0
61	FUA	CY	701	37/37	0.65	0.67	1.82	199,200,202,202	0
62	GDP	AY	702	28/28	0.92	0.19	1.21	78,82,83,84	0
63	MG	CY	703	1/1	0.98	0.18	-	1,1,1,1	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.