



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2017 – 11:35 PM EDT

PDB ID : 4W29
Title : 70S ribosome translocation intermediate containing elongation factor EFG/GDP/fusidic acid, mRNA, and tRNAs trapped in the AP/AP pe/E chimeric hybrid state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2014-07-02
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

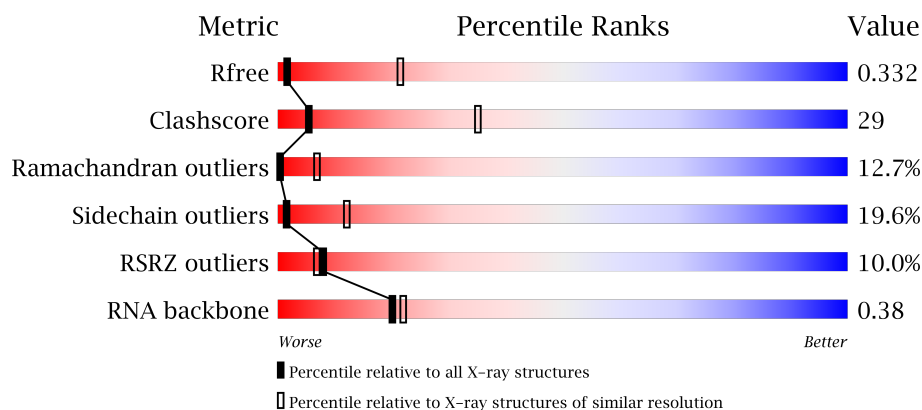
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)
RNA backbone	2435	1016 (4.70-2.90)

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

Mol	Chain	Length	Quality of chain
1	AB	235	<div> <div>5%</div> <div> <div>41%</div> <div>44%</div> <div>14%</div> </div> </div>
1	CB	235	<div> <div>6%</div> <div> <div>40%</div> <div>43%</div> <div>16%</div> </div> </div>
2	AC	207	<div> <div>18%</div> <div> <div>36%</div> <div>48%</div> <div>14%</div> </div> </div>
2	CC	207	<div> <div>6%</div> <div> <div>41%</div> <div>50%</div> <div>8%</div> </div> </div>

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AY	687	
20	CY	687	
21	AA	1511	
21	CA	1511	
22	AW	77	
22	CW	77	
23	AV	36	
23	CV	36	
24	AX	78	
24	CX	78	
25	BC	228	
25	DC	228	
26	BD	275	
26	DD	275	
27	BE	205	
27	DE	205	

Continued on next page...

Continued from previous page...

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	139	
33	DN	139	
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	

Continued on next page...

Continued from previous page...

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	B1	93	
47	D1	93	
48	B2	71	
48	D2	71	
49	B3	60	
49	D3	60	
50	B4	35	
50	D4	35	
51	B5	59	
51	D5	59	
52	B6	50	
52	D6	50	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	B7	49	
53	D7	49	
54	B8	64	
54	D8	64	
55	B9	37	
55	D9	37	
56	Be	103	
56	De	103	
57	Bf	31	
57	Bg	31	
57	Df	31	
57	Dg	31	
58	Bh	30	
58	Dh	30	
59	BA	2879	
59	DA	2879	
60	BB	119	
60	DB	119	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	GDP	CY	701	-	-	X	-
62	FUA	AY	702	-	-	X	X
62	FUA	CY	702	-	-	-	X
63	NMY	AA	1601	-	-	X	X
63	NMY	BA	2902	-	-	-	X
63	NMY	BA	2903	-	-	-	X
63	NMY	BA	2904	-	-	X	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
63	NMY	CA	1601	-	-	X	-
63	NMY	DA	2901	-	-	X	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 312066 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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			

Continued on next page...

Continued from previous page...

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	155	144	2			
16	CQ	100	Total	C	N	O	S	0	0	0
			835	534	155	144	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
			763	470	162	129	2			
19	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 20 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AY	661	Total	C	N	O	S	0	0	0
			5173	3288	884	983	18			
20	CY	661	Total	C	N	O	S	0	0	0
			5173	3288	884	983	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	40	THR	HIS	conflict	UNP Q72I01

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AY	129	LYS	HIS	conflict	UNP Q72I01
AY	226	ASN	HIS	conflict	UNP Q72I01
CY	40	THR	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 16S Ribosomal RNA.

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 tRNA.

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 mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AV	36	Total	C	N	O	P	0	0	0
			783	351	159	237	36			
23	CV	36	Total	C	N	O	P	0	0	0
			781	352	159	235	35			

- Molecule 24 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	78	Total	C	N	O	P	0	0	0
			1629	730	293	531	75			
24	CX	78	Total	C	N	O	P	0	0	0
			1629	730	293	531	75			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	77	VAL	-	expression tag	GB 1154835240

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AX	78	ACE	-	expression tag	GB 1154835240
CX	77	VAL	-	expression tag	GB 1154835240
CX	78	ACE	-	expression tag	GB 1154835240

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

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

- 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			

- 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			

Continued on next page...

Continued from previous page...

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

- 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	139	Total	C	N	O	S	0	0	0
			1114	717	207	186	4			
33	DN	139	Total	C	N	O	S	0	0	0
			1114	717	207	186	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			

- 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			

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Be	1	UNK	-	expression tag	UNP Q72GS2
Be	2	UNK	-	expression tag	UNP Q72GS2
Be	3	UNK	-	expression tag	UNP Q72GS2
Be	4	UNK	-	expression tag	UNP Q72GS2
Be	5	UNK	-	expression tag	UNP Q72GS2
Be	6	UNK	-	expression tag	UNP Q72GS2
Be	7	UNK	-	expression tag	UNP Q72GS2
Be	8	UNK	-	expression tag	UNP Q72GS2
Be	9	UNK	-	expression tag	UNP Q72GS2
Be	10	UNK	-	expression tag	UNP Q72GS2
Be	11	UNK	-	expression tag	UNP Q72GS2
Be	12	UNK	-	expression tag	UNP Q72GS2
Be	13	UNK	-	expression tag	UNP Q72GS2
Be	14	UNK	-	expression tag	UNP Q72GS2
Be	15	UNK	-	expression tag	UNP Q72GS2
Be	16	UNK	-	expression tag	UNP Q72GS2
Be	17	UNK	-	expression tag	UNP Q72GS2
Be	18	UNK	-	expression tag	UNP Q72GS2
Be	19	UNK	-	expression tag	UNP Q72GS2
Be	20	UNK	-	expression tag	UNP Q72GS2
Be	21	UNK	-	expression tag	UNP Q72GS2
Be	22	UNK	-	expression tag	UNP Q72GS2
Be	23	UNK	-	expression tag	UNP Q72GS2
Be	24	UNK	-	expression tag	UNP Q72GS2
Be	25	UNK	-	expression tag	UNP Q72GS2
Be	26	UNK	-	expression tag	UNP Q72GS2
Be	27	UNK	-	expression tag	UNP Q72GS2
Be	28	UNK	-	expression tag	UNP Q72GS2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Be	29	UNK	-	expression tag	UNP Q72GS2
Be	30	UNK	-	expression tag	UNP Q72GS2
Be	31	UNK	-	expression tag	UNP Q72GS2
De	1	UNK	-	expression tag	UNP Q72GS2
De	2	UNK	-	expression tag	UNP Q72GS2
De	3	UNK	-	expression tag	UNP Q72GS2
De	4	UNK	-	expression tag	UNP Q72GS2
De	5	UNK	-	expression tag	UNP Q72GS2
De	6	UNK	-	expression tag	UNP Q72GS2
De	7	UNK	-	expression tag	UNP Q72GS2
De	8	UNK	-	expression tag	UNP Q72GS2
De	9	UNK	-	expression tag	UNP Q72GS2
De	10	UNK	-	expression tag	UNP Q72GS2
De	11	UNK	-	expression tag	UNP Q72GS2
De	12	UNK	-	expression tag	UNP Q72GS2
De	13	UNK	-	expression tag	UNP Q72GS2
De	14	UNK	-	expression tag	UNP Q72GS2
De	15	UNK	-	expression tag	UNP Q72GS2
De	16	UNK	-	expression tag	UNP Q72GS2
De	17	UNK	-	expression tag	UNP Q72GS2
De	18	UNK	-	expression tag	UNP Q72GS2
De	19	UNK	-	expression tag	UNP Q72GS2
De	20	UNK	-	expression tag	UNP Q72GS2
De	21	UNK	-	expression tag	UNP Q72GS2
De	22	UNK	-	expression tag	UNP Q72GS2
De	23	UNK	-	expression tag	UNP Q72GS2
De	24	UNK	-	expression tag	UNP Q72GS2
De	25	UNK	-	expression tag	UNP Q72GS2
De	26	UNK	-	expression tag	UNP Q72GS2
De	27	UNK	-	expression tag	UNP Q72GS2
De	28	UNK	-	expression tag	UNP Q72GS2
De	29	UNK	-	expression tag	UNP Q72GS2
De	30	UNK	-	expression tag	UNP Q72GS2
De	31	UNK	-	expression tag	UNP Q72GS2

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

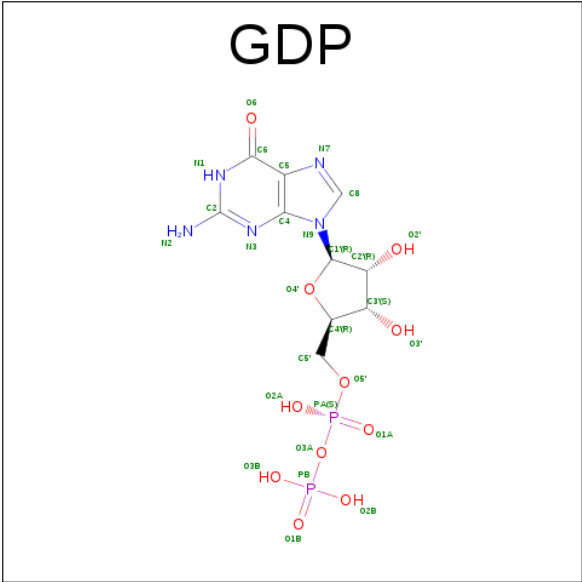
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1141A	U	C	conflict	GB 46197919
BA	2825	U	G	conflict	GB 46197919
DA	1141A	U	C	conflict	GB 46197919
DA	2825	U	G	conflict	GB 46197919

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

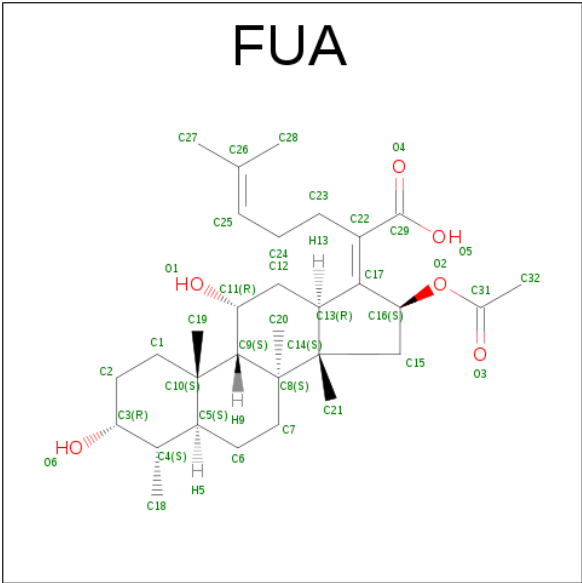
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
60	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



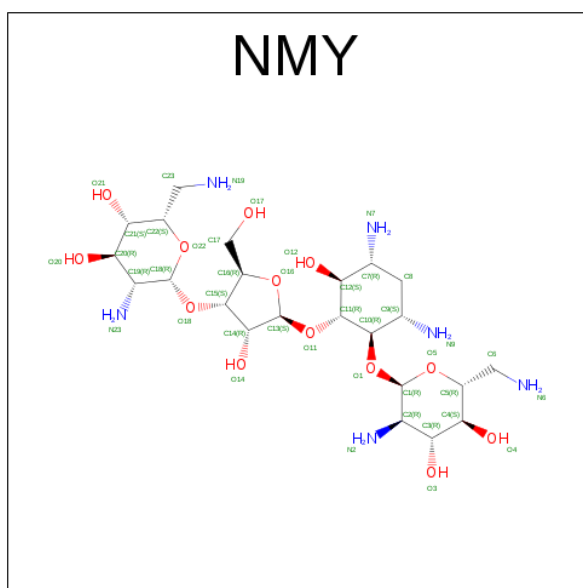
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
61	CY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 62 is FUSIDIC ACID (three-letter code: FUA) (formula: C₃₁H₄₈O₆).



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

- Molecule 63 is NEOMYCIN (three-letter code: NMY) (formula: $C_{23}H_{46}N_6O_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
63	AA	1	Total	C	N	O	0	0
			42	23	6	13		
63	BA	1	Total	C	N	O	0	0
			42	23	6	13		
63	BA	1	Total	C	N	O	0	0
			42	23	6	13		
63	BA	1	Total	C	N	O	0	0
			42	23	6	13		
63	CA	1	Total	C	N	O	0	0
			42	23	6	13		
63	DA	1	Total	C	N	O	0	0
			42	23	6	13		

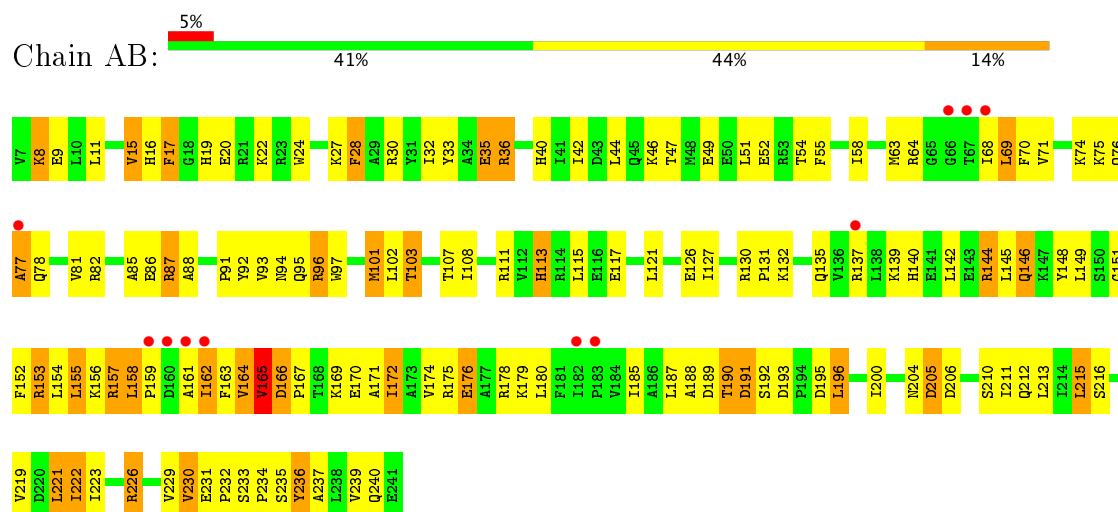
- Molecule 64 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	BA	1	Total	Mg	0	0
			1	1		
64	CY	1	Total	Mg	0	0
			1	1		

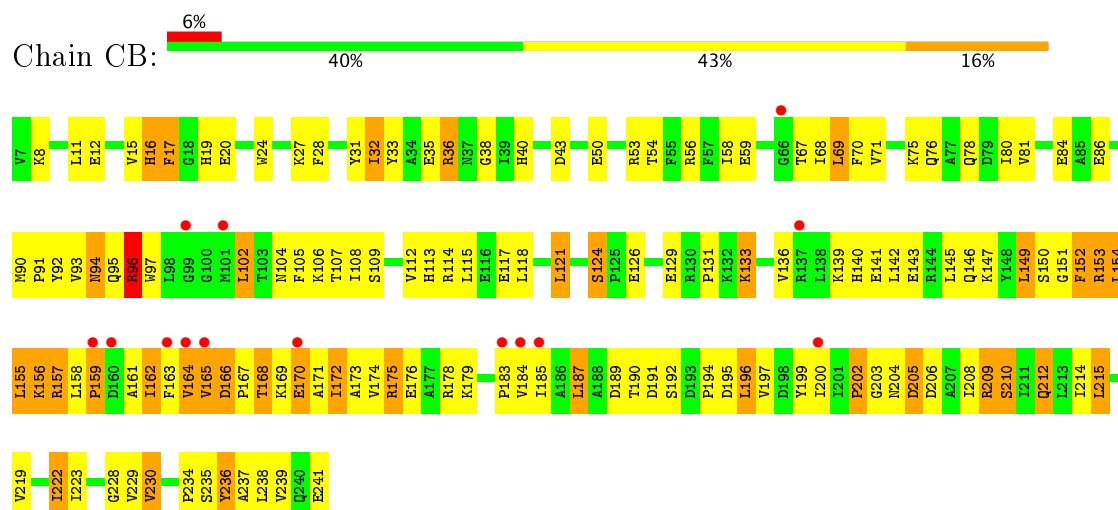
3 Residue-property plots

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

• Molecule 1: 30S ribosomal protein S2

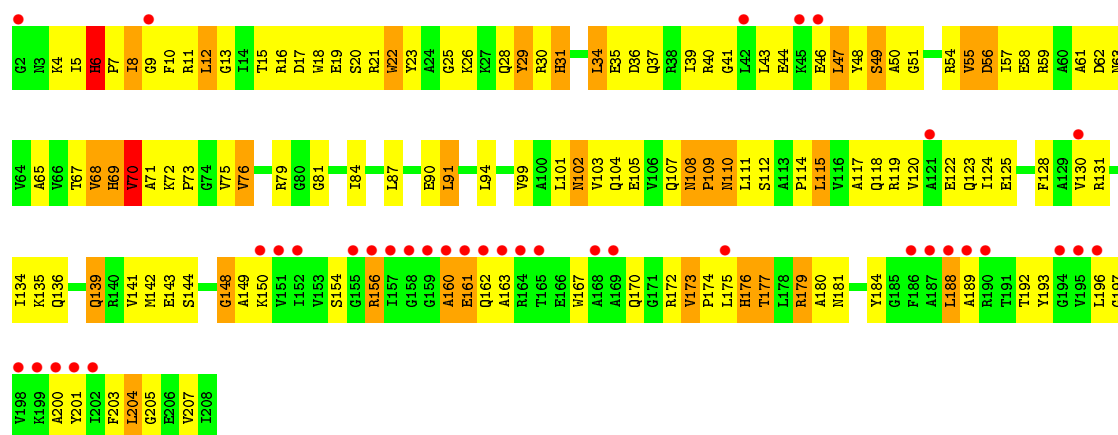


• Molecule 1: 30S ribosomal protein S2

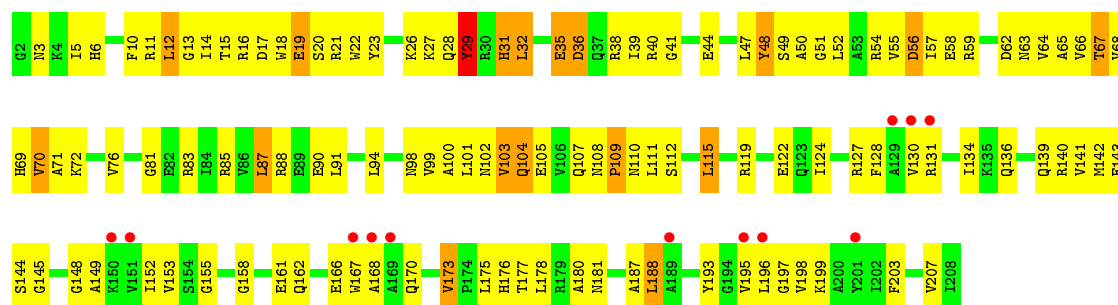
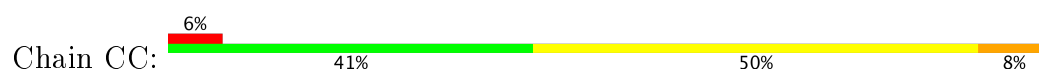


• Molecule 2: 30S ribosomal protein S3

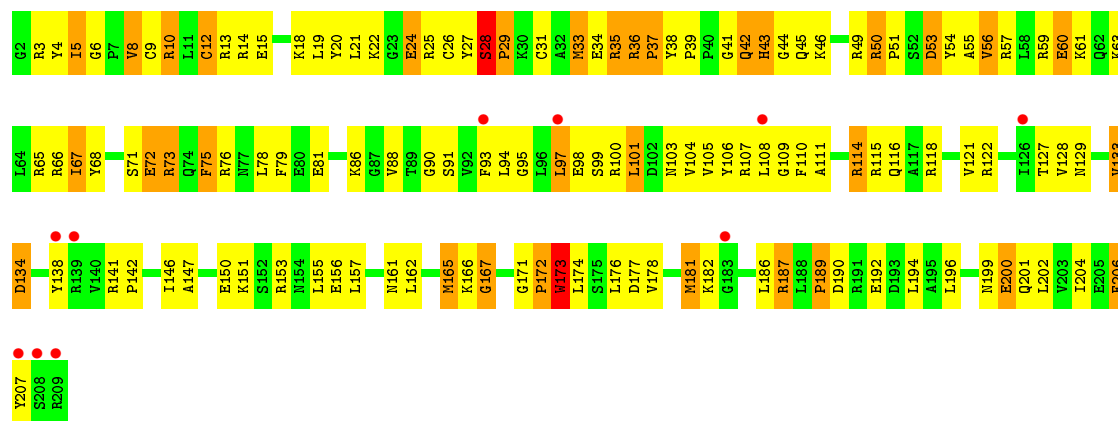




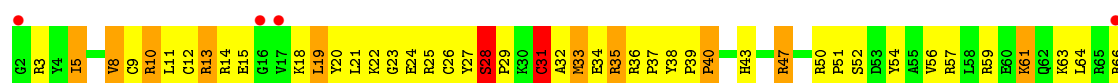
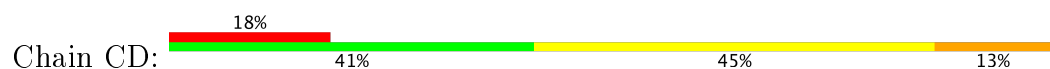
• Molecule 2: 30S ribosomal protein S3

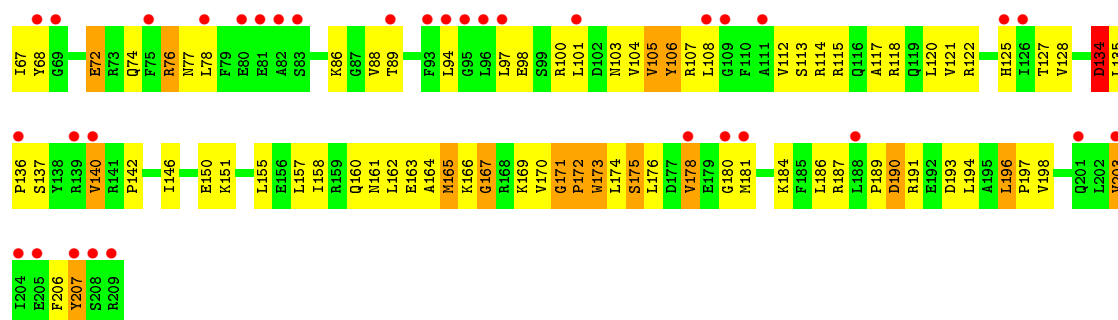


• Molecule 3: 30S ribosomal protein S4

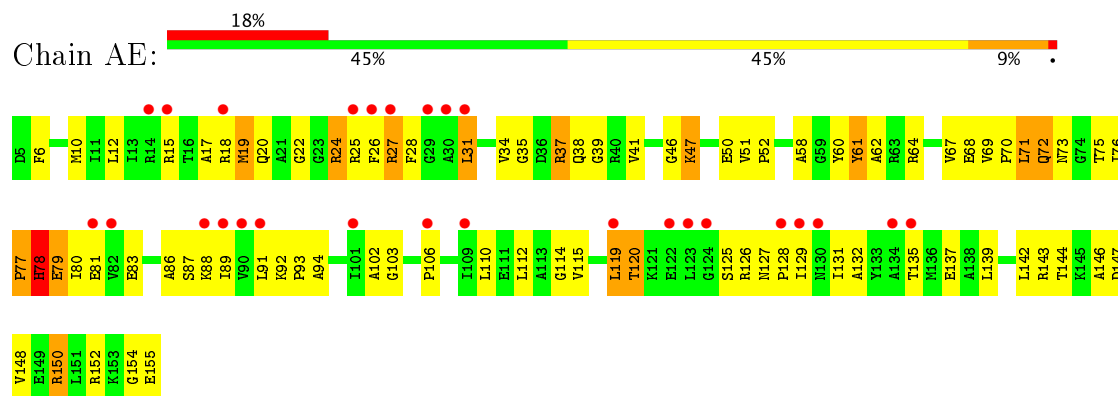


• Molecule 3: 30S ribosomal protein S4

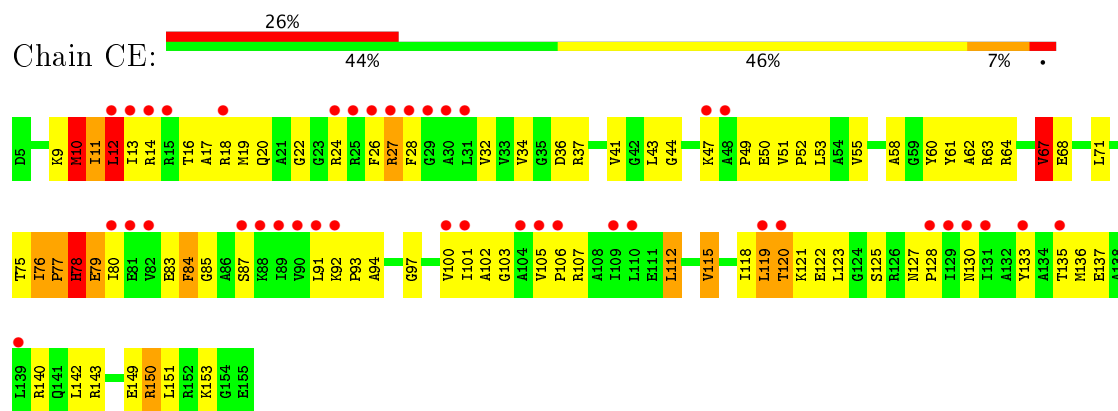




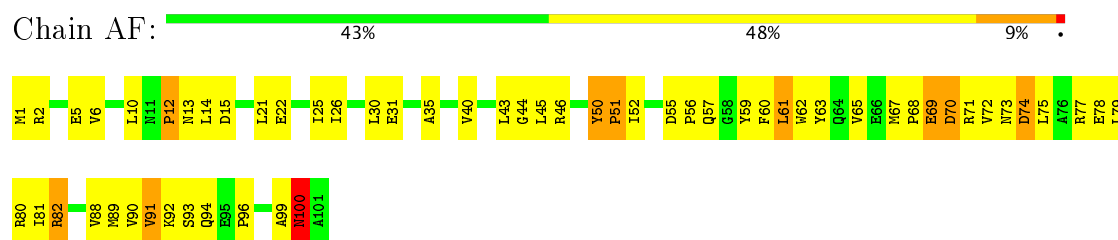
• Molecule 4: 30S ribosomal protein S5



• Molecule 4: 30S ribosomal protein S5

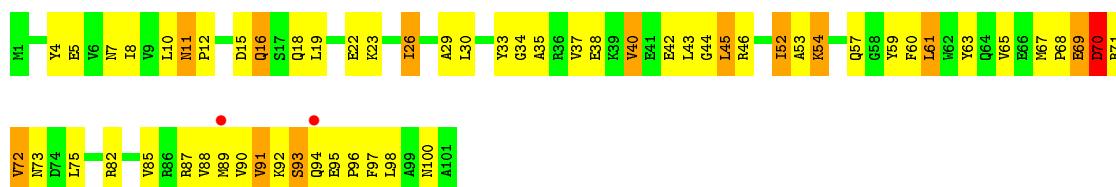


• Molecule 5: 30S ribosomal protein S6

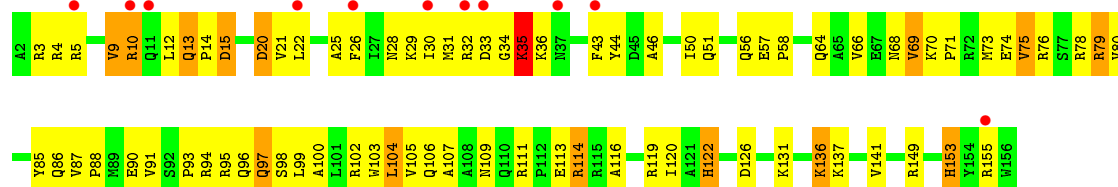


• Molecule 5: 30S ribosomal protein S6

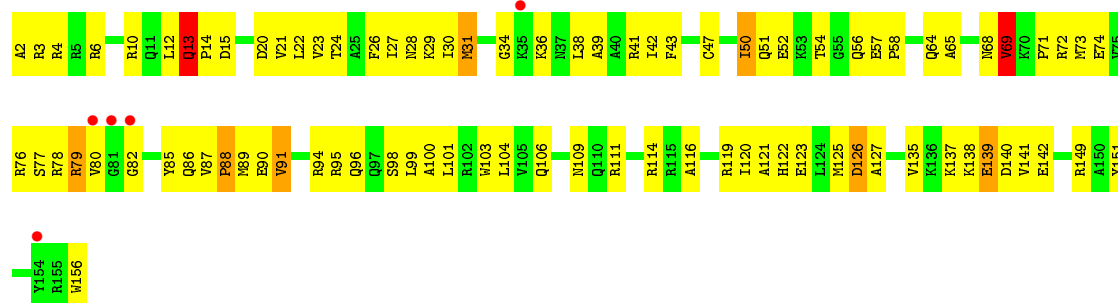
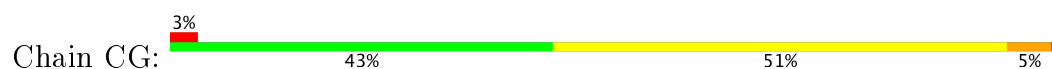




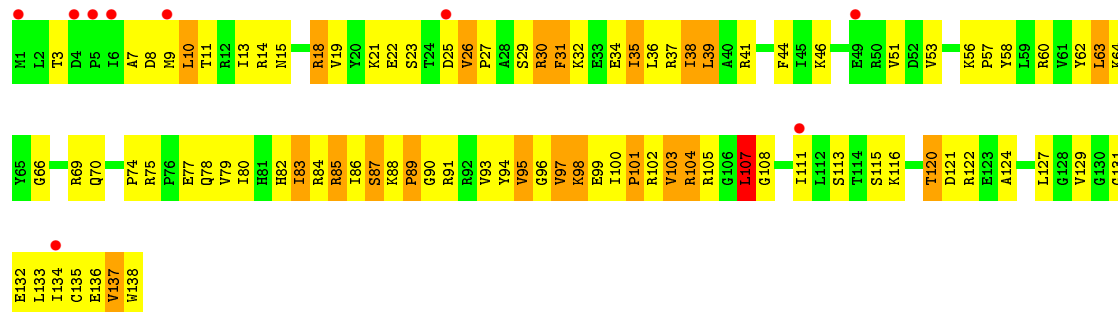
• Molecule 6: 30S ribosomal protein S7



• Molecule 6: 30S ribosomal protein S7

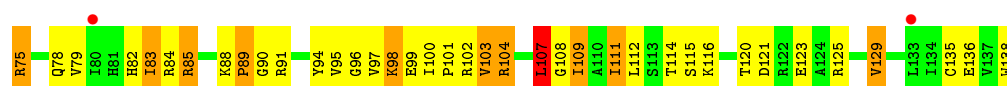


• Molecule 7: 30S ribosomal protein S8

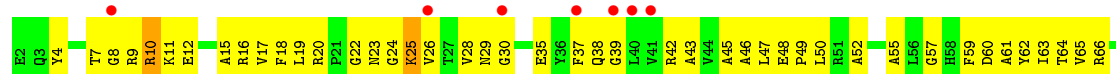


• Molecule 7: 30S ribosomal protein S8

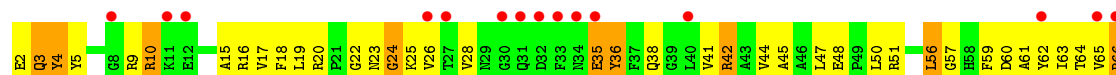




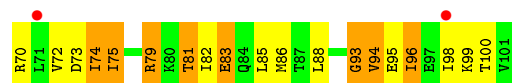
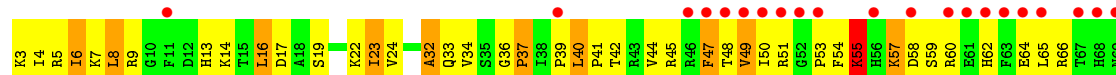
• Molecule 8: 30S ribosomal protein S9



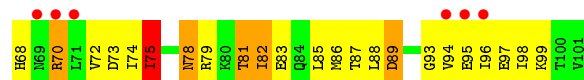
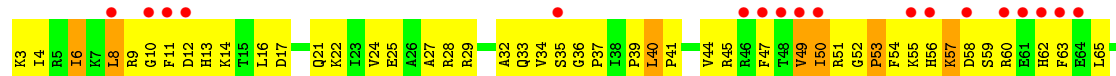
• Molecule 8: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S10

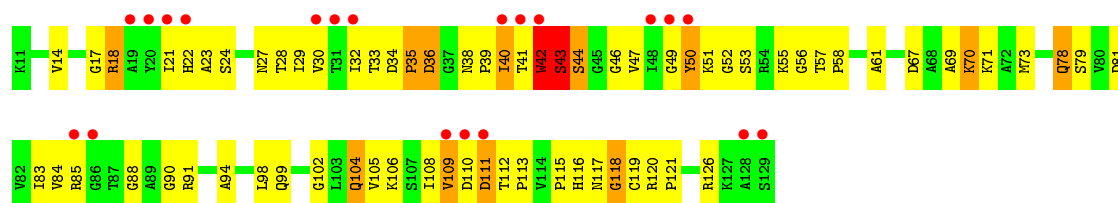


• Molecule 9: 30S ribosomal protein S10

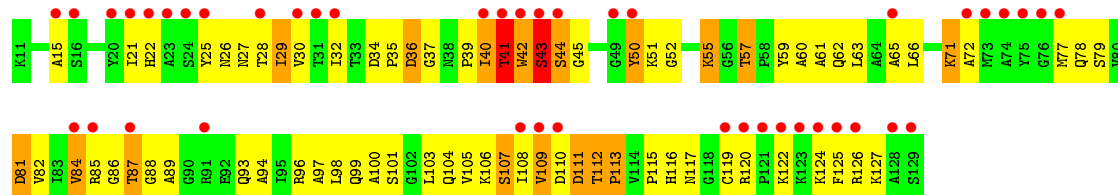


• Molecule 10: 30S ribosomal protein S11

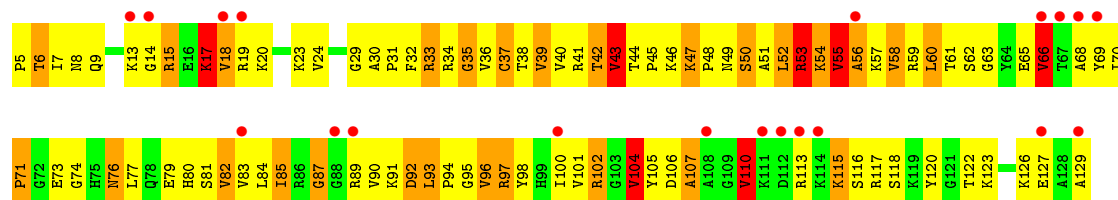




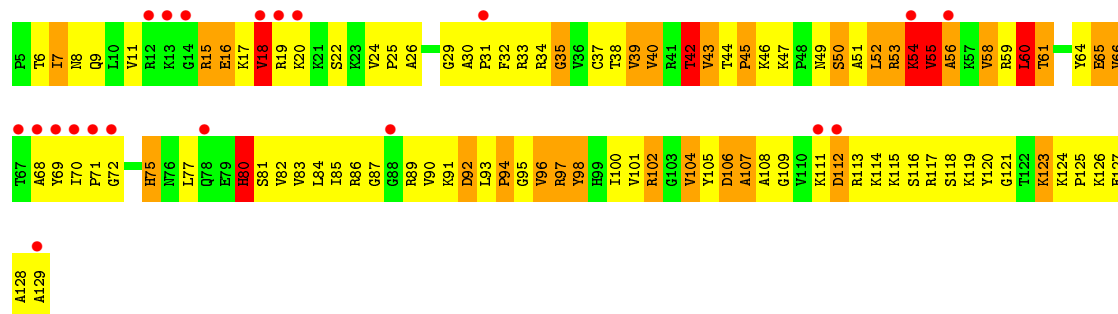
• Molecule 10: 30S ribosomal protein S11



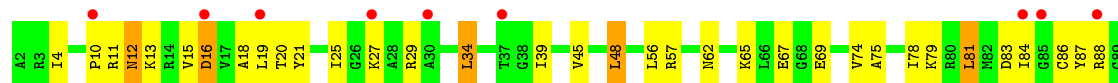
• Molecule 11: 30S ribosomal protein S12

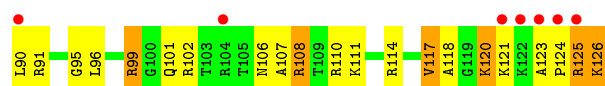


• Molecule 11: 30S ribosomal protein S12

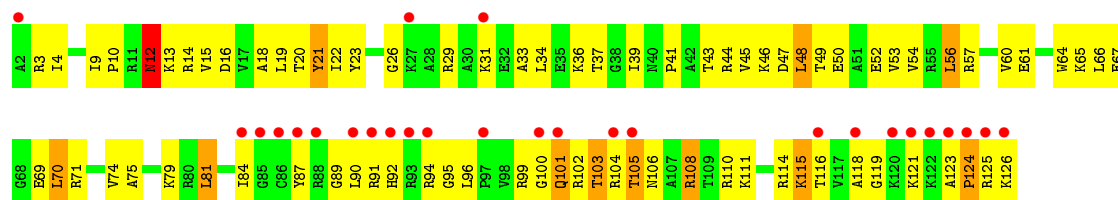


• Molecule 12: 30S ribosomal protein S13





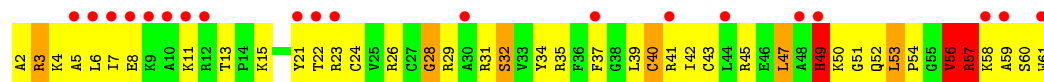
- Molecule 12: 30S ribosomal protein S13



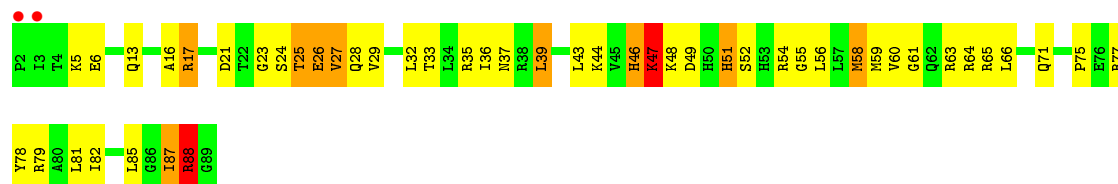
- Molecule 13: 30S ribosomal protein S14 type Z



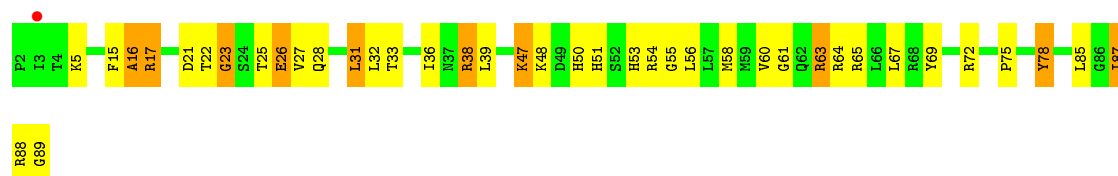
- Molecule 13: 30S ribosomal protein S14 type Z



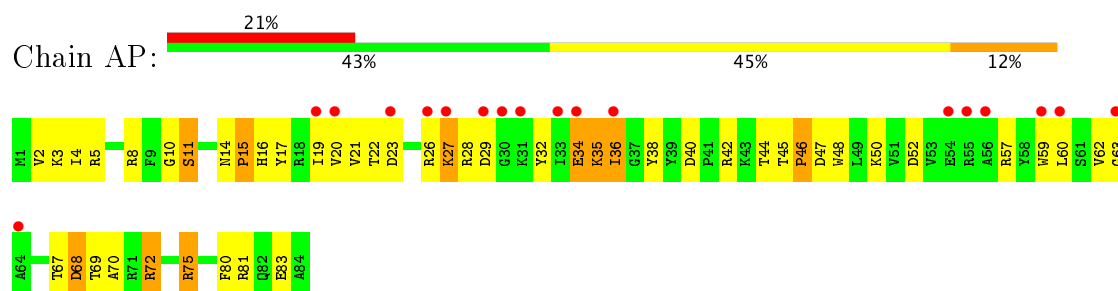
- Molecule 14: 30S ribosomal protein S15



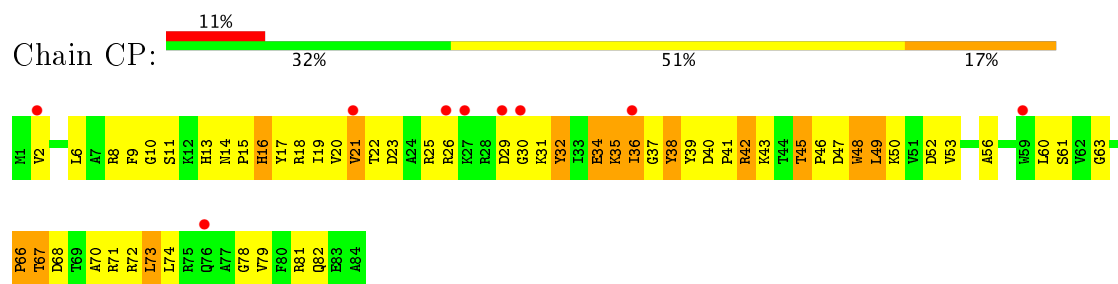
- Molecule 14: 30S ribosomal protein S15



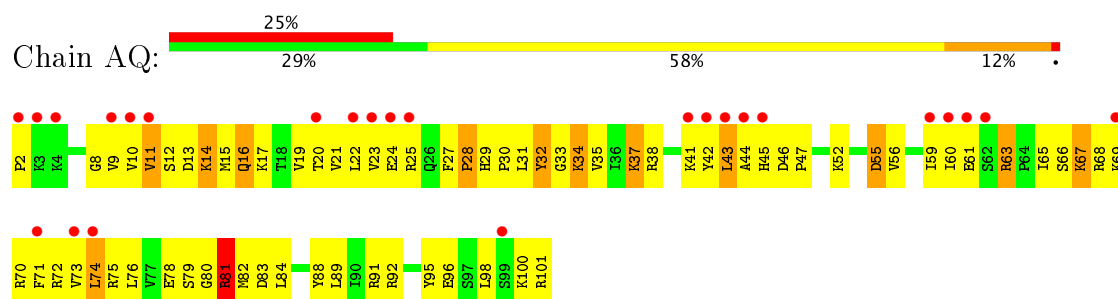
- Molecule 15: 30S ribosomal protein S16



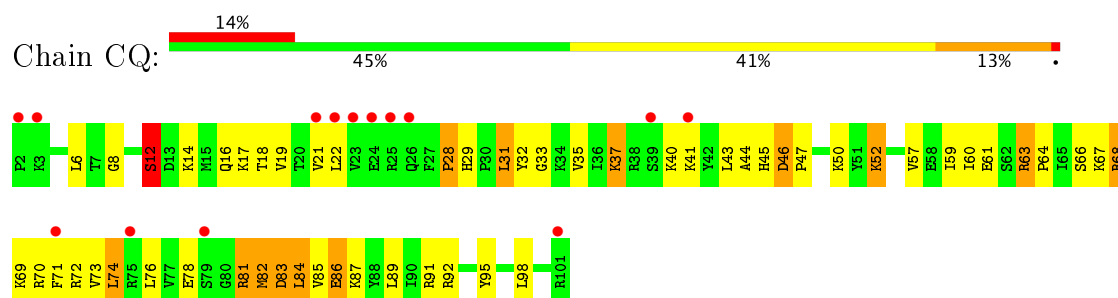
- Molecule 15: 30S ribosomal protein S16



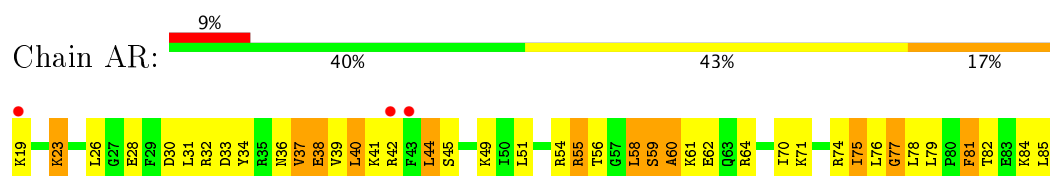
- Molecule 16: 30S ribosomal protein S17



- Molecule 16: 30S ribosomal protein S17

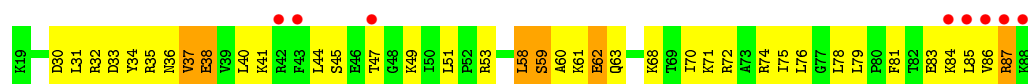


- Molecule 17: 30S ribosomal protein S18

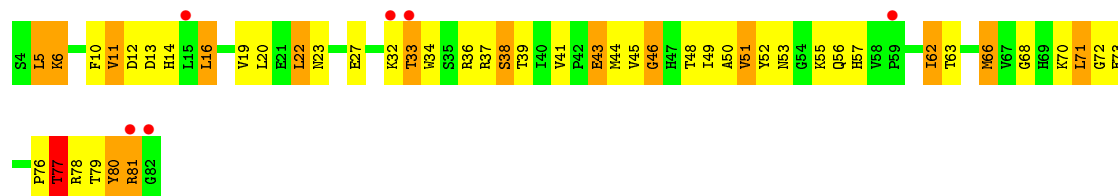


- Molecule 17: 30S ribosomal protein S18

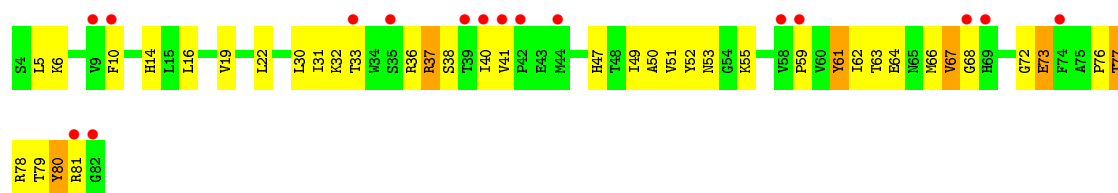




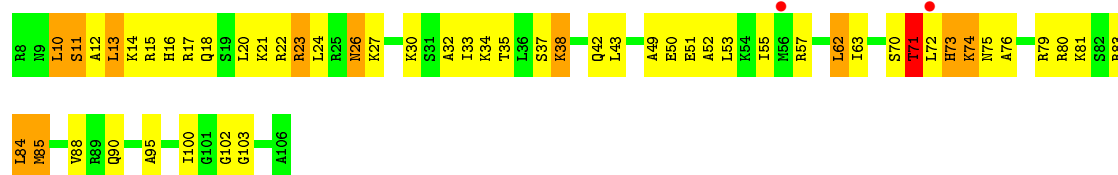
• Molecule 18: 30S ribosomal protein S19



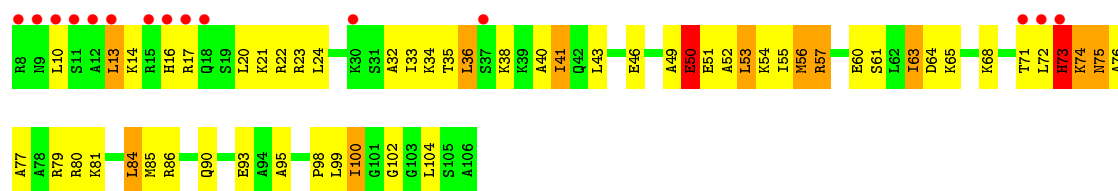
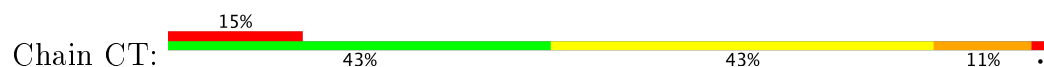
• Molecule 18: 30S ribosomal protein S19



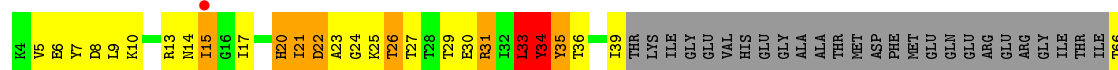
• Molecule 19: 30S ribosomal protein S20

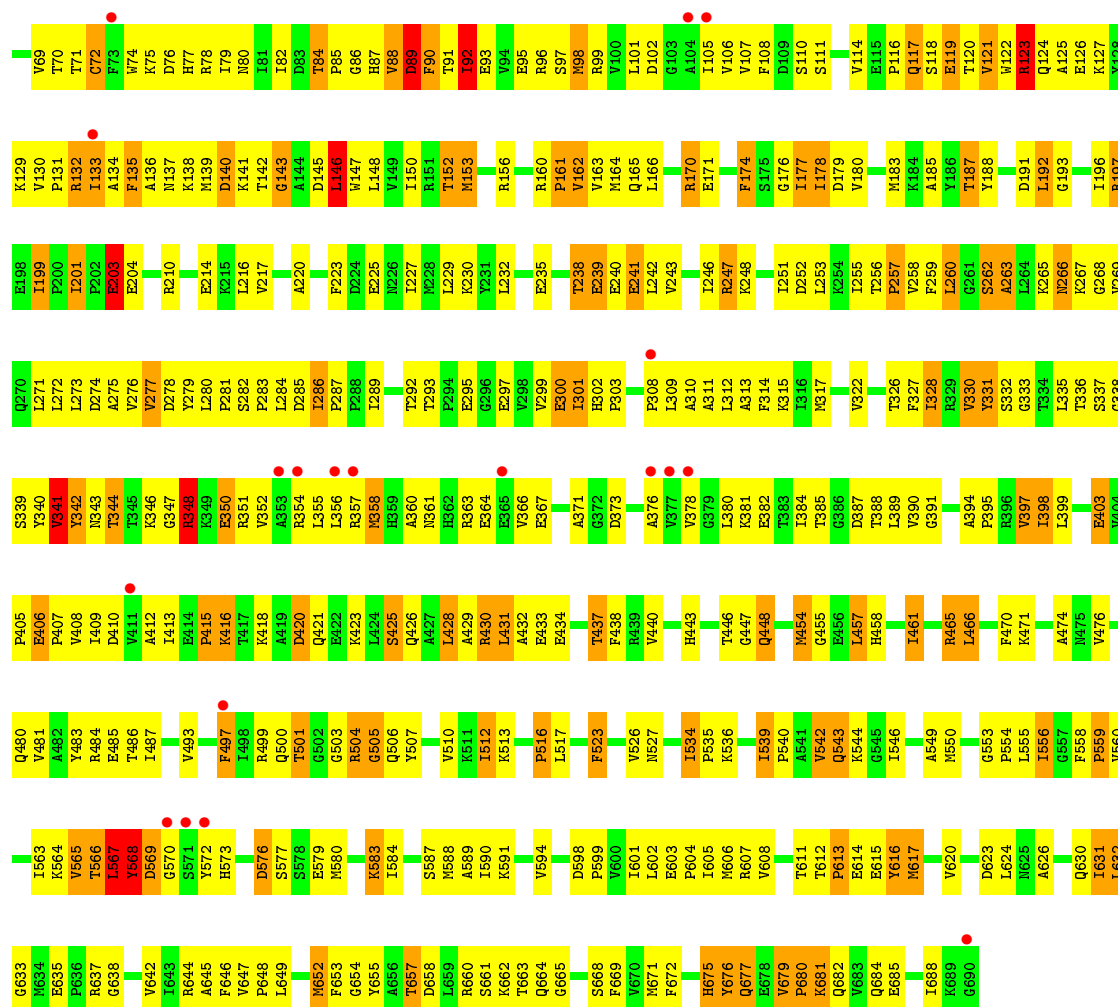


• Molecule 19: 30S ribosomal protein S20

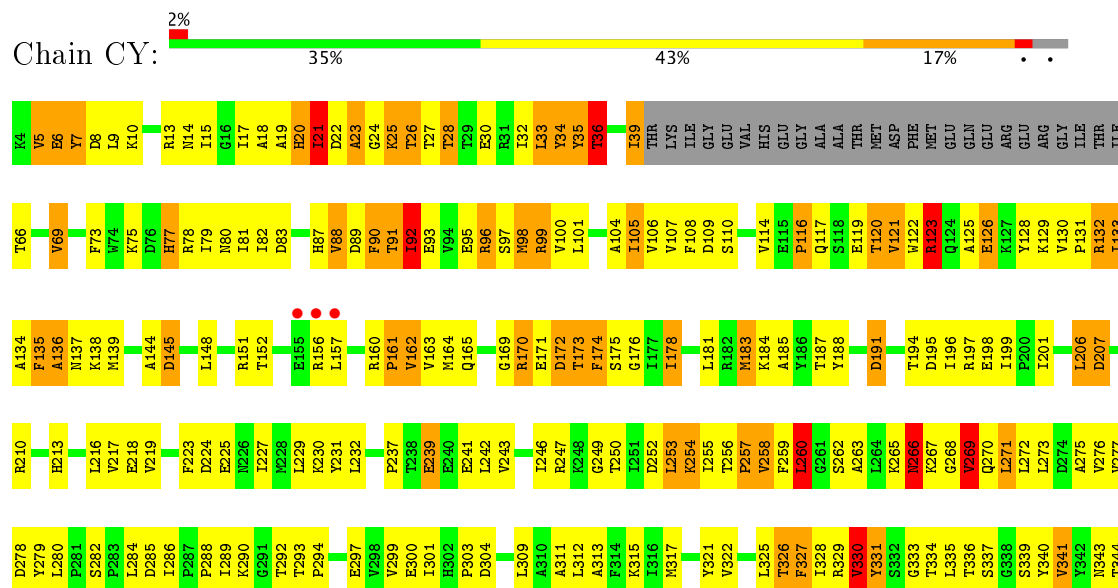


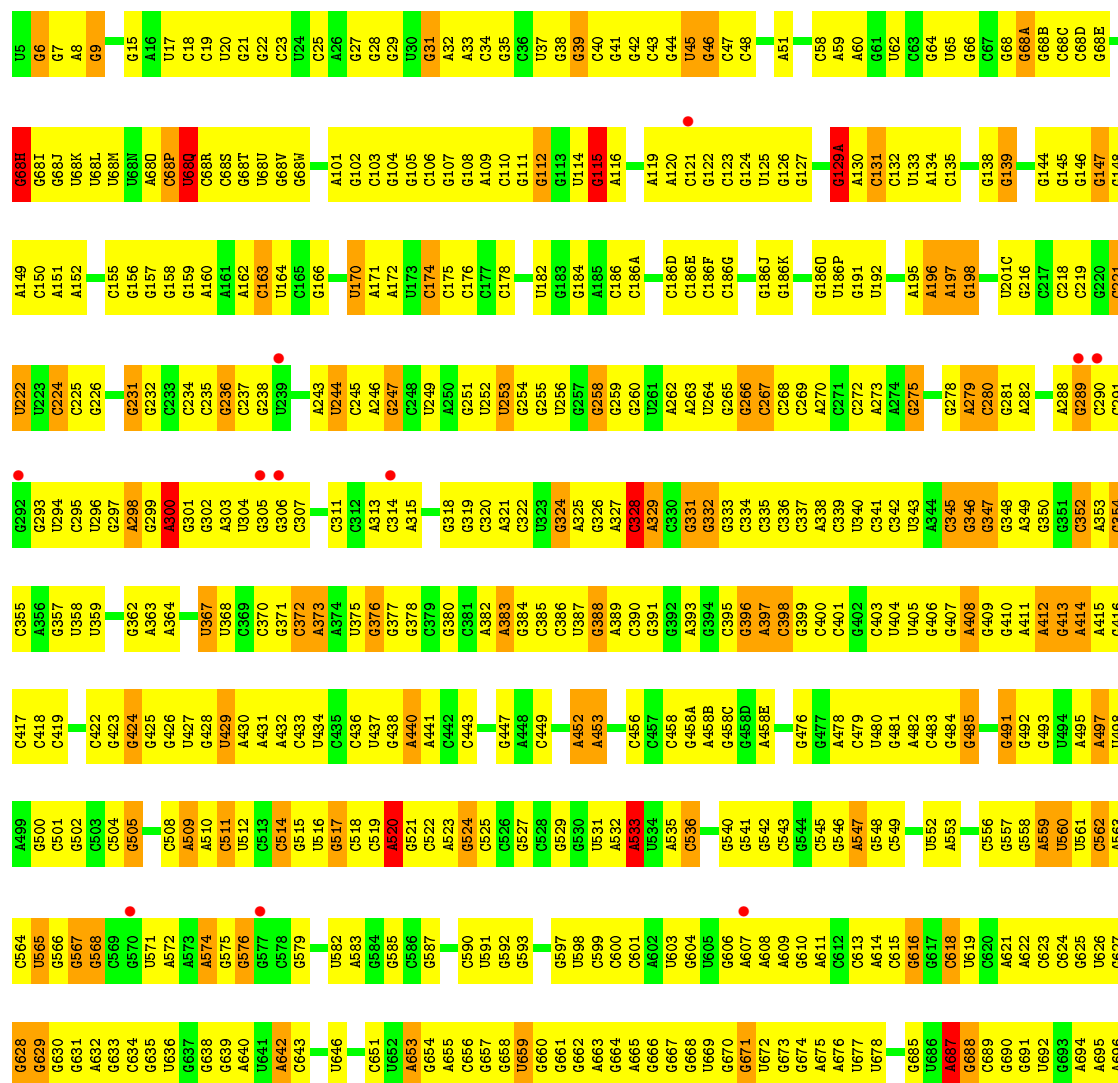
• Molecule 20: Elongation factor G

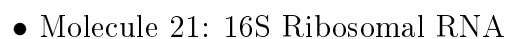




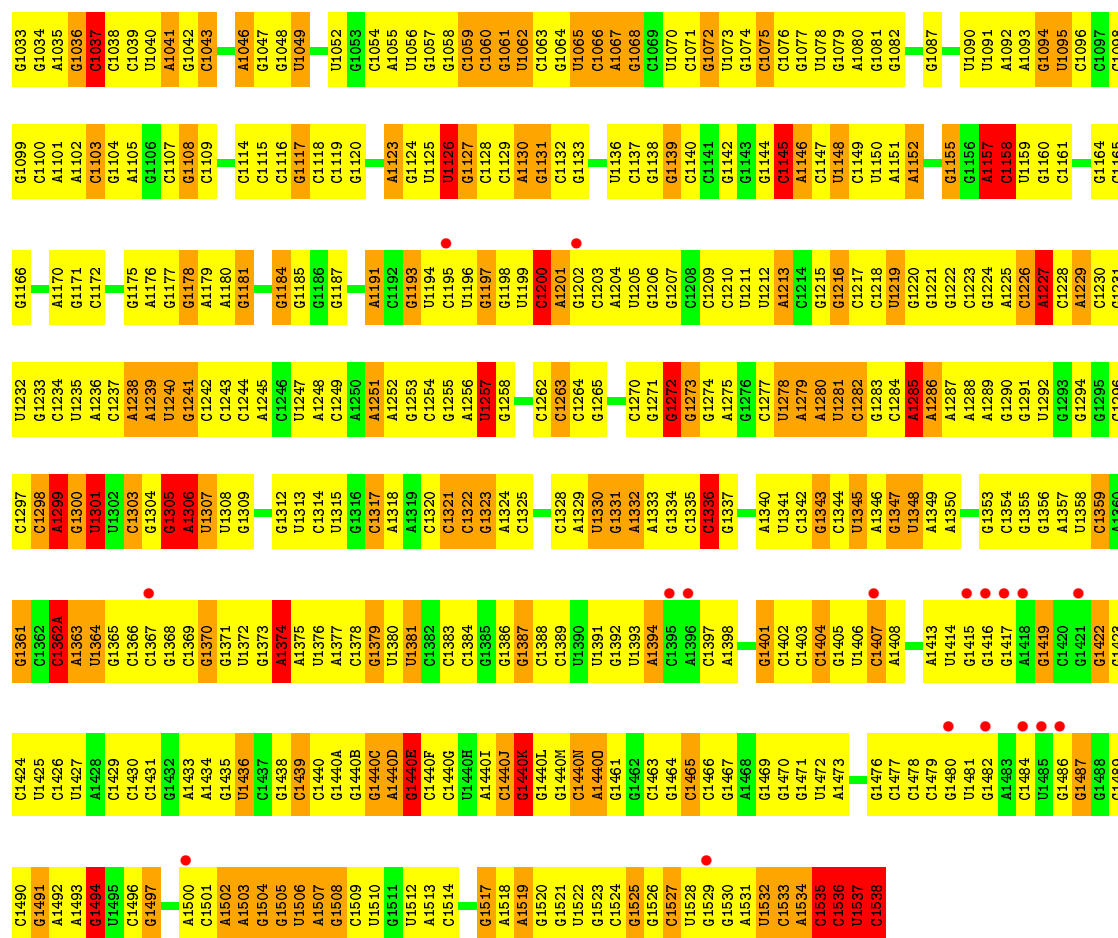
• Molecule 20: Elongation factor G



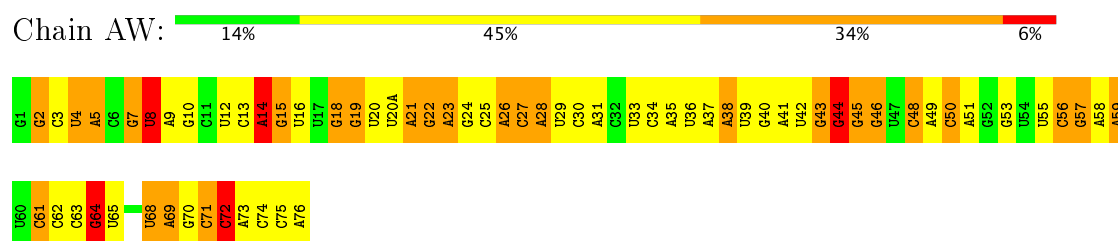




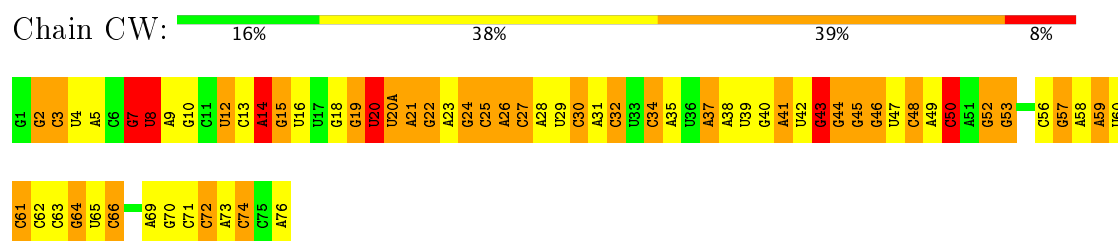




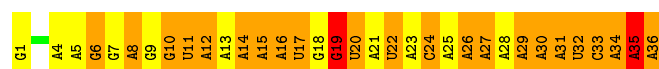
• Molecule 22: tRNA



• Molecule 22: tRNA



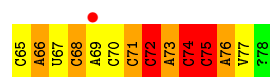
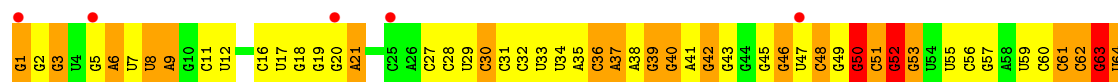
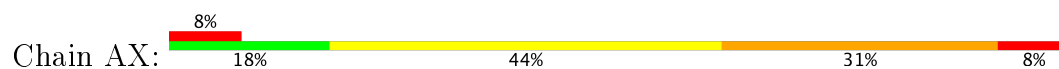
• Molecule 23: mRNA



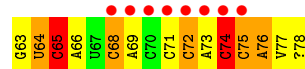
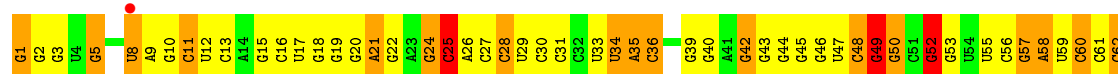
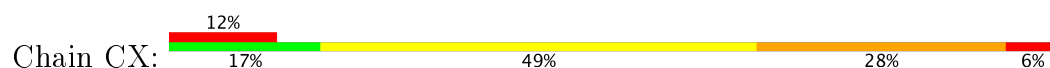
• Molecule 23: mRNA



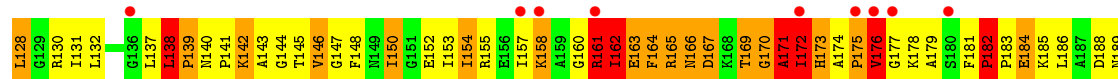
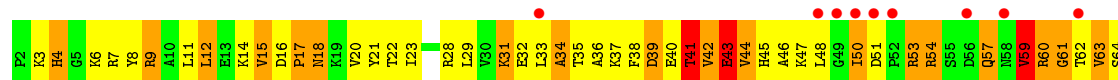
• Molecule 24: tRNA



• Molecule 24: tRNA

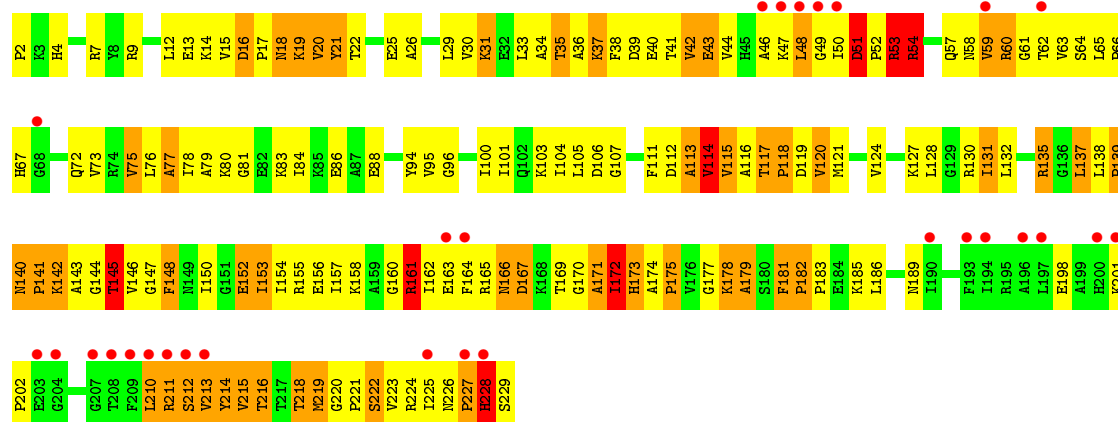


• Molecule 25: 50S ribosomal protein L1

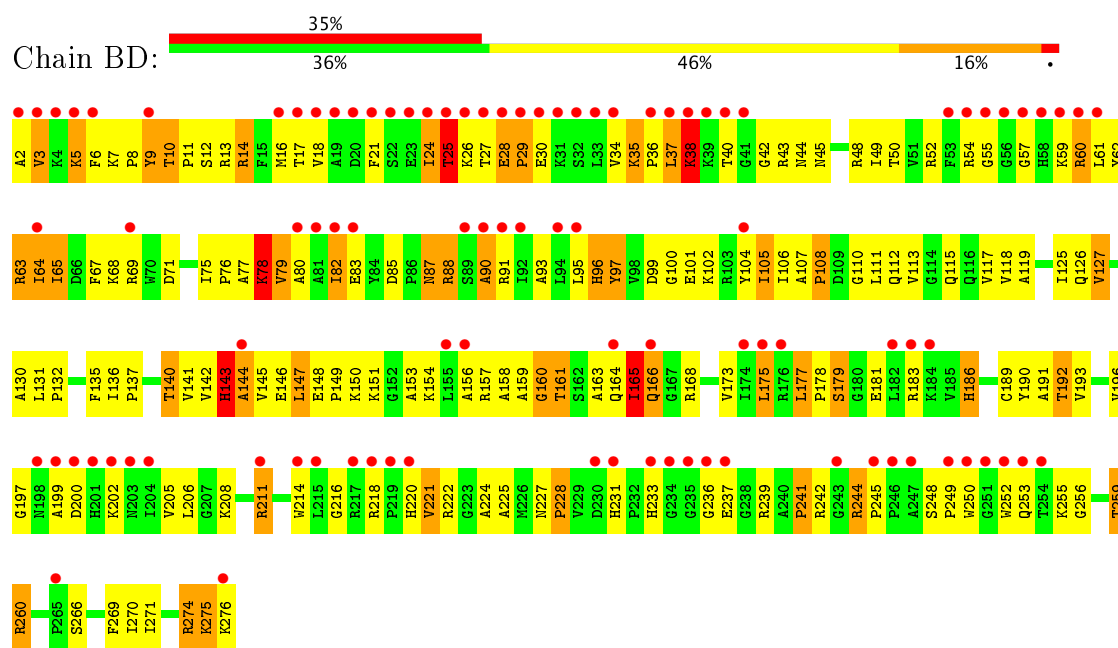


• Molecule 25: 50S ribosomal protein L1

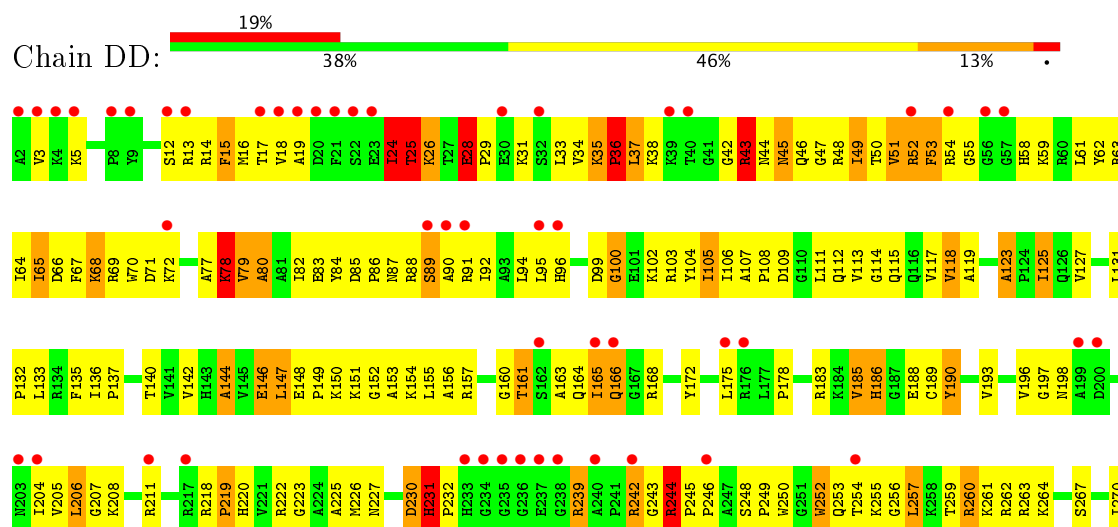




• Molecule 26: 50S ribosomal protein L2

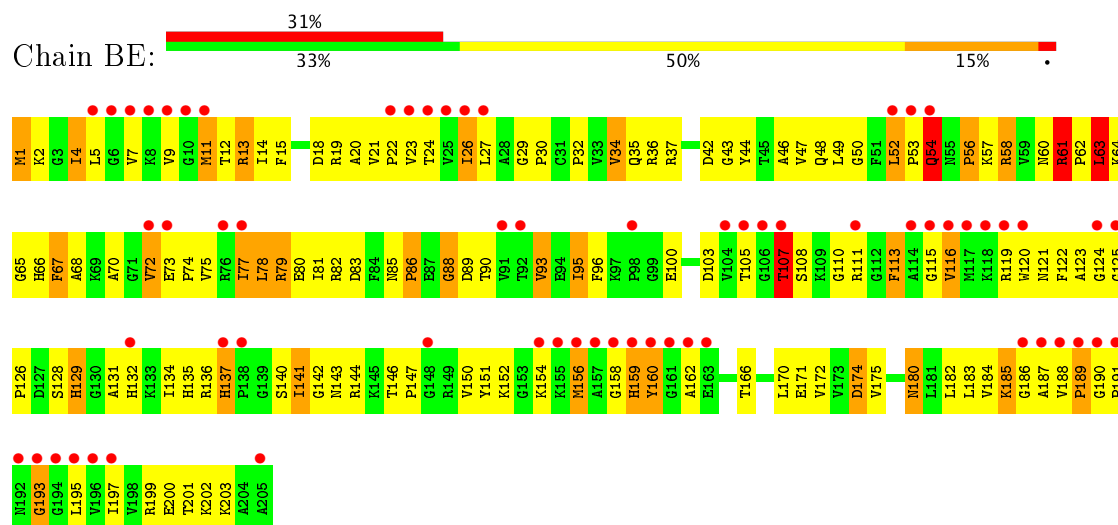


• Molecule 26: 50S ribosomal protein L2

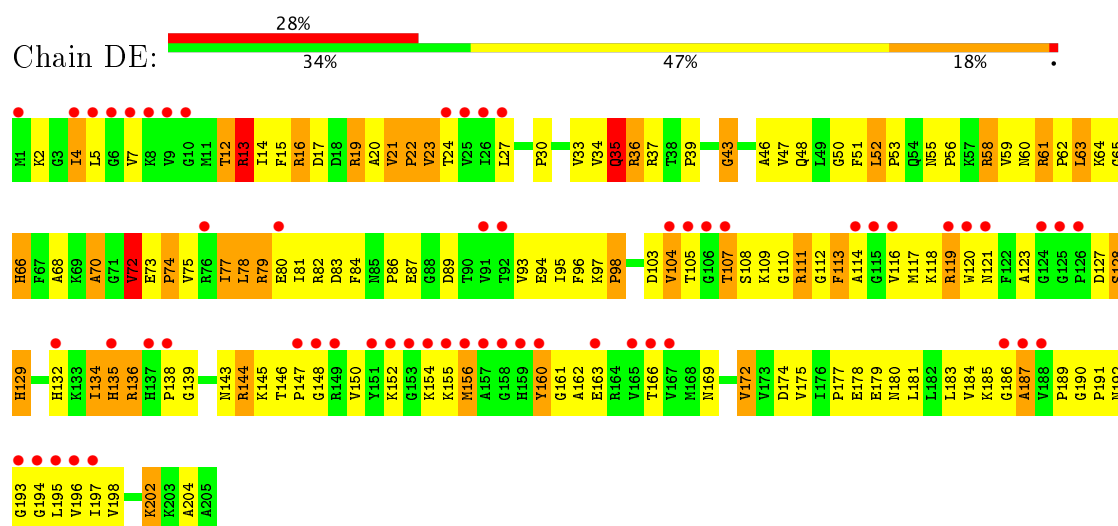




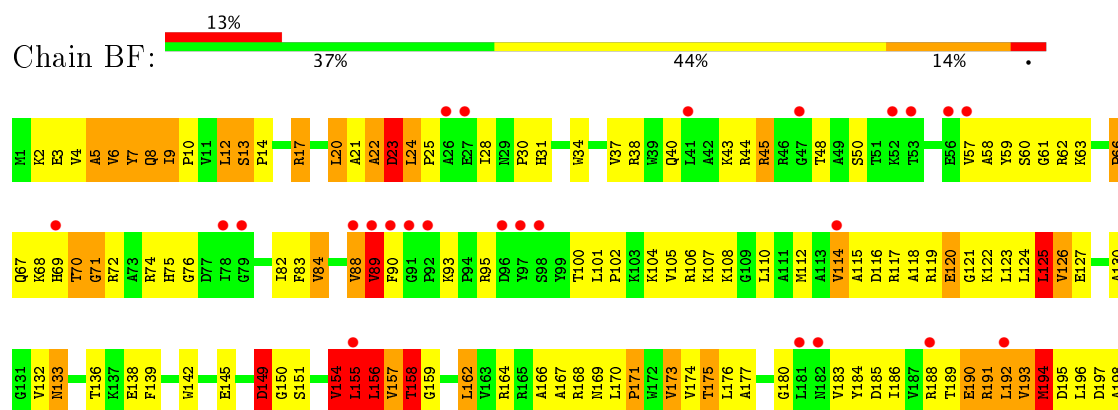
• Molecule 27: 50S ribosomal protein L3



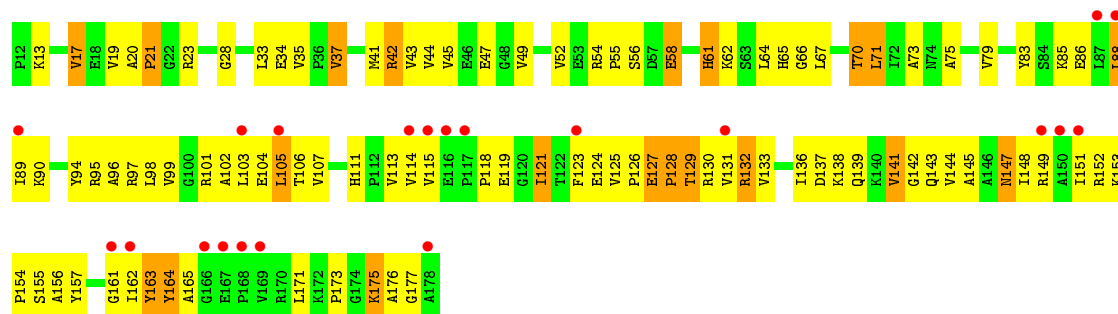
• Molecule 27: 50S ribosomal protein L3



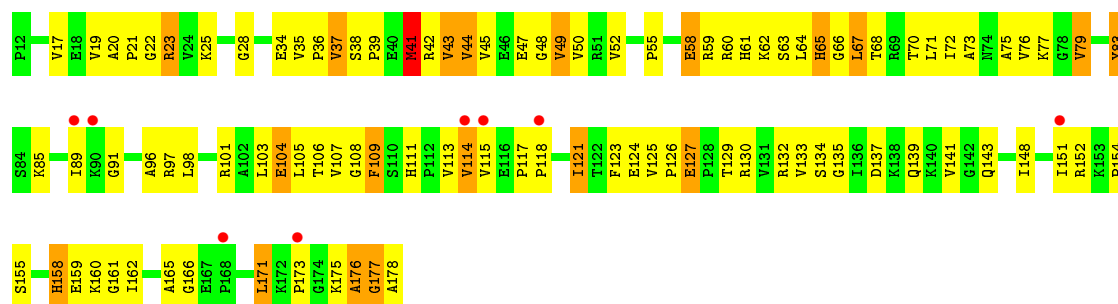
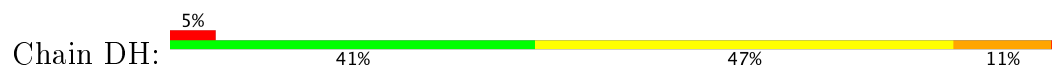
• Molecule 28: 50S ribosomal protein L4



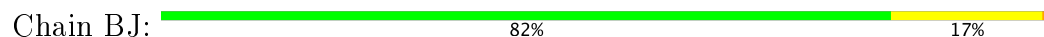




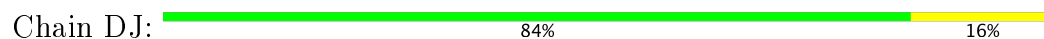
- Molecule 30: 50S ribosomal protein L6



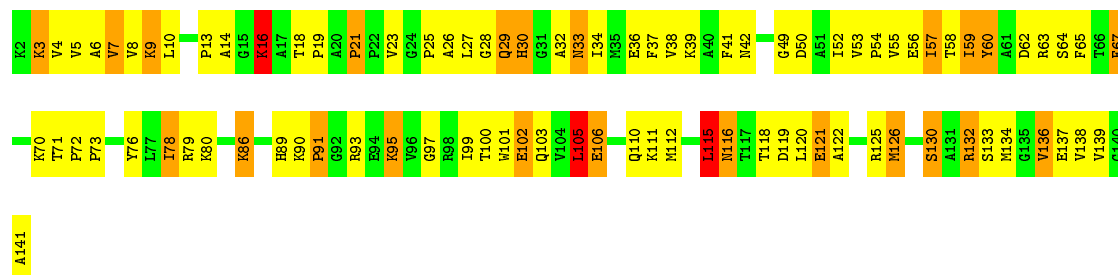
- Molecule 31: 50S ribosomal protein L10



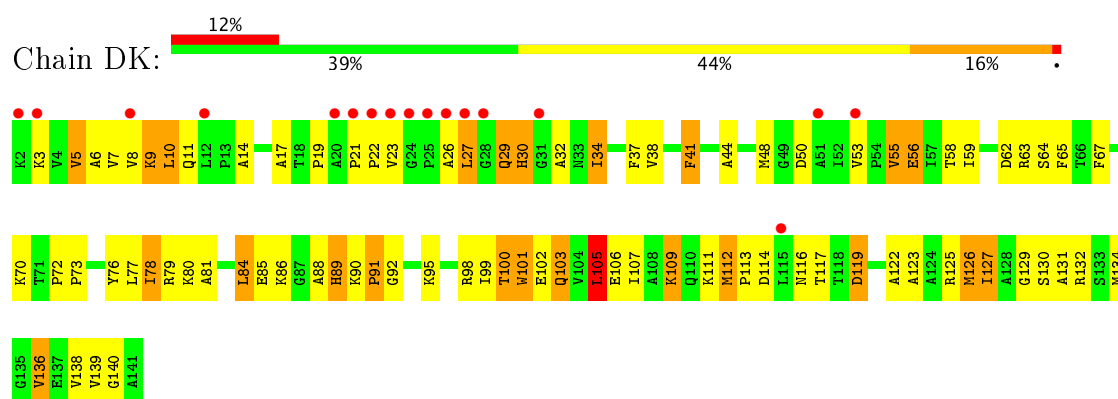
- Molecule 31: 50S ribosomal protein L10



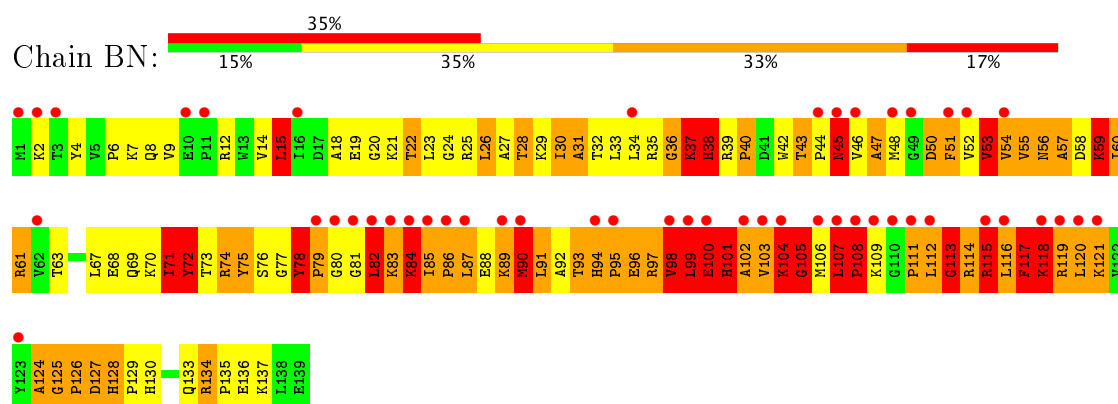
- Molecule 32: 50S ribosomal protein L11



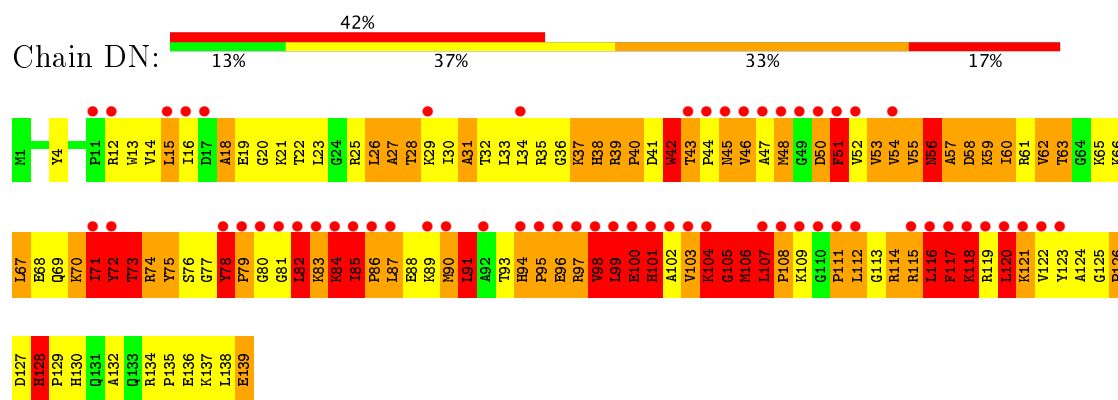
- Molecule 32: 50S ribosomal protein L11



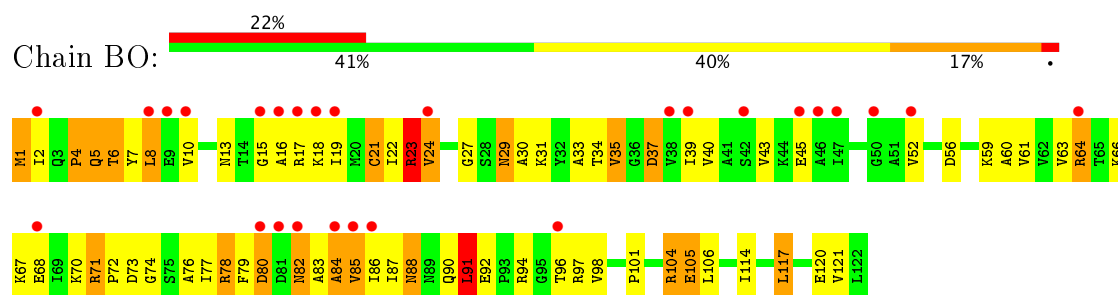
• Molecule 33: 50S ribosomal protein L13



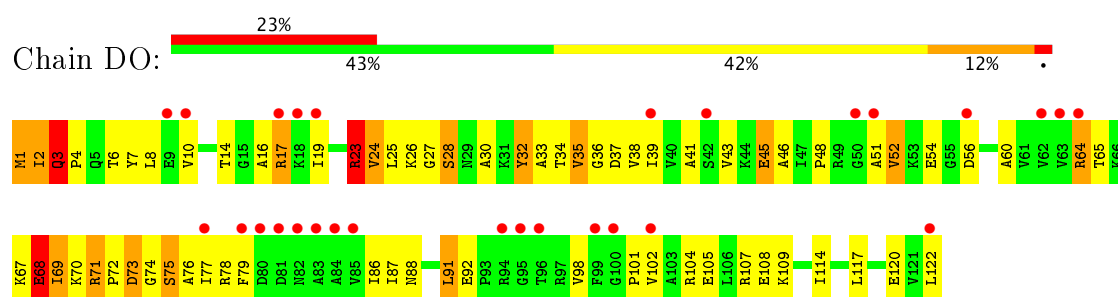
• Molecule 33: 50S ribosomal protein L13



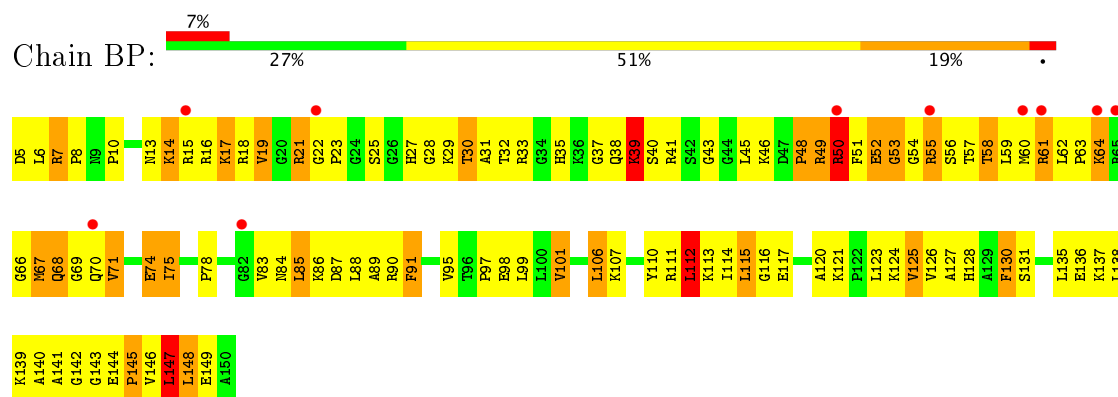
• Molecule 34: 50S ribosomal protein L14



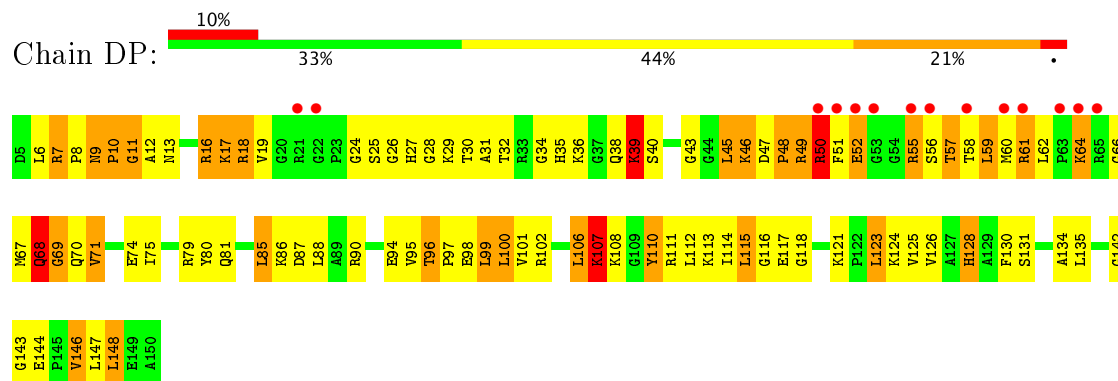
• Molecule 34: 50S ribosomal protein L14



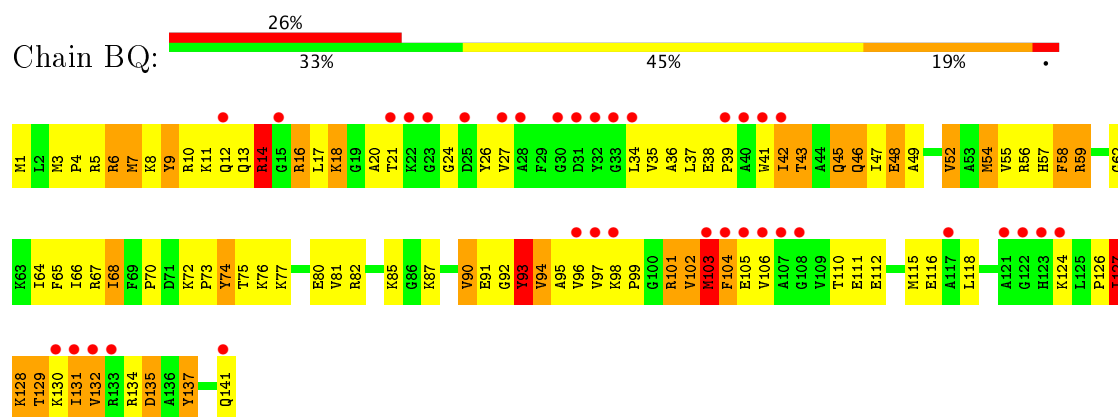
- Molecule 35: 50S ribosomal protein L15



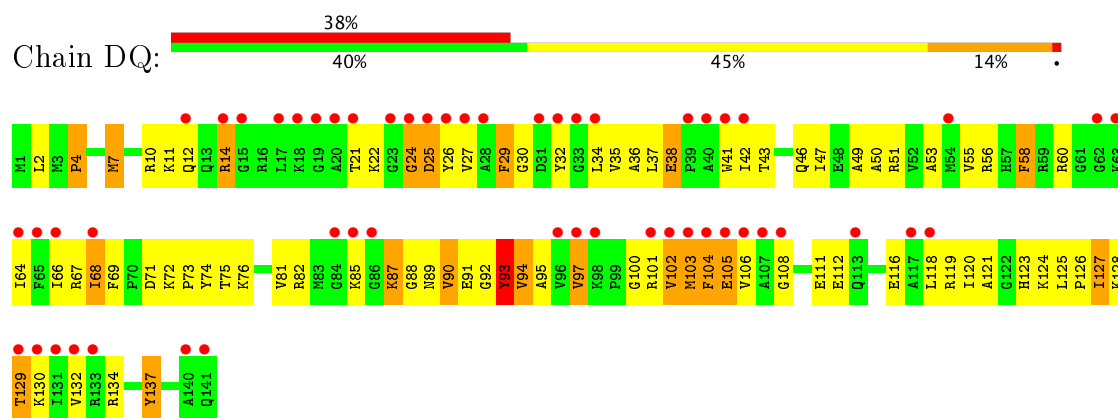
- Molecule 35: 50S ribosomal protein L15



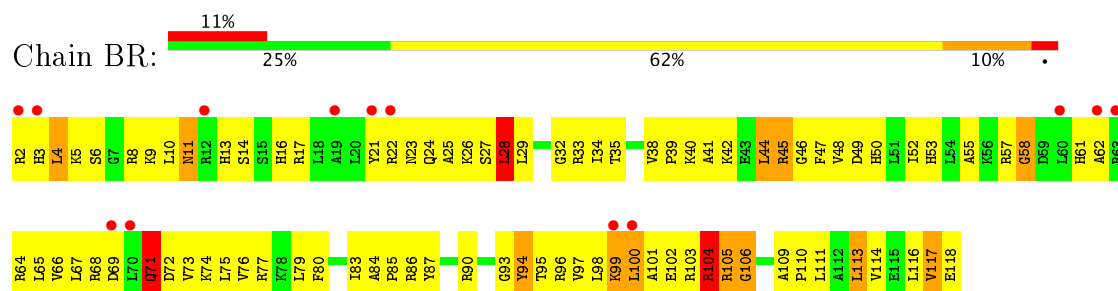
- Molecule 36: 50S ribosomal protein L16



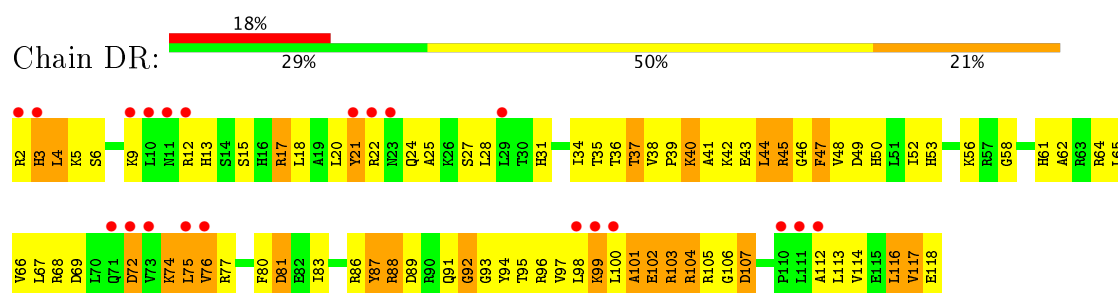
- Molecule 36: 50S ribosomal protein L16



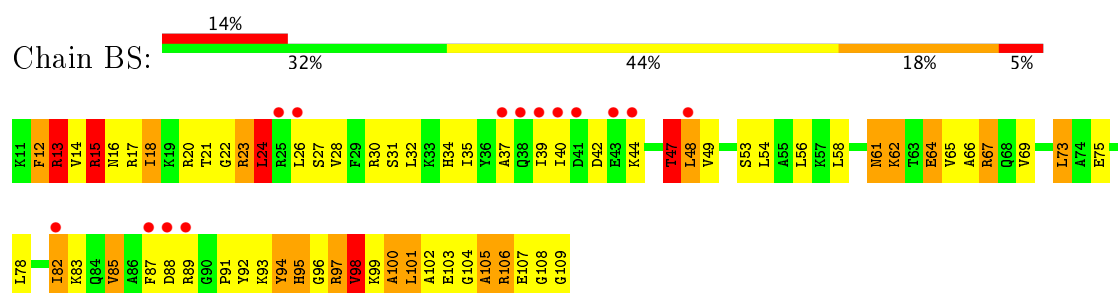
• Molecule 37: 50S ribosomal protein L17



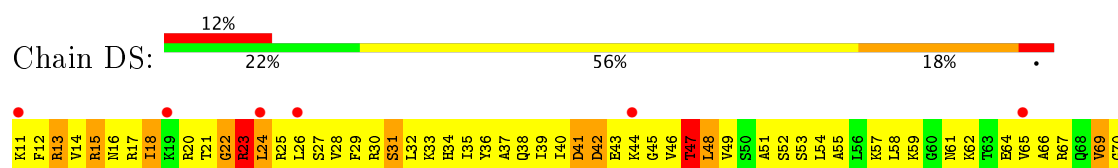
• Molecule 37: 50S ribosomal protein L17

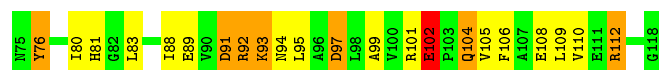


• Molecule 38: 50S ribosomal protein L18



• Molecule 38: 50S ribosomal protein L18






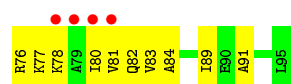
- Chain BV:

- Chain DV:
-
- | Chain DV | Percentage |
|----------|------------|
| 35% | 35% |
| 49% | 49% |
| 15% | 15% |
| 7% | 7% |

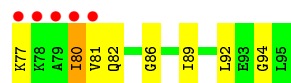
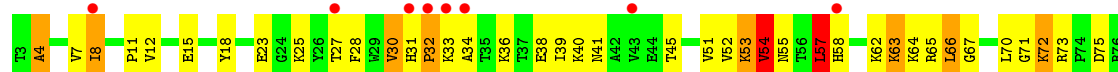
- Chain BW:
-
- 16% 31% 57% 12%
-
- M1 M2 M3 M4 M5 M6 M7 M8 M9 M10 M11 M12 M13 M14 M15 M16 M17 M18 M19 M20 M21 M22 M23 M24 M25 M26 M27 M28 M29 M30 M31 M32 M33 M34 M35 M36 M37 M38 M39 M40 M41 M42 M43 M44 M45 M46 M47 M48 M49 M50 M51 M52 M53 M54 M55 M56 M57 M58 M59 M60 M61 M62 M63
- L65 L66 L67 L68 L69 L70 L71 L72 L73 L74 L75 L76 L77 L78 L79 L80 L81 L82 L83 L84 L85 L86 L87 L88 L89 L90 L91 L92 L93 L94 L95 L96 L97 L98 L99 L100 L101 L102 L103 L104 L105 L106 L107 L108 L109 L110 L111 L112 L113

- Chain DW: 

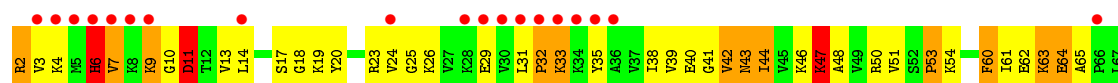
- Chain BX:
-
- 20% 45% 44% 9%



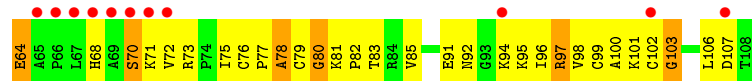
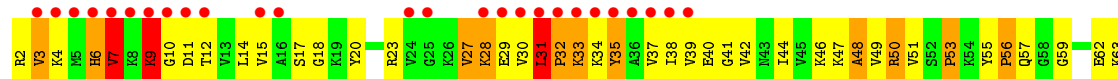
- Molecule 43: 50S ribosomal protein L23



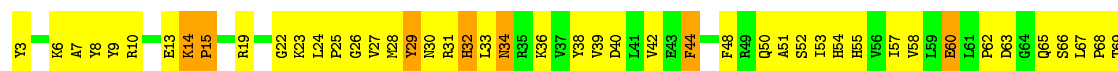
- Molecule 44: 50S ribosomal protein L24



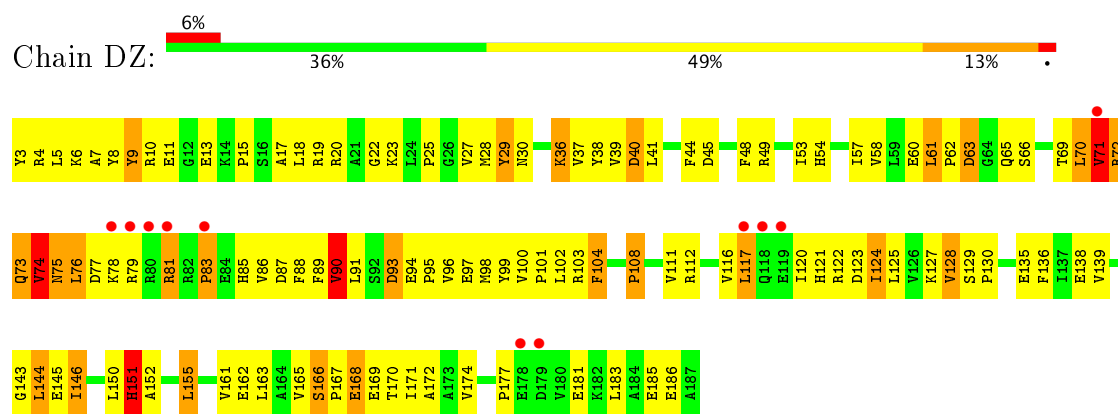
- Molecule 44: 50S ribosomal protein L24



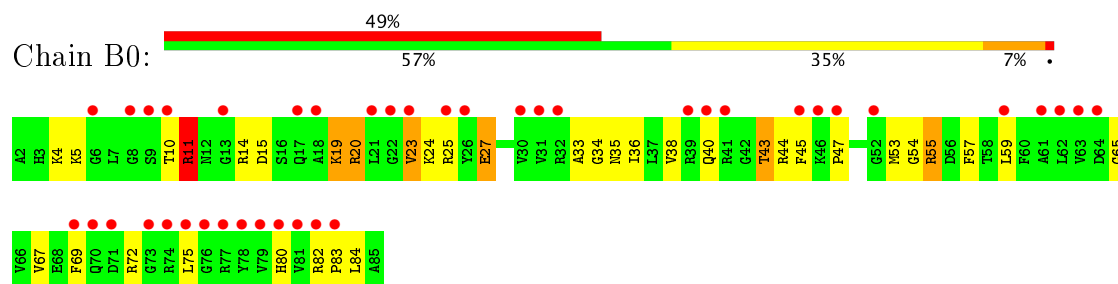
- Molecule 45: 50S ribosomal protein L25



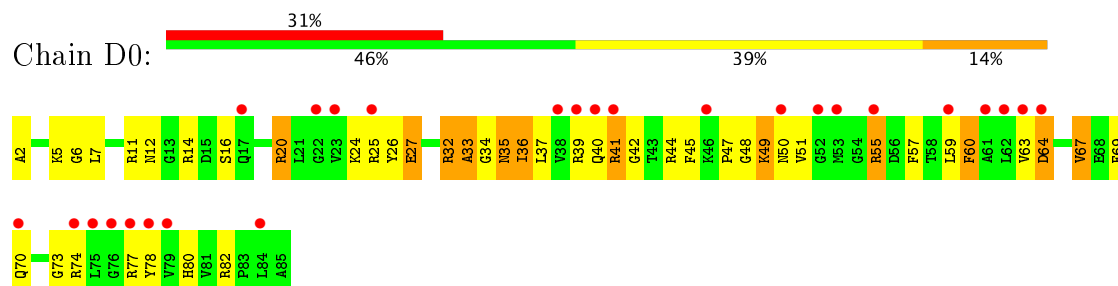
- Molecule 45: 50S ribosomal protein L25



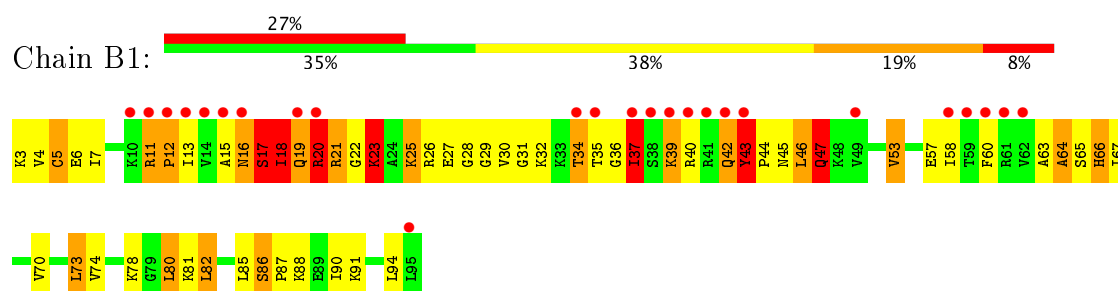
• Molecule 46: 50S ribosomal protein L27



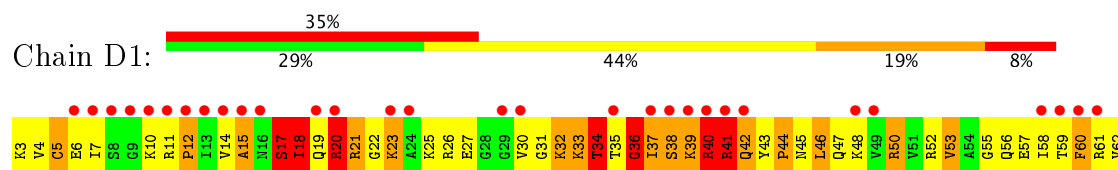
• Molecule 46: 50S ribosomal protein L27

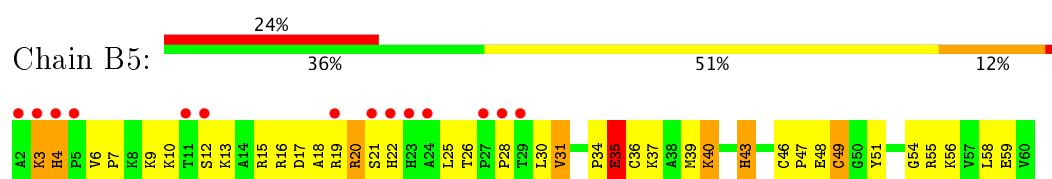


• Molecule 47: 50S ribosomal protein L28

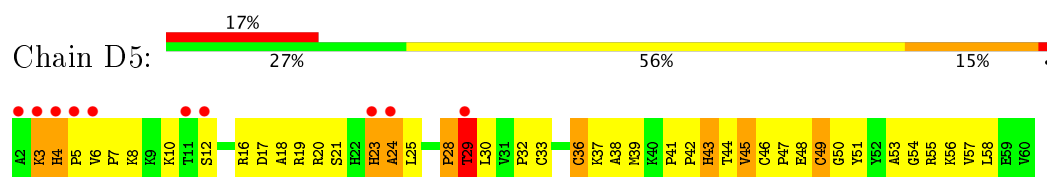


• Molecule 47: 50S ribosomal protein L28

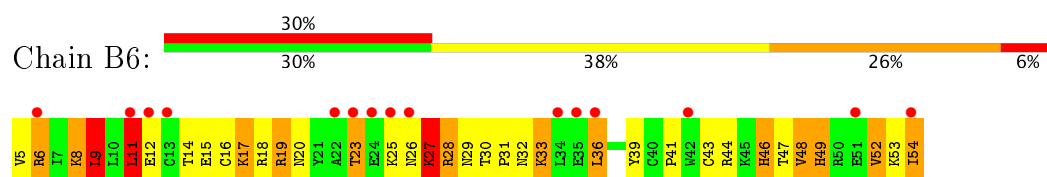




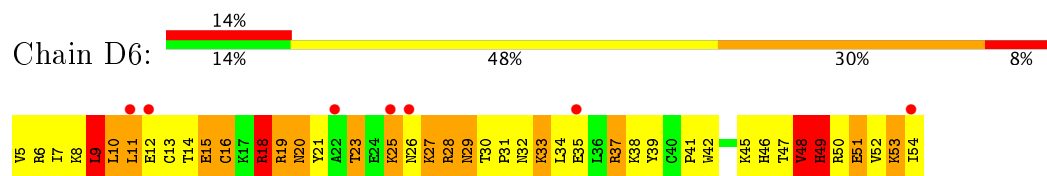
- Molecule 51: 50S ribosomal protein L32



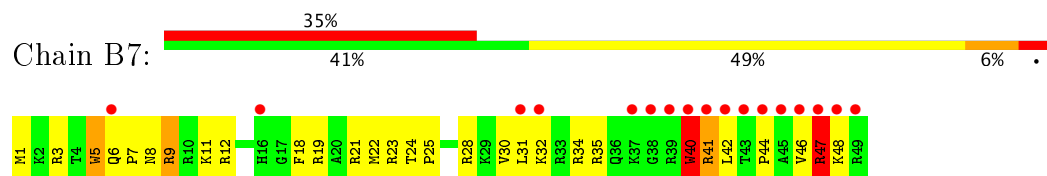
- Molecule 52: 50S ribosomal protein L33



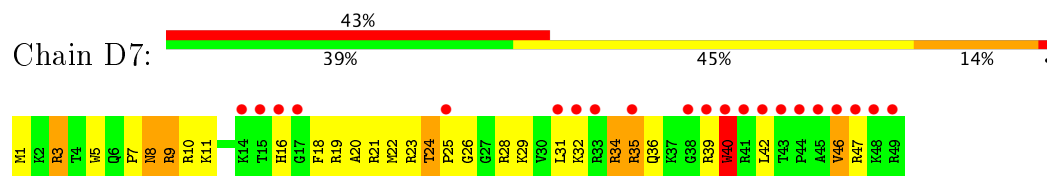
- Molecule 52: 50S ribosomal protein L33



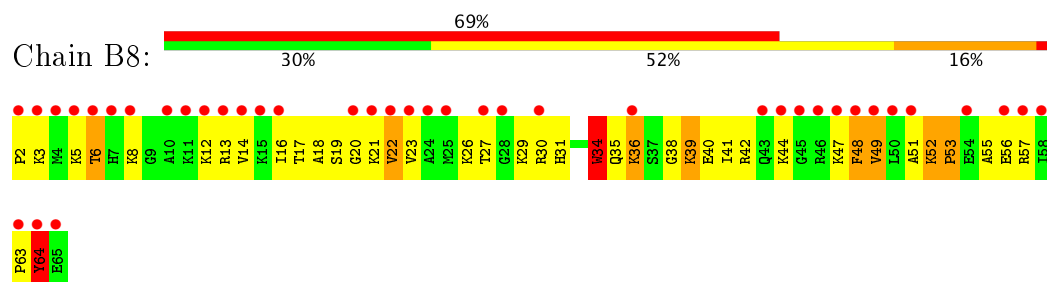
- Molecule 53: 50S ribosomal protein L34



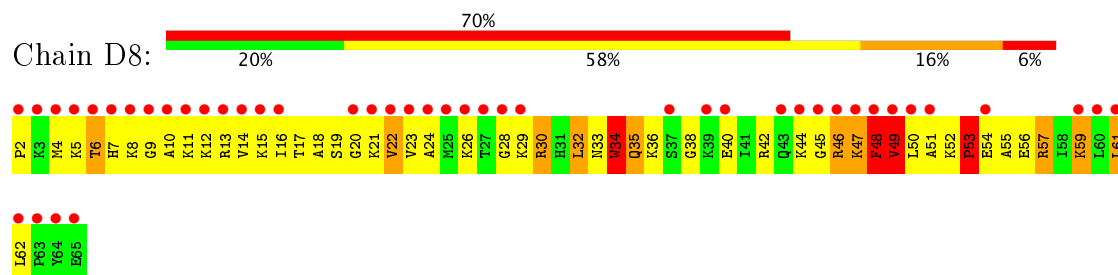
- Molecule 53: 50S ribosomal protein L34



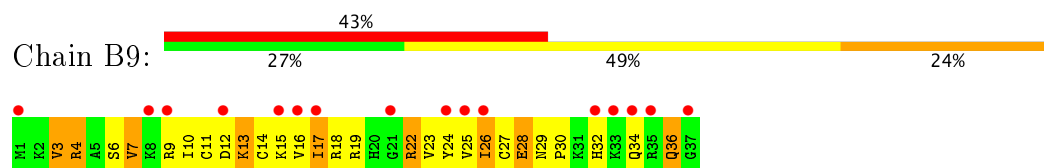
- Molecule 54: 50S ribosomal protein L35



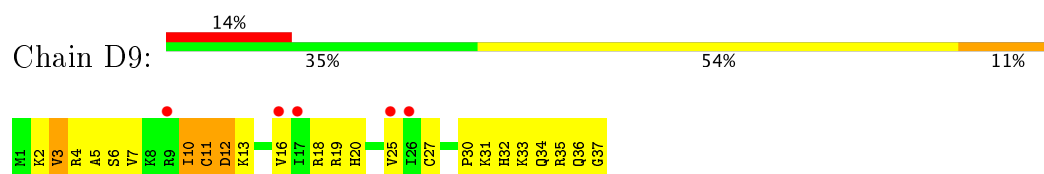
- Molecule 54: 50S ribosomal protein L35



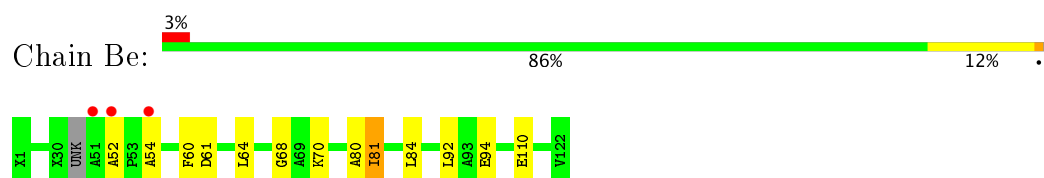
- Molecule 55: 50S ribosomal protein L36



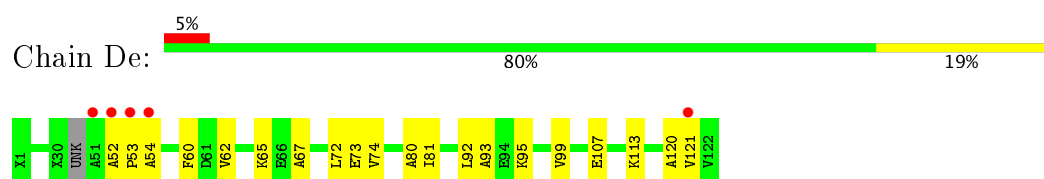
- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L7/L12



- Molecule 56: 50S ribosomal protein L7/L12



- Molecule 57: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Df:  100%

There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Dg:  100%

There are no outlier residues recorded for this chain.

- Molecule 58: 50S ribosomal protein L7/L12

Chain Bh:  100%

There are no outlier residues recorded for this chain.

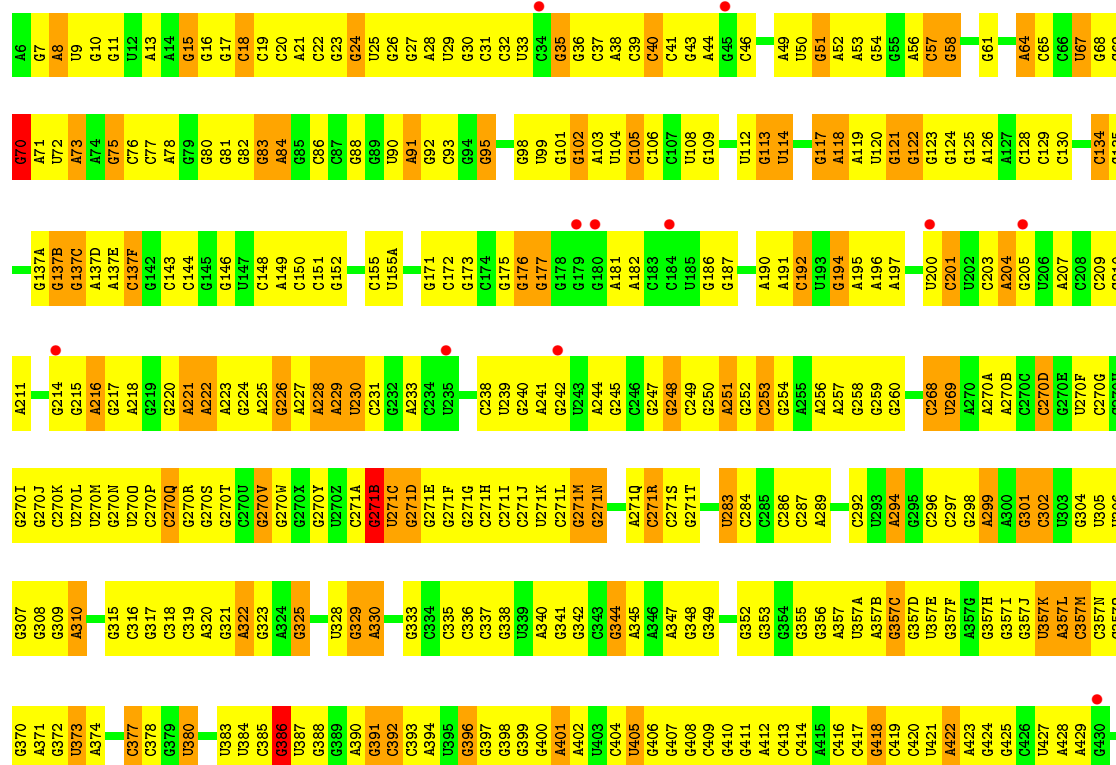
- Molecule 58: 50S ribosomal protein L7/L12

Chain Dh:  100%

There are no outlier residues recorded for this chain.

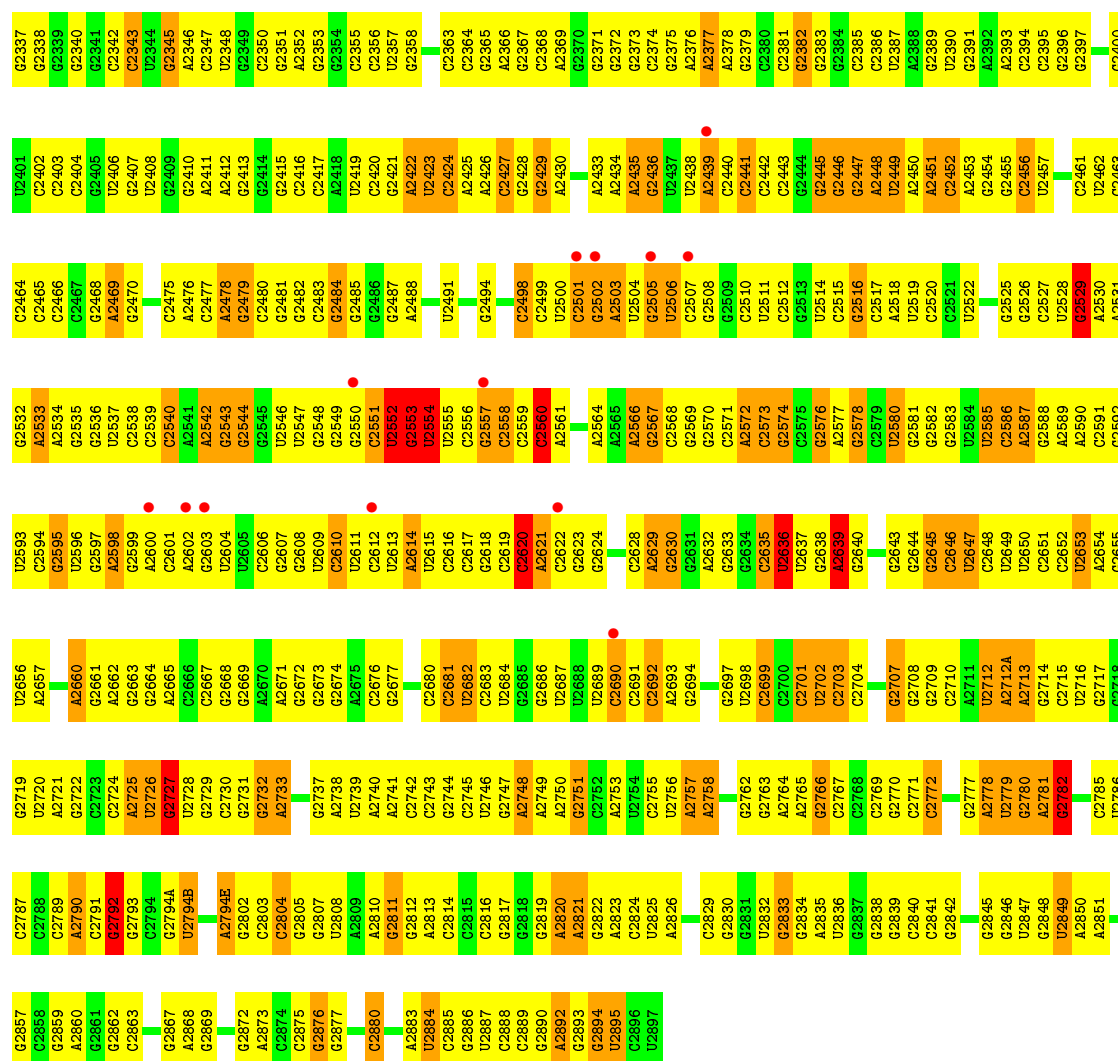
- Molecule 59: 23S Ribosomal RNA

Chain BA:  4% 23% 57% 19%

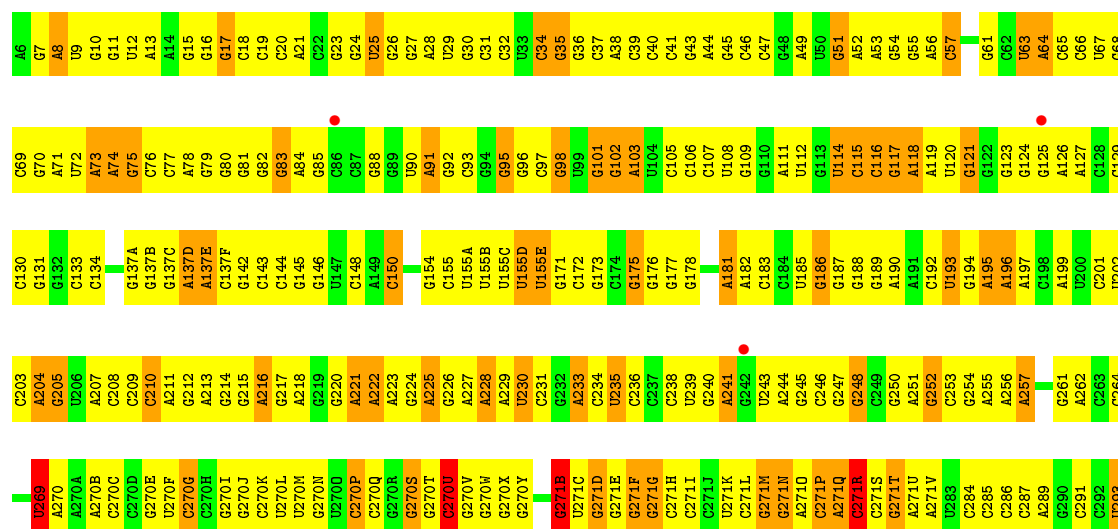


U1326	U1327	G1264	G1197	G1135	C1072	C1006	G944	G879	C815	C753	G691	G636	A501	U434
C1327	G1265	A1265	U1198	G1136	A1073	C1007	A945	G880	C816	C754	C692	A627	A502	C435
G1328	U1266	G1266	U1199	G1137	G1074	C1008	G946	G881	C817	C755	C693	U668	A503	C436
U1329	U1267	G1267	C1200	G1138	C1075	A1009	G947	G882	G818	C756	G694	G629	U504	G438
C1330	A1268	G1268	G1203	G1139	C1076	A1010	G948	G883	A819	U757	G695	G630	A505	G439
A1331	A1269	G1269	G1204	G1140	A1077	G1011	G949	G884	A820	C758	G696	A631	G506	G440
C1332	C1270	A1270	A1204	U1141	U1078	U1012	G952	C885	A821	C759	C697	A632	A507	U441
C1333	G1271	A1271	U1205	U1142	C1079	C1013	G953	C886	U826	A761	C698	A633	G508	G442
G1334	A1272	G1272	G1206	A1143	C1080	G1016	A953	A887	U827	A762	A699	G634	C509	A443
U1335	A1273	G1273	C1207	A1144	U1081	G1017	G954	C888	U828	G763	G700	G635	C510	C444
A1336	A1274	G1274	C1208	G1145	U1082	G1018	G955	C889	U829	G764	G701	G636	U511	C445
G1337	A1275	G1275	G1209	G1146	U1083	C1019	G956	A890	A830	A765	G702	A637	G512	G448
G1338	A1276	G1276	A1210	C1145	A1084	U1019	A957	G892	G831	C766	G703	G638	A513	U449
G1339	U1211	G1277	U1211	G1149	A1086	A1021	U958	C893	G832	C767	G704	U639	A514	A450
U1340	A1212	G1278	G1212	G1150	G1087	G1022	A959	C894	U833	U767	A706	U641	A705	G451
U1341	A1213	G1279	A1213	C1151	A1088	G1023	A960	U895	U834	G769	G707	G583	C516	G452
A1342	A1214	G1280	A1214	C1152	A1089	G1024	G961	A896	A835	G770	G708	G584	C517	G453
G1343	G1215	G1281	G1215	C1153	U1090	G1025	U963	C897	G836	G771	U709	G585	G518	G454
G1344	G1216	U1282	G1216	C1154	U1091	U1026	U964	C898	C837	C772	G710	A646	U519	G455
C1345	A1216	G1283	A1216	G1155	G1091	A1027	C965	A900	C838	U773	G711	C597	G520	C456
G1346	A1219A	A1284	A1219A	A1155	U1094	A1028	G966	A901	U839	A774	G712	G648	G521	A457
G1347	G1220	G1285	C1220	A1156	A1095	A1028	G967	A902	C840	G775	G713	U649	G522	G458
G1348	C1221	A1286	C1221	G1157	A1096	G1030	G968	C903	A841	G776	G714	C650	U524	A460
A1349	G1222	A1287	G1222	C1158	A1097	G1031	U969	C904	G842	A777	G715	G651	U525	G461
G1350	G1223	U1288	G1223	U1159	U1097	G1031	C970	U905	G843	G778	A716	U652	A526	G463
C1351	C1224	C1289	C1224	G1160	A1098	A1032	C971	G906	C844	U779	G717	C653	C527	G464
U1352	G1225	C1290	G1225	G1161	U1101	U1033	G972	G916	G845	G780	G718	U654	A528	G465
A1353	A1226	G1291	A1226	G1162	G1107	G1034	G973	C917	C846	A781	C719	G649	C529	A466
G1354	G1227	G1292	G1227	G1163	A1108	A1046	G974	A911	U847	A782	G720	G656	G530	G467
A1355	G1228	A1293	G1228	G1164	C1109	G1047	C974A	C912	G848	A783	G721	U657	C531	G468
G1356	G1229	U1294	G1229	U1165	C1110	G1043	G975	U913	A849	A784	A722	G658	G532	G469
U1357	G1230	G1295	G1230	C1166	U1105	C1043	G976	C914	C850	G785	G723	C659	A533	A470
G1358	U1234	G1296	U1234	G1167	G1106	G1044	G978	G920	U851	G786	G724	G660	U534	A471
A1359	G1235	C1297	G1235	G1168	U1107	A1045	G979	G921	G852	U787	G725	G661	C535	A472
A1360	A1236	G1298	G1236	G1169	A1108	A1046	A980	A917	G853	A788	A727	G662	A536	G473
G1364	A1237	U1299	A1237	G1170	C1109	G1047	A981	A918	G854	C790	G728	A603	C537	G474
A1365	G1238	U1300	G1238	G1171	G1110	A1043	C982	G919	A861	C791	G729	C664	G538	U475
A1366	U1240	A1301	U1240	G1172	A1111	C1049	A983	G920	G862	G792	C730	C665	G539	G476
A1367	A1241	G1302	A1241	U1174	G1112	A1050	A984	G921	U858	G793	C731	G666	C540	A477
G1368	G1242	G1303	A1242	G1175	G1113	C1052	C985	U922	G859	A794	G732	U667	C541	A478
G1369	U1243	G1306	G1243	A1177	G1115	C1053	G986	C923	U860	G794	G733	G668	C542	A479
U1370	G1244	A1307	G1244	C1177	G1116	A1054	G987	G924	A861	C797	A734	G669	C543	A480
G1371	G1245	G1308	G1245	C1179	G1117	G1055	A988	C925	G862	C798	A735	A670	G543	G481
U1372	A1246	G1309	A1246	C1180	C1118	G1056	G989	A926	A863	G799	C736	C673	A543D	A482
A1373	G1310	G1310	G1310	C1181	C1119	A1057	A990	G928	G864	G799	C737	C611	G550	A483
G1374	A1248	G1311	G1248	A1182	G1120	G1058	C991	G929	C865	A800	G738	G611A	G553	C484
C1375	U1249	U1312	G1249	G1183	C1121	G1059	C992	U930	A866	A801	G739	A675	U554	G487
C1376	G1250	U1313	G1250	G1184	G1122	U1060	G993	G931	C867	A802	U740	U611D	U555	G488
G1377	C1251	G1314	C1251	C1185	C1123	U1061	G994	G932	U868	U803	G741	G611E	G556	G489
A1378	G1252	C1315	G1252	G1186	C1124	G1062	A996	A933	A870	G805	G742	G681	G557	G491
A1379	A1253	U1316	A1253	G1187	G1125	G1063	G997	C936	U871	G806	G745	G682	U558	G492
G1380	U1254	A1317	A1254	U1188	A1126	C1064	C998	U937	A872	U807	G746	G683	G559	G493
G1383	U1255	C1318	U1255	A1189	A1127	U1065	U999	U937	G873	C806	G747	G684	G560	G494
A1384	C1257	A1321	C1257	G1190	A1128	U1066	A1001	G938	G874	U810	G748	A695	C561	G497
G1385	G1258	A1322	G1258	G1193	A1129	A1067	G1002	G940	G875	U811	C749	G686	U562	G498
C1386	U1323	G1324	G1259	A1194	U1130	G1068	C1003	G941	C876	C812	A750	U688	G563	G499
G1387	G1260	G1325	G1260	C1196	A1131	A1069	G1004	G942	U877	U813	G622	G689	G624	U499
G1388	G1325	G1325	G1325	G1196	U1133	G1071	C1005	U943	A878	C814	A752	G690	U566	G500

A2269	G2190	A2062	C1999	A1937	G1864B	A1803	G1712G	A1852	C1588	G1524	G1455	G1389
G2270	G2127	C2063	G2000	A1938	A1864C	C1804	A1712H	G1853	C1589	G1525		U1390
G2271	G2128	C2064	A2001	U1939	A1864D	U1805	U1712I	A1854	U1590	G1526	C1458	A1391
G2272	C2065	C2065	G2002	U1940	G1878	C1806	G1712J	A1855	G1591	G1527	A1459	A1392
C2275	G2130	C2066	G2003	C1941	C1979	G1807	G1712K	C1856	G1592	A1528	A1460	A1393
G2276	G2131	G2067	G2004	C1942	C1942	U1808	G1712L	C1857	G1593	A1529	G1461	U1394
G2277	U2132	U2068	A2005	U1943	C1882	A1809	C1712M	U1858	G1594	G1530	C1462	U1395
A2278	G2133	G2069	C2006	U1944	G1883	G1810	U1712N	U1859	G1595	C1531		U1396
G2279	A2134	G2070	C2007	U1945	A1884	A1811	G1712O	U1859	A1596	C1532	G1465	U1397
C2283	A2135	A2071	C2008	U1946	C1886	G1812	U1712P	U1859	A1597	C1533	G1466	C1398
C2284	C2136	G2072	C2009	C1947	C1887	G1813	C1712Q	U1859	C1598		C1467	C1399
C2285	C2137	C2073	G2012	G1948	C1888	A1815	G1750	C1662	C1599		G1468B	G1400
A2286	G2141	U2074	A2013	G1949	A1889	G1816	C1752	C1663	U1602	C1537		G1401
A2287	C2142	U2075	A2014	G1950	A1890	G1817		C1664	A1603	A1536	G1488B	
A2288	C2143	U2076	A2015	U1951	A1891	G1818	G1756	C1665	G1604	C1538	A1488C	U1406
A2288	U2144	A2077	U2016	A1952	G1891	A1819		G1666	C1605	G1540	G1468D	C1407
U2291	C2145	G2080	U2017	G1954	C1992	U1820	A1759	A1668	G1606	U1541	G1468E	C1408
C2292	C2146	C2081	G2018	U1955	C1895	A1821	A1760	C1670	G1607	G1542	G1468G	C1409
C2292	G2147	A2082	G2019	U1956	G1896	G1822	A1761	U1671	A1608	A1543		G1410
G2224	G2148	G2083	A2020	C1957	G1897	G1824	C1762	C1672	A1609	C1543A	G1488J	C1411
A2225	C2149	C2084	C2021	C1958	U1898	A1825	G1763	C1673	A1610	A1544	G1468K	A1412
C2226	U2150	G2085	U2022	G1959	G1899	G1826	G1764	C1674	C1611	A1545		G1413
C2297	G2151	U2086	U2022	A1960	A1900	G1826	C1765	C1675	C1612	C1546	G1483	G1414
G2228	G2152	G2087	G2024	A1961	A1901		U1766	A1676	G1613	C1547		U1415
G2229	C2153	G2088	G2025	C1962	C1902	A1829	C1767	C1678	C1615		A1486	G1416
G2300	G2154	U2089	G2026	U1963	G1903	G1830	U1768	U1679	G1551	C1551	G1487	C1417
C2301	G2155	G2090	G2027	G1964	G1904	G1831	U1769	U1680	G1552	G1552		G1418
G2302	C2156	U2091	G2028	C1965	C1905	G1832	G1770	G1681	A1553	A1490		A1419
G2303	G2157	G2092	U2029	A1966	G1906	U1833	C1771	G1619	A1554	G1491		U1420
G2304	G2158	A2096	A2030	C1967	G1907	U1834	G1772	C1686	G1555	G1492		G1421
A2305	G2159	U2096	A2031	G1968	C1908	G1835	U1773	U1687	C1556	C1493		G1422
G2306	G2160	U2097	G2032	A1969	C1909	G1836	C1774	U1688	U1621	A1494		G1423
G2307	C2161	U2098	U2033	A1970	G1910	C1837		A1690	G1622	A1495		
A2309	G2162	U2099	U2034	A1971	U1911	C1838	U1777	G1691	G1626	G1426		G1426
A2310	C2163	G2100	G2035	A1972	A1912	G1839	U1778	C1692	G1627	U1427		A1427
U2311	G2164	G2101	G2036	A1973	A1913	G1840	U1779	U1692	G1628	G1561		C1428
U2312	G2165	U2102	G2037	C1974	C1914	U1841	A1780	U1693	U1629	C1498		G1429
G2313	G2166	C2103	G2038	G1975	U1915	G1842	C1781	C1694	C1564	C1499		G1430
G2314	U2167	G2104	G2039		A1916	G1844	C1782	G1695	C1565	C1501		U1431
G2315	G2168	C2105	C2040		U1917	G1845	A1783	G1696	A1566	C1502		C1432
C2248	A2169	G2106	U2041	A1978	A1918	G1846	A1785	G1697	A1567	U1503		A1433
U2249	A2170	C2107	A2042	G1979	A1919	A1847	A1786	G1698	A1634	C1504		A1434
G2250	A2171	G2108	C2043	G1980	C1920	U1847	C1788	A1700	G1635	C1505		G1435
G2251	U2172	U2109	G2044	C1981	G1921	A1848	A1787	A1701	C1636	C1506		C1436
A2321	A2173	G2110	C2045	C1982	G1922	G1849	U1789	G1702	A1637	A1506A		U1438
A2322	C2174	G2111	G2046	G1983	C1923	G1850	A1789	G1703	C1638	A1506C		G1441
G2323	G2175	G2112	U2047	G1984	C1924	U1851	C1790	G1704	U1639	A1506D		G1444
G2324	C2176	U2113	G2048	G1985	C1925	G1852	A1791	G1705	C1640	A1506E		G1444
G2325	C2177	A2114	G2049	A1986	U1926	A1853	G1792		A1641	C1506F		G1444
U2257	C2178	G2115	G2050	G1987	A1927	A1854	C1793	U1709	G1642	U1576		G1444
A2328	C2179	G2116	A2051	C1990	A1928	G1855	U1794		G1643	C1506H		A1444A
G2329	U2180		G2052	U1991	G1929	G1856	C1795		C1644	U1577		C1445
G2330	G2181	U2109	G2053	G1992	G1930	G1857	U1796	C1712	A1580	A1579		G1448
U2331	G2182	G2120	C2055	U1993	U1931	A1858	G1797	U1712A	G1646	G1581		A1448A
U2332	G2121	G2121	G2056	C1994	U1932	A1859	U1798	G1712B	G1647	C1582		G1449
A2333	U2122	U2122		U1995	G1933	G1860	G1799	G1712C	C1648	A1583		C1450
G2334	G2123	G2123	A2059	C1996	C1934		C1800	G1712D	G1649	C1584		G1452
A2335	G2127	G2125	G2061	G1997	U1936	U1864	A1801	G1712E	A1586	G1650		A1453
A2336				G1998	A1936	G1864A	A1802	U1712F	U1651	U1506P		U1454

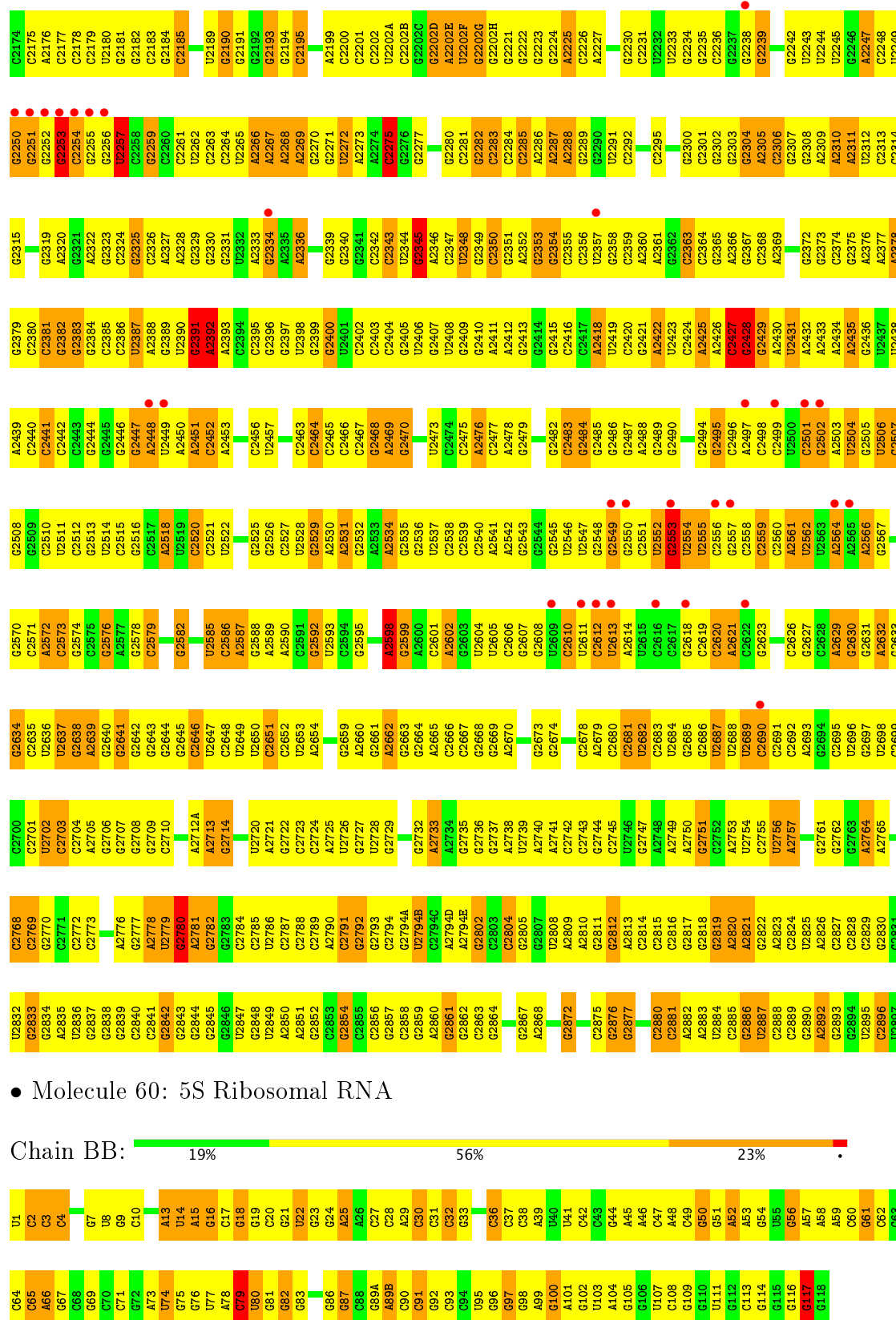


• Molecule 59: 23S Ribosomal RNA



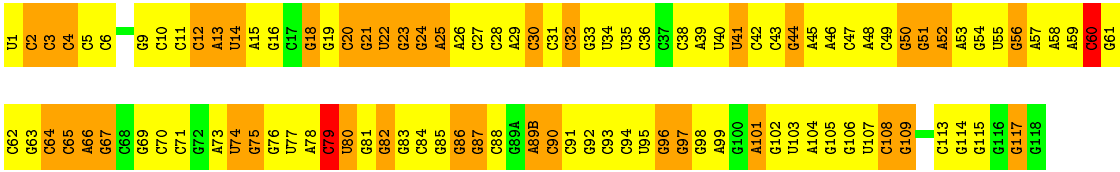
G1187	G1122	G1058	G993	U930	A866	G805	G745	G678	G611E	G553	G489	C420	G357F	A394
U1188	C1123	G1059	C994	G931	G869	C806	A746	C679	A611F	U554	G491	U421	A357G	C295
A1189	G1124	U1060	A995	A932	G870	U807	U747	G680	G611G	U555	A492	A422	G357H	C296
G1190	G1125	U1061	A996	G933	A870	U808	G748	G681	G617	G556	G493	A423	G357I	C297
G1191	A1126	G1062	G997	G934	U871	U809	C749	G682	C618	U557	G494		G357J	C298
G1192	A1127	G1063	G998	G935	U872	U810	A750	C683		G558	G495	U431	U357K	A299
G1193	A1128	C1064	U999	G936	G873	U811	A751	G684	A621	G559	G496	A432	A357L	A300
A1194	U1129	U1065	A1000	U937	G874	C812	A752	G685		C560	A497	C433	C357M	G301
G1195	U1130	A1001	A1001	G938	G875	U813	A753	G686	C624	G563	G498	U434	C357N	C302
G1196	C1135	A1067	G1002	G939	C876	C814	C754	G687	G625	G564	G499	C435	G357O	U305
G1197	U1196	G1068	G1003	G940	U877	C815	C755	U688	U626	C564	G500	G436	G370	U306
U1198	A1136	A1069	C1004	A941	G878	C816	C756	G689	A627	C565	A501	G437	A371	U307
U1199	G1137	A1070	G1005	G942	G879	C817	U757	G690	G628	C566	A502	G438	G372	G307
G1200	G1138	G1071	C1006	U943	G880	G818	C758	G691	G629	U567	A503	G440	U373	G308
C1201	G1139	A1072	C1007	G944	G881	A819	G759	C692	G630	U568	U504	U441	A374	G309
G1202	A1140	G1073	G1008	A945	G882	A820	G760	C693		U569	A505	G442	C375	A310
G1203	U1141	G1074	A1009	G946	G883	A821	A761	U694	A633	G571	G506	G443	C376	A311
A1204	U1141A	G1075	A1010	G947	C884	U822	U762		G634	A572	A507	C444	C377	G312
U1205	A1142	C1076	G1011	G948	C885	G823	G763	C697	C635	G573	G508	C445	C378	G317
G1206	A1143	A1077	U1012	G949	C886	A824	A764	C698	G636	G574	C509	C446	G379	C318
C1207	G1144	U1078	C1013	G950	A887	C825	G765	A699	G637	C574	C510	A447	U380	C319
G1208	C1145	C1079	G1014		C888	U826	U767	G700	G638	A575	U511	U448	G381	A320
G1209	C1146	C1080	U1015	G954	C889	U827	G768	G701	U639	U576	G512	U449	G382	A321
A1210		U1017	G1017	G955	A890	U928	G769	G702	C640	G577	A513	G450	U383	G321
G1211	G1149	U1081	G1018	G956	G892	A890	G770	U703	C641	G578	A514	C451	U384	A322
G1212	C1150	U1082	U1019	A957	C893	G831	G771	C708	A643	C580	C516		G386	G323
A1213	G1151	A1084	A1021	U958	C894	G832	C772	U709	A644	C581	C517	C455	U387	A324
C1214	C1152	A1085	G1022	A959	U895	U833	C773	G710	C645	G582	G518	C456	G388	U328
G1215	G1153	A1086	U1023	A960	A896	C834	U773	G711	C646	G583	U519	A457	G389	G329
G1216	G1154	G1087	G1024	C961	C897	A835	A774	G712	G647	C584	G520	U458	A390	A330
C1217	A1155	A1088	G1025	G962	C898	G836	G775	G713	G648	C585	G521	U459	G391	A331
G1218	A1156	U1026	U1026	U963	A899	C837	G776	G714	G649	A586	G522	A460	C392	
C1219	G1157	A1090	A1027	C964	A900	C838	A777	U714		C587	C523	C461	C393	C334
A1219A	U1158	A1028	G1028	C965	A901	U839	G778	G715	C850	C588	U524	C462	A394	C335
C1220	U1159	A1029	G1030	G966	C902	C840	U779	G716	U652	C589	U525	G463	U395	C336
G1221	G1160	U1095	G1031	C967	C903	G841	G780	G717	U652	C590	A526	U464	G396	C337
C1222	C1161	A1096	G1032	G968	C904	G842	A781	C719	U654	C591	C527	G465	G397	G338
G1223		U1097	A1032	U969	U905	G843	A782	C720	A655	G592	A528	A466	G398	U339
C1224	G1164	A1098	U1033	C970	G906	C844	A783	G721	G656	G593	A529	G467	G399	A340
G1225	U1165	G1099	G1034	C971	U907	G845	A784	G722	U657	U594	G530	G468	G400	G341
A1226	C1166	C1100	U1035	G972	C908	C846	G785	A722	U657	C595	C531	G469	A401	G342
G1227	U1167	U1101	G1036	A973	A909	U847	C786	G723	C658	G596	A532	A470	A402	C343
G1228	G1168	C1102	C1038	G974	A910	G848	U787	U724	C659	U597	G533		U403	G344
G1229	G1169	A1103	G1039	C974A	A911	A849	A788	G725	G660	G598	U534	G473	A345	A345
C1230	G1170	C1104	C1040	G975	C912	C850	A789		G661	G599	C535		U405	A346
G1231	U1105	G1171		C976	C915	U851	C790	G729	G662	G600		U475	G406	
G1232	G1172	G1106	C1043	G977	G916	G852	C791	G730	C665	G601	G538	U476	G407	G349
C1233	A1173	G1107	G1044		G917	G853	G792	C731	G666	G602	G539	A477	G408	
U1234	U1174	U1108	A1045	A980	A917	G854	A793	G732	U667	A803	C540	A478	C409	G352
G1235	G1175	C1109	A1046		A918	G855	G794	G733	G668	G604	C541	A479	G410	G353
	A1177	G1110	G1047	A983	G919	C856	C795	A734	G669	C605	C542	A480	G411	G354
G1238	C1178	A1111	A1048	A984	G920	C857	C796	A735	G670	C606	C543	A481	A412	G355
G1239	U1179	G1112	C985	C985	G921	U858	G797	C736	A670	U606	G543	A482	C413	G356
U1240	C1180	U1113	G986	G986	U922	G859	G798	C737	C671	U607	G543A	A483	C414	G357
A1241	C1181	G1114	C1052	G987	C923	U860	G799	G738	C672	A608	C543B	A484	A357	A357
A1242	A1182	G1115	C1053	A988	C924	A861	A800	G739	C673	A609	A543C	C484	A415	U357A
G1243	G1183	C1116	A1054	G989	C925	G862	G801	U740	G674	G610	A543D	C485	C416	A357B
G1244	C1184	U1055	G1055	A990	A926	A863	A802	G741	A675	C611	G550	C486	C417	G357C
G1245	C1185	G1056	G981	C991	G928	G864	U803	G742	A676	C611A	G551	C487	G418	G357D
A1246	G1186	A1057	C992	C992	G929	C865	A804	G744	A677		G552	G488	C419	U357E





• Molecule 60: 5S Ribosomal RNA

Chain DB: 11% 55% 33% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	306.92Å 677.00Å 356.78Å 90.00° 89.90° 90.00°	Depositor
Resolution (Å)	49.98 – 3.80 127.40 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.98-3.80) 60.2 (127.40-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.295 , 0.331 0.297 , 0.332	Depositor DCC
R_{free} test set	8483 reflections (1.98%)	DCC
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.17$, $\langle L^2 \rangle = 0.05$	Xtriage
Estimated twinning fraction	0.340 for h,-k,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	312066	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.41	0/1945	0.69	0/2621
1	CB	0.41	0/1945	0.69	1/2621 (0.0%)
2	AC	0.27	0/1645	0.55	0/2216
2	CC	0.29	0/1645	0.56	0/2216
3	AD	0.31	0/1733	0.59	0/2318
3	CD	0.29	0/1733	0.61	1/2318 (0.0%)
4	AE	0.30	0/1172	0.57	0/1576
4	CE	0.30	0/1172	0.61	1/1576 (0.1%)
5	AF	0.28	0/856	0.56	0/1154
5	CF	0.30	0/856	0.59	0/1154
6	AG	0.27	0/1276	0.51	0/1709
6	CG	0.28	0/1276	0.51	0/1709
7	AH	0.29	0/1136	0.60	0/1527
7	CH	0.28	0/1136	0.55	0/1527
8	AI	0.27	0/1029	0.56	0/1379
8	CI	0.27	0/1029	0.50	0/1379
9	AJ	0.27	0/815	0.54	0/1095
9	CJ	0.28	0/815	0.56	0/1095
10	AK	0.38	0/900	0.62	0/1213
10	CK	0.39	0/900	0.61	0/1213
11	AL	0.43	0/992	0.80	0/1327
11	CL	0.45	0/992	0.81	1/1327 (0.1%)
12	AM	0.27	0/1008	0.53	0/1347
12	CM	0.27	0/1008	0.58	0/1347
13	AN	0.29	0/501	0.51	0/664
13	CN	0.34	0/501	0.57	0/664
14	AO	0.34	0/745	0.61	0/992
14	CO	0.33	0/745	0.57	1/992 (0.1%)
15	AP	0.32	0/722	0.61	0/970
15	CP	0.32	0/722	0.60	0/970
16	AQ	0.35	0/848	0.67	1/1131 (0.1%)
16	CQ	0.36	0/848	0.68	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.29	0/579	0.58	0/768
17	CR	0.29	0/579	0.57	0/768
18	AS	0.29	0/647	0.56	0/870
18	CS	0.26	0/647	0.53	0/870
19	AT	0.30	0/765	0.54	0/1007
19	CT	0.31	0/765	0.51	0/1007
20	AY	0.37	0/5270	0.66	1/7135 (0.0%)
20	CY	0.36	0/5270	0.67	3/7135 (0.0%)
21	AA	0.39	9/36351 (0.0%)	1.12	149/56736 (0.3%)
21	CA	0.42	6/36351 (0.0%)	1.17	239/56736 (0.4%)
22	AW	0.52	0/1827	1.42	41/2845 (1.4%)
22	CW	0.48	0/1827	1.36	23/2845 (0.8%)
23	AV	1.27	1/881 (0.1%)	1.42	12/1372 (0.9%)
23	CV	0.82	7/880 (0.8%)	2.11	42/1372 (3.1%)
24	AX	0.62	1/1815 (0.1%)	1.56	47/2826 (1.7%)
24	CX	0.60	3/1815 (0.2%)	1.54	43/2826 (1.5%)
25	BC	0.51	1/1774 (0.1%)	0.86	2/2391 (0.1%)
25	DC	0.51	0/1774	0.80	0/2391
26	BD	0.40	2/2195 (0.1%)	0.62	1/2955 (0.0%)
26	DD	0.31	0/2195	0.60	0/2955
27	BE	0.35	0/1602	0.69	2/2160 (0.1%)
27	DE	0.33	0/1602	0.67	0/2160
28	BF	0.39	0/1663	0.81	6/2249 (0.3%)
28	DF	0.38	0/1663	0.78	4/2249 (0.2%)
29	BG	0.27	0/1499	0.54	0/2016
29	DG	0.29	0/1499	0.58	0/2016
30	BH	0.28	0/1298	0.58	0/1751
30	DH	0.28	0/1298	0.55	0/1751
32	BK	0.28	0/1054	0.55	1/1427 (0.1%)
32	DK	0.31	0/1054	0.58	1/1427 (0.1%)
33	BN	0.81	3/1141 (0.3%)	1.39	16/1537 (1.0%)
33	DN	0.81	2/1141 (0.2%)	1.28	13/1537 (0.8%)
34	BO	0.32	0/943	0.63	2/1269 (0.2%)
34	DO	0.32	0/943	0.65	0/1269
35	BP	0.28	0/1131	0.64	2/1504 (0.1%)
35	DP	0.29	0/1131	0.63	0/1504
36	BQ	0.36	0/1143	0.67	0/1527
36	DQ	0.33	0/1143	0.63	0/1527
37	BR	0.33	0/974	0.64	1/1302 (0.1%)
37	DR	0.32	0/974	0.59	0/1302
38	BS	0.35	0/783	0.69	0/1041
38	DS	0.36	0/783	0.71	0/1041
39	BT	0.30	0/1161	0.63	0/1549

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DT	0.30	0/1161	0.64	0/1549
40	BU	0.36	0/982	0.57	0/1306
40	DU	0.33	0/982	0.57	0/1306
41	BV	0.34	0/790	0.76	2/1057 (0.2%)
41	DV	0.31	0/790	0.65	1/1057 (0.1%)
42	BW	0.32	0/911	0.64	0/1220
42	DW	0.38	0/911	0.69	1/1220 (0.1%)
43	BX	0.28	0/748	0.56	1/1004 (0.1%)
43	DX	0.28	0/748	0.56	1/1004 (0.1%)
44	BY	0.28	0/831	0.54	0/1108
44	DY	0.27	0/831	0.57	1/1108 (0.1%)
45	BZ	0.28	0/1505	0.58	0/2042
45	DZ	0.29	0/1505	0.58	0/2042
46	B0	0.25	0/671	0.54	0/892
46	D0	0.25	0/671	0.50	0/892
47	B1	0.51	0/739	1.01	5/981 (0.5%)
47	D1	0.48	0/739	0.92	2/981 (0.2%)
48	B2	0.37	0/600	0.63	0/793
48	D2	0.34	0/600	0.65	0/793
49	B3	0.29	0/482	0.58	0/646
49	D3	0.26	0/482	0.58	0/646
50	B4	0.38	0/276	0.67	0/372
50	D4	0.37	0/276	0.68	0/372
51	B5	0.28	0/473	0.57	0/639
51	D5	0.32	0/473	0.62	0/639
52	B6	0.30	0/440	0.82	3/586 (0.5%)
52	D6	0.31	0/440	0.68	0/586
53	B7	1.14	6/438 (1.4%)	1.51	7/575 (1.2%)
53	D7	0.29	0/438	0.55	0/575
54	B8	0.31	0/525	0.58	0/691
54	D8	0.30	0/525	0.61	0/691
55	B9	0.28	0/310	0.55	0/407
55	D9	0.32	0/310	0.57	0/407
56	Be	0.25	0/538	0.53	0/715
56	De	0.27	0/538	0.51	0/715
59	BA	0.38	1/69437 (0.0%)	1.11	247/108401 (0.2%)
59	DA	0.40	2/69437 (0.0%)	1.14	333/108401 (0.3%)
60	BB	0.43	0/2853	1.28	29/4451 (0.7%)
60	DB	0.48	0/2853	1.34	49/4451 (1.1%)
All	All	0.40	44/334735 (0.0%)	1.04	1339/498724 (0.3%)

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	1
3	CD	0	1
10	AK	0	1
10	CK	0	1
15	AP	0	1
15	CP	0	1
20	AY	0	2
25	BC	0	6
25	DC	0	5
26	BD	0	1
26	DD	0	1
27	BE	0	1
28	BF	0	4
28	DF	0	2
29	DG	0	1
31	BJ	0	2
31	DJ	0	3
33	BN	0	17
33	DN	0	15
34	BO	0	1
34	DO	0	1
36	BQ	0	1
38	BS	0	1
38	DS	0	1
39	BT	0	1
39	DT	0	1
42	BW	0	1
42	DW	0	2
45	BZ	0	1
45	DZ	0	1
47	B1	0	4
47	D1	0	3
53	B7	0	1
All	All	0	86

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AV	1	G	P-O5'	35.77	1.95	1.59
53	B7	40	TRP	CD2-CE2	-12.82	1.25	1.41
21	AA	1126	U	C2-O2	-9.80	1.13	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	CA	1126	U	C2-O2	-9.32	1.14	1.22
53	B7	40	TRP	CE3-CZ3	8.92	1.53	1.38

The worst 5 of 1339 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AV	1	G	O5'-P-OP2	24.05	139.56	110.70
23	CV	10	G	N1-C6-O6	-22.12	106.63	119.90
21	AA	1126	U	N1-C2-N3	18.77	126.16	114.90
53	B7	40	TRP	CE2-CD2-CG	18.75	122.30	107.30
21	CA	1126	U	N1-C2-N3	18.50	126.00	114.90

There are no chirality outliers.

5 of 86 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	163	PHE	Peptide
10	AK	43	SER	Peptide
15	AP	34	GLU	Peptide
20	AY	34	TYR	Peptide
20	AY	630	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1910	0	1957	118	0
1	CB	1910	0	1957	112	0
2	AC	1621	0	1688	90	0
2	CC	1621	0	1688	85	0
3	AD	1703	0	1767	109	0
3	CD	1703	0	1767	92	0
4	AE	1156	0	1213	55	0
4	CE	1156	0	1213	57	0
5	AF	843	0	857	33	0
5	CF	843	0	857	49	0
6	AG	1257	0	1296	58	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	CG	1257	0	1296	61	0
7	AH	1116	0	1177	78	0
7	CH	1116	0	1177	76	0
8	AI	1010	0	1037	62	0
8	CI	1010	0	1037	59	0
9	AJ	802	0	849	48	0
9	CJ	802	0	849	57	0
10	AK	885	0	904	62	0
10	CK	885	0	904	63	0
11	AL	976	0	1062	107	0
11	CL	976	0	1062	105	0
12	AM	997	0	1072	35	0
12	CM	997	0	1072	68	0
13	AN	492	0	533	36	0
13	CN	492	0	533	40	0
14	AO	734	0	771	49	0
14	CO	734	0	771	32	0
15	AP	706	0	725	44	0
15	CP	706	0	725	45	0
16	AQ	835	0	904	69	0
16	CQ	835	0	904	63	0
17	AR	574	0	644	34	0
17	CR	574	0	644	35	0
18	AS	634	0	655	40	0
18	CS	634	0	655	28	0
19	AT	763	0	861	50	0
19	CT	763	0	861	44	0
20	AY	5173	0	5239	335	0
20	CY	5173	0	5239	330	0
21	AA	32474	0	16393	1202	0
21	CA	32474	0	16392	1570	0
22	AW	1635	0	831	83	0
22	CW	1635	0	831	86	0
23	AV	783	0	391	43	0
23	CV	781	0	393	75	0
24	AX	1629	0	832	75	0
24	CX	1629	0	832	93	0
25	BC	1742	0	1798	155	0
25	DC	1742	0	1798	126	0
26	BD	2145	0	2234	174	0
26	DD	2145	0	2234	154	0
27	BE	1569	0	1634	135	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	DE	1569	0	1634	124	0
28	BF	1628	0	1680	156	0
28	DF	1628	0	1680	128	0
29	BG	1474	0	1535	78	0
29	DG	1474	0	1535	102	0
30	BH	1274	0	1342	65	0
30	DH	1274	0	1342	75	0
31	BJ	851	0	207	26	0
31	DJ	851	0	207	18	0
32	BK	1035	0	1082	63	0
32	DK	1035	0	1082	72	0
33	BN	1114	0	1185	281	0
33	DN	1114	0	1185	309	0
34	BO	933	0	996	71	0
34	DO	933	0	996	60	0
35	BP	1114	0	1187	105	0
35	DP	1114	0	1187	106	0
36	BQ	1122	0	1179	91	0
36	DQ	1122	0	1179	85	0
37	BR	960	0	1021	85	0
37	DR	960	0	1021	85	0
38	BS	775	0	835	74	0
38	DS	775	0	835	82	0
39	BT	1147	0	1207	89	0
39	DT	1147	0	1207	92	0
40	BU	964	0	1022	77	0
40	DU	964	0	1022	69	0
41	BV	779	0	852	70	0
41	DV	779	0	852	54	0
42	BW	900	0	964	71	0
42	DW	900	0	964	58	0
43	BX	734	0	789	31	0
43	DX	734	0	789	28	0
44	BY	818	0	908	54	0
44	DY	818	0	908	62	0
45	BZ	1473	0	1497	85	0
45	DZ	1473	0	1497	80	0
46	B0	662	0	688	31	0
46	D0	662	0	688	47	0
47	B1	732	0	808	58	0
47	D1	732	0	808	67	0
48	B2	598	0	653	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	D2	598	0	653	52	0
49	B3	477	0	529	25	0
49	D3	477	0	529	29	0
50	B4	271	0	284	11	0
50	D4	271	0	284	21	0
51	B5	459	0	480	28	0
51	D5	459	0	480	36	0
52	B6	433	0	461	34	0
52	D6	433	0	461	43	0
53	B7	430	0	480	29	0
53	D7	430	0	480	33	0
54	B8	517	0	582	44	0
54	D8	517	0	582	43	0
55	B9	307	0	338	31	0
55	D9	307	0	338	26	0
56	Be	686	0	620	0	0
56	De	686	0	621	0	0
57	Bf	156	0	47	0	0
57	Bg	156	0	47	0	0
57	Df	156	0	48	0	0
57	Dg	156	0	46	0	0
58	Bh	151	0	41	0	0
58	Dh	151	0	48	0	0
59	BA	61997	0	31250	2492	0
59	DA	61997	0	31250	2828	0
60	BB	2551	0	1295	143	0
60	DB	2551	0	1295	164	0
61	AY	28	0	12	8	0
61	CY	28	0	12	14	0
62	AY	37	0	47	21	0
62	CY	37	0	47	14	0
63	AA	42	0	46	26	0
63	BA	126	0	138	60	0
63	CA	42	0	46	34	0
63	DA	42	0	46	23	0
64	BA	1	0	0	0	0
64	CY	1	0	0	0	0
All	All	312066	0	215233	14870	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

The worst 5 of 14870 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)
33:DN:114:ARG:HH21	59:DA:527:C:C1'	1.22	1.51
24:CX:75:C:N4	59:DA:2553:G:H1	1.11	1.47
59:DA:2681:C:N4	59:DA:2725:A:H62	1.09	1.47
33:DN:114:ARG:NH2	59:DA:527:C:H1'	1.12	1.44
21:CA:1538:C:C2	23:CV:7:G:N2	1.88	1.41

There are no symmetry-related clashes.

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%)	168 (72%)	45 (19%)	20 (9%)	1	16
1	CB	233/235 (99%)	171 (73%)	45 (19%)	17 (7%)	1	21
2	AC	205/207 (99%)	137 (67%)	39 (19%)	29 (14%)	0	5
2	CC	205/207 (99%)	150 (73%)	35 (17%)	20 (10%)	1	13
3	AD	206/208 (99%)	140 (68%)	41 (20%)	25 (12%)	0	7
3	CD	206/208 (99%)	152 (74%)	33 (16%)	21 (10%)	1	12
4	AE	149/151 (99%)	122 (82%)	20 (13%)	7 (5%)	3	31
4	CE	149/151 (99%)	115 (77%)	24 (16%)	10 (7%)	1	23
5	AF	99/101 (98%)	76 (77%)	15 (15%)	8 (8%)	1	17
5	CF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	1	15
6	AG	153/155 (99%)	123 (80%)	22 (14%)	8 (5%)	2	29
6	CG	153/155 (99%)	118 (77%)	23 (15%)	12 (8%)	1	19
7	AH	136/138 (99%)	102 (75%)	23 (17%)	11 (8%)	1	17
7	CH	136/138 (99%)	96 (71%)	30 (22%)	10 (7%)	1	20
8	AI	125/127 (98%)	97 (78%)	22 (18%)	6 (5%)	2	30
8	CI	125/127 (98%)	98 (78%)	21 (17%)	6 (5%)	2	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	97/99 (98%)	71 (73%)	15 (16%)	11 (11%)	0	9
9	CJ	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1	21
10	AK	117/119 (98%)	83 (71%)	21 (18%)	13 (11%)	0	9
10	CK	117/119 (98%)	79 (68%)	21 (18%)	17 (14%)	0	5
11	AL	123/125 (98%)	41 (33%)	44 (36%)	38 (31%)	0	0
11	CL	123/125 (98%)	49 (40%)	37 (30%)	37 (30%)	0	0
12	AM	123/125 (98%)	94 (76%)	19 (15%)	10 (8%)	1	17
12	CM	123/125 (98%)	95 (77%)	17 (14%)	11 (9%)	1	15
13	AN	58/60 (97%)	38 (66%)	17 (29%)	3 (5%)	2	29
13	CN	58/60 (97%)	35 (60%)	14 (24%)	9 (16%)	0	4
14	AO	86/88 (98%)	72 (84%)	12 (14%)	2 (2%)	7	46
14	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	4	38
15	AP	82/84 (98%)	58 (71%)	16 (20%)	8 (10%)	1	13
15	CP	82/84 (98%)	62 (76%)	13 (16%)	7 (8%)	1	16
16	AQ	98/100 (98%)	70 (71%)	22 (22%)	6 (6%)	2	25
16	CQ	98/100 (98%)	76 (78%)	16 (16%)	6 (6%)	2	25
17	AR	68/70 (97%)	50 (74%)	9 (13%)	9 (13%)	0	6
17	CR	68/70 (97%)	56 (82%)	8 (12%)	4 (6%)	2	26
18	AS	77/79 (98%)	43 (56%)	23 (30%)	11 (14%)	0	5
18	CS	77/79 (98%)	47 (61%)	27 (35%)	3 (4%)	3	35
19	AT	97/99 (98%)	72 (74%)	17 (18%)	8 (8%)	1	17
19	CT	97/99 (98%)	82 (84%)	10 (10%)	5 (5%)	2	29
20	AY	657/687 (96%)	407 (62%)	174 (26%)	76 (12%)	0	8
20	CY	657/687 (96%)	437 (66%)	135 (20%)	85 (13%)	0	6
25	BC	226/228 (99%)	107 (47%)	63 (28%)	56 (25%)	0	1
25	DC	226/228 (99%)	114 (50%)	52 (23%)	60 (26%)	0	1
26	BD	273/275 (99%)	174 (64%)	60 (22%)	39 (14%)	0	5
26	DD	273/275 (99%)	180 (66%)	59 (22%)	34 (12%)	0	7
27	BE	203/205 (99%)	134 (66%)	41 (20%)	28 (14%)	0	5
27	DE	203/205 (99%)	124 (61%)	49 (24%)	30 (15%)	0	5
28	BF	206/208 (99%)	139 (68%)	43 (21%)	24 (12%)	0	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	DF	206/208 (99%)	127 (62%)	51 (25%)	28 (14%)	0	5
29	BG	179/181 (99%)	131 (73%)	37 (21%)	11 (6%)	2	25
29	DG	179/181 (99%)	127 (71%)	37 (21%)	15 (8%)	1	16
30	BH	165/167 (99%)	117 (71%)	31 (19%)	17 (10%)	0	11
30	DH	165/167 (99%)	116 (70%)	30 (18%)	19 (12%)	0	8
32	BK	138/140 (99%)	91 (66%)	32 (23%)	15 (11%)	0	10
32	DK	138/140 (99%)	77 (56%)	44 (32%)	17 (12%)	0	7
33	BN	137/139 (99%)	52 (38%)	32 (23%)	53 (39%)	0	0
33	DN	137/139 (99%)	55 (40%)	28 (20%)	54 (39%)	0	0
34	BO	120/122 (98%)	89 (74%)	21 (18%)	10 (8%)	1	17
34	DO	120/122 (98%)	86 (72%)	22 (18%)	12 (10%)	1	12
35	BP	144/146 (99%)	84 (58%)	36 (25%)	24 (17%)	0	4
35	DP	144/146 (99%)	82 (57%)	39 (27%)	23 (16%)	0	4
36	BQ	139/141 (99%)	84 (60%)	35 (25%)	20 (14%)	0	5
36	DQ	139/141 (99%)	94 (68%)	34 (24%)	11 (8%)	1	18
37	BR	115/117 (98%)	80 (70%)	20 (17%)	15 (13%)	0	6
37	DR	115/117 (98%)	80 (70%)	22 (19%)	13 (11%)	0	9
38	BS	97/99 (98%)	52 (54%)	26 (27%)	19 (20%)	0	2
38	DS	97/99 (98%)	51 (53%)	27 (28%)	19 (20%)	0	2
39	BT	136/138 (99%)	81 (60%)	27 (20%)	28 (21%)	0	2
39	DT	136/138 (99%)	79 (58%)	31 (23%)	26 (19%)	0	2
40	BU	115/117 (98%)	88 (76%)	17 (15%)	10 (9%)	1	16
40	DU	115/117 (98%)	90 (78%)	17 (15%)	8 (7%)	1	22
41	BV	99/101 (98%)	56 (57%)	28 (28%)	15 (15%)	0	5
41	DV	99/101 (98%)	64 (65%)	21 (21%)	14 (14%)	0	5
42	BW	111/113 (98%)	74 (67%)	25 (22%)	12 (11%)	0	10
42	DW	111/113 (98%)	76 (68%)	23 (21%)	12 (11%)	0	10
43	BX	91/93 (98%)	71 (78%)	13 (14%)	7 (8%)	1	19
43	DX	91/93 (98%)	67 (74%)	10 (11%)	14 (15%)	0	4
44	BY	105/107 (98%)	54 (51%)	31 (30%)	20 (19%)	0	2
44	DY	105/107 (98%)	59 (56%)	26 (25%)	20 (19%)	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BZ	183/185 (99%)	121 (66%)	43 (24%)	19 (10%)	0	11
45	DZ	183/185 (99%)	109 (60%)	45 (25%)	29 (16%)	0	4
46	B0	82/84 (98%)	63 (77%)	14 (17%)	5 (6%)	2	25
46	D0	82/84 (98%)	59 (72%)	18 (22%)	5 (6%)	2	25
47	B1	91/93 (98%)	48 (53%)	24 (26%)	19 (21%)	0	2
47	D1	91/93 (98%)	52 (57%)	20 (22%)	19 (21%)	0	2
48	B2	69/71 (97%)	51 (74%)	12 (17%)	6 (9%)	1	16
48	D2	69/71 (97%)	53 (77%)	12 (17%)	4 (6%)	2	27
49	B3	58/60 (97%)	49 (84%)	7 (12%)	2 (3%)	4	38
49	D3	58/60 (97%)	47 (81%)	8 (14%)	3 (5%)	2	29
50	B4	33/35 (94%)	15 (46%)	13 (39%)	5 (15%)	0	5
50	D4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	5
51	B5	57/59 (97%)	36 (63%)	14 (25%)	7 (12%)	0	7
51	D5	57/59 (97%)	38 (67%)	6 (10%)	13 (23%)	0	1
52	B6	48/50 (96%)	24 (50%)	15 (31%)	9 (19%)	0	2
52	D6	48/50 (96%)	20 (42%)	17 (35%)	11 (23%)	0	1
53	B7	47/49 (96%)	33 (70%)	11 (23%)	3 (6%)	1	25
53	D7	47/49 (96%)	26 (55%)	14 (30%)	7 (15%)	0	5
54	B8	62/64 (97%)	34 (55%)	16 (26%)	12 (19%)	0	2
54	D8	62/64 (97%)	35 (56%)	13 (21%)	14 (23%)	0	1
55	B9	35/37 (95%)	29 (83%)	5 (14%)	1 (3%)	5	41
55	D9	35/37 (95%)	25 (71%)	7 (20%)	3 (9%)	1	16
56	Be	70/103 (68%)	39 (56%)	23 (33%)	8 (11%)	0	9
56	De	70/103 (68%)	40 (57%)	17 (24%)	13 (19%)	0	2
All	All	13246/13568 (98%)	8764 (66%)	2800 (21%)	1682 (13%)	0	7

5 of 1682 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	76	GLN
1	AB	190	THR
2	AC	12	LEU
2	AC	110	ASN
2	AC	130	VAL

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%)	163 (80%)	40 (20%)	1	12
1	CB	203/203 (100%)	158 (78%)	45 (22%)	1	8
2	AC	161/161 (100%)	129 (80%)	32 (20%)	1	11
2	CC	161/161 (100%)	128 (80%)	33 (20%)	1	10
3	AD	180/180 (100%)	142 (79%)	38 (21%)	1	10
3	CD	180/180 (100%)	148 (82%)	32 (18%)	2	16
4	AE	116/116 (100%)	92 (79%)	24 (21%)	1	10
4	CE	116/116 (100%)	89 (77%)	27 (23%)	1	7
5	AF	90/90 (100%)	73 (81%)	17 (19%)	2	13
5	CF	90/90 (100%)	77 (86%)	13 (14%)	4	25
6	AG	126/126 (100%)	111 (88%)	15 (12%)	6	32
6	CG	126/126 (100%)	110 (87%)	16 (13%)	5	29
7	AH	119/119 (100%)	98 (82%)	21 (18%)	2	16
7	CH	119/119 (100%)	94 (79%)	25 (21%)	1	10
8	AI	98/98 (100%)	83 (85%)	15 (15%)	3	22
8	CI	98/98 (100%)	78 (80%)	20 (20%)	1	11
9	AJ	89/89 (100%)	71 (80%)	18 (20%)	1	11
9	CJ	89/89 (100%)	68 (76%)	21 (24%)	1	7
10	AK	90/90 (100%)	80 (89%)	10 (11%)	7	35
10	CK	90/90 (100%)	79 (88%)	11 (12%)	6	30
11	AL	104/104 (100%)	82 (79%)	22 (21%)	1	9
11	CL	104/104 (100%)	82 (79%)	22 (21%)	1	9
12	AM	100/100 (100%)	84 (84%)	16 (16%)	3	20
12	CM	100/100 (100%)	79 (79%)	21 (21%)	1	10
13	AN	49/49 (100%)	40 (82%)	9 (18%)	2	14
13	CN	49/49 (100%)	38 (78%)	11 (22%)	1	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	79/79 (100%)	61 (77%)	18 (23%)	1	8
14	CO	79/79 (100%)	68 (86%)	11 (14%)	4	27
15	AP	72/72 (100%)	68 (94%)	4 (6%)	25	62
15	CP	72/72 (100%)	60 (83%)	12 (17%)	2	19
16	AQ	95/95 (100%)	80 (84%)	15 (16%)	3	21
16	CQ	95/95 (100%)	81 (85%)	14 (15%)	3	24
17	AR	61/61 (100%)	49 (80%)	12 (20%)	1	12
17	CR	61/61 (100%)	54 (88%)	7 (12%)	6	34
18	AS	69/69 (100%)	52 (75%)	17 (25%)	1	6
18	CS	69/69 (100%)	53 (77%)	16 (23%)	1	7
19	AT	76/76 (100%)	64 (84%)	12 (16%)	3	21
19	CT	76/76 (100%)	58 (76%)	18 (24%)	1	6
20	AY	558/579 (96%)	450 (81%)	108 (19%)	1	12
20	CY	558/579 (96%)	446 (80%)	112 (20%)	1	11
25	BC	180/180 (100%)	130 (72%)	50 (28%)	0	4
25	DC	180/180 (100%)	146 (81%)	34 (19%)	2	13
26	BD	217/217 (100%)	182 (84%)	35 (16%)	3	20
26	DD	217/217 (100%)	173 (80%)	44 (20%)	1	11
27	BE	165/165 (100%)	134 (81%)	31 (19%)	2	13
27	DE	165/165 (100%)	127 (77%)	38 (23%)	1	7
28	BF	165/165 (100%)	129 (78%)	36 (22%)	1	9
28	DF	165/165 (100%)	132 (80%)	33 (20%)	1	11
29	BG	155/155 (100%)	140 (90%)	15 (10%)	9	40
29	DG	155/155 (100%)	131 (84%)	24 (16%)	3	22
30	BH	136/136 (100%)	111 (82%)	25 (18%)	2	14
30	DH	136/136 (100%)	117 (86%)	19 (14%)	4	26
32	BK	105/105 (100%)	77 (73%)	28 (27%)	0	4
32	DK	105/105 (100%)	81 (77%)	24 (23%)	1	7
33	BN	118/118 (100%)	88 (75%)	30 (25%)	0	5
33	DN	118/118 (100%)	84 (71%)	34 (29%)	0	3
34	BO	100/100 (100%)	79 (79%)	21 (21%)	1	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DO	100/100 (100%)	82 (82%)	18 (18%)	2	15
35	BP	112/112 (100%)	84 (75%)	28 (25%)	1	6
35	DP	112/112 (100%)	88 (79%)	24 (21%)	1	9
36	BQ	111/111 (100%)	78 (70%)	33 (30%)	0	3
36	DQ	111/111 (100%)	91 (82%)	20 (18%)	2	15
37	BR	100/100 (100%)	82 (82%)	18 (18%)	2	15
37	DR	100/100 (100%)	78 (78%)	22 (22%)	1	8
38	BS	77/77 (100%)	64 (83%)	13 (17%)	2	18
38	DS	77/77 (100%)	58 (75%)	19 (25%)	1	6
39	BT	120/120 (100%)	93 (78%)	27 (22%)	1	8
39	DT	120/120 (100%)	91 (76%)	29 (24%)	1	6
40	BU	93/93 (100%)	78 (84%)	15 (16%)	3	20
40	DU	93/93 (100%)	76 (82%)	17 (18%)	2	14
41	BV	82/82 (100%)	59 (72%)	23 (28%)	0	4
41	DV	82/82 (100%)	68 (83%)	14 (17%)	2	18
42	BW	92/92 (100%)	79 (86%)	13 (14%)	4	26
42	DW	92/92 (100%)	72 (78%)	20 (22%)	1	9
43	BX	75/75 (100%)	58 (77%)	17 (23%)	1	8
43	DX	75/75 (100%)	59 (79%)	16 (21%)	1	9
44	BY	88/88 (100%)	65 (74%)	23 (26%)	0	5
44	DY	88/88 (100%)	74 (84%)	14 (16%)	3	21
45	BZ	162/162 (100%)	127 (78%)	35 (22%)	1	9
45	DZ	162/162 (100%)	135 (83%)	27 (17%)	2	19
46	B0	66/66 (100%)	59 (89%)	7 (11%)	8	37
46	D0	66/66 (100%)	53 (80%)	13 (20%)	1	12
47	B1	78/78 (100%)	56 (72%)	22 (28%)	0	3
47	D1	78/78 (100%)	57 (73%)	21 (27%)	0	4
48	B2	66/66 (100%)	56 (85%)	10 (15%)	3	22
48	D2	66/66 (100%)	57 (86%)	9 (14%)	4	27
49	B3	52/52 (100%)	44 (85%)	8 (15%)	3	22
49	D3	52/52 (100%)	45 (86%)	7 (14%)	4	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B4	31/31 (100%)	23 (74%)	8 (26%)	0	5
50	D4	31/31 (100%)	22 (71%)	9 (29%)	0	3
51	B5	51/51 (100%)	38 (74%)	13 (26%)	0	5
51	D5	51/51 (100%)	45 (88%)	6 (12%)	6	32
52	B6	49/49 (100%)	35 (71%)	14 (29%)	0	3
52	D6	49/49 (100%)	31 (63%)	18 (37%)	0	0
53	B7	42/42 (100%)	35 (83%)	7 (17%)	2	19
53	D7	42/42 (100%)	36 (86%)	6 (14%)	4	25
54	B8	54/54 (100%)	45 (83%)	9 (17%)	2	19
54	D8	54/54 (100%)	42 (78%)	12 (22%)	1	8
55	B9	34/34 (100%)	26 (76%)	8 (24%)	1	7
55	D9	34/34 (100%)	31 (91%)	3 (9%)	12	46
56	Be	54/54 (100%)	48 (89%)	6 (11%)	7	35
56	De	54/54 (100%)	47 (87%)	7 (13%)	5	28
All	All	11130/11172 (100%)	8951 (80%)	2179 (20%)	1	12

5 of 2179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	B0	80	HIS
4	CE	112	LEU
43	DX	23	GLU
48	B2	44	LEU
1	CB	121	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
3	CD	125	HIS
12	CM	101	GLN
44	DY	68	HIS
5	CF	7	ASN
10	CK	116	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1510/1511 (99%)	358 (23%)	16 (1%)
21	CA	1511/1511 (100%)	377 (24%)	16 (1%)
22	AW	76/77 (98%)	37 (48%)	1 (1%)
22	CW	76/77 (98%)	42 (55%)	2 (2%)
23	AV	35/36 (97%)	24 (68%)	9 (25%)
23	CV	35/36 (97%)	27 (77%)	7 (20%)
24	AX	75/78 (96%)	29 (38%)	1 (1%)
24	CX	75/78 (96%)	30 (40%)	0
59	BA	2878/2879 (99%)	748 (25%)	28 (0%)
59	DA	2878/2879 (99%)	715 (24%)	29 (1%)
60	BB	118/119 (99%)	27 (22%)	0
60	DB	118/119 (99%)	32 (27%)	0
All	All	9385/9400 (99%)	2446 (26%)	109 (1%)

5 of 2446 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	G
21	AA	9	G
21	AA	31	G
21	AA	32	A

5 of 109 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
59	BA	2250	G
21	CA	748	C
59	DA	2438	U
59	BA	2422	A
21	CA	5	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
63	NMY	AA	1601	-	45,45,45	0.58	0	59,67,67	1.00	4 (6%)
61	GDP	AY	701	-	25,30,30	1.30	3 (12%)	26,47,47	2.27	8 (30%)
62	FUA	AY	702	-	37,40,40	1.70	6 (16%)	45,64,64	1.72	6 (13%)
63	NMY	BA	2902	-	45,45,45	0.58	0	59,67,67	1.00	4 (6%)
63	NMY	BA	2903	-	45,45,45	0.60	0	59,67,67	1.00	4 (6%)
63	NMY	BA	2904	-	45,45,45	0.58	0	59,67,67	1.00	4 (6%)
63	NMY	CA	1601	-	45,45,45	0.58	0	59,67,67	1.00	4 (6%)
61	GDP	CY	701	-	25,30,30	1.26	3 (12%)	26,47,47	2.11	7 (26%)
62	FUA	CY	702	-	37,40,40	1.71	6 (16%)	45,64,64	1.72	6 (13%)
63	NMY	DA	2901	-	45,45,45	0.58	0	59,67,67	1.00	4 (6%)

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
63	NMY	AA	1601	-	-	1/18/94/94	0/4/4/4
61	GDP	AY	701	-	-	0/12/32/32	0/3/3/3
62	FUA	AY	702	-	-	0/10/92/92	0/4/4/4
63	NMY	BA	2902	-	-	1/18/94/94	0/4/4/4
63	NMY	BA	2903	-	-	1/18/94/94	0/4/4/4
63	NMY	BA	2904	-	-	1/18/94/94	0/4/4/4
63	NMY	CA	1601	-	-	1/18/94/94	0/4/4/4
61	GDP	CY	701	-	-	0/12/32/32	0/3/3/3
62	FUA	CY	702	-	-	0/10/92/92	0/4/4/4
63	NMY	DA	2901	-	-	1/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	CY	702	FUA	C23-C22	-6.41	1.39	1.51
62	AY	702	FUA	C23-C22	-6.32	1.40	1.51
62	AY	702	FUA	C23-C24	-4.15	1.39	1.53
62	CY	702	FUA	C23-C24	-4.13	1.39	1.53
62	AY	702	FUA	C24-C25	-3.13	1.39	1.50

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AY	701	GDP	N3-C2-N1	-5.60	119.28	127.46
61	CY	701	GDP	N3-C2-N1	-4.84	120.39	127.46
62	CY	702	FUA	C13-C12-C11	-4.40	105.84	111.97
62	AY	702	FUA	C13-C12-C11	-4.39	105.87	111.97
62	AY	702	FUA	C16-O2-C31	-3.85	111.13	117.10

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	BA	2903	NMY	C15-O18-C18-C19
63	CA	1601	NMY	C15-O18-C18-C19
63	AA	1601	NMY	C15-O18-C18-C19
63	BA	2902	NMY	C15-O18-C18-C19
63	DA	2901	NMY	C15-O18-C18-C19

There are no ring outliers.

10 monomers are involved in 199 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	AA	1601	NMY	26	0
61	AY	701	GDP	8	0
62	AY	702	FUA	21	0
63	BA	2902	NMY	13	0
63	BA	2903	NMY	15	0
63	BA	2904	NMY	32	0
63	CA	1601	NMY	34	0
61	CY	701	GDP	14	0
62	CY	702	FUA	14	0
63	DA	2901	NMY	23	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	AB	235/235 (100%)	-0.03	11 (4%)	32	25	17, 55, 103, 129	0
1	CB	235/235 (100%)	-0.01	14 (5%)	23	16	17, 63, 111, 140	0
2	AC	207/207 (100%)	0.65	37 (17%)	2	2	18, 52, 99, 118	0
2	CC	207/207 (100%)	0.02	12 (5%)	24	18	15, 58, 99, 132	0
3	AD	208/208 (100%)	-0.00	10 (4%)	31	25	14, 59, 107, 137	0
3	CD	208/208 (100%)	0.86	38 (18%)	1	2	20, 52, 102, 136	0
4	AE	151/151 (100%)	0.58	27 (17%)	2	2	26, 62, 96, 129	0
4	CE	151/151 (100%)	1.12	40 (26%)	1	1	19, 56, 99, 143	0
5	AF	101/101 (100%)	-0.19	0	100	100	22, 57, 111, 128	0
5	CF	101/101 (100%)	-0.31	2 (1%)	65	56	19, 56, 106, 128	0
6	AG	155/155 (100%)	0.16	11 (7%)	17	12	26, 78, 122, 150	0
6	CG	155/155 (100%)	-0.31	5 (3%)	48	38	38, 85, 120, 147	0
7	AH	138/138 (100%)	0.15	9 (6%)	20	14	16, 43, 87, 109	0
7	CH	138/138 (100%)	0.15	7 (5%)	29	23	10, 49, 86, 102	0
8	AI	127/127 (100%)	0.53	14 (11%)	6	6	30, 64, 101, 127	0
8	CI	127/127 (100%)	0.65	21 (16%)	2	3	9, 77, 108, 134	0
9	AJ	99/99 (100%)	0.99	23 (23%)	1	1	34, 64, 104, 146	0
9	CJ	99/99 (100%)	0.97	24 (24%)	1	1	22, 57, 107, 115	0
10	AK	119/119 (100%)	0.80	20 (16%)	2	2	13, 74, 139, 160	0
10	CK	119/119 (100%)	1.58	43 (36%)	0	1	21, 71, 125, 161	0
11	AL	125/125 (100%)	0.90	20 (16%)	2	3	15, 73, 145, 164	0
11	CL	125/125 (100%)	0.82	20 (16%)	2	3	27, 85, 148, 170	0
12	AM	125/125 (100%)	0.78	16 (12%)	4	5	43, 86, 129, 159	0
12	CM	125/125 (100%)	0.77	27 (21%)	1	1	27, 63, 103, 139	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	2.27	33 (55%)	0 1	33, 70, 116, 128	0
13	CN	60/60 (100%)	1.53	20 (33%)	0 1	30, 58, 105, 128	0
14	AO	88/88 (100%)	-0.13	2 (2%)	61 51	26, 53, 99, 110	0
14	CO	88/88 (100%)	-0.12	1 (1%)	80 72	8, 44, 84, 109	0
15	AP	84/84 (100%)	1.00	18 (21%)	1 1	33, 71, 110, 143	0
15	CP	84/84 (100%)	0.47	9 (10%)	7 6	39, 69, 111, 165	0
16	AQ	100/100 (100%)	1.02	25 (25%)	1 1	27, 62, 107, 131	0
16	CQ	100/100 (100%)	0.70	14 (14%)	3 4	22, 66, 120, 135	0
17	AR	70/70 (100%)	0.42	6 (8%)	11 9	19, 61, 102, 130	0
17	CR	70/70 (100%)	0.34	8 (11%)	6 6	24, 56, 100, 125	0
18	AS	79/79 (100%)	0.25	6 (7%)	15 11	17, 69, 111, 124	0
18	CS	79/79 (100%)	1.01	16 (20%)	1 2	28, 65, 108, 130	0
19	AT	99/99 (100%)	0.33	2 (2%)	65 56	17, 51, 85, 128	0
19	CT	99/99 (100%)	0.62	15 (15%)	2 3	26, 69, 110, 139	0
20	AY	661/687 (96%)	-0.26	20 (3%)	51 40	19, 64, 113, 178	0
20	CY	661/687 (96%)	-0.28	11 (1%)	70 61	11, 66, 108, 152	0
21	AA	1511/1511 (100%)	0.07	40 (2%)	56 46	10, 90, 161, 248	0
21	CA	1511/1511 (100%)	-0.00	23 (1%)	74 65	10, 88, 160, 242	0
22	AW	77/77 (100%)	-0.08	0	100 100	15, 71, 130, 150	0
22	CW	77/77 (100%)	-0.18	0	100 100	30, 88, 145, 178	0
23	AV	36/36 (100%)	0.33	0	100 100	32, 89, 137, 186	0
23	CV	36/36 (100%)	0.59	3 (8%)	12 10	23, 139, 232, 237	0
24	AX	77/78 (98%)	0.67	6 (7%)	14 11	3, 65, 233, 320	0
24	CX	77/78 (98%)	0.82	9 (11%)	5 5	37, 123, 185, 285	0
25	BC	228/228 (100%)	0.44	24 (10%)	7 6	55, 104, 139, 159	0
25	DC	228/228 (100%)	0.43	29 (12%)	4 5	37, 90, 130, 169	0
26	BD	275/275 (100%)	1.52	97 (35%)	0 1	10, 61, 103, 125	0
26	DD	275/275 (100%)	0.90	51 (18%)	1 2	16, 57, 100, 127	0
27	BE	205/205 (100%)	1.46	64 (31%)	0 1	21, 60, 107, 131	0
27	DE	205/205 (100%)	1.18	58 (28%)	1 1	22, 57, 97, 142	0
28	BF	208/208 (100%)	0.53	26 (12%)	4 5	20, 67, 108, 149	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	DF	208/208 (100%)	0.75	45 (21%)	1 1	23, 75, 120, 140	0
29	BG	181/181 (100%)	-0.09	5 (2%)	53 43	28, 69, 113, 148	0
29	DG	181/181 (100%)	-0.22	4 (2%)	62 53	25, 71, 113, 148	0
30	BH	167/167 (100%)	0.35	21 (12%)	4 5	29, 65, 108, 121	0
30	DH	167/167 (100%)	0.09	8 (4%)	31 25	24, 59, 100, 132	0
31	BJ	0/170	-	-	-	-	-
31	DJ	0/170	-	-	-	-	-
32	BK	140/140 (100%)	-0.32	0	100 100	32, 71, 114, 126	0
32	DK	140/140 (100%)	0.23	17 (12%)	5 5	34, 77, 113, 138	0
33	BN	139/139 (100%)	1.86	49 (35%)	0 1	23, 105, 298, 334	0
33	DN	139/139 (100%)	2.99	59 (42%)	0 1	16, 116, 252, 312	0
34	BO	122/122 (100%)	0.98	27 (22%)	1 1	12, 50, 93, 111	0
34	DO	122/122 (100%)	1.17	28 (22%)	1 1	28, 59, 103, 132	0
35	BP	146/146 (100%)	0.16	10 (6%)	18 13	25, 63, 106, 123	0
35	DP	146/146 (100%)	0.29	14 (9%)	9 7	25, 67, 104, 131	0
36	BQ	141/141 (100%)	1.30	36 (25%)	1 1	5, 54, 93, 109	0
36	DQ	141/141 (100%)	1.81	53 (37%)	0 1	27, 70, 113, 141	0
37	BR	117/117 (100%)	0.63	13 (11%)	6 6	29, 65, 116, 145	0
37	DR	117/117 (100%)	0.88	21 (17%)	2 2	27, 62, 97, 126	0
38	BS	99/99 (100%)	0.68	14 (14%)	3 4	14, 70, 108, 117	0
38	DS	99/99 (100%)	0.74	12 (12%)	5 5	19, 52, 96, 120	0
39	BT	138/138 (100%)	0.35	19 (13%)	3 4	16, 59, 101, 123	0
39	DT	138/138 (100%)	0.12	16 (11%)	5 5	15, 51, 109, 140	0
40	BU	117/117 (100%)	0.31	5 (4%)	36 28	20, 56, 96, 121	0
40	DU	117/117 (100%)	0.14	0	100 100	13, 53, 94, 142	0
41	BV	101/101 (100%)	0.74	15 (14%)	3 3	21, 66, 108, 127	0
41	DV	101/101 (100%)	0.49	7 (6%)	18 13	15, 65, 101, 126	0
42	BW	113/113 (100%)	0.65	18 (15%)	2 3	13, 54, 99, 111	0
42	DW	113/113 (100%)	0.37	11 (9%)	8 7	15, 64, 116, 148	0
43	BX	93/93 (100%)	1.04	19 (20%)	1 2	20, 54, 96, 115	0
43	DX	93/93 (100%)	0.77	13 (13%)	3 4	13, 45, 87, 126	0
44	BY	107/107 (100%)	0.76	21 (19%)	1 2	29, 58, 109, 149	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DY	107/107 (100%)	1.46	37 (34%) 0 1	25, 62, 97, 138	0
45	BZ	185/185 (100%)	-0.25	3 (1%) 72 63	17, 58, 97, 113	0
45	DZ	185/185 (100%)	-0.05	11 (5%) 23 17	33, 64, 101, 138	0
46	B0	84/84 (100%)	2.12	41 (48%) 0 1	26, 75, 117, 131	0
46	D0	84/84 (100%)	1.70	26 (30%) 0 1	19, 65, 108, 116	0
47	B1	93/93 (100%)	1.26	25 (26%) 1 1	21, 84, 140, 156	0
47	D1	93/93 (100%)	2.03	33 (35%) 0 1	31, 103, 148, 181	0
48	B2	71/71 (100%)	-0.02	1 (1%) 75 67	23, 55, 95, 116	0
48	D2	71/71 (100%)	0.26	3 (4%) 37 29	35, 61, 103, 118	0
49	B3	60/60 (100%)	-0.08	1 (1%) 70 61	29, 60, 99, 112	0
49	D3	60/60 (100%)	0.14	5 (8%) 12 10	36, 68, 94, 110	0
50	B4	35/35 (100%)	0.42	5 (14%) 3 3	27, 71, 110, 122	0
50	D4	35/35 (100%)	-0.32	0 100 100	64, 109, 144, 185	0
51	B5	59/59 (100%)	0.76	14 (23%) 1 1	25, 63, 106, 123	0
51	D5	59/59 (100%)	0.55	10 (16%) 2 2	31, 68, 113, 138	0
52	B6	50/50 (100%)	0.76	15 (30%) 1 1	13, 57, 107, 154	0
52	D6	50/50 (100%)	0.27	7 (14%) 3 4	26, 65, 120, 154	0
53	B7	49/49 (100%)	1.88	17 (34%) 0 1	46, 91, 136, 164	0
53	D7	49/49 (100%)	2.00	21 (42%) 0 1	51, 73, 109, 134	0
54	B8	64/64 (100%)	2.66	44 (68%) 0 1	26, 58, 109, 132	0
54	D8	64/64 (100%)	3.01	45 (70%) 0 0	30, 64, 104, 118	0
55	B9	37/37 (100%)	1.79	16 (43%) 0 1	39, 64, 109, 116	0
55	D9	37/37 (100%)	0.71	5 (13%) 3 4	34, 65, 116, 134	0
56	Be	72/103 (69%)	-0.09	3 (4%) 37 29	15, 49, 122, 163	0
56	De	72/103 (69%)	-0.00	5 (6%) 18 13	14, 57, 118, 157	0
57	Bf	0/31	-	-	-	-
57	Bg	0/31	-	-	-	-
57	Df	0/31	-	-	-	-
57	Dg	0/31	-	-	-	-
58	Bh	0/30	-	-	-	-
58	Dh	0/30	-	-	-	-
59	BA	2879/2879 (100%)	0.21	111 (3%) 40 32	11, 89, 164, 284	0
59	DA	2879/2879 (100%)	0.24	123 (4%) 36 28	9, 88, 171, 274	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	BB	119/119 (100%)	-0.38	0 100 100	18, 80, 158, 172	0
60	DB	119/119 (100%)	-0.28	0 100 100	30, 88, 150, 175	0
All	All	22852/23492 (97%)	0.39	2294 (10%) 8 7	3, 73, 146, 334	0

The worst 5 of 2294 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	DN	108	PRO	21.8
33	DN	81	GLY	18.9
33	DN	95	PRO	15.6
33	DN	86	PRO	14.8
33	DN	107	LEU	14.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
62	FUA	AY	702	37/37	0.74	0.63	4.35	198,199,200,201	0
62	FUA	CY	702	37/37	0.80	0.64	3.75	194,196,197,197	0
63	NMY	AA	1601	42/42	0.76	0.43	3.18	16,27,36,38	42
63	NMY	BA	2902	42/42	0.74	0.44	1.86	14,24,43,44	42
63	NMY	CA	1601	42/42	0.82	0.34	1.54	14,25,34,37	42
61	GDP	CY	701	28/28	0.77	0.21	1.41	104,108,109,110	0
63	NMY	DA	2901	42/42	0.77	0.37	1.29	31,42,51,53	42
61	GDP	AY	701	28/28	0.69	0.24	1.01	179,183,185,185	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
63	NMY	BA	2903	42/42	0.74	0.56	0.76	18,29,38,41	42
63	NMY	BA	2904	42/42	0.67	0.52	0.71	42,50,59,62	42
64	MG	CY	703	1/1	0.91	0.19	-0.08	6,6,6,6	0
64	MG	BA	2901	1/1	0.56	0.14	-1.28	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.