



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:08 PM GMT

PDB ID : 4V9K
Title : 70S ribosome translocation intermediate GDPNP-I containing elongation factor EFG/GDPNP, mRNA, and tRNA bound in the pe^{*}/E state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-24
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

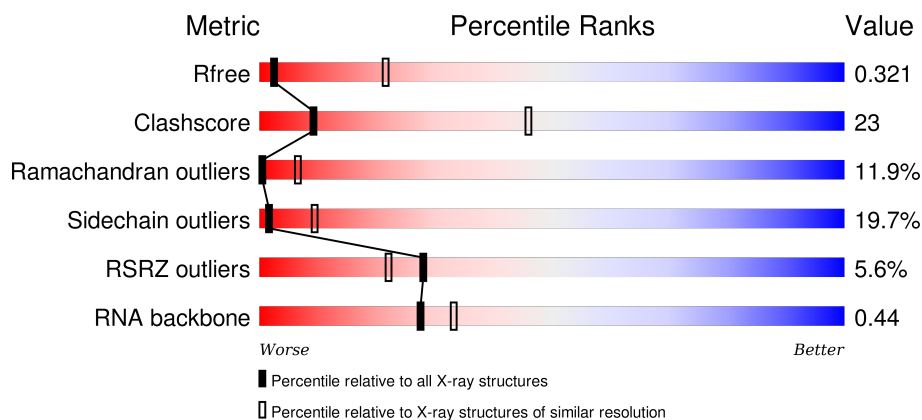
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>5%</div> <div>37%</div> <div>45%</div> <div>15%</div> <div>•</div> </div>
1	CB	235	<div> <div>12%</div> <div>40%</div> <div>48%</div> <div>10%</div> <div>•</div> </div>
2	AC	207	<div> <div>3%</div> <div>40%</div> <div>43%</div> <div>16%</div> <div>•</div> </div>
2	CC	207	<div> <div>9%</div> <div>44%</div> <div>43%</div> <div>12%</div> <div>•</div> </div>

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

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Mol	Chain	Length	Quality of chain
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AY	687	
20	CY	687	
21	AA	1511	
21	CA	1511	
22	AW	77	
22	CW	77	
23	AV	23	
23	CV	23	
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	Bf	31	
54	Bg	31	
54	Df	31	
54	Dg	31	
55	Bh	30	
55	Dh	30	
56	B1	93	
56	D1	93	
57	B4	35	
57	D4	35	
58	Be	102	
58	De	102	
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
24	5OH	CU	6	-	-	X	-
61	GNP	AY	701	-	-	X	-
61	GNP	CY	701	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 308422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
8	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
19	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 20 is a protein called Elongation factor G.

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

- Molecule 21 is a RNA chain called ribosomal RNA 16S.

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

- Molecule 22 is a RNA chain called transfer RNA.

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

- Molecule 23 is a RNA chain called messenger RNA.

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

- Molecule 24 is a protein called VIOMYCIN.

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 10 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

- Molecule 33 is a protein called 50S ribosomal protein 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			
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			

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

- 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			

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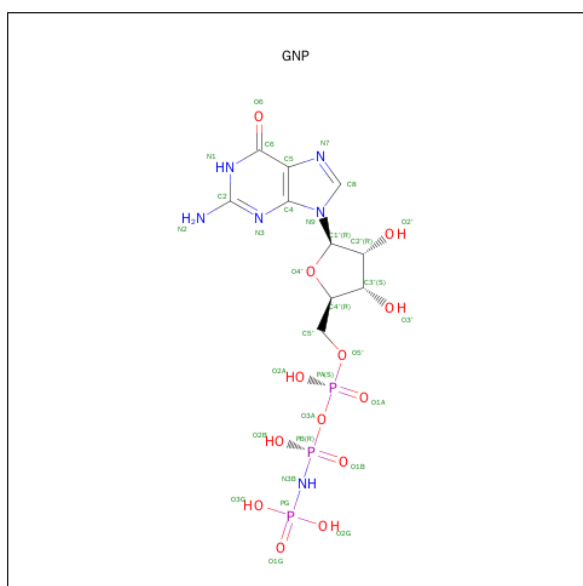
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	DA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AY	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
61	CY	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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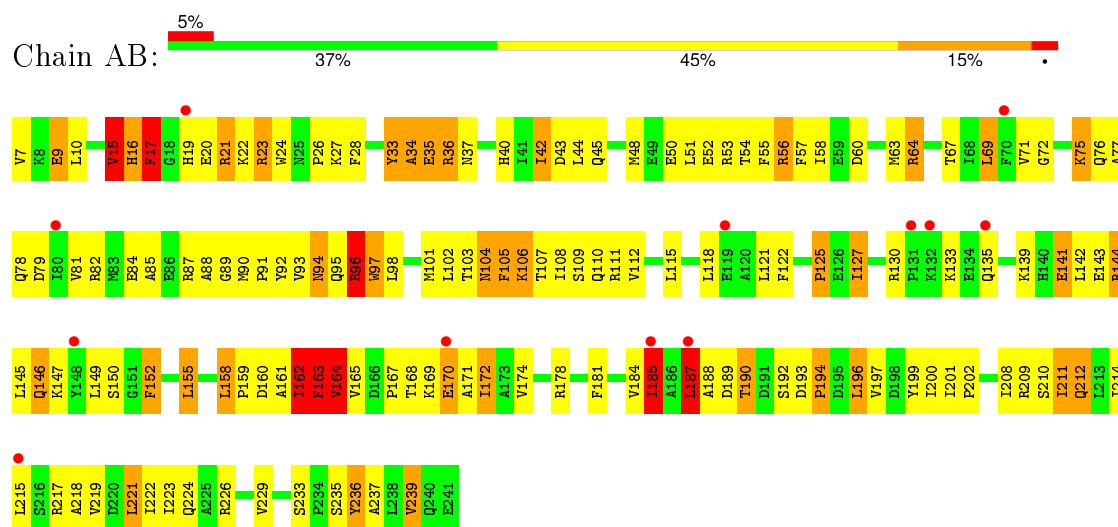
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CY	1	Total	Mg	0	0
			1	1		

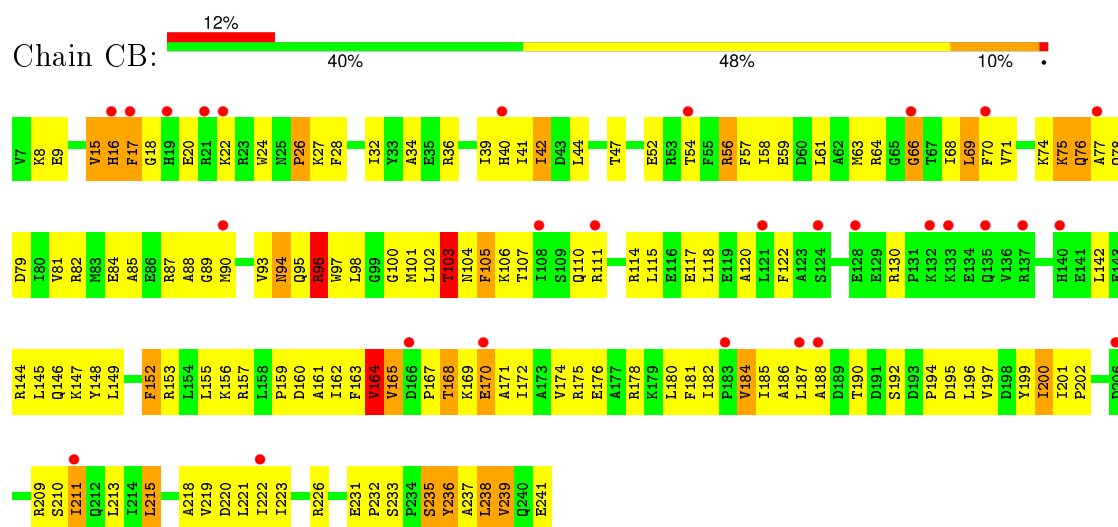
3 Residue-property plots [i](#)

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

• Molecule 1: 30S ribosomal protein S2

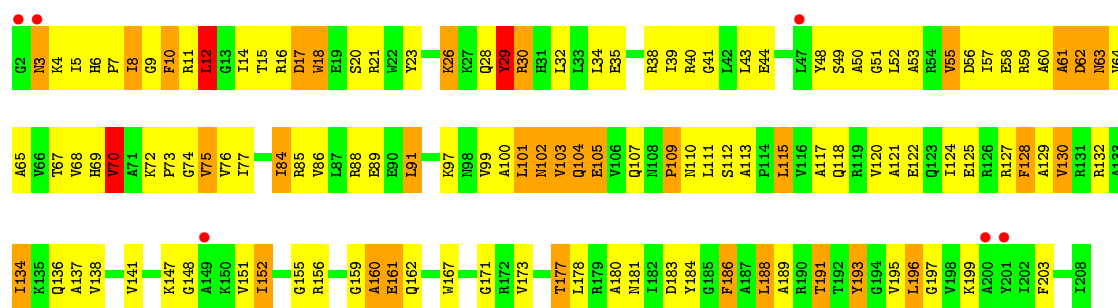


• Molecule 1: 30S ribosomal protein S2

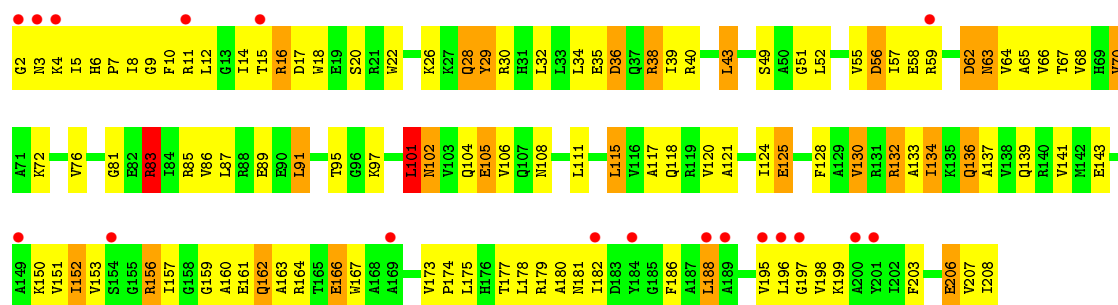


• Molecule 2: 30S ribosomal protein S3

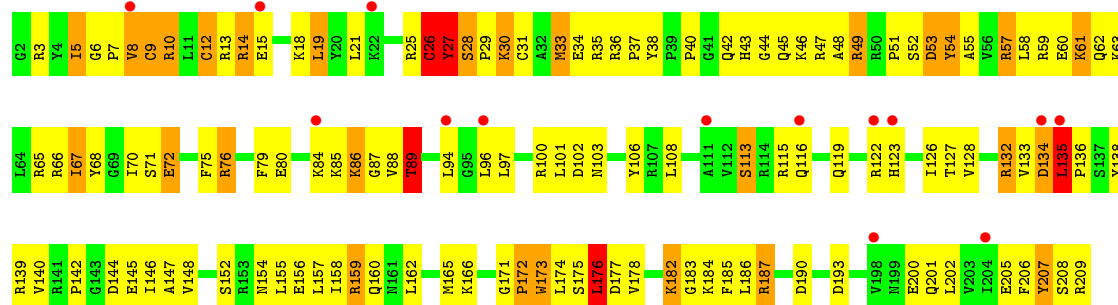




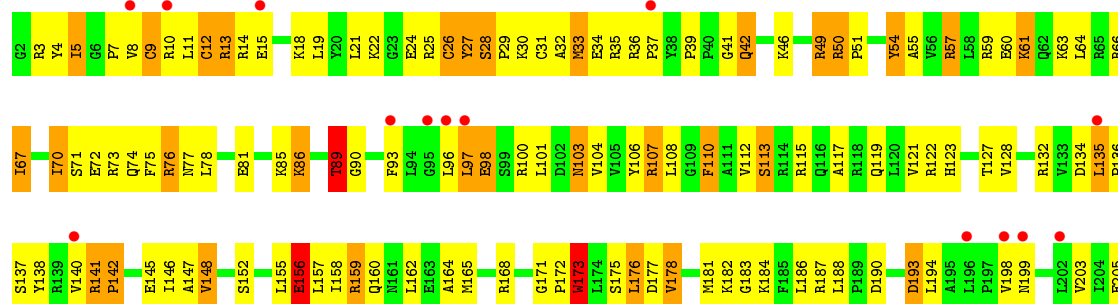
• Molecule 2: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S4

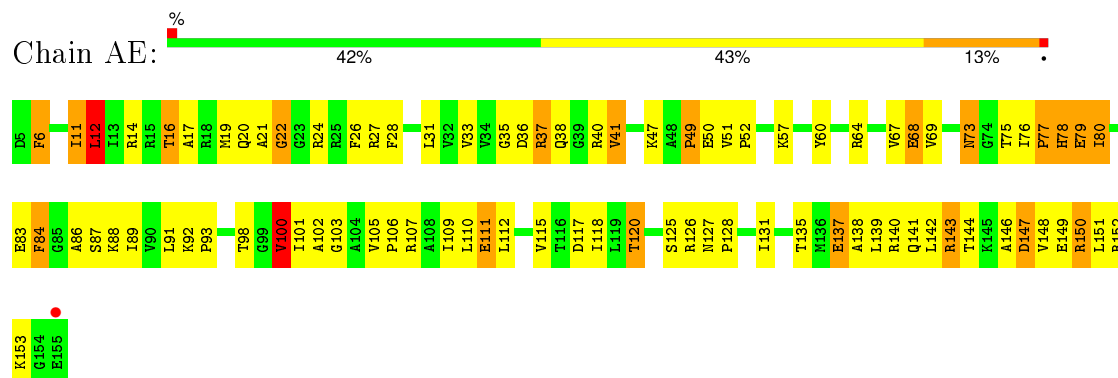


• Molecule 3: 30S ribosomal protein S4

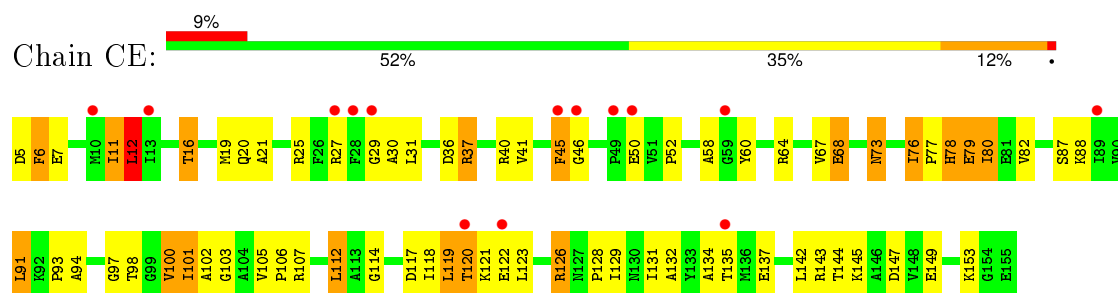




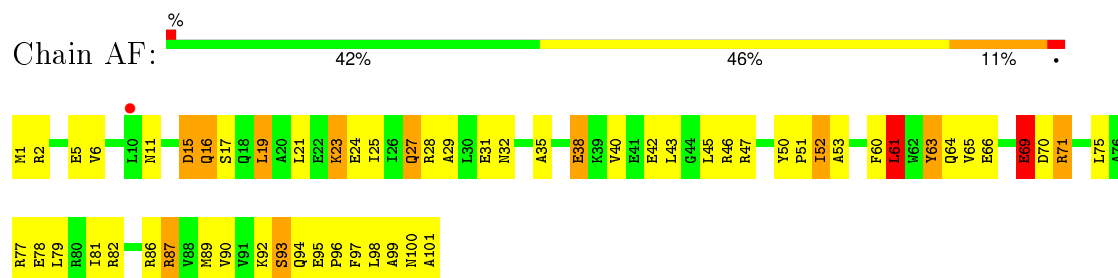
• Molecule 4: 30S ribosomal protein S5



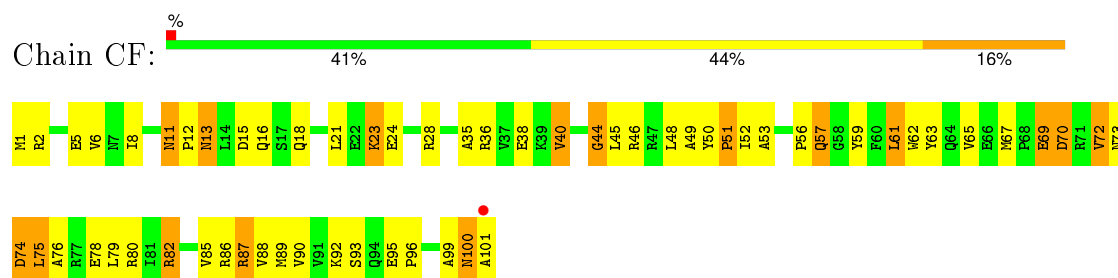
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6

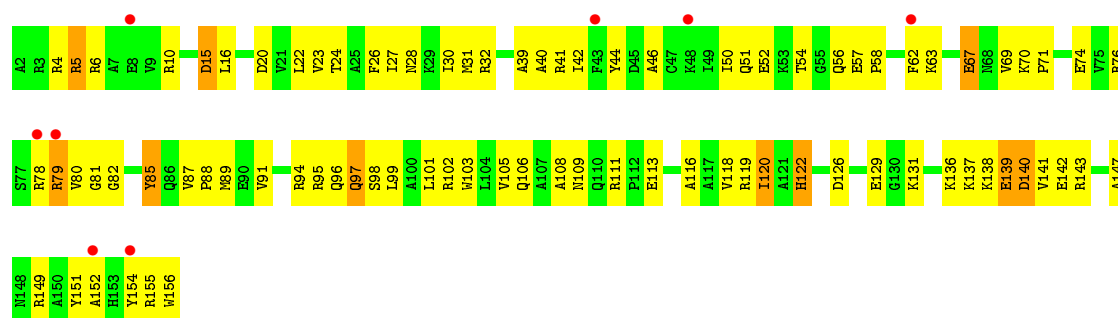


• Molecule 5: 30S ribosomal protein S6

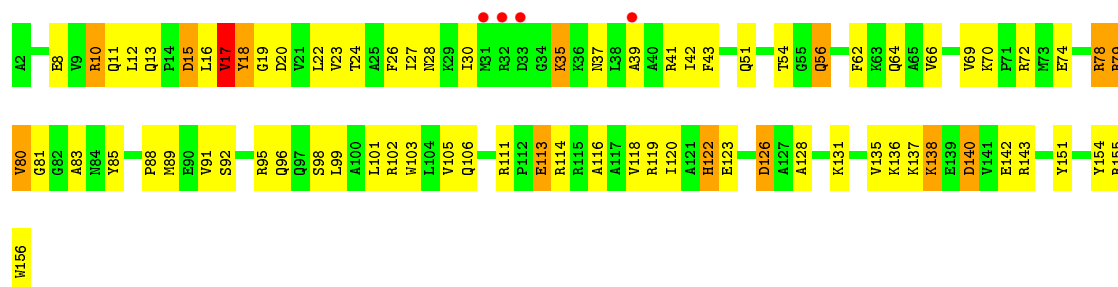


• Molecule 6: 30S ribosomal protein S7

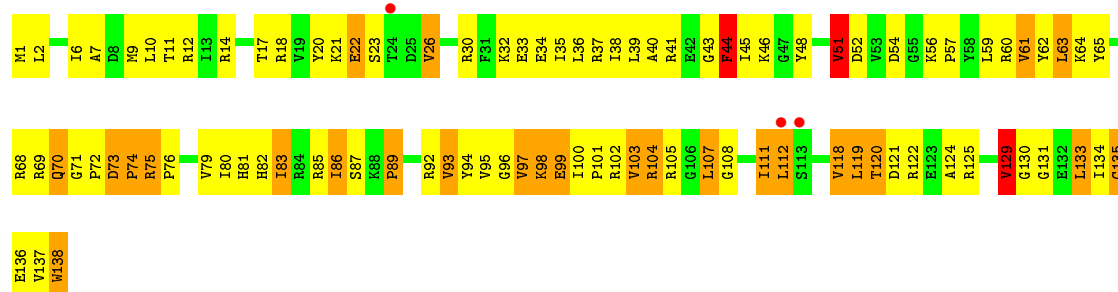




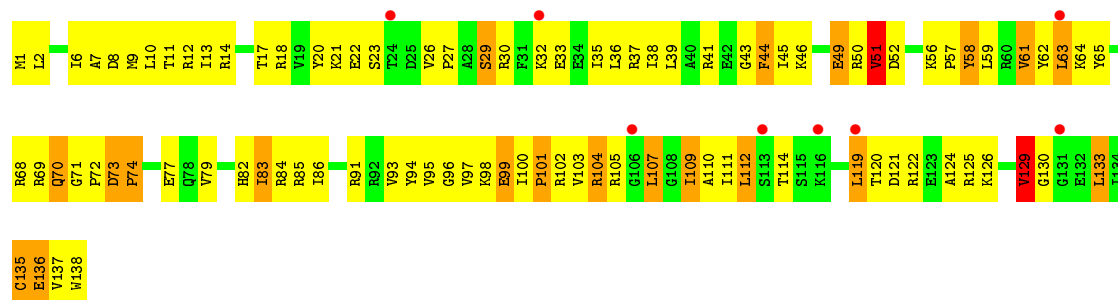
- Molecule 6: 30S ribosomal protein S7



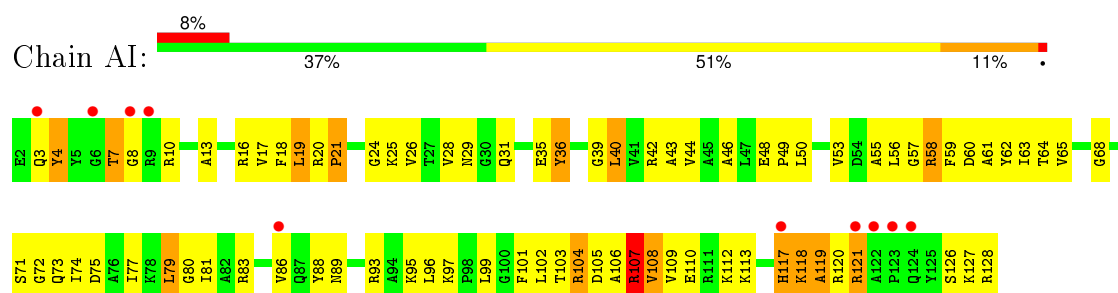
- Molecule 7: 30S ribosomal protein S8



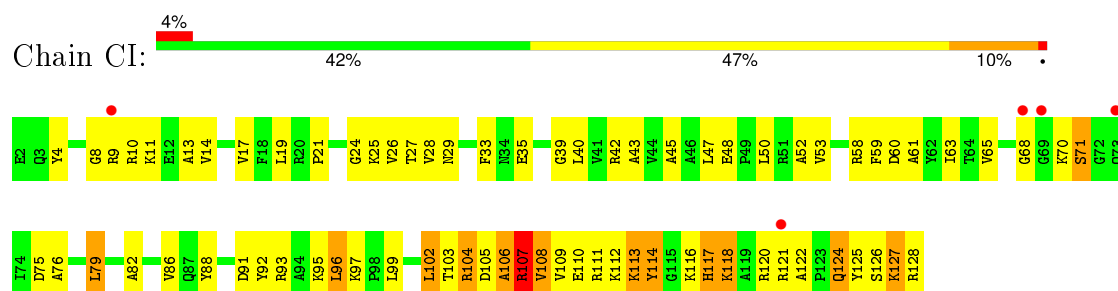
- Molecule 7: 30S ribosomal protein S8



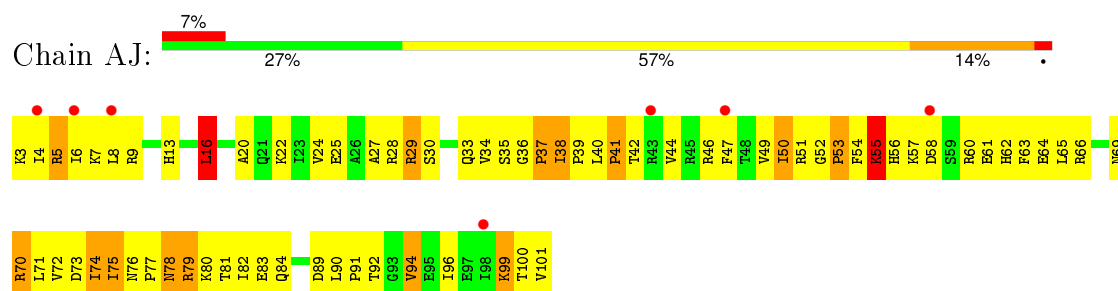
- Molecule 8: 30S ribosomal protein S9



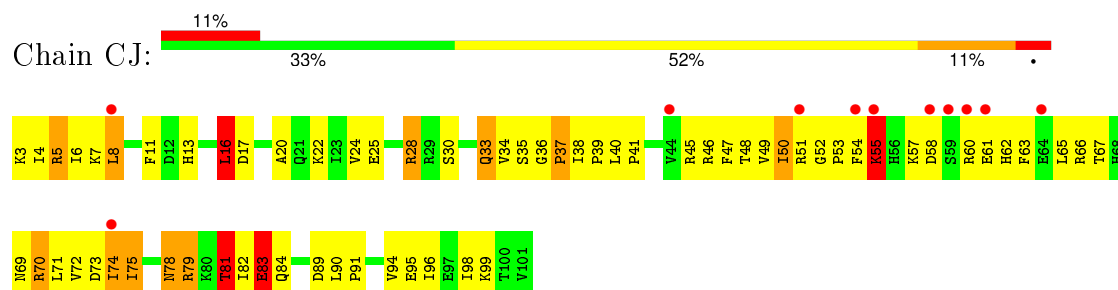
• Molecule 8: 30S ribosomal protein S9



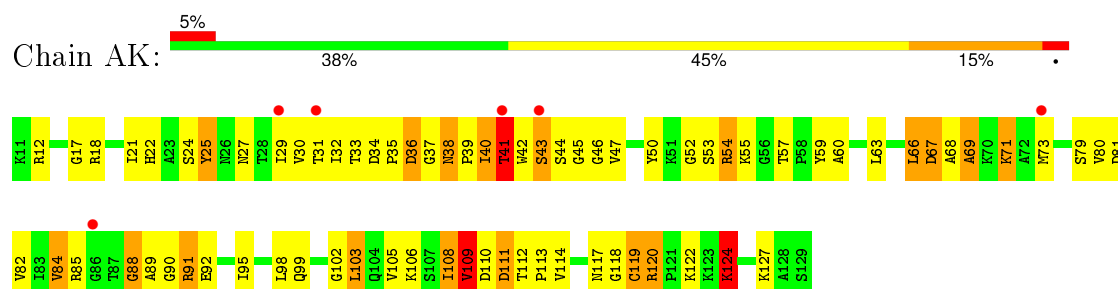
• Molecule 9: 30S ribosomal protein S10



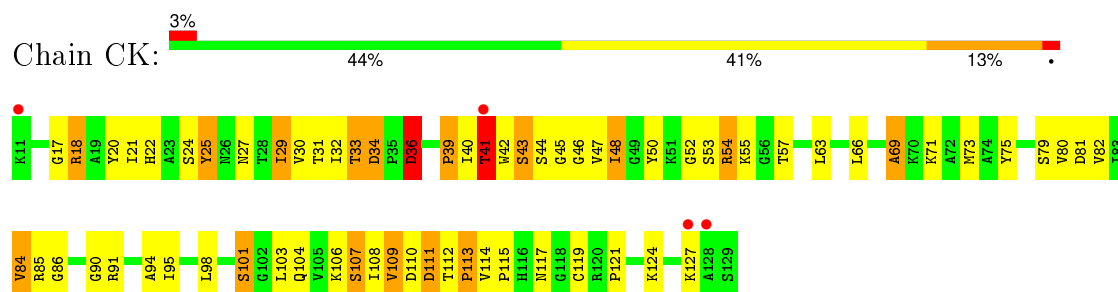
• Molecule 9: 30S ribosomal protein S10



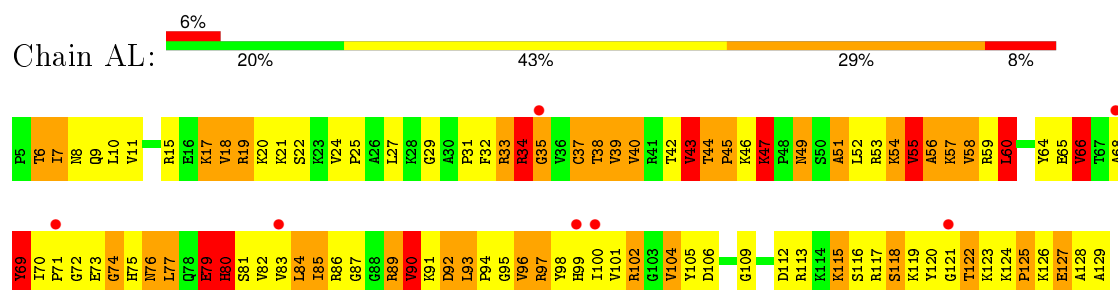
• Molecule 10: 30S ribosomal protein S11



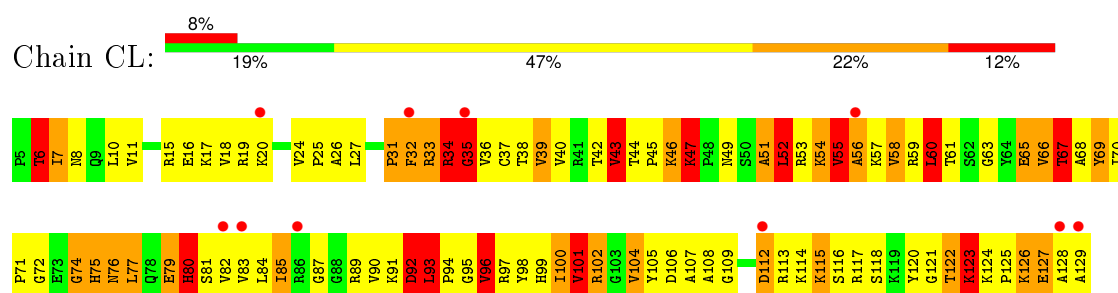
- Molecule 10: 30S ribosomal protein S11



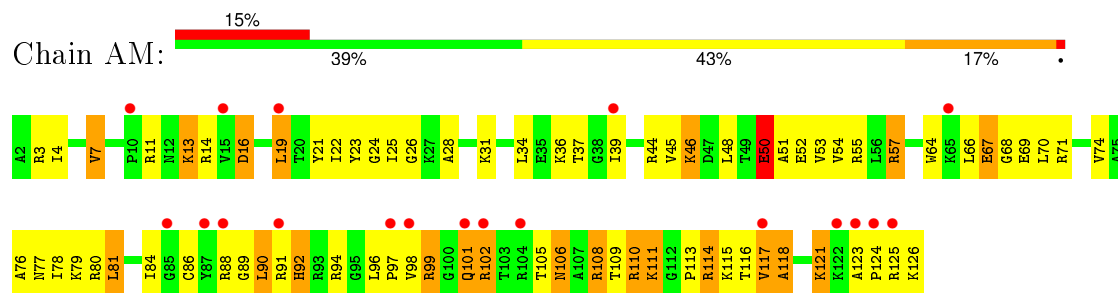
- Molecule 11: 30S ribosomal protein S12



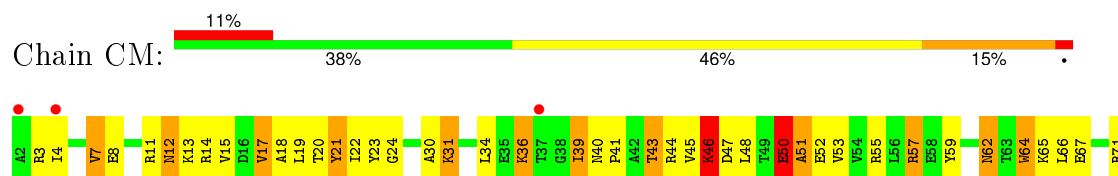
- Molecule 11: 30S ribosomal protein S12

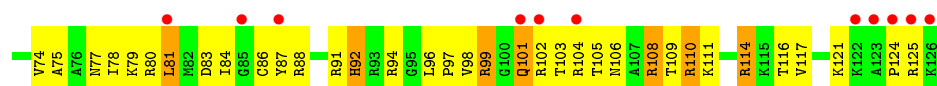


- Molecule 12: 30S ribosomal protein S13

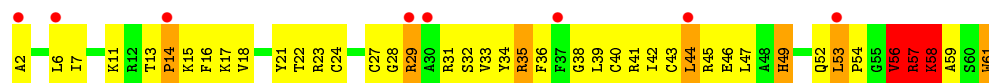


- Molecule 12: 30S ribosomal protein S13





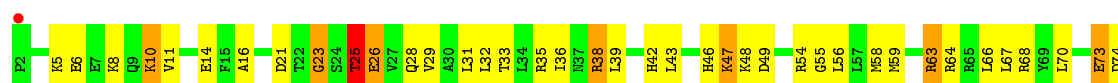
- Molecule 13: 30S ribosomal protein S14 type Z



- Molecule 13: 30S ribosomal protein S14 type Z



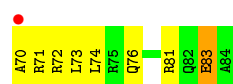
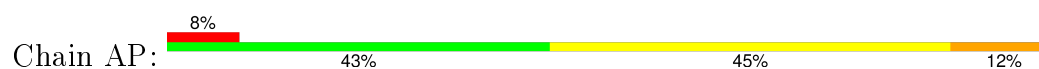
- Molecule 14: 30S ribosomal protein S15



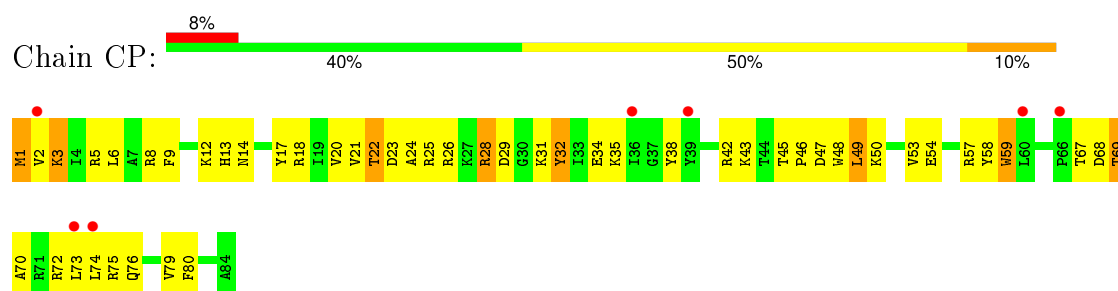
- Molecule 14: 30S ribosomal protein S15



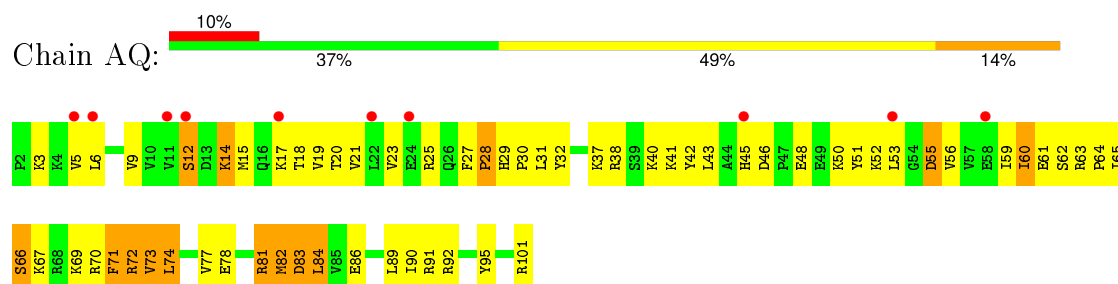
- Molecule 15: 30S ribosomal protein S16



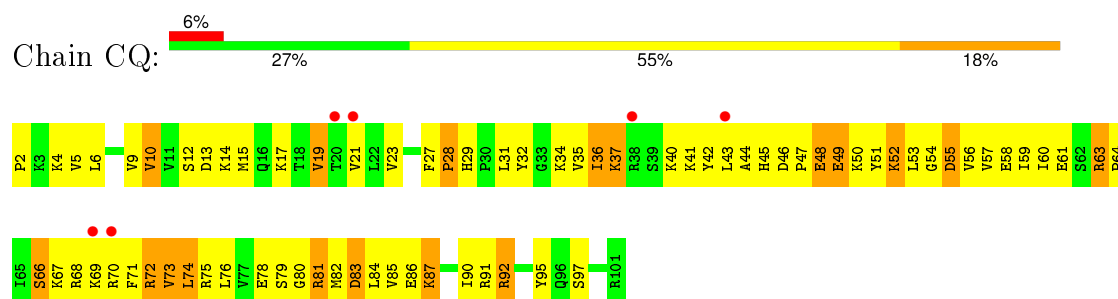
- Molecule 15: 30S ribosomal protein S16



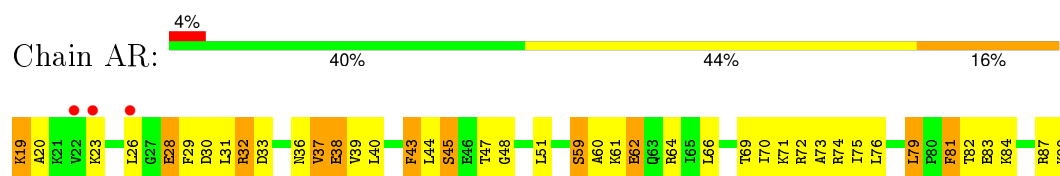
- Molecule 16: 30S ribosomal protein S17



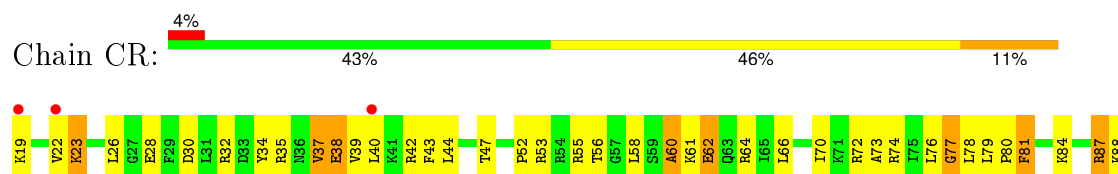
- Molecule 16: 30S ribosomal protein S17



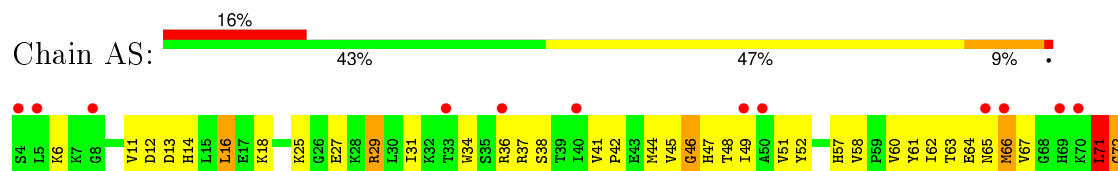
- Molecule 17: 30S ribosomal protein S18

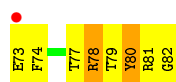


- Molecule 17: 30S ribosomal protein S18

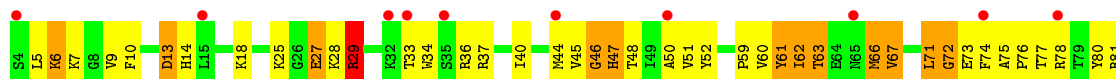


- Molecule 18: 30S ribosomal protein S19

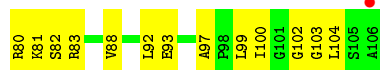
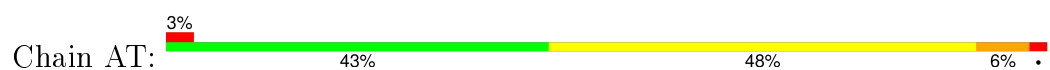




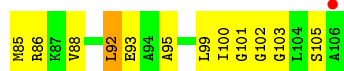
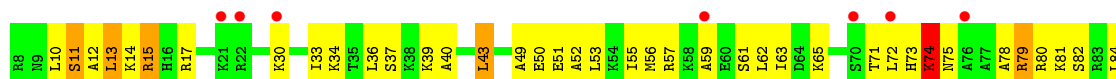
• Molecule 18: 30S ribosomal protein S19



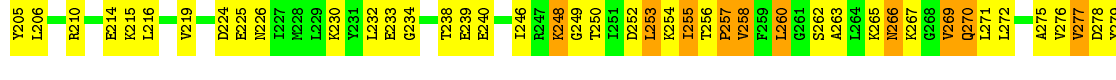
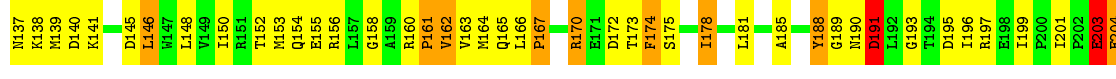
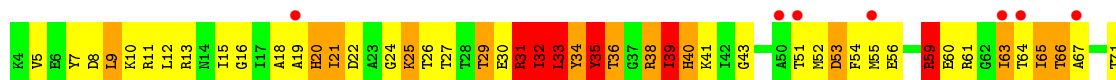
• Molecule 19: 30S ribosomal protein S20



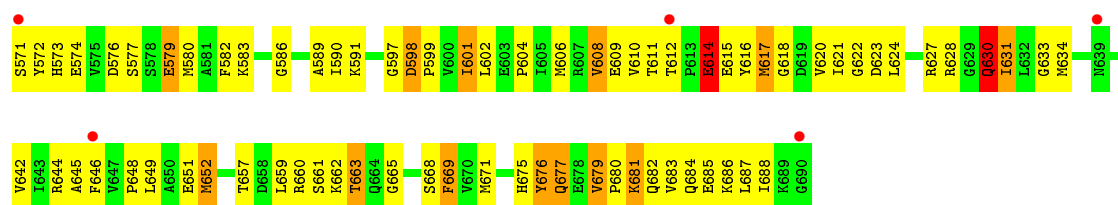
• Molecule 19: 30S ribosomal protein S20



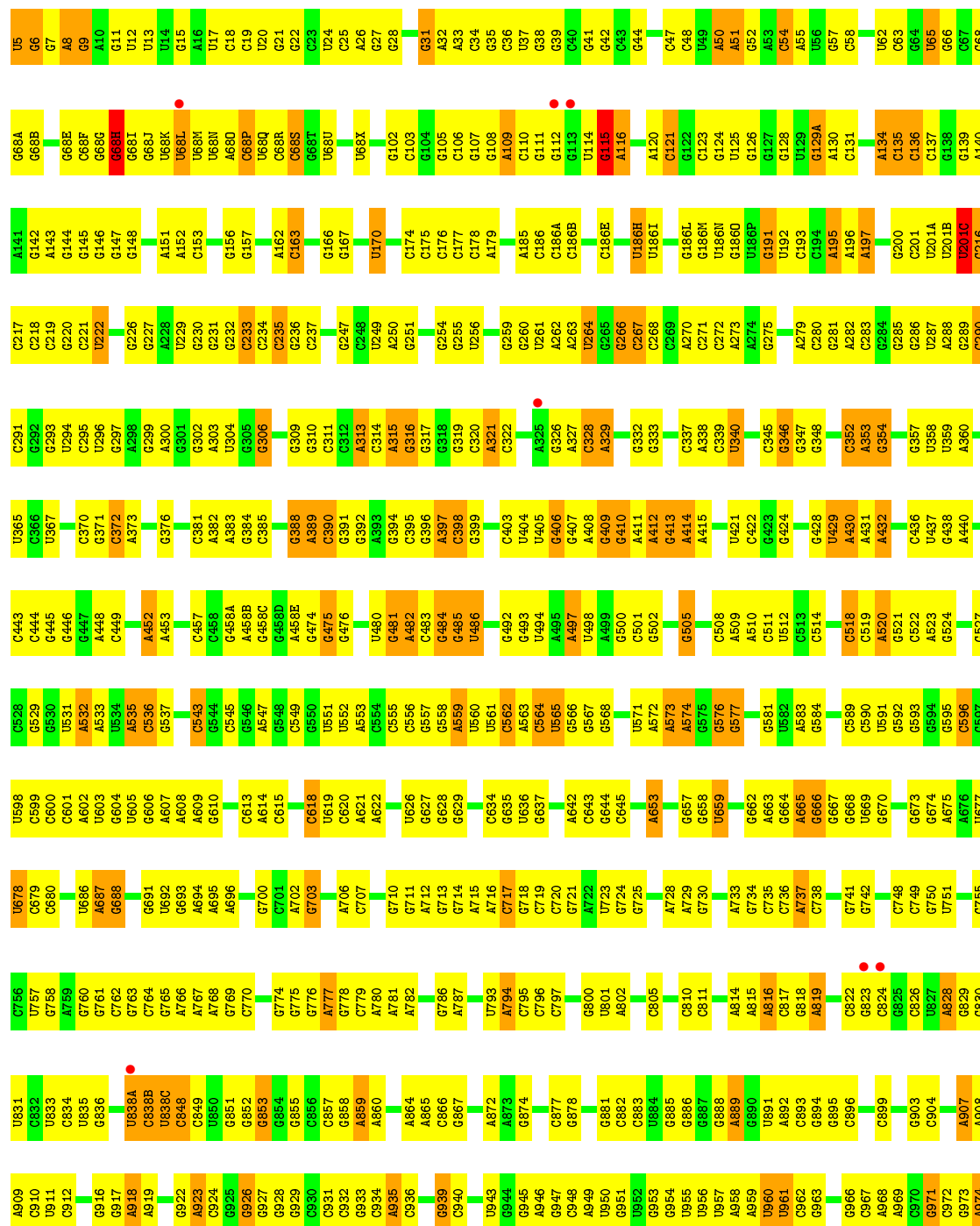
• Molecule 20: Elongation factor G







• Molecule 21: ribosomal RNA 16S





Category	Percentage
Very good	36%
Good	51%
Not good	13%

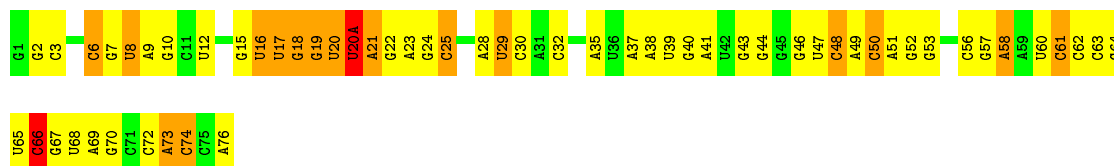


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C1403	G1210	C1128	A1044	G976	A907	G829	C756	C680	C599	G530	A441	
C1404	U1211	C1129	A1045	A977	A908	G829	C757	C680	C500	U531	C442	U365
G1405	U1212	A1130	C1045	A978	A909	U833	G758			A532	C443	C366
	A1213	G1131	U1049	C980	C911	U834	C762	A637	U603	A533	C444	U367
A1408	G1214	G1134	U1049	U981	C912	U835	C763	G688	G604	U534	G445	U368
C1409	G1215	U1135	G1053	C985	G916	C836	C764	G689	G605	A535	C446	
C1410	G1216	U1136	C1054	A986	G917	G837	C765	G690	G606	C536	G447	
A1346	C1217	C1137	U1056	A986	G918	G838	A766	G691	A608	G537	A448	C372
C1412	G1218	C1138	U1056	U982	A918	U838B	A767	U692	U609	U538	A449	A374
A1413	U1219	G1139	G1057	U983	A919	U838C	A768	U693	A609	A450	A451	C373
A1285	G1220	C1140	G1058	G993	U920	C948	G769	A695	G610	A452	A453	U375
A1286	G1221	C1141	C1059	A994	U921	C849	C770	A696	A611	C454	C455	C374
U1351	G1222	C1142	C1060	C995	G922	U851	C771	U697	C512	C456	C457	G376
A1287	G1223	G1143	G1061	U999	A923	G858	G773		C513	C458	C459	
A1288	G1224	C1144	U1062	A1000	C924	U859	G774	C701	C514	C460	C461	A382
A1289	G1225	C1145	C1063	A1001	G925	A860	G775	A702	C515	C462	C463	A383
G1290	C1226	C1146	G1064	G1002	G926	A861	G776	G703	C516	C464	C465	C385
C1423	G1227	A1146	U1065	G1003	G927	G862	A777	A704	G547	C466	C467	C386
U1292	C1228	C1147	U1065	G1004	G928	G863	A778	G705	G548	A458A	A459	C387
G1293	G1229	U1148	C1068	A1005	G929	U864	C779	A706	C549	A458B	A460	U387
U1294	C1230	U1149	G1069	A1006	G930	U865	A780	C707	C550	G458C	G461	C388
G1295	G1231	U1150	U1070	A1007	C931	A864	A781		U551		U480	A389
	U1232	A1151	U1070	C1007	C932	A865			U552		G481	C390
C1298	G1233	A1152	G1079	C1008	A935	C866	C784	G710	C553	C482	C483	C391
A1299	C1234		A1080	C1009	C936	G867	C785	G711	C554	C484	C485	C392
G1300	U1235	A1157	U1085	G1010	C937	G868	G786	A712	C555	C486	C487	
U1301	C1236	C1158	U1085	G1011	A938	G869	G787	G713	C556	C488	C489	C386
C1302	G1237	U1159	U1086	G1012	G939	U870	G788	A714	C557	C490	C491	A397
C1303	C1238	C1160	G1087	U1013	C940	U871	G789	A715	C558	C492	C493	C398
G1304	A1239	C1161	U1088	A1014	G941	A872		G716	C559	C494	C495	
G1305	U1240	C1162	G1089	A1015	G942	A873	A792	C717	C560	C496	C497	C401
A1306	G1241		U1089	A1016	U943	G874	G793	G721	C561	C498	C499	C402
	A1245	G1171	G1094	G1017	U944	C875	A794	G722	C562	C499	C500	C403
G1309	U1246	C1172	U1095	C1018	G945	G876		G723	C563	C501	C502	
G1310	G1247	G1173	C1096	C1019	A946	C877	A802	G724	C564	C503	C504	
	U1248	C1178	C1097	U1020	G947	G878	G803	G725	C565	C505	C506	
U1313	A1249	A1179	A1101	G1021	U950	C879	U804	A728	C566	C507	C508	
C1314	C1250	A1180	A1102	G1022	C951	C880	C805	A729	C567	C509	C510	
U1315	A1251	G1181	C1103	G1023	U952	C881	C806	G730	C568	C511	C512	
C1317	C1252		C1104	U1025	G953	C882	G809		C569	C513	C514	
A1318	G1253	G1187	A1105	G1026	C954	U884	C810	C735	C570	C515	C516	
A1319	C1254	A1188	A1106	G1027	U955	G885	C811	C736	C571	C517	C518	
C1320	G1255	C1189	G1107	C1028	U956		C812	A737	C572	C519	C520	
C1321	A1256	G1190	C1028A	C1028	U960	A889	C813	C738	C573	C521	C522	
C1322	U1257	A1191	G1108	C1028B	U961	G890	U813	C739	C574	C523	C524	
G1323	G1258	C1192	C1109	G1028C	C962	U891	A814		C575	C525	C526	
A1324	C1259	G1193	A1110	C1028D	G963	A892	A815	G741	C576	C527	C528	
C1325	U1260	U1194	A1111	C1028E	G964	C893	A816	G742	C577	C529	C530	
C1326	A1261	C1195		G1028F	G966	G894	C817	U743	C578	C531	C532	
C1327	C1262	U1196	C1114	G1028G	C967	C895	C818	U744	C579	C533	C534	
C1328	C1263	G1197	C1115	G1028H	C968	G896	G819	C745	C580	C535	C536	
A1329	U1264	G1198	C1118	G1028I	A969	C899	U820	C746	C581	C537	C538	
U1330	G1265		C1119	A1035	C970	A900	G821	C747	C582	C539	C540	
A1331		A1204	C1119	A1036	G971	A901	C824	C748	C583	C541	C542	
A1332		U1205	G1036	C1037	C972	G902	G825	U750	C584	C543	C544	
A1333	C1269	G1206	C1037		C973	G903	G826		C585	C545	C546	
G1334	C1270	U1125	U1125	U1040	G974		U827	A753	C586	C547	C548	
C1335	C1271	C1208	U1126					C754	C587	C549	C550	



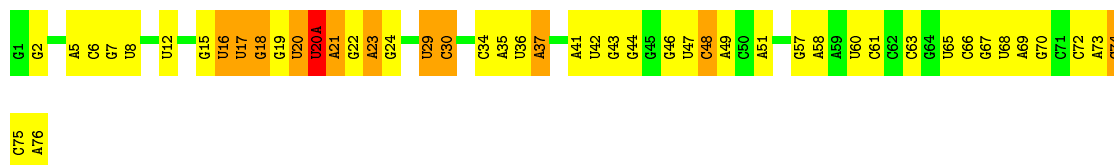
- Molecule 22: transfer RNA

Chain AW: 25% 52% 21%



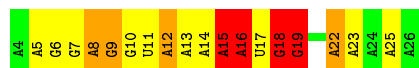
- Molecule 22: transfer RNA

Chain CW: 38% 47% 14%



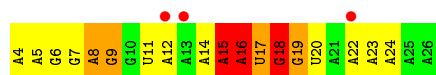
- Molecule 23: messenger RNA

Chain AV: 22% 43% 17% 17%



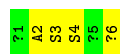
- Molecule 23: messenger RNA

Chain CV: 13% 22% 48% 17% 13%



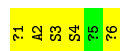
- Molecule 24: VIOMYCIN

Chain AU: 33% 67%

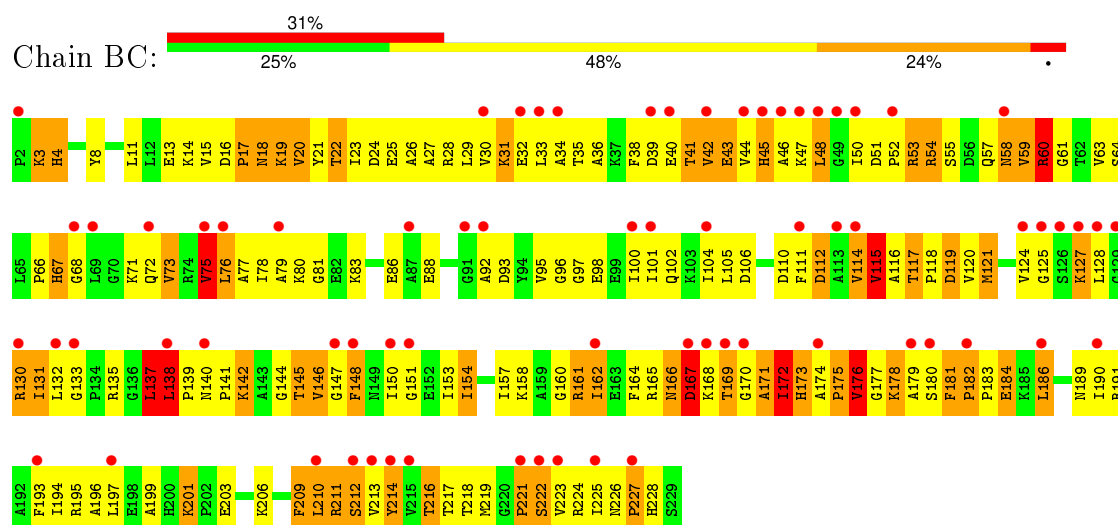


- Molecule 24: VIOMYCIN

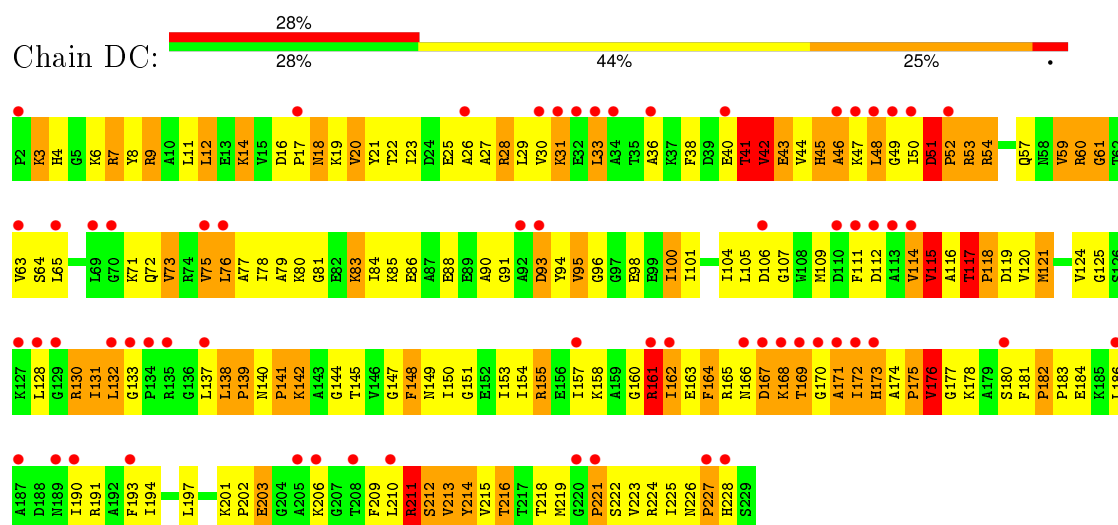
Chain CU: 17% 83%



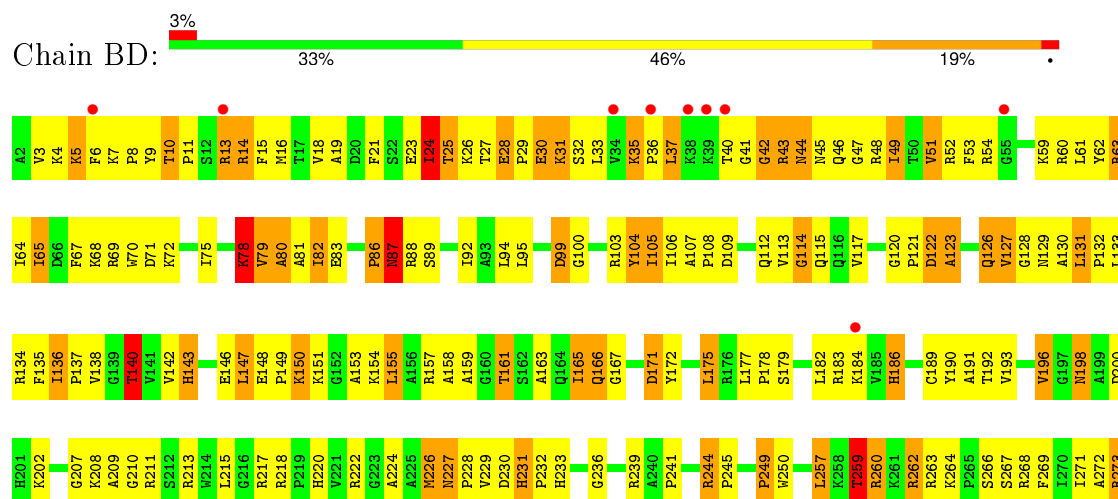
- Molecule 25: 50S ribosomal protein L1



• Molecule 25: 50S ribosomal protein L1

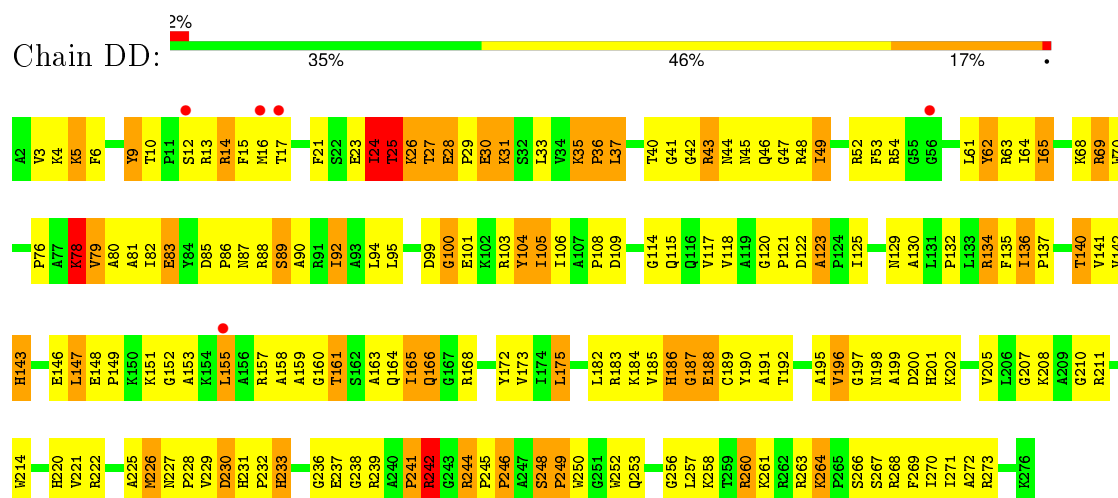


• Molecule 26: 50S ribosomal protein L2

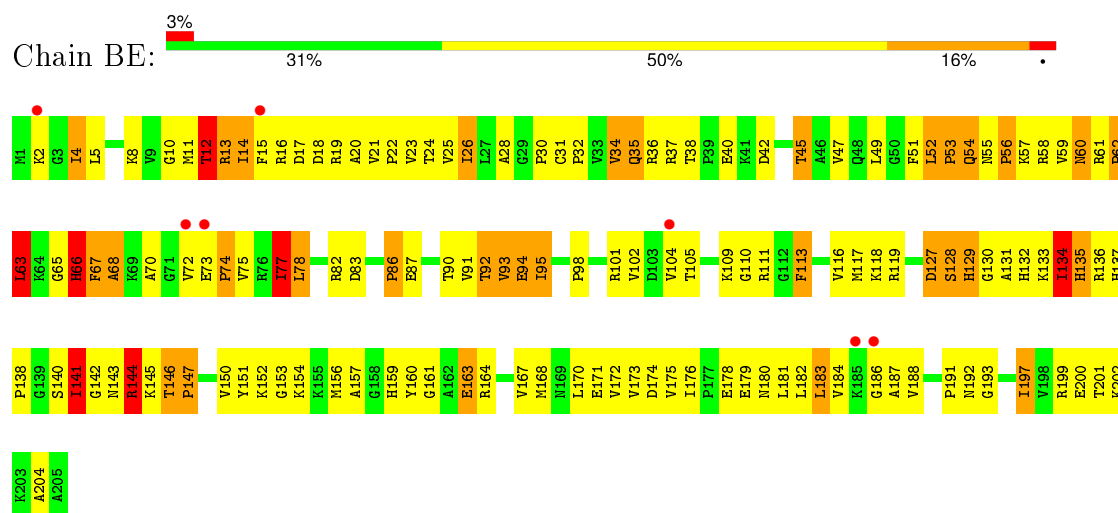


R274
R275
R276

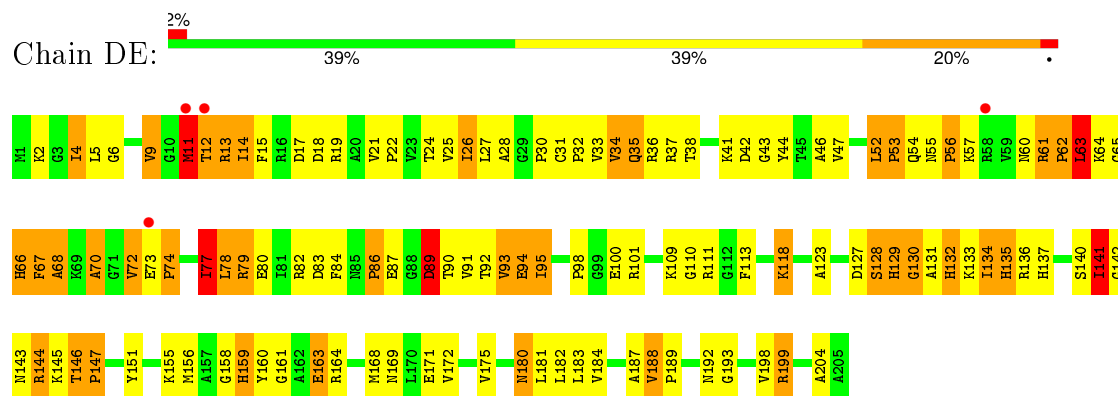
• Molecule 26: 50S ribosomal protein L2



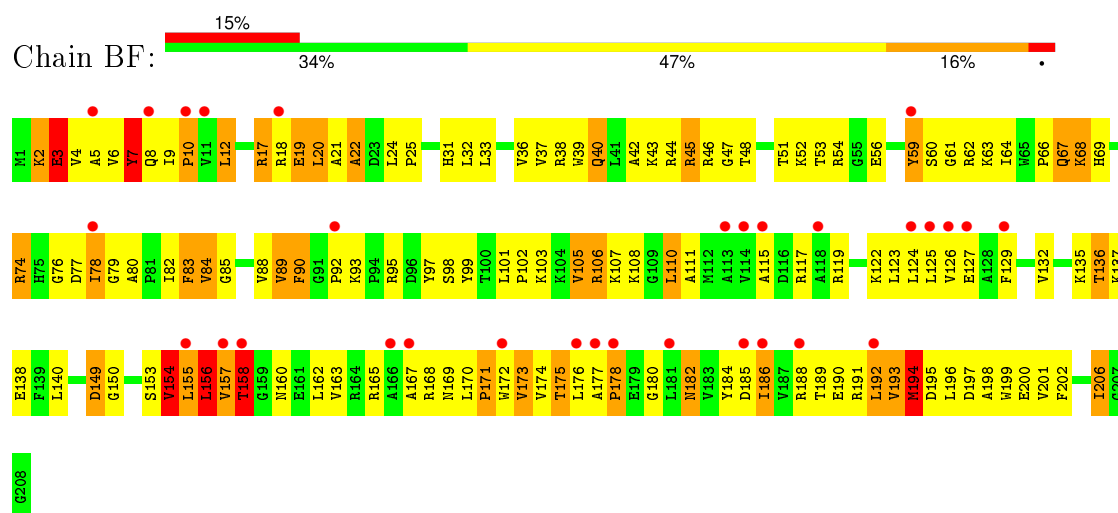
• Molecule 27: 50S ribosomal protein L3



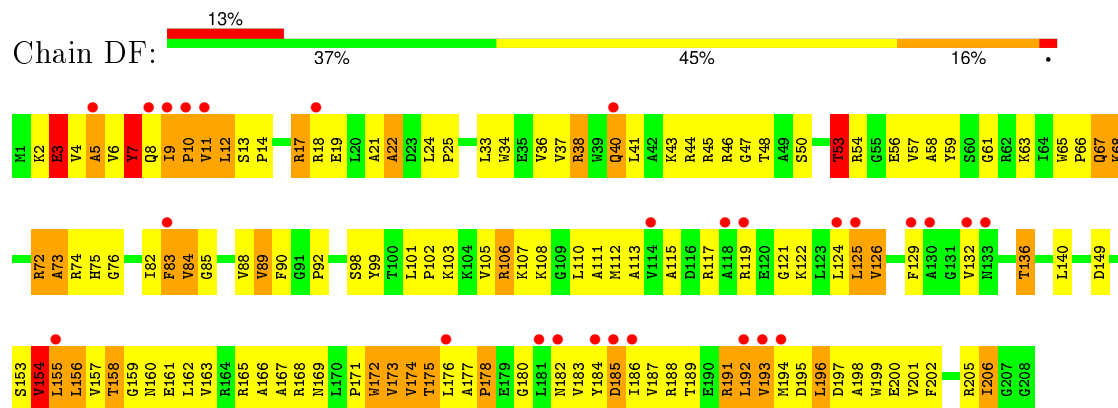
• Molecule 27: 50S ribosomal protein L3



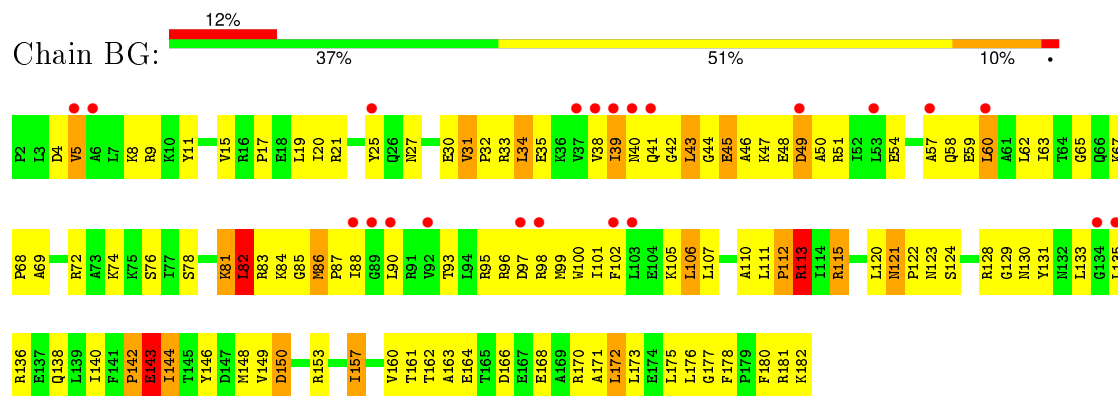
• Molecule 28: 50S ribosomal protein L4



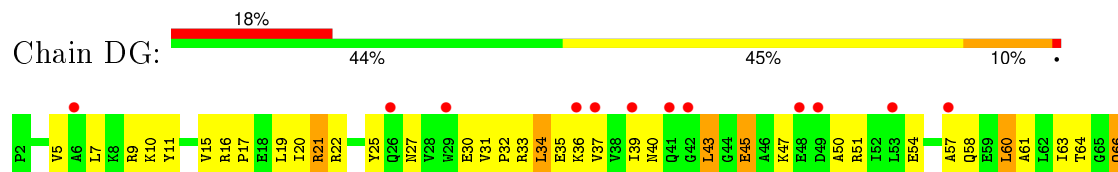
- Molecule 28: 50S ribosomal protein L4

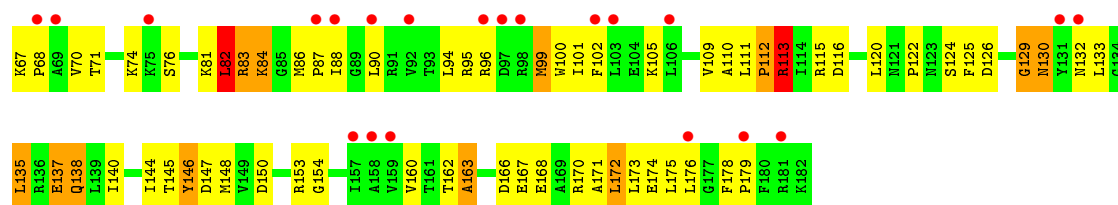


- Molecule 29: 50S ribosomal protein L5

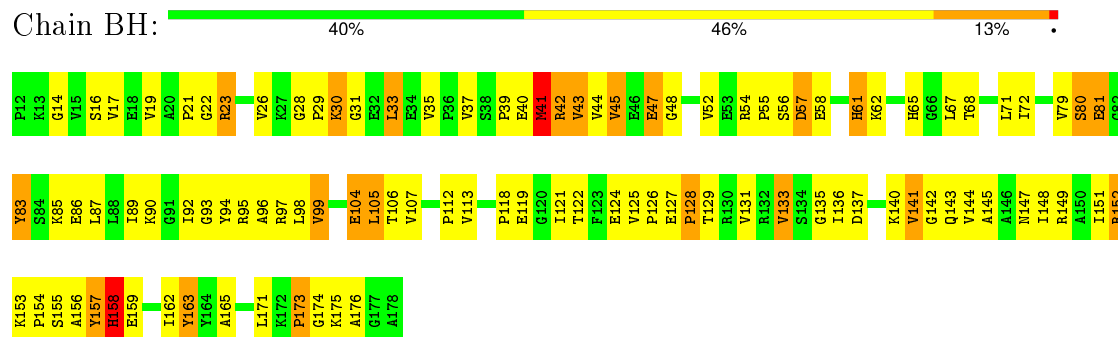


- Molecule 29: 50S ribosomal protein L5

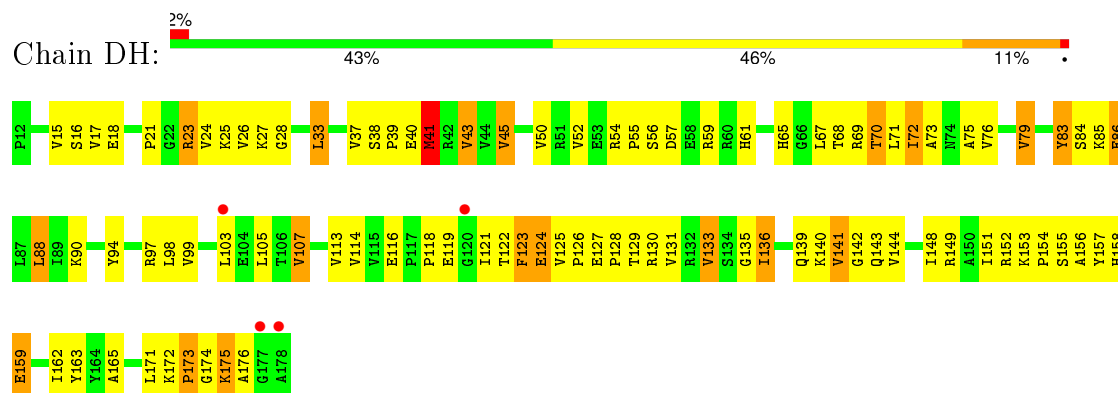




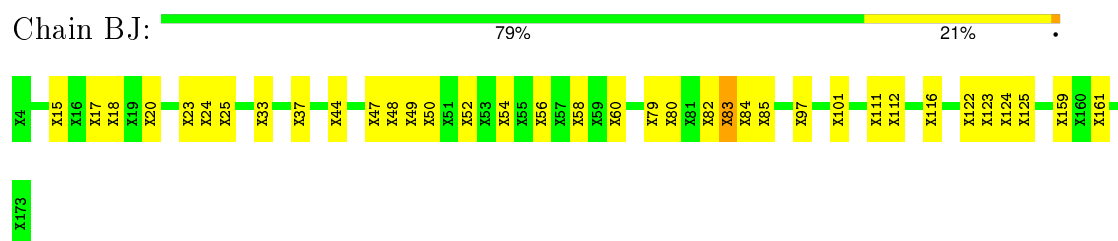
• Molecule 30: 50S ribosomal protein L6



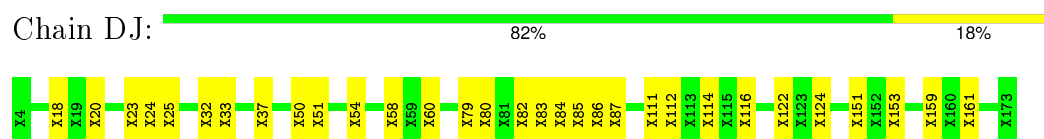
• Molecule 30: 50S ribosomal protein L6



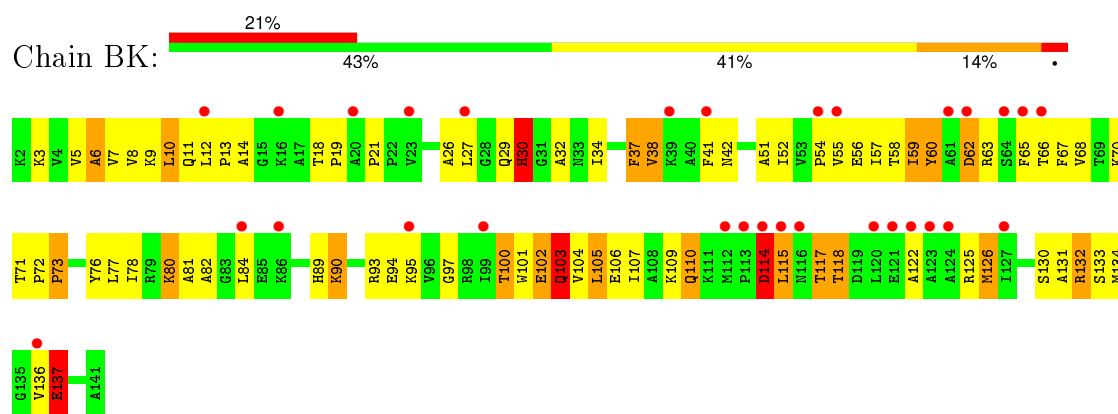
• Molecule 31: 50S RIBOSOMAL PROTEIN L10



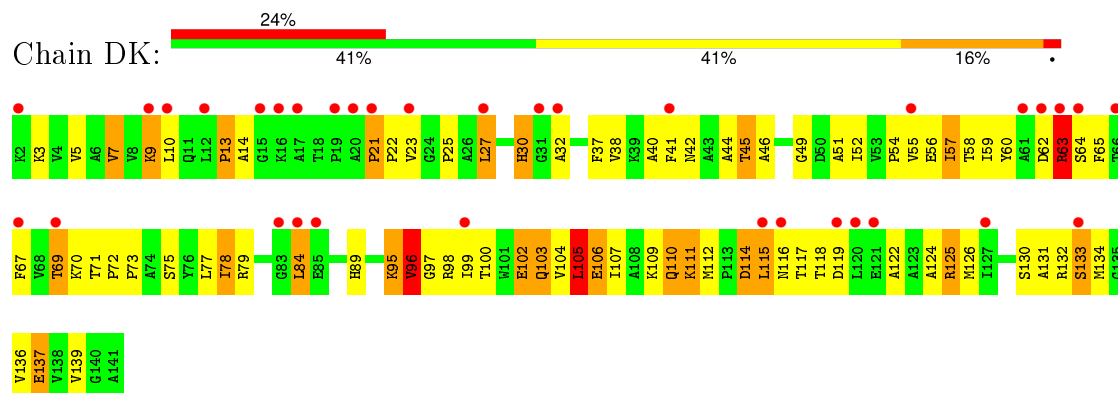
• Molecule 31: 50S RIBOSOMAL PROTEIN L10



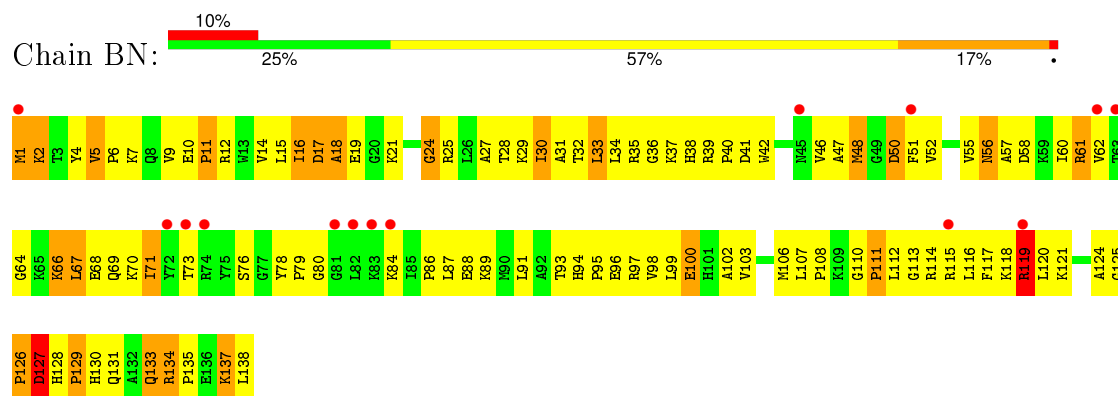
• Molecule 32: 50S ribosomal protein L11



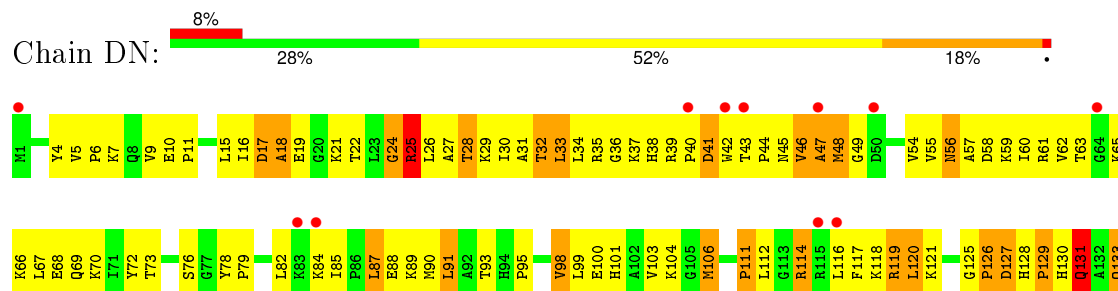
• Molecule 32: 50S ribosomal protein L11



• Molecule 33: 50S ribosomal protein L13



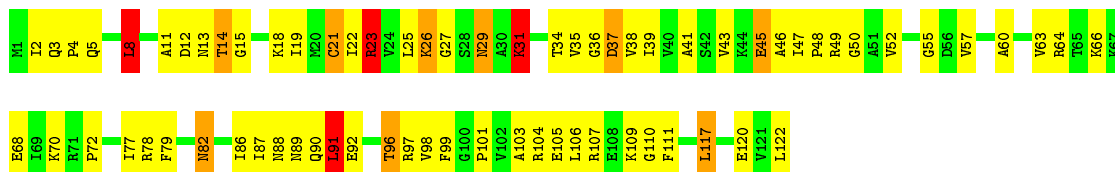
• Molecule 33: 50S ribosomal protein L13





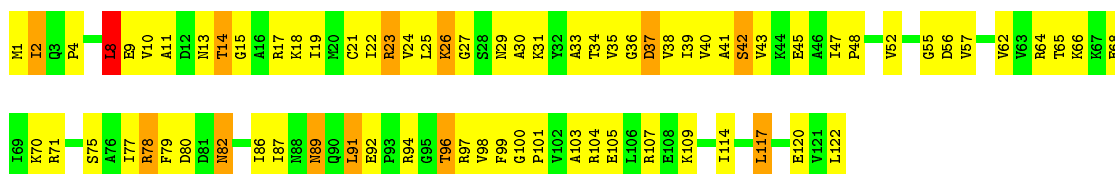
• Molecule 34: 50S ribosomal protein L14

Chain BO: 42% 48% 7% .



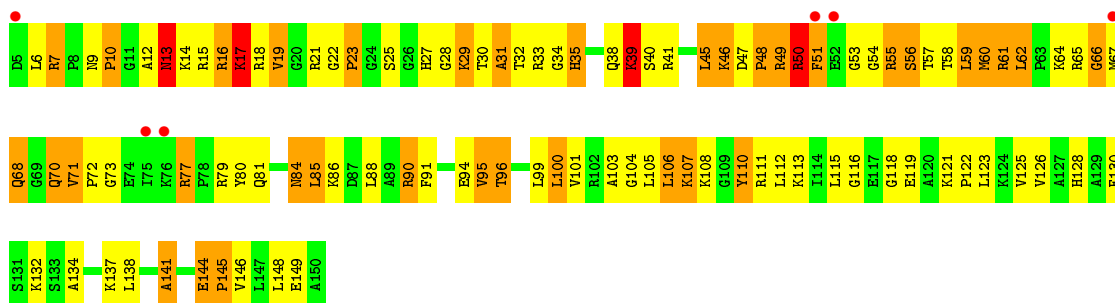
• Molecule 34: 50S ribosomal protein L14

Chain DO: 39% 51% 10% .



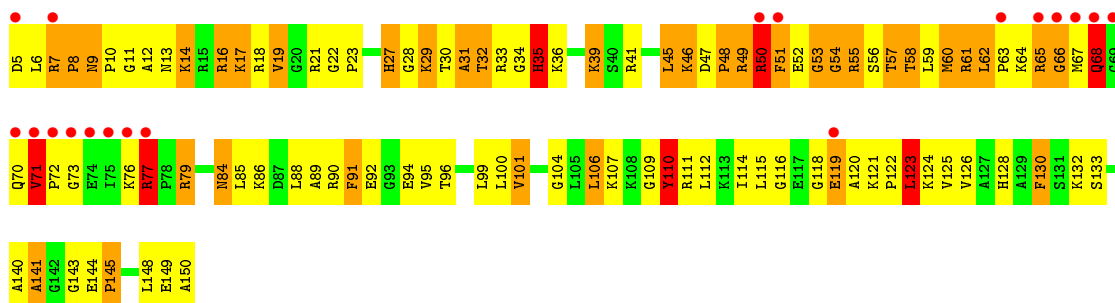
• Molecule 35: 50S ribosomal protein L15

Chain BP: 4% 30% 42% 25% .

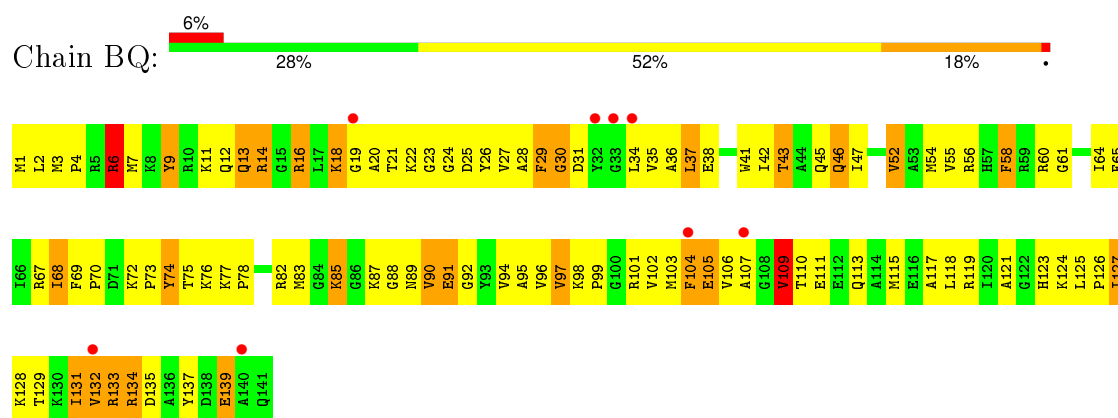


• Molecule 35: 50S ribosomal protein L15

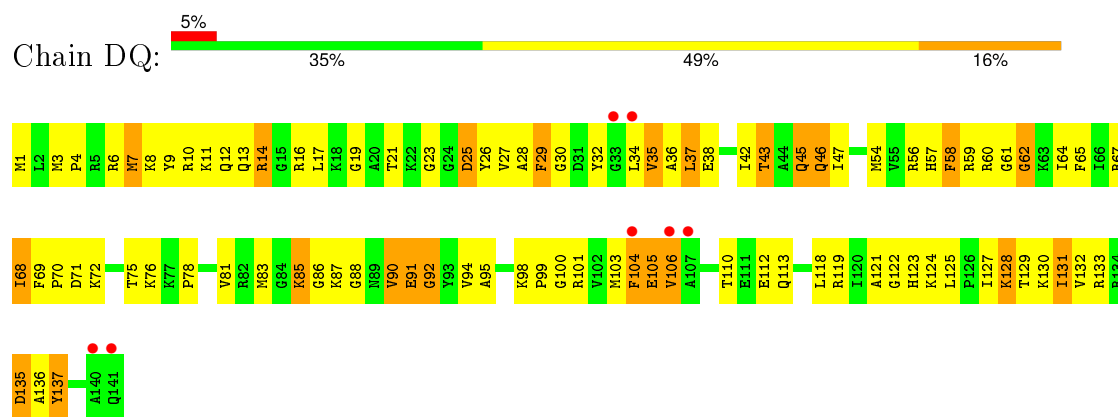
Chain DP: 13% 28% 42% 25% 5%



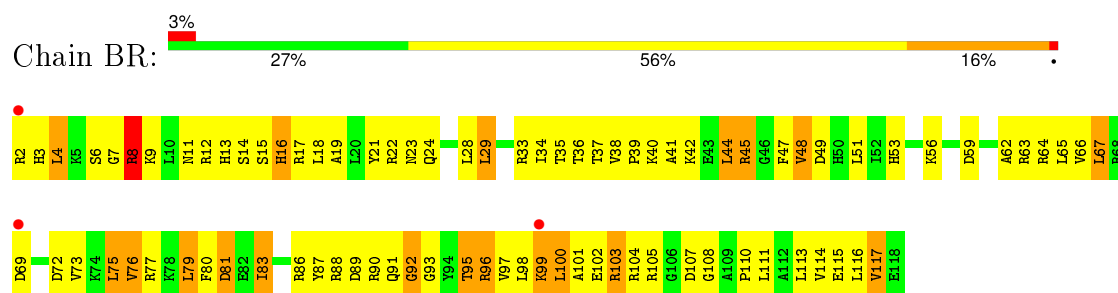
• Molecule 36: 50S ribosomal protein L16



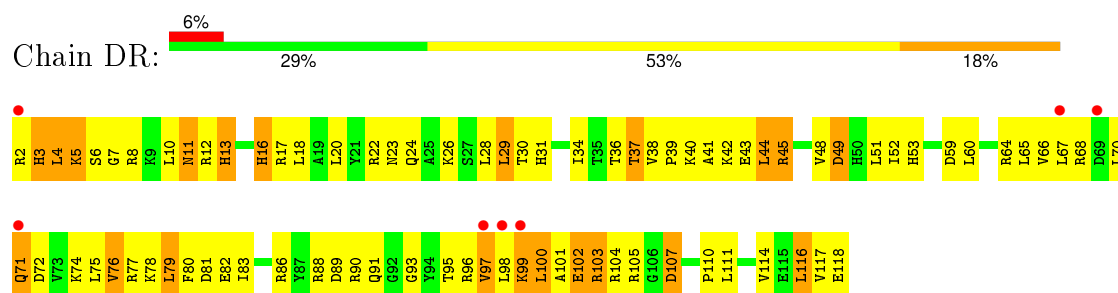
• Molecule 36: 50S ribosomal protein L16



• Molecule 37: 50S ribosomal protein L17

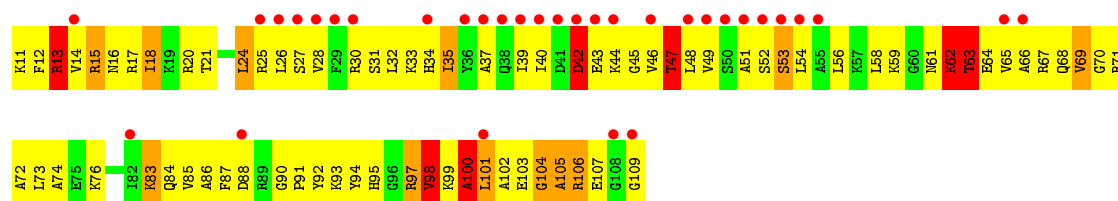


• Molecule 37: 50S ribosomal protein L17

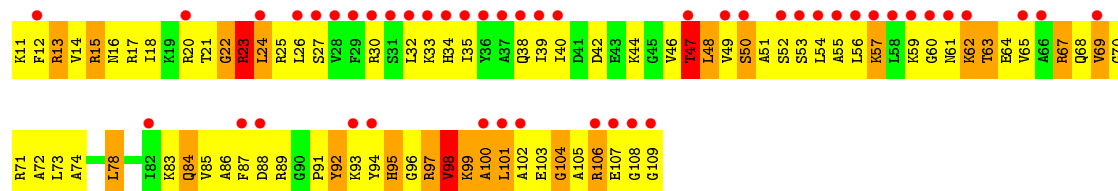


• Molecule 38: 50S ribosomal protein L18

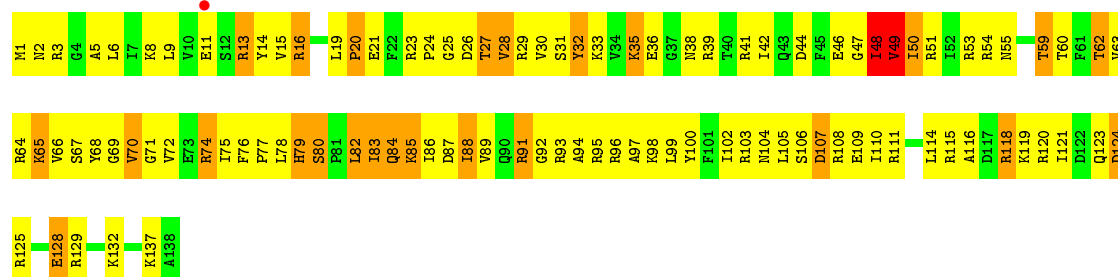




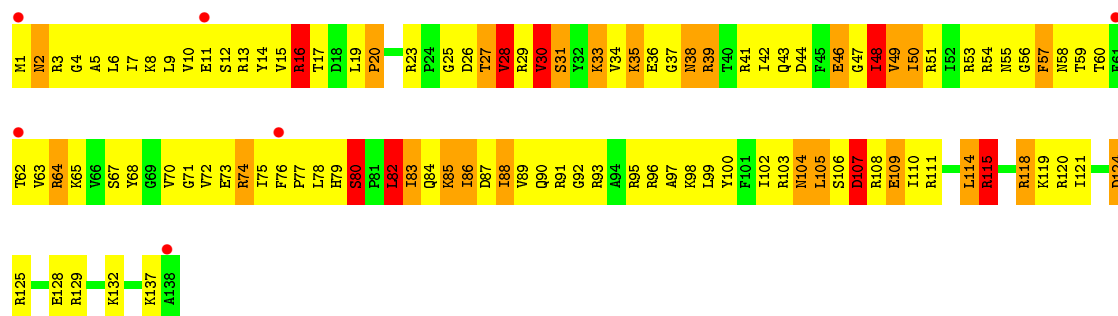
• Molecule 38: 50S ribosomal protein L18



• Molecule 39: 50S ribosomal protein L19

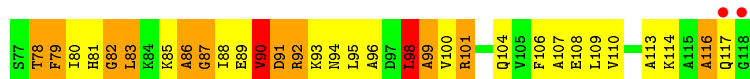


• Molecule 39: 50S ribosomal protein L19

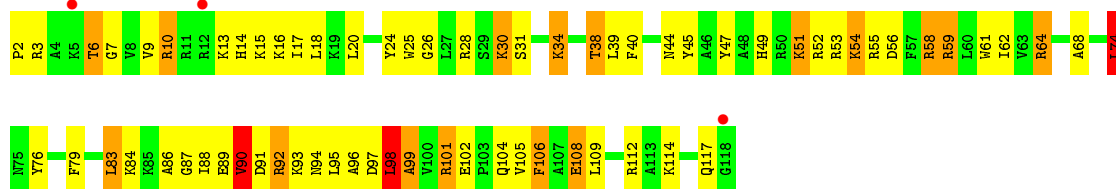
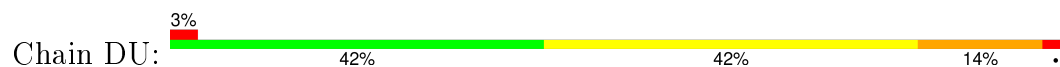


• Molecule 40: 50S ribosomal protein L20

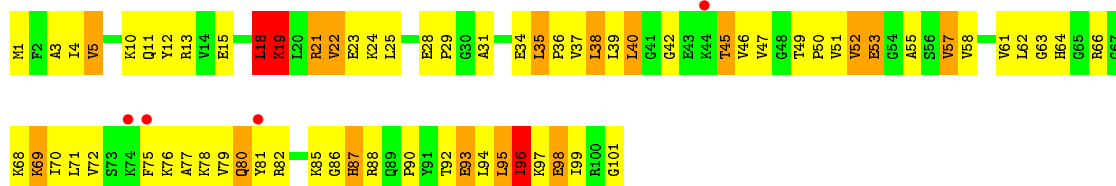




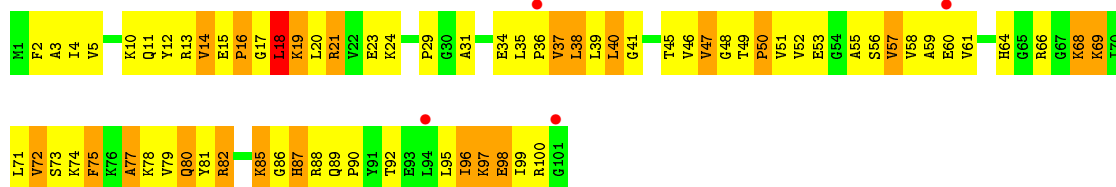
- Molecule 40: 50S ribosomal protein L20



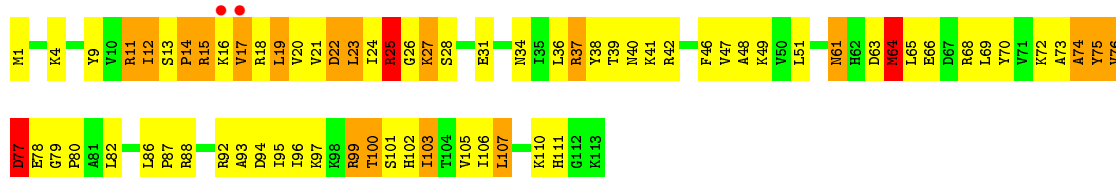
- Molecule 41: 50S ribosomal protein L21



- Molecule 41: 50S ribosomal protein L21

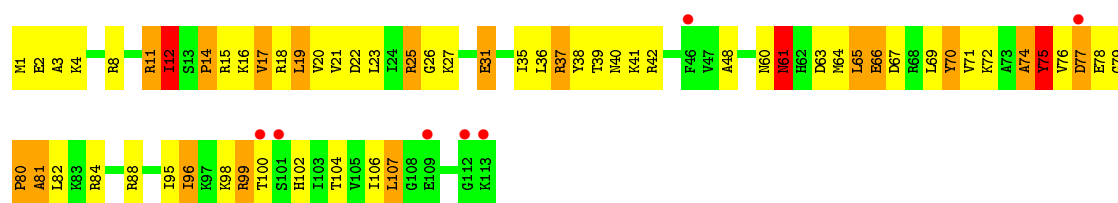


- Molecule 42: 50S ribosomal protein L22

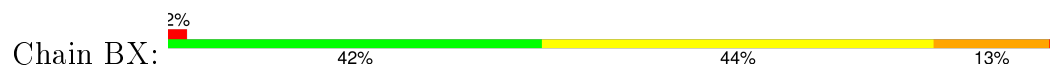


- Molecule 42: 50S ribosomal protein L22





- Molecule 43: 50S ribosomal protein L23



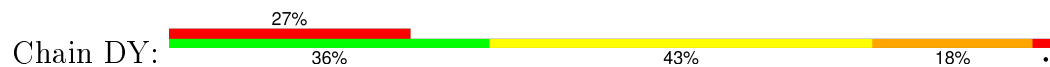
- Molecule 43: 50S ribosomal protein L23



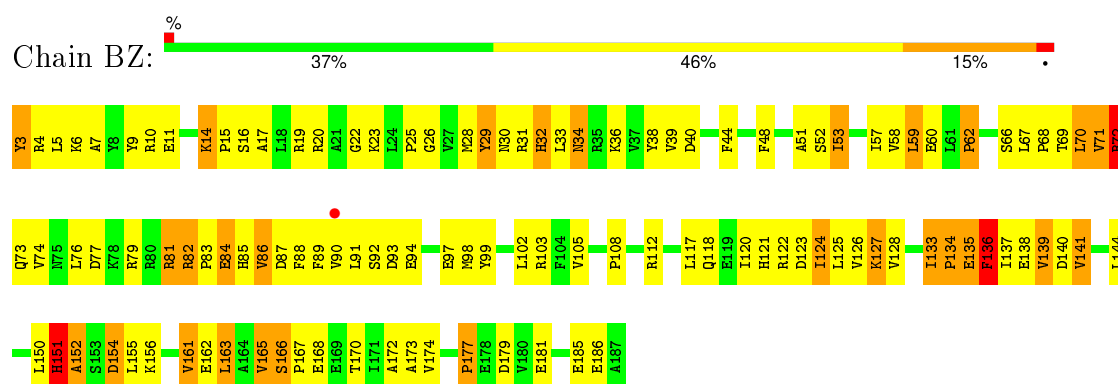
- Molecule 44: 50S ribosomal protein L24



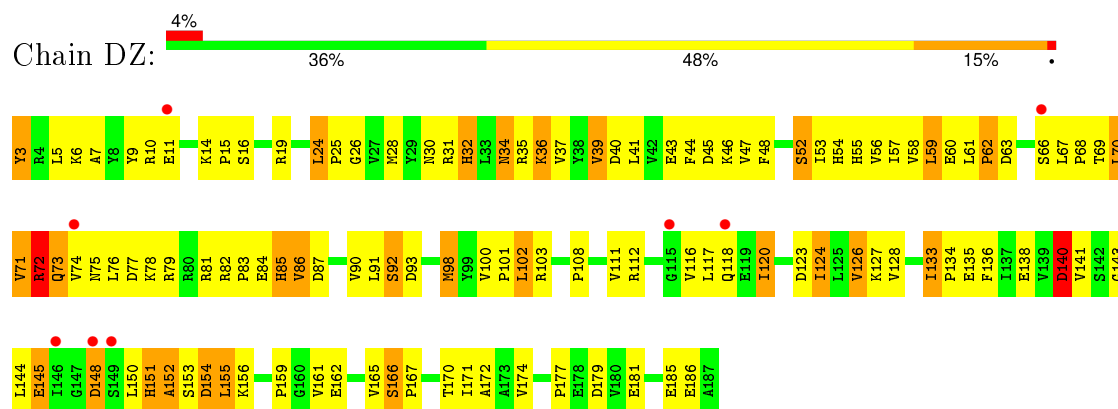
- Molecule 44: 50S ribosomal protein L24



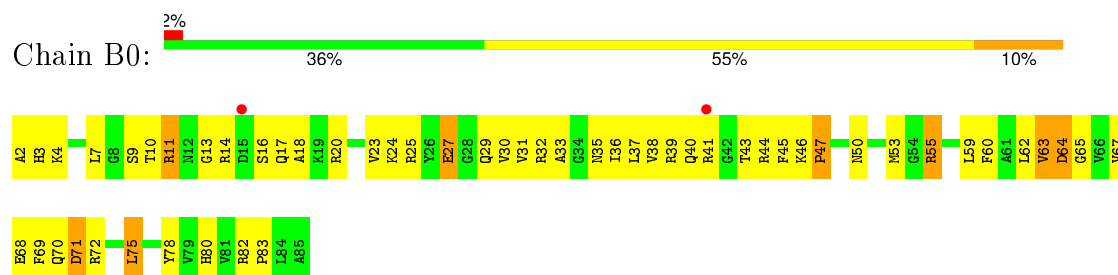
- Molecule 45: 50S ribosomal protein L25



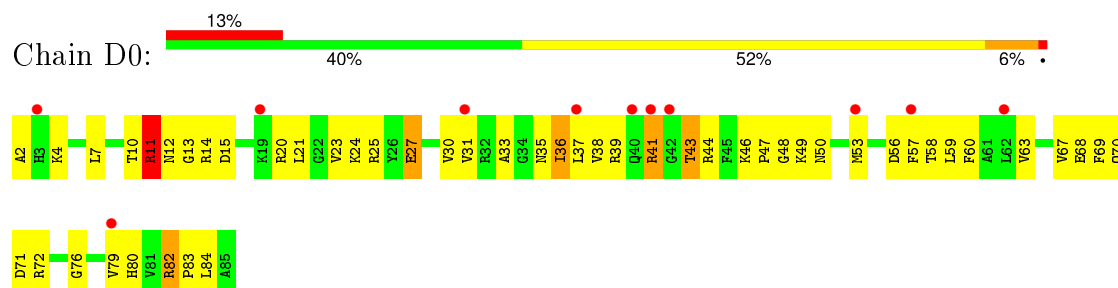
• Molecule 45: 50S ribosomal protein L25



• Molecule 46: 50S ribosomal protein L27

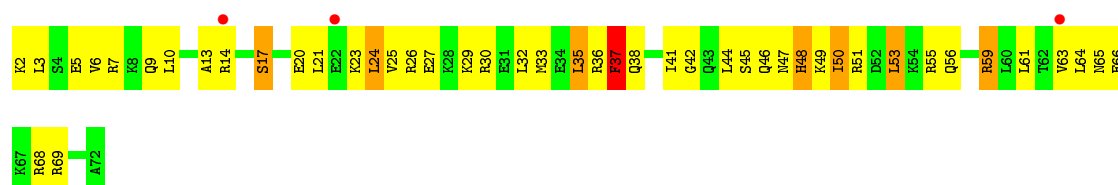


• Molecule 46: 50S ribosomal protein L27



• Molecule 47: 50S ribosomal protein L29

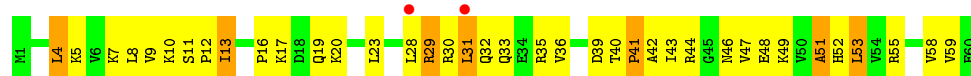




- Molecule 47: 50S ribosomal protein L29



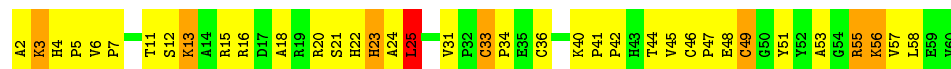
- Molecule 48: 50S ribosomal protein L30



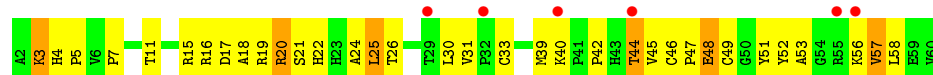
- Molecule 48: 50S ribosomal protein L30



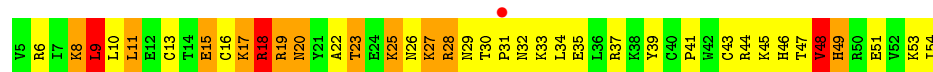
- Molecule 49: 50S ribosomal protein L32



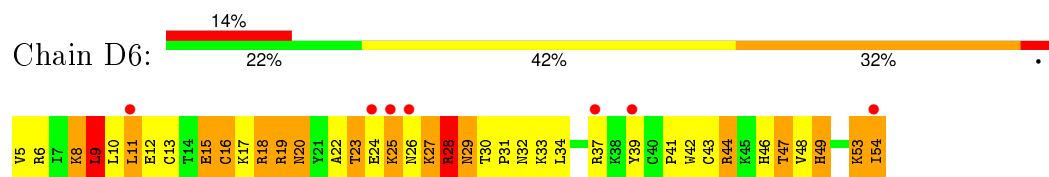
- Molecule 49: 50S ribosomal protein L32



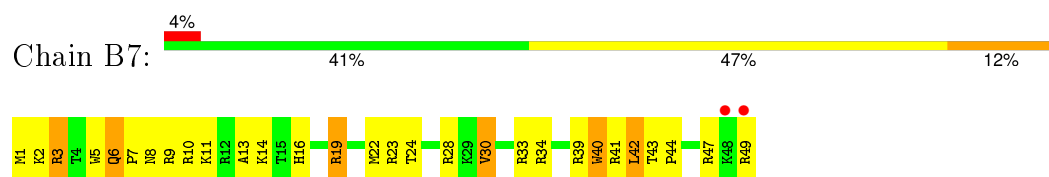
- Molecule 50: 50S ribosomal protein L33



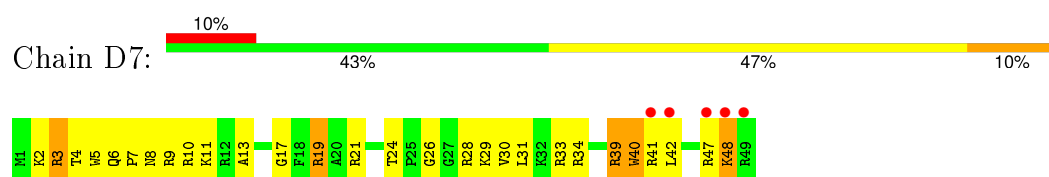
• Molecule 50: 50S ribosomal protein L33



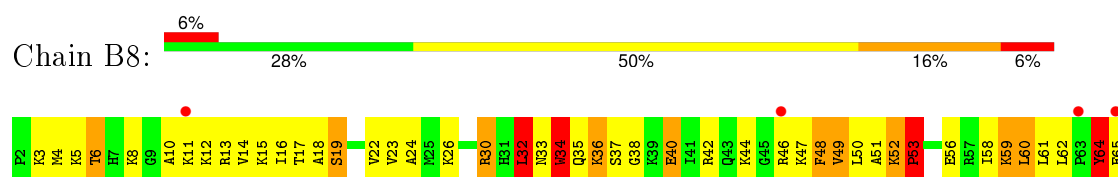
• Molecule 51: 50S ribosomal protein L34



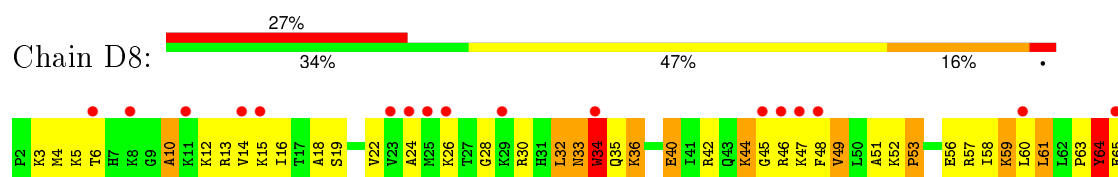
• Molecule 51: 50S ribosomal protein L34



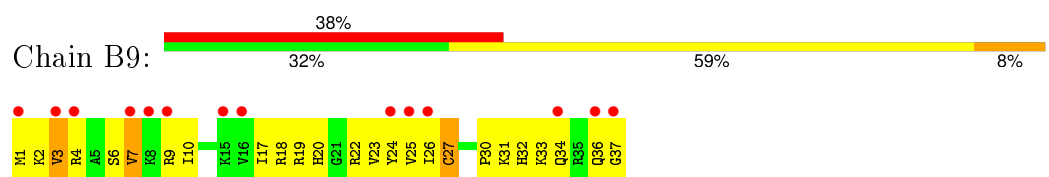
• Molecule 52: 50S ribosomal protein L35



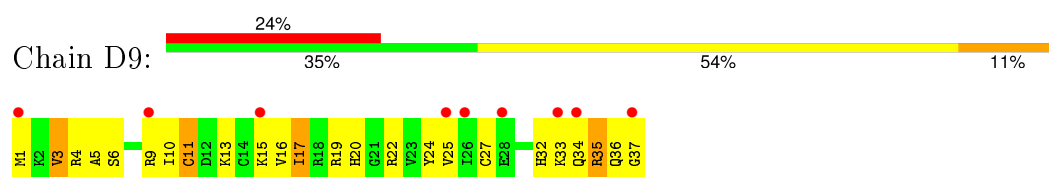
• Molecule 52: 50S ribosomal protein L35



• Molecule 53: 50S ribosomal protein L36



• Molecule 53: 50S ribosomal protein L36



- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bf:  100%

There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bg:  100%

There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Df:  100%

There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dg:  100%

There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bh:  100%

There are no outlier residues recorded for this chain.

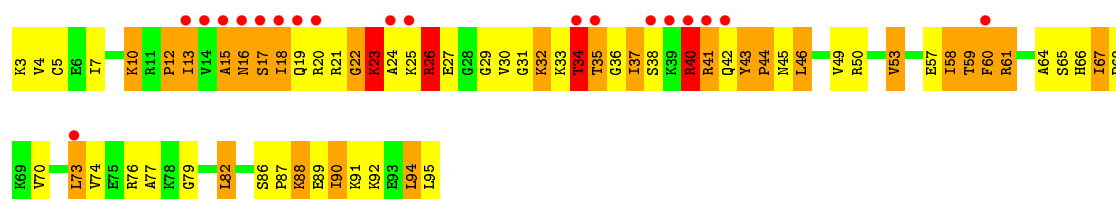
- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dh:  100%

There are no outlier residues recorded for this chain.

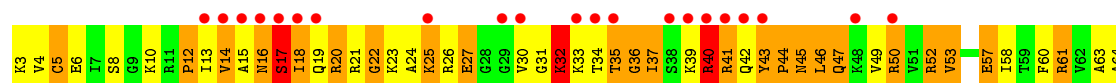
- Molecule 56: 50S ribosomal protein L28

Chain B1:  20% 29% 39% 28%



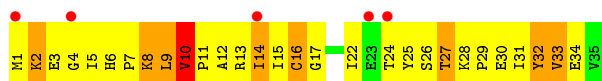
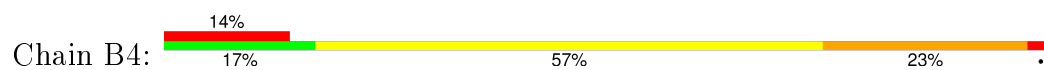
- Molecule 56: 50S ribosomal protein L28

Chain D1:  23% 29% 39% 28%





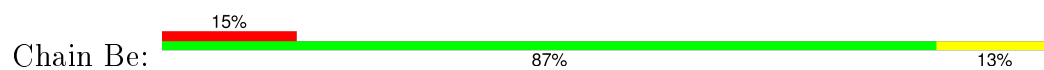
- Molecule 57: 50S ribosomal protein L31



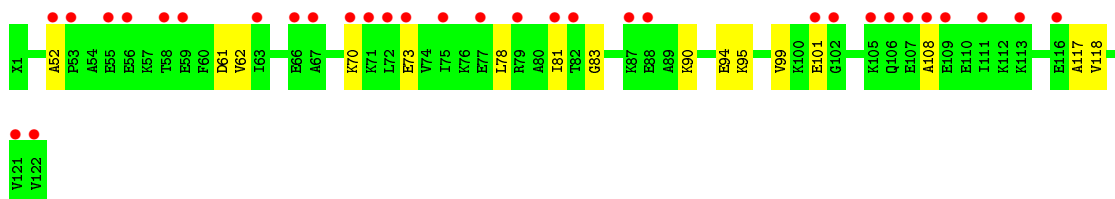
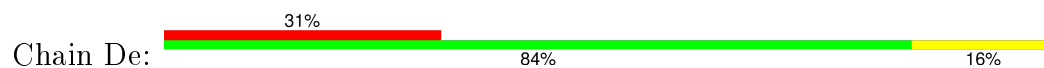
- Molecule 57: 50S ribosomal protein L31



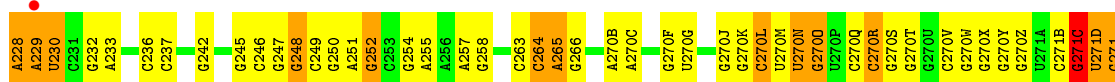
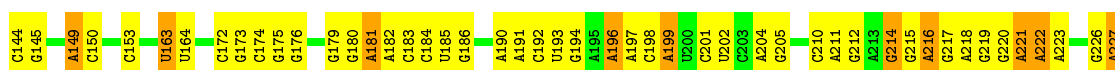
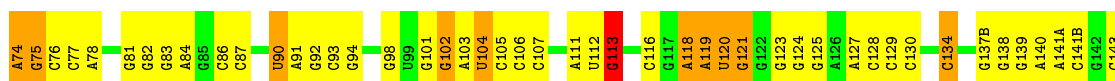
- Molecule 58: 50S ribosomal protein L7/L12



- Molecule 58: 50S ribosomal protein L7/L12

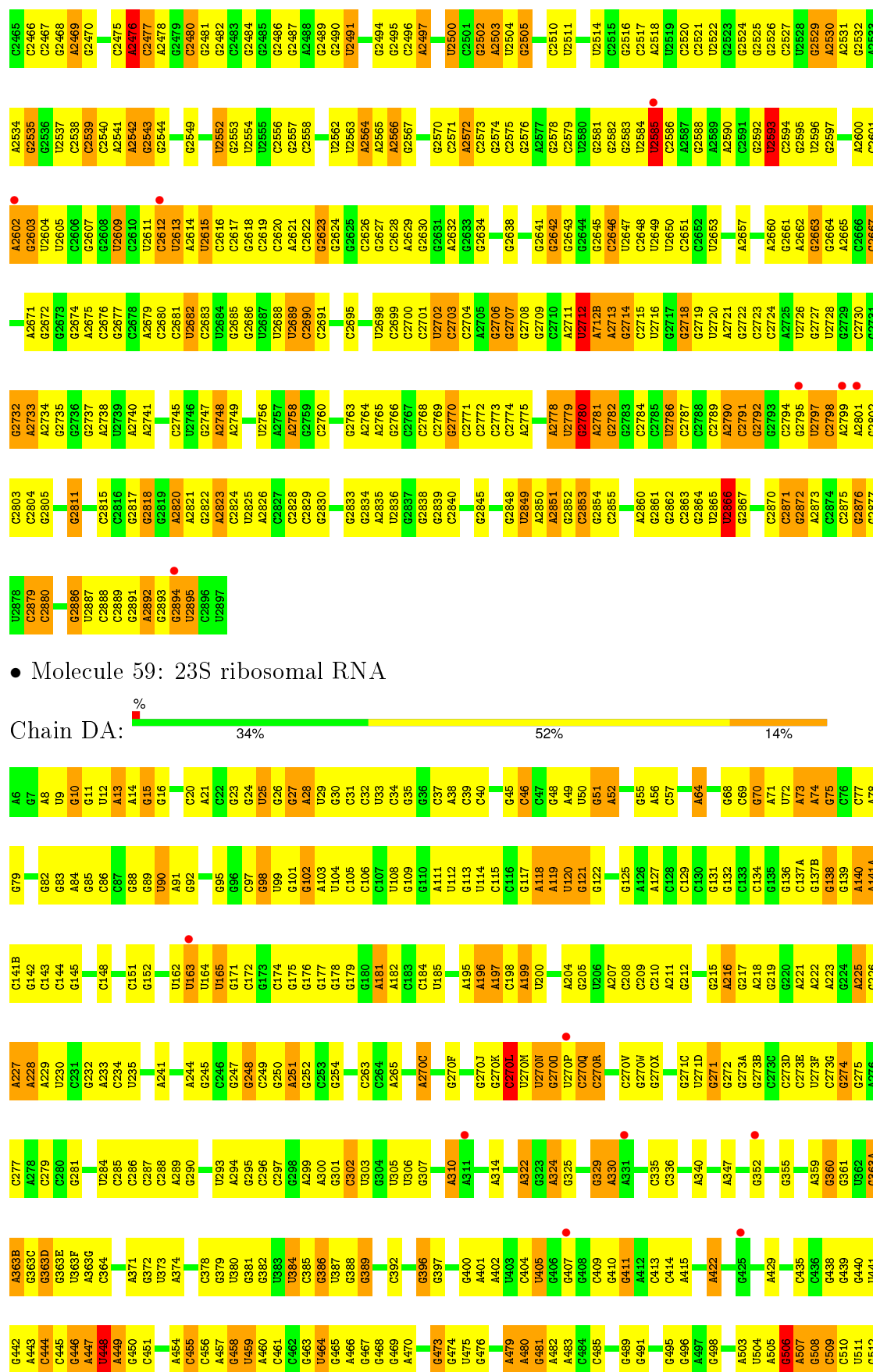


- Molecule 59: 23S ribosomal RNA



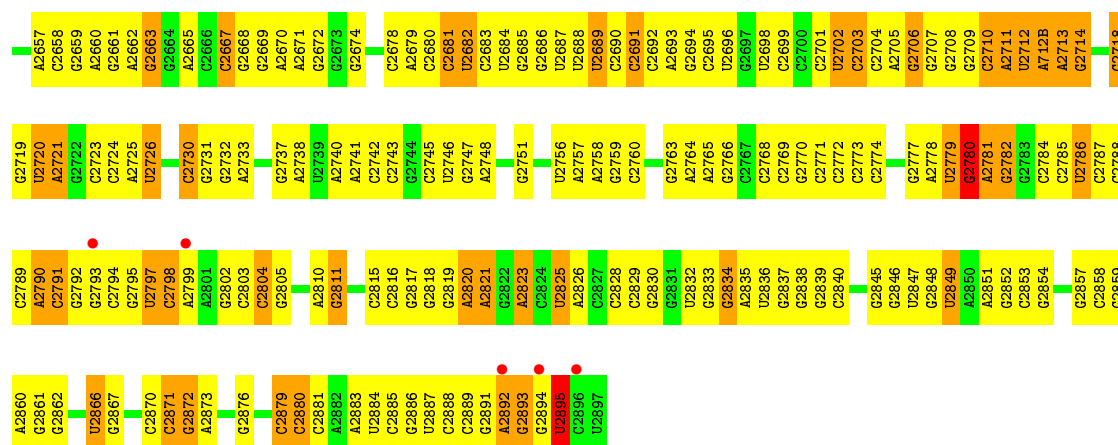




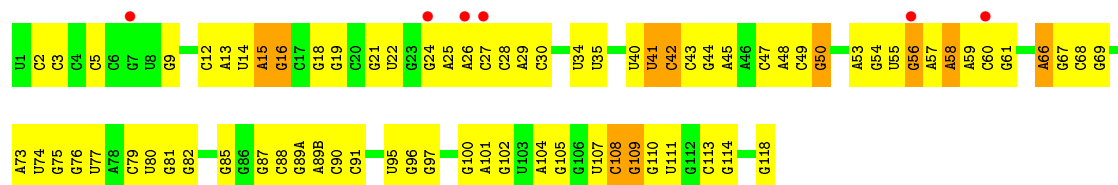


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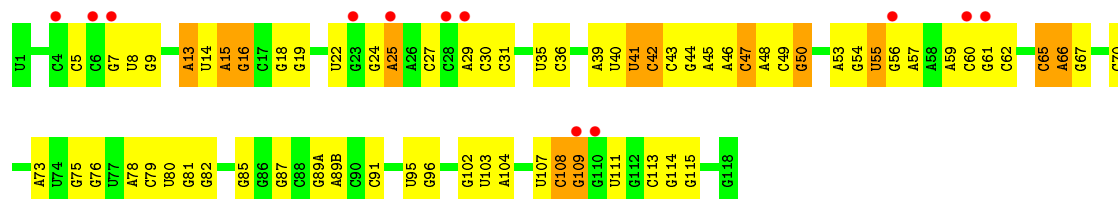
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C2501	A2369	A2369	A2369	U2291	U2291	A2225	U2144	U2079	G2012	A1938	G1858	A1784	C1674	C1606
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G2508	G2375	G2375	U2438	G2301	G2301	G2230	G2152	C2086	G2021	C1948	G1863	C1790	A1610	C1611
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G2512	G2379	G2379	C2442	A2305	A2305	G2335	G2156	G2092	G2024	C1949	G1867	C1794	U1681	C1615
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C2515	G2382	G2382	G2446	G2309	G2309	G2339	G2160	G2096	U2028	G1956	G1871	U1798	U1693	G1619
U2516	G2383	G2383	G2447	A2310	A2310	G2340	G2161	G2097	U2029	U1957	G1872	U1799	U1694	G1620
G2517	G2384	G2384	U2448	A2311	A2311	A2241	C2163	U2098	A2030	C1957	A1882	G1799	U1695	G1621
G2518	C2385	C2385	U2449	A2311	A2311	A2241	C2163	U2098	A2030	C1957	A1882	G1799	U1695	G1621



● 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, α , β , γ	306.01Å 673.49Å 351.98Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 131.34 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 86.0 (131.34-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.262 , 0.309 0.282 , 0.321	Depositor DCC
R_{free} test set	38154 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 59.8	EDS
Estimated twinning fraction	0.247 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	0 of 765681 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	308422	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, DPP, MG, KBE, UAL, 5OH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AB	0.42	0/1945	0.73	4/2621 (0.2%)
1	CB	0.40	0/1945	0.69	1/2621 (0.0%)
2	AC	0.35	0/1645	0.60	0/2216
2	CC	0.33	0/1645	0.58	1/2216 (0.0%)
3	AD	0.37	0/1733	0.60	0/2318
3	CD	0.34	0/1733	0.61	0/2318
4	AE	0.35	0/1172	0.63	1/1576 (0.1%)
4	CE	0.34	0/1172	0.63	1/1576 (0.1%)
5	AF	0.38	0/856	0.67	2/1154 (0.2%)
5	CF	0.35	0/856	0.64	1/1154 (0.1%)
6	AG	0.34	0/1276	0.58	0/1709
6	CG	0.35	0/1276	0.58	0/1709
7	AH	0.34	0/1136	0.58	0/1527
7	CH	0.33	0/1136	0.57	0/1527
8	AI	0.36	0/1029	0.63	1/1378 (0.1%)
8	CI	0.36	0/1029	0.61	1/1378 (0.1%)
9	AJ	0.37	0/815	0.64	1/1095 (0.1%)
9	CJ	0.33	0/815	0.65	1/1095 (0.1%)
10	AK	0.40	0/900	0.65	0/1213
10	CK	0.37	0/900	0.63	0/1213
11	AL	0.47	0/992	0.89	3/1327 (0.2%)
11	CL	0.47	0/992	0.88	4/1327 (0.3%)
12	AM	0.33	0/1008	0.61	0/1347
12	CM	0.32	0/1008	0.58	0/1347
13	AN	0.37	0/501	0.57	0/664
13	CN	0.35	0/501	0.57	0/664
14	AO	0.39	0/745	0.62	0/992
14	CO	0.35	0/745	0.59	0/992
15	AP	0.34	0/722	0.58	0/970
15	CP	0.33	0/722	0.56	0/970
16	AQ	0.45	0/848	0.75	0/1131
16	CQ	0.42	0/848	0.71	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.33	0/579	0.59	0/768
17	CR	0.31	0/579	0.57	0/768
18	AS	0.32	0/647	0.59	0/870
18	CS	0.31	0/647	0.56	0/870
19	AT	0.36	0/764	0.57	0/1006
19	CT	0.37	0/764	0.62	0/1006
20	AY	0.47	6/5481 (0.1%)	0.72	5/7418 (0.1%)
20	CY	0.52	7/5481 (0.1%)	0.76	12/7418 (0.2%)
21	AA	0.39	0/36351	0.97	36/56736 (0.1%)
21	CA	0.38	0/36351	0.95	35/56736 (0.1%)
22	AW	0.40	0/1827	1.06	9/2845 (0.3%)
22	CW	0.41	1/1827 (0.1%)	1.06	9/2845 (0.3%)
23	AV	0.78	1/568 (0.2%)	1.49	16/886 (1.8%)
23	CV	0.95	3/568 (0.5%)	1.74	19/886 (2.1%)
24	AU	1.05	0/11	1.28	0/13
24	CU	1.06	0/11	1.28	0/13
25	BC	0.44	0/1774	0.74	1/2391 (0.0%)
25	DC	0.50	1/1774 (0.1%)	0.76	0/2391
26	BD	0.38	0/2195	0.65	0/2955
26	DD	0.38	0/2195	0.67	0/2955
27	BE	0.39	0/1602	0.69	1/2160 (0.0%)
27	DE	0.35	0/1602	0.67	1/2160 (0.0%)
28	BF	0.41	0/1663	0.80	5/2249 (0.2%)
28	DF	0.41	0/1663	0.79	4/2249 (0.2%)
29	BG	0.57	1/1499 (0.1%)	0.60	0/2016
29	DG	0.59	1/1499 (0.1%)	0.67	3/2016 (0.1%)
30	BH	0.34	0/1298	0.59	0/1751
30	DH	0.34	0/1298	0.62	0/1751
32	BK	0.34	0/1054	0.60	0/1427
32	DK	0.34	0/1054	0.56	1/1427 (0.1%)
33	BN	0.58	0/1131	0.85	0/1525
33	DN	0.54	0/1131	0.80	0/1525
34	BO	0.36	0/943	0.65	1/1269 (0.1%)
34	DO	0.36	0/943	0.64	1/1269 (0.1%)
35	BP	0.34	0/1131	0.71	0/1504
35	DP	0.34	0/1131	0.71	0/1504
36	BQ	0.37	0/1143	0.64	0/1527
36	DQ	0.36	0/1143	0.60	0/1527
37	BR	0.38	0/974	0.65	0/1302
37	DR	0.34	0/974	0.62	1/1302 (0.1%)
38	BS	0.40	0/783	0.76	0/1041
38	DS	0.40	0/783	0.75	0/1041
39	BT	0.39	0/1161	0.76	3/1549 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DT	0.37	0/1161	0.67	0/1549
40	BU	0.39	0/982	0.67	1/1306 (0.1%)
40	DU	0.42	0/982	0.68	1/1306 (0.1%)
41	BV	0.37	0/790	0.66	0/1057
41	DV	0.38	0/790	0.71	0/1057
42	BW	0.38	0/911	0.65	0/1220
42	DW	0.37	0/911	0.65	0/1220
43	BX	0.35	0/748	0.59	1/1004 (0.1%)
43	DX	0.35	0/748	0.60	0/1004
44	BY	0.35	0/831	0.65	0/1108
44	DY	0.34	0/831	0.60	0/1108
45	BZ	0.33	0/1505	0.60	0/2042
45	DZ	0.32	0/1505	0.59	0/2042
46	B0	0.33	0/671	0.55	0/892
46	D0	0.31	0/671	0.56	0/892
47	B2	0.37	0/600	0.65	1/793 (0.1%)
47	D2	0.34	0/600	0.60	0/793
48	B3	0.34	0/482	0.63	0/646
48	D3	0.31	0/482	0.58	0/646
49	B5	0.33	0/473	0.58	0/639
49	D5	0.34	0/473	0.60	0/639
50	B6	0.38	0/440	0.81	0/586
50	D6	0.35	0/440	0.79	1/586 (0.2%)
51	B7	0.38	0/438	0.62	0/575
51	D7	0.48	0/438	0.69	0/575
52	B8	0.37	0/525	0.67	0/691
52	D8	0.36	0/525	0.64	0/691
53	B9	0.32	0/310	0.55	0/407
53	D9	0.29	0/310	0.55	0/407
56	B1	0.53	0/739	0.83	1/981 (0.1%)
56	D1	0.54	0/739	0.84	2/981 (0.2%)
57	B4	0.40	0/276	0.65	0/372
57	D4	0.45	0/276	0.66	0/372
58	Be	0.36	0/538	0.55	0/715
58	De	0.35	0/538	0.61	0/715
59	BA	0.41	2/69437 (0.0%)	0.99	82/108401 (0.1%)
59	DA	0.40	1/69437 (0.0%)	0.97	72/108401 (0.1%)
60	BB	0.34	0/2853	0.93	0/4451
60	DB	0.34	0/2853	0.90	1/4451 (0.0%)
All	All	0.40	24/330902 (0.0%)	0.90	348/492664 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	2
1	CB	0	1
10	AK	0	1
11	AL	0	1
11	CL	0	1
20	AY	0	3
20	CY	0	8
25	BC	0	3
25	DC	0	2
26	DD	0	1
28	BF	0	2
28	DF	0	2
29	BG	0	1
29	DG	0	1
31	BJ	0	1
31	DJ	0	1
38	BS	0	2
38	DS	0	2
39	BT	0	2
39	DT	0	1
42	DW	0	1
56	B1	0	2
56	D1	0	3
All	All	0	44

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CY	502	GLY	C-O	18.54	1.53	1.23
29	DG	112	PRO	CA-C	17.59	1.88	1.52
29	BG	112	PRO	CA-C	17.54	1.88	1.52
23	CV	16	A	O3'-P	-10.50	1.48	1.61
20	AY	499	ARG	C-N	9.84	1.56	1.34

The worst 5 of 348 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CW	37	A	P-O3'-C3'	19.49	143.09	119.70
23	CV	16	A	P-O3'-C3'	18.93	142.41	119.70
20	CY	502	GLY	O-C-N	-12.85	101.35	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CY	502	GLY	CA-C-N	12.59	141.38	116.20
20	CY	502	GLY	C-N-CA	11.35	146.14	122.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	162	ILE	Peptide
1	AB	163	PHE	Peptide
10	AK	109	VAL	Peptide
11	AL	57	LYS	Peptide
20	AY	31	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1910	0	1957	131	0
1	CB	1910	0	1957	98	0
2	AC	1621	0	1688	88	0
2	CC	1621	0	1688	67	0
3	AD	1703	0	1763	111	0
3	CD	1703	0	1763	120	0
4	AE	1156	0	1213	72	0
4	CE	1156	0	1213	54	0
5	AF	843	0	857	40	0
5	CF	843	0	857	40	0
6	AG	1257	0	1296	60	0
6	CG	1257	0	1296	61	0
7	AH	1116	0	1177	81	0
7	CH	1116	0	1177	73	0
8	AI	1011	0	1043	75	5
8	CI	1011	0	1043	54	0
9	AJ	802	0	849	71	0
9	CJ	802	0	849	61	0
10	AK	885	0	904	62	0
10	CK	885	0	904	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AL	976	0	1062	110	0
11	CL	976	0	1062	113	0
12	AM	997	0	1072	76	0
12	CM	997	0	1072	72	5
13	AN	492	0	529	39	0
13	CN	492	0	529	35	0
14	AO	734	0	771	42	0
14	CO	734	0	771	42	0
15	AP	706	0	725	38	0
15	CP	706	0	725	39	0
16	AQ	835	0	906	63	0
16	CQ	835	0	906	63	0
17	AR	574	0	644	44	0
17	CR	574	0	644	36	0
18	AS	634	0	655	38	0
18	CS	634	0	655	33	0
19	AT	762	0	859	48	0
19	CT	762	0	859	32	0
20	AY	5380	0	5433	360	0
20	CY	5380	0	5435	346	0
21	AA	32474	0	16393	910	0
21	CA	32474	0	16393	851	0
22	AW	1635	0	831	64	0
22	CW	1635	0	831	55	0
23	AV	503	0	252	25	0
23	CV	503	0	252	34	0
24	AU	48	0	39	9	0
24	CU	48	0	39	9	0
25	BC	1742	0	1798	160	0
25	DC	1742	0	1798	148	0
26	BD	2145	0	2234	172	0
26	DD	2145	0	2234	164	0
27	BE	1569	0	1634	147	0
27	DE	1569	0	1634	122	0
28	BF	1628	0	1680	146	0
28	DF	1628	0	1680	141	0
29	BG	1474	0	1535	102	0
29	DG	1474	0	1535	82	0
30	BH	1274	0	1342	76	0
30	DH	1274	0	1342	73	0
31	BJ	851	0	197	29	0
31	DJ	851	0	196	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BK	1035	0	1082	58	0
32	DK	1035	0	1082	57	0
33	BN	1104	0	1180	114	0
33	DN	1104	0	1180	115	0
34	BO	933	0	996	57	0
34	DO	933	0	996	71	0
35	BP	1114	0	1187	95	0
35	DP	1114	0	1187	111	0
36	BQ	1122	0	1179	81	0
36	DQ	1122	0	1179	65	0
37	BR	960	0	1021	77	0
37	DR	960	0	1021	71	0
38	BS	775	0	835	74	0
38	DS	775	0	835	76	0
39	BT	1147	0	1207	90	0
39	DT	1147	0	1207	111	0
40	BU	964	0	1022	85	0
40	DU	964	0	1022	76	0
41	BV	779	0	852	48	0
41	DV	779	0	852	62	0
42	BW	900	0	964	64	0
42	DW	900	0	964	57	0
43	BX	734	0	789	40	0
43	DX	734	0	789	42	0
44	BY	818	0	908	63	0
44	DY	818	0	908	58	0
45	BZ	1473	0	1497	89	0
45	DZ	1473	0	1497	81	0
46	B0	662	0	688	43	0
46	D0	662	0	688	40	0
47	B2	598	0	653	37	0
47	D2	598	0	653	28	0
48	B3	477	0	529	25	0
48	D3	477	0	529	25	0
49	B5	459	0	477	35	0
49	D5	459	0	477	34	0
50	B6	433	0	461	36	0
50	D6	433	0	461	36	0
51	B7	430	0	480	44	0
51	D7	430	0	480	32	0
52	B8	517	0	582	48	0
52	D8	517	0	582	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	B9	307	0	336	23	0
53	D9	307	0	335	20	0
54	Bf	156	0	41	0	0
54	Bg	156	0	39	0	0
54	Df	156	0	41	0	0
54	Dg	156	0	39	0	0
55	Bh	151	0	39	0	0
55	Dh	151	0	37	0	0
56	B1	732	0	808	88	0
56	D1	732	0	808	76	0
57	B4	271	0	284	31	0
57	D4	271	0	284	20	0
58	Be	686	0	620	0	0
58	De	686	0	619	0	0
59	BA	61997	0	31250	1815	0
59	DA	61997	0	31250	1738	0
60	BB	2551	0	1295	76	0
60	DB	2551	0	1295	70	0
61	AY	32	0	13	17	0
61	CY	32	0	13	32	0
62	AY	1	0	0	0	0
62	CY	1	0	0	0	0
All	All	308422	0	213301	11743	5

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 23.

The worst 5 of 11743 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)
22:CW:37:A:C2	23:CV:16:A:C2	1.85	1.57
20:AY:33:LEU:HD21	20:AY:34:TYR:CE2	1.42	1.54
20:AY:33:LEU:HD21	20:AY:34:TYR:CD2	1.54	1.43
20:AY:33:LEU:CD2	20:AY:34:TYR:CD2	2.00	1.42
20:AY:138:LYS:NZ	61:AY:701:GNP:N3	1.61	1.42

All (5) 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)
8:AI:58:ARG:CZ	12:CM:46:LYS:CG[2_555]	1.66	0.54
8:AI:58:ARG:CD	12:CM:47:ASP:OD1[2_555]	1.74	0.46
8:AI:58:ARG:NH2	12:CM:46:LYS:CG[2_555]	1.88	0.32
8:AI:58:ARG:NE	12:CM:46:LYS:CG[2_555]	2.01	0.19
8:AI:58:ARG:NH2	12:CM:46:LYS:CD[2_555]	2.04	0.16

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%)	173 (74%)	40 (17%)	20 (9%)	1	12
1	CB	233/235 (99%)	174 (75%)	36 (16%)	23 (10%)	1	10
2	AC	205/207 (99%)	137 (67%)	44 (22%)	24 (12%)	0	7
2	CC	205/207 (99%)	152 (74%)	34 (17%)	19 (9%)	1	11
3	AD	206/208 (99%)	146 (71%)	42 (20%)	18 (9%)	1	12
3	CD	206/208 (99%)	149 (72%)	46 (22%)	11 (5%)	2	25
4	AE	149/151 (99%)	107 (72%)	31 (21%)	11 (7%)	1	16
4	CE	149/151 (99%)	116 (78%)	24 (16%)	9 (6%)	2	21
5	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1	17
5	CF	99/101 (98%)	81 (82%)	7 (7%)	11 (11%)	0	7
6	AG	153/155 (99%)	120 (78%)	27 (18%)	6 (4%)	4	34
6	CG	153/155 (99%)	119 (78%)	27 (18%)	7 (5%)	3	29
7	AH	136/138 (99%)	98 (72%)	22 (16%)	16 (12%)	0	7
7	CH	136/138 (99%)	102 (75%)	21 (15%)	13 (10%)	1	10
8	AI	125/127 (98%)	88 (70%)	26 (21%)	11 (9%)	1	12
8	CI	125/127 (98%)	92 (74%)	25 (20%)	8 (6%)	2	20
9	AJ	97/99 (98%)	71 (73%)	17 (18%)	9 (9%)	1	11
9	CJ	97/99 (98%)	71 (73%)	16 (16%)	10 (10%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AK	117/119 (98%)	74 (63%)	25 (21%)	18 (15%)	0	3
10	CK	117/119 (98%)	78 (67%)	26 (22%)	13 (11%)	0	7
11	AL	123/125 (98%)	42 (34%)	46 (37%)	35 (28%)	0	0
11	CL	123/125 (98%)	39 (32%)	44 (36%)	40 (32%)	0	0
12	AM	123/125 (98%)	86 (70%)	24 (20%)	13 (11%)	0	8
12	CM	123/125 (98%)	91 (74%)	18 (15%)	14 (11%)	0	7
13	AN	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	0	6
13	CN	58/60 (97%)	40 (69%)	14 (24%)	4 (7%)	1	18
14	AO	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	13
14	CO	86/88 (98%)	66 (77%)	15 (17%)	5 (6%)	2	23
15	AP	82/84 (98%)	55 (67%)	18 (22%)	9 (11%)	0	8
15	CP	82/84 (98%)	59 (72%)	18 (22%)	5 (6%)	2	21
16	AQ	98/100 (98%)	68 (69%)	18 (18%)	12 (12%)	0	6
16	CQ	98/100 (98%)	68 (69%)	20 (20%)	10 (10%)	1	9
17	AR	68/70 (97%)	50 (74%)	12 (18%)	6 (9%)	1	12
17	CR	68/70 (97%)	52 (76%)	10 (15%)	6 (9%)	1	12
18	AS	77/79 (98%)	51 (66%)	18 (23%)	8 (10%)	1	8
18	CS	77/79 (98%)	56 (73%)	12 (16%)	9 (12%)	0	7
19	AT	97/99 (98%)	72 (74%)	17 (18%)	8 (8%)	1	13
19	CT	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	13
20	AY	685/687 (100%)	431 (63%)	168 (24%)	86 (13%)	0	6
20	CY	685/687 (100%)	457 (67%)	156 (23%)	72 (10%)	1	8
24	AU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
24	CU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
25	BC	226/228 (99%)	108 (48%)	70 (31%)	48 (21%)	0	1
25	DC	226/228 (99%)	105 (46%)	75 (33%)	46 (20%)	0	1
26	BD	273/275 (99%)	180 (66%)	54 (20%)	39 (14%)	0	4
26	DD	273/275 (99%)	188 (69%)	47 (17%)	38 (14%)	0	4
27	BE	203/205 (99%)	130 (64%)	43 (21%)	30 (15%)	0	4
27	DE	203/205 (99%)	133 (66%)	36 (18%)	34 (17%)	0	3
28	BF	206/208 (99%)	126 (61%)	54 (26%)	26 (13%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	DF	206/208 (99%)	137 (66%)	47 (23%)	22 (11%)	0	8
29	BG	179/181 (99%)	120 (67%)	46 (26%)	13 (7%)	1	16
29	DG	179/181 (99%)	127 (71%)	44 (25%)	8 (4%)	3	30
30	BH	165/167 (99%)	118 (72%)	29 (18%)	18 (11%)	0	8
30	DH	165/167 (99%)	118 (72%)	32 (19%)	15 (9%)	1	11
32	BK	138/140 (99%)	88 (64%)	33 (24%)	17 (12%)	0	6
32	DK	138/140 (99%)	86 (62%)	33 (24%)	19 (14%)	0	4
33	BN	136/138 (99%)	93 (68%)	24 (18%)	19 (14%)	0	4
33	DN	136/138 (99%)	91 (67%)	27 (20%)	18 (13%)	0	5
34	BO	120/122 (98%)	92 (77%)	20 (17%)	8 (7%)	1	19
34	DO	120/122 (98%)	95 (79%)	20 (17%)	5 (4%)	3	32
35	BP	144/146 (99%)	81 (56%)	36 (25%)	27 (19%)	0	2
35	DP	144/146 (99%)	76 (53%)	35 (24%)	33 (23%)	0	1
36	BQ	139/141 (99%)	87 (63%)	32 (23%)	20 (14%)	0	4
36	DQ	139/141 (99%)	91 (66%)	31 (22%)	17 (12%)	0	6
37	BR	115/117 (98%)	83 (72%)	21 (18%)	11 (10%)	1	10
37	DR	115/117 (98%)	91 (79%)	17 (15%)	7 (6%)	2	21
38	BS	97/99 (98%)	56 (58%)	25 (26%)	16 (16%)	0	3
38	DS	97/99 (98%)	57 (59%)	25 (26%)	15 (16%)	0	3
39	BT	136/138 (99%)	76 (56%)	41 (30%)	19 (14%)	0	4
39	DT	136/138 (99%)	82 (60%)	28 (21%)	26 (19%)	0	2
40	BU	115/117 (98%)	79 (69%)	25 (22%)	11 (10%)	1	10
40	DU	115/117 (98%)	80 (70%)	23 (20%)	12 (10%)	1	8
41	BV	99/101 (98%)	57 (58%)	28 (28%)	14 (14%)	0	4
41	DV	99/101 (98%)	64 (65%)	22 (22%)	13 (13%)	0	5
42	BW	111/113 (98%)	82 (74%)	14 (13%)	15 (14%)	0	4
42	DW	111/113 (98%)	81 (73%)	16 (14%)	14 (13%)	0	6
43	BX	91/93 (98%)	73 (80%)	12 (13%)	6 (7%)	1	19
43	DX	91/93 (98%)	70 (77%)	16 (18%)	5 (6%)	2	24
44	BY	105/107 (98%)	50 (48%)	30 (29%)	25 (24%)	0	1
44	DY	105/107 (98%)	50 (48%)	34 (32%)	21 (20%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BZ	183/185 (99%)	116 (63%)	46 (25%)	21 (12%)	0	7
45	DZ	183/185 (99%)	121 (66%)	44 (24%)	18 (10%)	1	10
46	B0	82/84 (98%)	59 (72%)	16 (20%)	7 (8%)	1	13
46	D0	82/84 (98%)	65 (79%)	13 (16%)	4 (5%)	3	27
47	B2	69/71 (97%)	49 (71%)	14 (20%)	6 (9%)	1	12
47	D2	69/71 (97%)	50 (72%)	17 (25%)	2 (3%)	6	42
48	B3	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	1	12
48	D3	58/60 (97%)	44 (76%)	9 (16%)	5 (9%)	1	12
49	B5	57/59 (97%)	44 (77%)	4 (7%)	9 (16%)	0	3
49	D5	57/59 (97%)	42 (74%)	11 (19%)	4 (7%)	1	18
50	B6	48/50 (96%)	28 (58%)	9 (19%)	11 (23%)	0	1
50	D6	48/50 (96%)	27 (56%)	8 (17%)	13 (27%)	0	0
51	B7	47/49 (96%)	30 (64%)	13 (28%)	4 (8%)	1	13
51	D7	47/49 (96%)	34 (72%)	11 (23%)	2 (4%)	3	31
52	B8	62/64 (97%)	42 (68%)	7 (11%)	13 (21%)	0	1
52	D8	62/64 (97%)	40 (64%)	11 (18%)	11 (18%)	0	2
53	B9	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	23
53	D9	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	2	23
56	B1	91/93 (98%)	56 (62%)	17 (19%)	18 (20%)	0	2
56	D1	91/93 (98%)	59 (65%)	18 (20%)	14 (15%)	0	3
57	B4	33/35 (94%)	15 (46%)	11 (33%)	7 (21%)	0	1
57	D4	33/35 (94%)	15 (46%)	9 (27%)	9 (27%)	0	0
58	Be	70/102 (69%)	36 (51%)	29 (41%)	5 (7%)	1	17
58	De	70/102 (69%)	40 (57%)	22 (31%)	8 (11%)	0	7
All	All	13304/13576 (98%)	8904 (67%)	2822 (21%)	1578 (12%)	0	6

5 of 1578 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	17	PHE
1	AB	22	LYS
1	AB	35	GLU
1	AB	75	LYS
1	AB	76	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	203/203 (100%)	164 (81%)	39 (19%)	2	10
1	CB	203/203 (100%)	177 (87%)	26 (13%)	5	28
2	AC	161/161 (100%)	125 (78%)	36 (22%)	1	6
2	CC	161/161 (100%)	122 (76%)	39 (24%)	1	5
3	AD	180/180 (100%)	143 (79%)	37 (21%)	1	8
3	CD	180/180 (100%)	142 (79%)	38 (21%)	1	8
4	AE	116/116 (100%)	96 (83%)	20 (17%)	2	15
4	CE	116/116 (100%)	95 (82%)	21 (18%)	2	12
5	AF	90/90 (100%)	76 (84%)	14 (16%)	3	20
5	CF	90/90 (100%)	74 (82%)	16 (18%)	2	13
6	AG	126/126 (100%)	111 (88%)	15 (12%)	6	31
6	CG	126/126 (100%)	112 (89%)	14 (11%)	8	35
7	AH	119/119 (100%)	94 (79%)	25 (21%)	1	8
7	CH	119/119 (100%)	91 (76%)	28 (24%)	1	5
8	AI	98/98 (100%)	82 (84%)	16 (16%)	3	17
8	CI	98/98 (100%)	77 (79%)	21 (21%)	1	7
9	AJ	89/89 (100%)	71 (80%)	18 (20%)	1	9
9	CJ	89/89 (100%)	66 (74%)	23 (26%)	0	4
10	AK	90/90 (100%)	73 (81%)	17 (19%)	2	10
10	CK	90/90 (100%)	72 (80%)	18 (20%)	1	9
11	AL	104/104 (100%)	74 (71%)	30 (29%)	0	3
11	CL	104/104 (100%)	77 (74%)	27 (26%)	0	4
12	AM	100/100 (100%)	83 (83%)	17 (17%)	2	15
12	CM	100/100 (100%)	86 (86%)	14 (14%)	4	24
13	AN	49/49 (100%)	39 (80%)	10 (20%)	1	8
13	CN	49/49 (100%)	35 (71%)	14 (29%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	79/79 (100%)	70 (89%)	9 (11%)	7	33
14	CO	79/79 (100%)	66 (84%)	13 (16%)	3	16
15	AP	72/72 (100%)	59 (82%)	13 (18%)	2	12
15	CP	72/72 (100%)	61 (85%)	11 (15%)	3	21
16	AQ	95/95 (100%)	82 (86%)	13 (14%)	4	25
16	CQ	95/95 (100%)	80 (84%)	15 (16%)	3	19
17	AR	61/61 (100%)	53 (87%)	8 (13%)	5	27
17	CR	61/61 (100%)	53 (87%)	8 (13%)	5	27
18	AS	69/69 (100%)	58 (84%)	11 (16%)	3	18
18	CS	69/69 (100%)	52 (75%)	17 (25%)	1	5
19	AT	76/76 (100%)	66 (87%)	10 (13%)	5	27
19	CT	76/76 (100%)	68 (90%)	8 (10%)	8	38
20	AY	579/579 (100%)	459 (79%)	120 (21%)	1	8
20	CY	579/579 (100%)	483 (83%)	96 (17%)	3	16
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%)	132 (73%)	48 (27%)	0	4
25	DC	180/180 (100%)	128 (71%)	52 (29%)	0	3
26	BD	217/217 (100%)	167 (77%)	50 (23%)	1	5
26	DD	217/217 (100%)	175 (81%)	42 (19%)	2	10
27	BE	165/165 (100%)	137 (83%)	28 (17%)	2	15
27	DE	165/165 (100%)	136 (82%)	29 (18%)	2	13
28	BF	165/165 (100%)	133 (81%)	32 (19%)	2	10
28	DF	165/165 (100%)	140 (85%)	25 (15%)	3	21
29	BG	155/155 (100%)	130 (84%)	25 (16%)	3	18
29	DG	155/155 (100%)	130 (84%)	25 (16%)	3	18
30	BH	136/136 (100%)	111 (82%)	25 (18%)	2	11
30	DH	136/136 (100%)	117 (86%)	19 (14%)	4	24
32	BK	105/105 (100%)	74 (70%)	31 (30%)	0	3
32	DK	105/105 (100%)	77 (73%)	28 (27%)	0	4
33	BN	117/117 (100%)	98 (84%)	19 (16%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DN	117/117 (100%)	93 (80%)	24 (20%)	1	8
34	BO	100/100 (100%)	85 (85%)	15 (15%)	3	21
34	DO	100/100 (100%)	86 (86%)	14 (14%)	4	24
35	BP	112/112 (100%)	82 (73%)	30 (27%)	0	4
35	DP	112/112 (100%)	85 (76%)	27 (24%)	1	5
36	BQ	111/111 (100%)	80 (72%)	31 (28%)	0	3
36	DQ	111/111 (100%)	84 (76%)	27 (24%)	1	5
37	BR	100/100 (100%)	79 (79%)	21 (21%)	1	8
37	DR	100/100 (100%)	78 (78%)	22 (22%)	1	7
38	BS	77/77 (100%)	60 (78%)	17 (22%)	1	6
38	DS	77/77 (100%)	59 (77%)	18 (23%)	1	5
39	BT	120/120 (100%)	94 (78%)	26 (22%)	1	7
39	DT	120/120 (100%)	93 (78%)	27 (22%)	1	6
40	BU	93/93 (100%)	75 (81%)	18 (19%)	2	10
40	DU	93/93 (100%)	70 (75%)	23 (25%)	1	5
41	BV	82/82 (100%)	60 (73%)	22 (27%)	0	4
41	DV	82/82 (100%)	62 (76%)	20 (24%)	1	5
42	BW	92/92 (100%)	69 (75%)	23 (25%)	1	4
42	DW	92/92 (100%)	76 (83%)	16 (17%)	2	14
43	BX	75/75 (100%)	56 (75%)	19 (25%)	1	4
43	DX	75/75 (100%)	58 (77%)	17 (23%)	1	6
44	BY	88/88 (100%)	69 (78%)	19 (22%)	1	7
44	DY	88/88 (100%)	73 (83%)	15 (17%)	2	15
45	BZ	162/162 (100%)	128 (79%)	34 (21%)	1	8
45	DZ	162/162 (100%)	125 (77%)	37 (23%)	1	6
46	B0	66/66 (100%)	56 (85%)	10 (15%)	3	21
46	D0	66/66 (100%)	56 (85%)	10 (15%)	3	21
47	B2	66/66 (100%)	59 (89%)	7 (11%)	8	38
47	D2	66/66 (100%)	58 (88%)	8 (12%)	6	30
48	B3	52/52 (100%)	42 (81%)	10 (19%)	2	10
48	D3	52/52 (100%)	45 (86%)	7 (14%)	5	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B5	51/51 (100%)	39 (76%)	12 (24%)	1	5
49	D5	51/51 (100%)	41 (80%)	10 (20%)	1	9
50	B6	49/49 (100%)	37 (76%)	12 (24%)	1	5
50	D6	49/49 (100%)	34 (69%)	15 (31%)	0	3
51	B7	42/42 (100%)	35 (83%)	7 (17%)	3	16
51	D7	42/42 (100%)	36 (86%)	6 (14%)	4	24
52	B8	54/54 (100%)	42 (78%)	12 (22%)	1	6
52	D8	54/54 (100%)	44 (82%)	10 (18%)	2	11
53	B9	34/34 (100%)	32 (94%)	2 (6%)	24	65
53	D9	34/34 (100%)	30 (88%)	4 (12%)	6	31
56	B1	78/78 (100%)	58 (74%)	20 (26%)	0	4
56	D1	78/78 (100%)	58 (74%)	20 (26%)	0	4
57	B4	31/31 (100%)	22 (71%)	9 (29%)	0	3
57	D4	31/31 (100%)	21 (68%)	10 (32%)	0	2
58	Be	54/54 (100%)	46 (85%)	8 (15%)	4	22
58	De	54/54 (100%)	46 (85%)	8 (15%)	4	22
All	All	11174/11174 (100%)	8972 (80%)	2202 (20%)	1	9

5 of 2202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BZ	124	ILE
4	CE	73	ASN
43	DX	68	ARG
47	B2	53	LEU
58	Be	106	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
50	B6	32	ASN
16	CQ	96	GLN
41	DV	89	GLN
3	CD	161	ASN
6	CG	148	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1511/1511 (100%)	326 (21%)	19 (1%)
21	CA	1511/1511 (100%)	310 (20%)	16 (1%)
22	AW	76/77 (98%)	22 (28%)	1 (1%)
22	CW	76/77 (98%)	19 (25%)	1 (1%)
23	AV	22/23 (95%)	11 (50%)	2 (9%)
23	CV	22/23 (95%)	9 (40%)	3 (13%)
59	BA	2878/2879 (99%)	666 (23%)	21 (0%)
59	DA	2878/2879 (99%)	629 (21%)	17 (0%)
60	BB	118/119 (99%)	20 (16%)	4 (3%)
60	DB	118/119 (99%)	19 (16%)	3 (2%)
All	All	9210/9218 (99%)	2031 (22%)	87 (0%)

5 of 2031 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	G
21	AA	8	A
21	AA	9	G
21	AA	13	U

5 of 87 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
59	BA	2092	U
21	CA	115	G
59	DA	2092	U
59	BA	2422	A
60	BB	56	G

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	1.37	1 (14%)
24	DPP	AU	2	24	3,5,6	0.40	0	1,5,7	0.89	0
24	UAL	AU	5	24	7,8,9	2.40	2 (28%)	4,9,11	1.16	1 (25%)
24	5OH	AU	6	24	7,12,13	0.66	0	7,16,18	0.98	0
24	KBE	CU	1	24	8,8,9	0.58	0	7,8,10	1.38	1 (14%)
24	DPP	CU	2	24	3,5,6	0.41	0	1,5,7	0.89	0
24	UAL	CU	5	24	7,8,9	2.41	2 (28%)	4,9,11	1.16	1 (25%)
24	5OH	CU	6	24	7,12,13	0.67	0	7,16,18	0.98	1 (14%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AU	5	UAL	C1-N1	-3.03	1.35	1.40
24	CU	5	UAL	C1-N1	-3.01	1.35	1.40
24	AU	5	UAL	C-CA	5.08	1.52	1.45
24	CU	5	UAL	C-CA	5.09	1.52	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AU	5	UAL	O-C-CA	-2.14	122.25	125.40
24	CU	5	UAL	O-C-CA	-2.14	122.25	125.40
24	CU	6	5OH	O-C-CA	-2.01	120.14	125.44
24	AU	1	KBE	CB-CA-C	3.02	117.11	112.32
24	CU	1	KBE	CB-CA-C	3.04	117.15	112.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AU	2	DPP	1	0
24	AU	6	5OH	4	0
24	CU	1	KBE	1	0
24	CU	2	DPP	1	0
24	CU	6	5OH	6	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	GNP	AY	701	62	28,34,34	1.78	4 (14%)	33,54,54	2.69	13 (39%)
61	GNP	CY	701	62	28,34,34	1.77	4 (14%)	33,54,54	2.68	13 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	GNP	AY	701	62	-	0/12/38/38	0/3/3/3
61	GNP	CY	701	62	-	0/12/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	GNP	PB-O3A	-2.43	1.56	1.59
61	CY	701	GNP	PB-O3A	-2.41	1.56	1.59
61	AY	701	GNP	PA-O2A	-2.27	1.45	1.54
61	CY	701	GNP	PA-O2A	-2.26	1.45	1.54
61	AY	701	GNP	C6-N1	3.34	1.39	1.33

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AY	701	GNP	C5-C6-N1	-8.70	111.69	123.59
61	CY	701	GNP	C5-C6-N1	-8.68	111.72	123.59
61	CY	701	GNP	PA-O3A-PB	-4.98	115.98	132.67
61	AY	701	GNP	PA-O3A-PB	-4.97	116.00	132.67
61	AY	701	GNP	C4'-O4'-C1'	-3.55	105.82	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AY	701	GNP	17	0
61	CY	701	GNP	32	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
58	Be	1
58	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	36.11
1	Be	30:UNK	C	51:ALA	N	35.10

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	235/235 (100%)	0.15	12 (5%) 32 24	30, 75, 127, 171	0
1	CB	235/235 (100%)	0.55	29 (12%) 5 6	34, 86, 153, 201	0
2	AC	207/207 (100%)	-0.17	6 (2%) 55 45	27, 59, 115, 156	0
2	CC	207/207 (100%)	0.31	18 (8%) 13 12	23, 75, 130, 190	0
3	AD	208/208 (100%)	0.03	14 (6%) 21 16	24, 72, 124, 159	0
3	CD	208/208 (100%)	0.25	14 (6%) 21 16	23, 85, 142, 184	0
4	AE	151/151 (100%)	-0.18	1 (0%) 89 82	17, 48, 101, 156	0
4	CE	151/151 (100%)	0.41	14 (9%) 11 10	14, 58, 106, 151	0
5	AF	101/101 (100%)	-0.27	1 (0%) 84 76	15, 50, 100, 133	0
5	CF	101/101 (100%)	-0.33	1 (0%) 84 76	29, 61, 123, 148	0
6	AG	155/155 (100%)	-0.15	8 (5%) 31 24	30, 80, 139, 199	0
6	CG	155/155 (100%)	-0.03	4 (2%) 59 49	38, 82, 137, 180	0
7	AH	138/138 (100%)	-0.05	3 (2%) 65 55	28, 59, 103, 142	0
7	CH	138/138 (100%)	0.18	8 (5%) 26 21	25, 75, 121, 155	0
8	AI	127/127 (100%)	0.25	10 (7%) 15 13	0, 71, 117, 134	0
8	CI	127/127 (100%)	0.20	5 (3%) 43 35	0, 84, 149, 220	0
9	AJ	99/99 (100%)	0.07	7 (7%) 19 15	25, 62, 116, 159	0
9	CJ	99/99 (100%)	0.51	11 (11%) 7 7	31, 75, 127, 166	0
10	AK	119/119 (100%)	0.15	6 (5%) 32 25	31, 69, 116, 157	0
10	CK	119/119 (100%)	-0.01	4 (3%) 49 40	38, 72, 133, 151	0
11	AL	125/125 (100%)	0.21	7 (5%) 28 22	10, 66, 120, 181	0
11	CL	125/125 (100%)	0.37	10 (8%) 15 12	29, 69, 136, 170	0
12	AM	125/125 (100%)	0.66	19 (15%) 3 3	49, 86, 144, 212	0
12	CM	125/125 (100%)	0.83	14 (11%) 7 7	53, 100, 158, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	0.44	8 (13%) 4 5	28, 52, 87, 120	0
13	CN	60/60 (100%)	0.52	3 (5%) 32 25	39, 69, 117, 135	0
14	AO	88/88 (100%)	-0.07	1 (1%) 82 73	22, 60, 114, 139	0
14	CO	88/88 (100%)	-0.01	2 (2%) 64 54	25, 68, 119, 170	0
15	AP	84/84 (100%)	0.48	7 (8%) 14 12	26, 66, 109, 117	0
15	CP	84/84 (100%)	0.38	7 (8%) 14 12	52, 81, 127, 153	0
16	AQ	100/100 (100%)	0.45	10 (10%) 9 9	0, 67, 117, 139	0
16	CQ	100/100 (100%)	0.31	6 (6%) 25 19	0, 68, 126, 150	0
17	AR	70/70 (100%)	0.02	3 (4%) 39 30	14, 54, 120, 154	0
17	CR	70/70 (100%)	0.11	3 (4%) 39 30	39, 63, 113, 155	0
18	AS	79/79 (100%)	0.95	13 (16%) 2 3	47, 92, 136, 169	0
18	CS	79/79 (100%)	0.69	10 (12%) 5 5	44, 99, 145, 189	0
19	AT	99/99 (100%)	0.24	3 (3%) 54 43	0, 77, 128, 159	0
19	CT	99/99 (100%)	0.50	8 (8%) 15 12	0, 79, 131, 166	0
20	AY	687/687 (100%)	0.11	38 (5%) 29 22	23, 84, 139, 174	0
20	CY	687/687 (100%)	0.18	49 (7%) 19 15	40, 92, 149, 204	0
21	AA	1511/1511 (100%)	-0.30	9 (0%) 90 85	15, 67, 145, 258	0
21	CA	1511/1511 (100%)	-0.28	9 (0%) 90 85	18, 70, 157, 272	0
22	AW	77/77 (100%)	-0.31	0 100 100	32, 90, 174, 205	0
22	CW	77/77 (100%)	-0.28	0 100 100	39, 101, 193, 240	0
23	AV	23/23 (100%)	0.01	0 100 100	41, 100, 156, 172	0
23	CV	23/23 (100%)	0.43	3 (13%) 5 5	41, 118, 186, 216	0
24	AU	2/6 (33%)	0.26	0 100 100	114, 114, 114, 114	0
24	CU	2/6 (33%)	-0.06	0 100 100	119, 119, 119, 119	0
25	BC	228/228 (100%)	1.45	70 (30%) 1 1	81, 124, 178, 222	0
25	DC	228/228 (100%)	1.33	63 (27%) 1 1	102, 162, 214, 247	0
26	BD	275/275 (100%)	-0.04	9 (3%) 50 41	11, 47, 102, 126	0
26	DD	275/275 (100%)	-0.05	5 (1%) 71 62	23, 54, 107, 147	0
27	BE	205/205 (100%)	-0.04	7 (3%) 49 40	19, 55, 101, 193	0
27	DE	205/205 (100%)	-0.03	4 (1%) 68 59	12, 60, 120, 175	0
28	BF	208/208 (100%)	0.68	31 (14%) 3 3	16, 69, 131, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	208/208 (100%)	0.56	27 (12%) 5 5	34, 83, 176, 205	0
29	BG	181/181 (100%)	0.65	22 (12%) 5 6	41, 90, 132, 195	0
29	DG	181/181 (100%)	0.84	33 (18%) 2 2	44, 104, 159, 196	0
30	BH	167/167 (100%)	-0.28	0 100 100	21, 68, 123, 159	0
30	DH	167/167 (100%)	-0.24	4 (2%) 62 52	36, 73, 140, 192	0
31	BJ	0/170	-	-	-	-
31	DJ	0/170	-	-	-	-
32	BK	140/140 (100%)	0.86	30 (21%) 1 1	60, 114, 165, 206	0
32	DK	140/140 (100%)	1.23	34 (24%) 1 1	72, 142, 197, 229	0
33	BN	138/138 (100%)	0.44	14 (10%) 9 9	59, 83, 108, 111	0
33	DN	138/138 (100%)	0.45	11 (7%) 15 12	61, 89, 110, 118	0
34	BO	122/122 (100%)	-0.21	0 100 100	23, 44, 90, 158	0
34	DO	122/122 (100%)	-0.02	0 100 100	26, 47, 96, 121	0
35	BP	146/146 (100%)	0.08	6 (4%) 41 32	23, 71, 132, 167	0
35	DP	146/146 (100%)	0.38	19 (13%) 5 5	19, 88, 140, 212	0
36	BQ	141/141 (100%)	0.08	8 (5%) 27 21	32, 53, 103, 155	0
36	DQ	141/141 (100%)	0.08	7 (4%) 32 25	34, 58, 126, 178	0
37	BR	117/117 (100%)	0.14	3 (2%) 59 49	22, 57, 106, 123	0
37	DR	117/117 (100%)	0.27	7 (5%) 25 19	34, 67, 108, 138	0
38	BS	99/99 (100%)	1.39	33 (33%) 0 0	41, 104, 177, 190	0
38	DS	99/99 (100%)	2.18	47 (47%) 0 0	44, 114, 168, 203	0
39	BT	138/138 (100%)	-0.42	1 (0%) 89 82	23, 68, 126, 162	0
39	DT	138/138 (100%)	-0.23	6 (4%) 39 30	25, 71, 133, 177	0
40	BU	117/117 (100%)	-0.10	2 (1%) 73 64	20, 45, 102, 140	0
40	DU	117/117 (100%)	0.02	3 (2%) 59 49	29, 54, 89, 222	0
41	BV	101/101 (100%)	-0.05	4 (3%) 42 33	22, 58, 105, 172	0
41	DV	101/101 (100%)	0.13	4 (3%) 42 33	28, 60, 114, 177	0
42	BW	113/113 (100%)	0.09	2 (1%) 71 62	14, 43, 101, 135	0
42	DW	113/113 (100%)	0.34	7 (6%) 24 19	11, 60, 133, 215	0
43	BX	93/93 (100%)	0.00	2 (2%) 65 55	16, 55, 107, 137	0
43	DX	93/93 (100%)	-0.16	0 100 100	16, 66, 134, 180	0
44	BY	107/107 (100%)	0.77	18 (16%) 2 2	38, 88, 141, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DY	107/107 (100%)	1.15	29 (27%) 1 1	45, 96, 167, 200	0
45	BZ	185/185 (100%)	-0.25	1 (0%) 91 88	36, 70, 124, 167	0
45	DZ	185/185 (100%)	0.03	8 (4%) 39 30	48, 82, 136, 193	0
46	B0	84/84 (100%)	0.18	2 (2%) 62 52	24, 65, 112, 142	0
46	D0	84/84 (100%)	0.89	11 (13%) 5 5	47, 77, 140, 162	0
47	B2	71/71 (100%)	0.07	3 (4%) 40 31	34, 64, 118, 140	0
47	D2	71/71 (100%)	0.13	5 (7%) 19 15	33, 85, 127, 141	0
48	B3	60/60 (100%)	-0.12	2 (3%) 50 41	28, 61, 116, 135	0
48	D3	60/60 (100%)	0.19	4 (6%) 21 16	32, 73, 137, 160	0
49	B5	59/59 (100%)	-0.02	0 100 100	22, 55, 125, 138	0
49	D5	59/59 (100%)	0.30	6 (10%) 9 8	29, 75, 130, 161	0
50	B6	50/50 (100%)	-0.18	1 (2%) 68 59	36, 74, 120, 139	0
50	D6	50/50 (100%)	0.50	7 (14%) 4 4	49, 81, 143, 164	0
51	B7	49/49 (100%)	0.34	2 (4%) 41 32	43, 53, 102, 126	0
51	D7	49/49 (100%)	0.35	5 (10%) 9 8	34, 61, 112, 165	0
52	B8	64/64 (100%)	0.35	4 (6%) 23 18	22, 66, 108, 137	0
52	D8	64/64 (100%)	1.22	17 (26%) 1 1	33, 70, 118, 139	0
53	B9	37/37 (100%)	1.66	14 (37%) 0 0	39, 60, 122, 134	0
53	D9	37/37 (100%)	1.20	9 (24%) 1 1	46, 60, 134, 159	0
54	Bf	0/31	-	-	-	-
54	Bg	0/31	-	-	-	-
54	Df	0/31	-	-	-	-
54	Dg	0/31	-	-	-	-
55	Bh	0/30	-	-	-	-
55	Dh	0/30	-	-	-	-
56	B1	93/93 (100%)	1.02	19 (20%) 1 2	22, 78, 160, 236	0
56	D1	93/93 (100%)	1.24	21 (22%) 1 1	41, 89, 159, 194	0
57	B4	35/35 (100%)	0.75	5 (14%) 4 4	67, 116, 167, 189	0
57	D4	35/35 (100%)	1.25	9 (25%) 1 1	73, 136, 168, 196	0
58	Be	72/102 (70%)	1.08	15 (20%) 1 1	77, 113, 160, 174	0
58	De	72/102 (70%)	1.86	32 (44%) 0 0	87, 141, 192, 236	0
59	BA	2879/2879 (100%)	-0.20	18 (0%) 90 85	9, 59, 146, 260	0
59	DA	2879/2879 (100%)	-0.14	34 (1%) 81 72	5, 63, 160, 308	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	BB	119/119 (100%)	0.04	6 (5%) 32 25	36, 103, 157, 192	0
60	DB	119/119 (100%)	0.24	12 (10%) 9 9	33, 108, 159, 193	0
All	All	22726/23318 (97%)	0.10	1262 (5%) 28 22	0, 72, 150, 308	0

The worst 5 of 1262 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	DK	62	ASP	11.3
44	DY	107	ASP	10.4
12	CM	123	ALA	9.9
56	B1	17	SER	9.5
28	DF	10	PRO	9.3

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	DPP	AU	2	6/7	0.80	0.24	-	114,114,114,114	0
24	5OH	AU	6	12/13	0.71	0.55	-	99,101,102,102	0
24	KBE	AU	1	9/10	0.80	0.61	-	114,114,114,114	0
24	5OH	CU	6	12/13	0.90	0.38	-	99,101,102,102	0
24	UAL	AU	5	9/10	0.89	0.31	-	114,114,114,114	0
24	UAL	CU	5	9/10	0.88	0.32	-	118,118,118,118	0
24	DPP	CU	2	6/7	0.77	0.35	-	118,118,118,118	0
24	KBE	CU	1	9/10	0.80	0.43	-	118,118,118,118	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
61	GNP	CY	701	32/32	0.80	0.32	0.15	58,71,81,83	0
61	GNP	AY	701	32/32	0.83	0.26	-0.25	58,71,81,83	0
62	MG	CY	702	1/1	0.95	0.09	-	135,135,135,135	0
62	MG	AY	702	1/1	0.92	0.14	-	88,88,88,88	0

6.5 Other polymers

There are no such residues in this entry.