



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:37 PM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

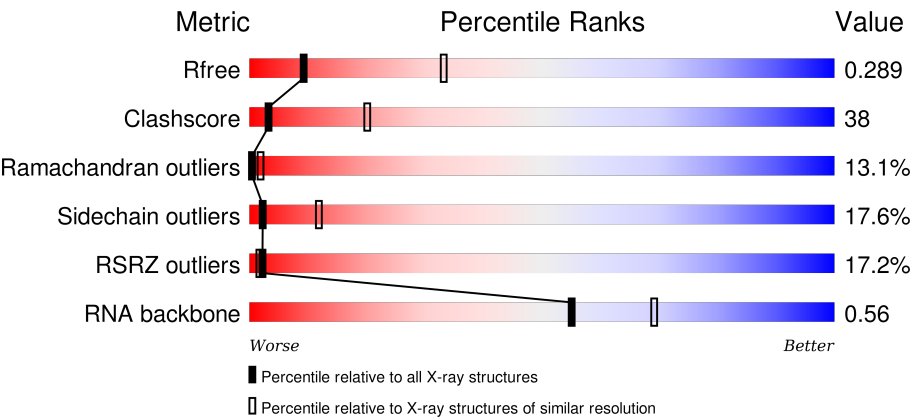
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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}	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)
RNA backbone	2183	1004 (3.72-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	<div><div>10%</div><div>19%65%15%..</div></div>
1	CA	1542	<div><div>%</div><div>20%64%15%. </div></div>
2	AW	17	<div><div>65%</div><div>47%53%</div></div>
2	CW	17	<div><div>6%</div><div>47%53%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AX	6	
3	CX	6	
4	AB	240	
4	CB	240	
5	AC	232	
5	CC	232	
6	AD	205	
6	CD	205	
7	AE	166	
7	CE	166	
8	AF	135	
8	CF	135	
9	AG	178	
9	CG	178	
10	AH	129	
10	CH	129	
11	AI	129	
11	CI	129	
12	AJ	103	
12	CJ	103	
13	AK	128	
13	CK	128	
14	AL	123	
14	CL	123	
15	AM	117	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CM	117	
16	AN	100	
16	CN	100	
17	AO	88	
17	CO	88	
18	AP	82	
18	CP	82	
19	AQ	83	
19	CQ	83	
20	AR	74	
20	CR	74	
21	AS	91	
21	CS	91	
22	AT	86	
22	CT	86	
23	AU	70	
23	CU	70	
24	BA	120	
24	DA	120	
25	BB	2904	
25	DB	2904	
26	BC	272	
26	DC	272	
27	BD	209	
27	DD	209	

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	
41	BR	103	
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	103	
44	DU	103	
45	BV	94	
45	DV	94	
46	BW	84	
46	DW	84	
47	BX	77	
47	DX	77	
48	BY	63	
48	DY	63	
49	BZ	58	
49	DZ	58	
50	B0	56	
50	D0	56	
51	B1	54	
51	D1	54	
52	B2	46	
52	D2	46	

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	1637	-	-	-	X
55	MG	AX	102	-	-	-	X
55	MG	BB	3016	-	-	-	X
55	MG	BB	3063	-	-	-	X
55	MG	DB	3109	-	-	-	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
1	AA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

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

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

- Molecule 3 is a RNA chain called MRNA.

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

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

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

- 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
10	CH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

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

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

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

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

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

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

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

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

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

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

- 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
26	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

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

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

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

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

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

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

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

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

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

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

- 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
42	DS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	BB	118	Total	Mg	0	0
			118	118		
55	CN	1	Total	Mg	0	0
			1	1		
55	CA	56	Total	Mg	0	0
			56	56		
55	AA	60	Total	Mg	0	0
			60	60		
55	AX	2	Total	Mg	0	0
			2	2		
55	BJ	1	Total	Mg	0	0
			1	1		
55	CX	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...

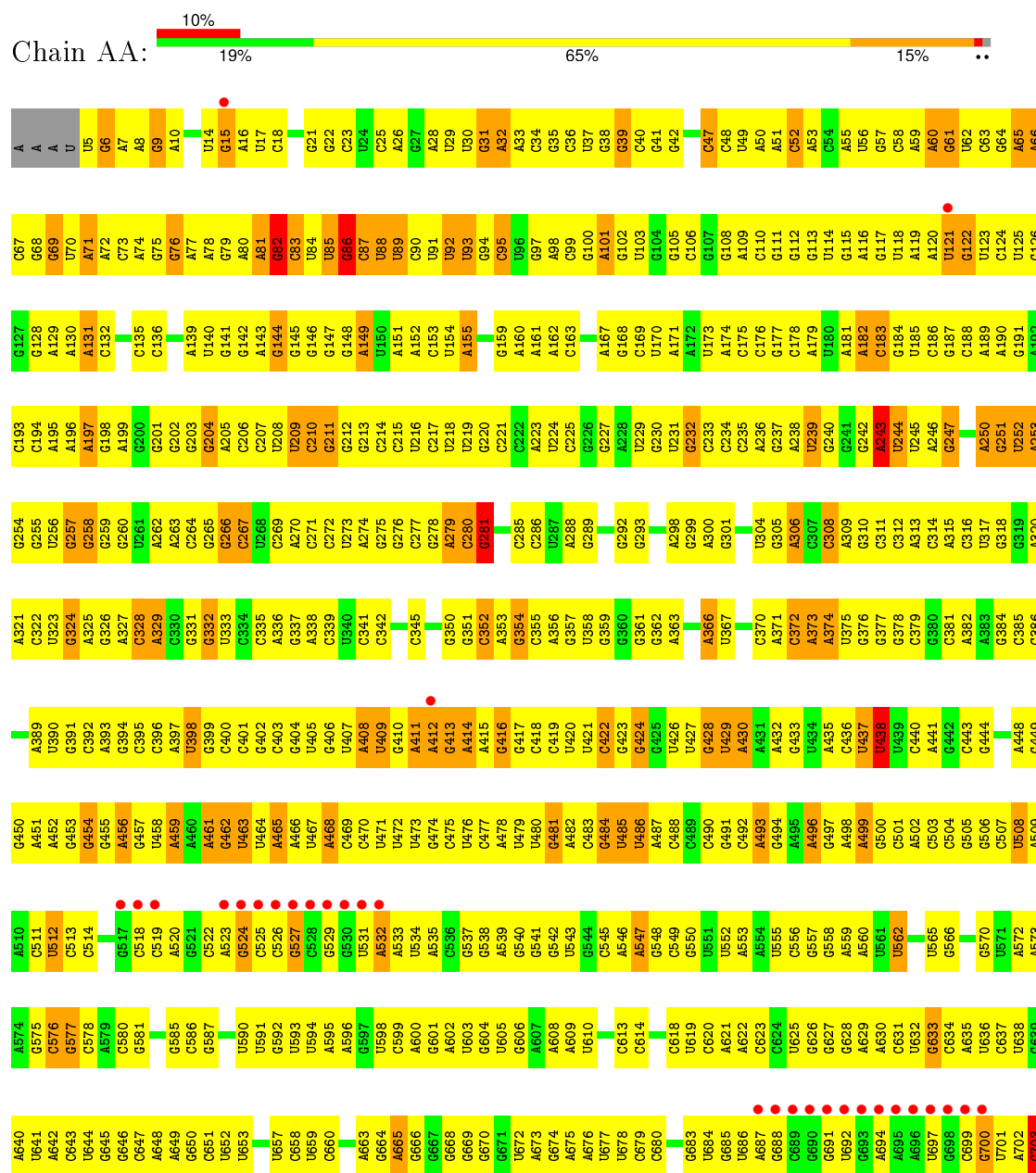
Continued from previous page...

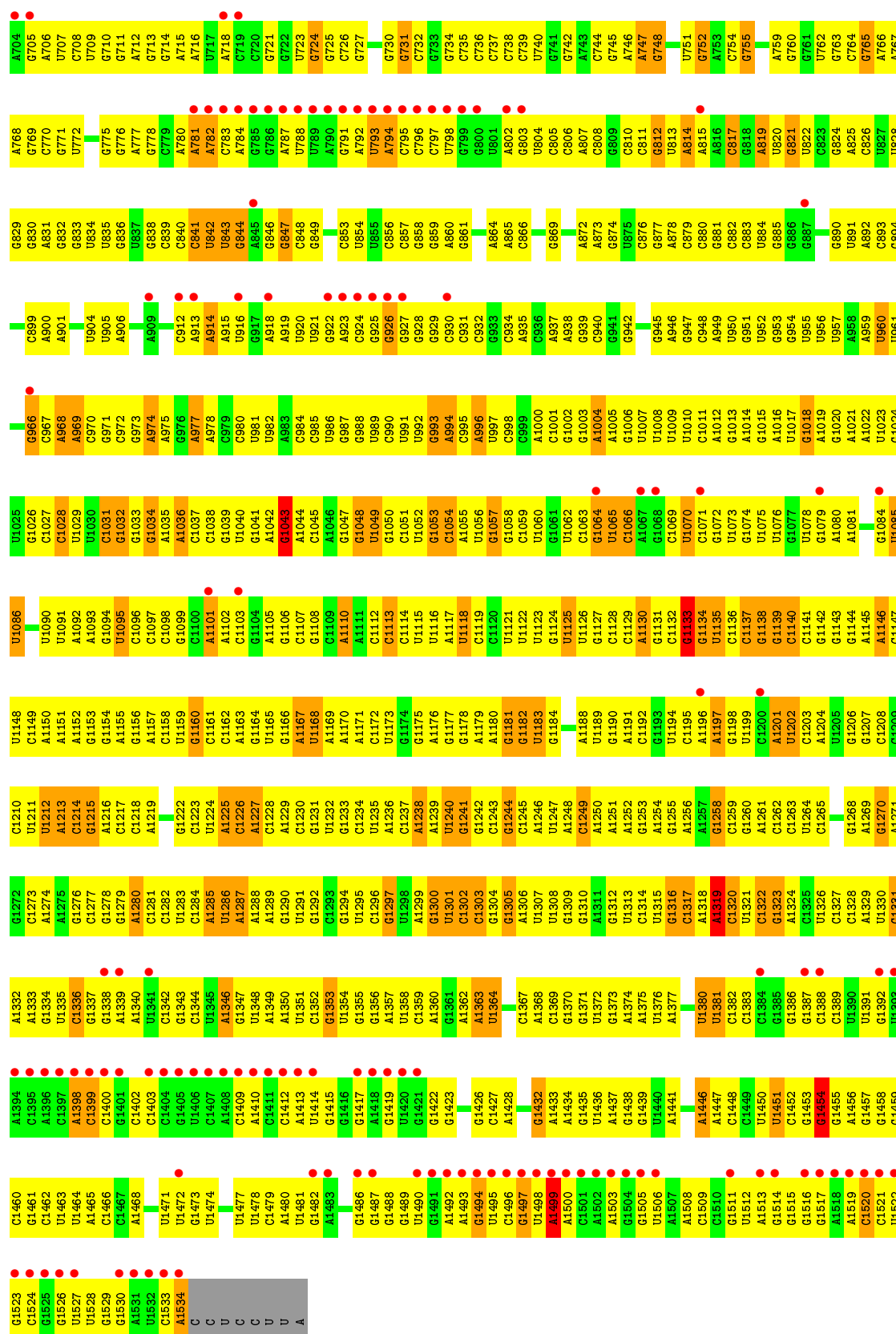
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CL	1	Total 1	O 1	0	0
57	CN	1	Total 1	O 1	0	0
57	CP	1	Total 1	O 1	0	0
57	CT	3	Total 3	O 3	0	0
57	CU	1	Total 1	O 1	0	0
57	DB	531	Total 531	O 531	0	0
57	DC	7	Total 7	O 7	0	0
57	DD	1	Total 1	O 1	0	0
57	DE	3	Total 3	O 3	0	0
57	DJ	2	Total 2	O 2	0	0
57	DL	3	Total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

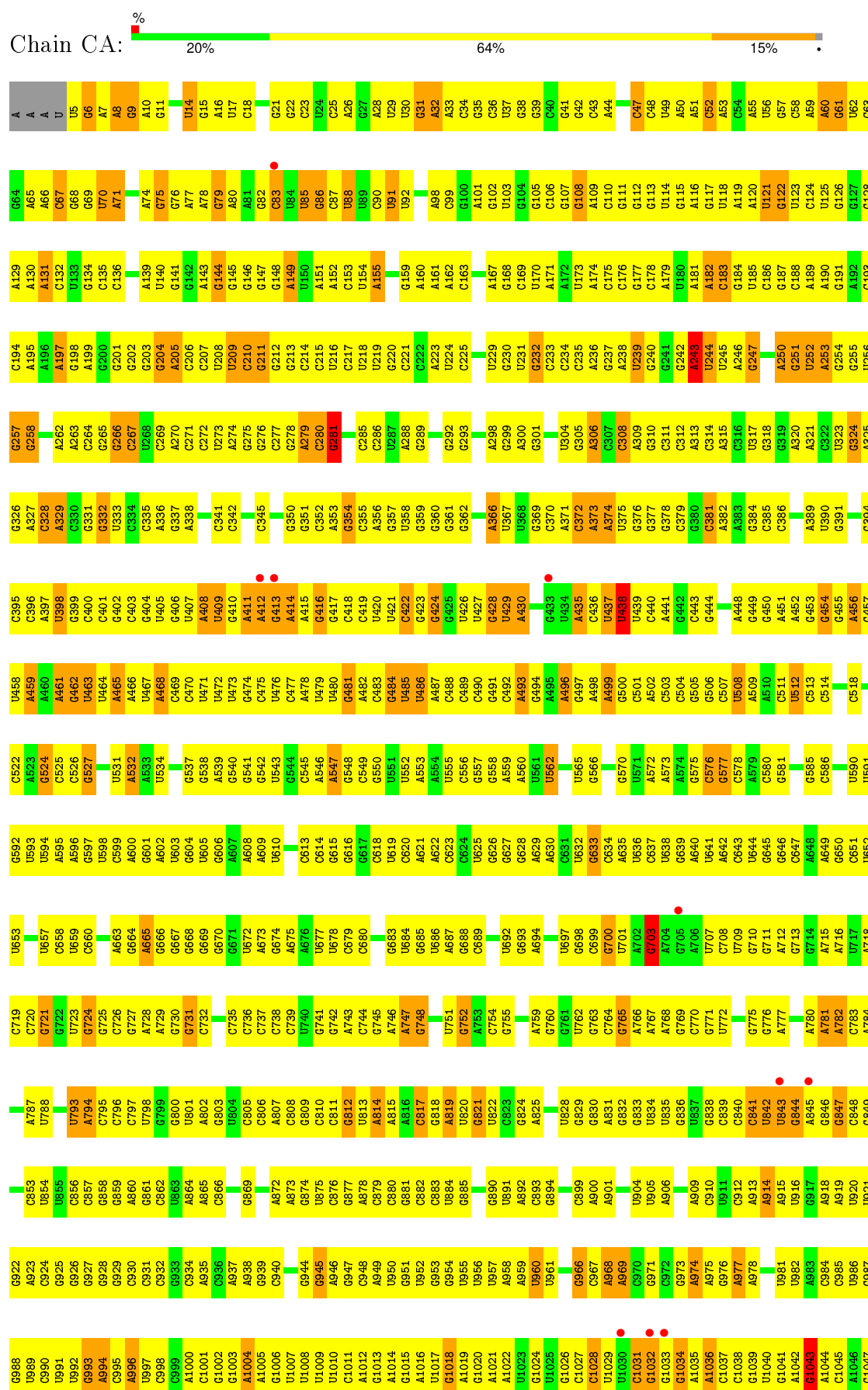
3 Residue-property plots

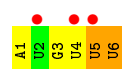
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: 16S ribosomal RNA

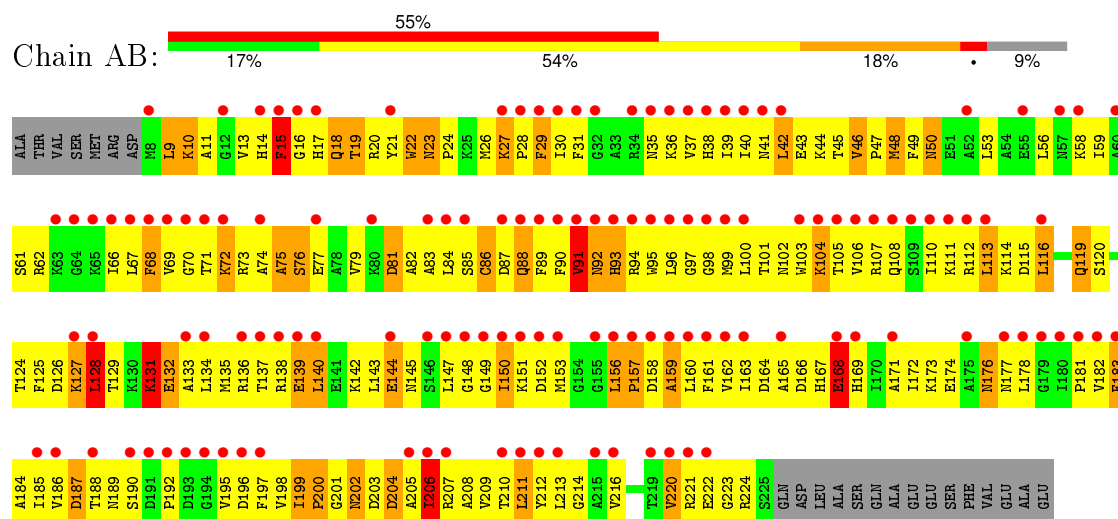




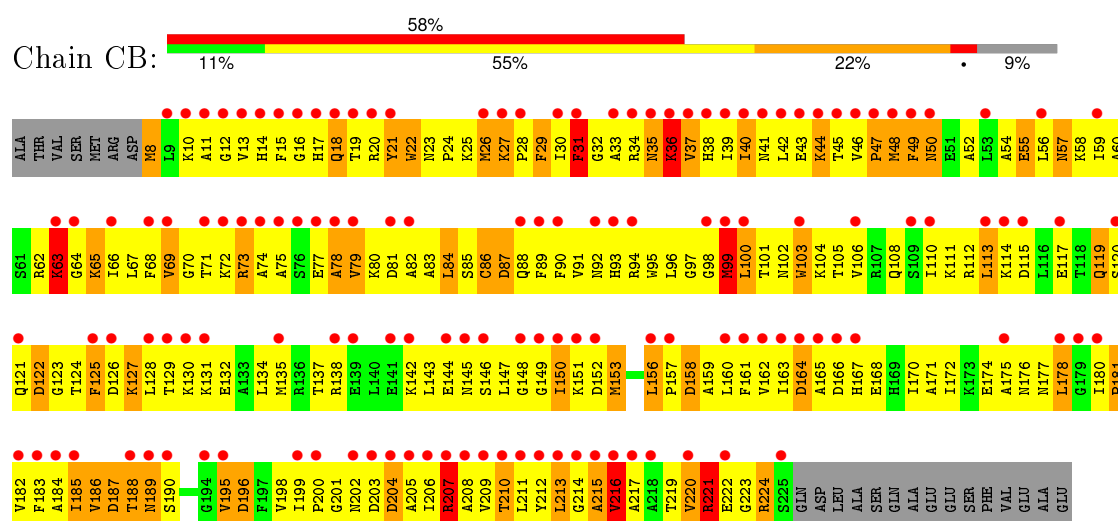




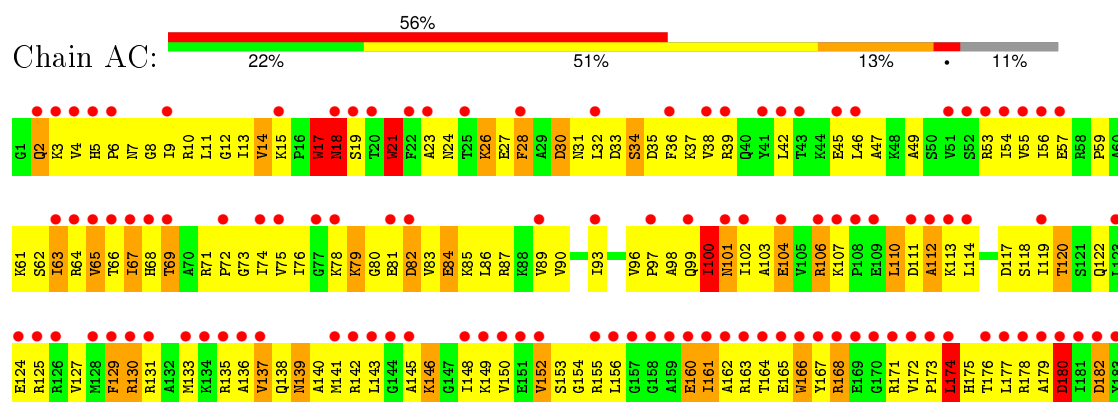
• Molecule 4: 30S ribosomal protein S2

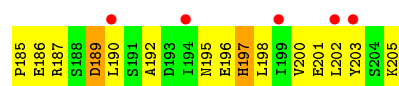


• Molecule 4: 30S ribosomal protein S2

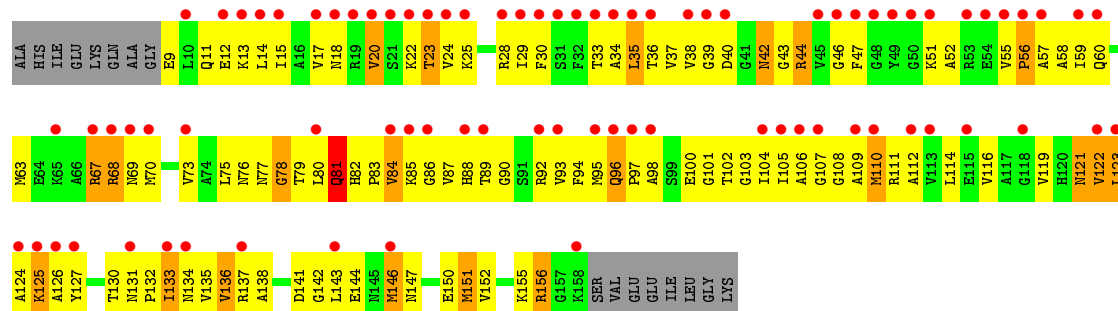


• Molecule 5: 30S ribosomal protein S3

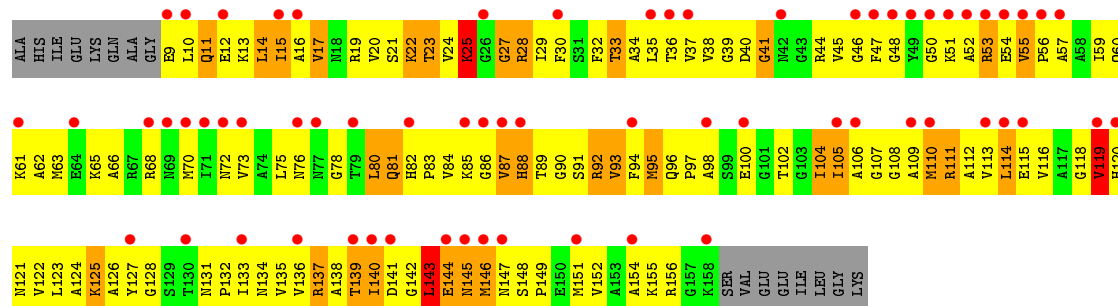
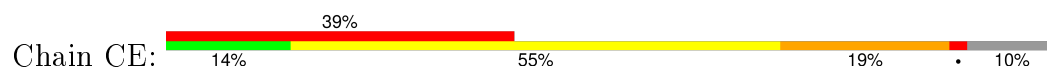




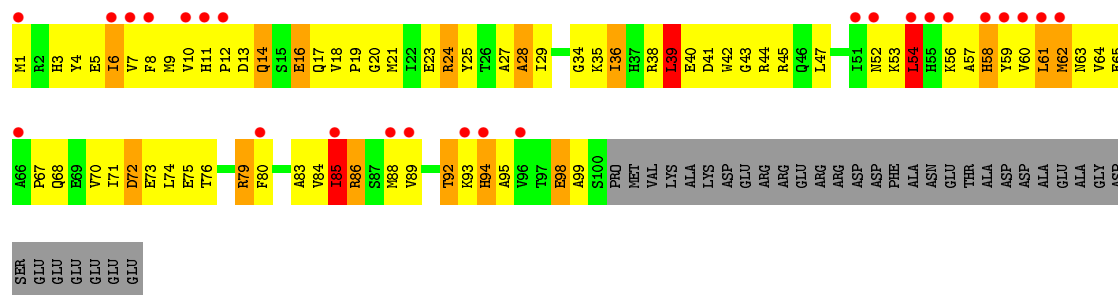
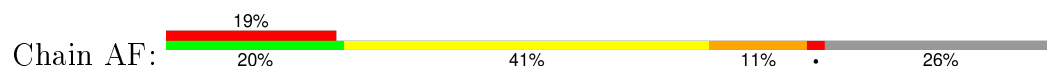
• Molecule 7: 30S ribosomal protein S5



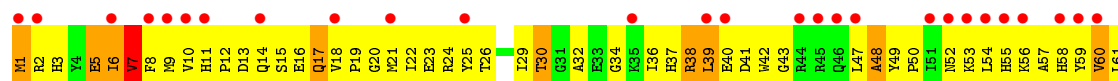
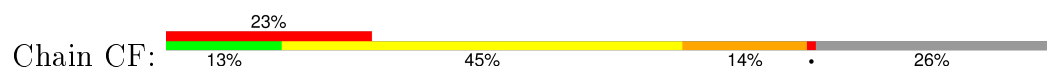
• Molecule 7: 30S ribosomal protein S5

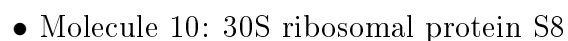
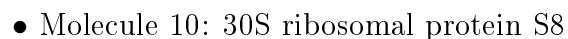
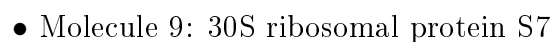
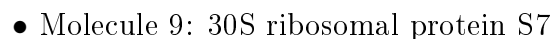


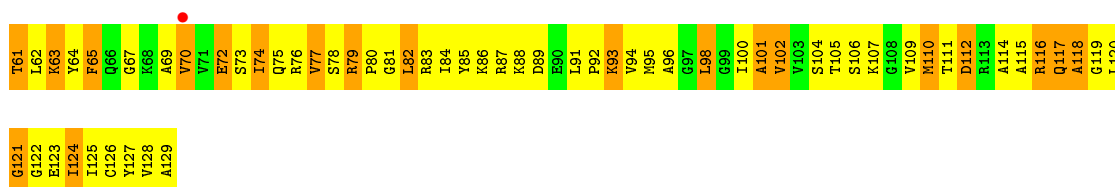
• Molecule 8: 30S ribosomal protein S6



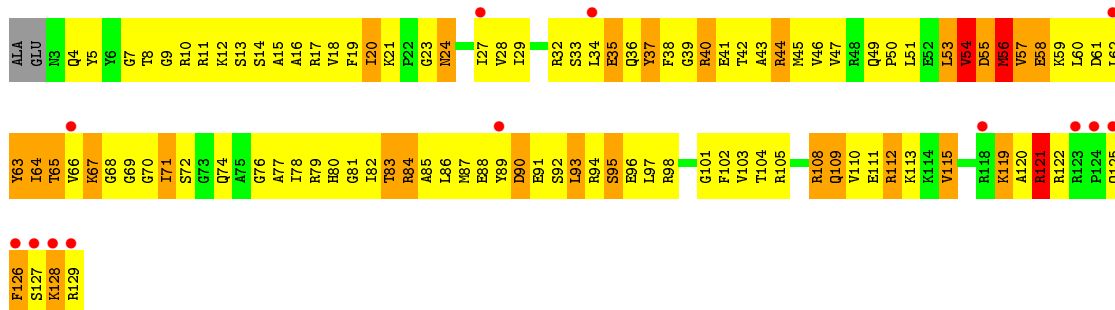
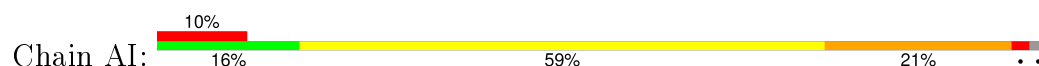
• Molecule 8: 30S ribosomal protein S6



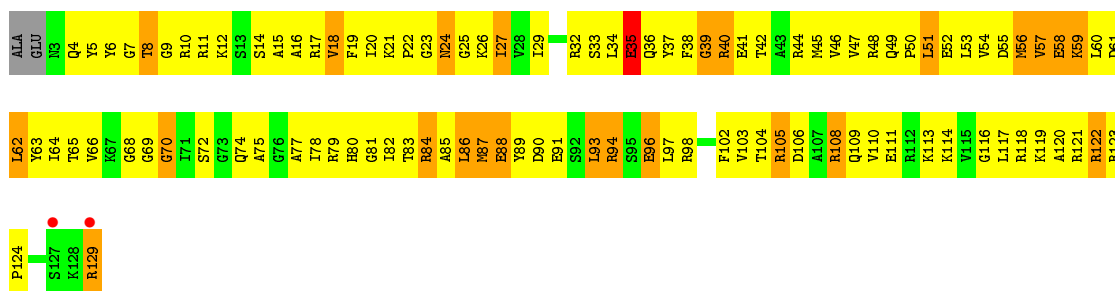




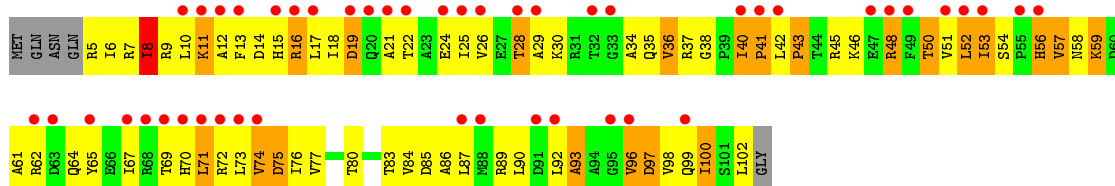
• Molecule 11: 30S ribosomal protein S9



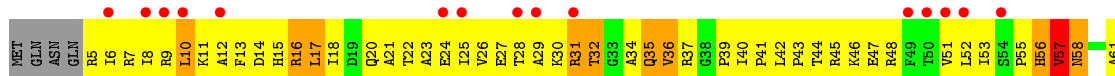
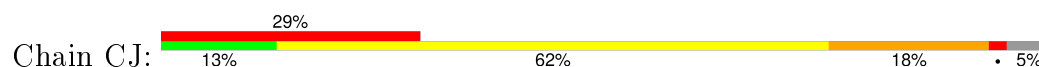
• Molecule 11: 30S ribosomal protein S9

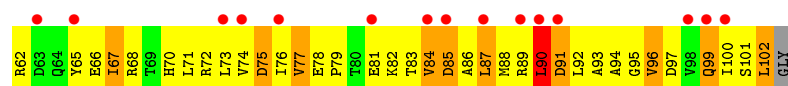


• Molecule 12: 30S ribosomal protein S10

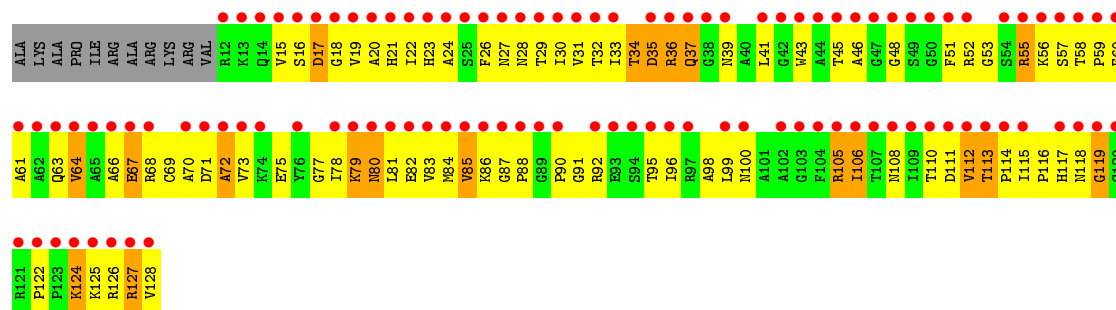
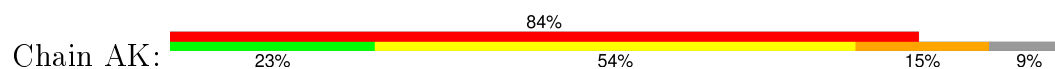


• Molecule 12: 30S ribosomal protein S10

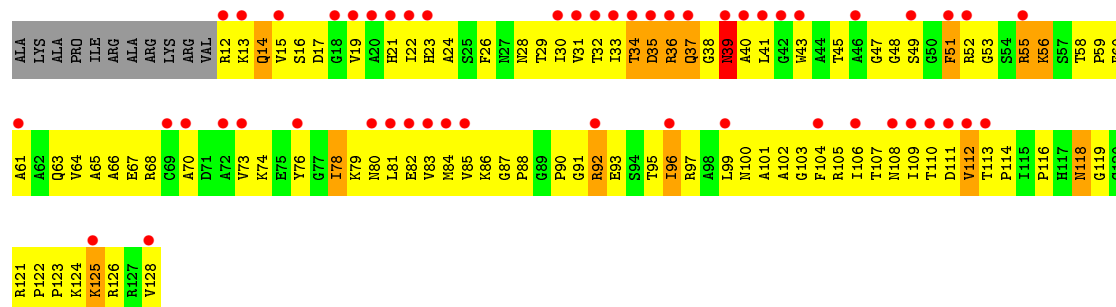




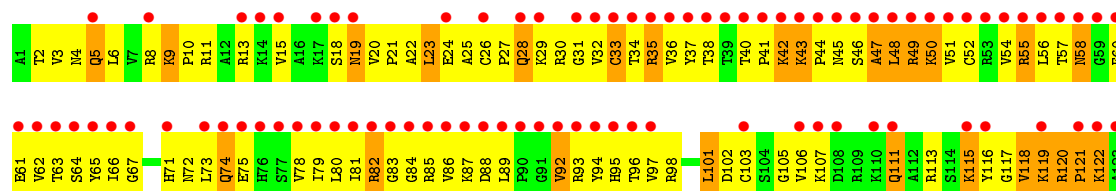
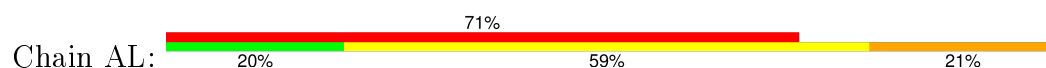
- Molecule 13: 30S ribosomal protein S11



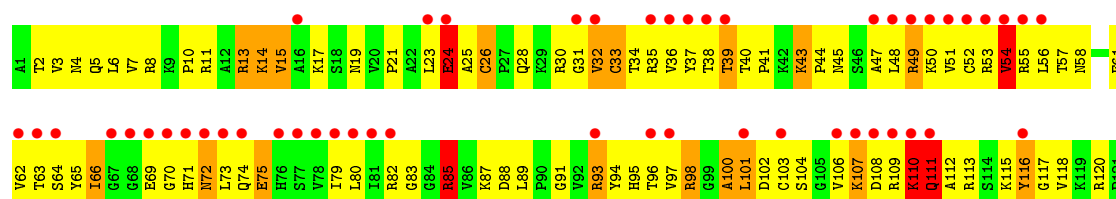
- Molecule 13: 30S ribosomal protein S11



- Molecule 14: 30S ribosomal protein S12

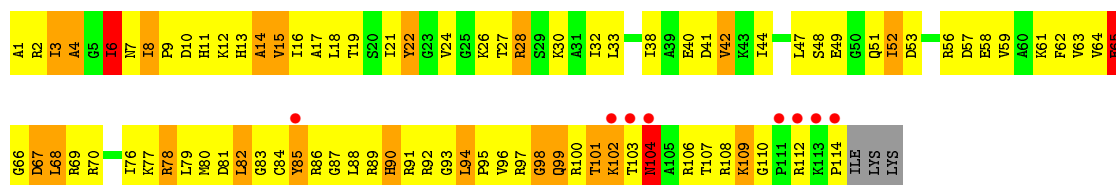


- Molecule 14: 30S ribosomal protein S12

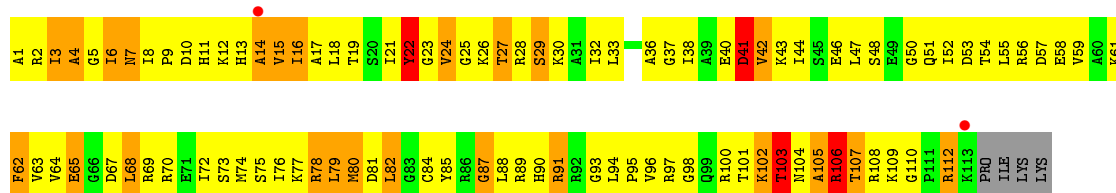
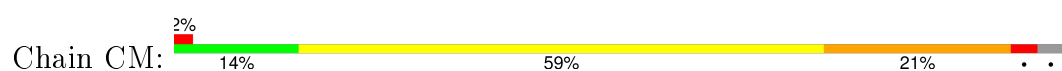




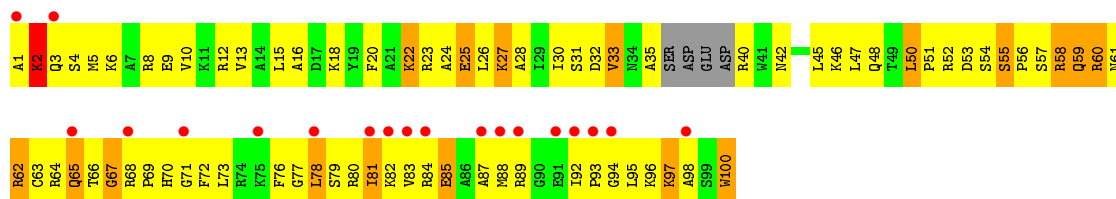
• Molecule 15: 30S ribosomal protein S13



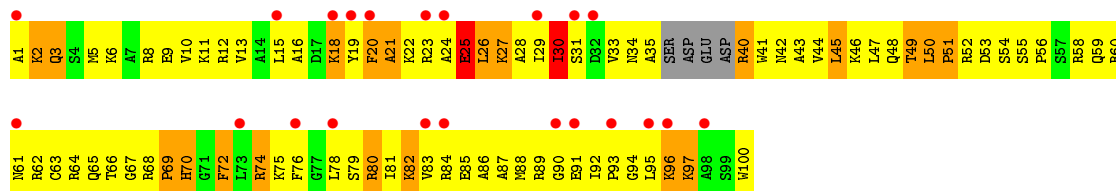
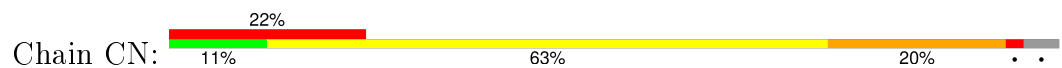
• Molecule 15: 30S ribosomal protein S13



• Molecule 16: 30S ribosomal protein S14

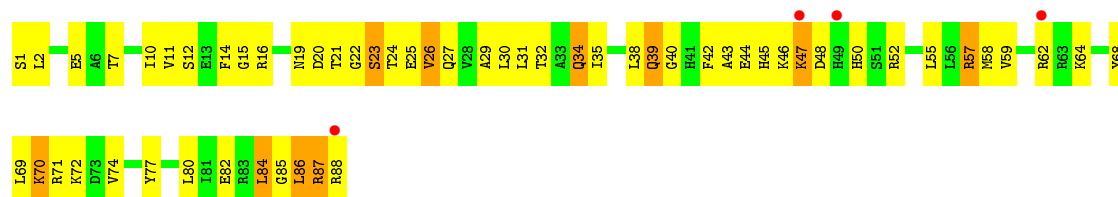


• Molecule 16: 30S ribosomal protein S14

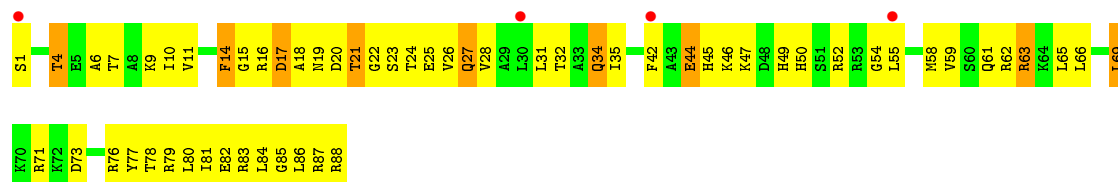
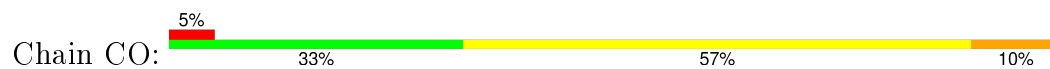


• Molecule 17: 30S ribosomal protein S15

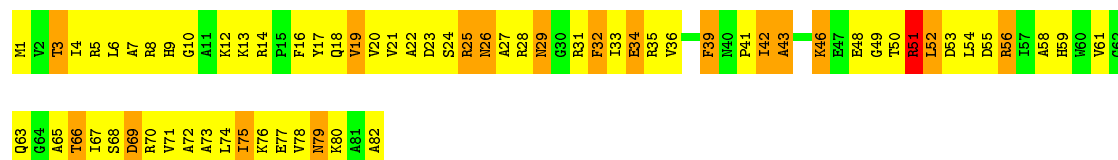
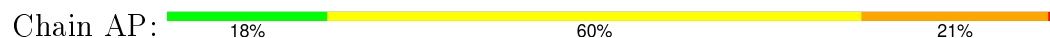




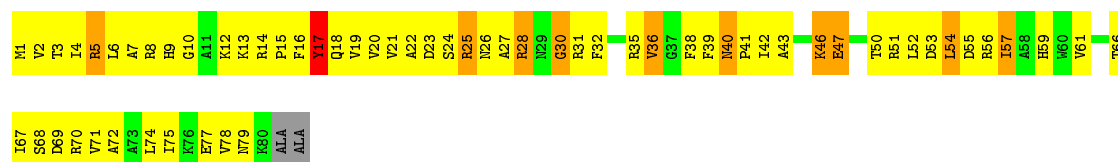
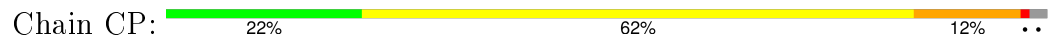
- Molecule 17: 30S ribosomal protein S15



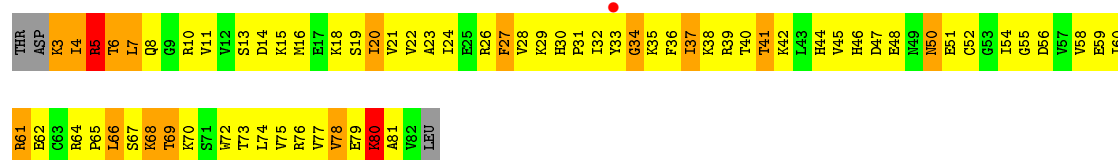
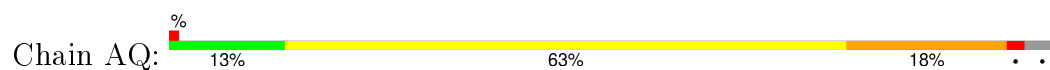
- Molecule 18: 30S ribosomal protein S16



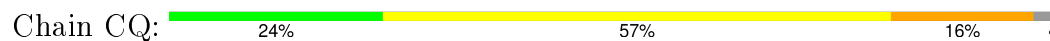
- Molecule 18: 30S ribosomal protein S16

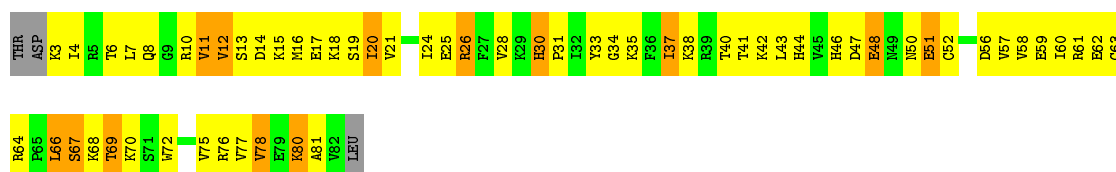


- Molecule 19: 30S ribosomal protein S17

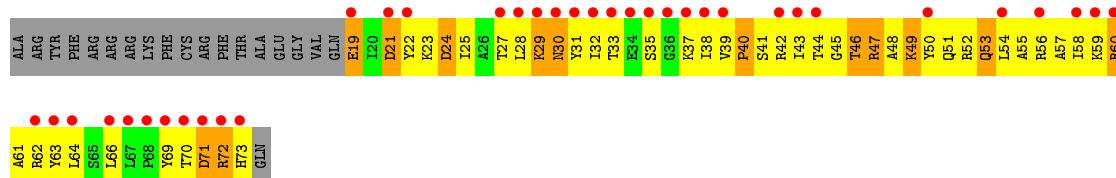


- Molecule 19: 30S ribosomal protein S17

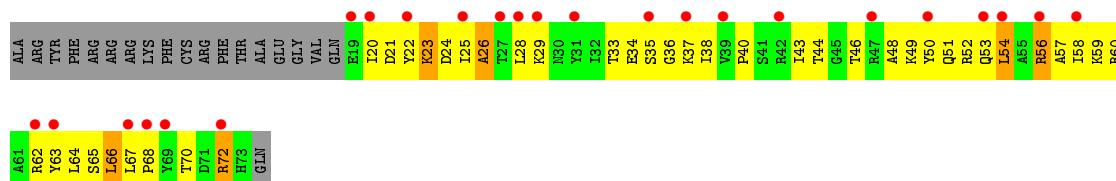
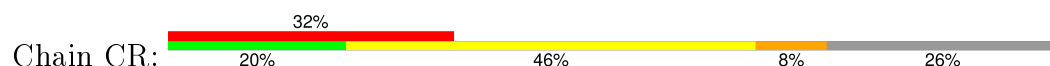




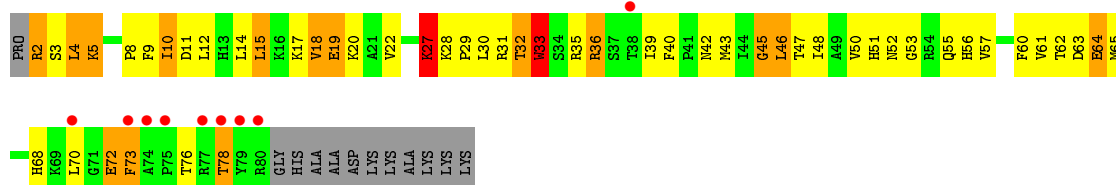
• Molecule 20: 30S ribosomal protein S18



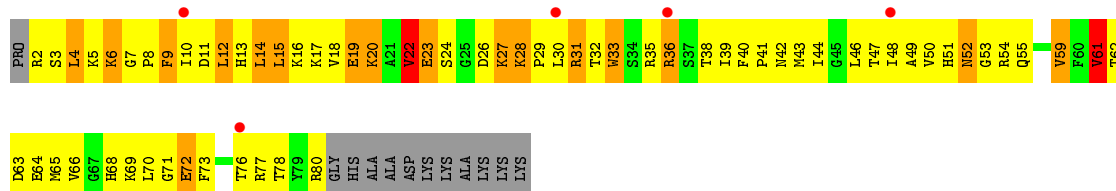
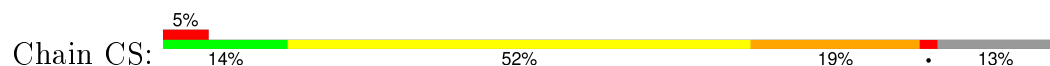
• Molecule 20: 30S ribosomal protein S18



• Molecule 21: 30S ribosomal protein S19

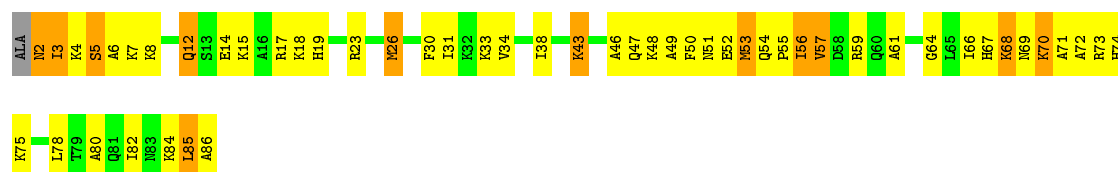


• Molecule 21: 30S ribosomal protein S19

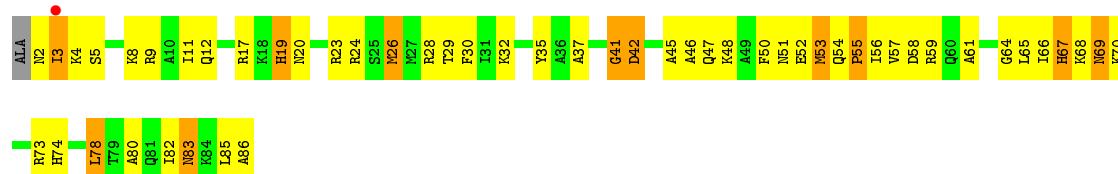


• Molecule 22: 30S ribosomal protein S20

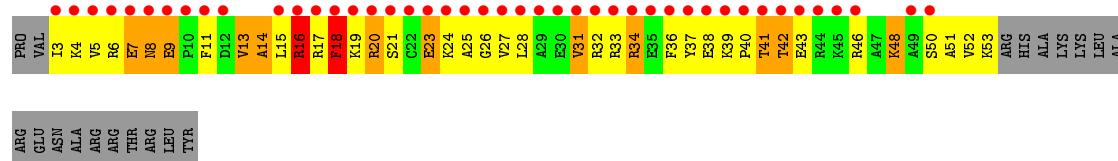




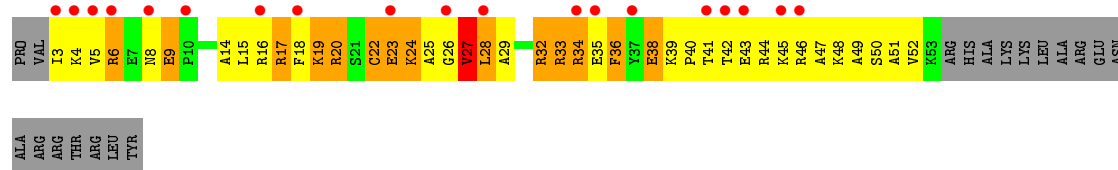
- Molecule 22: 30S ribosomal protein S20



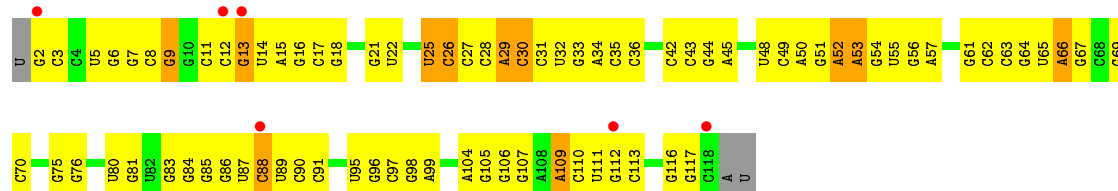
- Molecule 23: 30S ribosomal protein S21



- Molecule 23: 30S ribosomal protein S21

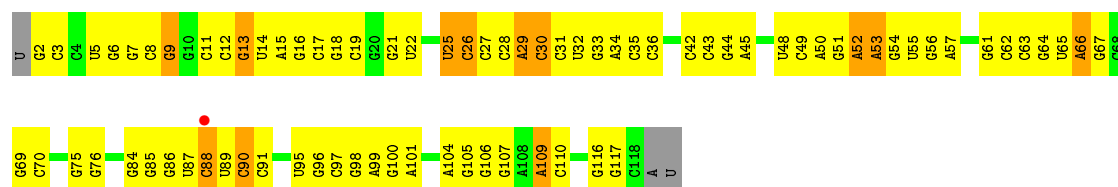


- Molecule 24: 5S ribosomal RNA

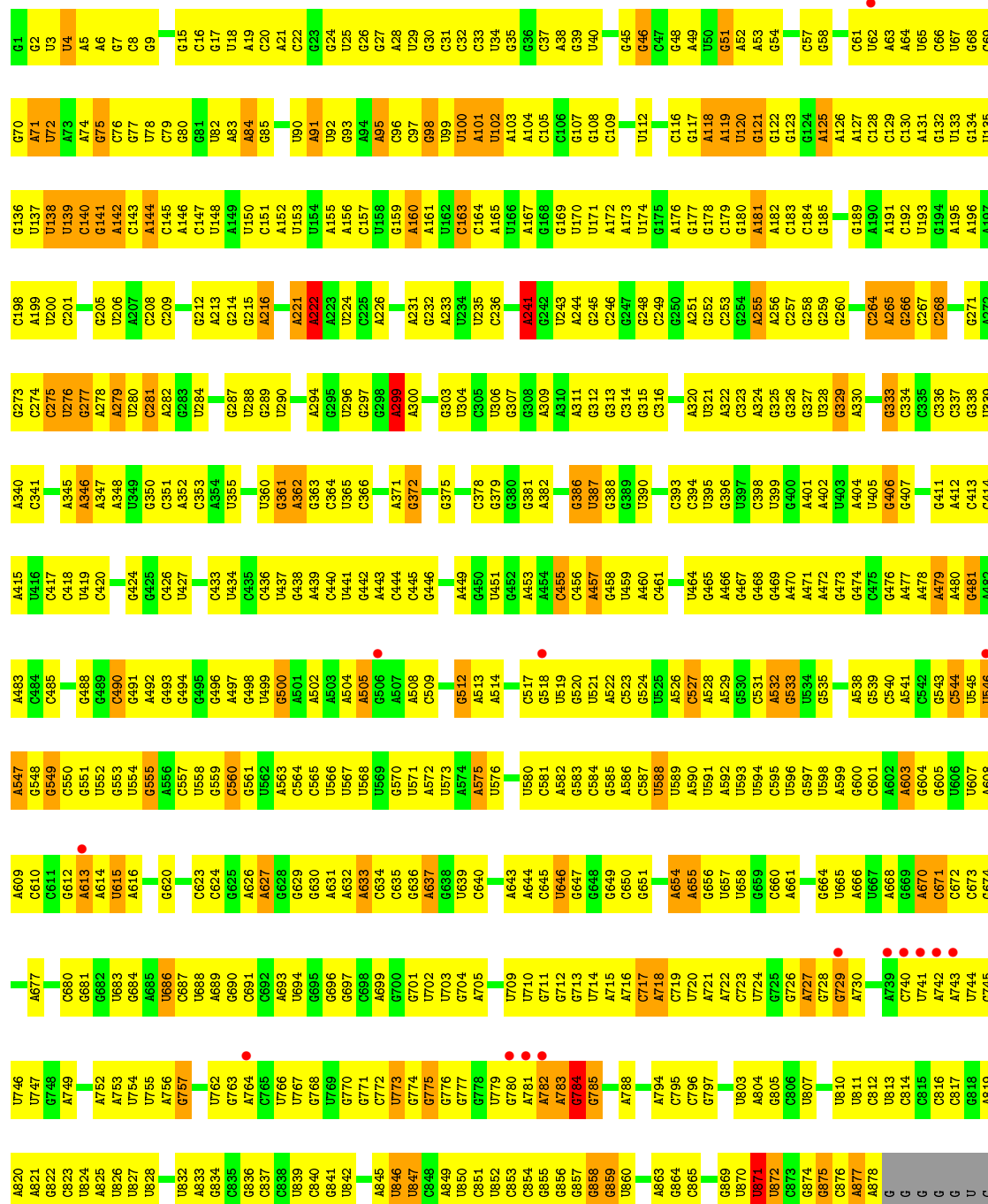


- Molecule 24: 5S ribosomal RNA



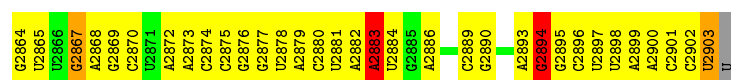


● Molecule 25: 23S ribosomal RNA



A	U	C	C	C	G	A	C	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A	C	A
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---

U2798	G2732	G2668	G2596	G2524	U2457	U2387	U2321	C2258	A2191	U	U	G1930	G1869
A2799	A2733	G2669	G2597	G2529	G2458	G2391	A2322	U2259	U2192	U	U	U1931	C1870
A2800	A2734	G2670	A2598	G2530	A2459	A2392	G2323	C2260	U2193	U	U	A1871	A1872
G2801	G2735	G2671	G2599	A2531	U2460	A2393	U2324	C2261	U2194	U	U	G1933	G1873
G2802	G2672	G2673	A2600	G2532	A2461	C2394	G2325	U2262	U2195	U	U	G1934	G1874
U2803	G2673	G2674	G2601	G2533	C2462	C2395	G2326	C2263	G2196	U	U	G1935	G1875
U2804	G2674	G2675	A2602	U2534	C2463	G2396	C2327	C2264	U2197	U	U	A1936	
C2805	A2675	A2676	G2603	A2535	C2464	G2396	A2328	U2265	A2198	U	U	A1937	
C2806	A2676	A2677	G2604	A2536	G2465	U2400	U2329	U2266	A2199	U	U	A1938	
U2807	G2677	G2678	U2605	U2537	C2466	G2401	G2330	A2267	C2200	U	U	U1939	
G2808	G2678	G2679	C2606	C2538	C2467	G2402	G2331	U2268	C2201	U	U	U1940	
A2809	A2679	A2680	G2607	C2539	A2468	U2403	C2332	G2269	U2203	U	U	U1941	
A2810	U2680	U2681	G2608	C2540	A2469	U2404	A2333	A2270	G2204	U	U	U1942	
G2811	G2681	G2682	U2609		G2470	U2405	U2334	G2271	U2205	U	U	U1943	
A2812	A2682	A2683	G2610	G2543	A2471	G2406	A2335	U2272	A2206	U	U	U1944	
G2813	G2683	G2684	U2611	G2544	G2472	A2407	A2336	C2273	C2207	U	U	G1945	
A2814	U2684	U2685	U2612		C2473	G2408	A2337	U2274	C2208	U	U	U1946	
C2815	U2685	U2686	U2613	A2547	C2474	U2409	G2338	G2275	U2209	U	U	C1947	
G2816	G2686	G2687	U2614	U2548	U2475	G2410	C2339	U2276	G2210	U	U	G1948	
U2817	U2687	U2688	U2615		U2476	G2411	A2340	A2277	A2211	U	U	G1949	
	U2754	U2689	U2616		U2477	G2412	C2342	U2278	A2212	U	U	U1955	
	U2755	G2688	G2617	U2549	U2478	A2413	C2343	G2279	A2213	U	U	U1956	
A2820	U2756	G2689	G2618	U2552	U2479	G2414	C2344	U2280	U2214	U	U	C1957	
A2821	A2757	U2690	G2619	G2553	C2480	G2415	C2345	G2281	G2215	U	U	G1958	
G2822	A2758	C2691	C2620	U2554	G2481	G2416	A2346	A2282	G2216	U	U	C1959	
A2823	G2621	G2692	G2621	U2555		G2417	C2347	C2283	G2217	U	U	G1960	
	U2622	G2693	U2622	C2556	G2485	C2418	U2348	C2284	G2218	U	U	A1961	
A2829	G2623	G2694	G2623	G2557	C2486	U2419	C2349	G2285	U2219	U	U	C1962	
C2830	G2624	U2695	G2624	U2558	U2487	G2420	C2350	G2286	U2220	U	U	G1963	
G2831	G2625	G2696	G2625	C2559	C2488	U2421	A2352	U2287	U2221	U	U	U1964	
U2832	G2626	G2697	C2626	A2560	U2489	G2422	G2353	G2288	G2222	U	U	G1965	
A2833	G2627	G2698	U2627	U2561	G2490	U2423	C2354	G2289	C2223	U	U	A1966	
	U2628	G2699	U2628	U2562	U2491	G2424	C2355	U2291	C2224	U	U	C1967	
C2834	G2629	G2700	G2629	U2563	U2492	A2425	U2356	U2292	A2225	U	U	A1968	
G2835	U2630	G2701	G2630	A2564	U2493	C2426	C2357	G2293	G2226	U	U	G1969	
U2836	G2631	A2705	G2631	U2565		C2427	G2358	U2294	U2227	U	U	U1970	
G2837	G2632	G2706	U2632	A2566	C2489	G2428	G2359	C2295	U2229	U	U	G1971	
U2838	G2633	U2707	U2633	G2567	U2498	G2429	G2360	U2296	U2230	U	U	G1972	
G2839	G2634	G2708	G2634	U2568	U2500	G2430	C2361	A2297	U2231	U	U	C1973	
C2840	G2635	G2709	G2635	U2569	C2501	U2431	G2362	U2298	G2232	U	U	G1974	
G2841	U2636	G2710	G2636	U2570	U2502	C2432	G2363	C2300	U2233	U	U	U1975	
G2842	G2637	G2711	G2637	U2571	A2503	U2433	G2364	G2301	G2234	U	U	G1980	
	U2778	U2713	G2640	A2572	U2504	A2434	A2365	C2302	G2235	U	U	A1981	
U2845	U2779	G2714	G2645		G2505	A2435	A2366	G2304	U2236	U	U	U1982	
G2846	G2780	C2715	U2646	A2577	U2506	G2436	G2367	U2305	G2237	U	U	G1983	
U2847	A2781	G2716	G2647	U2578	C2507	G2437	C2368	G2238	U2238	U	U	A1912	
G2848	G2782	C2717	U2648	C2579	G2508	U2438	A2369	G2239	U2239	U	U	C1913	
U2849	U2783	G2718	U2649	U2580	U2509	G2439	G2370	U2240	A2241	U	U	C1914	
A2850	U2784	G2719	U2650	C2651	U2510	C2440	U2371	G2242	G2242	U	U	U1915	
G2851	U2785	U2720	G2651	U2511	U2511	G2441	G2372	U2243	U2243	U	U	A1916	
U2852	U2786	G2721	U2652	A2512	C2512	C2442	C2373	A2244	U2244	U	U	U1917	
G2853	C2787	A2721	U2653	A2513	A2513	G2443	U2374	U2245	U2245	U	U	A1918	
U2854	G2788	G2722	G2654	U2514	U2514	G2444	U2375	U2246	U2246	U	U	A1919	
C2855	C2789	G2723	G2655	A2587	U2587	G2445	A2376	U2247	U2247	U	U	G1920	
G2856	U2790	U2724	U2656	U2588	C2588	G2446	G2377	A2248	U2248	U	U	U1921	
U2857	G2791	A2725	G2660	C2589	C2516	G2447	C2378	A2249	A2249	U	U	G1922	
G2858	A2792	G2726	G2661	A2590	C2517	G2448	C2379	U2250	U2250	U	U	U1923	
C2859	C2793	A2727	U2662	U2591	U2518	U2449	U2380	G2251	G2251	U	U	C1924	
A2860	G2794	U2728	G2663	C2592	A2519	A2450	G2381	A2317	G2252	U	U	U1925	
U2861	U2795	G2729	A2664	U2593	C2520	U2451	G2382	U2318	G2253	U	U	U1926	
G2862	U2796	C2730	U2665	C2594	U2521	U2452	U2383	G2319	U2254	U	U	A1927	
C2863	U2797	G2731	G2666	U2595	U2522	G2455	A2384	G2318	U2255	U	U	U1928	
			G2667	G2595	G2523	C2456	A2386	U2320	U2257	U	U	G1929	



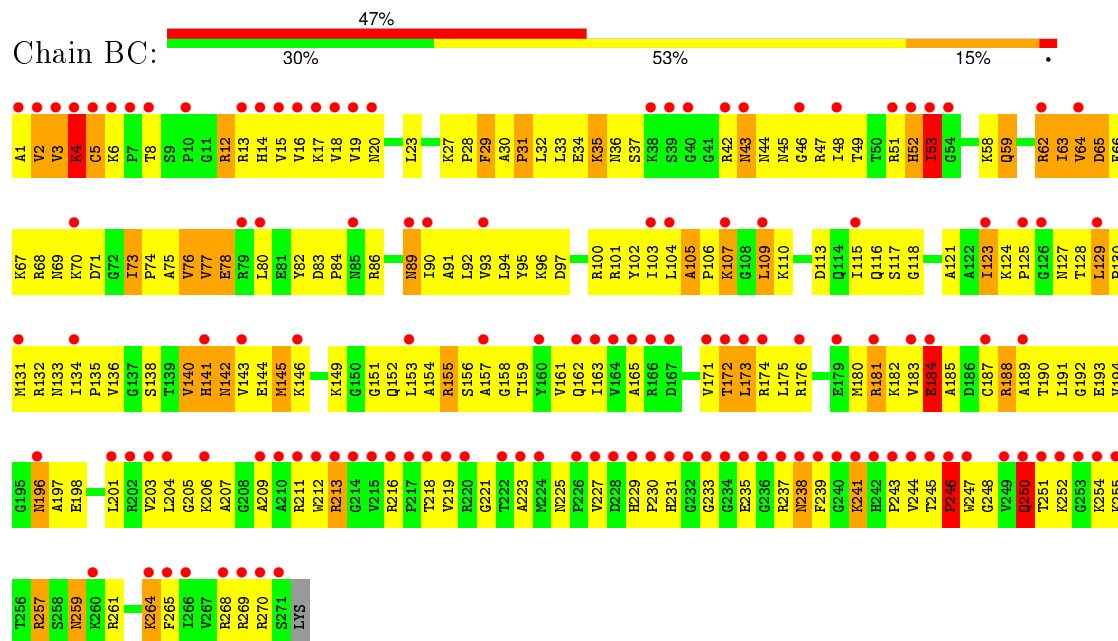
● Molecule 25: 23S ribosomal RNA



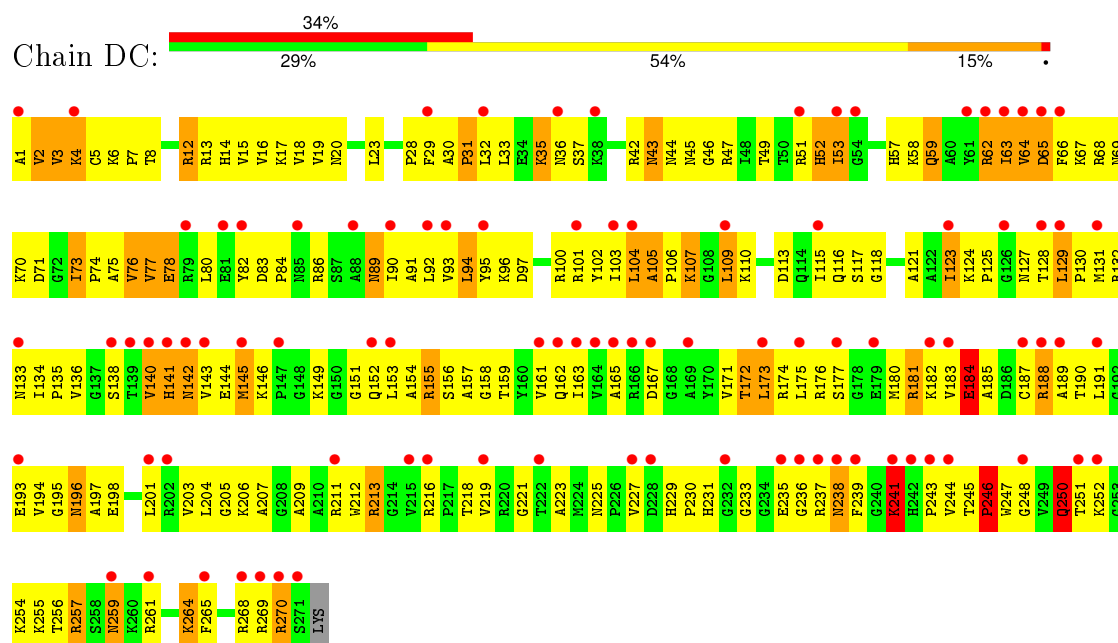
U1880	C1881	A1815	G1814	C1748	G1667	A1590	G1524	G1450	A1383	U1316	A1244	G1171	A1103	G1037	C961	A
U1882	C1883	G1750	G1816	A1749	A1668	A1591	A1525	C1451	A1384	U1317	G1245	C1172	C1104	G1038	G962	C
U1883	C1884	U1751	G1817	U1750	A1669	C1592	G1526	G1452	A1385	U1318	G1246	U1173	U1105	G1038	U963	U
A1884	C1885	G1752	G1818	G1674	G1674	C1593	G1527	C1453	A1386	C1320	U1249	U1174	G1106		C964	
U1885	C1886	G1753	U1819	U1594	C1595	U1594	A1532	C1454	A1387	A1321	U1250	U1175	G1107	G1041	U967	A
U1886	C1887	A1754	A1755	A1677	A1677	C1595	A1532	G1455	A1388	A1322	A1251	U1176	G1108	G1042	U967	C
A1887	C1888	U1756	G1756	U1680	U1680	U1599	C1533	U1458	A1389	A1323	A1252	G1177	G1109	C1043	C968	C898
A1888	C1889	A1757	G1757	G1681	G1681	U1599	U1534	G1459	U1394	C1324	A1253	G1178	A1110		C969	A899
A1890	C1890	U1758	U1758	G1682	G1682	C1600	A1535	U1460	U1395	A1324	A1254	U1179	A1111	A1046	U970	A900
G1891	C1891	U1759	G1824	U1683	U1683	G1601	A1536	C1461	U1396	U1325	G1255	U1180	G1112	G1047		C901
C1892	C1892	U1760	U1825	G1684	G1684	U1602	G1537	C1462	U1397	U1326	G1256	U1181	U1113		A973	C902
C1893	C1893	C1761	U1826	G1685	G1685	A1603	G1538	C1463	C1398	A1327	C1257	G1182	G1114		G974	C903
C1894	C1894	U1762	U1828	C1686	C1686	C1604	U1539	G1464	C1399	G1331	G1258	U1183	G1115	A1050	A975	G904
C1895	C1895	G1763	G1829	G1763	G1763	C1605	U1540	U1465	U1400	G1332	A1259	U1184	G1116	C1052		A905
G1896	C1896	U1764	A1829	U1764	U1764	C1606	G1541	U1466	U1401	G1333	A1260		G1120	A1054	A981	U906
G1897	C1897	U1765	A1830	U1765	U1765	C1607	U1542	U1467	U1402	G1334	G1261	U1188	G1121	A1055	C982	U907
U1898	C1898	G1766	A1831	U1766	U1766	A1608	G1543	A1470	U1403	C1335	G1262	A1199	G1056	G1056	A983	C908
A1899	C1899	G1767	U1834	U1767	U1767	A1609	A1544	A1471	A1404	A1336	A1263	G1191	G1057	A1057	C985	A909
						A1610	A1545	G1472	U1405	G1337	A1264	G1192	U1058	U1058	C986	A910
						G1613	G1546	G1473	U1406	G1338	C1270	G1193	A1126	U1059	C987	A911
						A1616	U1549	U1475	U1409	G1339	A1271	A1194	U1060	U1060	A988	U913
						G1617	C1550	U1476	G1410	G1340	A1272	G1195	U1130	U1061	A990	G916
						A1618	A1551	A1477	U1411	G1341	U1273	G1196	G1131	G1062	A991	A917
						A1652	A1553	G1478	U1412	U1344	A1276	U1198	A1133	C1064	C992	A918
						A1553	A1553		U1413	C1346	A1277	C1200	G1135	U1065		U919
						C1556	C1556	G1482	U1414	A1347	G1279	U1203	U1136	U1066	C995	A920
						C1557	C1557	U1483	U1415	G1348	G1280	U1204	G1137	G1067	A996	C921
						C1558	C1558	U1485	G1416	C1349	G1281	A1205	U1138	G1068	C997	C922
						U1559	U1559	U1486	C1417	C1350	U1282	A1069	G1139	A1069	C998	G923
						G1560	G1560	U1487	G1418	C1351	G1283	A1070	G1140	G1071	U999	G924
						C1561	C1561	U1488	A1419	A1352	A1284	U1141	C1072	G1072	A1000	A925
						G1562	U1562	C1489	U1420	A1353	A1285	U1142	A1143	U1076	A1001	G926
						U1563	U1563	A1490	G1421	C1354	A1286	C1211	A1144	A1076	A927	A928
						C1564	C1564	G1491		G1355	A1287	G1212	C1145	A1077	U929	U929
						U1565	U1565		G1426	G1356	G1288		C1146	A1080	G930	G930
						C1566	C1566	G1492	A1427	C1357		U1219	G1147	A1081	G1011	U931
						A1566	A1566	C1493	C1428	G1360	G1292	G1220	A1148	U1082	U1012	U932
						G1567	G1567	U1494	G1429	G1361	U1294	C1221	G1149	U1083	C1013	A933
						C1568	C1568	A1495	G1430	C1362	G1295	U1224	G1150	U1084	A1014	U934
						A1569	A1569	U1496	A1431	C1363	G1296	G1225	C1151	A1085	U1015	C935
						U1570	U1570	C1497	A1432	G1364	C1297	A1226	A1086	A1086	G1016	
						A1571	A1571	C1498	A1433	G1365	C1298	G1227	C1153	G1087	G1017	
						A1572	A1572		A1434	A1366	C1299	U1228	A1156	A1088	U1018	A941
						C1573	C1573	U1505	C1437	A1367	G1300	G1229	G1157	A1089	U1019	U942
						G1574	G1574	U1506	U1438	G1368	A1301	A1230	A1090	A1089	A1020	A943
						U1575	U1575	C1507	A1439	C1369	A1302	U1231	C1158	G1091	A1021	A945
						C1576	C1576	U1508	U1440	C1370		G1232	U1159	C1092	G1022	C946
						U1577	U1577	A1509	U1441	C1371	C1306		G1163	U1094	U1023	A947
						G1578	G1578	G1510	U1442	U1372	G1309	G1236	C1164	U1097	G1024	C948
						A1579	A1579	G1511	U1443	A1373	G1310	A1237	A1165	A1098	G1025	G950
						C1580	C1580	C1512	G1444	G1374	G1311	G1238	A1166	U1099	A1028	G956
						U1582	U1582	U1513	G1445		U1312	G1239	C1167	G1099	C1030	C957
						A1583	A1583	G1514	C1446	U1379	U1313	U1240	G1168	G1099	C1031	U958
						U1584	U1584	A1515	C1447	G1380	C1314	A1241	A1169	U1101	A1032	A959
						C1585	C1585	U1516	G1448	G1381	C1315	U1242	C1170	C1102	U1033	A960
						A1586	A1586	G1517	G1449	G1382		C1243				

C2889	C2890	A2823	C2760	U2698	G2623	U2552	G2485	G2415	G2345	A2284	G2215	A2154	C2091	G2024	C1947
G2893	G2894	A2829	A2761	G2699	G2624	G2553	C2486	G2416	A2346	C2285	G2216	U2155	U2092	C2025	G1948
G2895	G2896	G2831	A2765	U2555	G2625	U2554	G2487	C2417	C2347	G2286	G2217	G2156	A2094	U2026	G1949
U2897	U2898	G2832	C2767	G2556	G2626	G2557	U2489	U2418	U2348	A2287	G2218	G2157	A2095	U2027	A1952
U2899	U2900	U2833	U2768	C2558	G2627	C2558	U2491	C2420	A2352	G2288	U2219	G	C2096	U2028	A1953
C2901	C2902	U2834	U2769	C2559	U2628	U2560	U2492	C2421	C2353	G2289	U2220	C	A2030	U2029	U1955
U2903	U	G2842	U2770	U2561	G2629	U2561	U2493	C2422	C2354	U2291	G2221	C	A2100	A2031	U1956
			U2771	U2562	G2630	U2562	U2494	C2423	U2355	U2292	C2222	G	A2101	G2032	U1957
			U2772	U2563	G2631	U2563	C2498	C2424	U2356	U2293	A2225	C	G2102	A2033	C1958
			U2773	U2564	G2632	U2564	U2499	A2425	C2360	G2290	A2226	C	G2103	U2034	C1959
			U2774	U2565	G2633	U2565	U2500	C2426	C2361	U2295	A2227	C	C2104	G2035	A1960
			U2775	U2566	G2634	U2566	C2501	C2427	C2362	U2297	U2228	U	U2105	C2036	C1961
			U2776	U2567	G2635	U2567	G2502	C2428	C2363	A2298	U2229	G	U2106	A2037	C1962
			U2777	U2568	G2636	U2568	U2504	C2429	G2364	U2299	U2230	A	G2107	G2038	U1963
			U2778	U2569	G2637	U2569	U2505	U2431	G2365	U2299	U2231	A	A2108	U2039	C1964
			U2779	U2570	G2638	U2570	U2506	U2432	G2366	G2300	U2232	A	U2109	G2040	C1965
			U2780	U2571	G2639	U2571	U2511	U2433	G2367	C2301	U2233	A	G2110	U2041	A1966
			U2781	U2572	G2640	U2572	C2512	U2434	C2368	U2304	G2234	U	A2042	A2042	C1967
			U2782	C2573	G2641	U2573	C2513	U2435	A2369	U2305	G2235	A	C2043	G2043	G1968
			U2783	G2574	G2642	U2574	C2514	U2436	G2370	C2306	G2236	C	G2044	C2044	A1969
			U2784	G2575	G2643	U2575	U2515	U2437	G2371	U2307	G2237	C	G2045	C2045	A1970
			U2785	G2576	G2644	U2576	U2516	U2438	G2372	G2308	G2238	A	G2046	G2046	U1971
			U2786	G2577	G2645	U2577	U2517	U2439	G2373	G2309	U2239	C	G2047	C2047	G1972
			U2787	G2578	G2646	U2578	U2518	U2440	G2374	U2310	U2240	C	A	G2048	G1973
			U2788	G2579	G2647	U2579	U2519	U2441	G2375	C2311	A2241	U	U	G2049	C1974
			U2789	G2580	G2648	U2580	C2520	U2442	G2376	U2312	G2242	U	A	C2050	C1985
			U2790	G2581	G2649	U2581	U2521	U2443	G2377	U2313	U2243	G	A	A2051	C1986
			U2791	G2582	G2650	U2582	U2522	U2444	G2378	U2314	U2244	G	A	A2052	A1987
			U2792	G2583	G2651	U2583	U2523	U2445	G2379	U2315	U2245	U	G	G2055	G1988
			U2793	G2584	G2652	U2584	U2524	U2446	G2380	G2316	U2246	U	G	G2056	U1991
			U2794	G2585	G2653	U2585	U2525	U2447	G2381	U2317	U2247	A	A	A2060	G1992
			U2795	G2586	G2654	U2586	U2526	U2448	G2382	U2318	U2248	G	G	A2061	U1993
			U2796	G2587	G2655	U2587	U2527	U2449	G2383	U2319	U2249	G	G	A2062	C1994
			U2797	G2588	G2656	U2588	U2528	U2450	G2384	U2320	G2250	U	C	G2063	U1997
			U2798	G2589	G2657	U2589	U2529	U2451	G2385	U2321	U2251	U	U	C2064	A1998
			U2799	G2590	G2658	U2590	U2530	U2452	G2386	U2322	U2252	U	U	C2065	A1999
			U2800	G2591	G2659	U2591	U2531	U2453	G2387	U2323	C2253	U	U	C2066	C2000
			U2801	G2592	G2660	U2592	U2532	U2454	G2388	U2324	U2254	U	G2133	G2069	C2001
			U2802	G2593	G2661	U2593	U2533	U2455	G2389	U2325	U2255	U	A2134	A2070	G2002
			U2803	G2594	G2662	U2594	U2534	U2456	G2390	U2326	U2256	U	A2135	A2071	C2008
			U2804	G2595	G2663	U2595	U2535	U2457	G2391	U2327	U2257	U	G2136	C2072	A2009
			U2805	G2596	G2664	U2596	U2536	U2458	G2392	U2328	U2258	U	U2137	C2073	G2010
			U2806	G2597	G2665	U2597	U2537	U2459	G2393	U2329	U2259	U	G2138	U2074	U2011
			U2807	G2598	G2666	U2598	U2538	U2460	U2394	U2330	A2267	U	G2141	U2075	G2012
			U2808	G2599	G2667	U2599	U2539	U2461	U2395	U2331	A2268	U	A2142	U2076	A2013
			U2809	G2600	G2668	U2600	U2540	U2462	U2396	U2332	A2269	U	G2143	A2077	A2014
			U2810	G2601	G2669	U2601	U2541	U2463	G2396	U2333	A2270	U	A2144	A2082	A2015
			U2811	G2602	G2670	U2602	U2542	U2464	G2400	U2334	G2271	U	G2145	U2016	U2016
			U2812	G2603	G2671	U2603	U2543	U2465	U2401	U2335	U2272	U	C2146	U2017	U2017
			U2813	G2604	G2672	U2604	U2544	U2466	U2402	A2336	U2273	U	G2147	G2083	G2018
			U2814	G2605	G2673	U2605	U2545	U2467	U2403	A2337	A2274	U	G2148	U2085	G2019
			U2815	G2606	G2674	U2606	U2546	U2468	U2404	U2338	G2275	U	U2149	U2086	A2020
			U2816	G2607	G2675	U2607	U2547	U2469	G2405	U2339	U2276	U	G2150	G2087	A2021
			U2817	G2608	G2676	U2608	U2548	U2470	U2406	U2340	U2277	U	U2151	A2088	U2022
			U2818	G2609	G2677	U2609	U2549	U2471	G2407	U2341	U2278	U	G2152	G2089	C2023
			U2819	G2610	G2678	U2610	U2550	U2472	U2408	U2342	G2279	U	C2153	A2090	
			U2820	G2611	G2679	U2611	U2551	U2473	U2409	U2343	A2281	U			
			U2821	G2612	G2680	U2612	U2552	U2474	G2410	U2344	G2282	U			
			U2822	G2613	G2681	U2613	U2553	U2475	G2411	U2345	G2283	U			
			U2823	G2614	G2682	U2614	U2554	U2476	G2412	U2346		U			
			U2824	G2615	G2683	U2615	U2555	U2477	G2413	U2347		U			
			U2825	G2616	G2684	U2616	U2556	U2478	G2414	U2348		U			
			U2826	G2617	G2685	U2617	U2557	U2479	G2415	U2349		U			
			U2827	G2618	G2686	U2618	U2558	U2480	G2416	U2350		U			
			U2828	G2619	G2687	U2619	U2559	U2481	G2417	U2351		U			
			U2829	G2620	G2688	U2620	U2560	U2482	G2418	U2352		U			
			U2830	G2621	G2689	U2621	U2561	U2483	G2419	U2353		U			
			U2831	G2622	G2690	U2622	U2562	U2484	G2420	U2354		U			
			U2832	G2623	G2691	U2623	U2563	U2485	G2421	U2355		U			
			U2833	G2624	G2692	U2624	U2564	U2486	G2422	U2356		U			
			U2834	G2625	G2693	U2625	U2565	U2487	G2423	U2357		U			
			U2835	G2626	G2694	U2626	U2566	U2488	G2424	U2358		U			
			U2836	G2627	G2695	U2627	U2567	U2489	G2425	U2359		U			
			U2837	G2628	G2696	U2628	U2568	U2490	G2426	U2360		U			
			U2838	G2629	G2697	U2629	U2569	U2491	G2427	U2361		U			
			U2839	G2630	G2698	U2630	U2570	U2492	G2428	U2362		U			
			U2840	G2631	G2699	U2631	U2571	U2493	G2429	U2363		U			
			U2841	G2632	G2700	U2632	U2572	U2494	G2430	U2364		U			
			U2842	G2633	G2701	U2633	U2573	U2495	G2431	U2365		U			
			U2843	G2634	G2702	U2634	U2574	U2496	G2432	U2366		U			
			U2844	G2635	G2703	U2635	U2575	U2497	G2433	U2367		U			
			U2845	G2636	G2704	U2636	U2576	U2498	G2434	U2368		U			
			U2846	G2637	G2705	U2637	U2577	U2499	G2435	U2369		U			
			U2847	G2638	G2706	U2638	U2578	U2500	G2436	U2370		U			
			U2848	G2639	G2707	U2639	U2579	U2501	G2437	U2371		U			
			U2849	G2640	G2708	U2640	U2580	U2502	G2438	U2372		U			
			U2850	G2641	G2709	U2641	U2581	U2503	G2439	U2373		U			
			U2851	G2642	G2710	U2642	U2582	U2504	G2440	U2374		U			
			U2852	G2643	G2711	U2643	U2583	U2505	G2441	U2375		U			
			U2853	G2644	G2712	U2644	U2584	U2506	G2442	U2376		U			
			U2854	G2645	G2713	U2645	U2585	U2507	G2443	U2377		U			
			U2855	G2646	G2714	U2646	U2586	U2508	G2444	U2378		U			
			U2856	G2647	G2715	U2647	U2587	U2509	G2445	U2379		U			
			U2857	G2648	G2716	U2648	U2588	U2510	G2446	U2380		U			
			U2858	G2649	G2717	U2649	U2589	U2511	G2447	U2381		U			
			U2859	G2650	G2718	U2650	U2590	U2512	G2448	U2382		U			

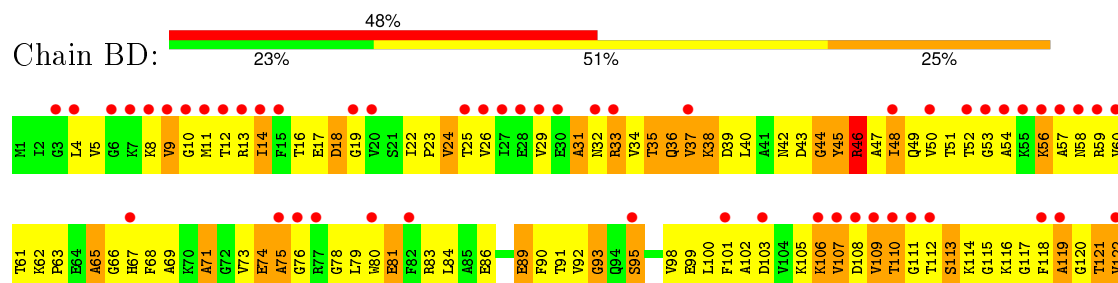
- Molecule 26: 50S ribosomal protein L2

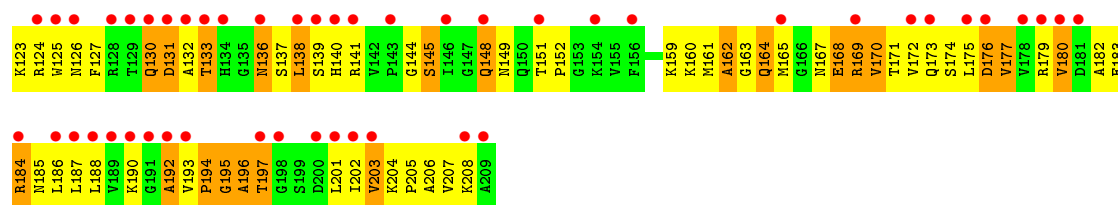


- Molecule 26: 50S ribosomal protein L2

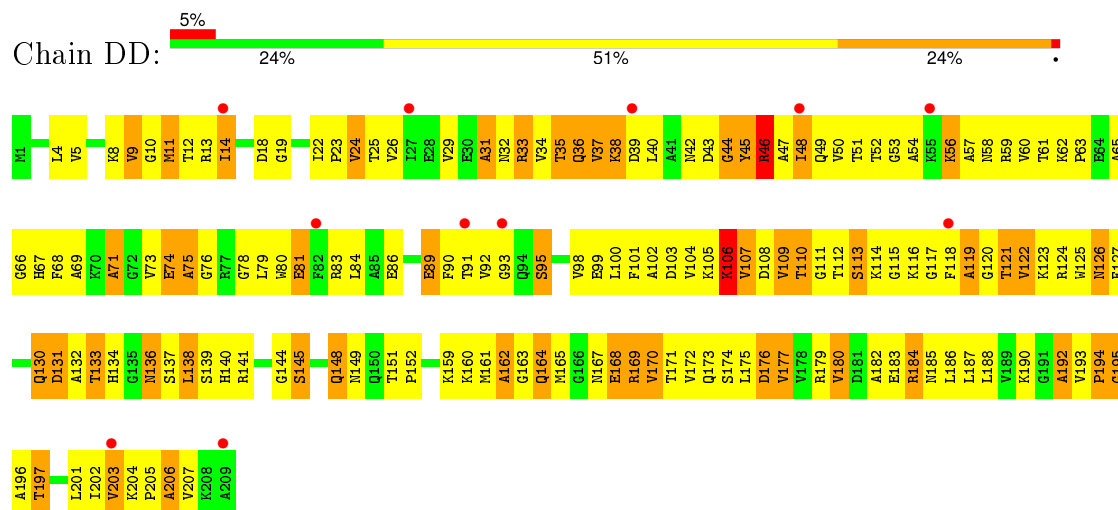


- Molecule 27: 50S ribosomal protein L3

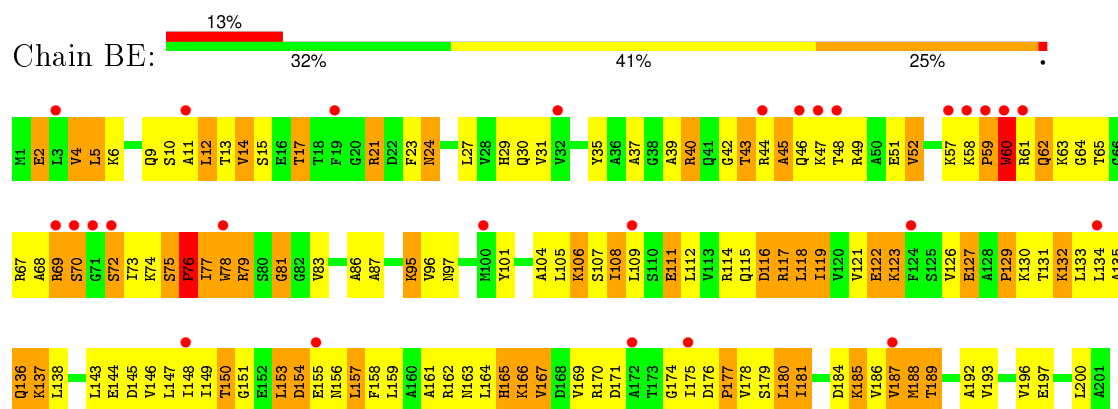




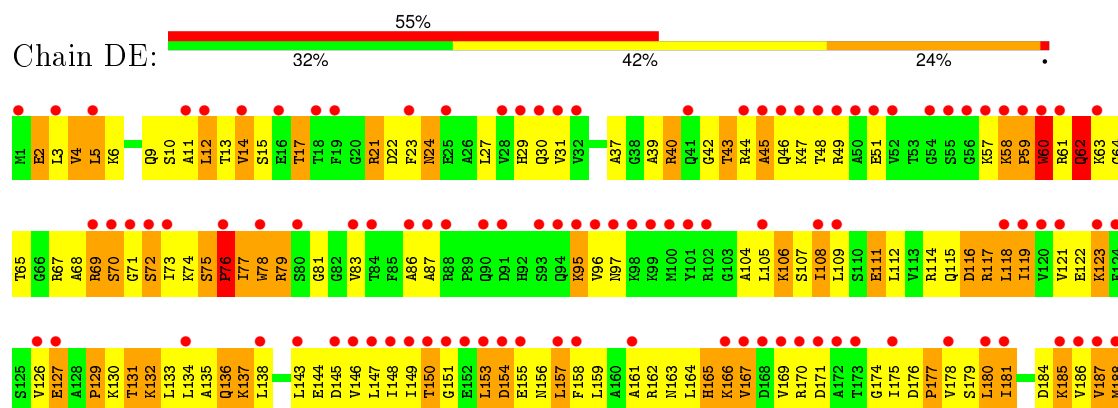
• Molecule 27: 50S ribosomal protein L3

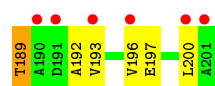


• Molecule 28: 50S ribosomal protein L4

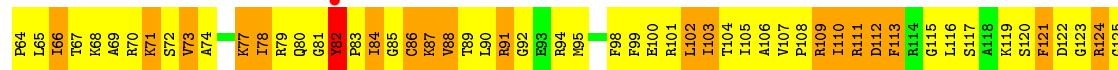
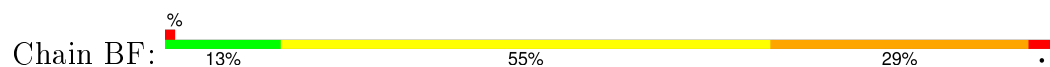


• Molecule 28: 50S ribosomal protein L4

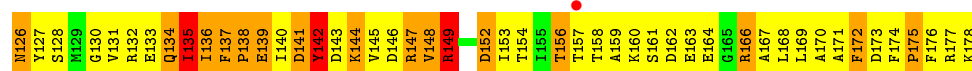
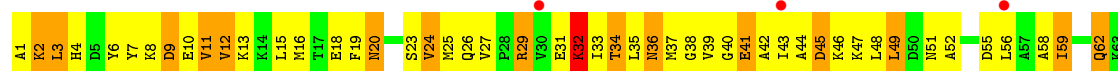
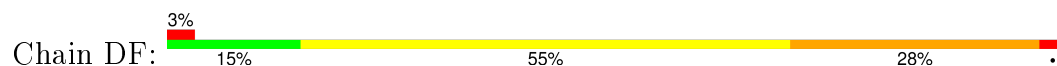




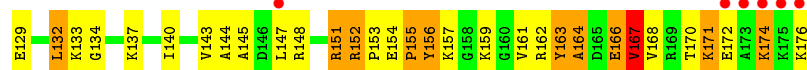
• Molecule 29: 50S ribosomal protein L5



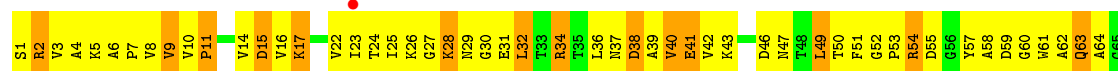
• Molecule 29: 50S ribosomal protein L5

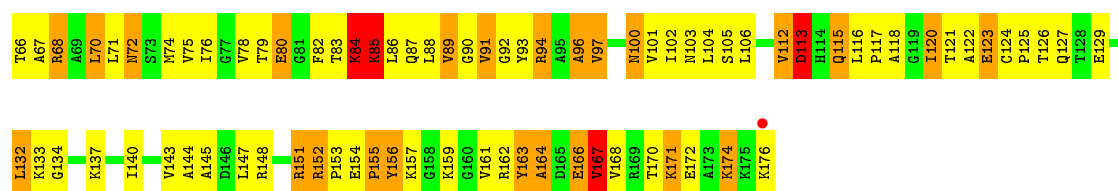


• Molecule 30: 50S ribosomal protein L6

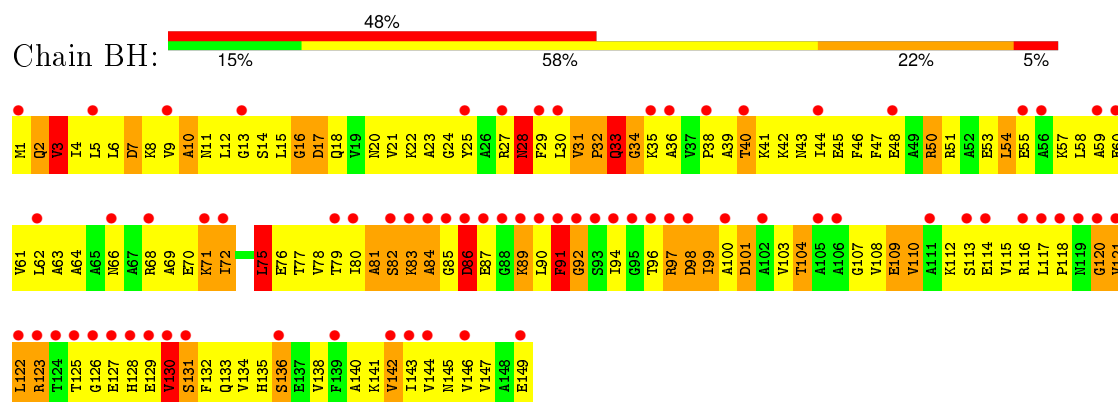


• Molecule 30: 50S ribosomal protein L6

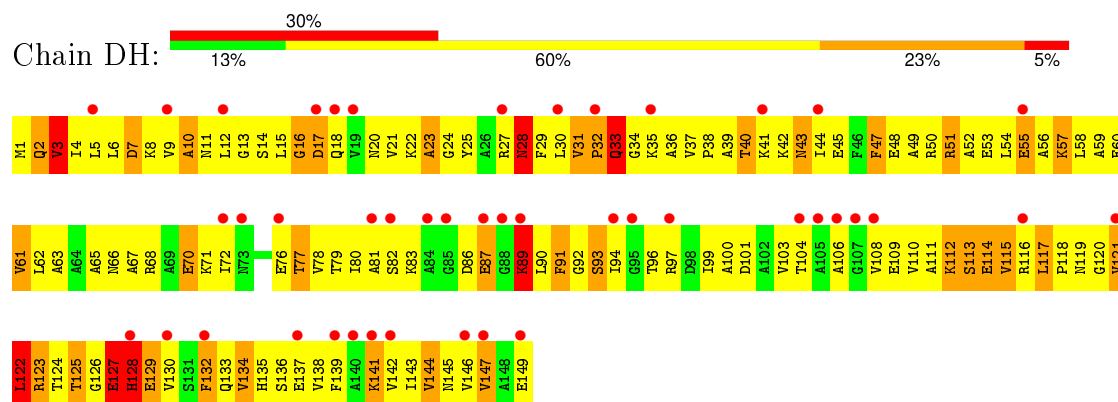




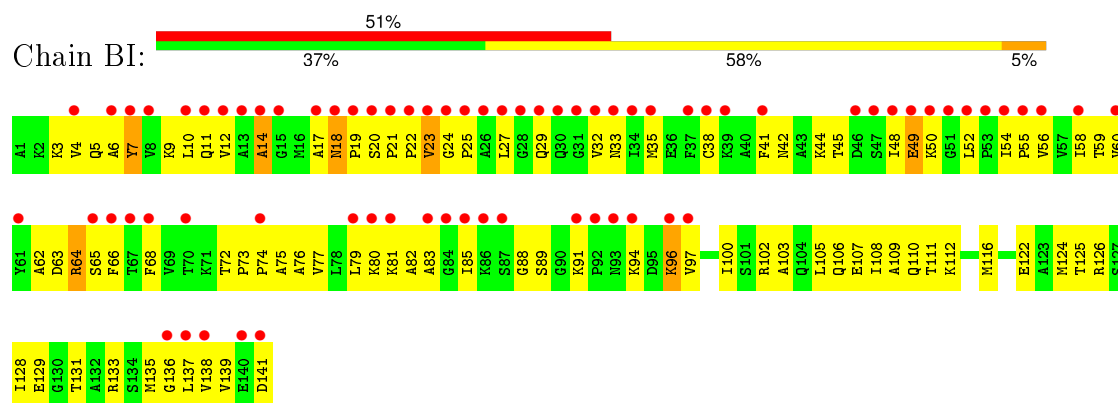
• Molecule 31: 50S ribosomal protein L9



• Molecule 31: 50S ribosomal protein L9



• Molecule 32: 50S ribosomal protein L11

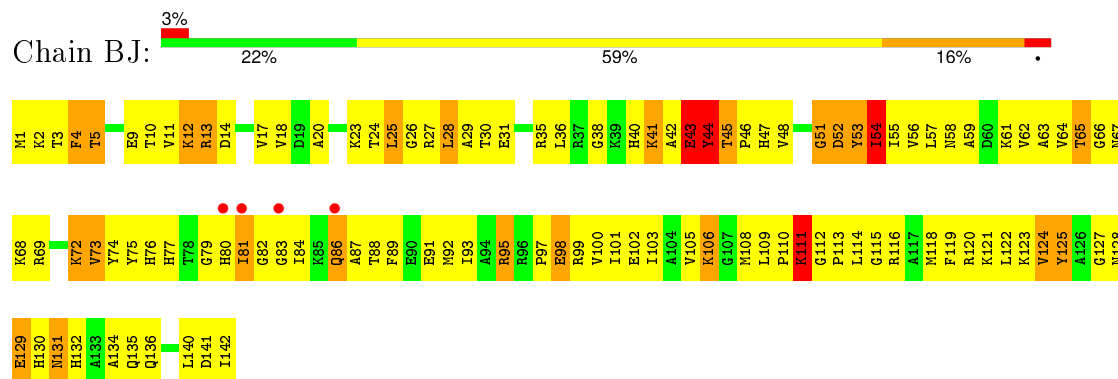


• Molecule 32: 50S ribosomal protein L11

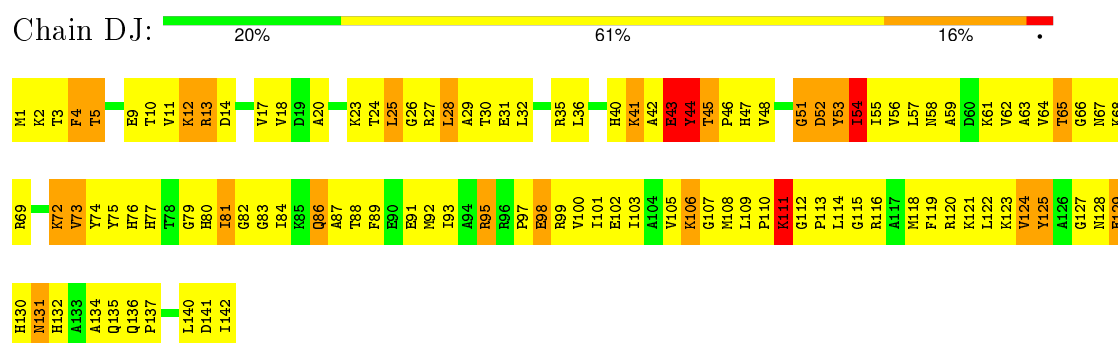




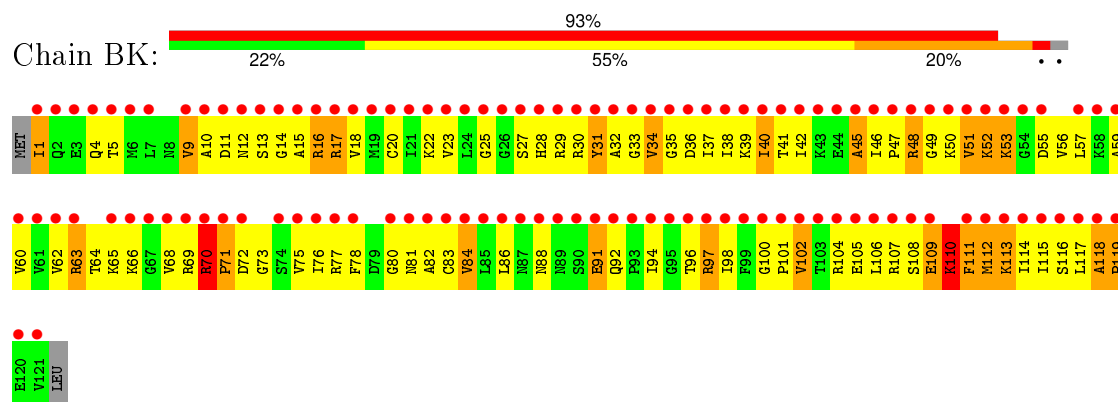
- Molecule 33: 50S ribosomal protein L13



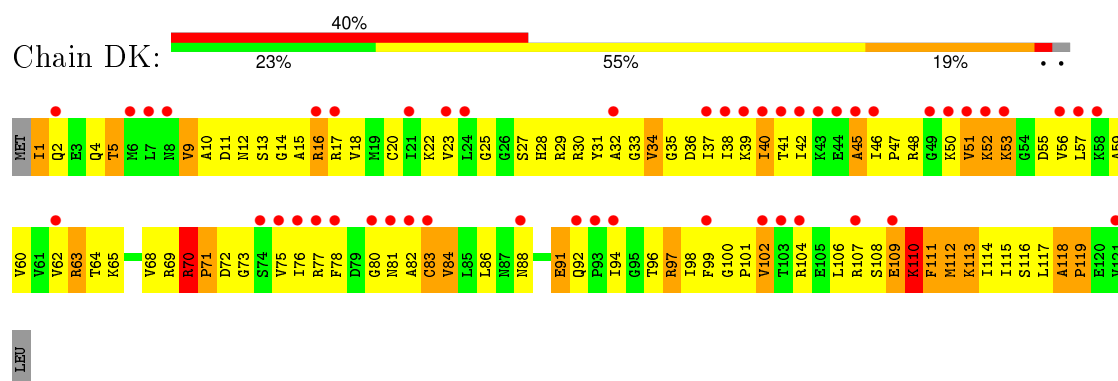
- Molecule 33: 50S ribosomal protein L13



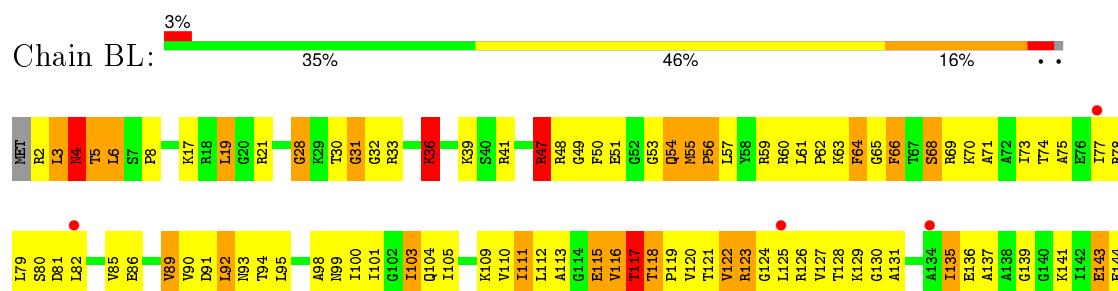
- Molecule 34: 50S ribosomal protein L14



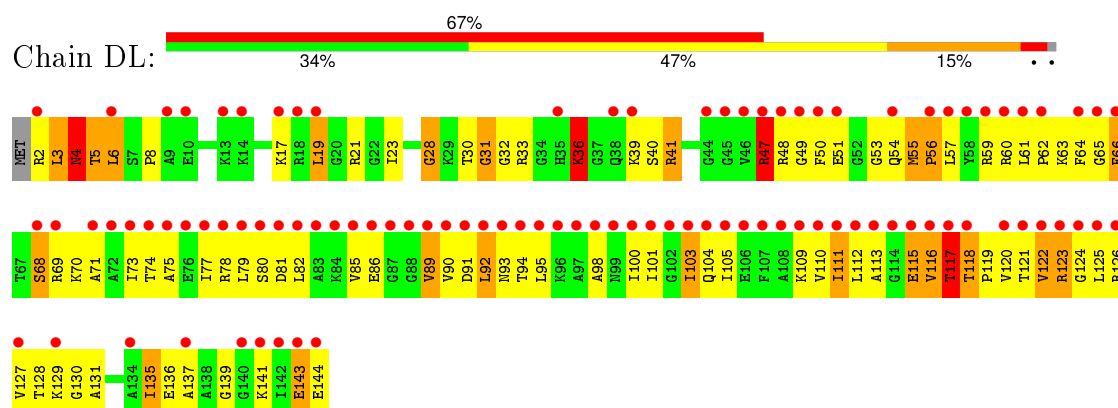
- Molecule 34: 50S ribosomal protein L14



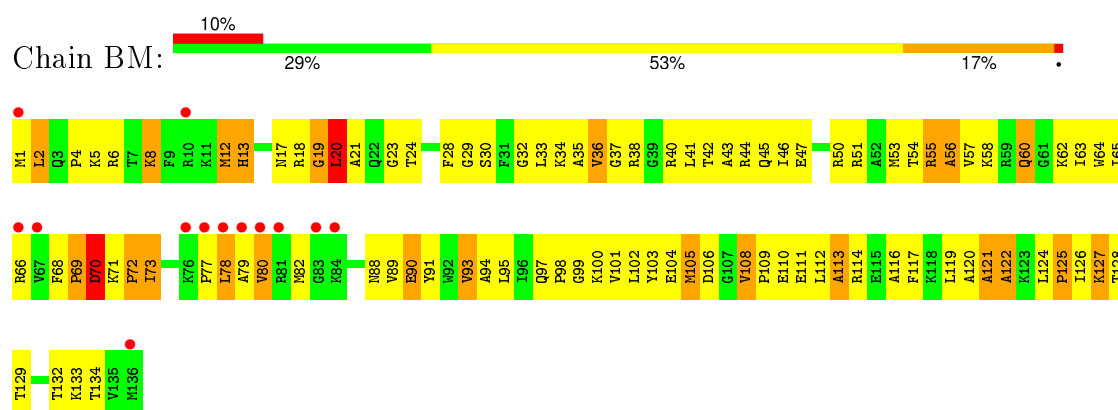
- Molecule 35: 50S ribosomal protein L15



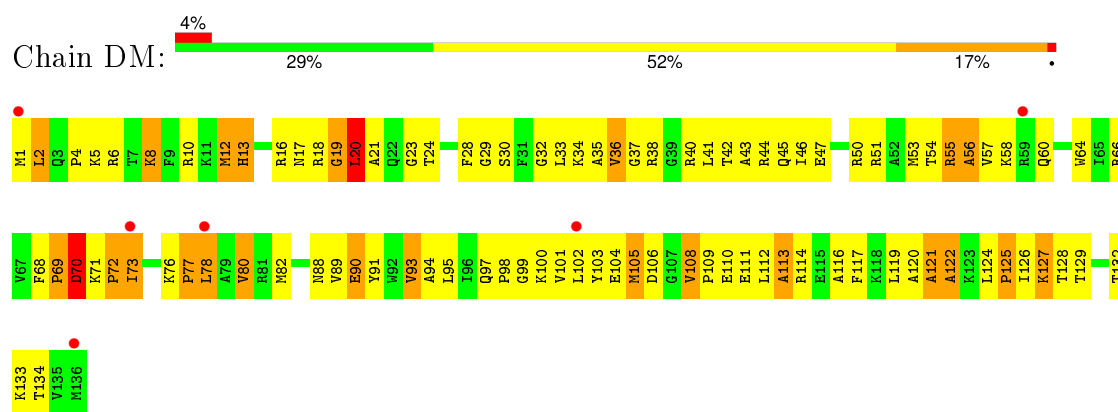
- Molecule 35: 50S ribosomal protein L15



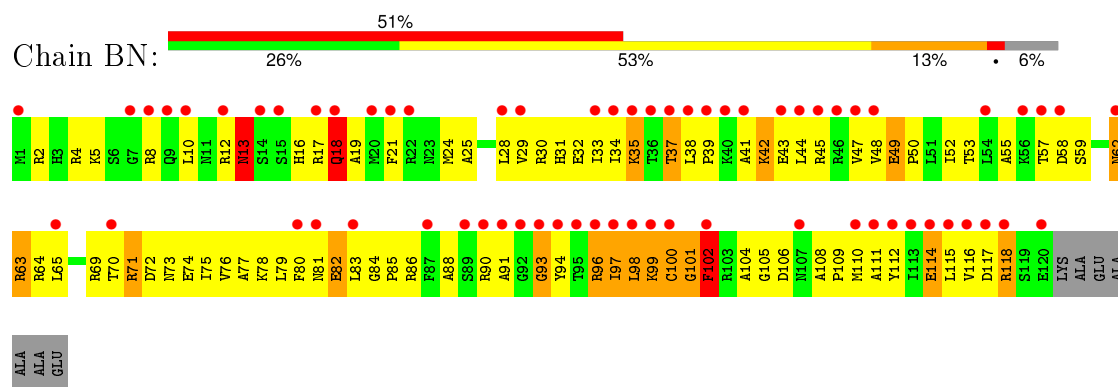
- Molecule 36: 50S ribosomal protein L16



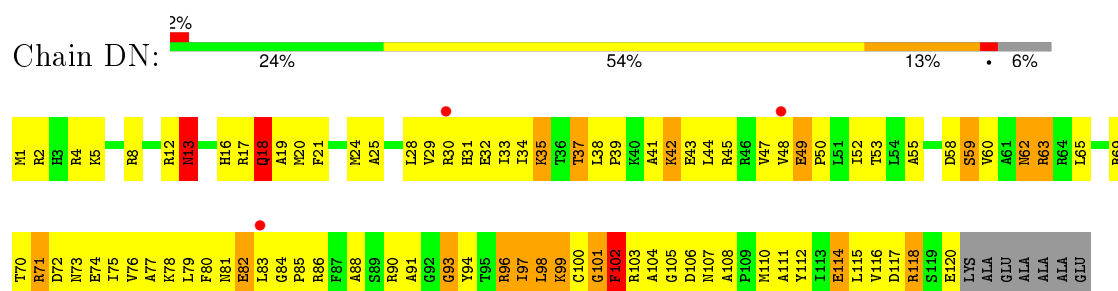
- Molecule 36: 50S ribosomal protein L16



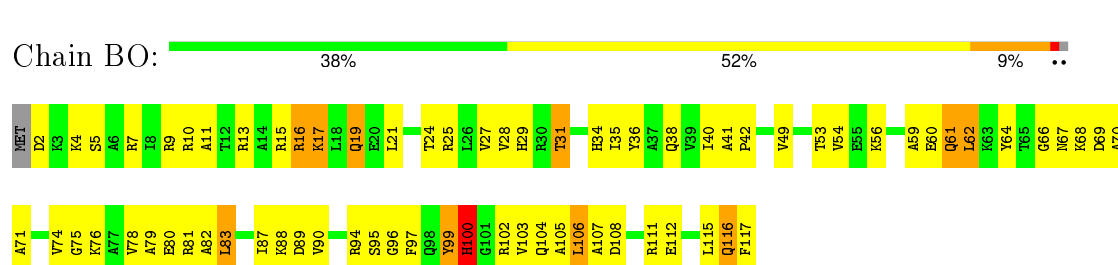
• Molecule 37: 50S ribosomal protein L17



• Molecule 37: 50S ribosomal protein L17

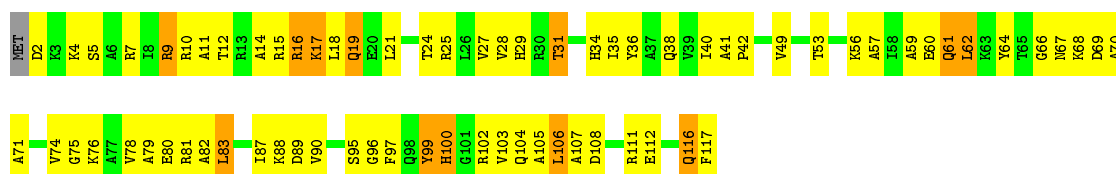


• Molecule 38: 50S ribosomal protein L18

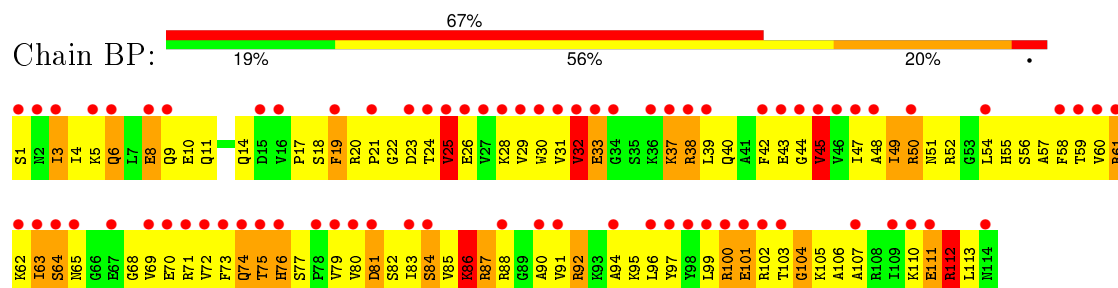


• Molecule 38: 50S ribosomal protein L18

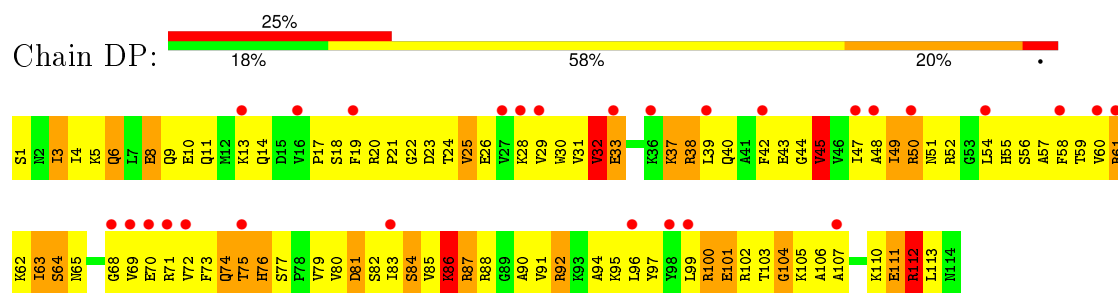




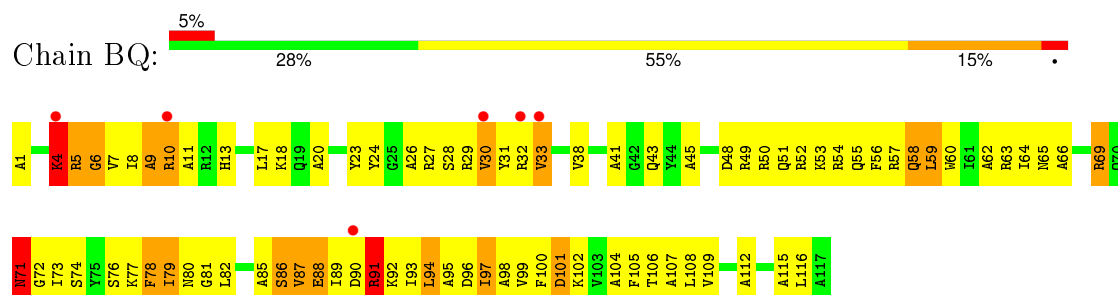
• Molecule 39: 50S ribosomal protein L19



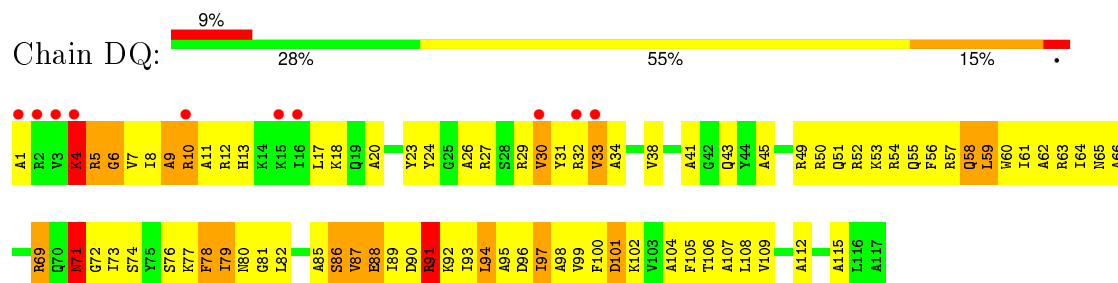
• Molecule 39: 50S ribosomal protein L19



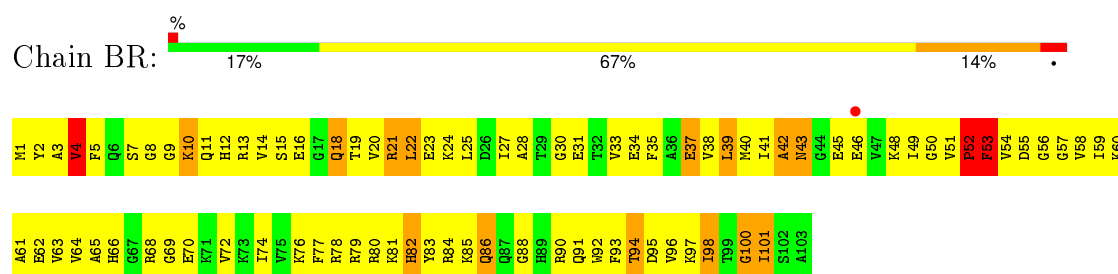
• Molecule 40: 50S ribosomal protein L20



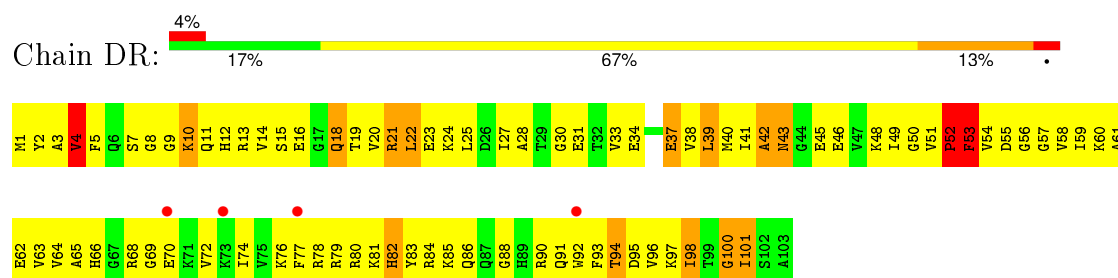
• Molecule 40: 50S ribosomal protein L20



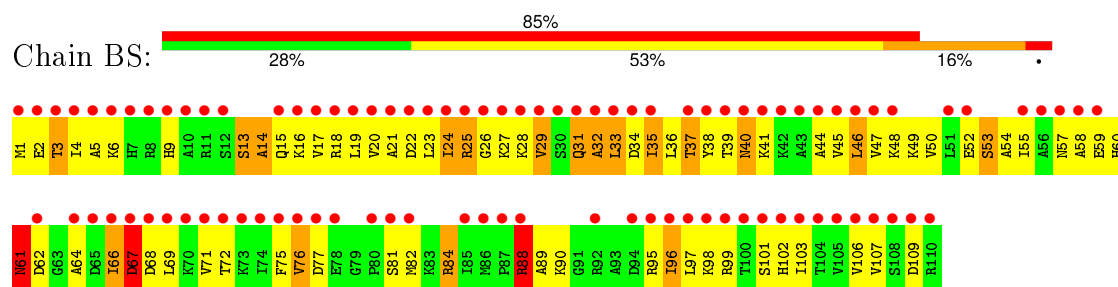
• Molecule 41: 50S ribosomal protein L21



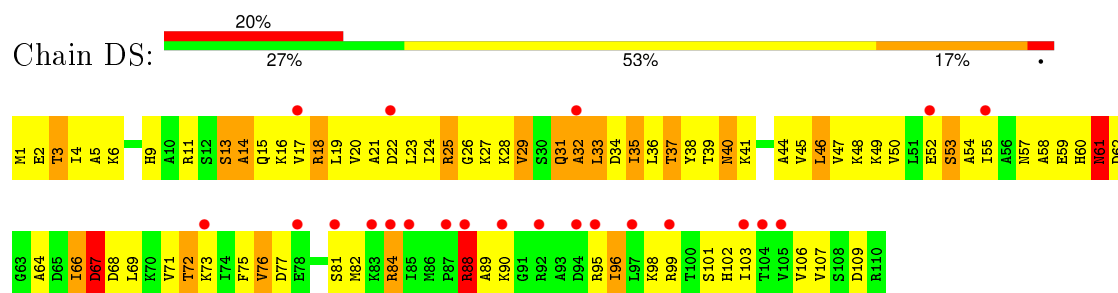
- Molecule 41: 50S ribosomal protein L21



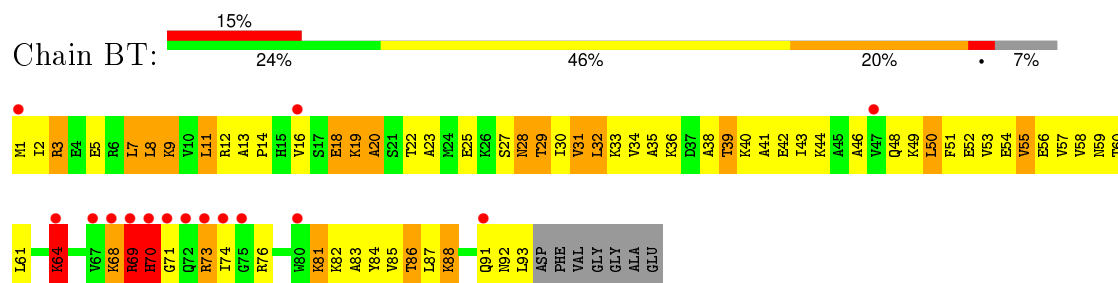
- Molecule 42: 50S ribosomal protein L22



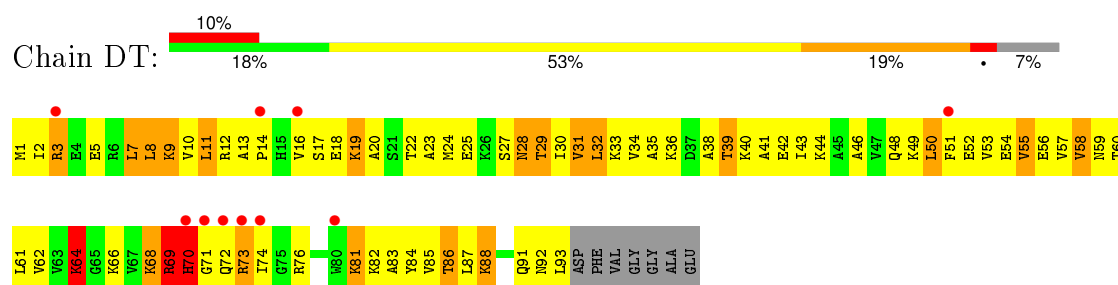
- Molecule 42: 50S ribosomal protein L22



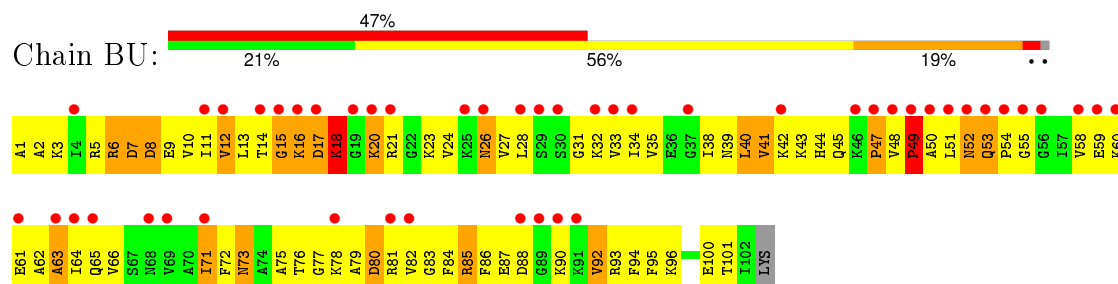
- Molecule 43: 50S ribosomal protein L23



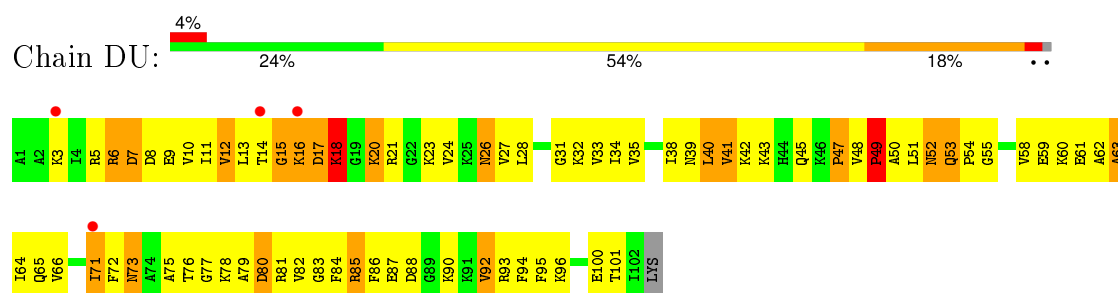
- Molecule 43: 50S ribosomal protein L23



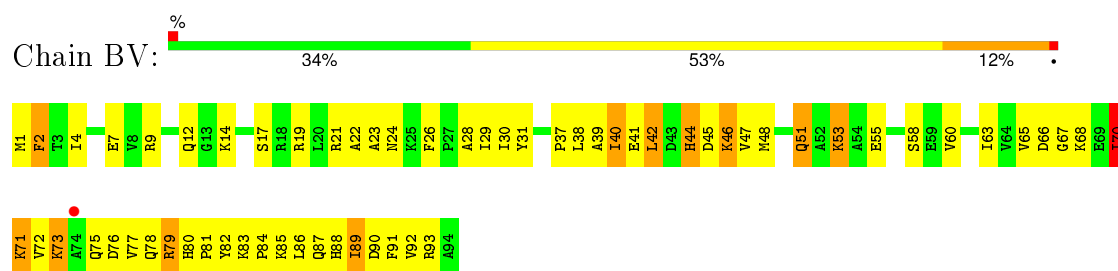
- Molecule 44: 50S ribosomal protein L24



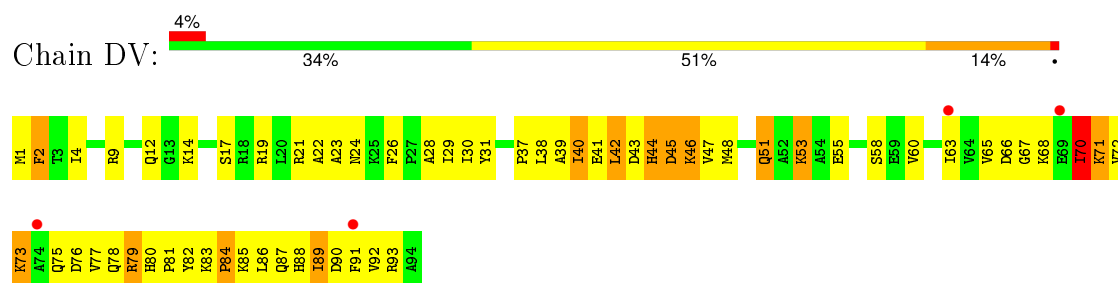
- Molecule 44: 50S ribosomal protein L24



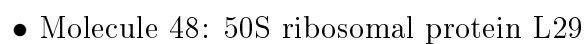
- Molecule 45: 50S ribosomal protein L25

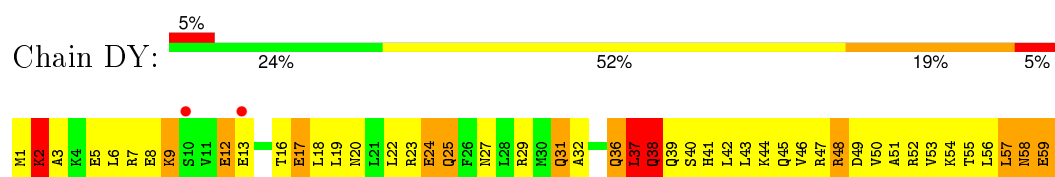


- Molecule 45: 50S ribosomal protein L25

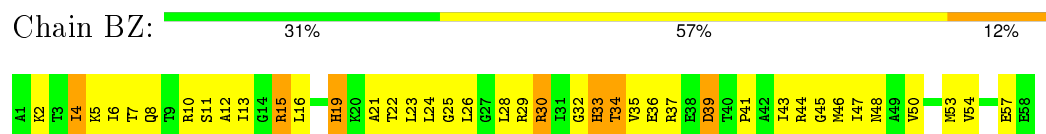


- Molecule 46: 50S ribosomal protein L27

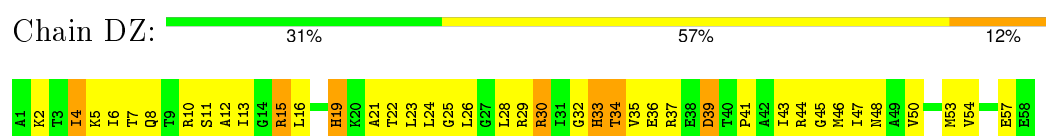




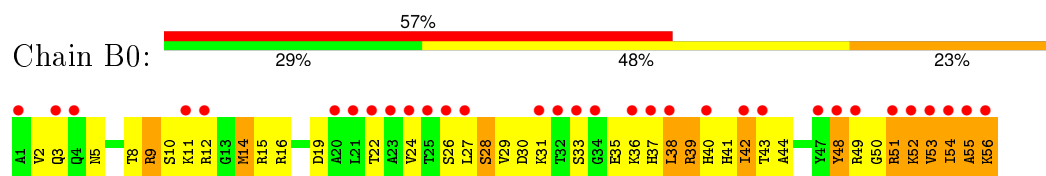
- Molecule 49: 50S ribosomal protein L30



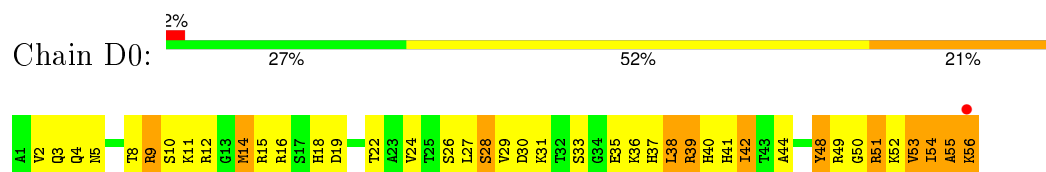
- Molecule 49: 50S ribosomal protein L30



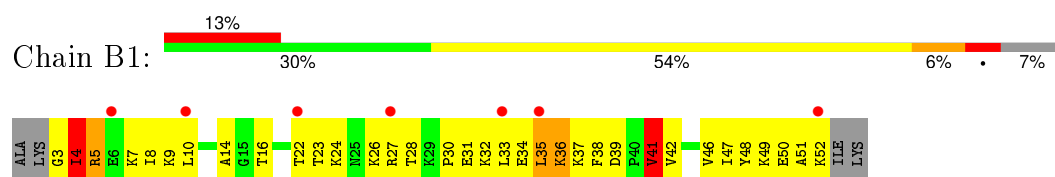
- Molecule 50: 50S ribosomal protein L32



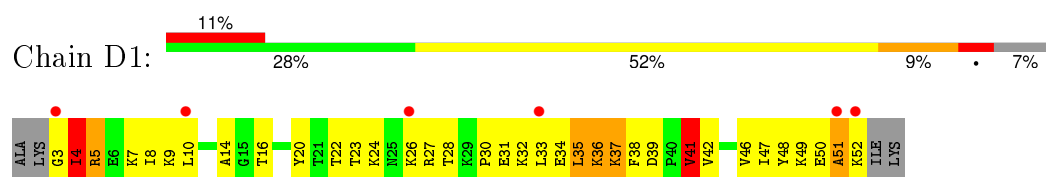
- Molecule 50: 50S ribosomal protein L32



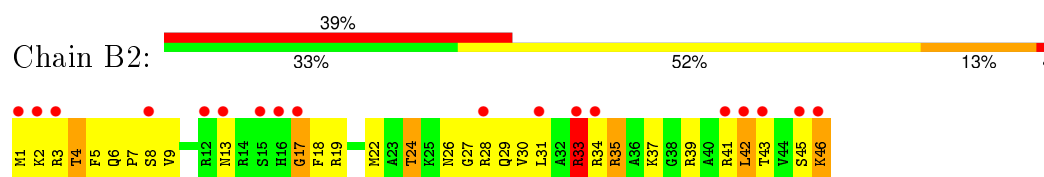
- Molecule 51: 50S ribosomal protein L33



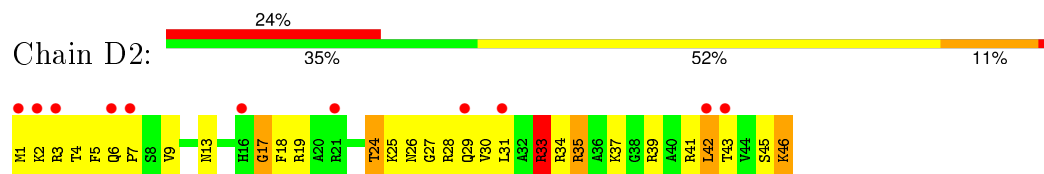
- Molecule 51: 50S ribosomal protein L33



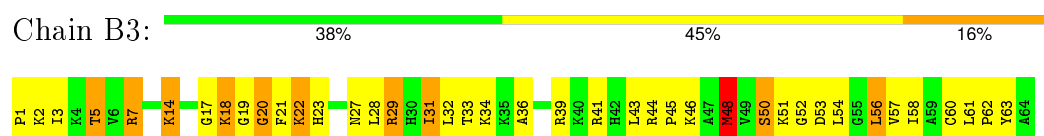
- Molecule 52: 50S ribosomal protein L34



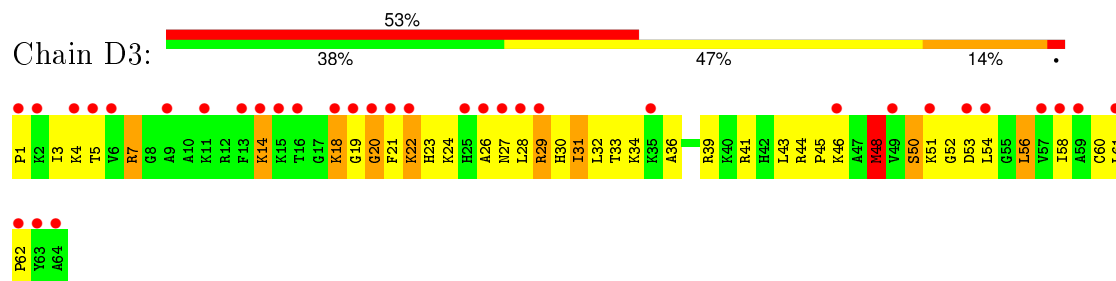
- Molecule 52: 50S ribosomal protein L34



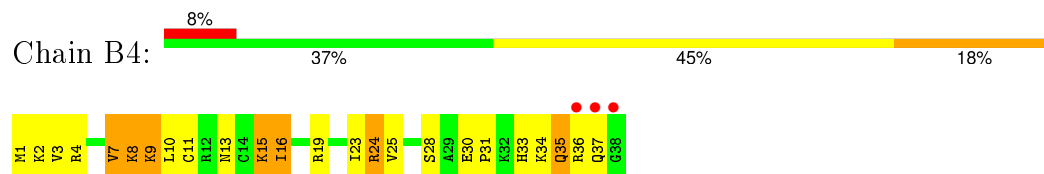
- Molecule 53: 50S ribosomal protein L35



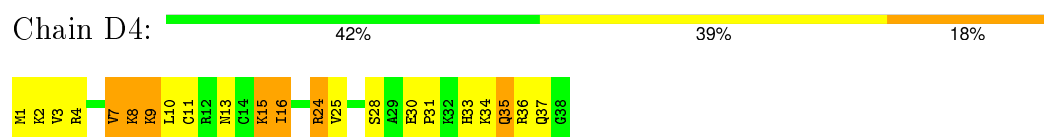
- Molecule 53: 50S ribosomal protein L35



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.287 , 0.320 0.260 , 0.289	Depositor DCC
R_{free} test set	37290 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.720	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 62.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 753156 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	285033	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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	3
4	CB	216/240 (90%)	106 (49%)	71 (33%)	39 (18%)	0	0
5	AC	204/232 (88%)	134 (66%)	50 (24%)	20 (10%)	1	4
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	3
6	CD	203/205 (99%)	122 (60%)	54 (27%)	27 (13%)	0	2
7	AE	148/166 (89%)	101 (68%)	38 (26%)	9 (6%)	2	15
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	3
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	11
9	CG	148/178 (83%)	89 (60%)	40 (27%)	19 (13%)	0	2
10	AH	127/129 (98%)	83 (65%)	31 (24%)	13 (10%)	1	4
10	CH	127/129 (98%)	78 (61%)	35 (28%)	14 (11%)	0	3
11	AI	125/129 (97%)	78 (62%)	33 (26%)	14 (11%)	0	3
11	CI	125/129 (97%)	74 (59%)	44 (35%)	7 (6%)	2	18
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	5
13	CK	115/128 (90%)	82 (71%)	25 (22%)	8 (7%)	1	10
14	AL	121/123 (98%)	80 (66%)	30 (25%)	11 (9%)	1	5
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	13
16	CN	94/100 (94%)	46 (49%)	29 (31%)	19 (20%)	0	0
17	AO	86/88 (98%)	69 (80%)	14 (16%)	3 (4%)	4	31
17	CO	86/88 (98%)	70 (81%)	14 (16%)	2 (2%)	8	44
18	AP	80/82 (98%)	46 (58%)	26 (32%)	8 (10%)	1	4
18	CP	78/82 (95%)	53 (68%)	17 (22%)	8 (10%)	1	4
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	5
20	AR	53/74 (72%)	39 (74%)	9 (17%)	5 (9%)	1	5
20	CR	53/74 (72%)	37 (70%)	12 (23%)	4 (8%)	1	9
21	AS	77/91 (85%)	53 (69%)	19 (25%)	5 (6%)	1	13
21	CS	77/91 (85%)	55 (71%)	18 (23%)	4 (5%)	2	19
22	AT	83/86 (96%)	63 (76%)	11 (13%)	9 (11%)	0	3
22	CT	83/86 (96%)	59 (71%)	20 (24%)	4 (5%)	3	22
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	2
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	1
32	BI	139/141 (99%)	118 (85%)	16 (12%)	5 (4%)	4	30

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%)	6	36
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%)	3	24
38	DO	114/117 (97%)	85 (75%)	24 (21%)	5 (4%)	3	24
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	3
40	DQ	115/117 (98%)	74 (64%)	28 (24%)	13 (11%)	0	3
41	BR	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	2
41	DR	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	2
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	9
45	DV	92/94 (98%)	73 (79%)	12 (13%)	7 (8%)	1	9
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	7
47	DX	75/77 (97%)	41 (55%)	27 (36%)	7 (9%)	1	5

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%)	1	4
48	DY	61/63 (97%)	34 (56%)	21 (34%)	6 (10%)	1	4
49	BZ	56/58 (97%)	42 (75%)	11 (20%)	3 (5%)	2	19
49	DZ	56/58 (97%)	42 (75%)	11 (20%)	3 (5%)	2	19
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	3
52	D2	44/46 (96%)	26 (59%)	14 (32%)	4 (9%)	1	5
53	B3	62/64 (97%)	42 (68%)	15 (24%)	5 (8%)	1	7
53	D3	62/64 (97%)	41 (66%)	17 (27%)	4 (6%)	1	13
54	B4	36/38 (95%)	21 (58%)	11 (31%)	4 (11%)	0	3
54	D4	36/38 (95%)	21 (58%)	11 (31%)	4 (11%)	0	3
All	All	11239/11910 (94%)	6961 (62%)	2802 (25%)	1476 (13%)	0	2

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 ⓘ

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	6
4	CB	180/198 (91%)	143 (79%)	37 (21%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AC	170/189 (90%)	134 (79%)	36 (21%)	1	7
5	CC	170/189 (90%)	138 (81%)	32 (19%)	2	10
6	AD	172/172 (100%)	146 (85%)	26 (15%)	3	17
6	CD	172/172 (100%)	130 (76%)	42 (24%)	1	3
7	AE	113/125 (90%)	95 (84%)	18 (16%)	3	15
7	CE	113/125 (90%)	87 (77%)	26 (23%)	1	5
8	AF	87/116 (75%)	74 (85%)	13 (15%)	4	17
8	CF	87/116 (75%)	76 (87%)	11 (13%)	5	26
9	AG	123/146 (84%)	99 (80%)	24 (20%)	2	9
9	CG	123/146 (84%)	100 (81%)	23 (19%)	2	10
10	AH	104/104 (100%)	89 (86%)	15 (14%)	4	19
10	CH	104/104 (100%)	81 (78%)	23 (22%)	1	6
11	AI	105/106 (99%)	83 (79%)	22 (21%)	1	7
11	CI	105/106 (99%)	83 (79%)	22 (21%)	1	7
12	AJ	86/90 (96%)	75 (87%)	11 (13%)	5	25
12	CJ	86/90 (96%)	71 (83%)	15 (17%)	2	12
13	AK	90/98 (92%)	75 (83%)	15 (17%)	3	13
13	CK	90/98 (92%)	77 (86%)	13 (14%)	4	19
14	AL	103/103 (100%)	83 (81%)	20 (19%)	2	9
14	CL	103/103 (100%)	80 (78%)	23 (22%)	1	5
15	AM	92/95 (97%)	75 (82%)	17 (18%)	2	10
15	CM	91/95 (96%)	71 (78%)	20 (22%)	1	6
16	AN	79/83 (95%)	60 (76%)	19 (24%)	1	3
16	CN	79/83 (95%)	66 (84%)	13 (16%)	3	13
17	AO	76/76 (100%)	65 (86%)	11 (14%)	4	19
17	CO	76/76 (100%)	67 (88%)	9 (12%)	6	29
18	AP	65/65 (100%)	52 (80%)	13 (20%)	1	8
18	CP	65/65 (100%)	58 (89%)	7 (11%)	8	34
19	AQ	74/77 (96%)	60 (81%)	14 (19%)	2	10
19	CQ	74/77 (96%)	66 (89%)	8 (11%)	8	34
20	AR	48/64 (75%)	37 (77%)	11 (23%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	CR	48/64 (75%)	43 (90%)	5 (10%)	9	35
21	AS	70/78 (90%)	55 (79%)	15 (21%)	1	7
21	CS	70/78 (90%)	51 (73%)	19 (27%)	0	2
22	AT	65/65 (100%)	56 (86%)	9 (14%)	4	21
22	CT	65/65 (100%)	55 (85%)	10 (15%)	3	16
23	AU	44/60 (73%)	37 (84%)	7 (16%)	3	15
23	CU	44/60 (73%)	32 (73%)	12 (27%)	0	2
26	BC	216/217 (100%)	182 (84%)	34 (16%)	3	15
26	DC	216/217 (100%)	182 (84%)	34 (16%)	3	15
27	BD	164/164 (100%)	136 (83%)	28 (17%)	2	13
27	DD	164/164 (100%)	137 (84%)	27 (16%)	3	13
28	BE	165/165 (100%)	130 (79%)	35 (21%)	1	7
28	DE	165/165 (100%)	130 (79%)	35 (21%)	1	7
29	BF	149/149 (100%)	116 (78%)	33 (22%)	1	6
29	DF	149/149 (100%)	117 (78%)	32 (22%)	1	7
30	BG	137/137 (100%)	110 (80%)	27 (20%)	1	8
30	DG	137/137 (100%)	110 (80%)	27 (20%)	1	8
31	BH	114/114 (100%)	85 (75%)	29 (25%)	1	2
31	DH	114/114 (100%)	86 (75%)	28 (25%)	1	3
32	BI	109/109 (100%)	107 (98%)	2 (2%)	66	89
32	DI	109/109 (100%)	104 (95%)	5 (5%)	33	73
33	BJ	116/116 (100%)	100 (86%)	16 (14%)	4	21
33	DJ	116/116 (100%)	100 (86%)	16 (14%)	4	21
34	BK	102/104 (98%)	84 (82%)	18 (18%)	2	12
34	DK	102/104 (98%)	83 (81%)	19 (19%)	2	10
35	BL	102/103 (99%)	87 (85%)	15 (15%)	4	18
35	DL	102/103 (99%)	88 (86%)	14 (14%)	4	21
36	BM	109/109 (100%)	93 (85%)	16 (15%)	4	18
36	DM	109/109 (100%)	93 (85%)	16 (15%)	4	18
37	BN	100/103 (97%)	85 (85%)	15 (15%)	3	17
37	DN	100/103 (97%)	84 (84%)	16 (16%)	3	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BO	86/87 (99%)	76 (88%)	10 (12%)	7	30
38	DO	86/87 (99%)	76 (88%)	10 (12%)	7	30
39	BP	99/99 (100%)	76 (77%)	23 (23%)	1	4
39	DP	99/99 (100%)	77 (78%)	22 (22%)	1	6
40	BQ	89/89 (100%)	73 (82%)	16 (18%)	2	11
40	DQ	89/89 (100%)	73 (82%)	16 (18%)	2	11
41	BR	84/84 (100%)	67 (80%)	17 (20%)	1	8
41	DR	84/84 (100%)	67 (80%)	17 (20%)	1	8
42	BS	93/93 (100%)	79 (85%)	14 (15%)	3	17
42	DS	93/93 (100%)	79 (85%)	14 (15%)	3	17
43	BT	80/84 (95%)	65 (81%)	15 (19%)	2	10
43	DT	80/84 (95%)	64 (80%)	16 (20%)	1	8
44	BU	83/84 (99%)	69 (83%)	14 (17%)	2	13
44	DU	83/84 (99%)	70 (84%)	13 (16%)	3	15
45	BV	78/78 (100%)	67 (86%)	11 (14%)	4	20
45	DV	78/78 (100%)	67 (86%)	11 (14%)	4	20
46	BW	59/62 (95%)	49 (83%)	10 (17%)	2	13
46	DW	59/62 (95%)	48 (81%)	11 (19%)	2	10
47	BX	67/67 (100%)	56 (84%)	11 (16%)	3	14
47	DX	67/67 (100%)	57 (85%)	10 (15%)	4	17
48	BY	55/55 (100%)	43 (78%)	12 (22%)	1	6
48	DY	55/55 (100%)	43 (78%)	12 (22%)	1	6
49	BZ	48/48 (100%)	43 (90%)	5 (10%)	9	35
49	DZ	48/48 (100%)	43 (90%)	5 (10%)	9	35
50	B0	47/47 (100%)	40 (85%)	7 (15%)	4	17
50	D0	47/47 (100%)	40 (85%)	7 (15%)	4	17
51	B1	45/48 (94%)	38 (84%)	7 (16%)	3	15
51	D1	45/48 (94%)	38 (84%)	7 (16%)	3	15
52	B2	38/38 (100%)	33 (87%)	5 (13%)	5	24
52	D2	38/38 (100%)	33 (87%)	5 (13%)	5	24
53	B3	51/51 (100%)	44 (86%)	7 (14%)	4	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	D3	51/51 (100%)	43 (84%)	8 (16%)	3	15
54	B4	34/34 (100%)	29 (85%)	5 (15%)	4	18
54	D4	34/34 (100%)	29 (85%)	5 (15%)	4	18
All	All	9329/9696 (96%)	7688 (82%)	1641 (18%)	2	12

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

Mol	Chain	Res	Type
45	BV	79	ARG
6	CD	170	LEU
41	DR	95	ASP
47	BX	77	TYR
4	CB	122	ASP

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

Mol	Chain	Res	Type
45	BV	88	HIS
7	CE	11	GLN
42	DS	57	ASN
48	BY	25	GLN
4	CB	121	GLN

5.3.3 RNA ⓘ

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	BB	2756	U
1	CA	366	A
25	DB	2308	G
1	CA	243	A
1	CA	428	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 carbohydrates 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	0.19	157 (10%) 9 6	41, 98, 164, 180	0
1	CA	1530/1542 (99%)	-0.32	15 (0%) 84 77	41, 109, 167, 180	0
2	AW	17/17 (100%)	3.00	11 (64%) 0 0	73, 87, 132, 177	0
2	CW	17/17 (100%)	0.25	1 (5%) 26 15	63, 86, 126, 150	0
3	AX	6/6 (100%)	6.59	6 (100%) 0 0	63, 78, 113, 127	0
3	CX	6/6 (100%)	1.55	3 (50%) 0 0	76, 83, 113, 115	0
4	AB	218/240 (90%)	2.91	132 (60%) 0 0	59, 127, 169, 180	0
4	CB	218/240 (90%)	3.85	138 (63%) 0 0	67, 141, 180, 180	0
5	AC	206/232 (88%)	2.99	130 (63%) 0 0	61, 104, 153, 180	0
5	CC	206/232 (88%)	2.37	98 (47%) 0 0	69, 121, 161, 180	0
6	AD	205/205 (100%)	1.91	80 (39%) 0 0	44, 106, 149, 180	0
6	CD	205/205 (100%)	2.00	81 (39%) 0 0	67, 120, 164, 180	0
7	AE	150/166 (90%)	2.39	81 (54%) 0 0	39, 98, 148, 180	0
7	CE	150/166 (90%)	2.60	65 (43%) 0 0	46, 129, 180, 180	0
8	AF	100/135 (74%)	1.27	25 (25%) 1 1	52, 100, 148, 180	0
8	CF	100/135 (74%)	1.53	31 (31%) 1 1	33, 101, 144, 165	0
9	AG	150/178 (84%)	2.17	65 (43%) 0 0	55, 113, 167, 180	0
9	CG	150/178 (84%)	-0.07	12 (8%) 15 9	71, 122, 165, 180	0
10	AH	129/129 (100%)	0.37	14 (10%) 7 5	51, 100, 143, 179	0
10	CH	129/129 (100%)	-0.45	1 (0%) 87 80	37, 106, 149, 176	0
11	AI	127/129 (98%)	0.39	13 (10%) 9 6	84, 120, 166, 180	0
11	CI	127/129 (98%)	-0.55	2 (1%) 74 64	68, 128, 167, 180	0
12	AJ	98/103 (95%)	1.80	47 (47%) 0 0	56, 124, 172, 180	0
12	CJ	98/103 (95%)	1.70	30 (30%) 1 1	76, 131, 164, 180	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AK	117/128 (91%)	5.31	107 (91%) 0 0	36, 91, 142, 180	0
13	CK	117/128 (91%)	2.17	52 (44%) 0 0	48, 91, 131, 159	0
14	AL	123/123 (100%)	3.79	87 (70%) 0 0	31, 80, 130, 169	0
14	CL	123/123 (100%)	1.77	52 (42%) 0 0	42, 91, 138, 172	0
15	AM	114/117 (97%)	-0.04	8 (7%) 19 12	63, 119, 165, 180	0
15	CM	113/117 (96%)	-0.44	2 (1%) 71 60	58, 121, 165, 176	0
16	AN	96/100 (96%)	0.74	19 (19%) 1 1	56, 112, 155, 180	0
16	CN	96/100 (96%)	1.11	22 (22%) 1 1	65, 124, 154, 180	0
17	AO	88/88 (100%)	0.09	4 (4%) 37 25	54, 91, 138, 180	0
17	CO	88/88 (100%)	0.25	4 (4%) 37 25	37, 96, 143, 160	0
18	AP	82/82 (100%)	-0.51	0 100 100	49, 95, 163, 180	0
18	CP	80/82 (97%)	-0.50	0 100 100	68, 113, 155, 180	0
19	AQ	80/83 (96%)	-0.07	1 (1%) 79 69	54, 107, 155, 169	0
19	CQ	80/83 (96%)	-0.49	0 100 100	50, 104, 145, 155	0
20	AR	55/74 (74%)	2.91	36 (65%) 0 0	52, 98, 134, 158	0
20	CR	55/74 (74%)	2.11	24 (43%) 0 0	46, 101, 144, 157	0
21	AS	79/91 (86%)	0.30	9 (11%) 7 4	80, 133, 169, 180	0
21	CS	79/91 (86%)	0.05	5 (6%) 23 14	75, 128, 160, 180	0
22	AT	85/86 (98%)	-0.76	0 100 100	62, 101, 151, 162	0
22	CT	85/86 (98%)	-0.43	1 (1%) 81 71	65, 104, 154, 180	0
23	AU	51/70 (72%)	5.22	44 (86%) 0 0	54, 110, 154, 180	0
23	CU	51/70 (72%)	1.95	19 (37%) 0 1	63, 125, 169, 180	0
24	BA	117/120 (97%)	0.98	6 (5%) 32 20	44, 75, 109, 180	0
24	DA	117/120 (97%)	-0.29	1 (0%) 85 79	33, 66, 105, 180	0
25	BB	2841/2904 (97%)	0.18	128 (4%) 37 25	13, 70, 147, 180	0
25	DB	2841/2904 (97%)	0.06	61 (2%) 67 54	12, 55, 149, 180	0
26	BC	271/272 (99%)	2.05	129 (47%) 0 0	16, 66, 111, 151	0
26	DC	271/272 (99%)	1.67	93 (34%) 0 1	9, 52, 97, 153	0
27	BD	209/209 (100%)	2.03	101 (48%) 0 0	25, 83, 146, 180	0
27	DD	209/209 (100%)	0.59	11 (5%) 30 19	20, 59, 119, 166	0
28	BE	201/201 (100%)	0.70	27 (13%) 4 3	22, 78, 139, 172	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	201/201 (100%)	2.50	110 (54%) 0 0	11, 76, 143, 178	0
29	BF	178/178 (100%)	-0.25	2 (1%) 82 73	49, 111, 174, 180	0
29	DF	178/178 (100%)	0.12	6 (3%) 49 35	49, 110, 166, 180	0
30	BG	176/176 (100%)	-0.17	8 (4%) 37 25	47, 112, 165, 176	0
30	DG	176/176 (100%)	-0.34	2 (1%) 82 73	38, 88, 155, 174	0
31	BH	149/149 (100%)	3.72	72 (48%) 0 0	52, 131, 180, 180	0
31	DH	149/149 (100%)	1.60	44 (29%) 1 1	35, 109, 150, 180	0
32	BI	141/141 (100%)	2.83	72 (51%) 0 0	110, 167, 180, 180	0
32	DI	141/141 (100%)	3.64	85 (60%) 0 0	105, 179, 180, 180	0
33	BJ	142/142 (100%)	0.02	4 (2%) 56 44	32, 86, 133, 180	0
33	DJ	142/142 (100%)	-0.14	0 100 100	19, 53, 108, 175	0
34	BK	121/123 (98%)	4.26	115 (95%) 0 0	32, 74, 148, 180	0
34	DK	121/123 (98%)	1.98	49 (40%) 0 0	27, 64, 130, 163	0
35	BL	143/144 (99%)	0.16	4 (2%) 56 44	27, 69, 121, 180	0
35	DL	143/144 (99%)	3.28	97 (67%) 0 0	17, 64, 115, 180	0
36	BM	136/136 (100%)	0.43	13 (9%) 10 7	33, 65, 132, 168	0
36	DM	136/136 (100%)	0.31	6 (4%) 38 26	11, 56, 109, 176	0
37	BN	120/127 (94%)	2.37	65 (54%) 0 0	43, 88, 131, 169	0
37	DN	120/127 (94%)	0.42	3 (2%) 61 49	19, 57, 97, 180	0
38	BO	116/117 (99%)	-0.12	0 100 100	34, 77, 118, 138	0
38	DO	116/117 (99%)	-0.38	0 100 100	28, 71, 129, 157	0
39	BP	114/114 (100%)	2.77	76 (66%) 0 0	43, 84, 145, 164	0
39	DP	114/114 (100%)	1.44	28 (24%) 1 1	26, 73, 123, 174	0
40	BQ	117/117 (100%)	-0.14	6 (5%) 32 20	34, 73, 135, 149	0
40	DQ	117/117 (100%)	0.39	10 (8%) 13 8	22, 53, 104, 158	0
41	BR	103/103 (100%)	-0.52	1 (0%) 84 77	44, 95, 146, 177	0
41	DR	103/103 (100%)	-0.06	4 (3%) 43 30	23, 72, 131, 156	0
42	BS	110/110 (100%)	3.85	93 (84%) 0 0	47, 84, 138, 180	0
42	DS	110/110 (100%)	1.21	22 (20%) 1 1	18, 53, 108, 152	0
43	BT	93/100 (93%)	0.97	15 (16%) 3 2	44, 93, 163, 180	0
43	DT	93/100 (93%)	0.69	10 (10%) 8 5	35, 72, 141, 178	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BU	102/103 (99%)	1.89	48 (47%) 0 0	48, 106, 162, 175	0
44	DU	102/103 (99%)	0.18	4 (3%) 43 30	41, 94, 154, 180	0
45	BV	94/94 (100%)	-0.06	1 (1%) 82 73	37, 84, 140, 180	0
45	DV	94/94 (100%)	0.30	4 (4%) 39 26	31, 70, 138, 156	0
46	BW	79/84 (94%)	0.17	1 (1%) 79 69	6, 53, 116, 154	0
46	DW	79/84 (94%)	0.08	1 (1%) 79 69	7, 42, 103, 180	0
47	BX	77/77 (100%)	1.07	13 (16%) 2 2	24, 63, 107, 157	0
47	DX	77/77 (100%)	1.03	14 (18%) 2 1	23, 60, 112, 152	0
48	BY	63/63 (100%)	0.93	11 (17%) 2 1	47, 108, 165, 180	0
48	DY	63/63 (100%)	-0.01	3 (4%) 34 23	34, 92, 158, 180	0
49	BZ	58/58 (100%)	-0.19	0 100 100	40, 74, 124, 150	0
49	DZ	58/58 (100%)	-0.42	0 100 100	22, 58, 110, 114	0
50	B0	56/56 (100%)	2.84	32 (57%) 0 0	35, 87, 152, 180	0
50	D0	56/56 (100%)	0.54	1 (1%) 71 60	19, 56, 118, 135	0
51	B1	50/54 (92%)	0.73	7 (14%) 4 3	43, 72, 122, 140	0
51	D1	50/54 (92%)	0.81	6 (12%) 6 4	26, 76, 119, 163	0
52	B2	46/46 (100%)	1.62	18 (39%) 0 0	42, 61, 97, 162	0
52	D2	46/46 (100%)	1.40	11 (23%) 1 1	17, 47, 97, 131	0
53	B3	64/64 (100%)	0.11	0 100 100	21, 56, 99, 136	0
53	D3	64/64 (100%)	2.36	34 (53%) 0 0	27, 49, 85, 105	0
54	B4	38/38 (100%)	0.30	3 (7%) 15 10	36, 86, 126, 146	0
54	D4	38/38 (100%)	-0.17	0 100 100	44, 68, 126, 165	0
All	All	20459/21088 (97%)	0.75	3525 (17%) 2 2	6, 86, 162, 180	0

The worst 5 of 3525 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	DI	82	ALA	28.3
31	BH	88	GLY	27.8
7	CE	114	LEU	27.2
32	DI	138	VAL	20.5
15	AM	114	PRO	19.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	AA	1637	1/1	0.63	2.78	61.61	134,134,134,134	0
55	MG	BB	3016	1/1	0.93	1.04	25.54	91,91,91,91	0
55	MG	BB	3063	1/1	0.91	0.46	9.05	95,95,95,95	0
55	MG	DB	3109	1/1	0.97	0.26	5.00	28,28,28,28	0
55	MG	DB	3091	1/1	0.90	0.20	1.56	39,39,39,39	0
55	MG	BB	3110	1/1	0.95	0.15	1.18	56,56,56,56	0
55	MG	CA	1654	1/1	0.80	0.31	1.06	78,78,78,78	0
55	MG	BB	3118	1/1	0.85	0.35	0.69	113,113,113,113	0
56	ZN	D4	401	1/1	0.97	0.17	-0.15	72,72,72,72	0
55	MG	AA	1653	1/1	0.80	0.13	-0.30	84,84,84,84	0
55	MG	BB	3083	1/1	0.91	0.19	-0.43	47,47,47,47	0
55	MG	DB	3119	1/1	0.85	0.19	-0.43	64,64,64,64	0
55	MG	DB	3069	1/1	0.98	0.24	-0.54	48,48,48,48	0
55	MG	DB	3012	1/1	0.96	0.18	-0.64	37,37,37,37	0
55	MG	AA	1635	1/1	0.17	0.11	-0.65	129,129,129,129	0
55	MG	CA	1637	1/1	0.82	0.17	-0.67	81,81,81,81	0
55	MG	DB	3089	1/1	0.94	0.17	-0.71	51,51,51,51	0
55	MG	DB	3035	1/1	0.98	0.18	-0.87	27,27,27,27	0
55	MG	CN	201	1/1	0.80	0.10	-0.89	104,104,104,104	0
55	MG	CA	1610	1/1	0.56	0.17	-0.95	130,130,130,130	0
55	MG	BB	3112	1/1	0.91	0.32	-1.03	27,27,27,27	0
55	MG	BB	3087	1/1	0.91	0.17	-1.05	63,63,63,63	0
55	MG	AX	102	1/1	0.96	0.41	-1.06	66,66,66,66	0
55	MG	AA	1621	1/1	0.76	0.28	-1.06	36,36,36,36	0
55	MG	AA	1636	1/1	0.96	0.07	-1.08	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BB	3099	1/1	0.93	0.23	-1.16	41,41,41,41	0
55	MG	BB	3113	1/1	0.97	0.19	-1.19	41,41,41,41	0
55	MG	CA	1620	1/1	0.88	0.12	-1.22	103,103,103,103	0
55	MG	DB	3113	1/1	0.98	0.17	-1.27	27,27,27,27	0
55	MG	DB	3093	1/1	0.95	0.12	-1.27	54,54,54,54	0
55	MG	CA	1603	1/1	0.81	0.12	-1.28	124,124,124,124	0
55	MG	DB	3088	1/1	0.92	0.16	-1.53	83,83,83,83	0
55	MG	AA	1641	1/1	0.61	0.09	-1.60	111,111,111,111	0
55	MG	BB	3005	1/1	0.95	0.16	-1.65	52,52,52,52	0
56	ZN	B4	101	1/1	0.96	0.04	-1.68	72,72,72,72	0
55	MG	BB	3012	1/1	0.95	0.10	-1.72	32,32,32,32	0
55	MG	BB	3029	1/1	0.91	0.09	-1.75	81,81,81,81	0
55	MG	DB	3067	1/1	0.89	0.15	-1.85	33,33,33,33	0
55	MG	AA	1620	1/1	0.98	0.10	-1.87	74,74,74,74	0
55	MG	BB	3094	1/1	0.91	0.17	-1.87	81,81,81,81	0
55	MG	DB	3003	1/1	0.97	0.06	-1.89	24,24,24,24	0
55	MG	BB	3082	1/1	0.92	0.16	-1.97	80,80,80,80	0
55	MG	DB	3059	1/1	0.72	0.13	-1.98	110,110,110,110	0
55	MG	BB	3002	1/1	0.98	0.16	-1.99	31,31,31,31	0
55	MG	DB	3010	1/1	0.96	0.09	-2.08	20,20,20,20	0
55	MG	BB	3049	1/1	0.96	0.09	-2.09	40,40,40,40	0
55	MG	CA	1609	1/1	0.84	0.09	-2.12	60,60,60,60	0
55	MG	BB	3090	1/1	0.86	0.11	-2.12	71,71,71,71	0
55	MG	BB	3116	1/1	0.99	0.08	-2.22	24,24,24,24	0
55	MG	BB	3040	1/1	0.93	0.12	-2.28	64,64,64,64	0
55	MG	BB	3035	1/1	0.98	0.14	-2.33	40,40,40,40	0
55	MG	DB	3030	1/1	0.89	0.16	-2.41	46,46,46,46	0
55	MG	BB	3048	1/1	0.91	0.08	-2.44	38,38,38,38	0
55	MG	DB	3077	1/1	0.95	0.15	-2.49	57,57,57,57	0
55	MG	DB	3117	1/1	0.95	0.06	-2.51	26,26,26,26	0
55	MG	CA	1617	1/1	0.85	0.11	-2.56	149,149,149,149	0
55	MG	BB	3066	1/1	0.96	0.16	-2.64	51,51,51,51	0
55	MG	BB	3097	1/1	0.79	0.08	-2.73	112,112,112,112	0
55	MG	CA	1630	1/1	0.96	0.08	-2.74	97,97,97,97	0
55	MG	AA	1607	1/1	0.94	0.09	-2.77	93,93,93,93	0
55	MG	CA	1608	1/1	0.88	0.08	-2.84	82,82,82,82	0
55	MG	BB	3021	1/1	0.98	0.13	-2.84	45,45,45,45	0
55	MG	BB	3085	1/1	0.99	0.05	-2.89	57,57,57,57	0
55	MG	DB	3086	1/1	0.99	0.12	-2.91	57,57,57,57	0
55	MG	CA	1605	1/1	0.85	0.08	-2.92	98,98,98,98	0
55	MG	DB	3047	1/1	0.91	0.10	-3.06	36,36,36,36	0
55	MG	DB	3095	1/1	0.96	0.11	-3.14	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BB	3103	1/1	0.98	0.10	-3.16	38,38,38,38	0
55	MG	DB	3107	1/1	0.84	0.11	-3.19	24,24,24,24	0
55	MG	BB	3098	1/1	0.98	0.11	-3.21	73,73,73,73	0
55	MG	AA	1638	1/1	0.86	0.09	-3.22	95,95,95,95	0
55	MG	DB	3056	1/1	0.96	0.13	-3.24	28,28,28,28	0
55	MG	DB	3006	1/1	0.97	0.15	-3.24	38,38,38,38	0
55	MG	BB	3042	1/1	0.87	0.08	-3.35	90,90,90,90	0
55	MG	DB	3068	1/1	0.84	0.08	-3.40	35,35,35,35	0
55	MG	AA	1633	1/1	0.87	0.06	-3.40	85,85,85,85	0
55	MG	AA	1610	1/1	0.97	0.05	-3.49	61,61,61,61	0
55	MG	BB	3096	1/1	0.88	0.17	-3.57	49,49,49,49	0
55	MG	DB	3116	1/1	0.95	0.04	-3.64	54,54,54,54	0
55	MG	AA	1629	1/1	0.93	0.08	-3.70	53,53,53,53	0
55	MG	BB	3086	1/1	0.97	0.11	-3.75	50,50,50,50	0
55	MG	AA	1654	1/1	0.97	0.05	-3.83	49,49,49,49	0
55	MG	AA	1615	1/1	0.85	0.08	-4.13	85,85,85,85	0
55	MG	BB	3092	1/1	0.93	0.14	-4.14	62,62,62,62	0
55	MG	AA	1609	1/1	0.96	0.07	-4.15	67,67,67,67	0
55	MG	BB	3081	1/1	0.91	0.09	-4.20	85,85,85,85	0
55	MG	AA	1601	1/1	0.91	0.04	-4.21	62,62,62,62	0
55	MG	DB	3083	1/1	0.96	0.12	-4.24	31,31,31,31	0
55	MG	BB	3074	1/1	0.89	0.08	-4.25	25,25,25,25	0
55	MG	BB	3011	1/1	0.91	0.10	-4.26	45,45,45,45	0
55	MG	BB	3079	1/1	0.99	0.14	-4.29	46,46,46,46	0
55	MG	CA	1616	1/1	0.98	0.08	-4.30	80,80,80,80	0
55	MG	DB	3009	1/1	0.99	0.05	-4.34	48,48,48,48	0
55	MG	CA	1649	1/1	0.58	0.08	-4.36	100,100,100,100	0
55	MG	CA	1631	1/1	0.77	0.09	-4.37	91,91,91,91	0
55	MG	AA	1606	1/1	0.86	0.08	-4.40	114,114,114,114	0
55	MG	BB	3032	1/1	0.92	0.07	-4.52	53,53,53,53	0
55	MG	DB	3087	1/1	0.85	0.10	-4.57	28,28,28,28	0
55	MG	DB	3112	1/1	0.94	0.14	-4.61	52,52,52,52	0
55	MG	DB	3073	1/1	0.98	0.12	-4.68	7,7,7,7	0
55	MG	DB	3084	1/1	0.98	0.12	-4.69	26,26,26,26	0
55	MG	DB	3051	1/1	0.96	0.09	-4.71	48,48,48,48	0
55	MG	DB	3071	1/1	0.92	0.08	-4.74	30,30,30,30	0
55	MG	DB	3020	1/1	0.95	0.08	-4.84	25,25,25,25	0
55	MG	BB	3088	1/1	0.93	0.08	-4.87	76,76,76,76	0
55	MG	BB	3056	1/1	0.92	0.07	-4.94	49,49,49,49	0
55	MG	CA	1601	1/1	0.95	0.09	-5.03	48,48,48,48	0
55	MG	BB	3013	1/1	0.95	0.05	-5.03	52,52,52,52	0
55	MG	DB	3014	1/1	0.98	0.05	-5.18	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DB	3098	1/1	0.97	0.09	-5.23	42,42,42,42	0
55	MG	DB	3102	1/1	0.99	0.09	-5.50	67,67,67,67	0
55	MG	BB	3052	1/1	0.98	0.07	-5.64	33,33,33,33	0
55	MG	DB	3055	1/1	0.95	0.05	-5.96	30,30,30,30	0
55	MG	BB	3065	1/1	0.97	0.06	-6.03	46,46,46,46	0
55	MG	BB	3019	1/1	0.62	0.10	-6.08	62,62,62,62	0
55	MG	BB	3018	1/1	0.96	0.07	-6.35	42,42,42,42	0
55	MG	BB	3023	1/1	0.96	0.06	-6.56	15,15,15,15	0
55	MG	BB	3037	1/1	0.95	0.09	-6.58	56,56,56,56	0
55	MG	BB	3069	1/1	0.94	0.14	-6.83	28,28,28,28	0
55	MG	DB	3026	1/1	0.89	0.08	-7.06	38,38,38,38	0
55	MG	DB	3079	1/1	0.98	0.08	-7.06	18,18,18,18	0
55	MG	BB	3062	1/1	0.98	0.06	-7.54	42,42,42,42	0
55	MG	BB	3108	1/1	0.90	0.09	-8.31	30,30,30,30	0
55	MG	DB	3019	1/1	0.98	0.08	-8.39	43,43,43,43	0
55	MG	DB	3007	1/1	0.94	0.08	-9.38	49,49,49,49	0
55	MG	DB	3001	1/1	0.97	0.06	-10.48	14,14,14,14	0
55	MG	BB	3059	1/1	0.91	0.07	-10.68	37,37,37,37	0
55	MG	DB	3002	1/1	0.94	0.09	-19.24	44,44,44,44	0
55	MG	AA	1647	1/1	0.77	0.39	-	79,79,79,79	0
55	MG	DB	3044	1/1	0.88	0.08	-	20,20,20,20	0
55	MG	DB	3057	1/1	0.94	0.16	-	63,63,63,63	0
55	MG	BJ	201	1/1	0.91	0.47	-	160,160,160,160	0
55	MG	BB	3100	1/1	0.89	0.20	-	128,128,128,128	0
55	MG	CA	1642	1/1	0.87	0.10	-	110,110,110,110	0
55	MG	CA	1606	1/1	0.79	0.13	-	139,139,139,139	0
55	MG	BB	3039	1/1	0.90	0.06	-	55,55,55,55	0
55	MG	BB	3109	1/1	0.98	0.13	-	52,52,52,52	0
55	MG	DB	3052	1/1	0.68	0.68	-	137,137,137,137	0
55	MG	CA	1625	1/1	0.76	0.07	-	54,54,54,54	0
55	MG	BB	3114	1/1	0.98	0.21	-	57,57,57,57	0
55	MG	DB	3032	1/1	0.86	0.43	-	111,111,111,111	0
55	MG	BB	3067	1/1	0.96	0.09	-	39,39,39,39	0
55	MG	AA	1602	1/1	0.93	0.28	-	83,83,83,83	0
55	MG	CA	1655	1/1	0.84	0.20	-	153,153,153,153	0
55	MG	BB	3075	1/1	0.98	0.10	-	44,44,44,44	0
55	MG	DB	3004	1/1	0.94	0.07	-	21,21,21,21	0
55	MG	AA	1626	1/1	0.55	0.75	-	139,139,139,139	0
55	MG	DB	3034	1/1	0.84	0.34	-	87,87,87,87	0
55	MG	DB	3015	1/1	0.97	0.10	-	49,49,49,49	0
55	MG	DB	3024	1/1	0.89	0.06	-	22,22,22,22	0
55	MG	AA	1659	1/1	0.93	0.19	-	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DB	3108	1/1	0.94	0.08	-	36,36,36,36	0
55	MG	BB	3084	1/1	0.93	0.09	-	61,61,61,61	0
55	MG	CA	1636	1/1	0.79	0.06	-	127,127,127,127	0
55	MG	DB	3058	1/1	0.83	0.60	-	136,136,136,136	0
55	MG	AA	1656	1/1	0.90	1.00	-	101,101,101,101	0
55	MG	AA	1604	1/1	0.93	0.07	-	45,45,45,45	0
55	MG	DB	3045	1/1	0.86	0.08	-	140,140,140,140	0
55	MG	CA	1619	1/1	0.96	0.07	-	79,79,79,79	0
55	MG	CA	1626	1/1	0.96	0.07	-	154,154,154,154	0
55	MG	BB	3111	1/1	0.97	0.09	-	43,43,43,43	0
55	MG	AA	1646	1/1	0.92	0.39	-	74,74,74,74	0
55	MG	DB	3096	1/1	0.94	0.09	-	46,46,46,46	0
55	MG	DB	3021	1/1	0.97	0.09	-	50,50,50,50	0
55	MG	DB	3118	1/1	0.97	0.06	-	35,35,35,35	0
55	MG	DB	3027	1/1	0.89	0.13	-	43,43,43,43	0
55	MG	BB	3028	1/1	0.90	0.15	-	54,54,54,54	0
55	MG	DB	3064	1/1	0.90	0.12	-	32,32,32,32	0
55	MG	CA	1634	1/1	0.84	0.20	-	80,80,80,80	0
55	MG	AA	1611	1/1	0.72	3.94	-	148,148,148,148	0
55	MG	BB	3115	1/1	0.77	0.18	-	106,106,106,106	0
55	MG	BB	3091	1/1	0.96	0.19	-	44,44,44,44	0
55	MG	AA	1623	1/1	0.85	0.18	-	115,115,115,115	0
55	MG	DB	3038	1/1	0.97	0.11	-	19,19,19,19	0
55	MG	BB	3093	1/1	0.78	0.69	-	120,120,120,120	0
55	MG	DB	3050	1/1	0.92	0.07	-	51,51,51,51	0
55	MG	CA	1629	1/1	0.61	0.09	-	94,94,94,94	0
55	MG	BB	3006	1/1	0.98	0.11	-	35,35,35,35	0
55	MG	DB	3092	1/1	0.96	0.16	-	44,44,44,44	0
55	MG	CA	1652	1/1	0.84	0.09	-	117,117,117,117	0
55	MG	DB	3078	1/1	0.97	0.05	-	28,28,28,28	0
55	MG	DB	3101	1/1	0.94	0.08	-	44,44,44,44	0
55	MG	DB	3053	1/1	0.93	0.07	-	37,37,37,37	0
55	MG	BB	3057	1/1	0.77	0.75	-	100,100,100,100	0
55	MG	DB	3080	1/1	0.97	0.12	-	29,29,29,29	0
55	MG	DB	3074	1/1	0.97	0.08	-	9,9,9,9	0
55	MG	AA	1614	1/1	-0.08	0.74	-	174,174,174,174	0
55	MG	DB	3062	1/1	0.93	0.11	-	54,54,54,54	0
55	MG	BB	3034	1/1	0.93	0.22	-	70,70,70,70	0
55	MG	AA	1632	1/1	0.88	0.55	-	106,106,106,106	0
55	MG	BB	3073	1/1	0.89	0.06	-	30,30,30,30	0
55	MG	BB	3117	1/1	0.93	0.18	-	82,82,82,82	0
55	MG	AA	1617	1/1	0.87	0.42	-	123,123,123,123	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DB	3017	1/1	0.96	0.10	-	34,34,34,34	0
55	MG	CA	1643	1/1	0.72	0.09	-	138,138,138,138	0
55	MG	DB	3090	1/1	0.95	0.12	-	62,62,62,62	0
55	MG	BB	3004	1/1	0.98	0.09	-	65,65,65,65	0
55	MG	AA	1645	1/1	0.93	0.19	-	127,127,127,127	0
55	MG	CA	1645	1/1	0.92	0.12	-	119,119,119,119	0
55	MG	DB	3099	1/1	0.97	0.06	-	19,19,19,19	0
55	MG	DB	3031	1/1	0.98	0.04	-	16,16,16,16	0
55	MG	DB	3106	1/1	0.97	0.06	-	29,29,29,29	0
55	MG	DB	3060	1/1	0.93	0.07	-	35,35,35,35	0
55	MG	BB	3089	1/1	0.99	0.06	-	51,51,51,51	0
55	MG	DB	3046	1/1	0.94	0.09	-	47,47,47,47	0
55	MG	DB	3104	1/1	0.91	0.09	-	50,50,50,50	0
55	MG	CA	1611	1/1	0.91	0.11	-	102,102,102,102	0
55	MG	BB	3054	1/1	0.92	0.13	-	56,56,56,56	0
55	MG	BB	3010	1/1	0.60	0.17	-	95,95,95,95	0
55	MG	CA	1633	1/1	0.92	0.09	-	136,136,136,136	0
55	MG	CA	1650	1/1	0.77	0.06	-	103,103,103,103	0
55	MG	BB	3026	1/1	0.98	0.09	-	26,26,26,26	0
55	MG	AA	1608	1/1	0.76	0.28	-	113,113,113,113	0
55	MG	AA	1652	1/1	0.73	0.39	-	103,103,103,103	0
55	MG	AA	1634	1/1	0.94	0.14	-	55,55,55,55	0
55	MG	DB	3054	1/1	0.95	0.22	-	53,53,53,53	0
55	MG	BB	3017	1/1	0.95	0.04	-	35,35,35,35	0
55	MG	AA	1640	1/1	0.85	0.09	-	99,99,99,99	0
55	MG	AA	1639	1/1	0.72	0.11	-	126,126,126,126	0
55	MG	BB	3102	1/1	0.94	0.14	-	71,71,71,71	0
55	MG	BB	3046	1/1	0.73	0.10	-	90,90,90,90	0
55	MG	BB	3001	1/1	0.95	0.10	-	57,57,57,57	0
55	MG	AA	1613	1/1	0.77	0.09	-	106,106,106,106	0
55	MG	AA	1643	1/1	0.69	0.52	-	112,112,112,112	0
55	MG	CA	1614	1/1	0.73	0.32	-	171,171,171,171	0
55	MG	CA	1647	1/1	0.89	0.07	-	109,109,109,109	0
55	MG	DB	3075	1/1	0.93	0.07	-	46,46,46,46	0
55	MG	BB	3030	1/1	0.94	0.08	-	111,111,111,111	0
55	MG	AA	1616	1/1	0.92	0.18	-	104,104,104,104	0
55	MG	BB	3053	1/1	0.96	0.05	-	43,43,43,43	0
55	MG	DB	3063	1/1	0.93	0.10	-	45,45,45,45	0
55	MG	DB	3037	1/1	0.89	0.09	-	32,32,32,32	0
55	MG	DB	3103	1/1	0.98	0.05	-	46,46,46,46	0
55	MG	AA	1658	1/1	0.23	0.53	-	147,147,147,147	0
55	MG	CA	1604	1/1	0.91	0.09	-	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1648	1/1	0.85	0.11	-	67,67,67,67	0
55	MG	CA	1646	1/1	0.55	0.51	-	155,155,155,155	0
55	MG	BB	3022	1/1	0.96	0.16	-	56,56,56,56	0
55	MG	AA	1622	1/1	0.94	0.28	-	87,87,87,87	0
55	MG	AA	1660	1/1	0.90	0.55	-	95,95,95,95	0
55	MG	DB	3061	1/1	0.92	0.14	-	97,97,97,97	0
55	MG	CA	1640	1/1	0.62	0.49	-	138,138,138,138	0
55	MG	CA	1618	1/1	0.63	0.12	-	87,87,87,87	0
55	MG	DB	3072	1/1	0.94	0.15	-	39,39,39,39	0
55	MG	CA	1653	1/1	0.71	0.12	-	149,149,149,149	0
55	MG	DB	3111	1/1	0.95	0.08	-	38,38,38,38	0
55	MG	DB	3043	1/1	0.95	0.20	-	49,49,49,49	0
55	MG	DB	3008	1/1	0.99	0.11	-	55,55,55,55	0
55	MG	BB	3078	1/1	0.92	0.11	-	71,71,71,71	0
55	MG	CA	1613	1/1	0.87	0.10	-	140,140,140,140	0
55	MG	BB	3031	1/1	0.91	0.28	-	83,83,83,83	0
55	MG	BB	3064	1/1	0.94	0.08	-	63,63,63,63	0
55	MG	BB	3107	1/1	0.86	0.09	-	86,86,86,86	0
55	MG	DB	3025	1/1	0.96	0.10	-	40,40,40,40	0
55	MG	BB	3061	1/1	0.96	0.12	-	57,57,57,57	0
55	MG	AA	1603	1/1	0.91	0.10	-	55,55,55,55	0
55	MG	DB	3042	1/1	0.98	0.06	-	56,56,56,56	0
55	MG	DB	3029	1/1	0.89	0.84	-	92,92,92,92	0
55	MG	BB	3047	1/1	0.88	0.08	-	131,131,131,131	0
55	MG	AA	1657	1/1	0.83	0.10	-	85,85,85,85	0
55	MG	DB	3036	1/1	0.93	0.09	-	36,36,36,36	0
55	MG	CA	1621	1/1	0.85	0.15	-	161,161,161,161	0
55	MG	BB	3070	1/1	0.91	0.08	-	52,52,52,52	0
55	MG	CA	1656	1/1	0.83	0.41	-	97,97,97,97	0
55	MG	DB	3041	1/1	0.91	0.08	-	32,32,32,32	0
55	MG	DB	3022	1/1	0.97	0.09	-	42,42,42,42	0
55	MG	BB	3051	1/1	0.79	0.14	-	94,94,94,94	0
55	MG	DB	3066	1/1	0.99	0.11	-	30,30,30,30	0
55	MG	AA	1642	1/1	0.81	0.09	-	63,63,63,63	0
55	MG	DB	3070	1/1	0.86	0.18	-	61,61,61,61	0
55	MG	CA	1623	1/1	0.91	0.16	-	136,136,136,136	0
55	MG	AA	1651	1/1	0.94	0.13	-	83,83,83,83	0
55	MG	AA	1631	1/1	0.94	0.10	-	91,91,91,91	0
55	MG	AA	1649	1/1	0.93	0.12	-	84,84,84,84	0
55	MG	BB	3106	1/1	0.95	0.24	-	53,53,53,53	0
55	MG	CA	1644	1/1	0.76	0.11	-	131,131,131,131	0
55	MG	DB	3105	1/1	0.96	0.06	-	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BB	3095	1/1	0.95	0.17	-	48,48,48,48	0
55	MG	BB	3044	1/1	0.94	0.13	-	62,62,62,62	0
55	MG	BB	3101	1/1	0.91	0.10	-	50,50,50,50	0
55	MG	DB	3100	1/1	0.95	0.09	-	10,10,10,10	0
55	MG	DB	3040	1/1	0.94	0.05	-	41,41,41,41	0
55	MG	DB	3081	1/1	0.98	0.07	-	36,36,36,36	0
55	MG	CA	1651	1/1	0.97	0.16	-	66,66,66,66	0
55	MG	DB	3065	1/1	0.77	0.29	-	67,67,67,67	0
55	MG	DB	3110	1/1	0.95	0.09	-	41,41,41,41	0
55	MG	BB	3020	1/1	0.96	0.22	-	45,45,45,45	0
55	MG	BB	3003	1/1	0.98	0.10	-	20,20,20,20	0
55	MG	CA	1607	1/1	0.70	0.09	-	108,108,108,108	0
55	MG	AX	101	1/1	0.92	1.02	-	84,84,84,84	0
55	MG	DB	3048	1/1	0.94	0.07	-	45,45,45,45	0
55	MG	BB	3077	1/1	0.92	0.17	-	50,50,50,50	0
55	MG	AA	1655	1/1	0.90	0.17	-	82,82,82,82	0
55	MG	BB	3055	1/1	0.98	0.09	-	72,72,72,72	0
55	MG	CA	1627	1/1	0.64	0.13	-	122,122,122,122	0
55	MG	AA	1628	1/1	0.79	0.32	-	100,100,100,100	0
55	MG	AA	1625	1/1	0.63	0.19	-	145,145,145,145	0
55	MG	BB	3038	1/1	0.94	0.08	-	125,125,125,125	0
55	MG	DB	3115	1/1	0.34	0.25	-	132,132,132,132	0
55	MG	DB	3028	1/1	0.91	0.06	-	42,42,42,42	0
55	MG	BB	3105	1/1	0.98	0.13	-	64,64,64,64	0
55	MG	BB	3050	1/1	0.88	0.09	-	54,54,54,54	0
55	MG	CA	1635	1/1	0.65	0.20	-	129,129,129,129	0
55	MG	BB	3060	1/1	0.93	0.17	-	33,33,33,33	0
55	MG	BB	3025	1/1	0.97	0.11	-	63,63,63,63	0
55	MG	BB	3027	1/1	0.97	0.44	-	40,40,40,40	0
55	MG	BB	3007	1/1	0.95	0.15	-	115,115,115,115	0
55	MG	CA	1628	1/1	0.88	0.06	-	106,106,106,106	0
55	MG	BB	3009	1/1	0.93	0.06	-	92,92,92,92	0
55	MG	DB	3018	1/1	0.95	0.15	-	32,32,32,32	0
55	MG	DB	3049	1/1	0.98	0.10	-	42,42,42,42	0
55	MG	CA	1624	1/1	0.91	0.07	-	103,103,103,103	0
55	MG	CA	1641	1/1	0.82	0.12	-	123,123,123,123	0
55	MG	BB	3071	1/1	0.99	0.10	-	41,41,41,41	0
55	MG	CA	1612	1/1	0.94	0.16	-	95,95,95,95	0
55	MG	AA	1605	1/1	0.87	0.06	-	87,87,87,87	0
55	MG	AA	1630	1/1	0.35	0.18	-	114,114,114,114	0
55	MG	AA	1618	1/1	0.69	0.12	-	92,92,92,92	0
55	MG	BB	3008	1/1	0.93	0.10	-	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1639	1/1	0.86	0.37	-	99,99,99,99	0
55	MG	DB	3097	1/1	0.98	0.11	-	39,39,39,39	0
55	MG	CA	1632	1/1	0.44	0.18	-	154,154,154,154	0
55	MG	AA	1612	1/1	0.89	0.09	-	117,117,117,117	0
55	MG	DB	3011	1/1	0.97	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	3043	1/1	0.98	0.13	-	107,107,107,107	0
55	MG	DB	3039	1/1	0.95	0.08	-	95,95,95,95	0
55	MG	DB	3023	1/1	0.92	0.12	-	46,46,46,46	0
55	MG	BB	3014	1/1	0.74	0.31	-	76,76,76,76	0
55	MG	AA	1650	1/1	0.95	0.09	-	92,92,92,92	0
55	MG	BB	3104	1/1	0.96	0.08	-	38,38,38,38	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	DB	3016	1/1	0.98	0.07	-	43,43,43,43	0
55	MG	CA	1602	1/1	0.96	0.12	-	87,87,87,87	0
55	MG	BB	3024	1/1	0.94	0.14	-	47,47,47,47	0
55	MG	BB	3045	1/1	0.92	0.10	-	60,60,60,60	0
55	MG	DB	3005	1/1	0.85	0.17	-	66,66,66,66	0
55	MG	BB	3033	1/1	0.87	0.07	-	86,86,86,86	0
55	MG	DB	3114	1/1	0.94	0.27	-	43,43,43,43	0
55	MG	BB	3058	1/1	0.95	0.09	-	62,62,62,62	0
55	MG	BB	3041	1/1	0.94	0.15	-	28,28,28,28	0
55	MG	AA	1619	1/1	0.71	0.36	-	92,92,92,92	0
55	MG	AA	1644	1/1	0.86	0.10	-	99,99,99,99	0
55	MG	BB	3080	1/1	0.96	0.20	-	65,65,65,65	0
55	MG	CA	1615	1/1	0.82	0.10	-	156,156,156,156	0
55	MG	AA	1624	1/1	0.89	0.05	-	88,88,88,88	0
55	MG	BB	3072	1/1	0.98	0.11	-	58,58,58,58	0
55	MG	DB	3033	1/1	0.89	0.11	-	43,43,43,43	0
55	MG	DB	3085	1/1	0.98	0.09	-	21,21,21,21	0
55	MG	BB	3068	1/1	0.82	0.10	-	40,40,40,40	0
55	MG	AA	1627	1/1	0.95	0.40	-	91,91,91,91	0
55	MG	DB	3076	1/1	0.96	0.07	-	49,49,49,49	0
55	MG	CA	1638	1/1	0.97	0.57	-	102,102,102,102	0
55	MG	CX	101	1/1	0.90	0.12	-	73,73,73,73	0
55	MG	DB	3082	1/1	0.78	0.22	-	104,104,104,104	0
55	MG	BB	3015	1/1	0.94	0.10	-	69,69,69,69	0
55	MG	BB	3036	1/1	0.93	0.08	-	52,52,52,52	0
55	MG	CA	1648	1/1	0.94	0.10	-	119,119,119,119	0
55	MG	DB	3013	1/1	0.76	0.10	-	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.