



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2023 – 05:04 PM EDT

PDB ID : 4V50  
Title : Crystal Structure of Ribosome with messenger RNA and the Anticodon stem-loop of P-site tRNA.  
Authors : Berk, V.; Zhang, W.; Pai, R.D.; Cate, J.H.D.  
Deposited on : 2006-08-16  
Resolution : 3.22 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

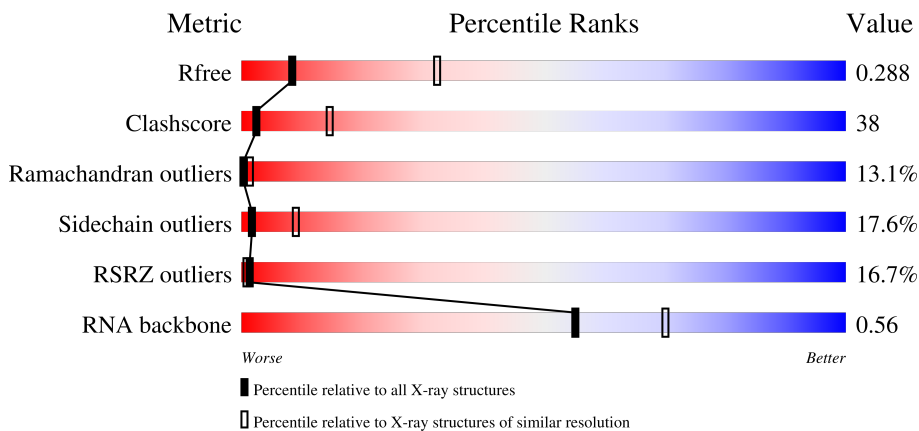
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.22 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))
$R_{free}$	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)
RNA backbone	3102	1023 (3.54-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	AA	1542	
1	CA	1542	
2	AW	17	
2	CW	17	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AX	6	100% 17% 50% 33%
3	CX	6	50% 17% 50% 33%
4	AB	240	54% 17% 54% 18% 9%
4	CB	240	57% 11% 55% 22% 9%
5	AC	232	55% 22% 51% 13% 11%
5	CC	232	42% 16% 52% 19% 11%
6	AD	205	39% 32% 50% 16%
6	CD	205	39% 20% 55% 23%
7	AE	166	49% 25% 52% 13% 10%
7	CE	166	38% 14% 55% 19% 10%
8	AF	135	19% 20% 41% 11% 26%
8	CF	135	21% 13% 45% 14% 26%
9	AG	178	35% 20% 47% 17% 16%
9	CG	178	7% 20% 43% 20% 16%
10	AH	129	10% 26% 53% 19%
10	CH	129	% 18% 58% 24%
11	AI	129	9% 16% 59% 21%
11	CI	129	2% 17% 62% 19%
12	AJ	103	46% 23% 50% 21% 5%
12	CJ	103	27% 13% 62% 18% 5%
13	AK	128	84% 23% 54% 15% 9%
13	CK	128	41% 18% 62% 11% 9%
14	AL	123	71% 20% 59% 21%
14	CL	123	41% 24% 57% 15%
15	AM	117	5% 22% 55% 18%

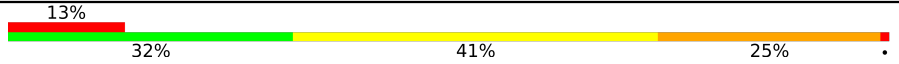
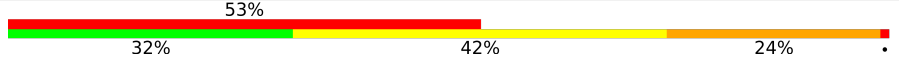
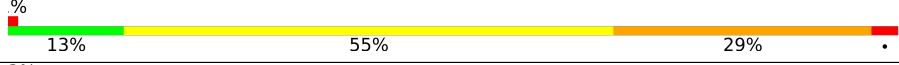
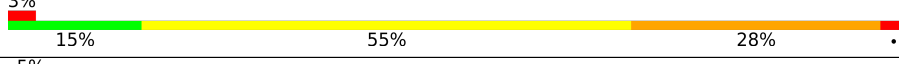
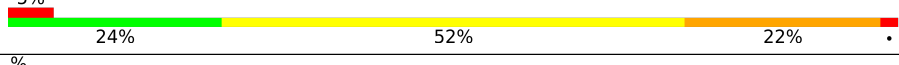
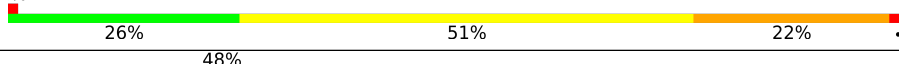



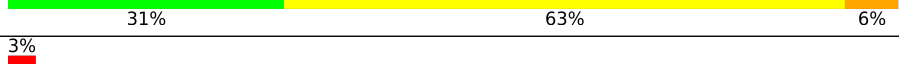
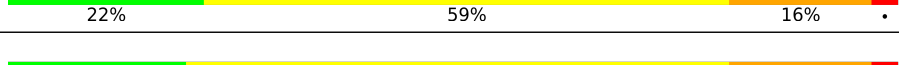
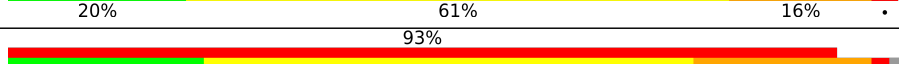
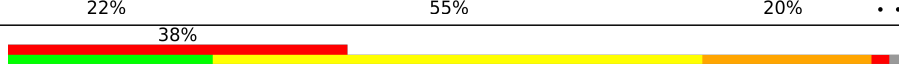
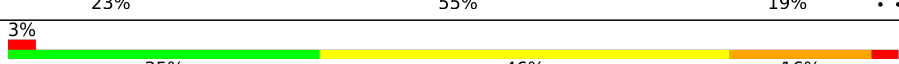

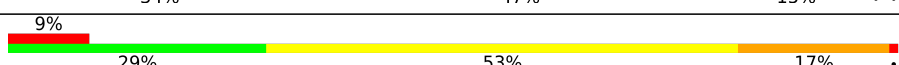
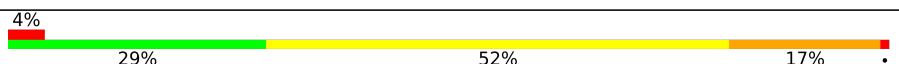
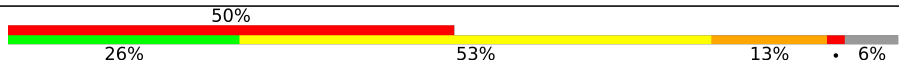
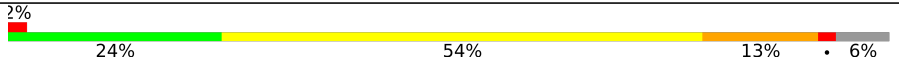


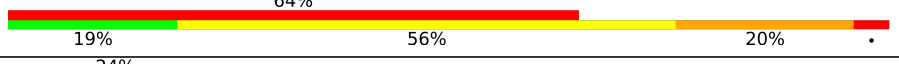
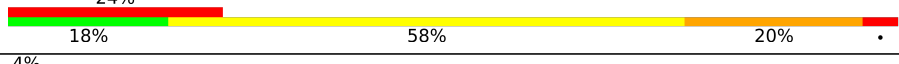
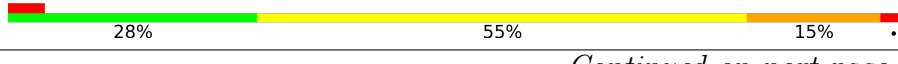

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CM	117	2% 14% 59% 21% . .
16	AN	100	19% 18% 60% 17% . .
16	CN	100	21% 11% 63% 20% . .
17	AO	88	5% 35% 53% 11%
17	CO	88	5% 33% 57% 10%
18	AP	82	18% 60% 21% .
18	CP	82	22% 62% 12% . .
19	AQ	83	% 13% 63% 18% . .
19	CQ	83	24% 57% 16% .
20	AR	74	47% 9% 47% 18% 26%
20	CR	74	32% 20% 46% 8% 26%
21	AS	91	9% 30% 38% 16% . 13%
21	CS	91	4% 14% 52% 19% . 13%
22	AT	86	38% 47% 14% .
22	CT	86	38% 48% 13% .
23	AU	70	61% 14% 39% 17% . 27%
23	CU	70	26% 14% 37% 20% . 27%
24	BA	120	4% 30% 58% 9% .
24	DA	120	% 32% 55% 10% .
25	BB	2904	4% 29% 58% 10% . .
25	DB	2904	2% 29% 59% 10% . .
26	BC	272	45% 30% 53% 15% .
26	DC	272	32% 29% 54% 15% .
27	BD	209	45% 23% 51% 25%
27	DD	209	5% 24% 51% 24% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	BE	201	
28	DE	201	
29	BF	178	
29	DF	178	
30	BG	176	
30	DG	176	
31	BH	149	
31	DH	149	
32	BI	141	
32	DI	141	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN	127	
38	BO	117	
38	DO	117	
39	BP	114	
39	DP	114	
40	BQ	117	



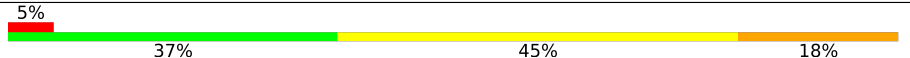
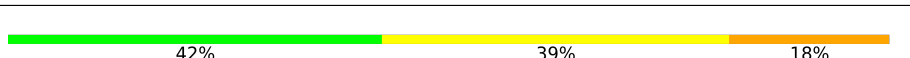
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DQ	117	9% 28% 55% 15% .
41	BR	103	% 17% 67% 14% .
41	DR	103	3% 17% 67% 13% .
42	BS	110	84% 28% 53% 16% .
42	DS	110	18% 27% 53% 17% .
43	BT	100	14% 24% 46% 20% . 7%
43	DT	100	10% 18% 53% 19% . 7%
44	BU	103	47% 21% 56% 19% ..
44	DU	103	3% 24% 54% 18% ..
45	BV	94	% 34% 53% 12% .
45	DV	94	4% 34% 51% 14% .
46	BW	84	% 20% 40% 29% 5% 6%
46	DW	84	% 18% 43% 30% . 6%
47	BX	77	14% 25% 61% 10% .
47	DX	77	17% 26% 60% 10% .
48	BY	63	16% 19% 57% 19% 5%
48	DY	63	3% 24% 52% 19% 5%
49	BZ	58	31% 57% 12%
49	DZ	58	31% 57% 12%
50	B0	56	50% 29% 48% 23%
50	D0	56	2% 27% 52% 21%
51	B1	54	13% 30% 54% 6% . 7%
51	D1	54	11% 28% 52% 9% . 7%
52	B2	46	39% 33% 52% 13% .
52	D2	46	24% 35% 52% 11% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	B3	64	
53	D3	64	
54	B4	38	
54	D4	38	

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
55	MG	AA	1611	-	-	-	X
55	MG	AA	1614	-	-	-	X
55	MG	AA	1626	-	-	-	X
55	MG	AA	1637	-	-	-	X
55	MG	AA	1643	-	-	-	X
55	MG	AA	1658	-	-	-	X
55	MG	BB	3057	-	-	-	X
55	MG	BB	3093	-	-	-	X
55	MG	CA	1640	-	-	-	X
55	MG	CA	1646	-	-	-	X
55	MG	DB	3052	-	-	-	X

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 285033 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1530	Total 32831	C 14642	N 6024	O 10635	P 1530	0	0	0
1	CA	1530	Total 32831	C 14642	N 6024	O 10635	P 1530	0	0	0

- Molecule 2 is a RNA chain called PHE TRNA (UNMODIFIED BASES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AW	17	Total 360	C 161	N 64	O 118	P 17	0	0	0
2	CW	17	Total 360	C 161	N 64	O 118	P 17	0	0	0

- Molecule 3 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	AX	6	Total 125	C 56	N 18	O 45	P 6	0	0	0
3	CX	6	Total 125	C 56	N 18	O 45	P 6	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AB	218	Total 1704	C 1081	N 305	O 311	S 7	0	0	0
4	CB	218	Total 1704	C 1081	N 305	O 311	S 7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S3.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
5	CC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
6	CD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
7	CE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
8	CF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
9	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	CH	129	979	616	173	184	6	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AI	127	1022	634	206	179	3	0	0	0
11	CI	127	1022	634	206	179	3	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AJ	98	786	493	150	142	1	0	0	0
12	CJ	98	786	493	150	142	1	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AK	117	877	540	174	160	3	0	0	0
13	CK	117	877	540	174	160	3	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AL	123	955	590	196	165	4	0	0	0
14	CL	123	955	590	196	165	4	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AM	114	883	546	178	156	3	0	0	0
15	CM	113	876	541	177	155	3	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
16	CN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			
17	CO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
18	CP	80	Total	C	N	O	S	0	0	0
			638	400	126	111	1			

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
19	CQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
20	CR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
21	CS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
22	CT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 23 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
23	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
24	DA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
25	DB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	DC	271	2082	1288	423	364	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	BD	209	1565	979	288	294	4	0	0	0
27	DD	209	1565	979	288	294	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	BE	201	1552	974	283	290	5	0	0	0
28	DE	201	1552	974	283	290	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	BF	178	1420	905	251	258	6	0	0	0
29	DF	178	1420	905	251	258	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	BG	176	1323	832	243	246	2	0	0	0
30	DG	176	1323	832	243	246	2	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	BH	149	1111	699	197	214	1	0	0	0
31	DH	149	1111	699	197	214	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
32	DI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
33	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			
34	DK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
35	DL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
36	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
37	DN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BO	116	Total	C	N	O	S	0	0	0
			892	552	178	162				
38	DO	116	Total	C	N	O	S	0	0	0
			892	552	178	162				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
39	DP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				
40	DQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
41	DR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	DS	110	857	532	166	156	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	BT	93	738	466	139	131	2	0	0	0
43	DT	93	738	466	139	131	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				
44	BU	102	779	492	146	141		0	0	0
44	DU	102	779	492	146	141		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BV	94	753	479	137	134	3	0	0	0
45	DV	94	753	479	137	134	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	BW	79	596	367	120	108	1	0	0	0
46	DW	79	596	367	120	108	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	BX	77	625	388	129	106	2	0	0	0
47	DX	77	625	388	129	106	2	0	0	0



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	BY	63	Total 509	C 313	N 99	O 95	S 2	0	0	0
48	DY	63	Total 509	C 313	N 99	O 95	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	BZ	58	Total 449	C 281	N 87	O 79	S 2	0	0	0
49	DZ	58	Total 449	C 281	N 87	O 79	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	B0	56	Total 444	C 269	N 94	O 80	S 1	0	0	0
50	D0	56	Total 444	C 269	N 94	O 80	S 1	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
51	B1	50	Total 409	C 263	N 75	O 71	0	0	0
51	D1	50	Total 409	C 263	N 75	O 71	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	B2	46	Total 377	C 228	N 90	O 57	S 2	0	0	0
52	D2	46	Total 377	C 228	N 90	O 57	S 2	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
53	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
54	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	60	Total	Mg	0	0
			60	60		
55	AX	2	Total	Mg	0	0
			2	2		
55	BB	118	Total	Mg	0	0
			118	118		
55	BJ	1	Total	Mg	0	0
			1	1		
55	CA	56	Total	Mg	0	0
			56	56		
55	CX	1	Total	Mg	0	0
			1	1		
55	CN	1	Total	Mg	0	0
			1	1		
55	DB	119	Total	Mg	0	0
			119	119		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B4	1	Total	Zn	0	0
			1	1		
56	D4	1	Total	Zn	0	0
			1	1		

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	287	Total O 287 287	0	0
57	AX	9	Total O 9 9	0	0
57	AE	3	Total O 3 3	0	0
57	AI	1	Total O 1 1	0	0
57	AK	2	Total O 2 2	0	0
57	AL	2	Total O 2 2	0	0
57	AN	1	Total O 1 1	0	0
57	AP	1	Total O 1 1	0	0
57	AT	2	Total O 2 2	0	0
57	BB	532	Total O 532 532	0	0
57	BC	7	Total O 7 7	0	0
57	BE	3	Total O 3 3	0	0
57	BH	3	Total O 3 3	0	0
57	BJ	3	Total O 3 3	0	0
57	BL	2	Total O 2 2	0	0
57	BN	3	Total O 3 3	0	0
57	B2	1	Total O 1 1	0	0
57	B4	5	Total O 5 5	0	0
57	CA	264	Total O 264 264	0	0
57	CX	6	Total O 6 6	0	0
57	CE	2	Total O 2 2	0	0
57	CI	3	Total O 3 3	0	0

*Continued on next page...*

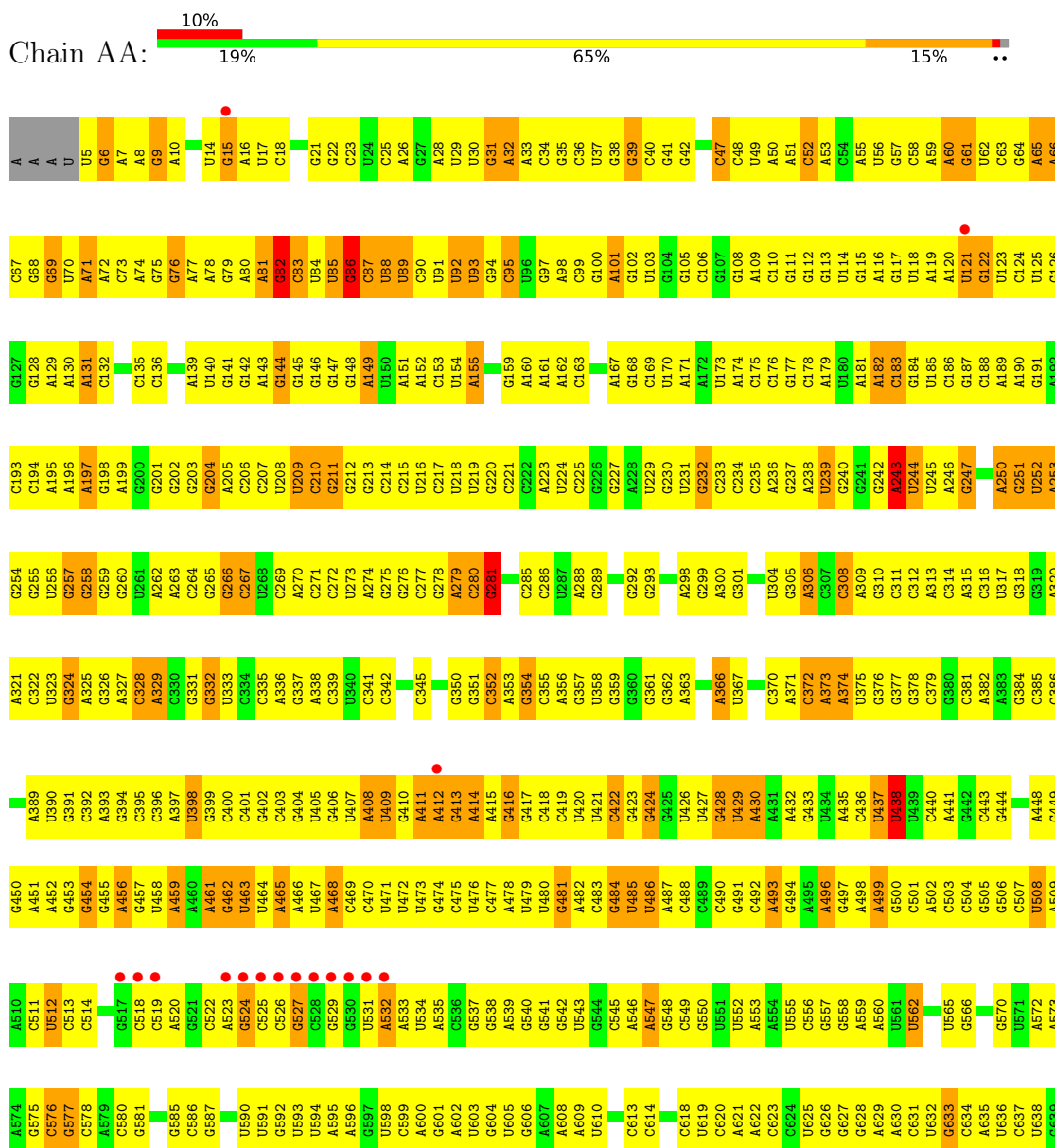
*Continued from previous page...*

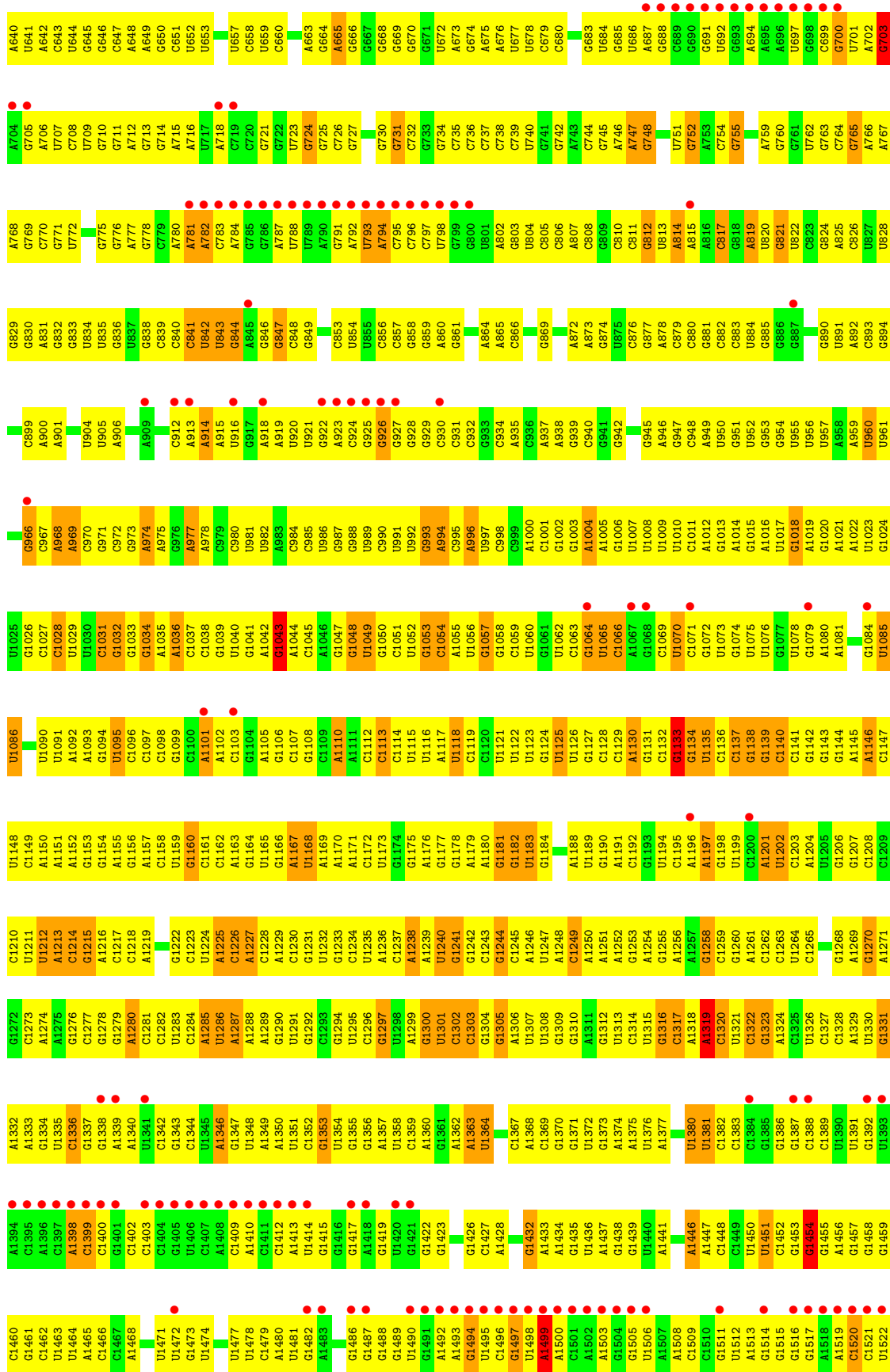
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	CL	1	Total O 1 1	0	0
57	CN	1	Total O 1 1	0	0
57	CP	1	Total O 1 1	0	0
57	CT	3	Total O 3 3	0	0
57	CU	1	Total O 1 1	0	0
57	DB	531	Total O 531 531	0	0
57	DC	7	Total O 7 7	0	0
57	DD	1	Total O 1 1	0	0
57	DE	3	Total O 3 3	0	0
57	DJ	2	Total O 2 2	0	0
57	DL	3	Total O 3 3	0	0
57	DN	3	Total O 3 3	0	0
57	DT	1	Total O 1 1	0	0
57	D2	1	Total O 1 1	0	0
57	D4	4	Total O 4 4	0	0

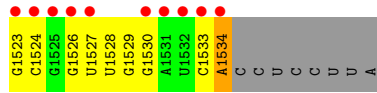
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

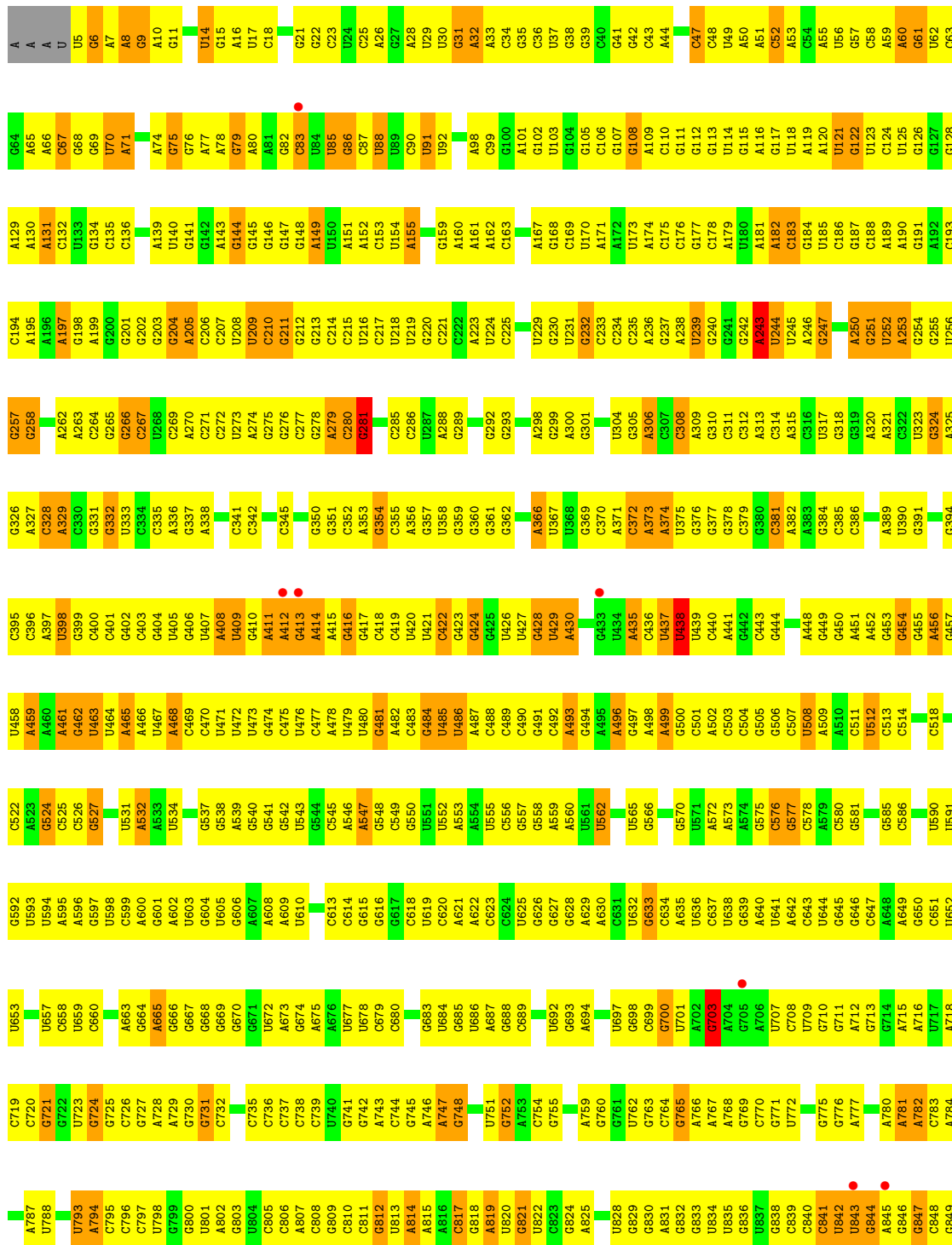
- Molecule 1: 16S ribosomal RNA

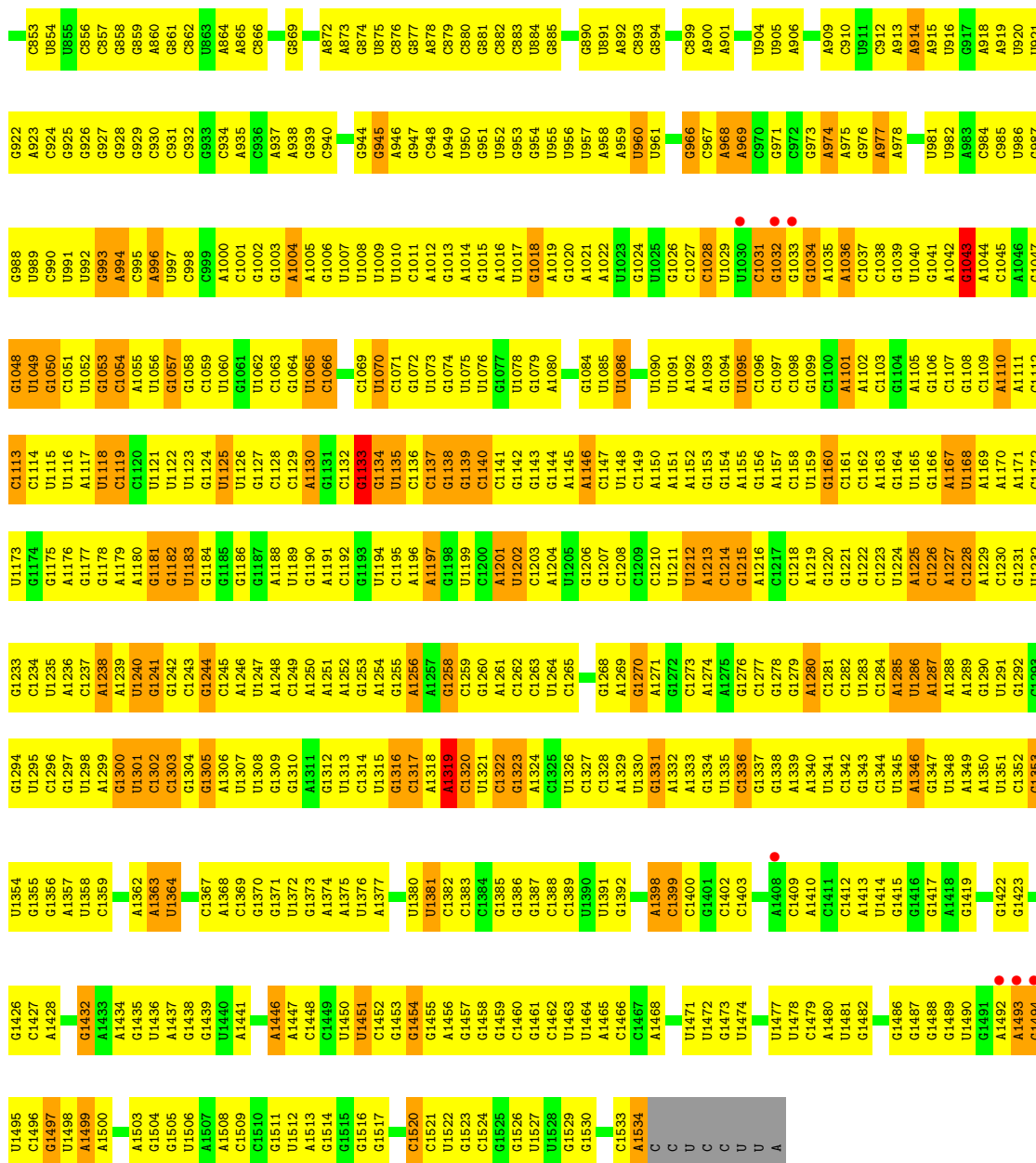




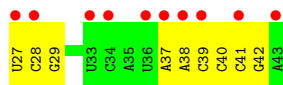


● Molecule 1: 16S ribosomal RNA





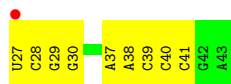
● Molecule 2: PHE TRNA (UNMODIFIED BASES)



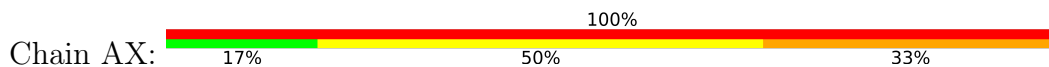
● Molecule 2: PHE TRNA (UNMODIFIED BASES)



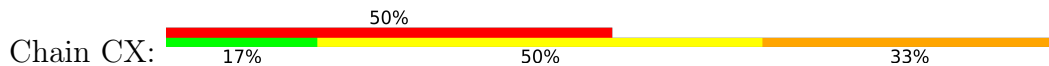




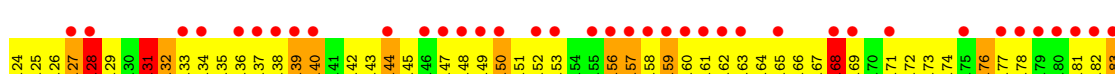
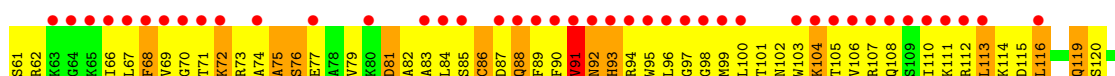
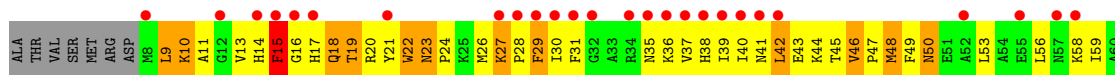
• Molecule 3: MRNA



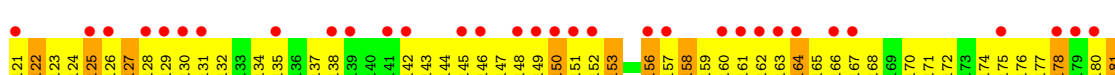
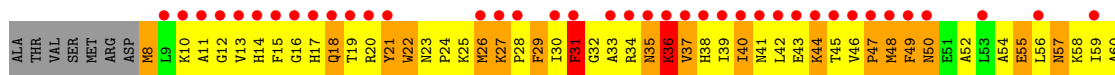
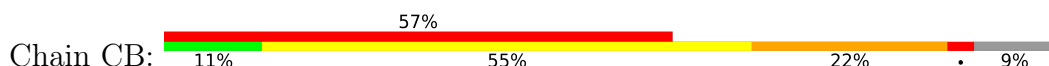
• Molecule 3: MRNA

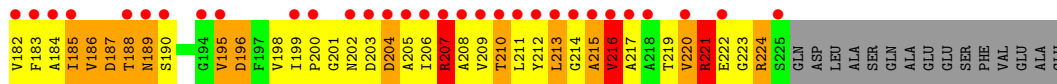


• Molecule 4: 30S ribosomal protein S2

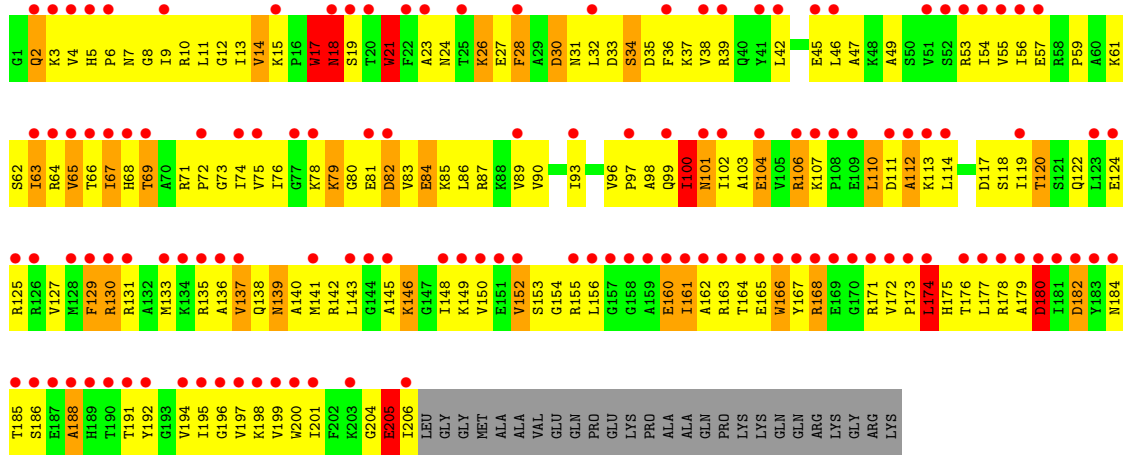


• Molecule 4: 30S ribosomal protein S2

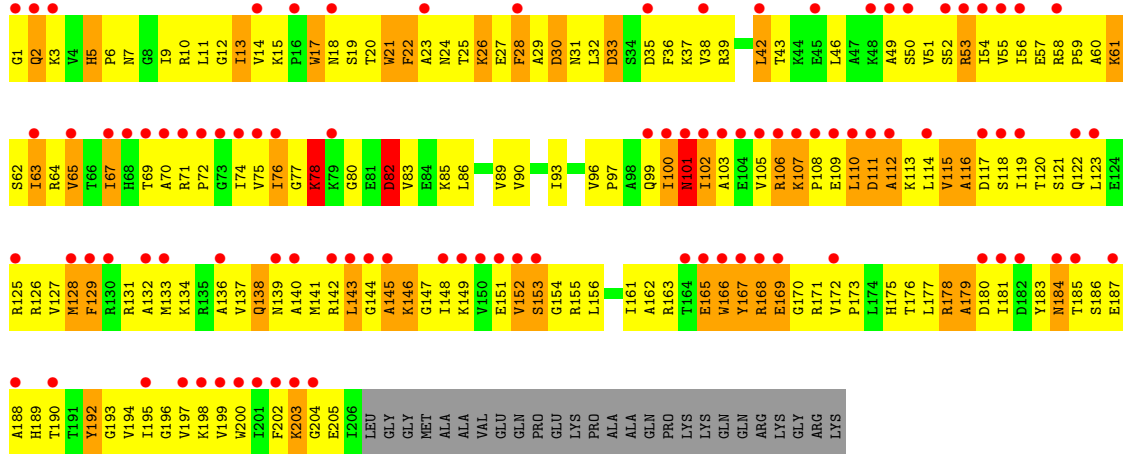
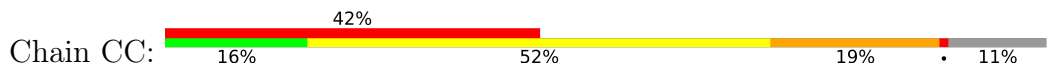




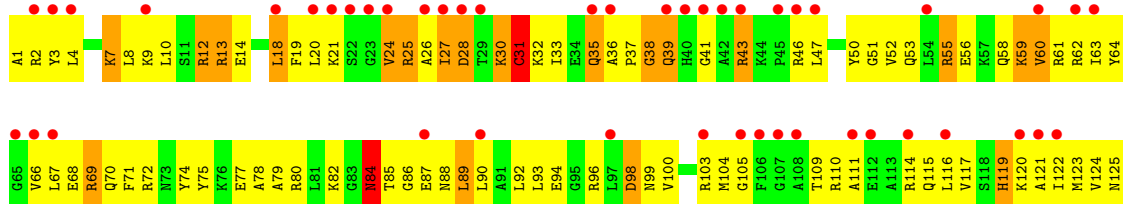
• Molecule 5: 30S ribosomal protein S3

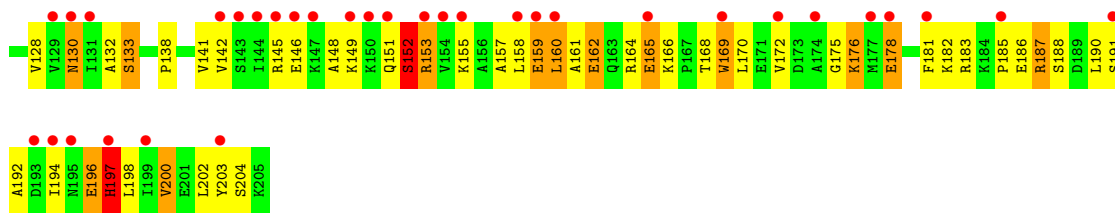


• Molecule 5: 30S ribosomal protein S3

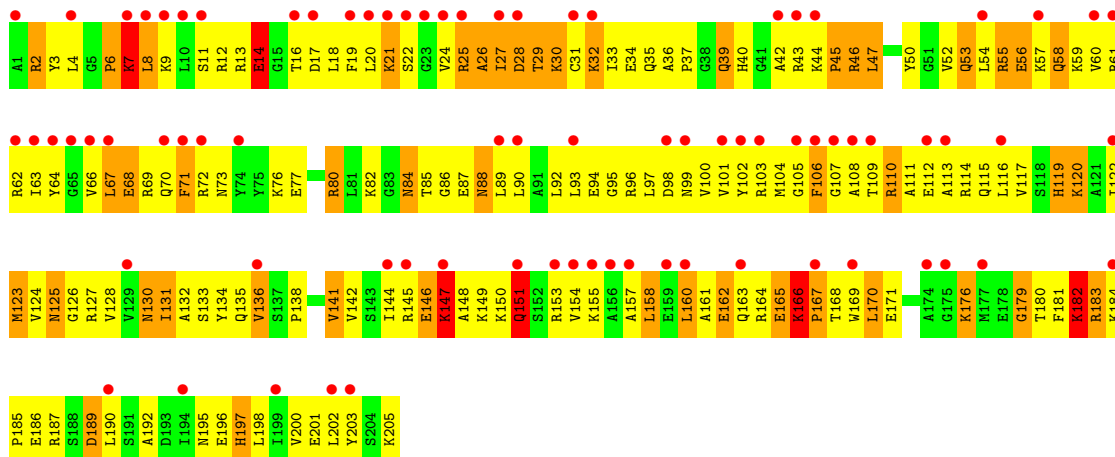


• Molecule 6: 30S ribosomal protein S4

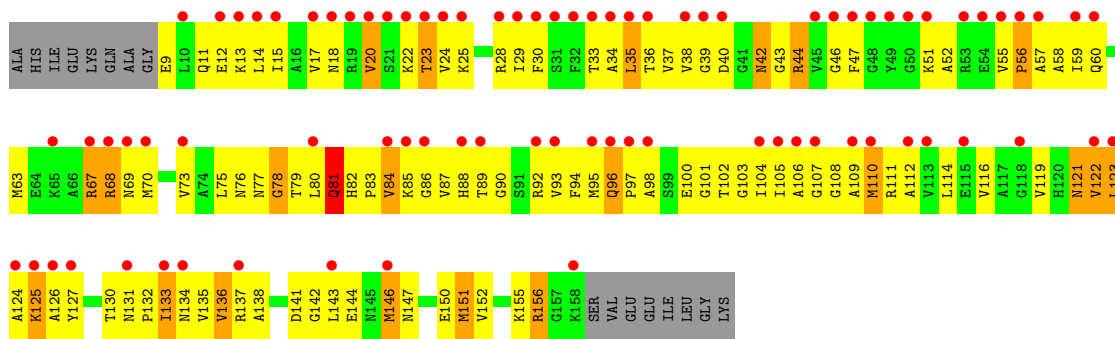




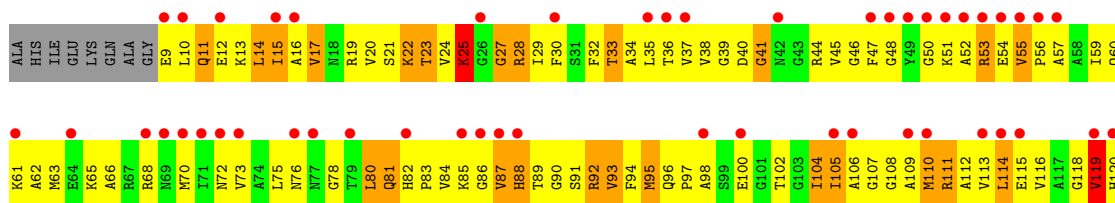
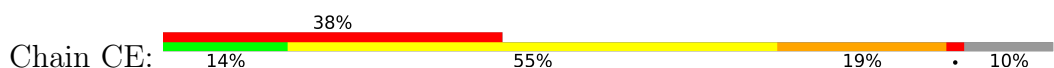
• Molecule 6: 30S ribosomal protein S4



• Molecule 7: 30S ribosomal protein S5

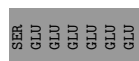
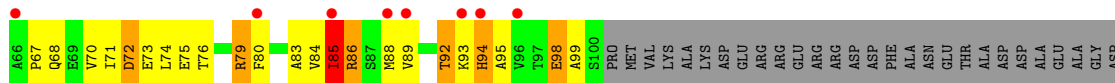
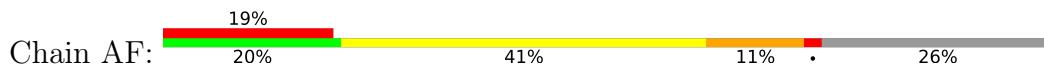


• Molecule 7: 30S ribosomal protein S5

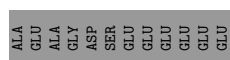
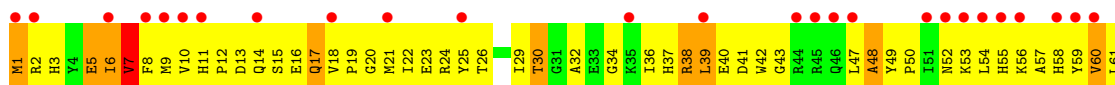
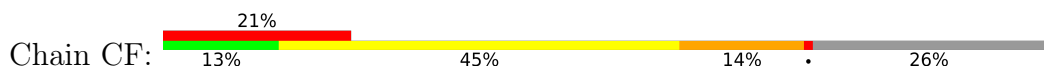




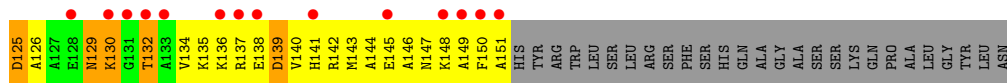
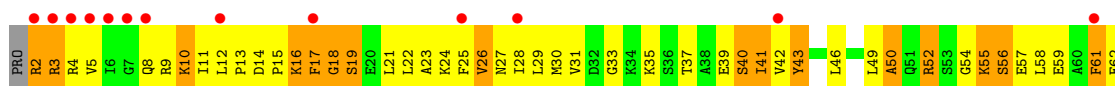
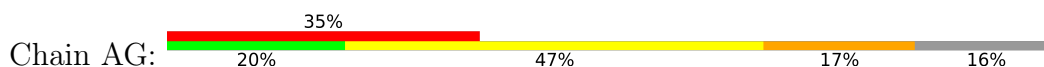
• Molecule 8: 30S ribosomal protein S6



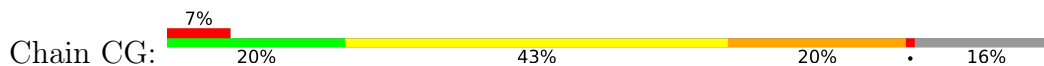
• Molecule 8: 30S ribosomal protein S6

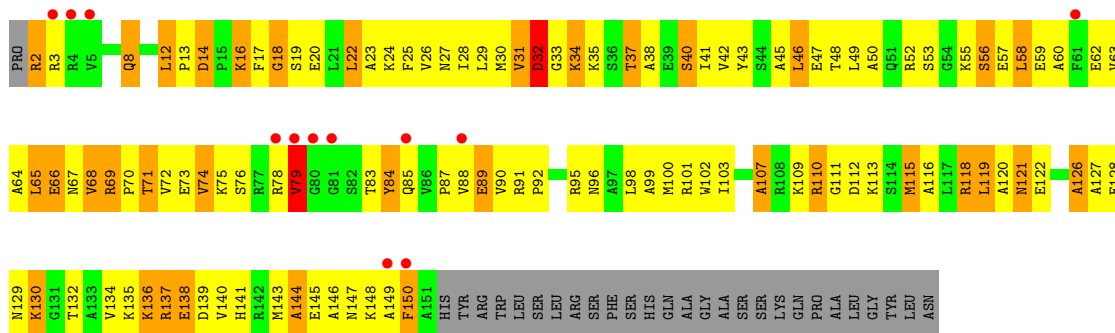


• Molecule 9: 30S ribosomal protein S7

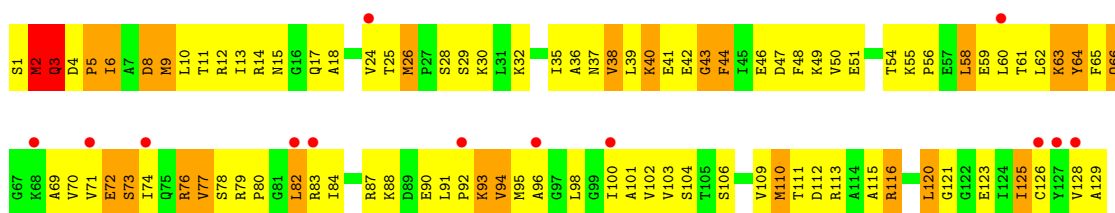


• Molecule 9: 30S ribosomal protein S7





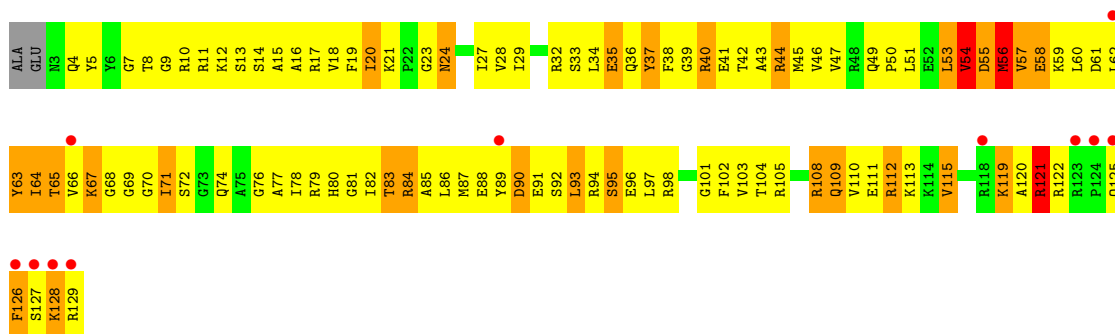
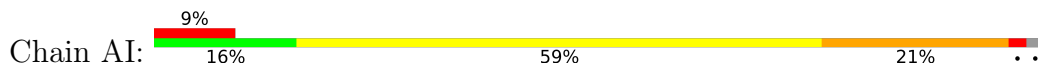
• Molecule 10: 30S ribosomal protein S8



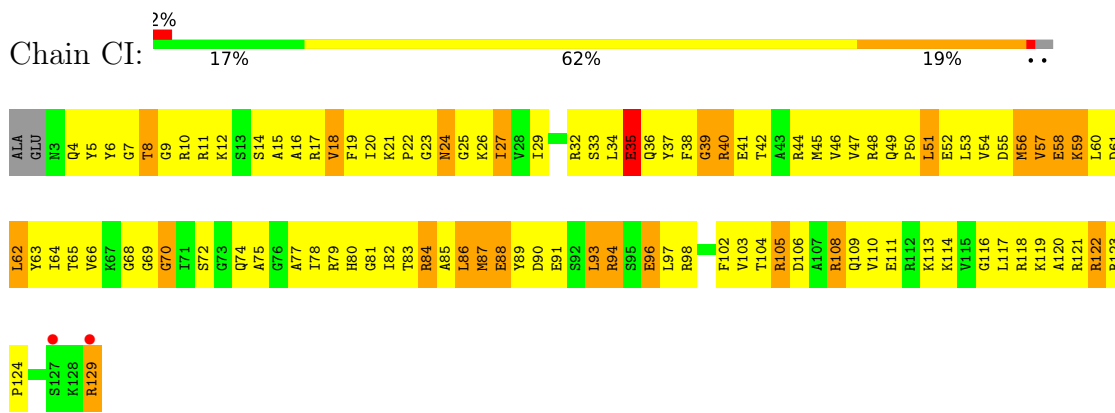
• Molecule 10: 30S ribosomal protein S8



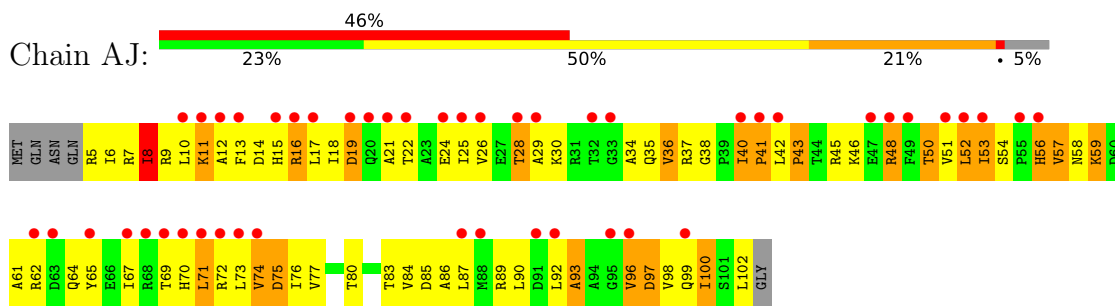
• Molecule 11: 30S ribosomal protein S9



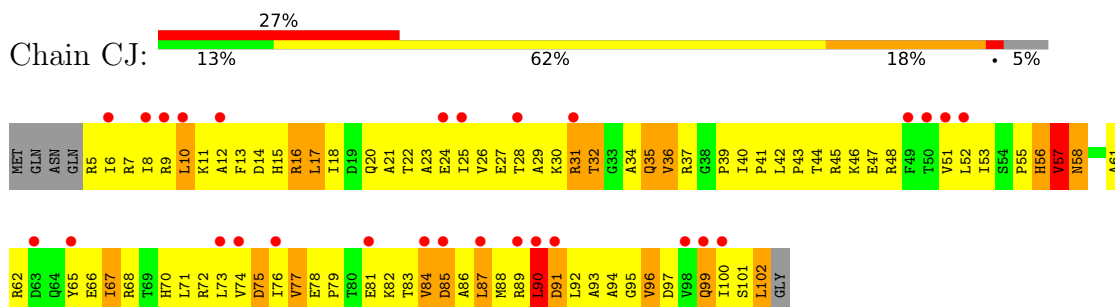
• Molecule 11: 30S ribosomal protein S9



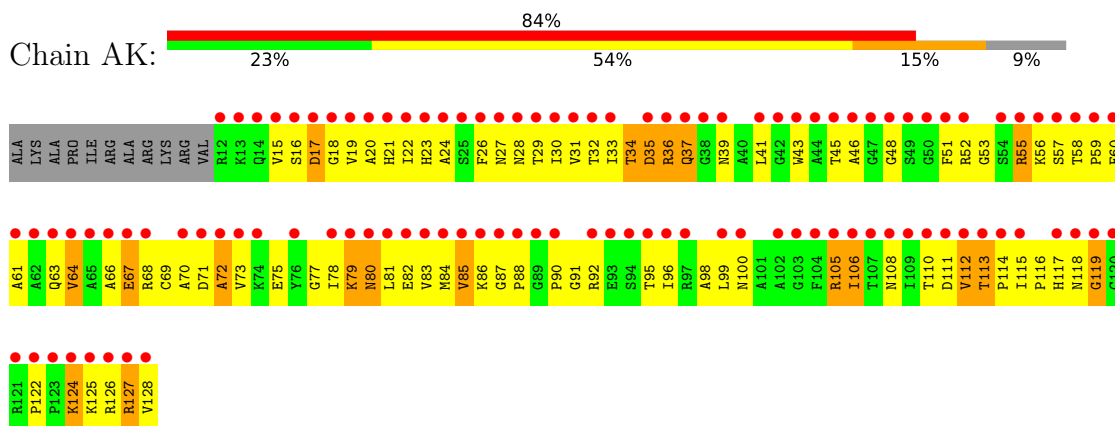
• Molecule 12: 30S ribosomal protein S10



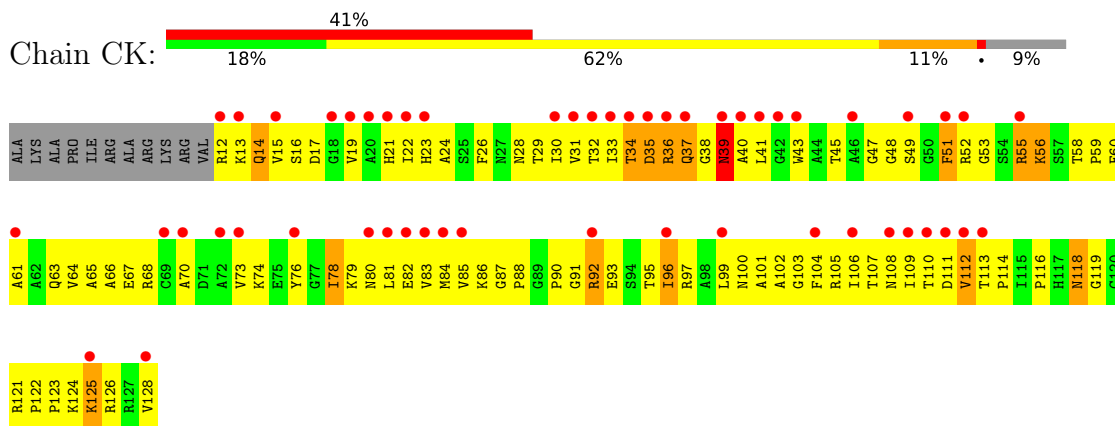
• Molecule 12: 30S ribosomal protein S10



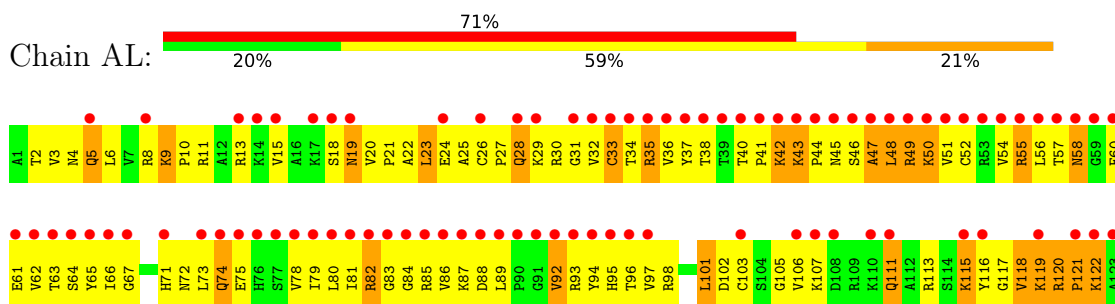
• Molecule 13: 30S ribosomal protein S11



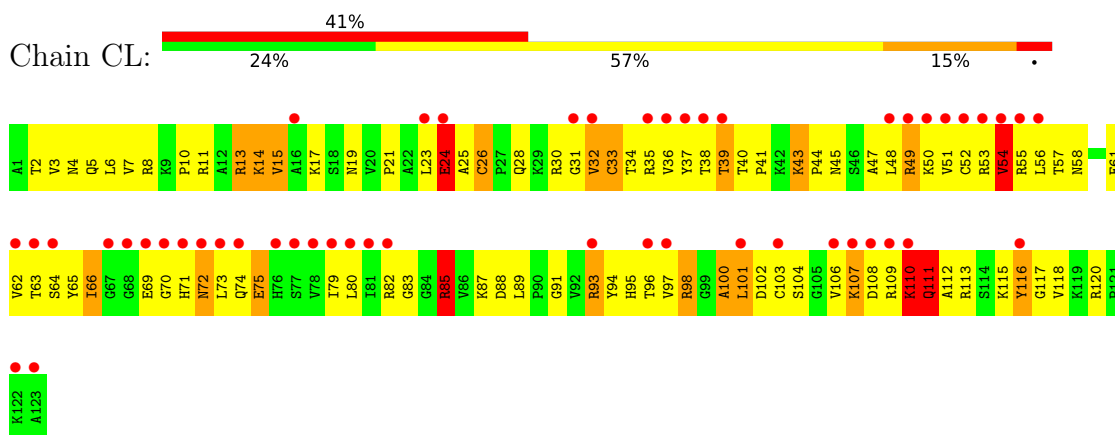
• Molecule 13: 30S ribosomal protein S11



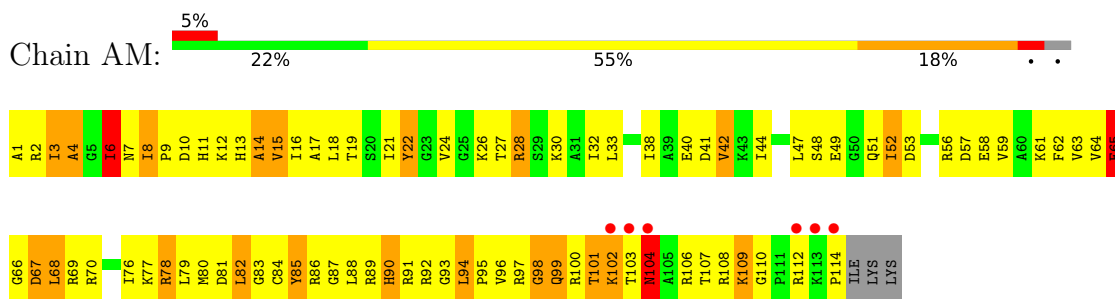
• Molecule 14: 30S ribosomal protein S12



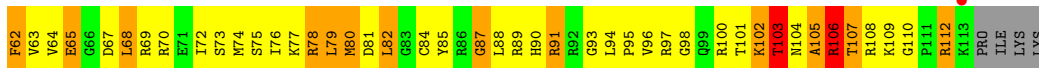
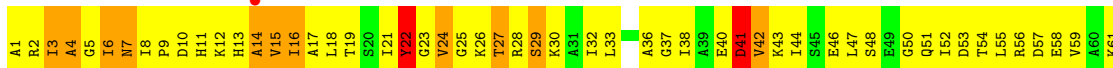
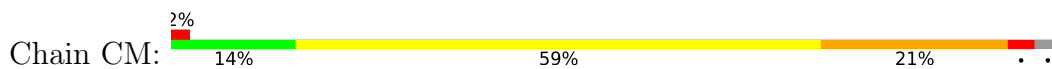
• Molecule 14: 30S ribosomal protein S12



• Molecule 15: 30S ribosomal protein S13



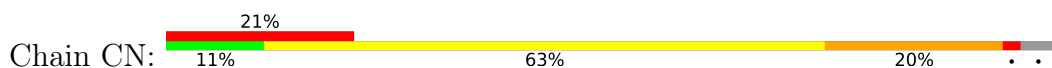
• Molecule 15: 30S ribosomal protein S13



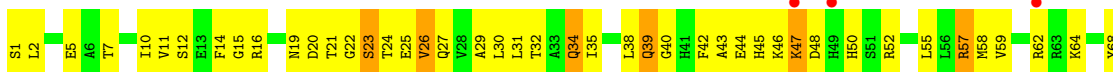
- Molecule 16: 30S ribosomal protein S14



- Molecule 16: 30S ribosomal protein S14



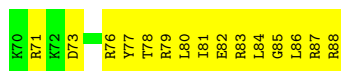
- Molecule 17: 30S ribosomal protein S15



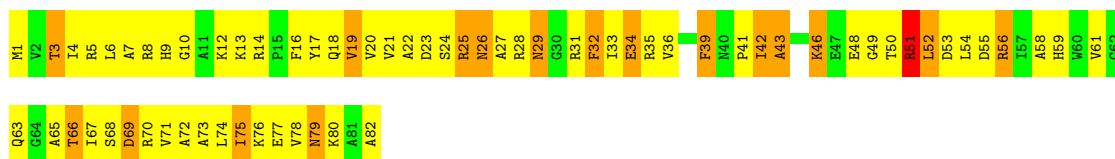
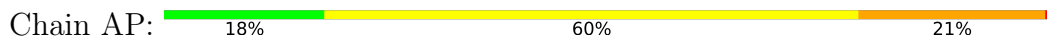
- Molecule 17: 30S ribosomal protein S15



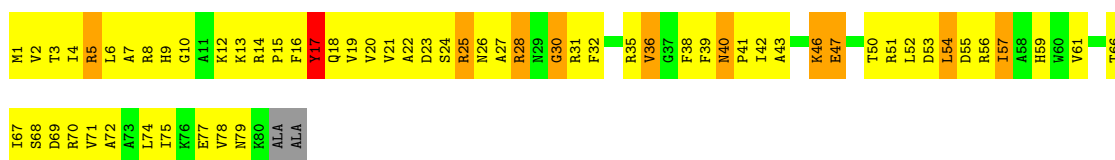




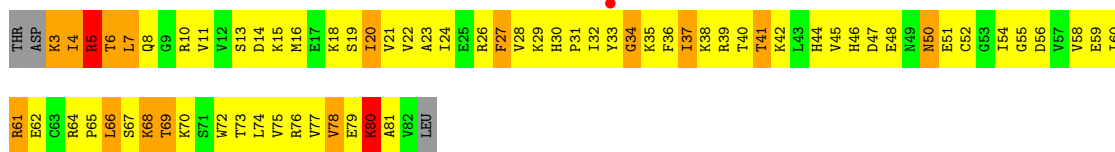
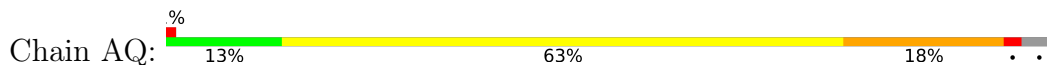
- Molecule 18: 30S ribosomal protein S16



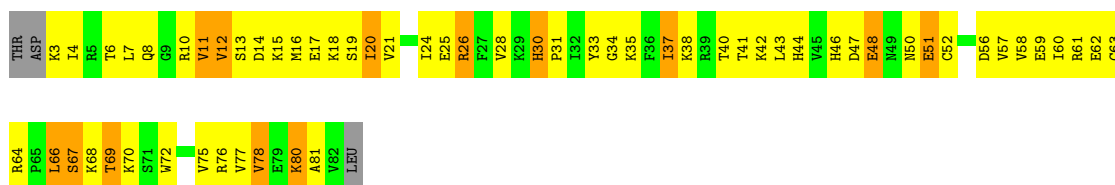
- Molecule 18: 30S ribosomal protein S16



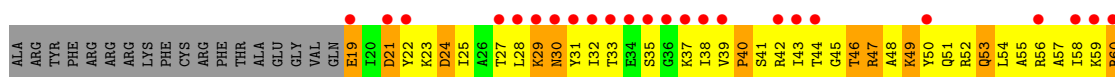
- Molecule 19: 30S ribosomal protein S17

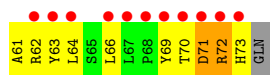


- Molecule 19: 30S ribosomal protein S17

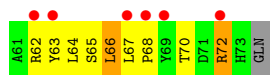
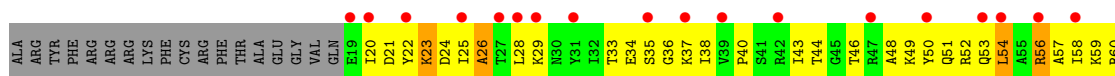
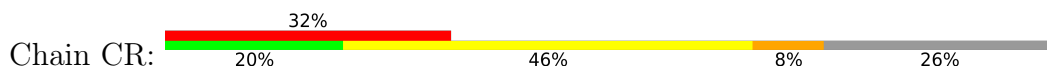


- Molecule 20: 30S ribosomal protein S18

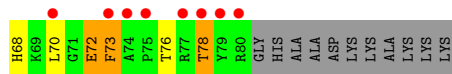




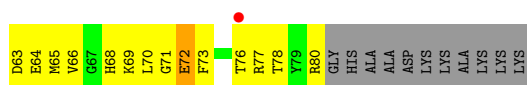
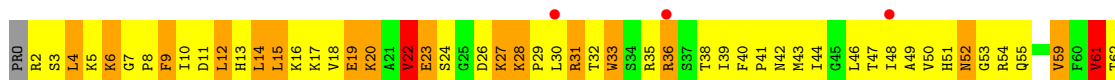
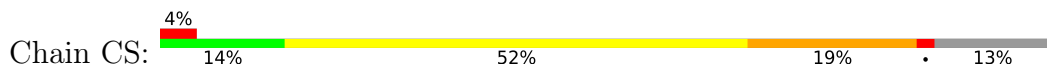
- Molecule 20: 30S ribosomal protein S18



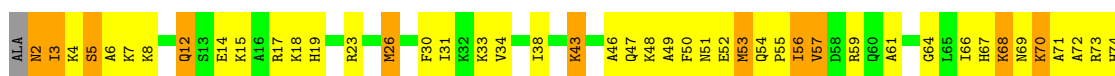
- Molecule 21: 30S ribosomal protein S19



- Molecule 21: 30S ribosomal protein S19

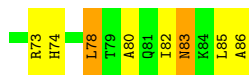


- Molecule 22: 30S ribosomal protein S20

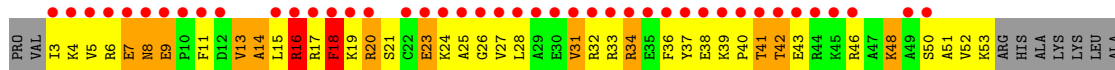


- Molecule 22: 30S ribosomal protein S20

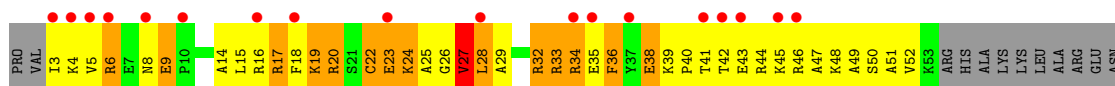




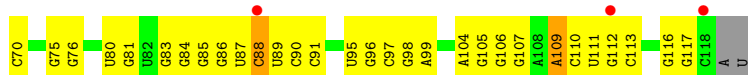
• Molecule 23: 30S ribosomal protein S21



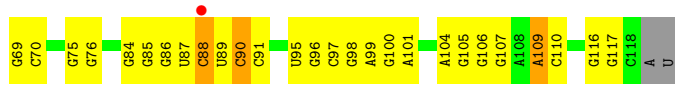
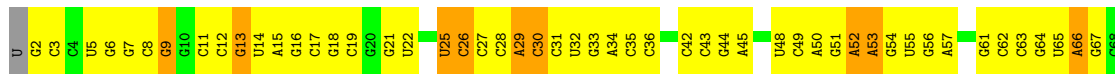
• Molecule 23: 30S ribosomal protein S21



• Molecule 24: 5S ribosomal RNA



• Molecule 24: 5S ribosomal RNA



• Molecule 25: 23S ribosomal RNA

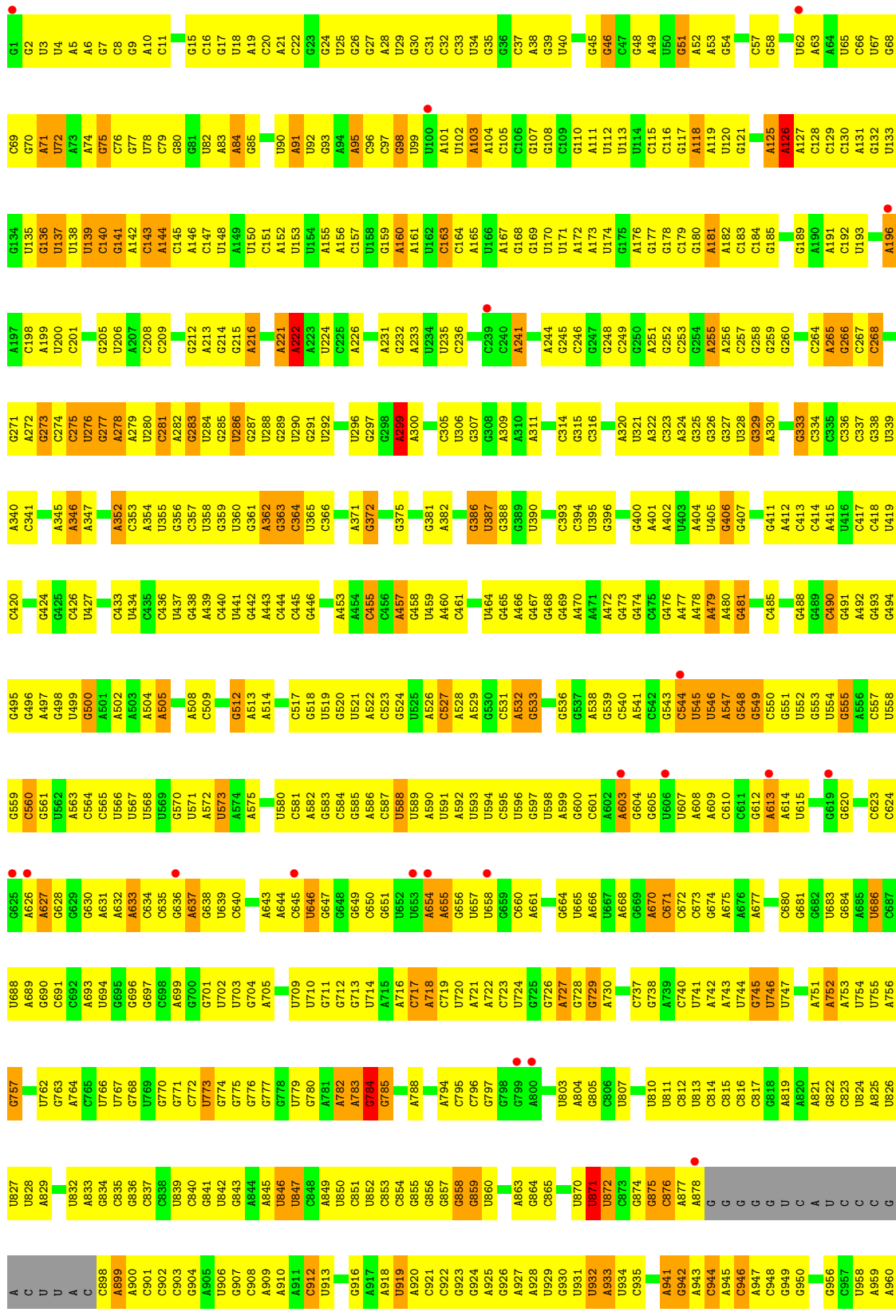


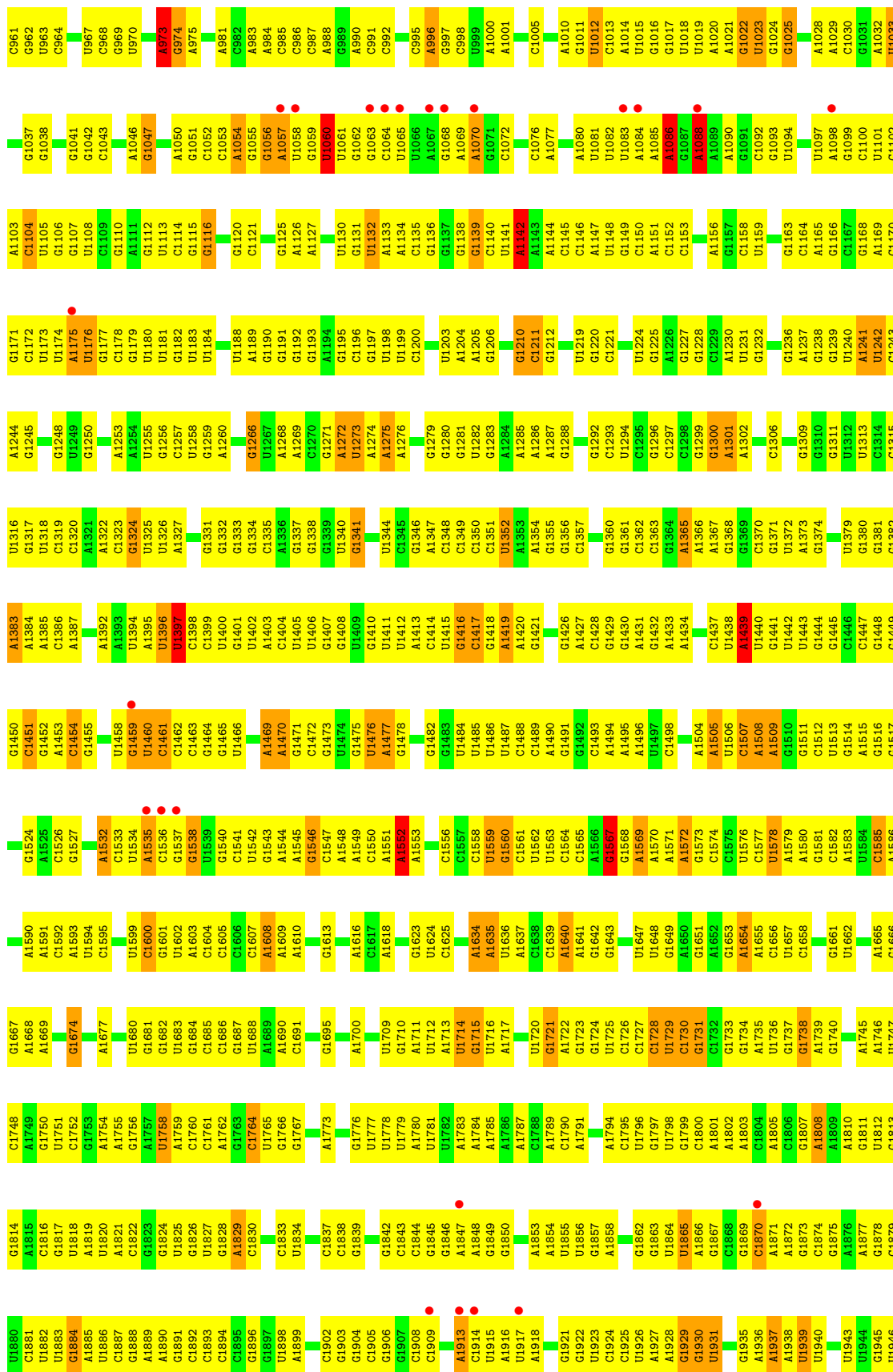
The table displays validation metrics for residues G957 through G1031. Each residue is represented by a horizontal bar divided into segments corresponding to different validation metrics: A (All atoms), U (Unmodelled side chains), C (Close contacts), G (Good geometry), B (Bad geometry), O (Outliers), and D (Disordered). The length of each segment indicates the count of residues failing that specific metric. Outliers are marked with a red dot above the bar, and disordered residues are marked with a 'D' in a grey box.



U2886	A2800	A2734	A2670	A2598	G2529	A2459	G2391	G2323	G2260	G2193	U	C2008
G2867	G2801	G2735	G2671	G2599	A2550	U2460	A2392	U2324	C2261	U2194	G2153	A2009
G2868	G2802	U2739	U2672	A2551	G2551	A2461	U2393	G2325	U2262	A2071	A2134	G2010
G2869	G2803	G2745	G2673	G2552	G2552	C2462	C2394	C2326	C2263	C2072	A2135	U2011
G2870	U2804	A2740	A2674	U2553	U2553	A2463	G2395	A2327	G2264	U2074	G2136	G2012
G2871	G2805	A2741	A2675	A2534	G2534	G2464	G2396	A2328	U2265	U2075	A2137	A2013
A2872	G2806	G2742	C2465	U2604	G2535	C2465	G2396	U2329	U2266	U2076	U2139	A2014
A2873	U2807	U2743	G2466	U2605	G2536	C2466	G2400	G2330	A2267	A2077	G2140	A2015
G2874	G2808	G2744	C2467	G2606	U2537	A2467	U2401	G2331	A2268	G2078	G2141	U2016
G2875	A2809	C2745	U2678	G2607	C2538	A2468	U2402	C2332	A2269	U2079	A2142	G2017
G2876	G2810	U2746	U2680	C2539	C2539	A2469	G2403	A2333	A2270	G2082	C2143	G2018
G2877	G2811	G2747	A2681	U2609	C2540	G2470	U2404	U2334	G2271	A2082	G2144	A2019
G2878	A2812	A2748	A2682	G2610	G2541	A2471	U2405	A2335	U2272	G2083	G2145	A2020
A2879	G2813	G2685	G2685	G2611	G2542	G2472	A2406	A2336	A2273	C2084	C2146	C2021
G2880	A2814	U2684	C2475	U2543	G2543	A2473	A2407	G2337	A2274	U2085	G2147	U2022
U2881	G2815	G2685	C2476	U2544	G2544	C2476	U2408	C2338	A2275	G2086	A2148	C2023
A2882	G2816	U2686	A2476	U2547	U2547	A2476	G2409	C2339	A2276	U2087	G2149	G2024
U2883	U2817	U2687	G2410	U2548	U2548	U2477	G2410	A2340	G2279	A2088	C2150	C2025
G2884	G2688	U2617	A2411	A2411	A2411	A2478	A2411	G2341	G2280	U2026	U2151	U2026
G2885	U2689	U2552	A2412	A2412	U2552	U2479	A2412	C2342	A2281	G2091	G2152	G2027
G2886	U2690	G2553	A2413	A2413	G2553	G2480	G2413	G2345	A2282	U2092	C2153	U2028
G2887	G2691	U2554	G2414	G2414	U2554	G2481	G2414	G2346	C2283	U2093	A2154	G2029
G2888	G2692	U2555	G2415	G2415	U2555	G2482	G2415	G2347	A2284	A2094	U2155	A2030
G2889	G2693	G2556	G2416	G2416	G2556	G2483	A2416	C2347	C2285	A2095	G2156	G2031
G2890	G2694	G2557	C2417	C2417	G2557	U2484	C2417	U2348	G2286	G2096	G2157	G2032
G2891	G2695	C2558	A2418	A2418	C2558	G2487	A2418	G2352	A2287	A2097	A	A2033
G2892	G2696	G2559	U2419	U2419	G2559	G2488	U2419	A2353	A2288	U2098	G	U2034
G2893	G2697	A2560	G2420	G2420	A2560	G2489	G2420	G2354	G2289	U2099	C	U2035
G2894	G2698	U2561	U2421	U2421	U2561	G2490	U2421	G2355	G2290	G2100	G	C2036
G2895	G2699	U2562	A2422	A2422	U2562	U2491	A2422	G2356	U2291	A2101	C	A2037
G2896	G2702	U2563	A2423	A2423	U2563	U2492	A2423	U2357	U2292	G2102	A	G2038
G2897	C2703	A2564	U2424	U2424	A2564	U2493	A2424	G2358	G2293	G2103	C	U2039
G2898	C2704	A2565	G2425	G2425	A2565	C2494	G2425	G2359	G2294	C2104	C	G2040
G2899	U2705	A2566	G2426	A2426	A2566	C2495	A2426	G2360	G2295	U2105	U	U2041
A2900	A2706	A2567	G2427	G2427	A2567	G2496	G2427	G2361	U2296	U2106	U	A2042
C2901	G2707	G2568	U2430	U2430	G2568	G2497	U2430	G2362	U2297	G2107	G	C2043
C2902	G2708	G2569	A2431	A2431	U2569	G2501	U2431	G2363	A2298	A2108	A	C2044
C2903	G2709	G2570	G2432	G2432	G2570	G2502	G2432	G2364	U2299	U2109	A	G2045
C2904	C2710	U2571	A2433	A2433	U2571	A2503	A2433	G2365	C2300	G2110	A	G2046
C2905	U2713	A2572	U2511	U2511	A2572	U2504	U2441	A2366	G2301	U	U	C2047
C2906	G2714	G2645	C2512	C2512	A2573	G2505	G2442	A2367	G2302	G	A	G2048
C2907	C2715	G2648	A2513	A2513	G2574	U2506	G2443	C2368	G2303	U	C	G2049
C2908	C2716	G2649	U2514	U2514	G2575	C2507	U2444	A2369	U2304	A	A	C2050
C2909	G2717	U2650	C2515	C2515	G2576	G2508	A2439	G2370	U2240	C	A	A2051
C2910	G2651	G2651	G2516	G2516	C2579	G2509	G2440	G2371	A2241	C	C	A2052
C2911	G2652	G2655	U2517	U2517	U2583	U2511	U2441	G2372	G2308	A	C	C2055
C2912	G2653	G2656	A2518	A2518	U2584	C2512	G2442	C2373	A2309	U	U	G2056
C2913	G2654	U2657	U2519	U2519	U2585	A2513	G2443	G2374	C2310	A	A	G2057
C2914	A2659	G2658	C2514	C2514	U2586	U2514	G2444	A2377	A2311	G	U	A2058
C2915	G2660	G2659	A2515	A2515	U2587	G2515	G2445	G2378	U2312	U	U	A2059
C2916	G2661	A2660	G2516	G2516	G2588	A2516	G2446	G2379	C2313	A	A	A2060
C2917	A2662	G2661	U2517	U2517	A2589	C2517	G2447	C2380	A2314	G	G	A2061
C2918	A2663	A2662	A2518	A2518	A2590	A2448	A2448	C2381	G2315	G	G	G2062
C2919	A2664	A2663	U2519	U2519	U2591	A2449	A2449	G2382	G2250	U	U	C2063
C2920	G2728	A2665	C2520	C2520	C2592	A2450	A2450	A2383	A2317	A	A	G2064
C2921	G2729	A2665	U2593	U2593	U2593	U2384	U2384	U2384	G2318	G	C	C2065
C2922	C2730	G2666	U2594	U2594	C2594	U2385	U2385	C2385	G2319	C	C	G2066
C2923	G2731	G2667	G2595	G2595	U2595	A2386	A2386	A2386	U2320	U	U	C2067
C2924	A2733	G2668	U2596	U2596	U2596	U2457	U2457	A2387	U2321	U	U	C2068
C2925	G2733	G2669	G2597	G2597	G2597	G2524	G2524	G2387	U2322	U	U	C2069

● Molecule 25: 23S ribosomal RNA



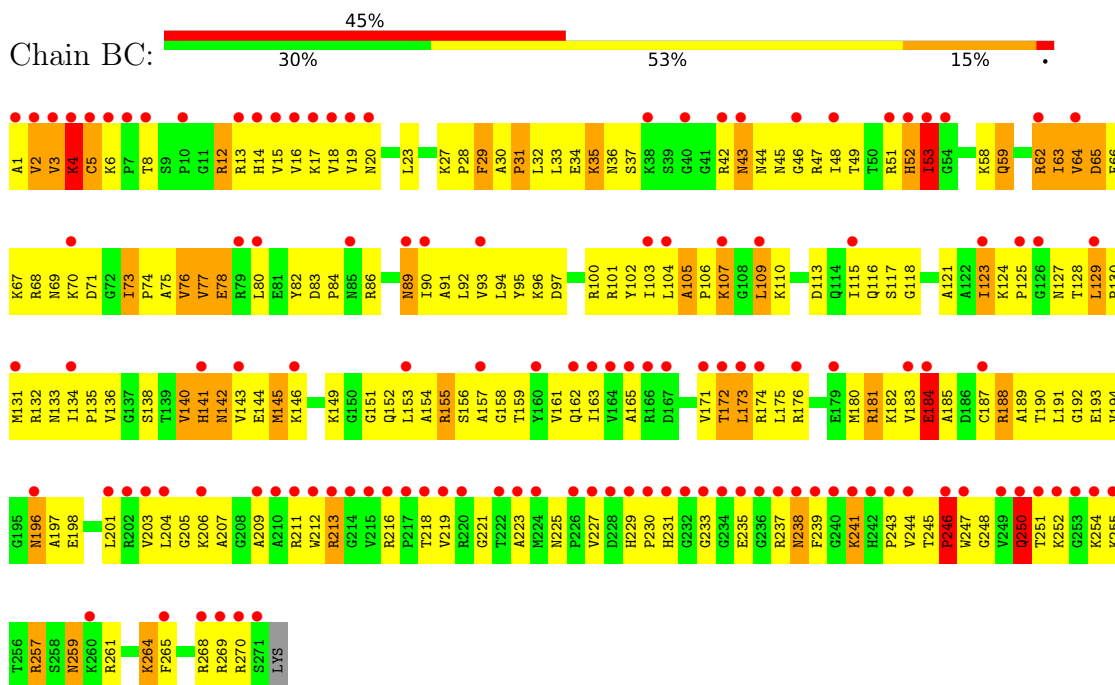




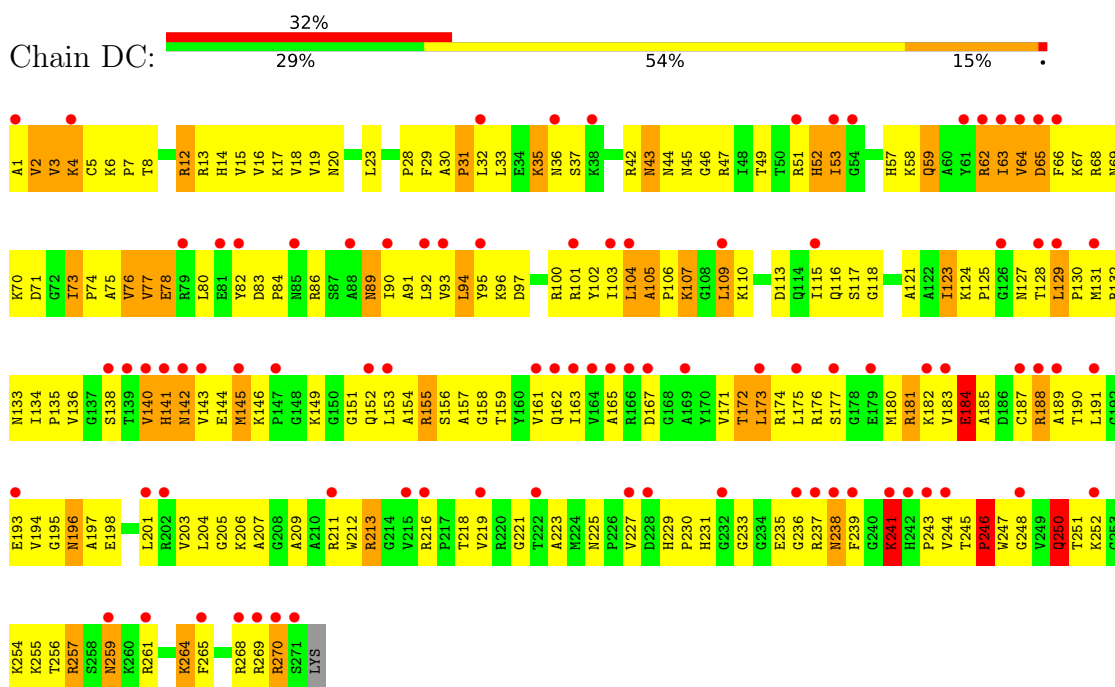
C1947	G2024	C2091	A2154	C2215	G2345	G2415	G2485	U2552	G2623	G2760	A2823
G1948	C2025	U2092	U2155	G2216	A2346	C2416	C2486	G2553	G2624	A2761	A2829
G1949	U2026	G2093	G2156	G2217	A2347	C2417	C2487	U2554	G2625	A2765	C2830
A1952	G2027	A2094	G2157	G2218	U2348	C2418	G2488	U2555	G2626	A2766	G2831
U1955	U2028	G2095	A	U2219	A2352	C2419	U2489	G2556	G2627	G2702	G2832
U1956	G2029	C2096	G	U2220	G2353	U2420	U2490	C2557	G2628	G2703	U2833
C1957	A2030	U	C	G2221	G2354	G2421	U2491	C2558	U2629	G2704	G2834
C1958	A2031	G2100	C	G2222	C2354	G2422	U2492	C2559	G2630	A2705	A2835
G1959	G2032	A2101	G	A2225	U2356	A2423	U2493	U2560	G2631	A2706	A2836
A1960	A2033	G2102	A	U2226	G2360	A2424	C2498	U2561	G2632	U2707	U2837
C1961	U2034	C2103	C	C2227	G2361	A2425	C2499	U2562	U2633	G2708	C2838
C1962	U2035	G2104	C	A2228	G2362	A2426	U2500	U2563	U2634	G2709	G2839
U1963	G2036	U2105	U	U2229	C2362	C2427	G2501	U2564	G2635	C2710	C2840
U1964	A2037	U2106	G	G2230	C2363	G2428	G2502	A2565	A2636	A2711	C2841
C1965	G2038	A2107	A	U2231	C2364	A2429	A2503	A2566	A2637	C2712	C2842
C1966	U2039	G2108	G	U2232	U2364	A2430	A2504	U2567	G2638	U2713	A2778
A1966	G2040	U2109	A	U2233	A2365	U2431	U2505	U2568	G2639	G2714	U2779
C1967	U2041	G2110	A	U2234	G2366	A2432	G2506	U2569	G2640	C2715	U2780
U1968	A2042	U	U	G2235	C2366	A2433	U	G2570	G2641	C2716	A2781
A1969	C2043	G	C	U2236	C2367	A2434	U2511	U2571	G2642	C2717	G2782
A1970	G2044	U	C	U2237	C2368	A2435	C2512	A2572	G2643	G2718	U2783
U1971	C2045	A	C	G2238	G2370	G2436	A2513	C2573	C2644	C2649	U2784
G1972	G2046	A	A	G2239	G2371	G2437	A2514	G2574	A2645	U2785	U2785
G1973	U2047	C	A	U2240	G2372	U2438	U2515	G2575	G2646	C2720	C2785
C1974	G2048	C	C	U2241	C2373	A2439	C2516	C2576	G2647	G2721	C2786
U1985	U2049	U	C2179	A2242	U2374	G2440	A2516	U2577	G2648	C2722	C2787
C1986	A2050	G	U2180	G2243	A2377	U2441	C2517	G2578	C2649	C2723	C2788
A1987	G2051	A	U2181	U2244	A2378	C2442	A2518	G2579	C2650	U2724	C2789
G1988	U2052	U	U2182	U2245	G2379	C2443	U2519	U2580	U2651	A2725	C2855
U1991	G2055	G	U2183	G2246	C2380	A2444	U2520	U2581	G2652	A2726	A2856
U1992	C2056	G	A2184	U2247	C2381	G2445	C2521	G2582	G2653	U2727	G2857
U1993	A2060	A	U2185	C2248	G2382	G2446	U2522	G2583	G2654	C2728	C2858
C1994	G2061	G	U2186	U2249	C2383	A2447	G2523	A2584	A2655	C2729	C2859
C1997	C2063	C	U2187	G2250	C2384	A2448	G2524	G2585	G2656	C2730	A2860
A1998	U2064	U	U2188	U2257	C2385	U2449	G2525	G2586	G2657	U2731	G2861
C1999	C2065	U	U2189	C2258	C2386	G2455	G2526	C2587	G2658	A2732	C2862
C2000	G2066	U	A2191	U2261	A2387	U2456	G2529	U2588	A2659	A2733	C2863
C2001	U2069	G	U2192	U2262	A2389	G2457	A2530	U2589	G2660	A2734	U2864
G2002	A2070	A2134	U2193	U2263	A2392	A2458	A2531	G2590	G2661	G2735	U2865
C2008	A2071	G2136	U2194	C2263	A2393	A2459	A2532	A2591	U2662	U2736	G2866
A2009	C2072	U2137	U2195	U2264	U2394	A2460	U2533	A2592	G2663	U2737	A2867
A2010	G2073	G2138	U2196	U2265	C2395	A2461	U2534	G2593	U2664	A2738	A2868
G2010	U2074	U	U2197	U2266	G2396	C2462	U2535	G2594	U2665	C2739	C2869
U2011	U2075	A2142	U2198	A2266	U2400	G2463	G2536	C2595	G2666	U2740	C2870
G2012	A2076	G2143	U2199	A2267	U2401	U2464	A2537	A2596	U2667	G2741	U2871
A2013	A2077	C2144	U2203	A2268	U2402	A2465	U2538	A2597	U2668	A2742	A2872
A2014	A2082	G2144	A2204	U2272	A2405	G2472	A2542	U2598	G2669	U2743	C2873
U2016	C2083	C2145	C2205	A2273	A2406	C2473	A2543	U2600	U2669	C2744	C2874
U2017	G2084	A2146	C2206	A2274	A2407	C2474	G2544	U2601	U2670	C2745	C2875
G2018	C2085	C2147	C2207	C2274	U2408	A2475	G2545	U2602	U2671	A2746	G2876
G2019	U2085	A2148	C2208	U2275	U2409	U2476	U2546	U2603	U2672	G2747	C2877
A2020	U2086	U2149	G2209	A2276	G2410	U2477	U2547	C2604	U2673	U2748	U2878
A2021	G2087	U2150	U2210	G2266	A2411	U2478	U2548	G2605	C2674	A2749	C2879
U2022	C2088	C2151	A2211	G2267	A2412	U2479	G2549	U2606	U2675	C2750	A2880
C2022	C2089	U2152	A2212	G2268	A2413	G2481	G2550	C2607	U2676	A2751	C2881
C2033	A2090	C2153	C2214	C2283	U2344	G2481	C2551	G2608	C2677	G2752	U2882



- Molecule 26: 50S ribosomal protein L2

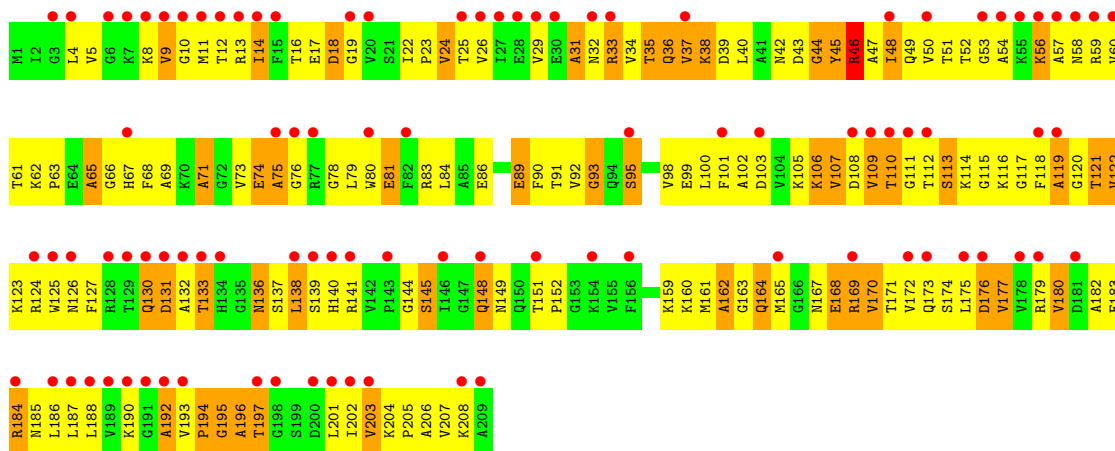


- Molecule 26: 50S ribosomal protein L2

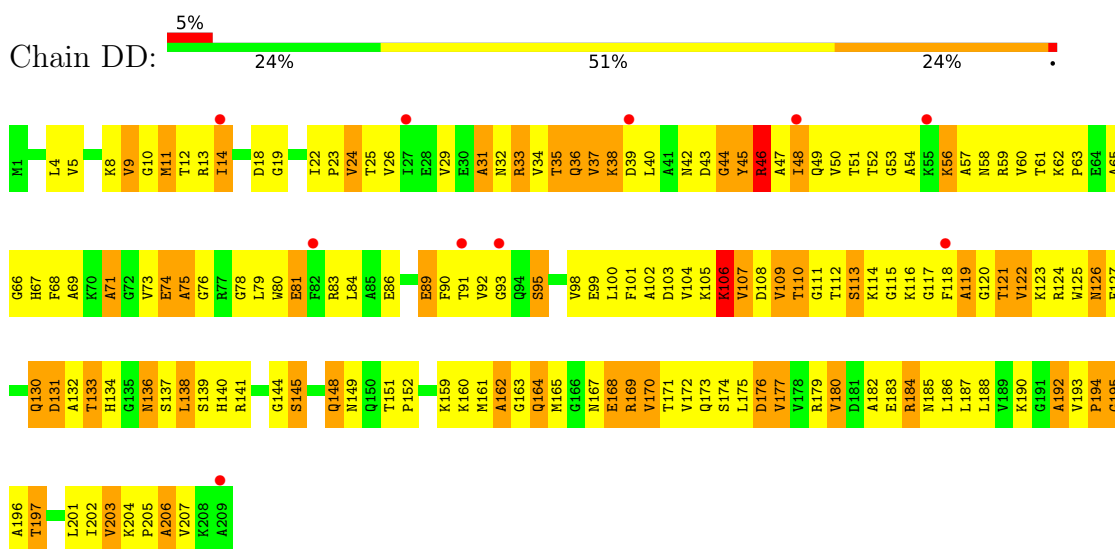


- Molecule 27: 50S ribosomal protein L3

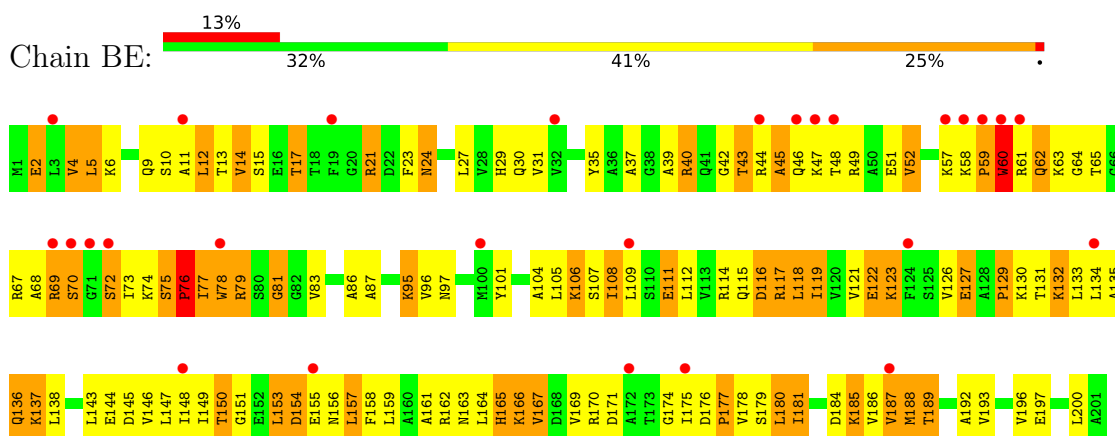




• Molecule 27: 50S ribosomal protein L3

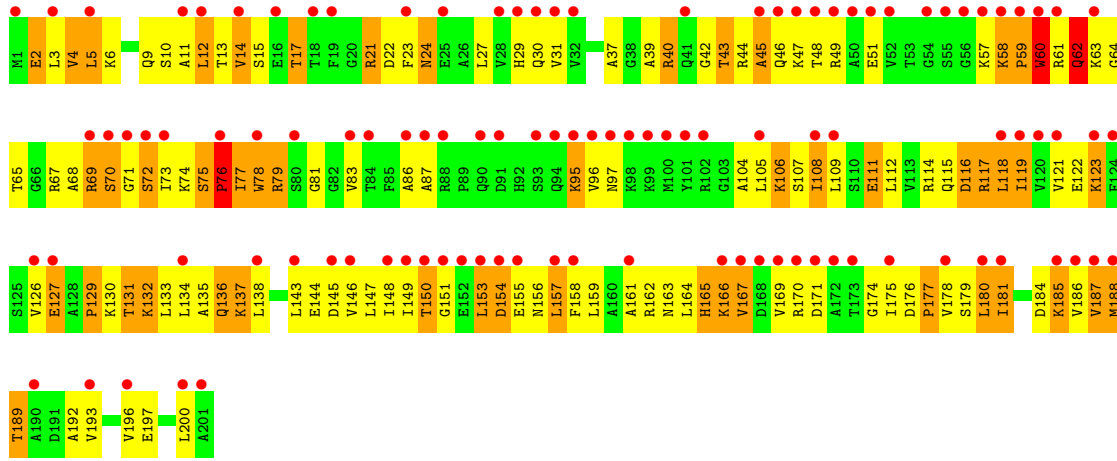


• Molecule 28: 50S ribosomal protein L4

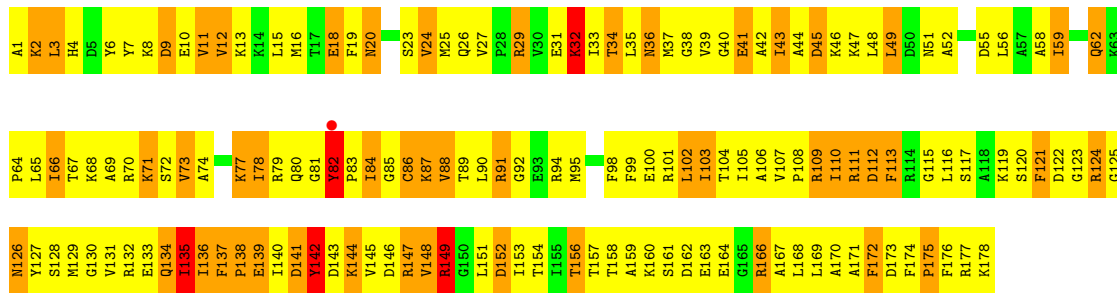
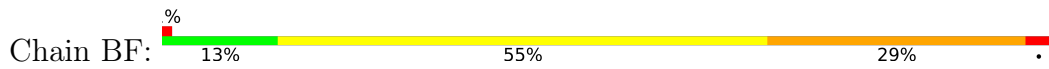


• Molecule 28: 50S ribosomal protein L4

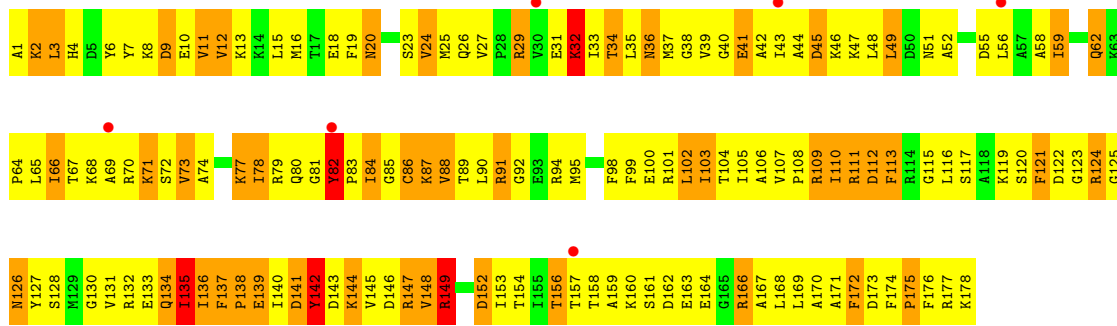
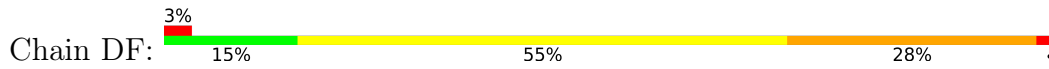




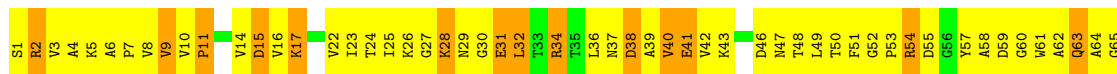
• Molecule 29: 50S ribosomal protein L5

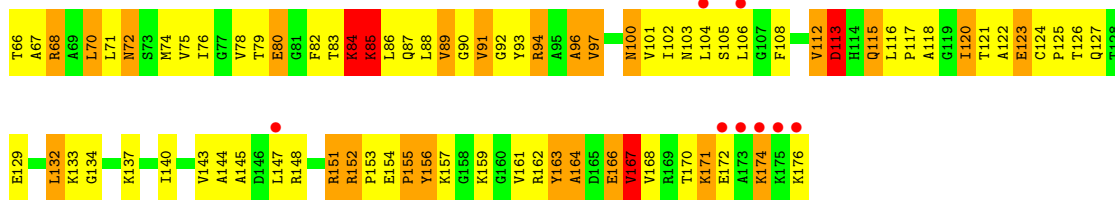


• Molecule 29: 50S ribosomal protein L5

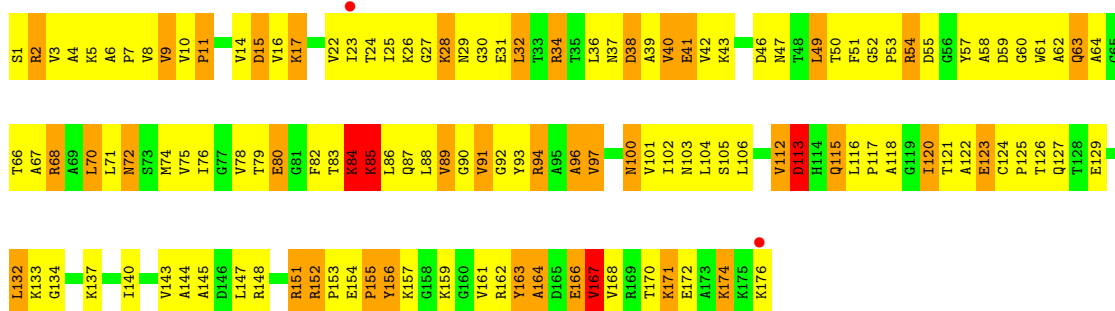


• Molecule 30: 50S ribosomal protein L6

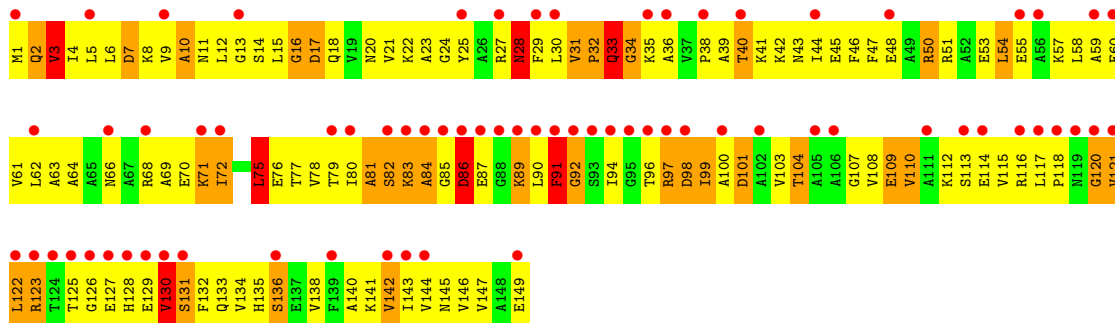
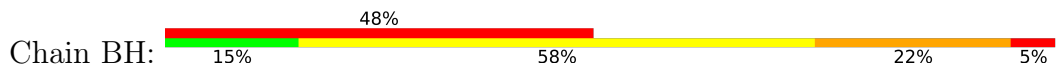




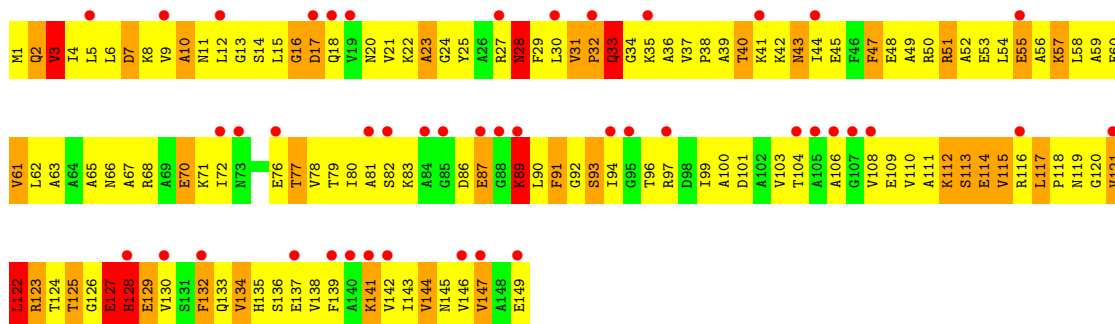
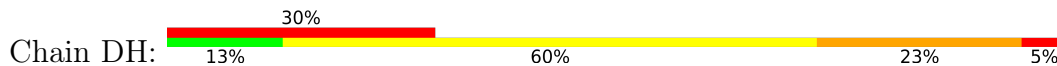
● Molecule 30: 50S ribosomal protein L6



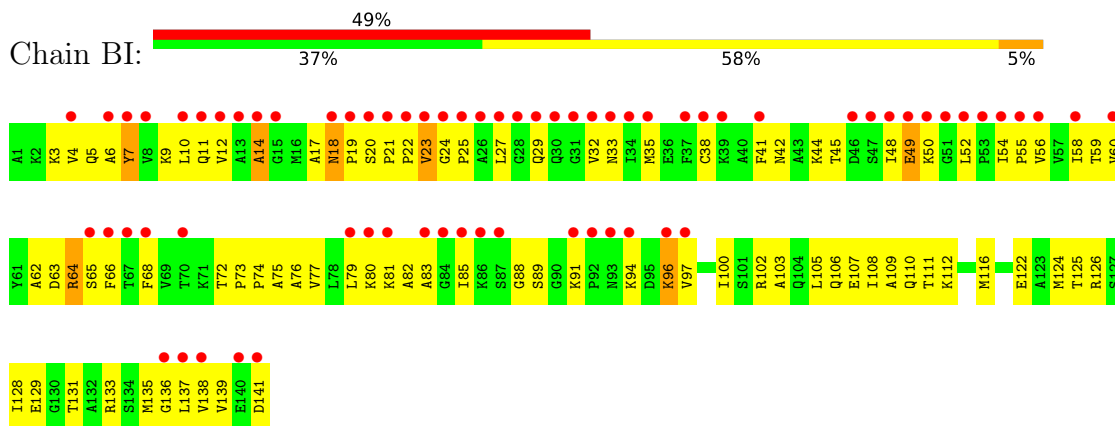
● Molecule 31: 50S ribosomal protein L9



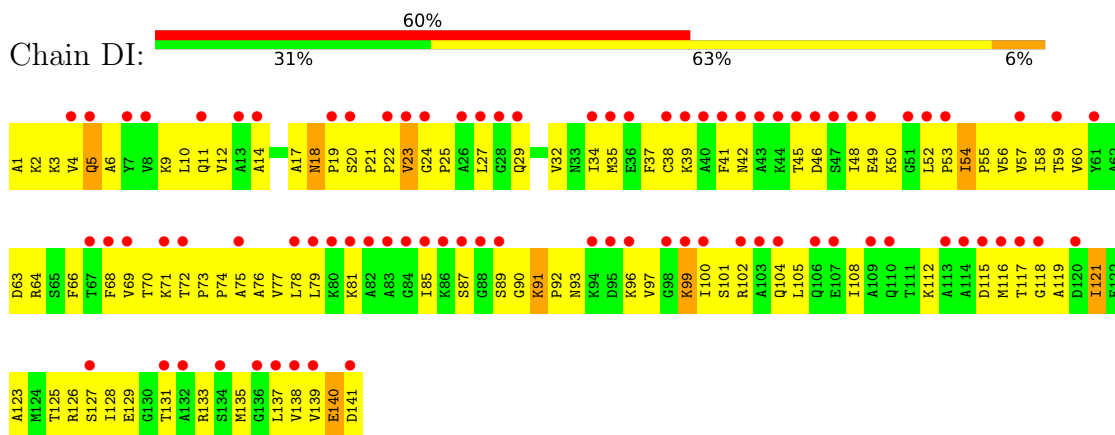
● Molecule 31: 50S ribosomal protein L9



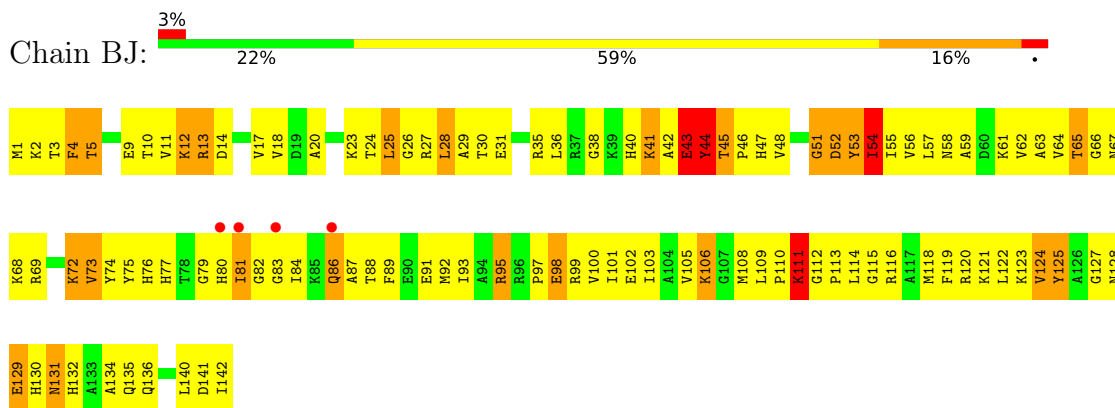
● Molecule 32: 50S ribosomal protein L11



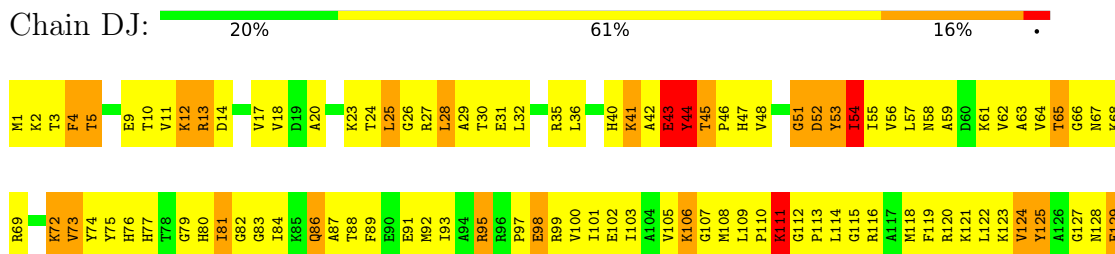
• Molecule 32: 50S ribosomal protein L11

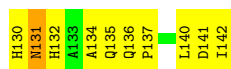


• Molecule 33: 50S ribosomal protein L13

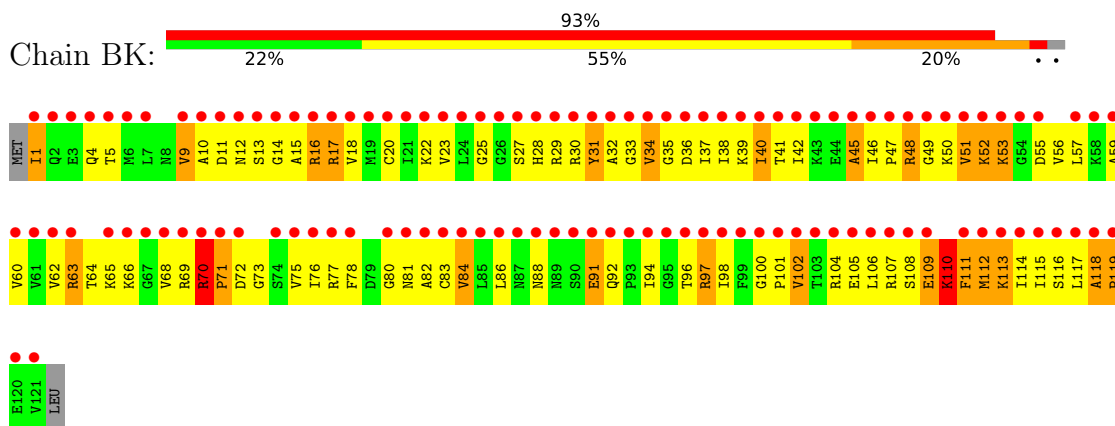


• Molecule 33: 50S ribosomal protein L13

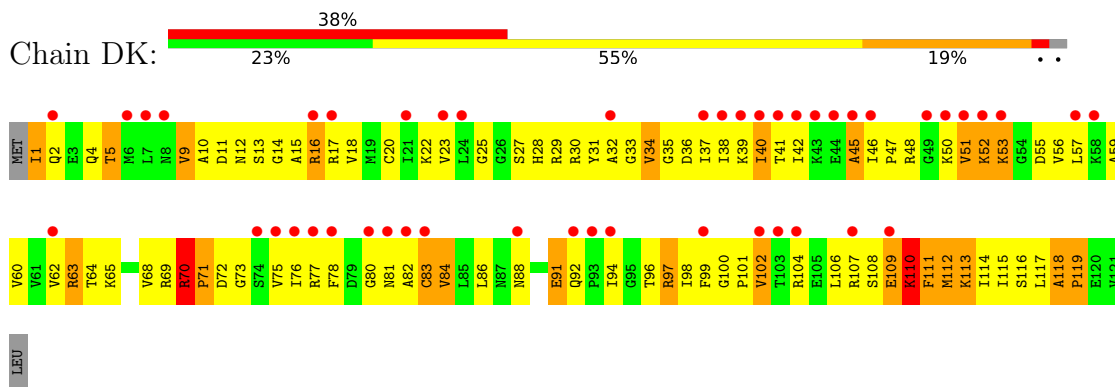




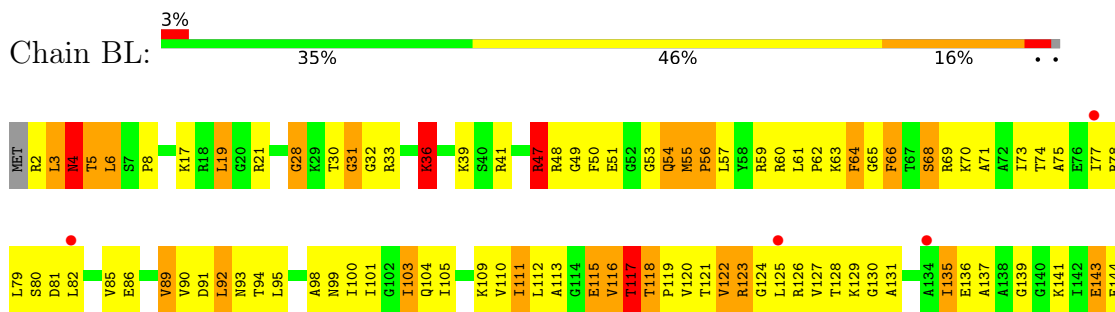
• Molecule 34: 50S ribosomal protein L14



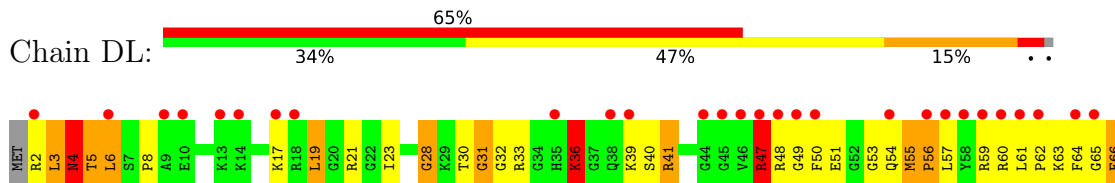
• Molecule 34: 50S ribosomal protein L14

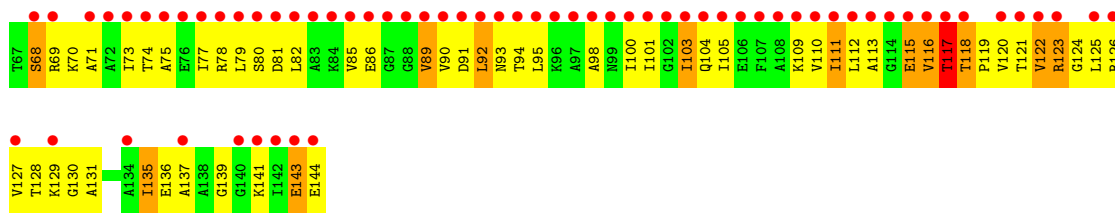


• Molecule 35: 50S ribosomal protein L15

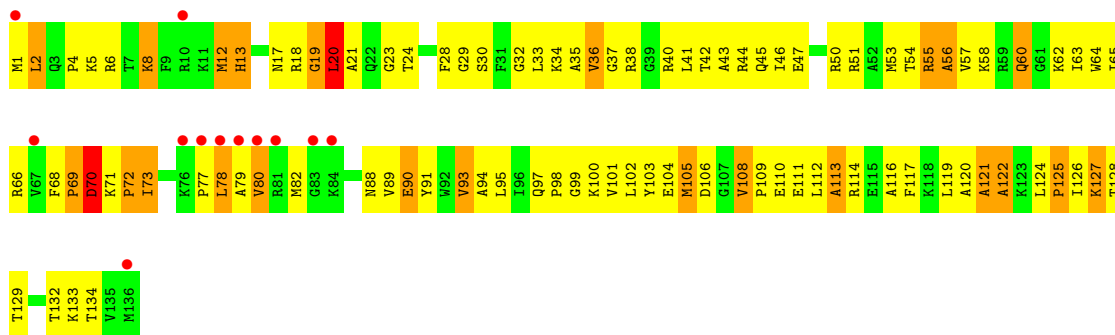
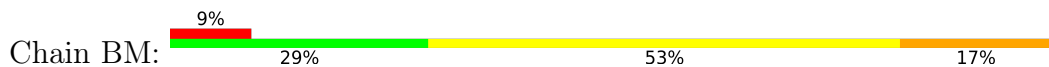


• Molecule 35: 50S ribosomal protein L15





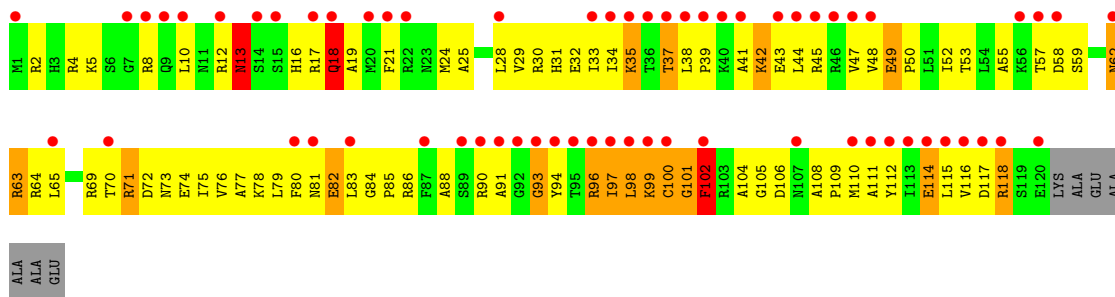
● Molecule 36: 50S ribosomal protein L16



● Molecule 36: 50S ribosomal protein L16

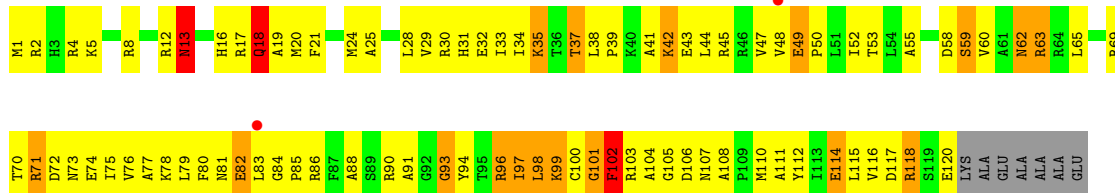
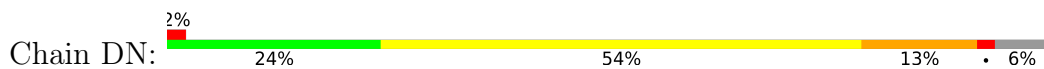


● Molecule 37: 50S ribosomal protein L17

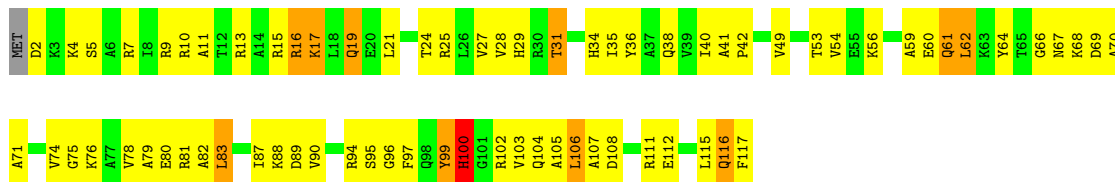
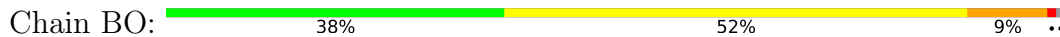


● Molecule 37: 50S ribosomal protein L17

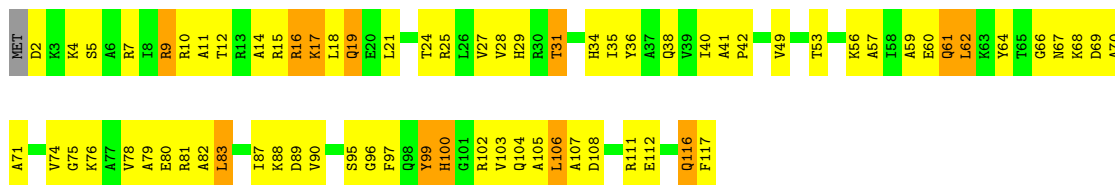




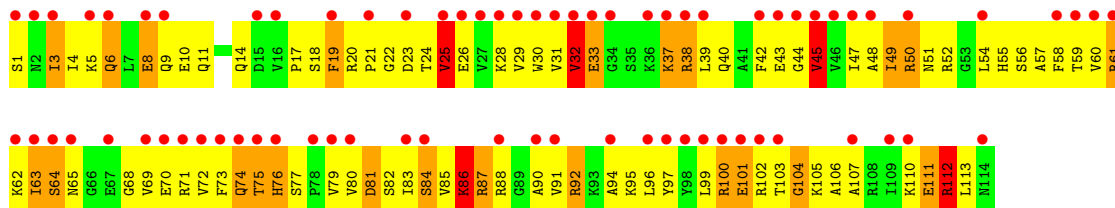
● Molecule 38: 50S ribosomal protein L18



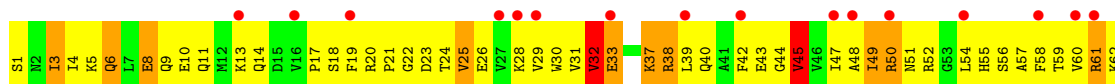
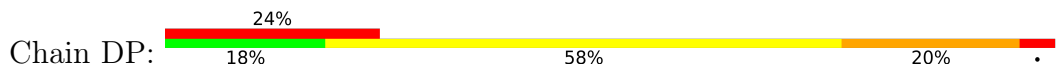
● Molecule 38: 50S ribosomal protein L18



● Molecule 39: 50S ribosomal protein L19

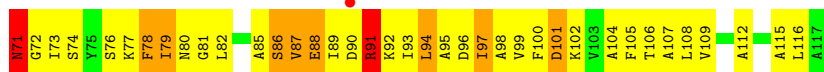
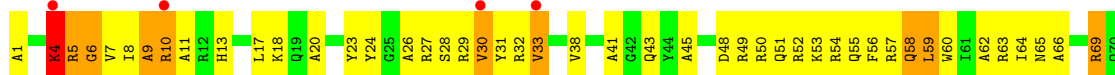


● Molecule 39: 50S ribosomal protein L19





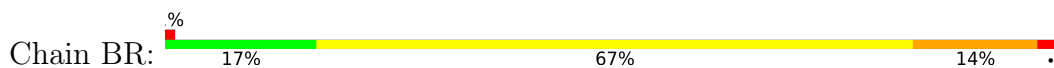
• Molecule 40: 50S ribosomal protein L20



• Molecule 40: 50S ribosomal protein L20



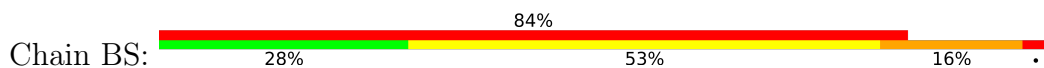
• Molecule 41: 50S ribosomal protein L21

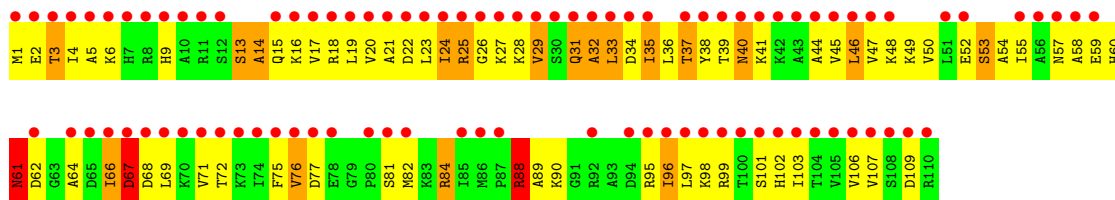


• Molecule 41: 50S ribosomal protein L21

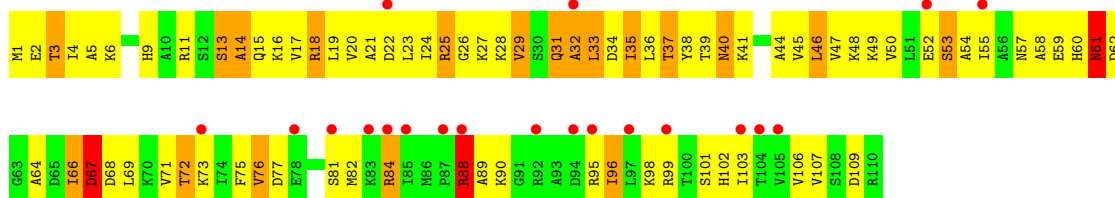


• Molecule 42: 50S ribosomal protein L22

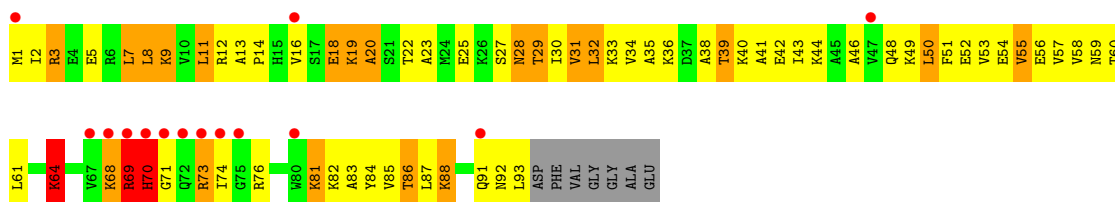
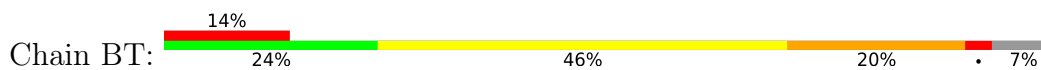




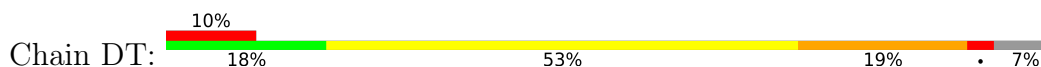
- Molecule 42: 50S ribosomal protein L22



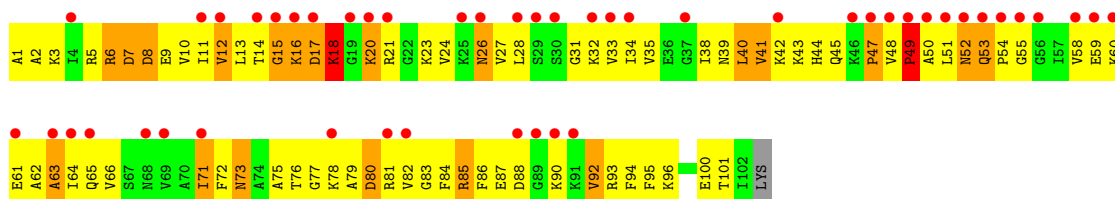
- Molecule 43: 50S ribosomal protein L23



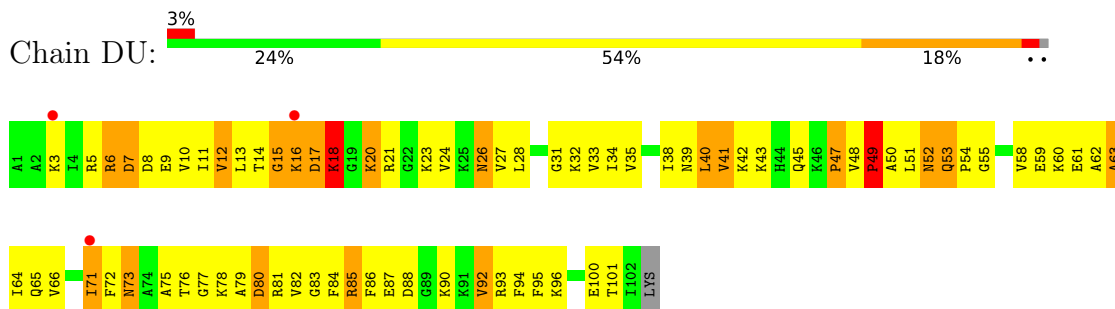
- Molecule 43: 50S ribosomal protein L23



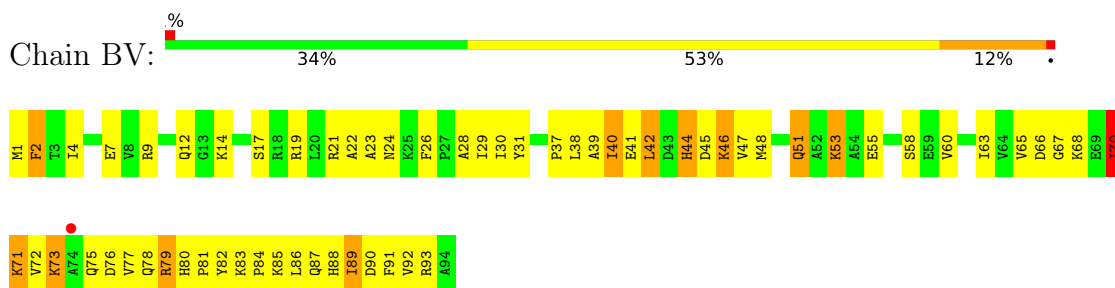
- Molecule 44: 50S ribosomal protein L24



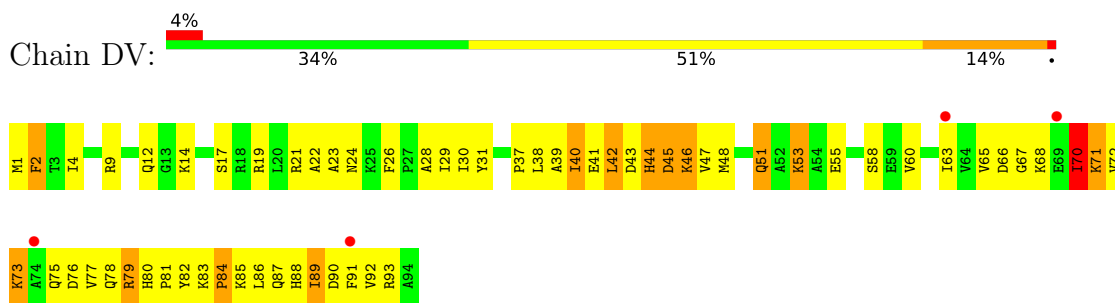
- Molecule 44: 50S ribosomal protein L24



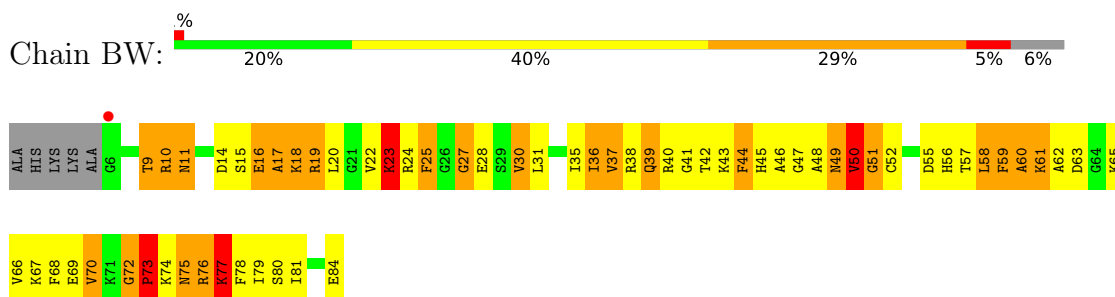
- Molecule 45: 50S ribosomal protein L25



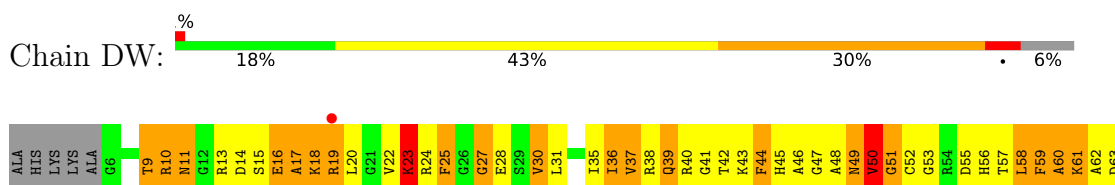
- Molecule 45: 50S ribosomal protein L25



- Molecule 46: 50S ribosomal protein L27

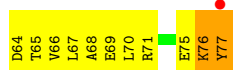
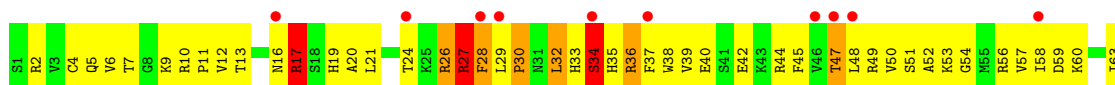


- Molecule 46: 50S ribosomal protein L27

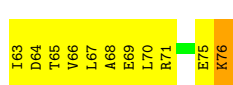
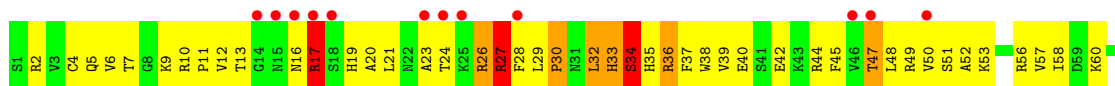




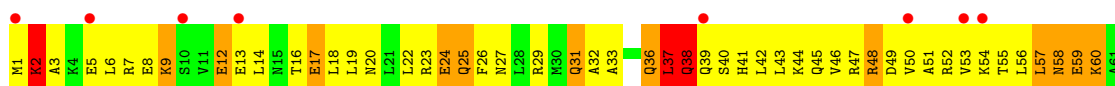
• Molecule 47: 50S ribosomal protein L28



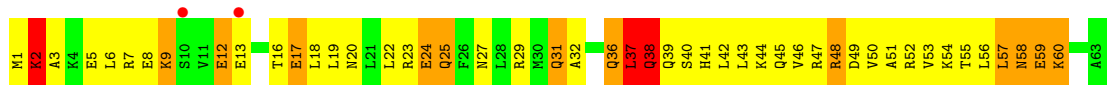
• Molecule 47: 50S ribosomal protein L28



• Molecule 48: 50S ribosomal protein L29



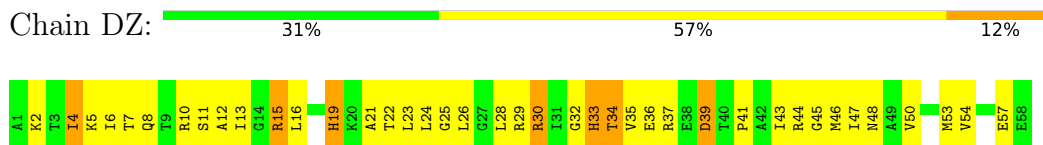
• Molecule 48: 50S ribosomal protein L29



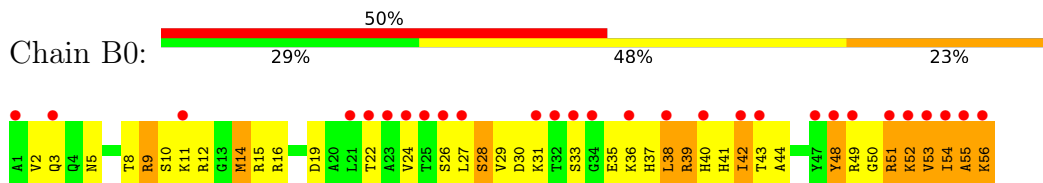
• Molecule 49: 50S ribosomal protein L30



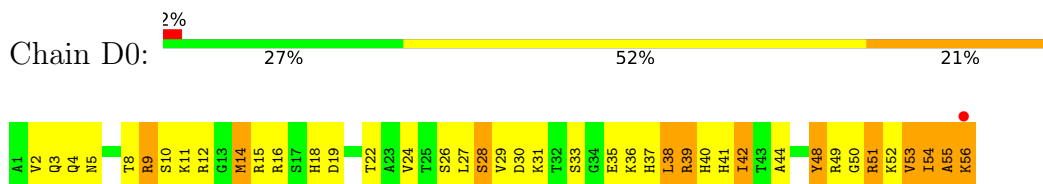
- Molecule 49: 50S ribosomal protein L30



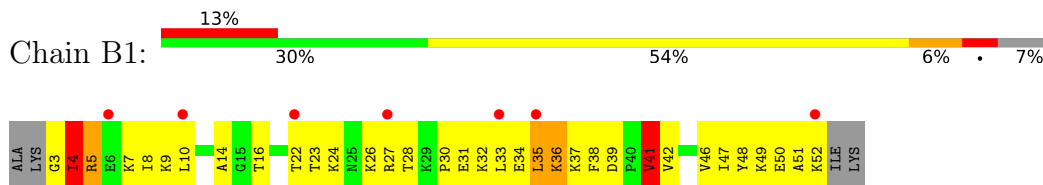
- Molecule 50: 50S ribosomal protein L32



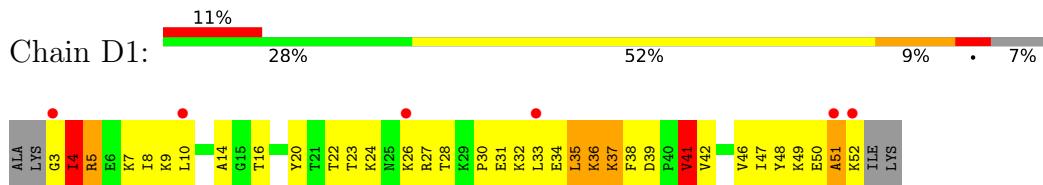
- Molecule 50: 50S ribosomal protein L32



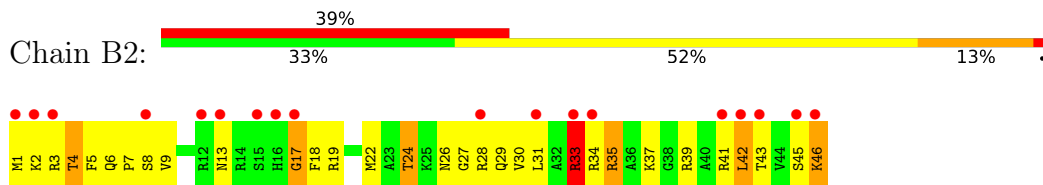
- Molecule 51: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L33

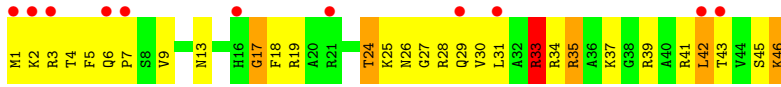


- Molecule 52: 50S ribosomal protein L34

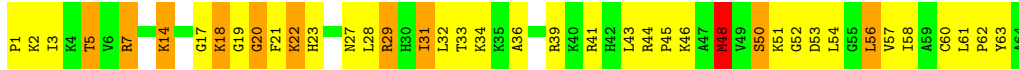


- Molecule 52: 50S ribosomal protein L34

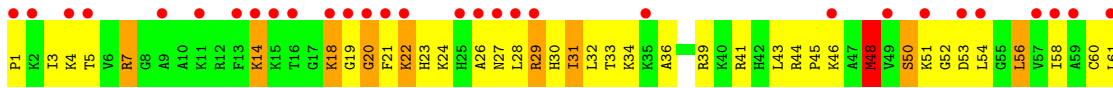




- Molecule 53: 50S ribosomal protein L35



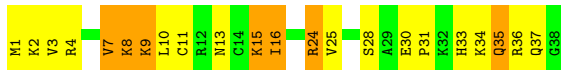
- Molecule 53: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L36



- Molecule 54: 50S ribosomal protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.78Å 395.22Å 744.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.22 184.07 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.22) 75.6 (184.07-3.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 3.19Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.287 , 0.320 0.260 , 0.288	Depositor DCC
$R_{free}$ test set	37294 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.0	Xtrriage
Anisotropy	0.720	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 62.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	285033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	AA	0.25	0/36762	0.74	11/57350 (0.0%)
1	CA	0.25	0/36762	0.73	7/57350 (0.0%)
2	AW	0.32	0/401	0.75	0/622
2	CW	0.31	0/401	0.74	0/622
3	AX	0.48	0/138	0.88	0/212
3	CX	0.49	0/138	0.88	0/212
4	AB	0.25	0/1735	0.44	0/2338
4	CB	0.25	0/1735	0.45	0/2338
5	AC	0.23	0/1651	0.44	0/2225
5	CC	0.23	0/1651	0.44	0/2225
6	AD	0.23	0/1665	0.44	0/2227
6	CD	0.23	0/1665	0.45	0/2227
7	AE	0.23	0/1118	0.45	0/1504
7	CE	0.23	0/1118	0.47	0/1504
8	AF	0.24	0/835	0.44	0/1128
8	CF	0.24	0/835	0.45	0/1128
9	AG	0.23	0/1187	0.43	0/1591
9	CG	0.23	0/1187	0.44	0/1591
10	AH	0.23	0/989	0.47	0/1326
10	CH	0.23	0/989	0.46	0/1326
11	AI	0.24	0/1034	0.45	0/1375
11	CI	0.24	0/1034	0.44	0/1375
12	AJ	0.22	0/796	0.47	0/1077
12	CJ	0.22	0/796	0.47	0/1077
13	AK	0.24	0/893	0.46	0/1205
13	CK	0.24	0/893	0.45	0/1205
14	AL	0.22	0/969	0.46	0/1300
14	CL	0.22	0/969	0.46	0/1300
15	AM	0.21	0/892	0.46	0/1193
15	CM	0.22	0/884	0.46	0/1181
16	AN	0.24	0/785	0.43	0/1043
16	CN	0.24	0/786	0.44	0/1046

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AO	0.23	0/724	0.44	0/966
17	CO	0.23	0/724	0.44	0/966
18	AP	0.25	0/659	0.45	0/884
18	CP	0.25	0/648	0.43	0/870
19	AQ	0.23	0/657	0.46	0/881
19	CQ	0.24	0/657	0.46	0/881
20	AR	0.23	0/462	0.45	0/621
20	CR	0.23	0/462	0.46	0/621
21	AS	0.25	0/652	0.43	0/877
21	CS	0.25	0/652	0.45	0/877
22	AT	0.23	0/671	0.42	0/888
22	CT	0.23	0/671	0.41	0/888
23	AU	0.26	0/430	0.45	0/570
23	CU	0.26	0/430	0.44	0/570
24	BA	0.24	0/2803	0.72	0/4371
24	DA	0.24	0/2803	0.73	0/4371
25	BB	0.27	7/68314 (0.0%)	0.77	53/106569 (0.0%)
25	DB	0.28	7/68314 (0.0%)	0.77	62/106569 (0.1%)
26	BC	0.22	0/2121	0.52	0/2852
26	DC	0.22	0/2121	0.52	0/2852
27	BD	0.25	0/1586	0.60	0/2134
27	DD	0.25	0/1586	0.60	0/2134
28	BE	0.24	0/1571	0.61	2/2113 (0.1%)
28	DE	0.24	0/1571	0.61	2/2113 (0.1%)
29	BF	0.26	0/1444	0.59	0/1937
29	DF	0.27	0/1444	0.59	0/1937
30	BG	0.23	0/1343	0.52	0/1816
30	DG	0.23	0/1343	0.52	0/1816
31	BH	0.28	0/1122	0.56	1/1515 (0.1%)
31	DH	0.26	0/1122	0.52	0/1515
32	BI	0.24	0/1046	0.46	0/1410
32	DI	0.24	0/1046	0.46	0/1410
33	BJ	0.24	0/1152	0.59	0/1551
33	DJ	0.24	0/1152	0.59	0/1551
34	BK	0.25	0/939	0.81	2/1258 (0.2%)
34	DK	0.25	0/939	0.81	2/1258 (0.2%)
35	BL	0.23	0/1054	0.58	0/1403
35	DL	0.23	0/1054	0.58	0/1403
36	BM	0.26	0/1093	0.56	0/1460
36	DM	0.26	0/1093	0.56	0/1460
37	BN	0.25	0/973	0.62	0/1301
37	DN	0.25	0/973	0.62	0/1301
38	BO	0.24	0/902	0.55	0/1209

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DO	0.23	0/902	0.55	0/1209
39	BP	0.25	0/929	0.60	0/1242
39	DP	0.25	0/929	0.60	0/1242
40	BQ	0.26	0/960	0.65	0/1278
40	DQ	0.26	0/960	0.65	0/1278
41	BR	0.26	0/829	0.58	0/1107
41	DR	0.26	0/829	0.58	0/1107
42	BS	0.23	0/864	0.61	1/1156 (0.1%)
42	DS	0.23	0/864	0.61	1/1156 (0.1%)
43	BT	0.23	0/744	0.73	2/994 (0.2%)
43	DT	0.23	0/744	0.73	2/994 (0.2%)
44	BU	0.26	0/787	0.56	0/1051
44	DU	0.26	0/787	0.56	0/1051
45	BV	0.25	0/766	0.46	0/1025
45	DV	0.25	0/766	0.46	0/1025
46	BW	0.31	0/603	0.65	0/797
46	DW	0.31	0/603	0.65	0/797
47	BX	0.25	0/635	0.58	0/848
47	DX	0.25	0/635	0.58	0/848
48	BY	0.24	0/510	0.64	0/677
48	DY	0.25	0/510	0.64	0/677
49	BZ	0.24	0/453	0.55	0/605
49	DZ	0.23	0/453	0.55	0/605
50	B0	0.23	0/450	0.65	0/599
50	D0	0.22	0/450	0.65	0/599
51	B1	0.27	0/416	0.55	0/554
51	D1	0.27	0/416	0.55	0/554
52	B2	0.26	0/380	0.58	0/498
52	D2	0.26	0/380	0.58	0/498
53	B3	0.26	0/513	0.66	2/676 (0.3%)
53	D3	0.26	0/513	0.66	2/676 (0.3%)
54	B4	0.24	0/303	0.54	0/397
54	D4	0.23	0/303	0.54	0/397
All	All	0.26	14/307402 (0.0%)	0.70	152/459589 (0.0%)

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	AA	0	16

*Continued on next page...*

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	CA	0	15
25	BB	0	37
25	DB	0	36
All	All	0	104

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BB	1086	A	C5-C6	-16.31	1.26	1.41
25	DB	1086	A	C5-C6	-16.20	1.26	1.41
25	DB	1088	A	C6-N1	-10.54	1.28	1.35
25	BB	1088	A	C6-N1	-10.43	1.28	1.35
25	DB	1060	U	C2-N3	7.83	1.43	1.37

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	DB	2204	G	O5'-P-OP1	-29.28	75.56	110.70
25	DB	2791	G	O5'-P-OP2	-29.23	75.63	110.70
25	BB	2791	G	O5'-P-OP1	-28.43	76.59	110.70
25	BB	2204	G	O5'-P-OP2	-27.54	77.65	110.70
25	DB	2204	G	O5'-P-OP2	18.17	132.50	110.70

There are no chirality outliers.

5 of 104 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	437	U	Sidechain
1	AA	82	G	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1479	0
1	CA	32831	0	16521	1483	0
2	AW	360	0	185	9	0
2	CW	360	0	185	9	0
3	AX	125	0	63	6	0
3	CX	125	0	63	5	0
4	AB	1704	0	1732	269	0
4	CB	1704	0	1732	320	0
5	AC	1624	0	1699	212	0
5	CC	1624	0	1699	251	0
6	AD	1643	0	1710	195	0
6	CD	1643	0	1710	260	0
7	AE	1105	0	1148	159	0
7	CE	1105	0	1148	217	0
8	AF	817	0	808	94	0
8	CF	817	0	808	123	0
9	AG	1174	0	1230	146	0
9	CG	1174	0	1230	167	0
10	AH	979	0	1034	120	0
10	CH	979	0	1034	166	0
11	AI	1022	0	1070	188	0
11	CI	1022	0	1070	193	0
12	AJ	786	0	828	125	0
12	CJ	786	0	828	121	0
13	AK	877	0	887	117	0
13	CK	877	0	887	141	0
14	AL	955	0	1019	139	0
14	CL	955	0	1019	119	0
15	AM	883	0	944	127	0
15	CM	876	0	937	165	0
16	AN	774	0	827	128	0
16	CN	774	0	828	133	0
17	AO	716	0	742	62	0
17	CO	716	0	742	70	0
18	AP	649	0	666	101	0
18	CP	638	0	656	103	0
19	AQ	648	0	691	97	0
19	CQ	648	0	691	75	0
20	AR	455	0	478	76	0
20	CR	455	0	478	54	0
21	AS	637	0	665	83	0
21	CS	637	0	665	109	0
22	AT	665	0	714	57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CT	665	0	714	60	0
23	AU	425	0	449	77	0
23	CU	425	0	449	88	0
24	BA	2507	0	1270	87	0
24	DA	2507	0	1270	76	0
25	BB	60995	0	30678	2083	0
25	DB	60995	0	30678	2153	0
26	BC	2082	0	2157	218	0
26	DC	2082	0	2157	215	0
27	BD	1565	0	1616	219	0
27	DD	1565	0	1616	215	0
28	BE	1552	0	1619	163	0
28	DE	1552	0	1619	165	0
29	BF	1420	0	1460	254	0
29	DF	1420	0	1460	241	0
30	BG	1323	0	1374	181	0
30	DG	1323	0	1374	175	0
31	BH	1111	0	1148	203	0
31	DH	1111	0	1148	174	0
32	BI	1032	0	1088	108	0
32	DI	1032	0	1088	184	0
33	BJ	1129	0	1162	155	0
33	DJ	1129	0	1162	167	0
34	BK	930	0	1003	99	0
34	DK	930	0	1003	96	0
35	BL	1045	0	1117	123	0
35	DL	1045	0	1117	123	0
36	BM	1074	0	1157	109	0
36	DM	1074	0	1157	105	0
37	BN	960	0	1000	103	0
37	DN	960	0	1000	102	0
38	BO	892	0	923	77	0
38	DO	892	0	923	73	0
39	BP	917	0	965	118	0
39	DP	917	0	965	111	0
40	BQ	947	0	1022	133	0
40	DQ	947	0	1022	140	0
41	BR	816	0	839	111	0
41	DR	816	0	839	114	0
42	BS	857	0	922	95	0
42	DS	857	0	922	96	0
43	BT	738	0	807	109	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DT	738	0	807	118	0
44	BU	779	0	834	111	0
44	DU	779	0	834	105	0
45	BV	753	0	780	75	0
45	DV	753	0	780	71	0
46	BW	596	0	610	149	0
46	DW	596	0	610	146	0
47	BX	625	0	655	79	0
47	DX	625	0	655	78	0
48	BY	509	0	543	84	0
48	DY	509	0	543	75	0
49	BZ	449	0	491	47	0
49	DZ	449	0	491	40	0
50	B0	444	0	461	45	0
50	D0	444	0	461	48	0
51	B1	409	0	440	31	0
51	D1	409	0	440	32	0
52	B2	377	0	418	32	0
52	D2	377	0	418	29	0
53	B3	504	0	574	49	0
53	D3	504	0	574	48	0
54	B4	302	0	340	27	0
54	D4	302	0	340	28	0
55	AA	60	0	0	0	0
55	AX	2	0	0	0	0
55	BB	118	0	0	0	0
55	BJ	1	0	0	0	0
55	CA	56	0	0	0	0
55	CN	1	0	0	0	0
55	CX	1	0	0	0	0
55	DB	119	0	0	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	287	0	0	5	0
57	AE	3	0	0	0	0
57	AI	1	0	0	0	0
57	AK	2	0	0	0	0
57	AL	2	0	0	0	0
57	AN	1	0	0	0	0
57	AP	1	0	0	0	0
57	AT	2	0	0	0	0
57	AX	9	0	0	1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B2	1	0	0	0	0
57	B4	5	0	0	0	0
57	BB	532	0	0	7	0
57	BC	7	0	0	0	0
57	BE	3	0	0	0	0
57	BH	3	0	0	0	0
57	BJ	3	0	0	0	0
57	BL	2	0	0	1	0
57	BN	3	0	0	0	0
57	CA	264	0	0	4	0
57	CE	2	0	0	0	0
57	CI	3	0	0	1	0
57	CL	1	0	0	0	0
57	CN	1	0	0	0	0
57	CP	1	0	0	0	0
57	CT	3	0	0	0	0
57	CU	1	0	0	0	0
57	CX	6	0	0	1	0
57	D2	1	0	0	0	0
57	D4	4	0	0	0	0
57	DB	531	0	0	5	0
57	DC	7	0	0	0	0
57	DD	1	0	0	0	0
57	DE	3	0	0	0	0
57	DJ	2	0	0	0	0
57	DL	3	0	0	0	0
57	DN	3	0	0	0	0
57	DT	1	0	0	0	0
All	All	285033	0	191150	17782	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 38.

The worst 5 of 17782 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)
37:DN:101:GLY:HA2	37:DN:110:MET:H	1.04	1.18
27:BD:148:GLN:HG3	27:BD:152:PRO:HG2	1.29	1.15
34:BK:70:ARG:HB3	34:BK:71:PRO:CD	1.76	1.14
37:BN:101:GLY:HA2	37:BN:110:MET:H	1.06	1.13
28:DE:46:GLN:HG3	28:DE:87:ALA:HB3	1.31	1.12



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	
4	AB	216/240 (90%)	133 (62%)	59 (27%)	24 (11%)	0	2
4	CB	216/240 (90%)	106 (49%)	71 (33%)	39 (18%)	0	0
5	AC	204/232 (88%)	134 (66%)	50 (24%)	20 (10%)	0	3
5	CC	204/232 (88%)	119 (58%)	57 (28%)	28 (14%)	0	1
6	AD	203/205 (99%)	123 (61%)	56 (28%)	24 (12%)	0	2
6	CD	203/205 (99%)	122 (60%)	54 (27%)	27 (13%)	0	1
7	AE	148/166 (89%)	101 (68%)	38 (26%)	9 (6%)	1	11
7	CE	148/166 (89%)	78 (53%)	50 (34%)	20 (14%)	0	1
8	AF	98/135 (73%)	63 (64%)	24 (24%)	11 (11%)	0	2
8	CF	98/135 (73%)	52 (53%)	30 (31%)	16 (16%)	0	1
9	AG	148/178 (83%)	107 (72%)	31 (21%)	10 (7%)	1	8
9	CG	148/178 (83%)	89 (60%)	40 (27%)	19 (13%)	0	1
10	AH	127/129 (98%)	83 (65%)	31 (24%)	13 (10%)	0	3
10	CH	127/129 (98%)	78 (61%)	35 (28%)	14 (11%)	0	2
11	AI	125/129 (97%)	78 (62%)	33 (26%)	14 (11%)	0	2
11	CI	125/129 (97%)	74 (59%)	44 (35%)	7 (6%)	2	13
12	AJ	96/103 (93%)	55 (57%)	27 (28%)	14 (15%)	0	1
12	CJ	96/103 (93%)	60 (62%)	22 (23%)	14 (15%)	0	1
13	AK	115/128 (90%)	75 (65%)	30 (26%)	10 (9%)	1	4
13	CK	115/128 (90%)	82 (71%)	25 (22%)	8 (7%)	1	7
14	AL	121/123 (98%)	80 (66%)	30 (25%)	11 (9%)	1	3
14	CL	121/123 (98%)	80 (66%)	24 (20%)	17 (14%)	0	1

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	AM	112/117 (96%)	75 (67%)	22 (20%)	15 (13%)	0	1
15	CM	111/117 (95%)	66 (60%)	29 (26%)	16 (14%)	0	1
16	AN	92/100 (92%)	61 (66%)	25 (27%)	6 (6%)	1	9
16	CN	94/100 (94%)	46 (49%)	29 (31%)	19 (20%)	0	0
17	AO	86/88 (98%)	69 (80%)	14 (16%)	3 (4%)	3	23
17	CO	86/88 (98%)	70 (81%)	14 (16%)	2 (2%)	6	33
18	AP	80/82 (98%)	46 (58%)	26 (32%)	8 (10%)	0	3
18	CP	78/82 (95%)	53 (68%)	17 (22%)	8 (10%)	0	3
19	AQ	78/83 (94%)	51 (65%)	16 (20%)	11 (14%)	0	1
19	CQ	78/83 (94%)	51 (65%)	20 (26%)	7 (9%)	1	4
20	AR	53/74 (72%)	39 (74%)	9 (17%)	5 (9%)	0	3
20	CR	53/74 (72%)	37 (70%)	12 (23%)	4 (8%)	1	6
21	AS	77/91 (85%)	53 (69%)	19 (25%)	5 (6%)	1	9
21	CS	77/91 (85%)	55 (71%)	18 (23%)	4 (5%)	2	14
22	AT	83/86 (96%)	63 (76%)	11 (13%)	9 (11%)	0	2
22	CT	83/86 (96%)	59 (71%)	20 (24%)	4 (5%)	2	16
23	AU	49/70 (70%)	21 (43%)	17 (35%)	11 (22%)	0	0
23	CU	49/70 (70%)	27 (55%)	16 (33%)	6 (12%)	0	2
26	BC	269/272 (99%)	166 (62%)	68 (25%)	35 (13%)	0	1
26	DC	269/272 (99%)	168 (62%)	63 (23%)	38 (14%)	0	1
27	BD	207/209 (99%)	113 (55%)	56 (27%)	38 (18%)	0	0
27	DD	207/209 (99%)	110 (53%)	56 (27%)	41 (20%)	0	0
28	BE	199/201 (99%)	126 (63%)	43 (22%)	30 (15%)	0	1
28	DE	199/201 (99%)	127 (64%)	42 (21%)	30 (15%)	0	1
29	BF	176/178 (99%)	97 (55%)	40 (23%)	39 (22%)	0	0
29	DF	176/178 (99%)	95 (54%)	43 (24%)	38 (22%)	0	0
30	BG	174/176 (99%)	94 (54%)	54 (31%)	26 (15%)	0	1
30	DG	174/176 (99%)	93 (53%)	55 (32%)	26 (15%)	0	1
31	BH	147/149 (99%)	69 (47%)	50 (34%)	28 (19%)	0	0
31	DH	147/149 (99%)	68 (46%)	54 (37%)	25 (17%)	0	0
32	BI	139/141 (99%)	118 (85%)	16 (12%)	5 (4%)	3	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	DI	139/141 (99%)	114 (82%)	21 (15%)	4 (3%)	4	27
33	BJ	140/142 (99%)	88 (63%)	30 (21%)	22 (16%)	0	1
33	DJ	140/142 (99%)	88 (63%)	30 (21%)	22 (16%)	0	1
34	BK	119/123 (97%)	75 (63%)	26 (22%)	18 (15%)	0	1
34	DK	119/123 (97%)	75 (63%)	26 (22%)	18 (15%)	0	1
35	BL	141/144 (98%)	81 (57%)	37 (26%)	23 (16%)	0	1
35	DL	141/144 (98%)	81 (57%)	37 (26%)	23 (16%)	0	1
36	BM	134/136 (98%)	77 (58%)	32 (24%)	25 (19%)	0	0
36	DM	134/136 (98%)	77 (58%)	33 (25%)	24 (18%)	0	0
37	BN	118/127 (93%)	75 (64%)	27 (23%)	16 (14%)	0	1
37	DN	118/127 (93%)	75 (64%)	27 (23%)	16 (14%)	0	1
38	BO	114/117 (97%)	85 (75%)	24 (21%)	5 (4%)	2	18
38	DO	114/117 (97%)	85 (75%)	24 (21%)	5 (4%)	2	18
39	BP	112/114 (98%)	71 (63%)	20 (18%)	21 (19%)	0	0
39	DP	112/114 (98%)	71 (63%)	20 (18%)	21 (19%)	0	0
40	BQ	115/117 (98%)	74 (64%)	28 (24%)	13 (11%)	0	2
40	DQ	115/117 (98%)	74 (64%)	28 (24%)	13 (11%)	0	2
41	BR	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	1
41	DR	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	1
42	BS	108/110 (98%)	66 (61%)	26 (24%)	16 (15%)	0	1
42	DS	108/110 (98%)	66 (61%)	26 (24%)	16 (15%)	0	1
43	BT	91/100 (91%)	54 (59%)	23 (25%)	14 (15%)	0	1
43	DT	91/100 (91%)	52 (57%)	25 (28%)	14 (15%)	0	1
44	BU	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	1
44	DU	100/103 (97%)	57 (57%)	28 (28%)	15 (15%)	0	1
45	BV	92/94 (98%)	74 (80%)	11 (12%)	7 (8%)	1	6
45	DV	92/94 (98%)	73 (79%)	12 (13%)	7 (8%)	1	6
46	BW	77/84 (92%)	29 (38%)	23 (30%)	25 (32%)	0	0
46	DW	77/84 (92%)	29 (38%)	22 (29%)	26 (34%)	0	0
47	BX	75/77 (97%)	43 (57%)	26 (35%)	6 (8%)	1	5
47	DX	75/77 (97%)	41 (55%)	27 (36%)	7 (9%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	BY	61/63 (97%)	37 (61%)	18 (30%)	6 (10%)	0	3
48	DY	61/63 (97%)	34 (56%)	21 (34%)	6 (10%)	0	3
49	BZ	56/58 (97%)	42 (75%)	11 (20%)	3 (5%)	2	13
49	DZ	56/58 (97%)	42 (75%)	11 (20%)	3 (5%)	2	13
50	B0	54/56 (96%)	35 (65%)	8 (15%)	11 (20%)	0	0
50	D0	54/56 (96%)	34 (63%)	10 (18%)	10 (18%)	0	0
51	B1	48/54 (89%)	33 (69%)	7 (15%)	8 (17%)	0	1
51	D1	48/54 (89%)	33 (69%)	6 (12%)	9 (19%)	0	0
52	B2	44/46 (96%)	26 (59%)	13 (30%)	5 (11%)	0	2
52	D2	44/46 (96%)	26 (59%)	14 (32%)	4 (9%)	1	3
53	B3	62/64 (97%)	42 (68%)	15 (24%)	5 (8%)	1	5
53	D3	62/64 (97%)	41 (66%)	17 (27%)	4 (6%)	1	9
54	B4	36/38 (95%)	21 (58%)	11 (31%)	4 (11%)	0	2
54	D4	36/38 (95%)	21 (58%)	11 (31%)	4 (11%)	0	2
All	All	11239/11910 (94%)	6961 (62%)	2802 (25%)	1476 (13%)	0	1

5 of 1476 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AB	19	THR
4	AB	22	TRP
4	AB	75	ALA
4	AB	76	SER
4	AB	91	VAL

### 5.3.2 Protein sidechains [i](#)

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	
4	AB	180/198 (91%)	140 (78%)	40 (22%)	1	4
4	CB	180/198 (91%)	143 (79%)	37 (21%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AC	170/189 (90%)	134 (79%)	36 (21%)	1	5
5	CC	170/189 (90%)	138 (81%)	32 (19%)	1	8
6	AD	172/172 (100%)	146 (85%)	26 (15%)	3	13
6	CD	172/172 (100%)	130 (76%)	42 (24%)	0	2
7	AE	113/125 (90%)	95 (84%)	18 (16%)	2	11
7	CE	113/125 (90%)	87 (77%)	26 (23%)	1	3
8	AF	87/116 (75%)	74 (85%)	13 (15%)	3	13
8	CF	87/116 (75%)	76 (87%)	11 (13%)	4	20
9	AG	123/146 (84%)	99 (80%)	24 (20%)	1	7
9	CG	123/146 (84%)	100 (81%)	23 (19%)	1	8
10	AH	104/104 (100%)	89 (86%)	15 (14%)	3	14
10	CH	104/104 (100%)	81 (78%)	23 (22%)	1	4
11	AI	105/106 (99%)	83 (79%)	22 (21%)	1	5
11	CI	105/106 (99%)	83 (79%)	22 (21%)	1	5
12	AJ	86/90 (96%)	75 (87%)	11 (13%)	4	19
12	CJ	86/90 (96%)	71 (83%)	15 (17%)	2	9
13	AK	90/98 (92%)	75 (83%)	15 (17%)	2	10
13	CK	90/98 (92%)	77 (86%)	13 (14%)	3	14
14	AL	103/103 (100%)	83 (81%)	20 (19%)	1	7
14	CL	103/103 (100%)	80 (78%)	23 (22%)	1	4
15	AM	92/95 (97%)	75 (82%)	17 (18%)	1	8
15	CM	91/95 (96%)	71 (78%)	20 (22%)	1	4
16	AN	79/83 (95%)	60 (76%)	19 (24%)	0	3
16	CN	79/83 (95%)	66 (84%)	13 (16%)	2	10
17	AO	76/76 (100%)	65 (86%)	11 (14%)	3	14
17	CO	76/76 (100%)	67 (88%)	9 (12%)	5	22
18	AP	65/65 (100%)	52 (80%)	13 (20%)	1	6
18	CP	65/65 (100%)	58 (89%)	7 (11%)	6	26
19	AQ	74/77 (96%)	60 (81%)	14 (19%)	1	8
19	CQ	74/77 (96%)	66 (89%)	8 (11%)	6	26
20	AR	48/64 (75%)	37 (77%)	11 (23%)	1	4

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	CR	48/64 (75%)	43 (90%)	5 (10%)	7	28
21	AS	70/78 (90%)	55 (79%)	15 (21%)	1	5
21	CS	70/78 (90%)	51 (73%)	19 (27%)	0	1
22	AT	65/65 (100%)	56 (86%)	9 (14%)	3	16
22	CT	65/65 (100%)	55 (85%)	10 (15%)	2	12
23	AU	44/60 (73%)	37 (84%)	7 (16%)	2	11
23	CU	44/60 (73%)	32 (73%)	12 (27%)	0	1
26	BC	216/217 (100%)	182 (84%)	34 (16%)	2	11
26	DC	216/217 (100%)	182 (84%)	34 (16%)	2	11
27	BD	164/164 (100%)	136 (83%)	28 (17%)	2	9
27	DD	164/164 (100%)	137 (84%)	27 (16%)	2	10
28	BE	165/165 (100%)	130 (79%)	35 (21%)	1	5
28	DE	165/165 (100%)	130 (79%)	35 (21%)	1	5
29	BF	149/149 (100%)	116 (78%)	33 (22%)	1	4
29	DF	149/149 (100%)	117 (78%)	32 (22%)	1	5
30	BG	137/137 (100%)	110 (80%)	27 (20%)	1	6
30	DG	137/137 (100%)	110 (80%)	27 (20%)	1	6
31	BH	114/114 (100%)	85 (75%)	29 (25%)	0	2
31	DH	114/114 (100%)	86 (75%)	28 (25%)	0	2
32	BI	109/109 (100%)	107 (98%)	2 (2%)	59	81
32	DI	109/109 (100%)	104 (95%)	5 (5%)	27	62
33	BJ	116/116 (100%)	100 (86%)	16 (14%)	3	16
33	DJ	116/116 (100%)	100 (86%)	16 (14%)	3	16
34	BK	102/104 (98%)	84 (82%)	18 (18%)	2	9
34	DK	102/104 (98%)	83 (81%)	19 (19%)	1	8
35	BL	102/103 (99%)	87 (85%)	15 (15%)	3	14
35	DL	102/103 (99%)	88 (86%)	14 (14%)	3	16
36	BM	109/109 (100%)	93 (85%)	16 (15%)	3	14
36	DM	109/109 (100%)	93 (85%)	16 (15%)	3	14
37	BN	100/103 (97%)	85 (85%)	15 (15%)	3	13
37	DN	100/103 (97%)	84 (84%)	16 (16%)	2	11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BO	86/87 (99%)	76 (88%)	10 (12%)	5	23
38	DO	86/87 (99%)	76 (88%)	10 (12%)	5	23
39	BP	99/99 (100%)	76 (77%)	23 (23%)	1	3
39	DP	99/99 (100%)	77 (78%)	22 (22%)	1	4
40	BQ	89/89 (100%)	73 (82%)	16 (18%)	1	8
40	DQ	89/89 (100%)	73 (82%)	16 (18%)	1	8
41	BR	84/84 (100%)	67 (80%)	17 (20%)	1	6
41	DR	84/84 (100%)	67 (80%)	17 (20%)	1	6
42	BS	93/93 (100%)	79 (85%)	14 (15%)	3	13
42	DS	93/93 (100%)	79 (85%)	14 (15%)	3	13
43	BT	80/84 (95%)	65 (81%)	15 (19%)	1	8
43	DT	80/84 (95%)	64 (80%)	16 (20%)	1	6
44	BU	83/84 (99%)	69 (83%)	14 (17%)	2	10
44	DU	83/84 (99%)	70 (84%)	13 (16%)	2	11
45	BV	78/78 (100%)	67 (86%)	11 (14%)	3	15
45	DV	78/78 (100%)	67 (86%)	11 (14%)	3	15
46	BW	59/62 (95%)	49 (83%)	10 (17%)	2	10
46	DW	59/62 (95%)	48 (81%)	11 (19%)	1	8
47	BX	67/67 (100%)	56 (84%)	11 (16%)	2	10
47	DX	67/67 (100%)	57 (85%)	10 (15%)	3	13
48	BY	55/55 (100%)	43 (78%)	12 (22%)	1	5
48	DY	55/55 (100%)	43 (78%)	12 (22%)	1	5
49	BZ	48/48 (100%)	43 (90%)	5 (10%)	7	28
49	DZ	48/48 (100%)	43 (90%)	5 (10%)	7	28
50	B0	47/47 (100%)	40 (85%)	7 (15%)	3	13
50	D0	47/47 (100%)	40 (85%)	7 (15%)	3	13
51	B1	45/48 (94%)	38 (84%)	7 (16%)	2	11
51	D1	45/48 (94%)	38 (84%)	7 (16%)	2	11
52	B2	38/38 (100%)	33 (87%)	5 (13%)	4	18
52	D2	38/38 (100%)	33 (87%)	5 (13%)	4	18
53	B3	51/51 (100%)	44 (86%)	7 (14%)	3	16

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	D3	51/51 (100%)	43 (84%)	8 (16%)	2	11
54	B4	34/34 (100%)	29 (85%)	5 (15%)	3	14
54	D4	34/34 (100%)	29 (85%)	5 (15%)	3	14
All	All	9329/9696 (96%)	7688 (82%)	1641 (18%)	2	9

5 of 1641 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	CE	11	GLN
21	CS	14	LEU
48	DY	48	ARG
8	CF	13	ASP
7	CE	10	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 364 such sidechains are listed below:

Mol	Chain	Res	Type
13	CK	14	GLN
28	DE	163	ASN
14	CL	28	GLN
22	CT	67	HIS
32	DI	5	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	278 (18%)	20 (1%)
1	CA	1529/1542 (99%)	272 (17%)	19 (1%)
2	AW	16/17 (94%)	0	0
2	CW	16/17 (94%)	0	0
24	BA	116/120 (96%)	19 (16%)	2 (1%)
24	DA	116/120 (96%)	19 (16%)	2 (1%)
25	BB	2837/2904 (97%)	416 (14%)	13 (0%)
25	DB	2837/2904 (97%)	420 (14%)	17 (0%)
3	AX	5/6 (83%)	3 (60%)	0
3	CX	5/6 (83%)	3 (60%)	0
All	All	9006/9178 (98%)	1430 (15%)	73 (0%)

5 of 1430 RNA backbone outliers are listed below:



Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	14	U
1	AA	15	G

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	DB	544	C
25	DB	2756	U
25	DB	784	G
25	DB	2076	U
25	BB	858	G

#### 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 monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

Of 360 ligands modelled in this entry, 360 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1530/1542 (99%)	0.16	153 (10%) 7 4	41, 98, 164, 180	0
1	CA	1530/1542 (99%)	-0.34	14 (0%) 84 76	41, 109, 167, 180	0
2	AW	17/17 (100%)	2.89	10 (58%) 0 0	73, 87, 132, 177	0
2	CW	17/17 (100%)	0.22	1 (5%) 22 13	63, 86, 126, 150	0
3	AX	6/6 (100%)	6.38	6 (100%) 0 0	63, 78, 113, 127	0
3	CX	6/6 (100%)	1.48	3 (50%) 0 0	76, 83, 113, 115	0
4	AB	218/240 (90%)	2.82	129 (59%) 0 0	59, 127, 169, 180	0
4	CB	218/240 (90%)	3.74	136 (62%) 0 0	67, 141, 180, 180	0
5	AC	206/232 (88%)	2.89	128 (62%) 0 0	61, 104, 153, 180	0
5	CC	206/232 (88%)	2.29	97 (47%) 0 0	69, 121, 161, 180	0
6	AD	205/205 (100%)	1.85	79 (38%) 0 0	44, 106, 149, 180	0
6	CD	205/205 (100%)	1.93	79 (38%) 0 0	67, 120, 164, 180	0
7	AE	150/166 (90%)	2.31	81 (54%) 0 0	39, 98, 148, 180	0
7	CE	150/166 (90%)	2.52	63 (42%) 0 0	46, 129, 180, 180	0
8	AF	100/135 (74%)	1.21	25 (25%) 0 0	52, 100, 148, 180	0
8	CF	100/135 (74%)	1.47	29 (29%) 0 0	33, 101, 144, 165	0
9	AG	150/178 (84%)	2.10	63 (42%) 0 0	55, 113, 167, 180	0
9	CG	150/178 (84%)	-0.09	12 (8%) 12 7	71, 122, 165, 180	0
10	AH	129/129 (100%)	0.34	13 (10%) 7 4	51, 100, 143, 179	0
10	CH	129/129 (100%)	-0.46	1 (0%) 86 79	37, 106, 149, 176	0
11	AI	127/129 (98%)	0.35	11 (8%) 10 6	84, 120, 166, 180	0
11	CI	127/129 (98%)	-0.56	2 (1%) 72 60	68, 128, 167, 180	0
12	AJ	98/103 (95%)	1.73	47 (47%) 0 0	56, 124, 172, 180	0
12	CJ	98/103 (95%)	1.63	28 (28%) 0 0	76, 131, 164, 180	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AK	117/128 (91%)	5.16	107 (91%) 0 0	36, 91, 142, 180	0
13	CK	117/128 (91%)	2.09	52 (44%) 0 0	48, 91, 131, 159	0
14	AL	123/123 (100%)	3.68	87 (70%) 0 0	31, 80, 130, 169	0
14	CL	123/123 (100%)	1.70	50 (40%) 0 0	42, 91, 138, 172	0
15	AM	114/117 (97%)	-0.06	6 (5%) 26 15	63, 119, 165, 180	0
15	CM	113/117 (96%)	-0.46	2 (1%) 68 56	58, 121, 165, 176	0
16	AN	96/100 (96%)	0.70	19 (19%) 1 0	56, 112, 155, 180	0
16	CN	96/100 (96%)	1.06	21 (21%) 0 0	65, 124, 154, 180	0
17	AO	88/88 (100%)	0.07	4 (4%) 33 21	54, 91, 138, 180	0
17	CO	88/88 (100%)	0.22	4 (4%) 33 21	37, 96, 143, 160	0
18	AP	82/82 (100%)	-0.52	0 100 100	49, 95, 163, 180	0
18	CP	80/82 (97%)	-0.52	0 100 100	68, 113, 155, 180	0
19	AQ	80/83 (96%)	-0.10	1 (1%) 77 66	54, 107, 155, 169	0
19	CQ	80/83 (96%)	-0.50	0 100 100	50, 104, 145, 155	0
20	AR	55/74 (74%)	2.82	35 (63%) 0 0	52, 98, 134, 158	0
20	CR	55/74 (74%)	2.03	24 (43%) 0 0	46, 101, 144, 157	0
21	AS	79/91 (86%)	0.27	8 (10%) 7 4	80, 133, 169, 180	0
21	CS	79/91 (86%)	0.02	4 (5%) 28 17	75, 128, 160, 180	0
22	AT	85/86 (98%)	-0.77	0 100 100	62, 101, 151, 162	0
22	CT	85/86 (98%)	-0.44	0 100 100	65, 104, 154, 180	0
23	AU	51/70 (72%)	5.08	43 (84%) 0 0	54, 110, 154, 180	0
23	CU	51/70 (72%)	1.88	18 (35%) 0 0	63, 125, 169, 180	0
24	BA	117/120 (97%)	0.93	5 (4%) 35 23	44, 75, 109, 180	0
24	DA	117/120 (97%)	-0.31	1 (0%) 84 76	33, 66, 105, 180	0
25	BB	2841/2904 (97%)	0.15	119 (4%) 36 24	13, 70, 147, 180	0
25	DB	2841/2904 (97%)	0.04	53 (1%) 66 54	12, 55, 149, 180	0
26	BC	271/272 (99%)	1.98	123 (45%) 0 0	16, 66, 111, 151	0
26	DC	271/272 (99%)	1.61	88 (32%) 0 0	9, 52, 97, 153	0
27	BD	209/209 (100%)	1.96	95 (45%) 0 0	25, 83, 146, 180	0
27	DD	209/209 (100%)	0.56	10 (4%) 30 19	20, 59, 119, 166	0
28	BE	201/201 (100%)	0.66	27 (13%) 3 2	22, 78, 139, 172	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DE	201/201 (100%)	2.42	107 (53%) 0 0	11, 76, 143, 178	0
29	BF	178/178 (100%)	-0.27	1 (0%) 89 84	49, 111, 174, 180	0
29	DF	178/178 (100%)	0.09	6 (3%) 45 31	49, 110, 166, 180	0
30	BG	176/176 (100%)	-0.19	8 (4%) 33 21	47, 112, 165, 176	0
30	DG	176/176 (100%)	-0.36	2 (1%) 80 70	38, 88, 155, 174	0
31	BH	149/149 (100%)	3.61	71 (47%) 0 0	52, 131, 180, 180	0
31	DH	149/149 (100%)	1.54	44 (29%) 0 0	35, 109, 150, 180	0
32	BI	141/141 (100%)	2.74	69 (48%) 0 0	110, 167, 180, 180	0
32	DI	141/141 (100%)	3.53	84 (59%) 0 0	105, 179, 180, 180	0
33	BJ	142/142 (100%)	-0.00	4 (2%) 53 39	32, 86, 133, 180	0
33	DJ	142/142 (100%)	-0.16	0 100 100	19, 53, 108, 175	0
34	BK	121/123 (98%)	4.14	115 (95%) 0 0	32, 74, 148, 180	0
34	DK	121/123 (98%)	1.91	47 (38%) 0 0	27, 64, 130, 163	0
35	BL	143/144 (99%)	0.13	4 (2%) 53 39	27, 69, 121, 180	0
35	DL	143/144 (99%)	3.19	93 (65%) 0 0	17, 64, 115, 180	0
36	BM	136/136 (100%)	0.39	12 (8%) 10 6	33, 65, 132, 168	0
36	DM	136/136 (100%)	0.28	5 (3%) 41 28	11, 56, 109, 176	0
37	BN	120/127 (94%)	2.29	63 (52%) 0 0	43, 88, 131, 169	0
37	DN	120/127 (94%)	0.39	2 (1%) 70 58	19, 57, 97, 180	0
38	BO	116/117 (99%)	-0.14	0 100 100	34, 77, 118, 138	0
38	DO	116/117 (99%)	-0.39	0 100 100	28, 71, 129, 157	0
39	BP	114/114 (100%)	2.68	73 (64%) 0 0	43, 84, 145, 164	0
39	DP	114/114 (100%)	1.38	27 (23%) 0 0	26, 73, 123, 174	0
40	BQ	117/117 (100%)	-0.16	5 (4%) 35 23	34, 73, 135, 149	0
40	DQ	117/117 (100%)	0.36	10 (8%) 10 6	22, 53, 104, 158	0
41	BR	103/103 (100%)	-0.53	1 (0%) 82 73	44, 95, 146, 177	0
41	DR	103/103 (100%)	-0.09	3 (2%) 51 37	23, 72, 131, 156	0
42	BS	110/110 (100%)	3.74	92 (83%) 0 0	47, 84, 138, 180	0
42	DS	110/110 (100%)	1.16	20 (18%) 1 1	18, 53, 108, 152	0
43	BT	93/100 (93%)	0.93	14 (15%) 2 1	44, 93, 163, 180	0
43	DT	93/100 (93%)	0.65	10 (10%) 5 4	35, 72, 141, 178	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BU	102/103 (99%)	1.83	48 (47%) 0 0	48, 106, 162, 175	0
44	DU	102/103 (99%)	0.15	3 (2%) 51 37	41, 94, 154, 180	0
45	BV	94/94 (100%)	-0.08	1 (1%) 80 70	37, 84, 140, 180	0
45	DV	94/94 (100%)	0.27	4 (4%) 35 23	31, 70, 138, 156	0
46	BW	79/84 (94%)	0.14	1 (1%) 77 66	6, 53, 116, 154	0
46	DW	79/84 (94%)	0.05	1 (1%) 77 66	7, 42, 103, 180	0
47	BX	77/77 (100%)	1.02	11 (14%) 2 2	24, 63, 107, 157	0
47	DX	77/77 (100%)	0.98	13 (16%) 1 1	23, 60, 112, 152	0
48	BY	63/63 (100%)	0.89	10 (15%) 1 1	47, 108, 165, 180	0
48	DY	63/63 (100%)	-0.04	2 (3%) 47 33	34, 92, 158, 180	0
49	BZ	58/58 (100%)	-0.21	0 100 100	40, 74, 124, 150	0
49	DZ	58/58 (100%)	-0.44	0 100 100	22, 58, 110, 114	0
50	B0	56/56 (100%)	2.75	28 (50%) 0 0	35, 87, 152, 180	0
50	D0	56/56 (100%)	0.50	1 (1%) 68 56	19, 56, 118, 135	0
51	B1	50/54 (92%)	0.68	7 (14%) 2 2	43, 72, 122, 140	0
51	D1	50/54 (92%)	0.77	6 (12%) 4 3	26, 76, 119, 163	0
52	B2	46/46 (100%)	1.56	18 (39%) 0 0	42, 61, 97, 162	0
52	D2	46/46 (100%)	1.34	11 (23%) 0 0	17, 47, 97, 131	0
53	B3	64/64 (100%)	0.08	0 100 100	21, 56, 99, 136	0
53	D3	64/64 (100%)	2.28	33 (51%) 0 0	27, 49, 85, 105	0
54	B4	38/38 (100%)	0.27	2 (5%) 26 15	36, 86, 126, 146	0
54	D4	38/38 (100%)	-0.20	0 100 100	44, 68, 126, 165	0
All	All	20459/21088 (97%)	0.71	3408 (16%) 1 1	6, 86, 162, 180	0

The worst 5 of 3408 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	DI	82	ALA	27.6
31	BH	88	GLY	27.1
7	CE	114	LEU	26.5
32	DI	138	VAL	19.9
15	AM	114	PRO	19.3

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	AA	1614	1/1	-0.08	0.74	174,174,174,174	0
55	MG	AA	1635	1/1	0.16	0.12	129,129,129,129	0
55	MG	AA	1658	1/1	0.23	0.53	147,147,147,147	0
55	MG	AA	1630	1/1	0.34	0.18	114,114,114,114	0
55	MG	DB	3115	1/1	0.34	0.25	132,132,132,132	0
55	MG	CA	1632	1/1	0.44	0.17	154,154,154,154	0
55	MG	AA	1626	1/1	0.54	0.75	139,139,139,139	0
55	MG	CA	1646	1/1	0.55	0.52	155,155,155,155	0
55	MG	CA	1610	1/1	0.56	0.17	130,130,130,130	0
55	MG	CA	1649	1/1	0.58	0.08	100,100,100,100	0
55	MG	BB	3010	1/1	0.60	0.17	95,95,95,95	0
55	MG	AA	1641	1/1	0.61	0.09	111,111,111,111	0
55	MG	CA	1629	1/1	0.61	0.09	94,94,94,94	0
55	MG	CA	1640	1/1	0.62	0.49	138,138,138,138	0
55	MG	BB	3019	1/1	0.62	0.10	62,62,62,62	0
55	MG	AA	1625	1/1	0.63	0.19	145,145,145,145	0
55	MG	CA	1618	1/1	0.63	0.12	87,87,87,87	0
55	MG	AA	1637	1/1	0.64	2.75	134,134,134,134	0
55	MG	CA	1627	1/1	0.64	0.13	122,122,122,122	0
55	MG	CA	1635	1/1	0.65	0.20	129,129,129,129	0
55	MG	DB	3052	1/1	0.68	0.68	137,137,137,137	0
55	MG	AA	1643	1/1	0.69	0.52	112,112,112,112	0
55	MG	AA	1618	1/1	0.69	0.12	92,92,92,92	0
55	MG	CA	1622	1/1	0.69	0.09	98,98,98,98	0
55	MG	BB	3076	1/1	0.70	0.20	56,56,56,56	0
55	MG	CA	1607	1/1	0.70	0.09	108,108,108,108	0
55	MG	CA	1653	1/1	0.71	0.12	149,149,149,149	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1619	1/1	0.71	0.36	92,92,92,92	0
55	MG	CA	1643	1/1	0.71	0.09	138,138,138,138	0
55	MG	AA	1639	1/1	0.72	0.11	126,126,126,126	0
55	MG	AA	1611	1/1	0.72	3.92	148,148,148,148	0
55	MG	AA	1652	1/1	0.73	0.39	103,103,103,103	0
55	MG	CA	1614	1/1	0.73	0.33	171,171,171,171	0
55	MG	DB	3059	1/1	0.73	0.13	110,110,110,110	0
55	MG	BB	3046	1/1	0.73	0.10	90,90,90,90	0
55	MG	BB	3014	1/1	0.74	0.31	76,76,76,76	0
55	MG	AA	1608	1/1	0.75	0.28	113,113,113,113	0
55	MG	DB	3013	1/1	0.76	0.10	62,62,62,62	0
55	MG	AA	1621	1/1	0.76	0.28	36,36,36,36	0
55	MG	CA	1625	1/1	0.76	0.07	54,54,54,54	0
55	MG	CA	1644	1/1	0.76	0.11	131,131,131,131	0
55	MG	CA	1650	1/1	0.77	0.06	103,103,103,103	0
55	MG	AA	1613	1/1	0.77	0.09	106,106,106,106	0
55	MG	BB	3115	1/1	0.77	0.18	106,106,106,106	0
55	MG	CA	1631	1/1	0.77	0.09	91,91,91,91	0
55	MG	AA	1647	1/1	0.77	0.39	79,79,79,79	0
55	MG	DB	3065	1/1	0.77	0.29	67,67,67,67	0
55	MG	BB	3057	1/1	0.77	0.76	100,100,100,100	0
55	MG	DB	3082	1/1	0.78	0.22	104,104,104,104	0
55	MG	BB	3093	1/1	0.78	0.69	120,120,120,120	0
55	MG	BB	3051	1/1	0.79	0.14	94,94,94,94	0
55	MG	CA	1636	1/1	0.79	0.06	127,127,127,127	0
55	MG	CA	1606	1/1	0.79	0.13	139,139,139,139	0
55	MG	AA	1628	1/1	0.79	0.32	100,100,100,100	0
55	MG	BB	3097	1/1	0.79	0.08	112,112,112,112	0
55	MG	AA	1653	1/1	0.80	0.13	84,84,84,84	0
55	MG	CA	1654	1/1	0.80	0.31	78,78,78,78	0
55	MG	CN	201	1/1	0.80	0.10	104,104,104,104	0
55	MG	AA	1642	1/1	0.81	0.10	63,63,63,63	0
55	MG	CA	1603	1/1	0.81	0.12	124,124,124,124	0
55	MG	CA	1615	1/1	0.82	0.10	156,156,156,156	0
55	MG	CA	1641	1/1	0.82	0.12	123,123,123,123	0
55	MG	BB	3068	1/1	0.82	0.10	40,40,40,40	0
55	MG	CA	1637	1/1	0.82	0.17	81,81,81,81	0
55	MG	CA	1655	1/1	0.83	0.20	153,153,153,153	0
55	MG	CA	1656	1/1	0.83	0.41	97,97,97,97	0
55	MG	AA	1657	1/1	0.83	0.10	85,85,85,85	0
55	MG	DB	3058	1/1	0.84	0.60	136,136,136,136	0
55	MG	CA	1634	1/1	0.84	0.20	80,80,80,80	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1652	1/1	0.84	0.09	117,117,117,117	0
55	MG	DB	3068	1/1	0.84	0.08	35,35,35,35	0
55	MG	DB	3034	1/1	0.84	0.34	87,87,87,87	0
55	MG	DB	3107	1/1	0.84	0.11	24,24,24,24	0
55	MG	CA	1609	1/1	0.84	0.09	60,60,60,60	0
55	MG	DB	3119	1/1	0.84	0.19	64,64,64,64	0
55	MG	AA	1623	1/1	0.85	0.18	115,115,115,115	0
55	MG	BB	3118	1/1	0.85	0.36	113,113,113,113	0
55	MG	AA	1648	1/1	0.85	0.11	67,67,67,67	0
55	MG	CA	1605	1/1	0.85	0.08	98,98,98,98	0
55	MG	CA	1617	1/1	0.85	0.11	149,149,149,149	0
55	MG	AA	1615	1/1	0.85	0.08	85,85,85,85	0
55	MG	DB	3087	1/1	0.85	0.10	28,28,28,28	0
55	MG	DB	3005	1/1	0.85	0.17	66,66,66,66	0
55	MG	CA	1621	1/1	0.85	0.15	161,161,161,161	0
55	MG	AA	1640	1/1	0.85	0.09	99,99,99,99	0
55	MG	BB	3090	1/1	0.86	0.11	71,71,71,71	0
55	MG	AA	1605	1/1	0.86	0.06	87,87,87,87	0
55	MG	AA	1644	1/1	0.86	0.10	99,99,99,99	0
55	MG	CA	1639	1/1	0.86	0.37	99,99,99,99	0
55	MG	DB	3070	1/1	0.86	0.18	61,61,61,61	0
55	MG	BB	3107	1/1	0.86	0.09	86,86,86,86	0
55	MG	DB	3032	1/1	0.86	0.43	111,111,111,111	0
55	MG	AA	1638	1/1	0.86	0.09	95,95,95,95	0
55	MG	DB	3045	1/1	0.86	0.08	140,140,140,140	0
55	MG	AA	1606	1/1	0.86	0.09	114,114,114,114	0
55	MG	CA	1642	1/1	0.87	0.10	110,110,110,110	0
55	MG	AA	1633	1/1	0.87	0.06	85,85,85,85	0
55	MG	BB	3033	1/1	0.87	0.07	86,86,86,86	0
55	MG	CA	1608	1/1	0.87	0.08	82,82,82,82	0
55	MG	BB	3042	1/1	0.87	0.08	90,90,90,90	0
55	MG	AA	1617	1/1	0.87	0.42	123,123,123,123	0
55	MG	CA	1613	1/1	0.87	0.10	140,140,140,140	0
55	MG	BB	3047	1/1	0.88	0.08	131,131,131,131	0
55	MG	DB	3044	1/1	0.88	0.08	20,20,20,20	0
55	MG	BB	3050	1/1	0.88	0.09	54,54,54,54	0
55	MG	AA	1632	1/1	0.88	0.54	106,106,106,106	0
55	MG	CA	1620	1/1	0.88	0.12	103,103,103,103	0
55	MG	DB	3026	1/1	0.88	0.08	38,38,38,38	0
55	MG	CA	1628	1/1	0.88	0.06	106,106,106,106	0
55	MG	CA	1647	1/1	0.89	0.08	109,109,109,109	0
55	MG	BB	3100	1/1	0.89	0.21	128,128,128,128	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	AA	1612	1/1	0.89	0.09	117,117,117,117	0
55	MG	AA	1624	1/1	0.89	0.05	88,88,88,88	0
55	MG	DB	3024	1/1	0.89	0.06	22,22,22,22	0
55	MG	BB	3073	1/1	0.89	0.06	30,30,30,30	0
55	MG	DB	3067	1/1	0.89	0.15	33,33,33,33	0
55	MG	DB	3027	1/1	0.89	0.13	43,43,43,43	0
55	MG	DB	3029	1/1	0.89	0.84	92,92,92,92	0
55	MG	DB	3030	1/1	0.89	0.16	46,46,46,46	0
55	MG	BB	3096	1/1	0.89	0.17	49,49,49,49	0
55	MG	DB	3033	1/1	0.89	0.11	43,43,43,43	0
55	MG	BB	3074	1/1	0.89	0.07	25,25,25,25	0
55	MG	DB	3037	1/1	0.89	0.09	32,32,32,32	0
55	MG	AA	1656	1/1	0.90	1.00	101,101,101,101	0
55	MG	BB	3108	1/1	0.90	0.09	30,30,30,30	0
55	MG	CX	101	1/1	0.90	0.12	73,73,73,73	0
55	MG	AA	1660	1/1	0.90	0.54	95,95,95,95	0
55	MG	BB	3028	1/1	0.90	0.15	54,54,54,54	0
55	MG	DB	3091	1/1	0.90	0.20	39,39,39,39	0
55	MG	AA	1655	1/1	0.90	0.17	82,82,82,82	0
55	MG	DB	3064	1/1	0.90	0.12	32,32,32,32	0
55	MG	BB	3039	1/1	0.90	0.07	55,55,55,55	0
55	MG	BB	3070	1/1	0.91	0.08	52,52,52,52	0
55	MG	BB	3031	1/1	0.91	0.28	83,83,83,83	0
55	MG	BB	3112	1/1	0.91	0.32	27,27,27,27	0
55	MG	BB	3048	1/1	0.91	0.08	38,38,38,38	0
55	MG	AA	1603	1/1	0.91	0.10	55,55,55,55	0
55	MG	DB	3041	1/1	0.91	0.08	32,32,32,32	0
55	MG	CA	1623	1/1	0.91	0.16	136,136,136,136	0
55	MG	CA	1624	1/1	0.91	0.07	103,103,103,103	0
55	MG	DB	3047	1/1	0.91	0.10	36,36,36,36	0
55	MG	BJ	201	1/1	0.91	0.47	160,160,160,160	0
55	MG	BB	3081	1/1	0.91	0.09	85,85,85,85	0
55	MG	CA	1604	1/1	0.91	0.09	58,58,58,58	0
55	MG	BB	3083	1/1	0.91	0.19	47,47,47,47	0
55	MG	BB	3087	1/1	0.91	0.17	63,63,63,63	0
55	MG	AA	1601	1/1	0.91	0.04	62,62,62,62	0
55	MG	BB	3011	1/1	0.91	0.10	45,45,45,45	0
55	MG	BB	3094	1/1	0.91	0.17	81,81,81,81	0
55	MG	BB	3059	1/1	0.91	0.07	37,37,37,37	0
55	MG	CA	1611	1/1	0.91	0.11	102,102,102,102	0
55	MG	BB	3063	1/1	0.91	0.46	95,95,95,95	0
55	MG	BB	3029	1/1	0.91	0.09	81,81,81,81	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DB	3028	1/1	0.91	0.06	42,42,42,42	0
55	MG	BB	3101	1/1	0.91	0.10	50,50,50,50	0
55	MG	AX	101	1/1	0.92	1.02	84,84,84,84	0
55	MG	AA	1646	1/1	0.92	0.39	74,74,74,74	0
55	MG	DB	3061	1/1	0.92	0.14	97,97,97,97	0
55	MG	BB	3045	1/1	0.92	0.10	60,60,60,60	0
55	MG	BB	3054	1/1	0.92	0.13	56,56,56,56	0
55	MG	CA	1633	1/1	0.92	0.09	136,136,136,136	0
55	MG	CA	1645	1/1	0.92	0.12	119,119,119,119	0
55	MG	BB	3056	1/1	0.92	0.07	49,49,49,49	0
55	MG	DB	3071	1/1	0.92	0.08	30,30,30,30	0
55	MG	BB	3032	1/1	0.92	0.07	53,53,53,53	0
55	MG	DB	3023	1/1	0.92	0.12	46,46,46,46	0
55	MG	DB	3088	1/1	0.92	0.16	83,83,83,83	0
55	MG	BB	3077	1/1	0.92	0.17	50,50,50,50	0
55	MG	DB	3104	1/1	0.92	0.09	50,50,50,50	0
55	MG	AA	1616	1/1	0.92	0.18	104,104,104,104	0
55	MG	DB	3050	1/1	0.92	0.07	51,51,51,51	0
55	MG	BB	3082	1/1	0.92	0.16	80,80,80,80	0
55	MG	AA	1645	1/1	0.93	0.19	127,127,127,127	0
55	MG	BB	3016	1/1	0.93	1.04	91,91,91,91	0
55	MG	BB	3099	1/1	0.93	0.23	41,41,41,41	0
55	MG	DB	3053	1/1	0.93	0.07	37,37,37,37	0
55	MG	AA	1659	1/1	0.93	0.19	86,86,86,86	0
55	MG	AA	1602	1/1	0.93	0.28	83,83,83,83	0
55	MG	DB	3060	1/1	0.93	0.07	35,35,35,35	0
55	MG	AA	1604	1/1	0.93	0.07	45,45,45,45	0
55	MG	DB	3062	1/1	0.93	0.11	54,54,54,54	0
55	MG	DB	3063	1/1	0.93	0.10	45,45,45,45	0
55	MG	BB	3008	1/1	0.93	0.10	63,63,63,63	0
55	MG	BB	3078	1/1	0.93	0.11	71,71,71,71	0
55	MG	BB	3009	1/1	0.93	0.06	92,92,92,92	0
55	MG	BB	3117	1/1	0.93	0.18	82,82,82,82	0
55	MG	AA	1629	1/1	0.93	0.08	53,53,53,53	0
55	MG	BB	3034	1/1	0.93	0.22	70,70,70,70	0
55	MG	DB	3075	1/1	0.93	0.07	46,46,46,46	0
55	MG	BB	3084	1/1	0.93	0.09	61,61,61,61	0
55	MG	BB	3036	1/1	0.93	0.08	52,52,52,52	0
55	MG	BB	3088	1/1	0.93	0.08	76,76,76,76	0
55	MG	DB	3036	1/1	0.93	0.09	36,36,36,36	0
55	MG	AA	1649	1/1	0.93	0.12	84,84,84,84	0
55	MG	BB	3092	1/1	0.93	0.14	62,62,62,62	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BB	3060	1/1	0.93	0.17	33,33,33,33	0
55	MG	BB	3040	1/1	0.93	0.12	64,64,64,64	0
55	MG	DB	3057	1/1	0.94	0.16	63,63,63,63	0
55	MG	BB	3102	1/1	0.94	0.14	71,71,71,71	0
55	MG	BB	3044	1/1	0.94	0.13	62,62,62,62	0
55	MG	AA	1622	1/1	0.94	0.28	87,87,87,87	0
55	MG	CA	1612	1/1	0.94	0.16	95,95,95,95	0
55	MG	CA	1648	1/1	0.94	0.10	119,119,119,119	0
55	MG	BB	3064	1/1	0.94	0.08	63,63,63,63	0
55	MG	BB	3015	1/1	0.94	0.10	69,69,69,69	0
55	MG	BB	3069	1/1	0.94	0.14	28,28,28,28	0
55	MG	AA	1651	1/1	0.94	0.13	83,83,83,83	0
55	MG	AA	1607	1/1	0.94	0.09	93,93,93,93	0
55	MG	BB	3024	1/1	0.94	0.14	47,47,47,47	0
55	MG	BB	3038	1/1	0.94	0.08	125,125,125,125	0
55	MG	DB	3072	1/1	0.94	0.15	39,39,39,39	0
55	MG	AA	1634	1/1	0.94	0.14	55,55,55,55	0
55	MG	AA	1631	1/1	0.94	0.10	91,91,91,91	0
55	MG	DB	3002	1/1	0.94	0.09	44,44,44,44	0
55	MG	DB	3046	1/1	0.94	0.09	47,47,47,47	0
55	MG	DB	3089	1/1	0.94	0.17	51,51,51,51	0
55	MG	DB	3004	1/1	0.94	0.07	21,21,21,21	0
55	MG	DB	3096	1/1	0.94	0.09	46,46,46,46	0
55	MG	DB	3101	1/1	0.94	0.08	44,44,44,44	0
55	MG	DB	3048	1/1	0.94	0.07	45,45,45,45	0
55	MG	BB	3041	1/1	0.94	0.15	28,28,28,28	0
55	MG	DB	3108	1/1	0.94	0.08	36,36,36,36	0
55	MG	DB	3112	1/1	0.94	0.14	52,52,52,52	0
55	MG	DB	3114	1/1	0.94	0.27	43,43,43,43	0
55	MG	DB	3007	1/1	0.94	0.08	49,49,49,49	0
55	MG	BB	3030	1/1	0.94	0.08	111,111,111,111	0
55	MG	DB	3040	1/1	0.95	0.05	41,41,41,41	0
55	MG	BB	3037	1/1	0.95	0.09	56,56,56,56	0
55	MG	DB	3043	1/1	0.95	0.20	49,49,49,49	0
55	MG	BB	3012	1/1	0.95	0.10	32,32,32,32	0
55	MG	DB	3018	1/1	0.95	0.15	32,32,32,32	0
55	MG	DB	3020	1/1	0.95	0.08	25,25,25,25	0
55	MG	CA	1601	1/1	0.95	0.09	48,48,48,48	0
55	MG	DB	3077	1/1	0.95	0.15	57,57,57,57	0
55	MG	BB	3013	1/1	0.95	0.05	52,52,52,52	0
55	MG	BB	3007	1/1	0.95	0.15	115,115,115,115	0
55	MG	AA	1627	1/1	0.95	0.40	91,91,91,91	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1650	1/1	0.95	0.09	92,92,92,92	0
55	MG	DB	3090	1/1	0.95	0.12	62,62,62,62	0
55	MG	DB	3054	1/1	0.95	0.22	53,53,53,53	0
55	MG	DB	3093	1/1	0.95	0.12	54,54,54,54	0
55	MG	DB	3055	1/1	0.95	0.05	30,30,30,30	0
55	MG	DB	3100	1/1	0.95	0.09	10,10,10,10	0
55	MG	BB	3106	1/1	0.95	0.24	53,53,53,53	0
55	MG	BB	3017	1/1	0.95	0.04	35,35,35,35	0
55	MG	BB	3058	1/1	0.95	0.09	62,62,62,62	0
55	MG	BB	3110	1/1	0.95	0.15	56,56,56,56	0
55	MG	DB	3110	1/1	0.95	0.09	41,41,41,41	0
55	MG	DB	3111	1/1	0.95	0.08	38,38,38,38	0
55	MG	BB	3001	1/1	0.95	0.10	57,57,57,57	0
55	MG	BB	3005	1/1	0.95	0.16	52,52,52,52	0
55	MG	BB	3095	1/1	0.95	0.17	48,48,48,48	0
55	MG	DB	3116	1/1	0.95	0.04	54,54,54,54	0
55	MG	DB	3117	1/1	0.95	0.06	26,26,26,26	0
55	MG	DB	3039	1/1	0.95	0.08	95,95,95,95	0
55	MG	BB	3018	1/1	0.96	0.07	42,42,42,42	0
55	MG	DB	3017	1/1	0.96	0.10	34,34,34,34	0
55	MG	DB	3076	1/1	0.96	0.07	49,49,49,49	0
55	MG	CA	1626	1/1	0.96	0.07	154,154,154,154	0
55	MG	BB	3091	1/1	0.96	0.19	44,44,44,44	0
55	MG	DB	3083	1/1	0.96	0.12	31,31,31,31	0
55	MG	BB	3049	1/1	0.96	0.09	40,40,40,40	0
55	MG	DB	3051	1/1	0.96	0.09	48,48,48,48	0
55	MG	AA	1636	1/1	0.96	0.07	61,61,61,61	0
55	MG	DB	3025	1/1	0.96	0.10	40,40,40,40	0
55	MG	CA	1630	1/1	0.96	0.08	97,97,97,97	0
55	MG	DB	3092	1/1	0.96	0.16	44,44,44,44	0
55	MG	BB	3061	1/1	0.96	0.12	57,57,57,57	0
55	MG	DB	3095	1/1	0.96	0.11	26,26,26,26	0
55	MG	DB	3056	1/1	0.96	0.13	28,28,28,28	0
55	MG	BB	3020	1/1	0.96	0.22	45,45,45,45	0
55	MG	BB	3080	1/1	0.96	0.20	65,65,65,65	0
55	MG	BB	3053	1/1	0.96	0.05	43,43,43,43	0
55	MG	DB	3105	1/1	0.96	0.06	18,18,18,18	0
55	MG	BB	3066	1/1	0.96	0.16	51,51,51,51	0
55	MG	CA	1602	1/1	0.96	0.12	87,87,87,87	0
55	MG	CA	1619	1/1	0.96	0.07	79,79,79,79	0
55	MG	BB	3067	1/1	0.96	0.09	39,39,39,39	0
55	MG	BB	3022	1/1	0.96	0.16	56,56,56,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	BB	3023	1/1	0.96	0.06	15,15,15,15	0
55	MG	BB	3104	1/1	0.96	0.08	38,38,38,38	0
55	MG	AA	1609	1/1	0.96	0.07	67,67,67,67	0
55	MG	DB	3010	1/1	0.96	0.09	20,20,20,20	0
55	MG	DB	3012	1/1	0.96	0.18	37,37,37,37	0
56	ZN	B4	101	1/1	0.96	0.04	72,72,72,72	0
55	MG	DB	3038	1/1	0.97	0.11	19,19,19,19	0
55	MG	BB	3086	1/1	0.97	0.11	50,50,50,50	0
55	MG	AA	1610	1/1	0.97	0.05	61,61,61,61	0
55	MG	AX	102	1/1	0.97	0.41	66,66,66,66	0
55	MG	DB	3021	1/1	0.97	0.09	50,50,50,50	0
55	MG	DB	3022	1/1	0.97	0.09	42,42,42,42	0
55	MG	BB	3065	1/1	0.97	0.06	46,46,46,46	0
55	MG	DB	3098	1/1	0.97	0.09	42,42,42,42	0
55	MG	DB	3099	1/1	0.97	0.06	19,19,19,19	0
55	MG	DB	3001	1/1	0.97	0.06	14,14,14,14	0
55	MG	CA	1638	1/1	0.97	0.57	102,102,102,102	0
55	MG	DB	3003	1/1	0.97	0.06	24,24,24,24	0
55	MG	AA	1654	1/1	0.97	0.05	49,49,49,49	0
55	MG	DB	3106	1/1	0.97	0.06	29,29,29,29	0
55	MG	BB	3025	1/1	0.97	0.11	63,63,63,63	0
55	MG	DB	3074	1/1	0.97	0.08	9,9,9,9	0
55	MG	DB	3109	1/1	0.97	0.26	28,28,28,28	0
55	MG	DB	3006	1/1	0.97	0.15	38,38,38,38	0
55	MG	CA	1651	1/1	0.97	0.16	66,66,66,66	0
55	MG	BB	3111	1/1	0.97	0.09	43,43,43,43	0
55	MG	DB	3078	1/1	0.97	0.05	28,28,28,28	0
55	MG	DB	3080	1/1	0.97	0.12	29,29,29,29	0
55	MG	DB	3011	1/1	0.97	0.05	16,16,16,16	0
55	MG	BB	3027	1/1	0.97	0.44	40,40,40,40	0
55	MG	DB	3118	1/1	0.97	0.06	35,35,35,35	0
55	MG	BB	3113	1/1	0.97	0.19	41,41,41,41	0
55	MG	DB	3015	1/1	0.97	0.10	49,49,49,49	0
56	ZN	D4	401	1/1	0.97	0.17	72,72,72,72	0
55	MG	BB	3052	1/1	0.98	0.07	33,33,33,33	0
55	MG	DB	3084	1/1	0.98	0.12	26,26,26,26	0
55	MG	DB	3085	1/1	0.98	0.09	21,21,21,21	0
55	MG	BB	3043	1/1	0.98	0.14	107,107,107,107	0
55	MG	BB	3098	1/1	0.98	0.11	73,73,73,73	0
55	MG	BB	3035	1/1	0.98	0.14	40,40,40,40	0
55	MG	BB	3055	1/1	0.98	0.09	72,72,72,72	0
55	MG	BB	3021	1/1	0.98	0.13	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BB	3006	1/1	0.98	0.11	35,35,35,35	0
55	MG	DB	3031	1/1	0.98	0.05	16,16,16,16	0
55	MG	DB	3094	1/1	0.98	0.21	77,77,77,77	0
55	MG	BB	3103	1/1	0.98	0.10	38,38,38,38	0
55	MG	BB	3002	1/1	0.98	0.16	31,31,31,31	0
55	MG	DB	3097	1/1	0.98	0.11	39,39,39,39	0
55	MG	BB	3105	1/1	0.98	0.13	64,64,64,64	0
55	MG	DB	3035	1/1	0.98	0.18	27,27,27,27	0
55	MG	BB	3072	1/1	0.98	0.11	58,58,58,58	0
55	MG	BB	3003	1/1	0.98	0.10	20,20,20,20	0
55	MG	DB	3103	1/1	0.98	0.05	46,46,46,46	0
55	MG	BB	3004	1/1	0.98	0.09	65,65,65,65	0
55	MG	DB	3014	1/1	0.98	0.05	32,32,32,32	0
55	MG	BB	3109	1/1	0.98	0.13	52,52,52,52	0
55	MG	DB	3069	1/1	0.98	0.24	48,48,48,48	0
55	MG	DB	3016	1/1	0.98	0.07	43,43,43,43	0
55	MG	DB	3042	1/1	0.98	0.06	56,56,56,56	0
55	MG	BB	3075	1/1	0.98	0.10	44,44,44,44	0
55	MG	DB	3073	1/1	0.98	0.12	7,7,7,7	0
55	MG	BB	3026	1/1	0.98	0.09	26,26,26,26	0
55	MG	DB	3113	1/1	0.98	0.17	27,27,27,27	0
55	MG	DB	3019	1/1	0.98	0.08	43,43,43,43	0
55	MG	BB	3062	1/1	0.98	0.06	42,42,42,42	0
55	MG	AA	1620	1/1	0.98	0.10	74,74,74,74	0
55	MG	BB	3114	1/1	0.98	0.21	57,57,57,57	0
55	MG	DB	3079	1/1	0.98	0.08	18,18,18,18	0
55	MG	DB	3049	1/1	0.98	0.10	42,42,42,42	0
55	MG	DB	3081	1/1	0.98	0.07	36,36,36,36	0
55	MG	CA	1616	1/1	0.98	0.08	80,80,80,80	0
55	MG	DB	3102	1/1	0.99	0.09	67,67,67,67	0
55	MG	BB	3116	1/1	0.99	0.08	24,24,24,24	0
55	MG	BB	3085	1/1	0.99	0.05	57,57,57,57	0
55	MG	DB	3086	1/1	0.99	0.13	57,57,57,57	0
55	MG	BB	3089	1/1	0.99	0.06	51,51,51,51	0
55	MG	BB	3079	1/1	0.99	0.14	46,46,46,46	0
55	MG	DB	3008	1/1	0.99	0.11	55,55,55,55	0
55	MG	DB	3009	1/1	0.99	0.05	48,48,48,48	0
55	MG	DB	3066	1/1	0.99	0.11	30,30,30,30	0
55	MG	BB	3071	1/1	0.99	0.10	41,41,41,41	0



## 6.5 Other polymers

There are no such residues in this entry.