



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 11, 2022 – 01:51 pm BST

PDB ID : 4V5B
Title : Structure of PDF binding helix in complex with the ribosome
Authors : Bingel-Erlenmeyer, R.; Kohler, R.; Kramer, G.; Sandikci, A.; Antolic, S.;
Maier, T.; Schaffitzel, C.; Wiedmann, B.; Bukau, B.; Ban, N.
Deposited on : 2007-11-22
Resolution : 3.74 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

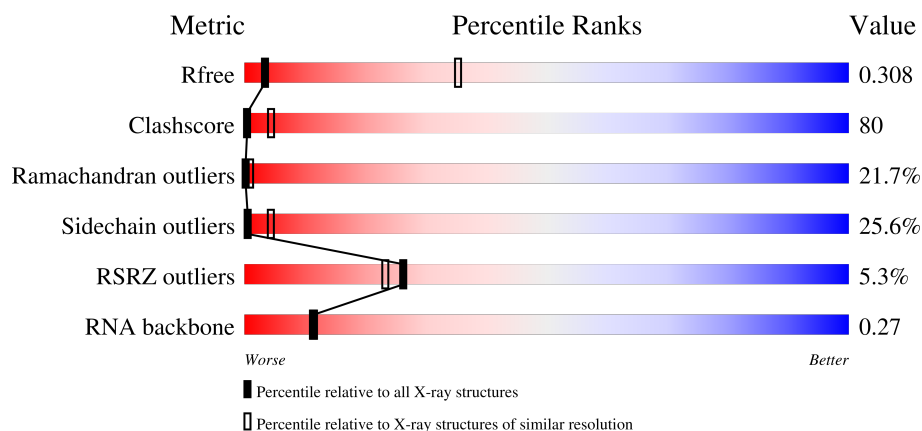
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.74 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1001 (3.90-3.58)
Clashscore	141614	1063 (3.90-3.58)
Ramachandran outliers	138981	1027 (3.90-3.58)
Sidechain outliers	138945	1023 (3.90-3.58)
RSRZ outliers	127900	1006 (3.92-3.56)
RNA backbone	3102	1028 (4.46-3.00)

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

Mol	Chain	Length	Quality of chain
1	A0	56	<div> <div>11%</div> <div>16%</div> <div>43%</div> <div>38%</div> <div>.</div> </div>
1	C0	56	<div> <div>11%</div> <div>12%</div> <div>41%</div> <div>46%</div> </div>
2	A1	54	<div> <div>19%</div> <div>15%</div> <div>48%</div> <div>33%</div> <div>.</div> </div>
2	C1	54	<div> <div>19%</div> <div>11%</div> <div>44%</div> <div>39%</div> <div>6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	A2	46	
3	C2	46	
4	A3	64	
4	C3	64	
5	A4	38	
5	C4	38	
6	A5	16	
7	AA	120	
7	CA	120	
8	AB	2904	
8	CB	2904	
9	AC	273	
9	CC	273	
10	AD	209	
10	CD	209	
11	AE	201	
11	CE	201	
12	AF	178	
12	CF	178	
13	AG	176	
13	CG	176	
14	AH	149	
14	CH	149	
15	AI	141	
15	CI	141	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	AJ	142	
16	CJ	142	
17	AK	123	
17	CK	123	
18	AL	144	
18	CL	144	
19	AM	136	
19	CM	136	
20	AN	127	
20	CN	127	
21	AO	117	
21	CO	117	
22	AP	114	
22	CP	114	
23	AQ	117	
23	CQ	117	
24	AR	103	
24	CR	103	
25	AS	110	
25	CS	110	
26	AT	100	
26	CT	100	
27	AU	103	
27	CU	103	
28	AV	94	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	CV	94	
29	AW	84	
29	CW	84	
30	AX	63	
30	CX	63	
31	AY	58	
31	CY	58	
32	AZ	70	
32	CZ	70	
33	BA	1542	
33	DA	1542	
34	BB	240	
34	DB	240	
35	BC	232	
35	DC	232	
36	BD	205	
36	DD	205	
37	BE	166	
37	DE	166	
38	BF	135	
38	DF	135	
39	BG	178	
39	DG	178	
40	BH	129	
40	DH	129	


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	BI	129	
41	DI	129	
42	BJ	103	
42	DJ	103	
43	BK	128	
43	DK	128	
44	BL	123	
44	DL	123	
45	BM	117	
45	DM	117	
46	BN	100	
46	DN	100	
47	BO	89	
47	DO	89	
48	BP	82	
48	DP	82	
49	BQ	83	
49	DQ	83	
50	BR	74	
50	DR	74	
51	BS	91	
51	DS	91	
52	BT	86	
52	DT	86	
53	BU	71	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	DU	71	

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
54	MG	BA	4053	-	-	-	X
54	MG	BA	4054	-	-	-	X
54	MG	DA	1612	-	-	-	X

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 284264 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
1	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A1	54	Total	C	N	O	0	0	0
			441	284	81	76			
2	C1	54	Total	C	N	O	0	0	0
			441	284	81	76			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
3	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
4	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
5	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 6 is a protein called C-TERM HELIX PDF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	A5	16	Total	C	N	O	0	0	0
			134	84	28	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A5	146	ALA	LEU	engineered mutation	UNP P0A6K3

- Molecule 7 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
7	CA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 8 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
8	CB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AC	268	Total	C	N	O	S	0	0	1
			2054	1271	417	359	7			
9	CC	268	Total	C	N	O	S	0	0	1
			2054	1271	417	359	7			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
10	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
11	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
12	CF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
13	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
14	CH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	CI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AJ	141	Total	C	N	O	S	0	0	1
			1113	704	211	194	4			
16	CJ	141	Total	C	N	O	S	0	0	1
			1113	704	211	194	4			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AK	122	Total	C	N	O	S	0	0	1
			931	582	180	164	5			
17	CK	122	Total	C	N	O	S	0	0	1
			931	582	180	164	5			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
18	CL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
19	CM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			
20	CN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			
21	CO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
22	CP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
23	CQ	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
24	CR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
25	CS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AT	100	Total	C	N	O	S	0	0	1
			778	491	146	139	2			
26	CT	100	Total	C	N	O	S	0	0	1
			778	491	146	139	2			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AU	103	Total	C	N	O	S	0	0	1
			780	492	147	141				
27	CU	103	Total	C	N	O	S	0	0	1
			780	492	147	141				

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
28	CV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AW	84	Total	C	N	O	S	0	0	0
			634	391	129	113	1			
29	CW	84	Total	C	N	O	S	0	0	0
			634	391	129	113	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
30	CX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AZ	70	Total	C	N	O	S	0	0	0
			549	339	104	100	6			
32	CZ	70	Total	C	N	O	S	0	0	0
			549	339	104	100	6			

- Molecule 33 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
33	DA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BB	219	Total	C	N	O	S	0	0	1
			1705	1081	306	311	7			
34	DB	219	Total	C	N	O	S	0	0	1
			1705	1081	306	311	7			

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BC	207	Total	C	N	O	S	0	0	1
			1625	1028	306	288	3			
35	DC	207	Total	C	N	O	S	0	0	1
			1625	1028	306	288	3			

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
36	DD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BE	151	Total	C	N	O	S	0	0	1
			1106	687	212	201	6			
37	DE	151	Total	C	N	O	S	0	0	1
			1106	687	212	201	6			

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BF	101	Total	C	N	O	S	0	0	1
			818	515	149	148	6			
38	DF	101	Total	C	N	O	S	0	0	1
			818	515	149	148	6			

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BG	151	Total	C	N	O	S	0	0	1
			1175	730	227	214	4			
39	DG	153	Total	C	N	O	S	0	0	1
			1197	745	231	217	4			

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
40	DH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
41	DI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BJ	99	Total	C	N	O	S	0	0	1
			787	493	151	142	1			
42	DJ	99	Total	C	N	O	S	0	0	1
			787	493	151	142	1			

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
43	DK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
44	DL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BM	115	Total	C	N	O	S	0	0	1
			884	546	179	156	3			
45	DM	114	Total	C	N	O	S	0	0	1
			877	541	178	155	3			

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
46	DN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	DO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
48	DP	81	Total	C	N	O	S	0	0	1
			639	400	127	111	1			

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	81	Total	C	N	O	S	0	0	1
			649	411	122	113	3			
49	DQ	81	Total	C	N	O	S	0	0	0
			657	417	122	115	3			

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BR	56	Total	C	N	O	0	0	1
			456	288	87	81			
50	DR	56	Total	C	N	O	0	0	1
			456	288	87	81			

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	80	Total	C	N	O	S	0	0	1
			638	408	121	107	2			
51	DS	81	Total	C	N	O	S	0	0	1
			645	413	122	108	2			

- Molecule 52 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
52	DT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 53 is a protein called 30S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	52	Total	C	N	O	S	0	0	1
			426	265	87	73	1			
53	DU	52	Total	C	N	O	S	0	0	1
			426	265	87	73	1			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AB	109	Total	Mg	0	0
			109	109		
54	AE	1	Total	Mg	0	0
			1	1		
54	BA	58	Total	Mg	0	0
			58	58		
54	BN	1	Total	Mg	0	0
			1	1		
54	BT	1	Total	Mg	0	0
			1	1		
54	CB	109	Total	Mg	0	0
			109	109		
54	CC	1	Total	Mg	0	0
			1	1		
54	CL	1	Total	Mg	0	0
			1	1		
54	DA	61	Total	Mg	0	0
			61	61		
54	DN	1	Total	Mg	0	0
			1	1		

- Molecule 55 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	A2	2	Total	O	0	0
			2	2		
55	AB	489	Total	O	0	0
			489	489		
55	AC	3	Total	O	0	0
			3	3		
55	AD	1	Total	O	0	0
			1	1		
55	AE	3	Total	O	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AJ	2	Total O 2 2	0	0
55	AL	3	Total O 3 3	0	0
55	BA	284	Total O 284 284	0	0
55	BE	3	Total O 3 3	0	0
55	BI	2	Total O 2 2	0	0
55	BK	1	Total O 1 1	0	0
55	BL	2	Total O 2 2	0	0
55	BN	3	Total O 3 3	0	0
55	BP	1	Total O 1 1	0	0
55	BT	2	Total O 2 2	0	0
55	C0	1	Total O 1 1	0	0
55	C2	2	Total O 2 2	0	0
55	CB	485	Total O 485 485	0	0
55	CC	3	Total O 3 3	0	0
55	CD	1	Total O 1 1	0	0
55	CE	1	Total O 1 1	0	0
55	CJ	2	Total O 2 2	0	0
55	CK	1	Total O 1 1	0	0
55	CL	5	Total O 5 5	0	0
55	CN	3	Total O 3 3	0	0
55	CP	1	Total O 1 1	0	0

Continued on next page...

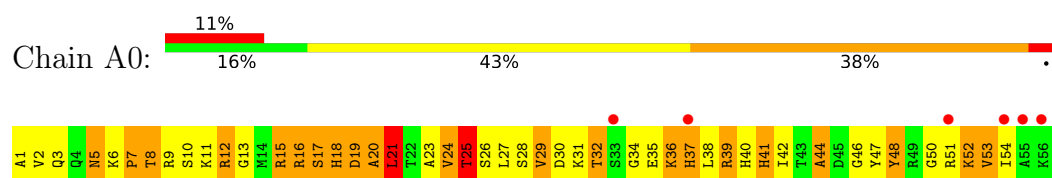
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CQ	1	Total 1	O 1	0	0
55	CT	2	Total 2	O 2	0	0
55	CU	1	Total 1	O 1	0	0
55	DA	293	Total 293	O 293	0	0
55	DD	1	Total 1	O 1	0	0
55	DE	2	Total 2	O 2	0	0
55	DG	1	Total 1	O 1	0	0
55	DL	4	Total 4	O 4	0	0
55	DN	2	Total 2	O 2	0	0
55	DP	1	Total 1	O 1	0	0
55	DT	3	Total 3	O 3	0	0

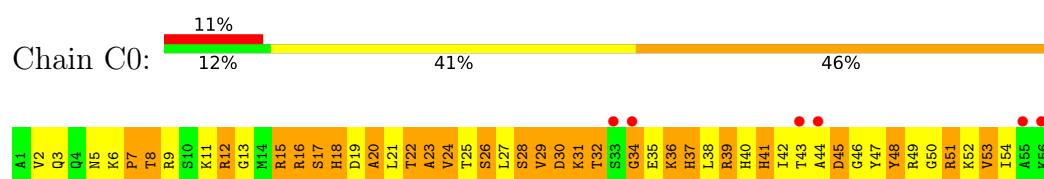
3 Residue-property plots [i](#)

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

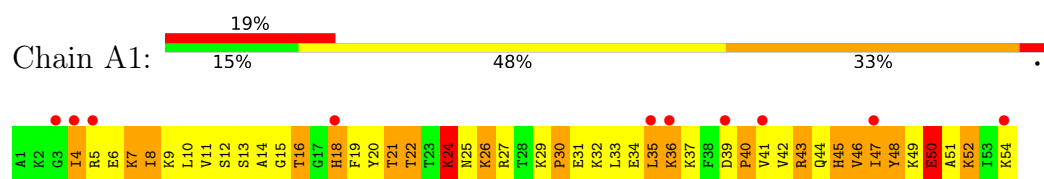
- Molecule 1: 50S RIBOSOMAL PROTEIN L32



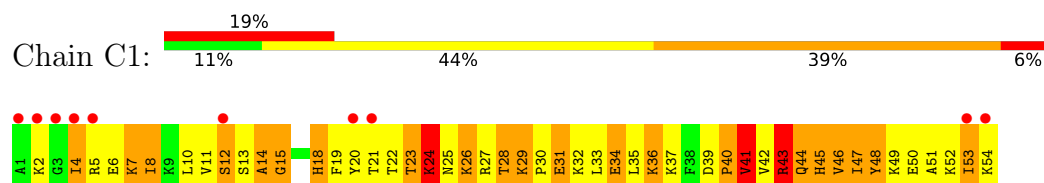
- Molecule 1: 50S RIBOSOMAL PROTEIN L32



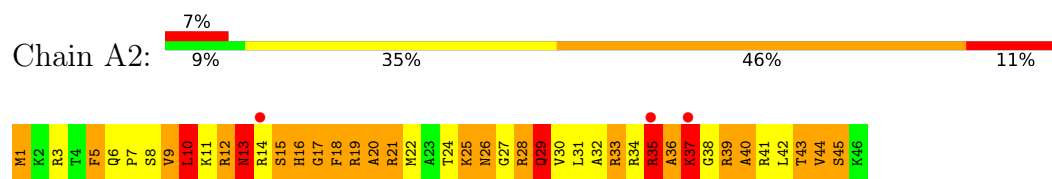
- Molecule 2: 50S RIBOSOMAL PROTEIN L33



- Molecule 2: 50S RIBOSOMAL PROTEIN L33



- Molecule 3: 50S RIBOSOMAL PROTEIN L34



- Molecule 3: 50S RIBOSOMAL PROTEIN L34





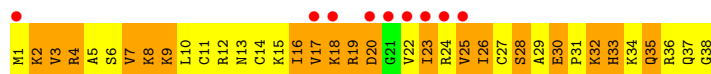
• Molecule 4: 50S RIBOSOMAL PROTEIN L35



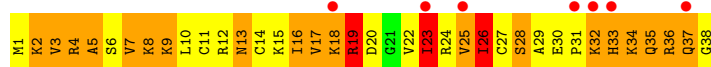
• Molecule 4: 50S RIBOSOMAL PROTEIN L35



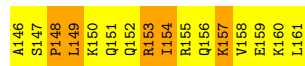
• Molecule 5: 50S RIBOSOMAL PROTEIN L36



• Molecule 5: 50S RIBOSOMAL PROTEIN L36

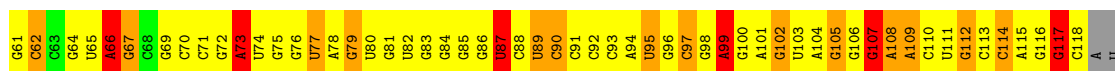


• Molecule 6: C-TERM HELIX PDF

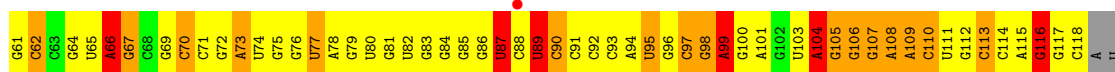


• Molecule 7: 5S RIBOSOMAL RNA

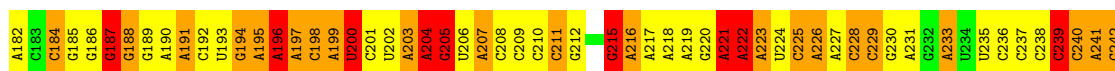
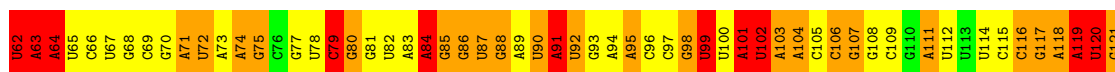
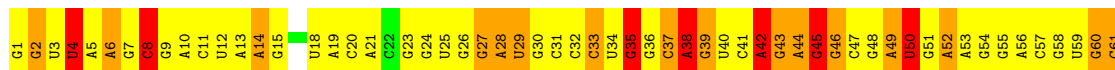




• Molecule 7: 5S RIBOSOMAL RNA

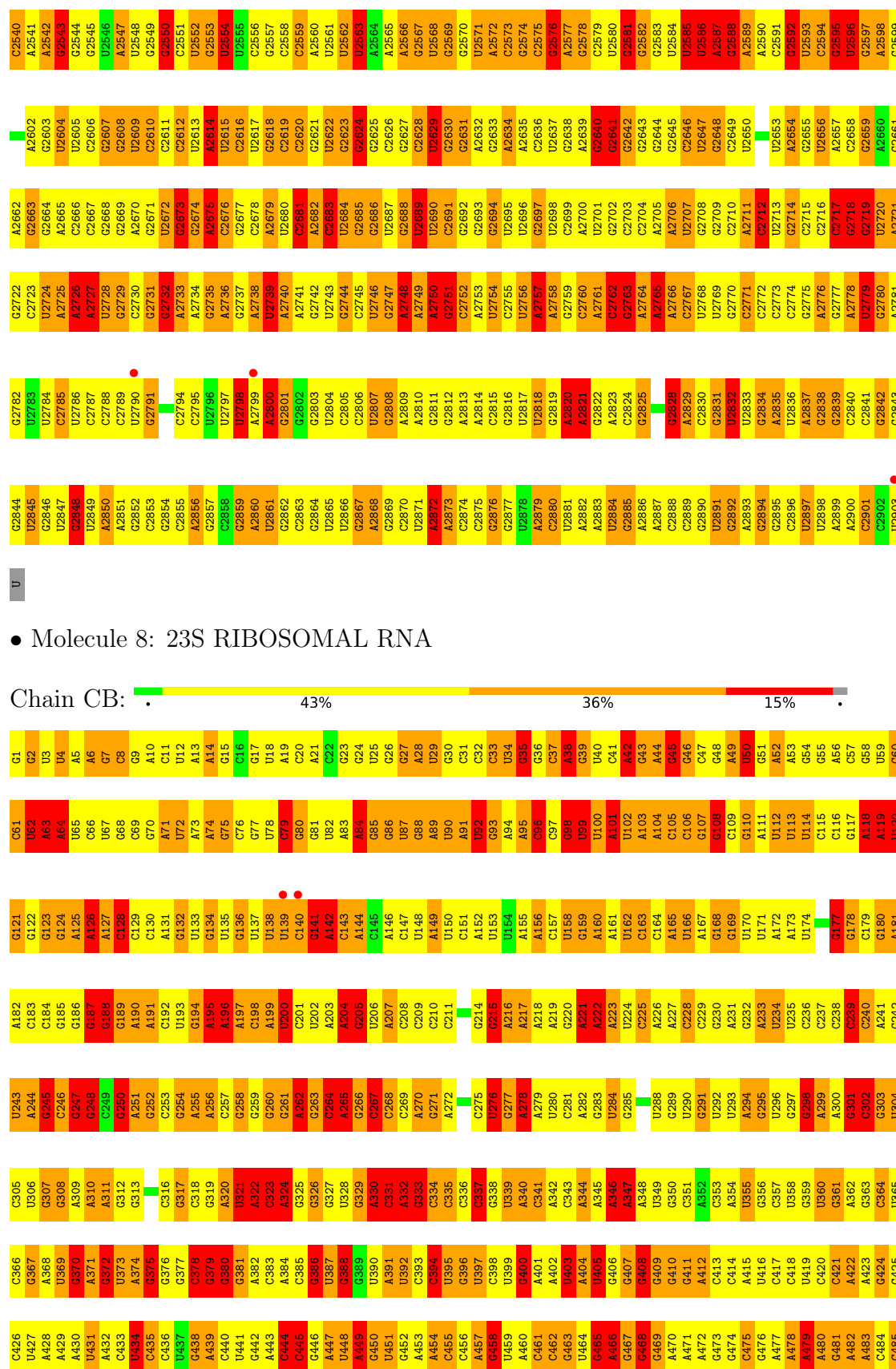


• Molecule 8: 23S RIBOSOMAL RNA



U1576	G1516	G1449	G1389	U1329	A1269	G1210	A1147	A1085	G1024	C964	G904	A844	G764	G664
C1577	G1517	G1450	U1390	C1330	C1270	G1211	A1148	A1086	G1025	C965	A905	A845	G765	U665
U1578	G1518	C1451	U1391	G1331	C1271	C1212	U1149	G1087	G1026	G966	U906	U846	G766	A666
G1579	G1519	G1452	A1392	G1332	A1272	G1213	U1150	A1088	A1027	G967	G907	U847	G767	U667
A1580	U1520	A1453	A1393	G1333	C1273	A1213	C1151	A1089	C988	C968	C908	C848	G768	A668
G1581	G1521	C1454	U1394	G1334	A1274	A1214	A1152	A1090	A1029	G969	A909	A849	G769	G669
C1582	A1522	G1455	A1385	C1335	A1275	G1215	C1153	G1091	C1030	U970	U910	U850	G770	A670
A1583	U1523	G1456	U1396	C1336	A1276	G1216	C1154	C1092	G1031	G971	A911	C851	G771	C671
U1584	G1524	U1457	U1397	C1337	C1277	U1217	U1154	G1093	A1032	A972	C912	U852	A792	C672
A1585	A1525	U1458	C1398	G1338	C1278	U1218	A1155	G1094	U1033	A973	U913	C853	A793	C673
A1586	C1526	G1459	C1399	G1339	C1279	U1219	A1156	A1095	G1034	G974	U914	C854	A794	G674
G1587	G1527	U1460	U1400	U1340	G1280	G1220	A1157	A1096	U1035	A975	C915	C855	C795	A675
G1588	G1401	C1461	G1401	G1341	G1281	C1221	C1158	U1097	U1036	G976	G916	C856	C796	A676
U1589	U1402	C1462	U1402	A1342	U1282	U1222	U1159	A1098	G1037	G977	A917	C857	C797	A677
A1590	G1530	G1463	A1403	G1343	G1283	G1223	G1160	G1099	U1038	G978	A918	C858	G798	C678
A1591	C1531	U1464	C1404	U1344	A1284	U1224	C1161	C1100	G1039	A979	U919	C859	A799	C679
C1592	U1405	U1466	U1405	G1345	A1285	G1225	G1162	A980	A1040	A980	A920	U860	C740	C680
A1593	C1533	G1467	U1406	G1346	A1286	A1226	G1163	U1101	G1041	A981	C921	U861	U741	G681
U1594	U1534	A1469	G1407	A1347	A1287	G1227	C1164	A1103	G1042	C982	C922	C862	A802	G682
C1595	A1535	A1470	G1408	C1348	G1288	G1228	A1165	C1104	C1043	A983	G923	A863	U803	U683
A1596	U1536	G1471	U1409	C1349	C1289	C1229	U1166	U1105	G1044	A984	U924	C864	A804	G684
A1597	G1537	C1472	G1410	C1350	C1290	U1230	C1167	G1106	C1045	C985	A925	C865	G805	A685
A1598	G1538	G1473	U1411	C1351	C1291	U1231	G1168	G1107	A1046	C986	G926	A866	C806	U686
U1599	U1539	U1474	U1412	U1352	G1292	G1232	A1169	G1108	U1047	C987	A927	C867	U807	C687
C1600	G1540	G1475	A1413	A1353	C1293	C1233	C1170	U1109	G1048	A988	A928	U868	G808	U688
G1601	G1541	U1476	G1414	A1354	U1294	U1234	C1172	G1110	C1049	C989	U929	C868	A809	A689
U1602	U1542	A1477	G1415	G1355	C1295	G1235	U1173	A1111	A1050	A990	G930	U870	U810	C690
A1603	G1543	G1478	G1416	G1356	G1296	U1236	U1174	G1112	G1051	C991	U931	U871	U811	C691
C1604	G1479	C1479	G1417	G1357	C1297	A1237	U1175	U1113	C1052	C992	U932	U872	C812	C692
A1605	A1545	C1480	G1418	G1358	C1298	G1238	U1176	C1114	C1053	C993	A933	C873	U813	A693
C1606	G1546	U1481	A1419	A1359	G1299	G1239	G1177	G1115	A1054	C994	U934	C874	C814	U694
G1607	C1547	G1482	G1420	G1360	G1300	U1240	C1178	G1116	G1055	C995	C935	C875	C815	G695
A1608	A1548	G1483	A1421	G1361	A1301	A1241	G1179	C1117	U1056	A996	A936	C876	C816	G696
A1609	U1549	U1484	G1422	C1362	A1302	U1242	U1180	C1118	U1058	G997	C937	A877	C817	G697
A1610	C1550	U1485	G1423	C1363	G1303	C1243	U1181	U1119	G1059	C998	G938	A878	G818	C698
C1611	G1424	U1486	G1424	G1364	A1304	A1244	U1182	G1120	G1060	U999	G939	G	A819	A699
G1612	U1487	U1487	G1425	A1365	C1305	G1245	U1183	C1121	U1061	A1000	G940	G	A820	G700
G1613	C1488	C1488	G1426	A1366	C1306	A1246	U1184	G1122	U1062	A1001	C941	G	A821	G701
A1614	C1489	C1489	A1427	A1367	A1307	A1247	G1185	C1123	G1063	G1002	G942	G	G822	U702
C1615	A1490	G1491	C1428	G1368	A1308	U1248	G1186	G1124	U1064	C	A943	G	C823	U703
A1616	G1492	G1492	G1429	G1369	C1309	G1249	G1187	G1125	C1064	U	C944	U	U824	G704
A1617	C1557	G1493	G1430	C1370	G1310	G1250	U1188	A1126	U1065	C1005	A945	C	A825	A705
A1618	U1558	A1494	A1431	G1371	G1311	G1251	A1189	A1127	U1066	C1006	C946	U	U826	A706
G1619	U1559	A1494	G1432	U1372	G1312	G1252	G1190	G1128	U1067	C1007	A947	A	U827	G707
G1620	G1560	A1495	A1433	A1373	U1313	A1253	G1191	A1129	G1068	A1008	C948	C	U828	G708
U1621	C1561	U1496	A1434	G1374	C1314	A1254	G1192	U1130	A1069	C	C949	C	A829	U709
G1622	U1562	U1497	G1435	U1375	C1315	U1255	G1193	G1131	A1070	A1010	G950	C	G830	U710
G1623	C1563	C1498	G1436	C1376	U1316	G1256	A1194	U1132	G1071	G1011	C951	G	G831	G711
U1624	U1564	C1499	C1437	G1377	G1317	G1257	G1195	A1133	C1072	U1012	G952	A	U832	G712
C1625	C1565	G1503	U1438	A1378	U1318	U1258	C1196	A1134	G1075	C1013	G953	C	A833	G713
A1626	A1566	A1503	A1439	U1379	C1319	G1259	G1197	C1135	C1076	A1014	G954	U	G834	U714
G1627	G1567	A1504	U1440	G1380	C1320	A1260	U1198	G1136	A1077	U1015	U955	U	C835	A715
G1628	U1568	A1505	G1441	A1381	A1321	C1261	U1199	G1137	U1078	G836	G956	A	G837	A716
U1629	A1569	U1506	U1442	G1382	A1322	A1262	C1200	G1138	U1079	G837	C957	C	C837	C717
A1630	U1570	C1507	U1443	A1383	C1323	U1263	U1201	G1139	G1079	U1018	U958	C898	C838	U718
G1631	A1571	A1508	G1444	A1384	G1324	A1264	G1202	C1140	A1080	U1019	A959	A899	U839	C719
A1632	A1572	A1509	G1445	A1385	U1325	A1265	U1203	U1141	U1081	A1020	A960	A900	C840	U720
G1633	G1573	U1510	C1446	C1386	U1326	G1266	A1204	A1142	U1082	A1021	C961	C901	G841	A721
A1634	C1477	G1574	C1447	A1387	A1327	U1267	A1205	A1143	U1083	U1022	G962	C902	U842	A722
A1635	C1575	A1515	G1448	G1388	A1328	A1268	G1206	A1144	A1084	U1023	U963	C903	G843	C723

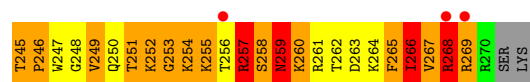




U1390	C1330	G1270	G1210	G1149	A1088	A1027	U967	G907	U847	C787	A727	U687	U607	A547	C486
U1391	G1331	G1271	C1211	C1150	A1089	A1028	C968	C908	C848	A788	G728	A688	A608	G548	C487
A1392	G1332	A1272	A1151	C1151	A1090	A1029	G969	A909	A849	A789	G729	G689	A609	G549	C488
A1393	G1333	U1273	C1213	C1152	G1091	C1030	U970	A910	U850	U790	A730	A670	C610	C550	C489
A1394	G1334	A1274	A1214	C1154	C1092	G1031	G971	A911	C851	C791	C731	C671	C611	G551	C490
A1395	C1335	A1275	G1215	C1155	G1093	A1032	A972	C912	U852	A792	C732	C672	G612	U552	C491
U1396	A1336	A1276	G1216	A1156	U1094	U1033	A973	U913	C853	A793	G733	G673	A613	G553	A492
U1397	G1337	G1277	U1217	A1157	A1095	U1034	A974	C914	C854	A794	G734	G674	A614	U554	A493
A1398	G1338	C1278	G1218	C1157	A1096	U1035	A975	C915	C855	A795	A735	A675	U615	G555	A494
A1399	G1339	G1279	U1219	C1158	A1097	G1036	G976	C916	C856	C796	G736	A676	A616	A556	A495
U1400	U1340	G1280	G1220	U1159	A1098	G1037	G977	A917	C857	C797	C737	A677	G617	G496	A496
G1401	G1341	G1281	C1221	G1160	G1099	A1038	A978	A918	C858	C798	G738	C678	G618	U558	A497
U1402	A1342	U1282	C1161	C1161	C1100	G1039	A979	U919	C859	C799	A739	C679	G619	G559	A498
A1403	G1343	G1283	G1223	G1162	U1101	A1040	A980	A920	U860	A800	C740	C680	G620	C560	U499
U1404	U1344	A1284	U1224	G1163	C1102	G1041	A981	C921	A861	G801	C741	G681	A621	U561	G500
U1405	C1345	A1285	G1225	C1164	A1103	G1042	C982	C922	C862	A802	A742	G682	G622	U562	A501
U1406	G1346	A1286	A1226	A1165	C1104	A1043	A983	G923	A863	U803	A743	U683	C623	A563	A502
G1407	A1347	A1287	G1227	G1166	U1105	C1044	A984	G924	G864	U804	U744	G684	C624	C564	A503
U1408	C1348	G1288	G1228	C1167	G1106	C1045	C985	A925	C865	G805	G745	A685	G625	C565	A504
U1409	C1349	C1289	C1229	G1168	G1107	A1046	C986	G926	A866	C806	U746	U686	A626	U566	A505
G1410	C1350	C1290	A1230	A1169	U1108	G1047	C987	A927	C867	U807	U747	U687	G627	U567	G506
U1411	C1351	C1291	U1231	C1170	C1109	A1048	A988	A928	U868	G808	G748	U688	G628	U568	A507
U1412	U1352	G1292	G1232	G1171	G1110	C1049	G989	U929	U869	C809	A749	A689	G629	U569	A508
A1413	A1353	C1293	C1233	C1172	A1111	A1050	A990	G930	U870	U810	A750	G690	G630	G570	C509
C1414	A1354	U1294	U1234	U1173	G1112	G1051	C991	U931	U871	U811	A751	C691	A631	U571	C510
U1415	G1355	C1295	G1235	U1174	U1113	C1052	C992	U932	U872	C812	A752	C692	A632	A572	U511
G1416	G1356	G1296	G1236	A1175	C1114	C1053	G993	A933	C873	U813	A753	A693	A633	U573	G512
C1417	C1357	C1297	A1237	U1176	G1115	A1054	C994	U934	C874	C814	U754	U694	C634	A574	A514
G1418	G1358	C1298	G1238	G1177	C1116	G1055	C995	G935	C875	C815	U755	G695	C635	A575	A515
A1419	A1359	G1299	G1239	C1178	C1117	G1056	A996	A936	C876	C816	A756	G696	G636	U576	A516
A1420	G1360	G1300	U1240	G1179	C1118	A1057	G997	C937	A877	C817	G757	G697	A637	G577	C516
G1421	G1361	A1301	A1241	U1180	U1119	U1058	C998	G938	A878	C818	C758	C698	G638	G578	C517
G1422	C1362	A1302	U1242	U1181	G1120	G1059	U999	G939	G	A819	G759	A699	U639	G579	G518
G1423	C1363	G1303	C1243	G1182	C1121	U1060	A1000	G940	G	A820	G760	G700	C640	U580	U519
G1424	G1364	A1304	A1244	U1183	G1122	A1061	A1001	A941	G	A821	A761	G701	U641	C581	G520
G1425	A1365	C1305	G1245	U1184	C1123	G1062	G1002	G942	G	G822	U762	U702	U642	A582	
G1426	A1366	C1306	G1246	G1185	G1124	G1063	G1003	A943	G	C823	G763	U703	A643	G583	C523
A1427	A1367	A1307	A1247	G1186	G1125	C1064	U1004	C944	U	U824	A764	G704	A644	C584	G524
G1428	G1368	A1308	G1248	G1187	A1126	U1065	C1005	A945	C	A825	C765	A705	C645	G585	U525
G1429	G1369	G1309	U1249	U1188	A1127	U1066	C1006	C946	A	U826	U766	U706	U646	A586	A526
G1430	C1370	G1310	G1250	A1189	G1128	A1067	C1007	A947	U	U827	U767	G707	G647	C587	C527
A1431	G1371	G1311	C1251	G1190	A1129	G1068	A1008	C948	C	U828	G768	G708	G648	U588	A528
G1432	U1372	U1312	C1252	G1191	U1130	A1069	A1009	G949	C	A829	U769	U709	G649	U589	A529
A1433	A1373	C1313	A1253	G1192	G1131	A1070	A1010	C950	C	C830	G770	U710	C650	A590	G530
A1434	G1374	C1314	U1254	G1193	U1132	G1071	G1011	C951	G	C831	G771	G711	G651	U591	C531
G1435	U1375	C1315	U1255	A1194	A1133	C1072	U1012	G952	A	A832	C772	G712	U652	A592	A532
G1436	C1376	G1316	G1256	G1195	A1134	A1073	C1013	G953	C	A833	U773	G713	U653	U593	G533
C1437	G1377	G1317	C1257	C1196	C1135	G1074	A1014	G954	U	G834	G774	U714	A654	U594	U534
U1438	A1378	U1318	U1258	G1197	G1136	C1075	U1015	G955	U	C835	G775	A715	A655	C595	G535
A1439	U1379	C1319	G1259	U1198	G1137	C1076	G1016	G956	A	C836	G776	A716	G656	U596	G536
U1440	G1380	A1320	A1260	U1199	G1138	A1077	G1017	C957	C	C837	G777	C717	U657	G597	G537
G1441	C1381	C1321	C1261	C1200	G1139		C998	U958	C998	C838	G778	A718	U658	U598	A538
U1442	G1382	A1322	U1262	U1201	A1080	A1081	U1019	A959	A899	U839	U779	C719	G659	A599	G539
U1443	A1383	C1323	G1263	G1202	U1141	U1082	U1020	A960	A900	C840	G780	U720	C660	G600	C540
G1444	G1384	G1324	A1264	U1203	A1083	U1083	A1021	C961	C901	C841	A781	A721	A661	C601	A541
G1445	A1385	A1265	A1265	A1204	A1142	A1084	G1022	G962	C902	U842	A782	A722	G662	A602	C542
C1446	C1386	U1326	G1266	A1205	A1144	A1084	U1023	U963	C903	G843	G783	G723	G663	A603	G543
G1447	A1387	A1327	U1267	C1206	A1147	A1085	G1024	C964	G904	A844	G784	U724	G664	G604	C544
G1448	G1388	A1328	A1268	G1207	A1148	A1086	G1025	C965	A905	G785	G785	G725	G665	G605	U545
G1449	G1389	U1329	A1269			G1087	G1026	G966	U906	U846	G786	G726	A666	U606	U546

U2299	G2239	C2179	A	A1938	A1877	A1815	A1755	G1695	A1634	C1574	G1513	G1450
C2300	U2240	U2180	G	U1939	G1878	C1816	G1756	G1696	A1635	C1575	A1514	C1451
U2301	G2241	U2181	G	U1940	C1879	G1817	A1757	G1697	A1636	U1576	G1516	G1452
G2302	A2242	G2061	U	C1941	U1880	U1818	A1758	A1698	A1637	C1577	G1517	A1453
G2303	U2243	A2062	G	C1942	U1881	C1819	A1759	G1699	A1638	U1577	C1518	C1454
C2304	G2244	C2063	G	U1943	U1882	U1820	C1760	A1700	C1639	A1578	G1519	G1455
U2305	U2245	C2064	G	C1944	U1883	A1821	C1761	A1701	A1640	A1580	U1520	G1456
C2306	G2246	C2065	G	U1945	U1884	A1822	A1762	G1702	A1641	G1581	G1521	A1457
G2307	A2247	G2066	A	U1946	G1885	G1823	G1763	U1703	A1642	G1582	U1522	U1458
G2308	U2248	U2067	G	C1947	A1886	G1824	C1764	C1704	G1643	A1583	U1523	G1459
A2309	U2249	G2068	G	U1948	C1887	U1825	U1765	A1705	A1644	U1584	G1524	U1460
G2310	G2250	A2070	U	G1949	G1888	G1826	G1766	C1706	G1645	C1585	A1525	C1461
A2311	A2251	U2071	U	U1950	A1889	U1827	G1767	G1707	C1646	A1586	C1526	C1462
U2312	G2252	C2072	U	U1951	A1890	G1828	C1768	C1708	U1647	G1587	G1527	
C2313	G2253	A2013	G	A1952	G1891	A1829	U1769	U1709	U1648	U1588	A1528	G1465
A2314	U2254	A2014	A	C1953	C1892	C1830	U1770	G1710	G1649	U1589	G1529	U1466
G2315	G2255	U2015	G	U1954		G1831	C1771	A1711	A1650	A1590	G1530	
G2316	G2256	U2016	G	G1955	C1895	C1832	A1772	U1712	G1651	A1591	A1531	A1469
G2317	U2257	U2017	U	U1956	G1896	C1833	A1773	G1713	A1652	C1592	A1532	A1470
A2318	C2258	C2078	G	C1957	G1897	U1834	C1774	U1714	G1653	A1593	G1533	G1471
G2319	U2259	A2019	U	U1958	U1898	G1835	U1775	G1715	A1654	U1594	U1534	C1472
C2320	C2260	A2020	G	A1959	A1899	C1836	G1776	U1716	A1655	C1595	A1535	G1473
U2321	C2261	C2081	G	U1960	A1900	C1837	U1777	A1717	C1656	A1596	G1474	U1475
A2322	U2262	U2022	G	C1961	A1901	C1838	U1778	G1718	U1657	A1597	G1537	G1476
G2323	C2263	A2082	U		C1902	G1839	U1779	G1719	C1658	A1598	U1538	U1477
U2324	C2264	C2083	G		G1903	G1840	A1780	U1720	G1659	U1599	U1539	A1478
C2325	U2265	C2084	G	G1964	G1904	U1841	U1781	U1721	G1660	C1600	G1540	G1479
G2326	A2266	U2085	G	C1965	G1905	G1842	U1782	A1722	G1661	C1601	C1541	C1480
A2327	U2267	U2086	U	A1966	C1906	C1843	G1783	G1723	U1662	A1602	U1542	C1481
C2328	C2268	G2087	G	C1967	G1907	C1844	A1784	G1724	G1663	A1603	G1543	U1482
A2329	A2269	C2089	U	A1969	C1908	G1845	A1785	U1725	A1664	C1604	A1544	G1483
G2330	U2270	A2090	U	U1970	C1909	G1846	A1786	G1726	A1665	C1605	A1545	U1484
C2331	G2271	A2031	G	U1971	G1910	A1847	A1787	C1727	G1666	C1606	G1547	U1485
G2332	U2272	U2032	U	G1972	U1911	C1848	C1788	C1728	G1667	C1607	C1547	U1486
A2333	C2273	C2093	G	C1973	A1912	A1849	A1789	U1729	A1668	A1608	A1548	U1487
U2334	A2274	A2094	U	C1974	A1913	G1850	C1790	G1730	A1669	A1609	A1549	U1488
C2335	C2275	G2035	G	G1975	C1914		A1791	G1731	C1670	A1610	C1550	C1489
A2336	G2276	C2096	G	U1976	U1915	A1853	G1792	C1732	U1671	C1611	A1551	C1490
G2337	U2277	A2097	A	A1977	A1916	A1854	C1793	G1733	A1672	C1612	A1552	G1491
C2338	A2278	U2098	G	A1978	U1917	U1855	A1794	G1734	G1673	G1613	U1553	C1492
U2339	G2279	U2099	U	U1979	A1918	U1856	C1795	A1735	G1674	A1614	U1554	G1493
G2340	U2280	G2100	C	G1980	A1919	G1857	U1796	U1736	C1675	C1615	G1555	A1494
C2341	C2281	A2101	C	U1981	C1920	A1858	G1797	G1737	A1676	A1616	G1556	A1495
G2342	G2282	G2102	G	U1982	G1921		U1798	G1738	A1677	C1617	C1557	A1496
U2343	C2283	C2103	A	G1983	G1922	G1861	G1799	A1739	A1678	A1618	C1558	U1497
G2344	A2284	C2104	C	U1984	U1923	G1862	C1800	G1740	A1679	G1619	U1559	U1498
C2345	G2285	G2105	C	C1985	C1924	G1863	A1801	C1741	U1680	G1620	G1560	C1499
A2346	G2286	G2106	U	C1986	C1925	U1864	A1802	U1742	G1681	U1621	C1561	
G2347	A2287	U2107	U	U1987	U1926	U1865	A1803	G1743	G1682	G1622	U1562	
U2348	U2288	A2108	G	G1988	A1927	A1866	C1804	A1744	U1683	G1623	U1563	A1503
G2349	G2289	G2048	A	U1989	A1928	G1867	A1805	A1745	G1684	U1624	C1564	A1504
C2350	U2290	C2050	A	C1990	G1929	C1868	C1806	U1746	C1685	C1625	C1565	A1505
G2351	U2291	A2051	A	U1991	G1930	G1869	G1807	U1747	A1696	A1626	U1566	U1506
A2352	U2292	C2052	U	G1992	U1931	C1870	A1808	C1748	G1686	G1627	G1567	U1507
G2353	C2293	U2053	U	U1993	A1932	A1871	A1809	U1749	U1688	G1628	G1568	A1508
C2354	G2294	A2054	C	C1994	G1933	A1872	A1810	G1750	U1689	U1629	A1569	A1509
G2355	C2295	C2055	C	U1995	C1934	G1873	G1811	U1751	C1691	A1630	A1570	G1510
U2356	U2296	G2056	G	C1996	C1935	C1874	U1812	C1752	U1692	G1631	A1571	G1511
G2357	A2297	G2057	A	U1997	G1936	A1875	G1813	G1753	U1693	A1632	A1572	C1512
A2358	U2298	A2058	C	A1998	A1937	A1876	G1814	A1754	C1694	G1633	G1573	U1513

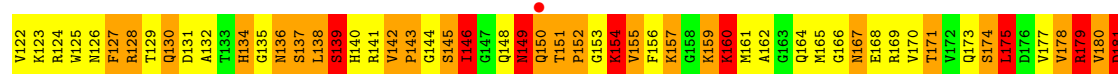
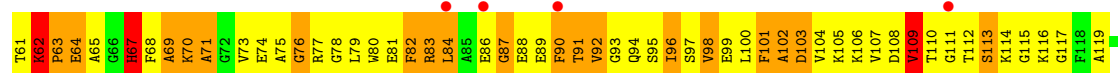




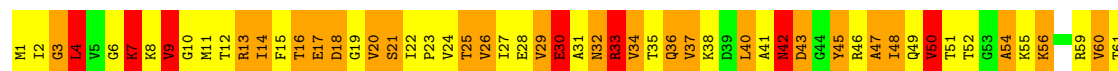
● Molecule 9: 50S RIBOSOMAL PROTEIN L2

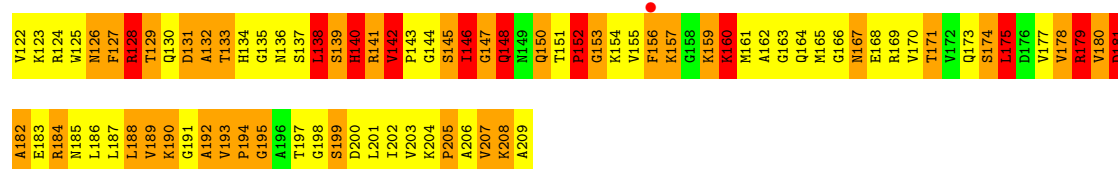


● Molecule 10: 50S RIBOSOMAL PROTEIN L3

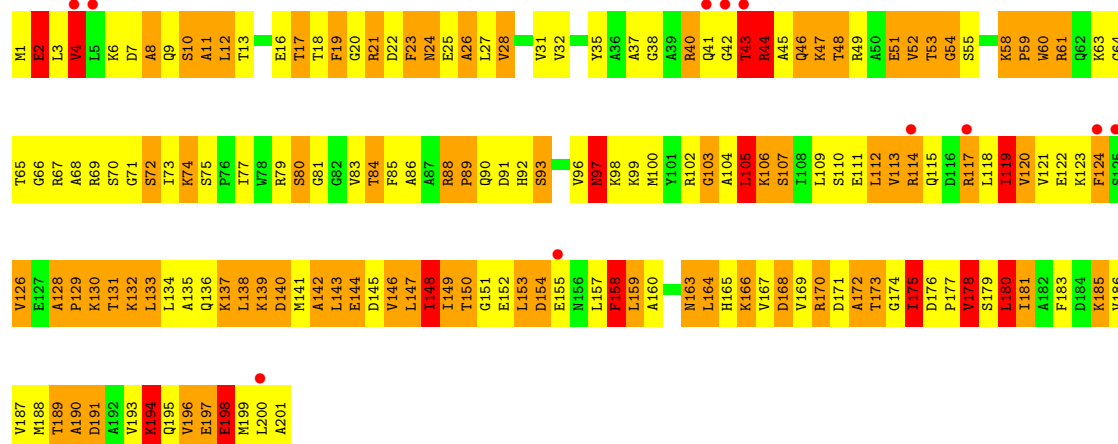
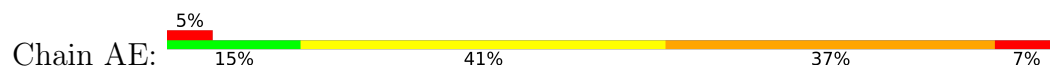


● Molecule 10: 50S RIBOSOMAL PROTEIN L3

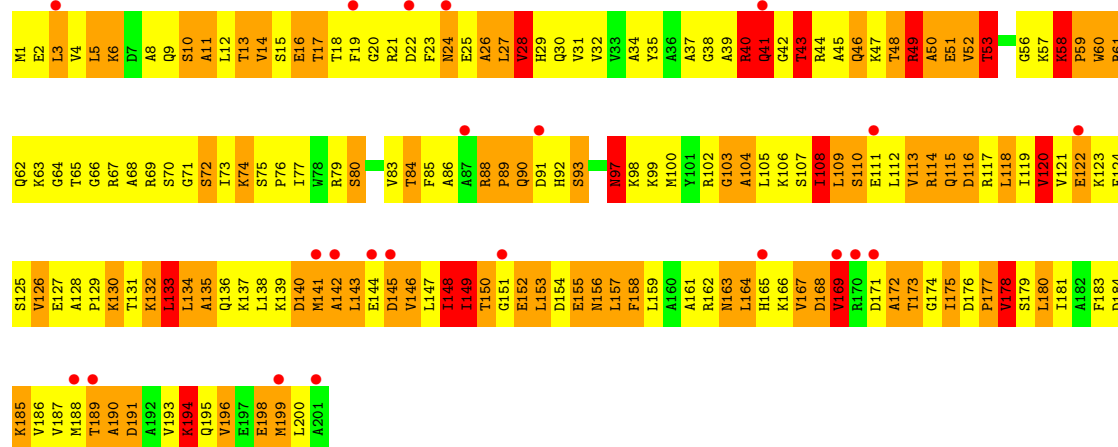




• Molecule 11: 50S RIBOSOMAL PROTEIN L4

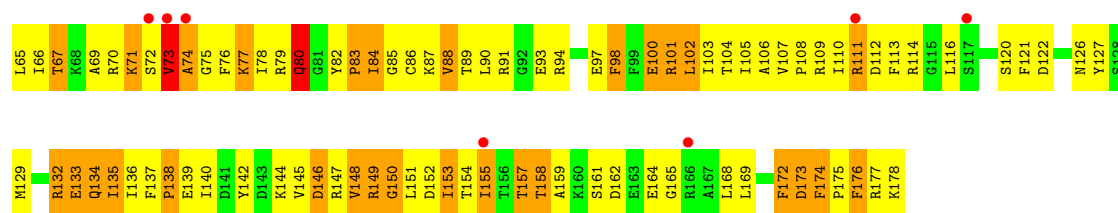


• Molecule 11: 50S RIBOSOMAL PROTEIN L4

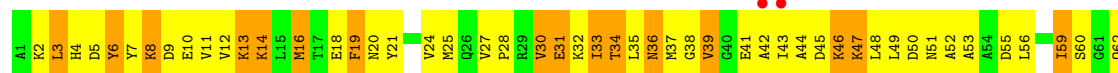


• Molecule 12: 50S RIBOSOMAL PROTEIN L5

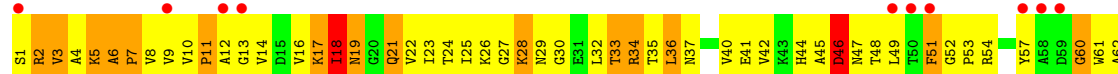
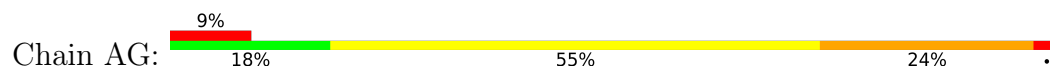




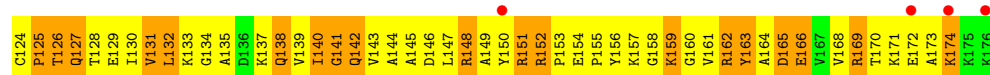
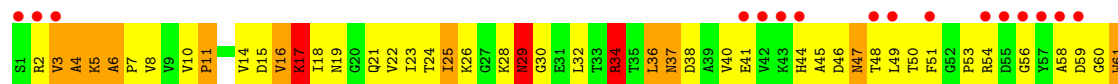
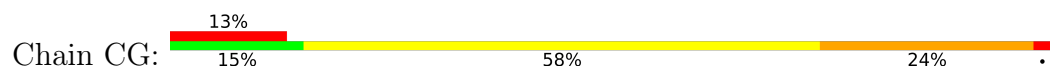
• Molecule 12: 50S RIBOSOMAL PROTEIN L5



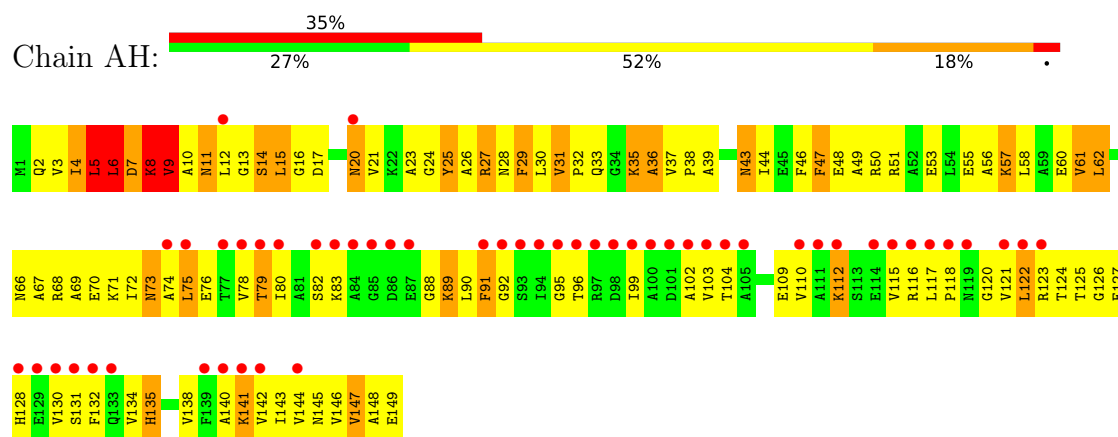
• Molecule 13: 50S RIBOSOMAL PROTEIN L6



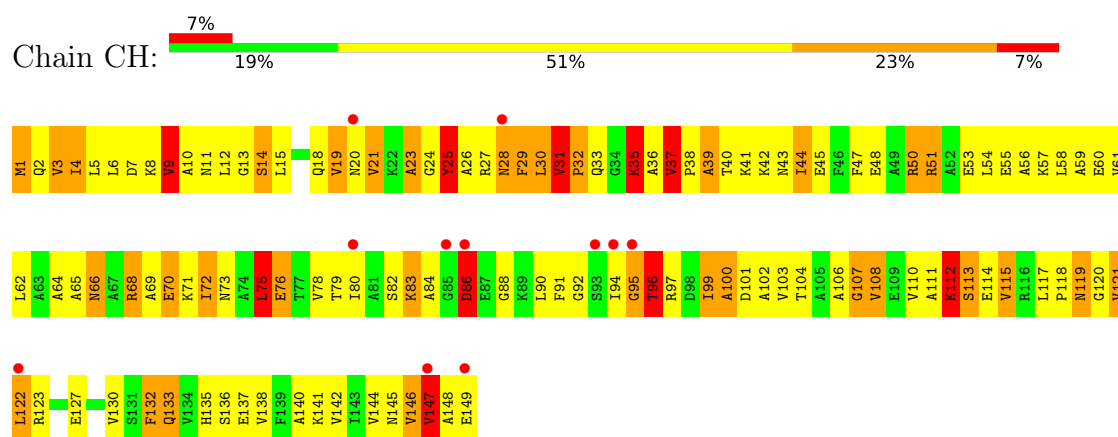
• Molecule 13: 50S RIBOSOMAL PROTEIN L6



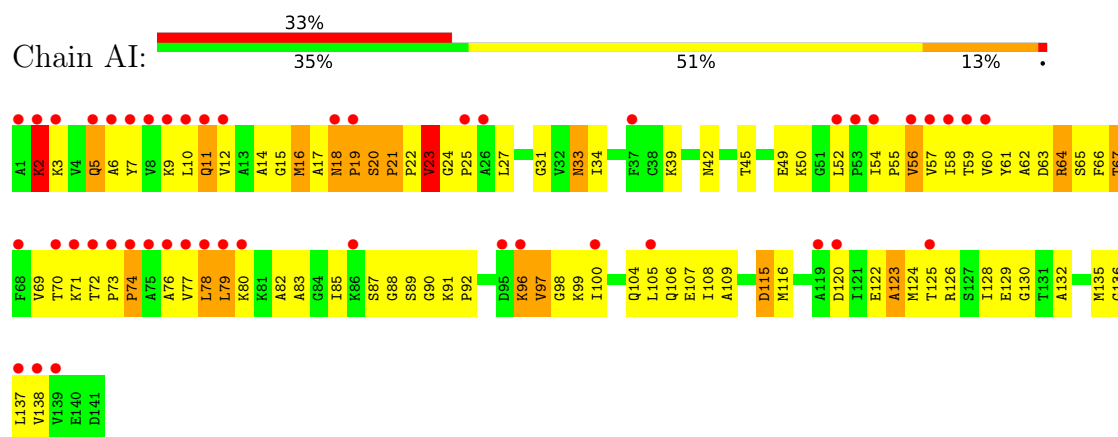
• Molecule 14: 50S RIBOSOMAL PROTEIN L9



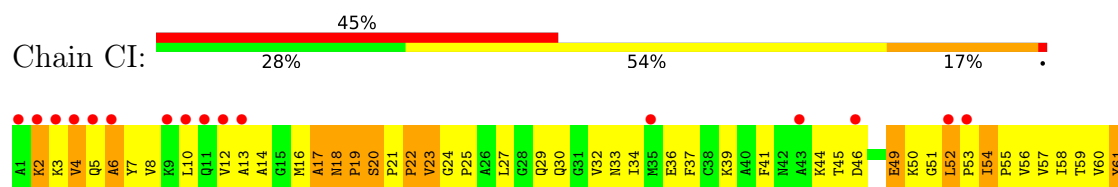
• Molecule 14: 50S RIBOSOMAL PROTEIN L9

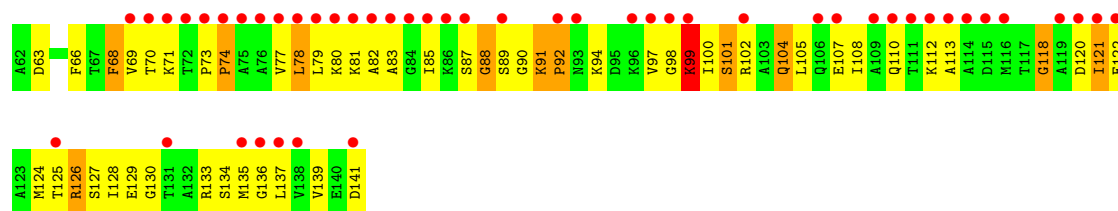


• Molecule 15: 50S RIBOSOMAL PROTEIN L11

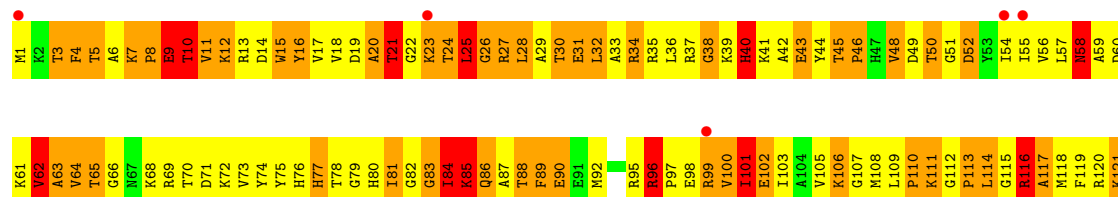


• Molecule 15: 50S RIBOSOMAL PROTEIN L11

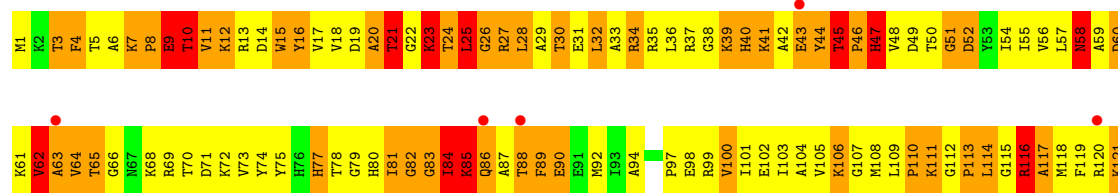




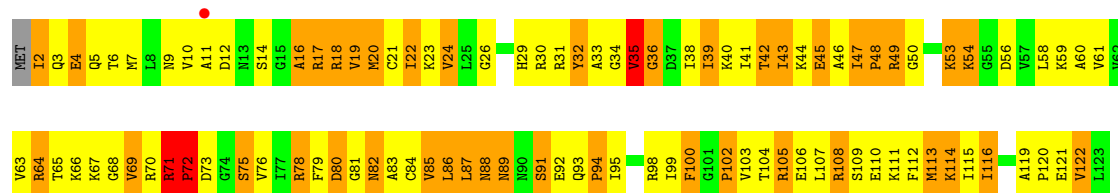
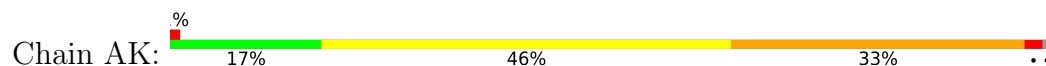
• Molecule 16: 50S RIBOSOMAL PROTEIN L13



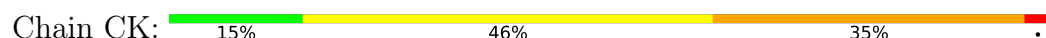
• Molecule 16: 50S RIBOSOMAL PROTEIN L13

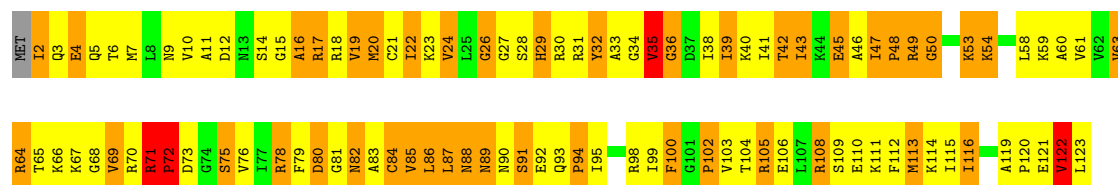


• Molecule 17: 50S RIBOSOMAL PROTEIN L14

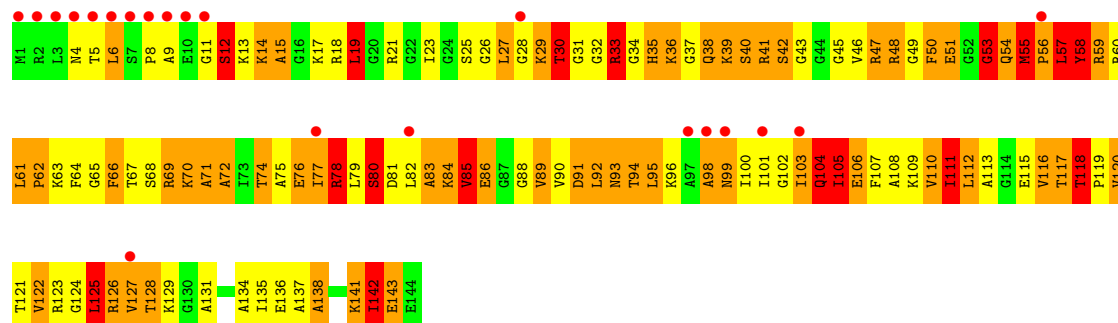


• Molecule 17: 50S RIBOSOMAL PROTEIN L14

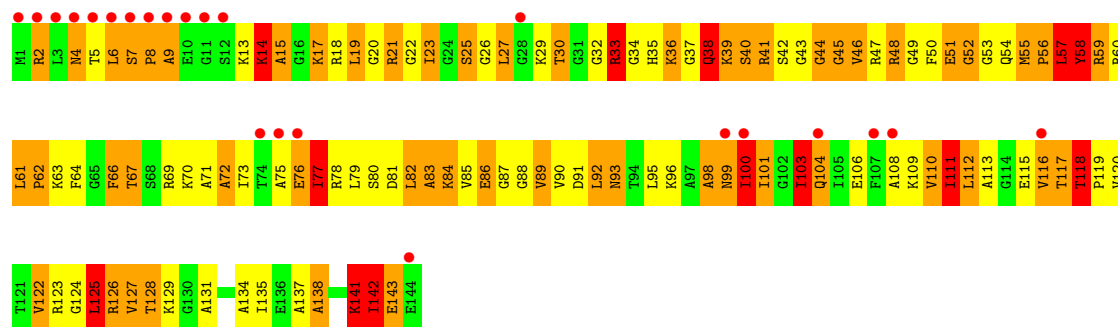
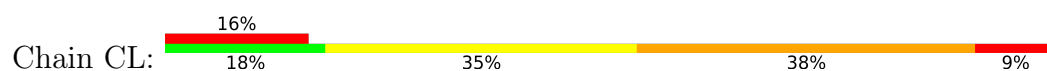




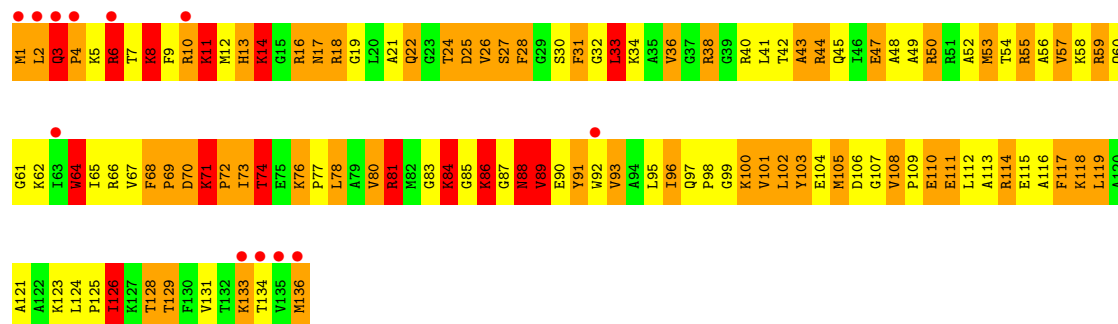
• Molecule 18: 50S RIBOSOMAL PROTEIN L15



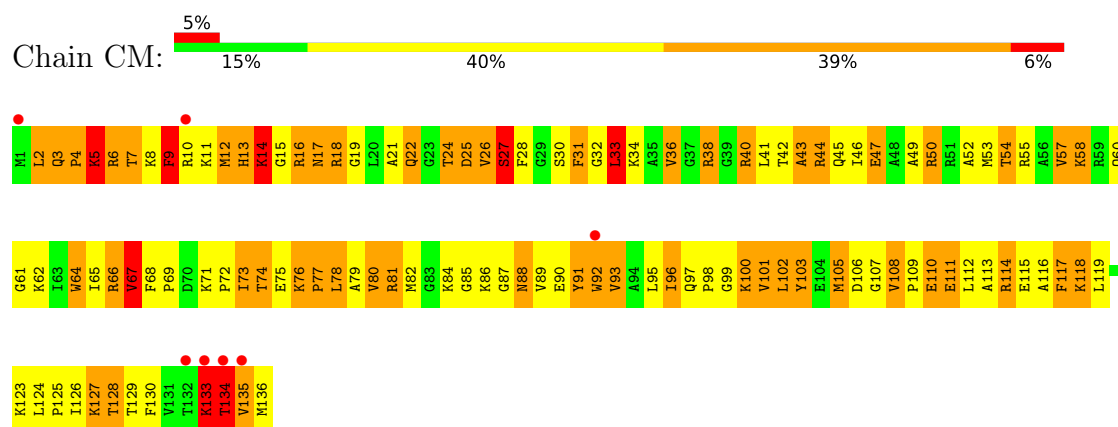
• Molecule 18: 50S RIBOSOMAL PROTEIN L15



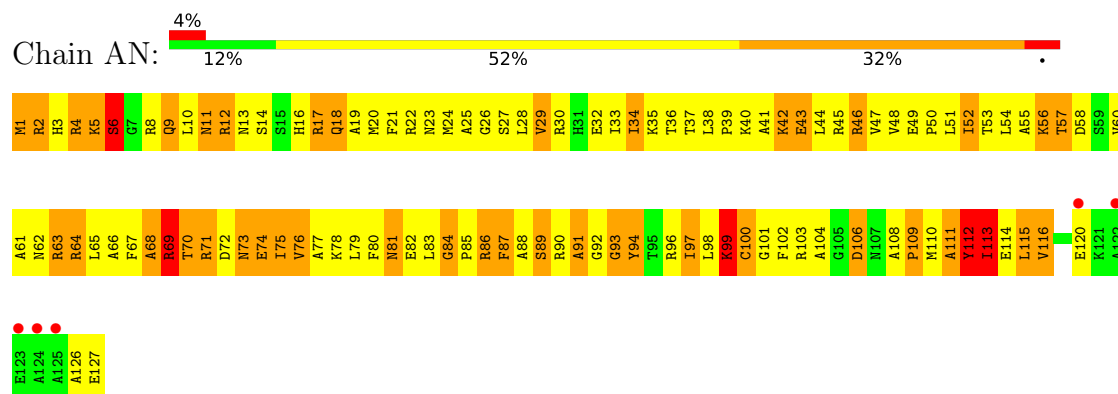
• Molecule 19: 50S RIBOSOMAL PROTEIN L16



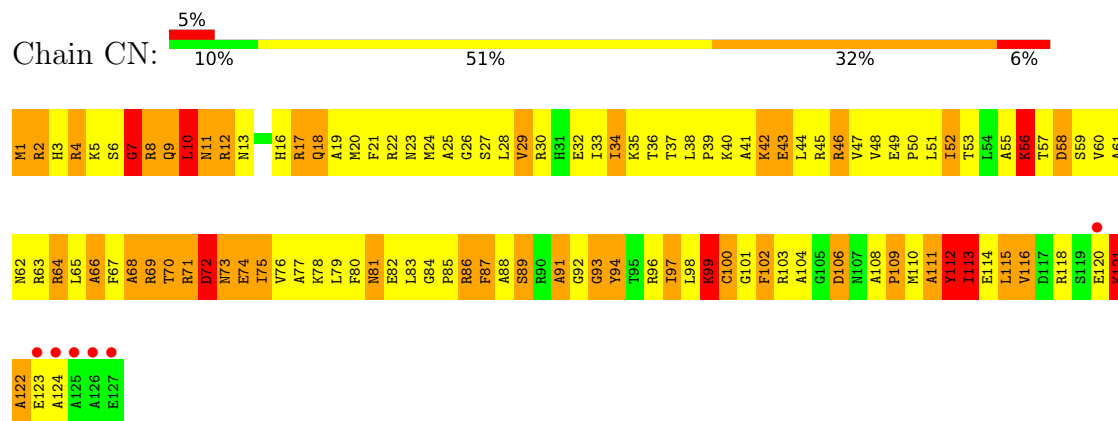
• Molecule 19: 50S RIBOSOMAL PROTEIN L16



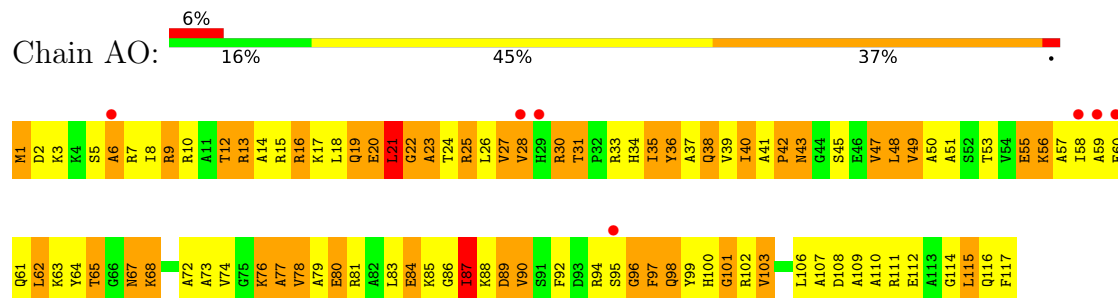
• Molecule 20: 50S RIBOSOMAL PROTEIN L17



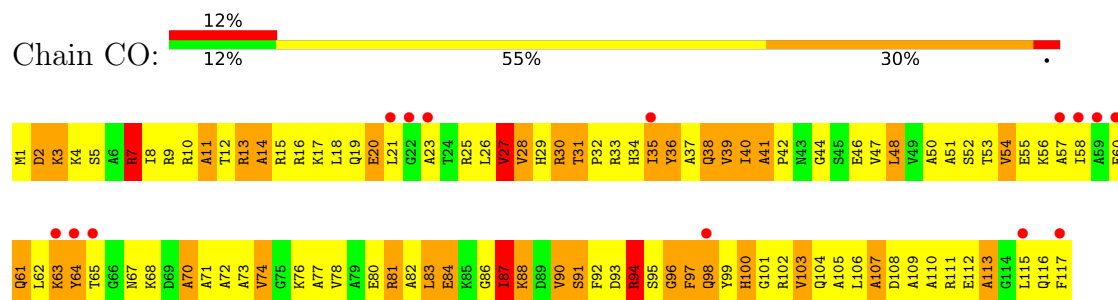
• Molecule 20: 50S RIBOSOMAL PROTEIN L17



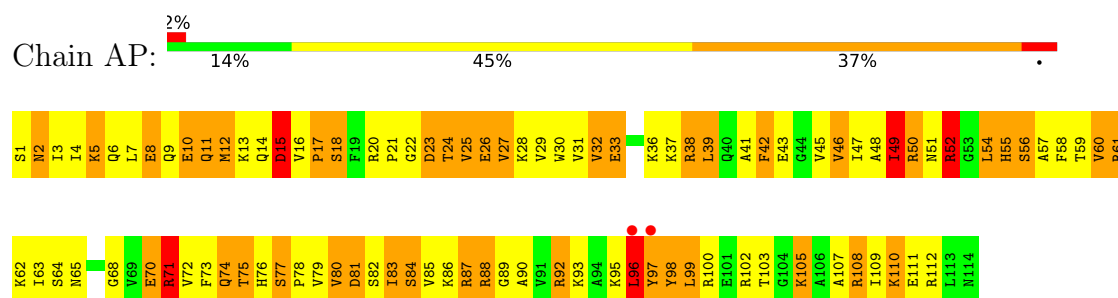
• Molecule 21: 50S RIBOSOMAL PROTEIN L18



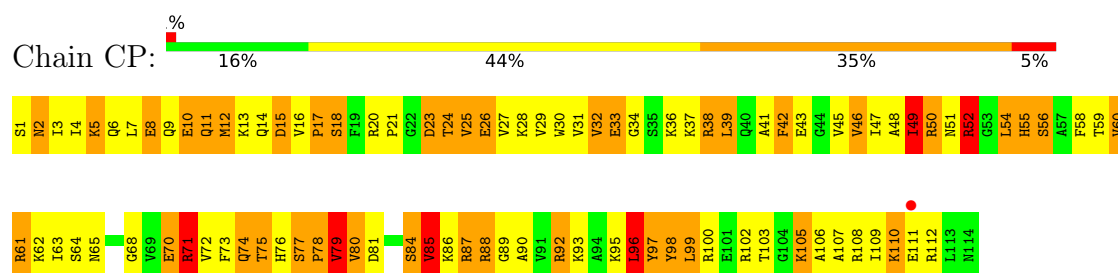
- Molecule 21: 50S RIBOSOMAL PROTEIN L18



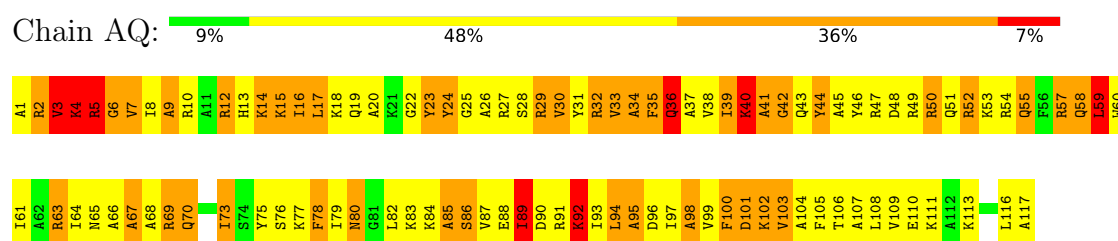
- Molecule 22: 50S RIBOSOMAL PROTEIN L19



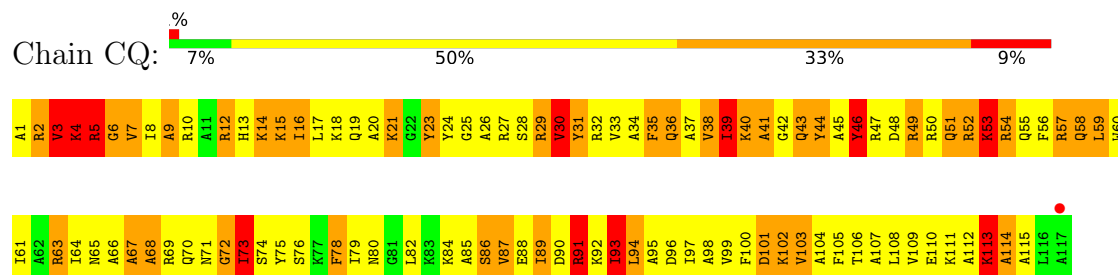
- Molecule 22: 50S RIBOSOMAL PROTEIN L19



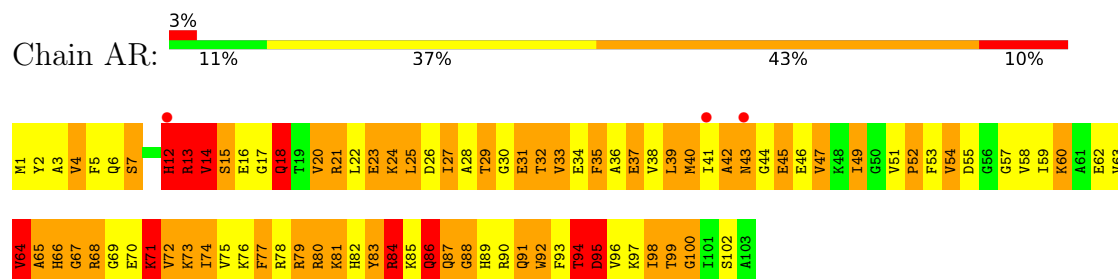
- Molecule 23: 50S RIBOSOMAL PROTEIN L20



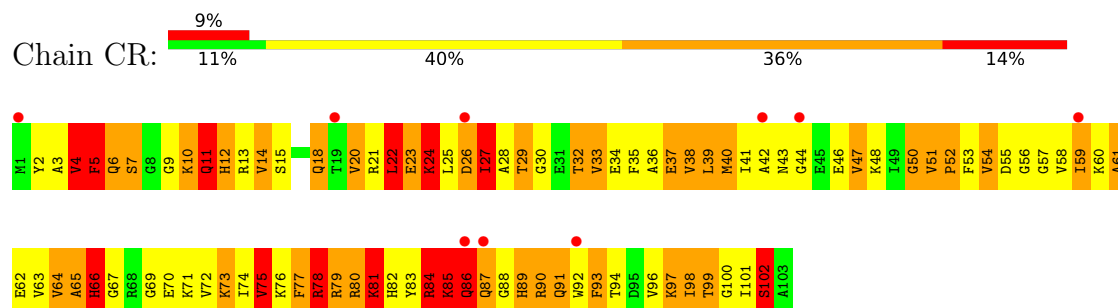
- Molecule 23: 50S RIBOSOMAL PROTEIN L20



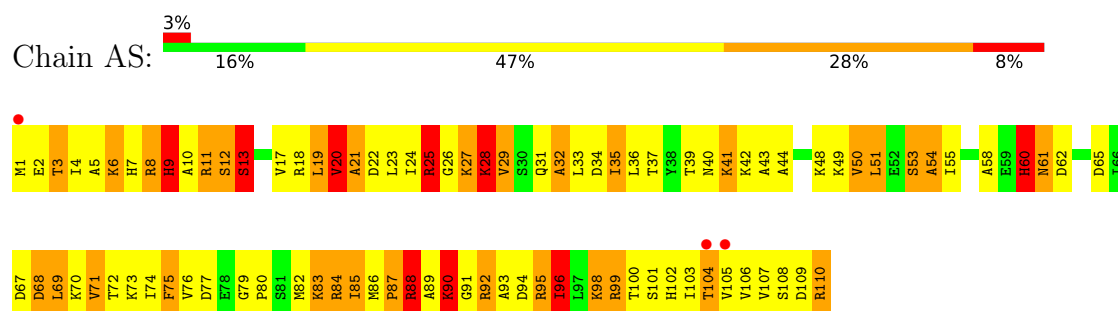
• Molecule 24: 50S RIBOSOMAL PROTEIN L21



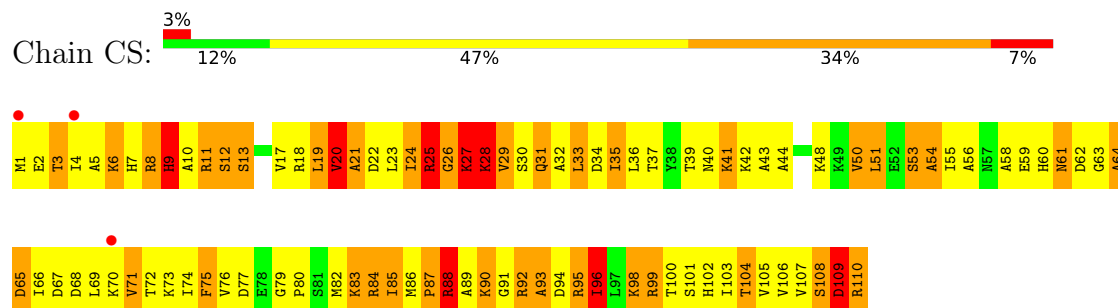
• Molecule 24: 50S RIBOSOMAL PROTEIN L21



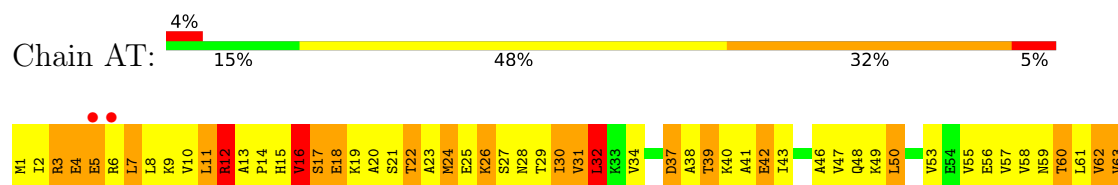
• Molecule 25: 50S RIBOSOMAL PROTEIN L22

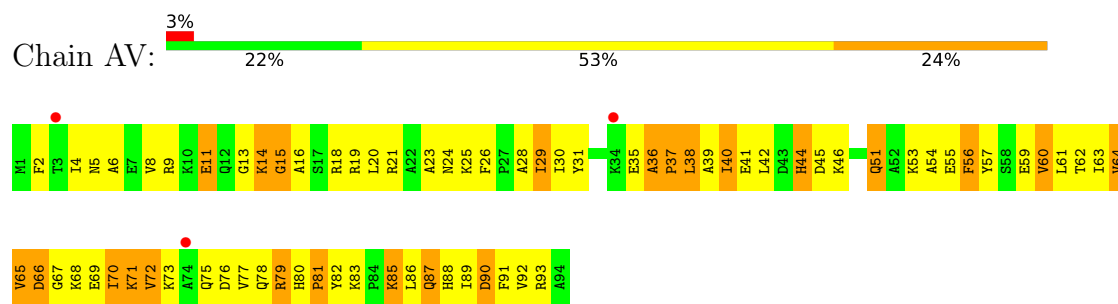
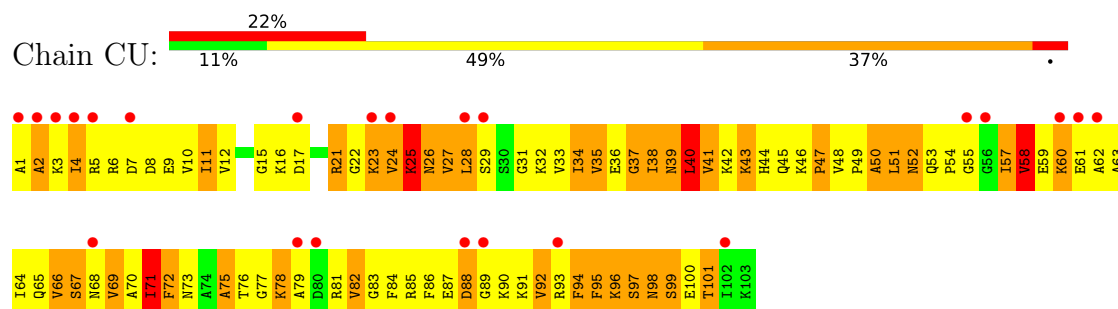
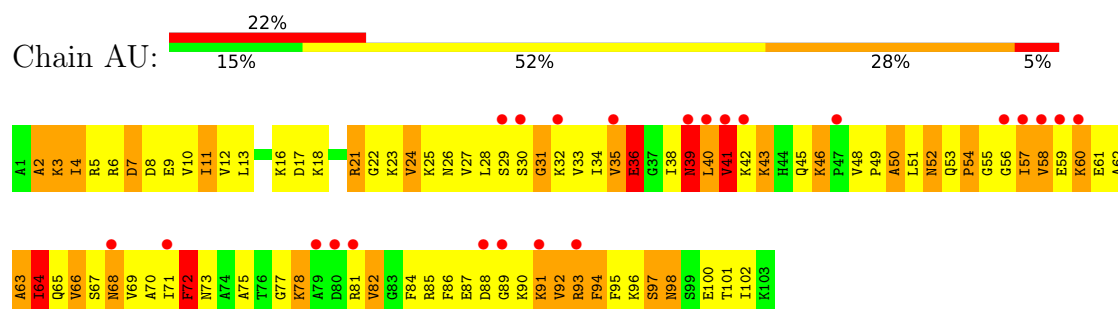
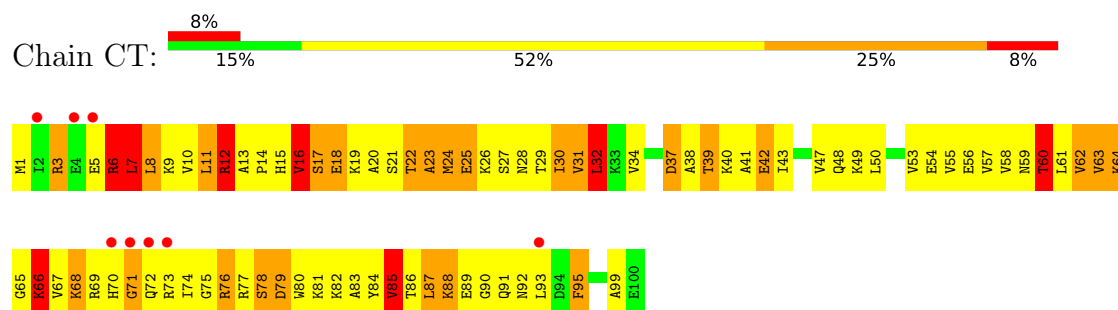
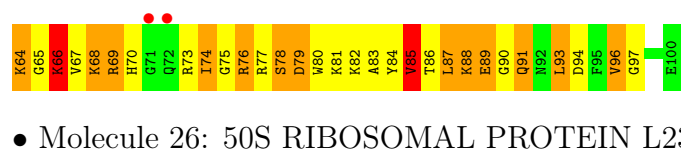


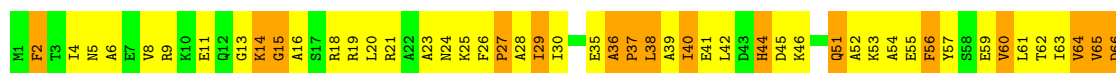
• Molecule 25: 50S RIBOSOMAL PROTEIN L22



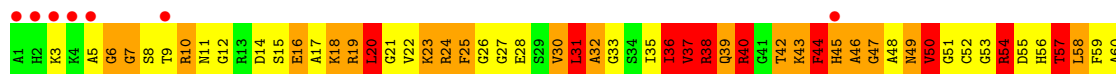
• Molecule 26: 50S RIBOSOMAL PROTEIN L23



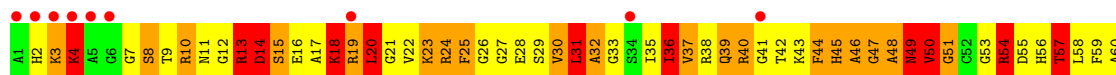




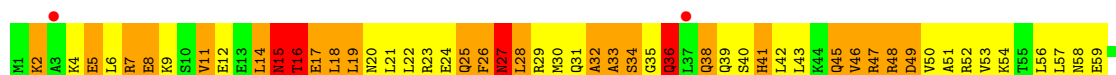
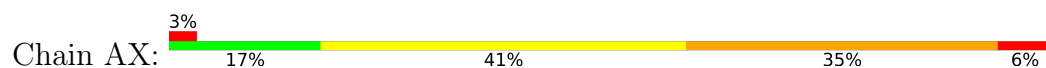
- Molecule 29: 50S RIBOSOMAL PROTEIN L27



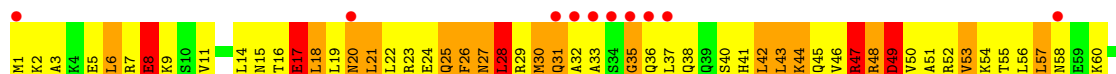
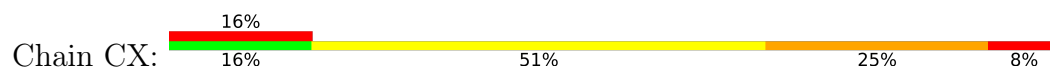
- Molecule 29: 50S RIBOSOMAL PROTEIN L27



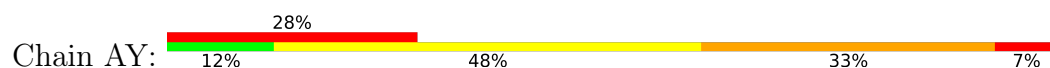
- Molecule 30: 50S RIBOSOMAL PROTEIN L29

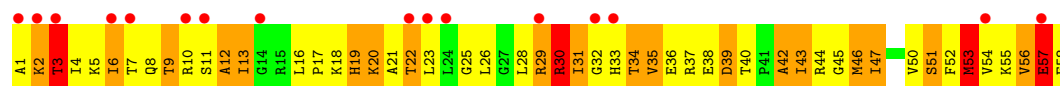


- Molecule 30: 50S RIBOSOMAL PROTEIN L29

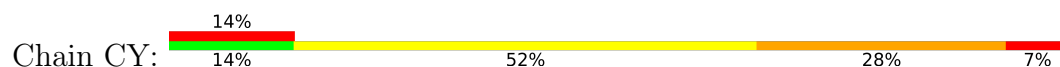


- Molecule 31: 50S RIBOSOMAL PROTEIN L30

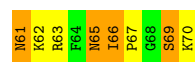
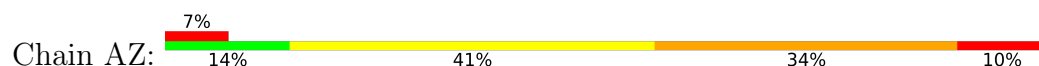




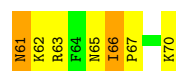
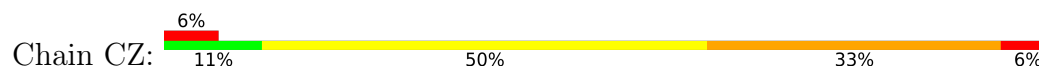
• Molecule 31: 50S RIBOSOMAL PROTEIN L30



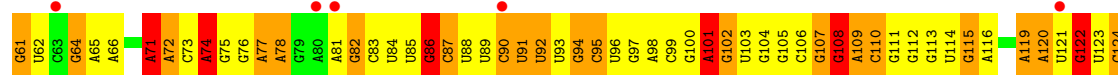
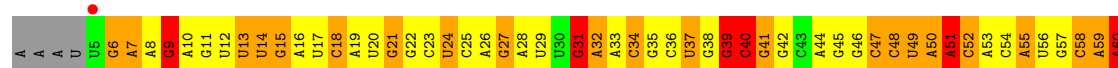
• Molecule 32: 50S RIBOSOMAL PROTEIN L31



• Molecule 32: 50S RIBOSOMAL PROTEIN L31

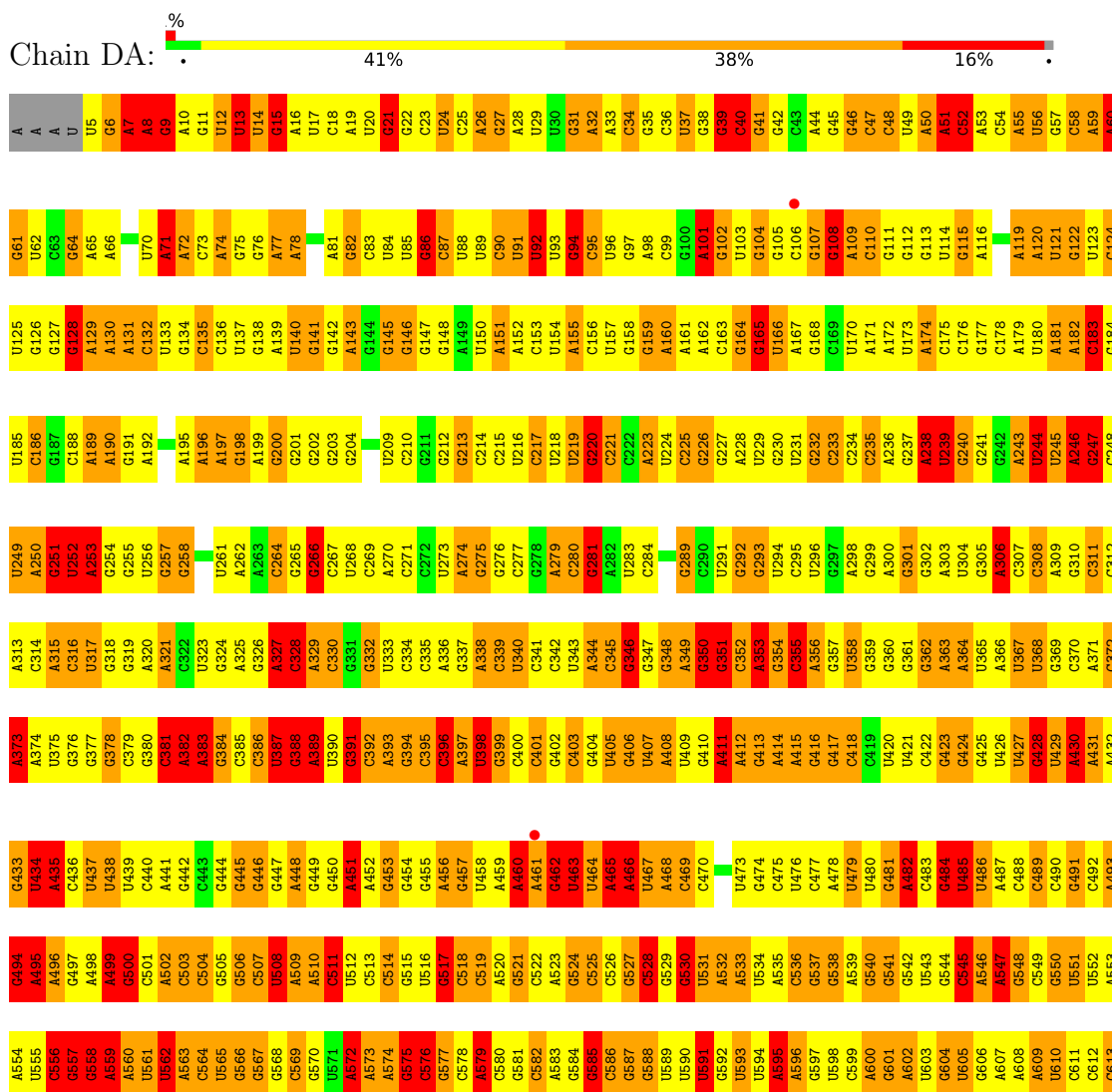


• Molecule 33: 16S RIBOSOMAL RNA



A1216	A1155	U1095	A1035	A974	U854	A794	G734	G674	C613	A553	A493	G433	A373	A313
C1217	G1156	C1096	A1036	A975	U855	C795	C735	A675	C614	A554	A494	U434	A374	C314
C1218	C1157	C1097	A1037	G976	C856	C796	C736	A676	G615	U555	A495	A435	U375	A315
A1219	C1158	C1098	C1038	A977	C857	C797	C737	U677	G616	C556	A496	A436	G376	C316
G1220	U1159	G1099	G1039	A978	G858	U798	C738	U678	G617	G557	A497	U437	G377	U317
G1221	U1160	G1100	U1040	C979	G859	G799	C739	C679	C618	G558	A498	U438	G378	G318
G1222	C1162	A1101	G1041	C980	U860	G800	U740	C680	U619	A559	A499	U439	C379	G319
C1223	A1163	A1102	A1042	C981	G861	U801	G741	A681	C620	A560	G500	U440	C380	A320
U1224	G1164	C1103	G1043	U982	C862	A802	G742	G682	A621	U561	C501	A441	C381	A321
A1225	A1165	A1104	A1044	C983	U863	G803	A743	G683	A622	U562	A502	G442	A382	C322
C1226	G1166	A1105	C1045	A984	U864	U804	C744	U684	C623	A563	C503	G443	A383	U323
A1227	A1167	G1106	A1046	C985	A865	C805	G745	G685	G624	C564	C504	G444	G384	G324
C1228	U1168	C1107	G1047	U986	C866	C806	A746	U686	U625	U565	C505	G445	A325	A325
A1229	A1169	G1108	G1048	G987	G867	A807	A747	A687	G626	G566	G506	G446	C386	G326
C1230	A1170	C1109	U1049	G988	C868	C808	G748	G688	G627	G567	C507	A447	U387	A327
G1231	A1171	A1110	G1050	U989	C869	G809	A749	G689	G628	G568	U508	A448	C388	C328
U1232	C1172	A1111	C1051	C990	U870	C810	C750	G690	A629	C569	A509	G449	A389	A329
G1233	U1173	C1112	U1052	U991	U871	C811	G751	G691	U632	G570	A510	G450	U390	C330
C1234	G1174	C1113	G1053	U992	A872	G812	G752	U692	G633	U571	C511	A451	G391	G331
U1235	G1175	C1114	C1054	G993	A873	U813	A753	G693	G634	A572	U512	A452	C392	G332
A1236	A1176	U1115	A1055	A994	G874	A814	C754	A694	C635	A573	C513	G453	U393	U333
C1237	G1177	U1116	U1056	C995	U875	A815	G755	A695	A636	A574	C514	G454	G394	C334
A1238	G1178	A1117	G1057	C996	C876	A816	C756	A696	U637	G575	C515	G455	C395	C335
U1239	A1179	U1118	G1058	C997	G877	C817	U757	U697	G638	C576	U516	G456	C396	A336
A1240	A1180	C1119	C1059	C998	A878	G818	C758	G698	U639	G577	G517	A457	A397	G337
G1241	G1181	C1120	U1060	A1000	C879	A819	A759	C699	G639	C578	C518	U458	U398	A338
C1242	G1182	U1121	G1061	C1001	C880	U820	G760	G700	A640	A579	C519	A459	G399	C339
G1243	U1183	U1122	U1062	G881	G881	G821	G761	U701	U641	C580	A520	A460	C400	U340
C1244	G1184	G1123	C1063	G942	C882	U822	U762	A702	A642	G581	C521	A461	A401	C341
G1245	A1185	U124	G1064	A1004	C883	C823	G763	G703	C643	G582	C522	G462	G402	C342
U1246	G1186	U1125	U1065	G944	U884	G824	C764	A704	U644	A583	A523	U463	G403	U343
A1247	G1187	U1126	C1066	G945	G885	A825	G765	G705	G645	G584	C524	U464	G404	A344
U1248	A1188	U1127	A1067	U1007	G886	C826	A766	A706	G646	G585	C525	A465	A405	C345
C1249	U1189	C1128	G1068	G947	G887	U827	A767	U707	C647	C586	C526	U467	U407	G347
A1250	G1190	C1129	C1069	C948	G888	U828	A768	C708	A648	G587	C527	A468	A408	G348
A1251	A1191	A1130	U1070	A949	A889	G829	G769	U709	A649	G588	C528	A469	A409	A349
C1252	C1192	G1131	C1071	U950	G890	G830	C770	G710	G650	U589	G529	C469	U409	A349
G1253	G1193	C1132	G1072	U951	U891	A831	G771	G711	C651	U590	G530	C470	G410	G350
A1254	U1194	G1133	U1073	G952	A892	G832	U772	A712	U652	G591	U531	U471	A411	G351
G1255	C1195	G1134	G1074	G953	C893	G833	G773	G713	U653	G592	A532	G472	A412	C352
A1256	A1196	U1135	U1075	G954	G894	U834	G774	A714	G654	U594	A533	U473	G413	A353
A1257	A1197	C1136	U1076	G955	G895	U835	G775	A715	A655	U594	U534	G474	A414	G354
G1258	U1198	C1137	G1077	U956	C896	G836	G776	A716	G656	A595	A535	U475	A415	C355
C1259	U1199	G1138	U1078	U957	C897	U837	A777	U717	U657	A596	C536	U476	A416	A356
G1260	C1200	G1139	G1079	A958	G898	G838	G778	A718	C658	G597	G537	C477	G417	G357
A1261	U1201	C1140	A1080	A959	C899	C839	C779	C719	U659	U598	G538	A478	C418	U358
C1262	U1202	C1141	A1081	U960	A900	C940	A780	C720	C660	C599	A539	U479	C419	G359
C1263	C1203	G1142	A1082	U961	A901	C941	G721	G661	G661	A600	G540	U480	U420	G360
U1264	A1204	G1143	U1083	C962	G902	U842	A782	G722	U662	G601	G541	U481	U421	G361
C1265	U1205	G1144	G1084	G963	G903	U843	C783	U723	A663	A602	G542	A482	G422	G362
G1266	G1206	A1145	U1085	A964	U904	G844	A784	G724	G664	U603	U543	C483	G423	A363
C1267	U1207	A1146	U1086	G965	U905	A845	G725	G725	A665	G604	G544	G484	G424	A364
A1268	C1208	C1147	G1087	G966	A906	G846	G726	C726	G666	U605	C545	U485	G425	U365
G1269	U1209	U1148	G1088	C967	A907	G847	A787	G727	G667	G606	A546	U486	U426	A366
C1270	C1210	C1149	U1089	A968	A908	C848	A788	A728	G668	A607	A547	A487	U427	U367
A1271	U1211	A1150	U1090	A969	A909	G849	U789	A729	G669	A608	G548	C488	G428	U368
G1272	U1212	A1151	U1091	C970	C910	U850	A790	G730	G670	A609	C549	C489	U429	G369
C1273	A1213	A1152	A1092	G971	U911	G851	A791	C731	G671	U610	G550	C490	A450	C370
A1274	G1214	C1153	A1093	C972	U912	G852	A792	C732	U672	C611	U551	C491	A451	A371
A1275	G1215	G1154	G1094	G973	A913	C853	U793	G733	A673	C612	U552	C492	A452	C372

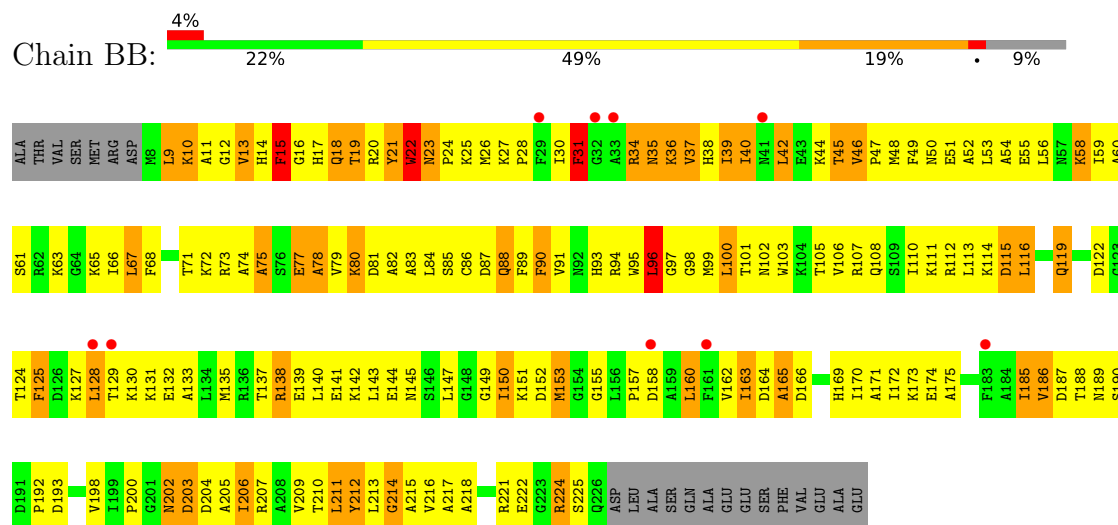
- Molecule 33: 16S RIBOSOMAL RNA



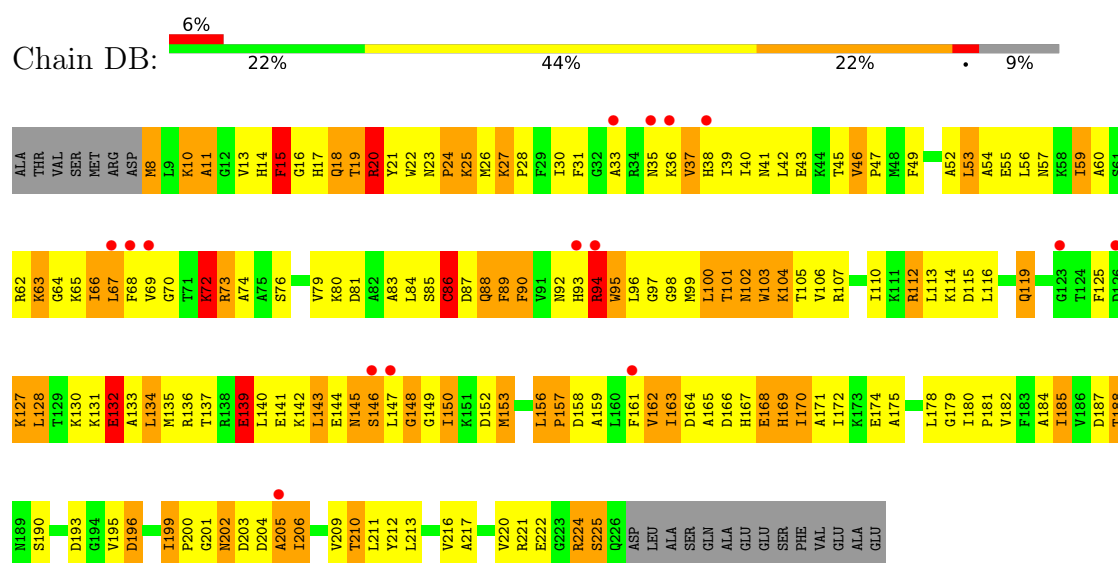


WORLD WIDE
PDB
PROTEIN DATA BANK

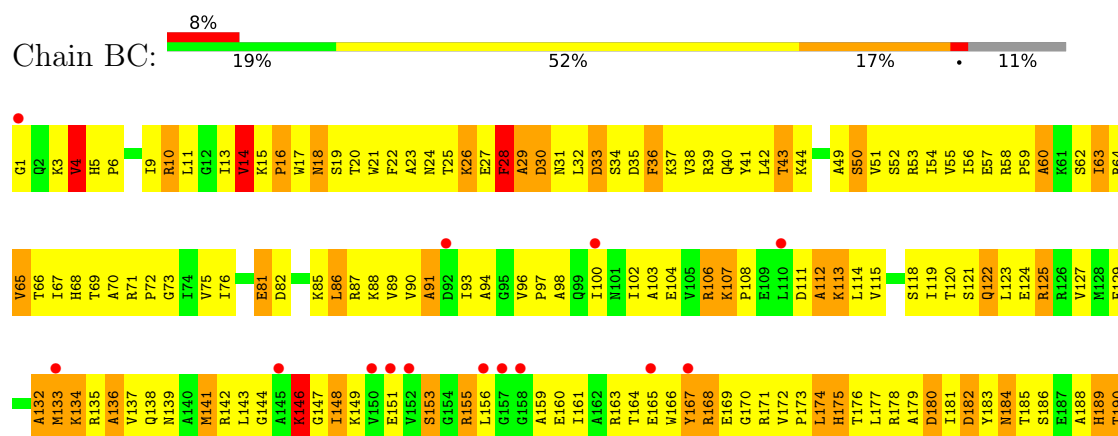
• Molecule 34: 30S RIBOSOMAL PROTEIN S2

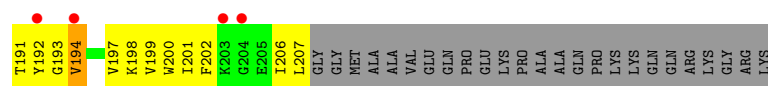


• Molecule 34: 30S RIBOSOMAL PROTEIN S2

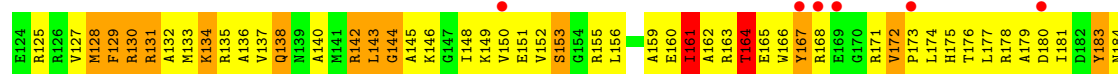
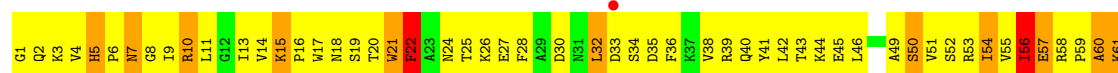
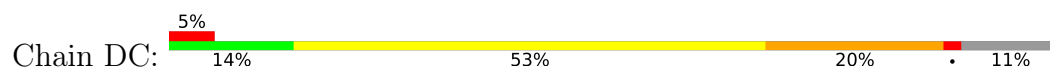


• Molecule 35: 30S RIBOSOMAL PROTEIN S3

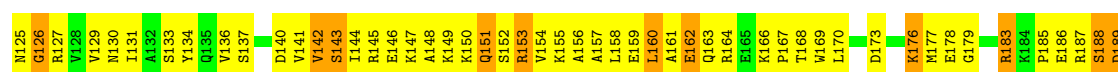
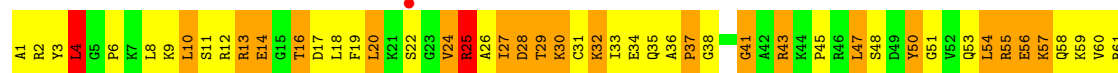




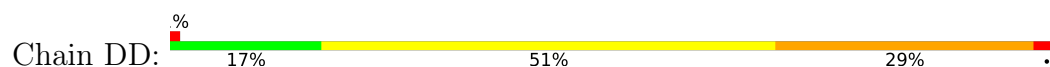
• Molecule 35: 30S RIBOSOMAL PROTEIN S3



• Molecule 36: 30S RIBOSOMAL PROTEIN S4

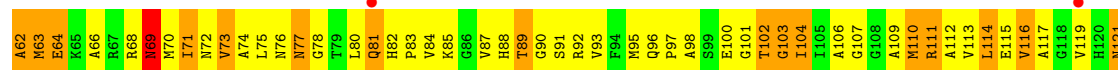
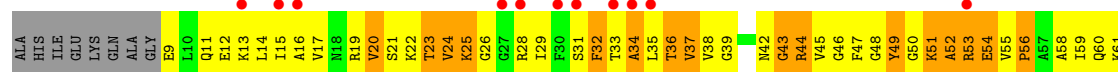
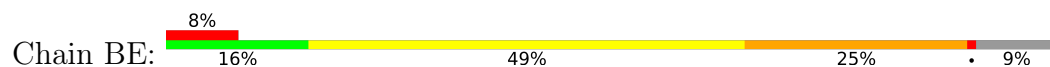


• Molecule 36: 30S RIBOSOMAL PROTEIN S4

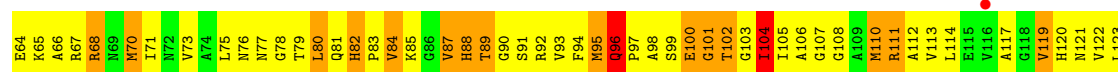
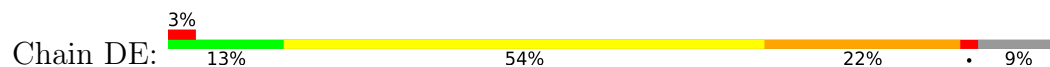




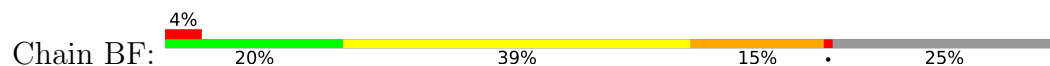
• Molecule 37: 30S RIBOSOMAL PROTEIN S5



• Molecule 37: 30S RIBOSOMAL PROTEIN S5

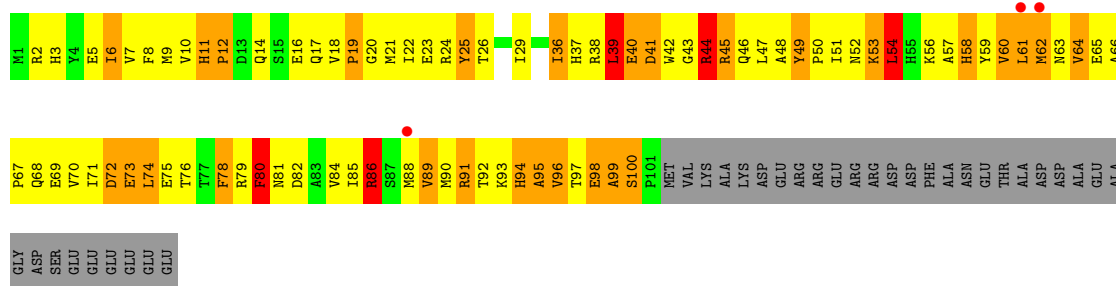


• Molecule 38: 30S RIBOSOMAL PROTEIN S6

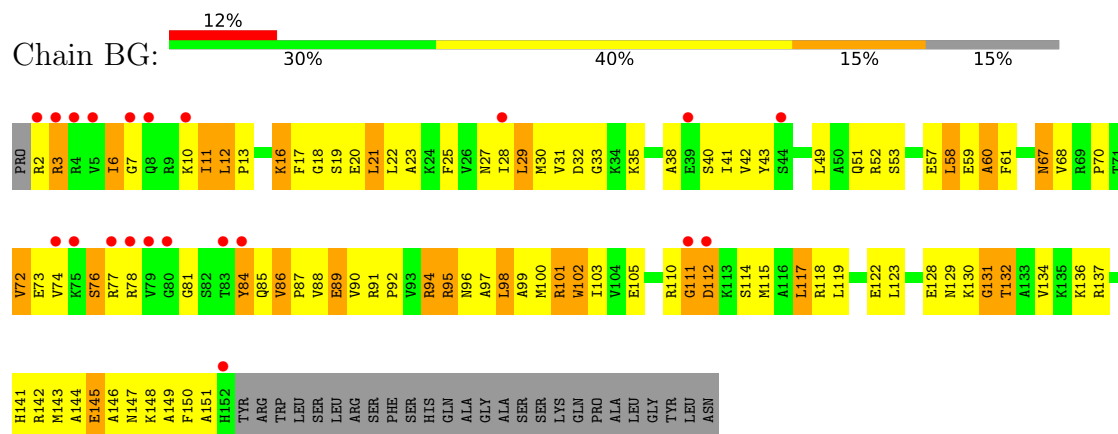


• Molecule 38: 30S RIBOSOMAL PROTEIN S6

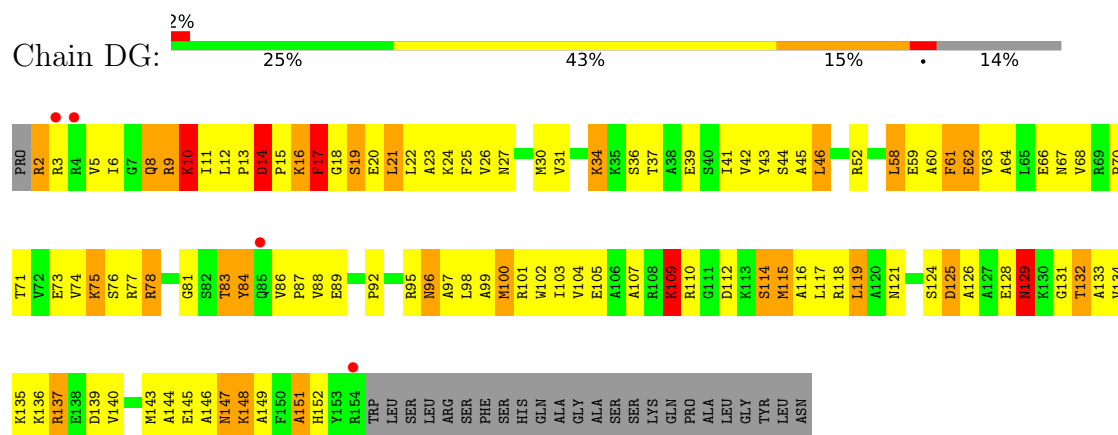




• Molecule 39: 30S RIBOSOMAL PROTEIN S7



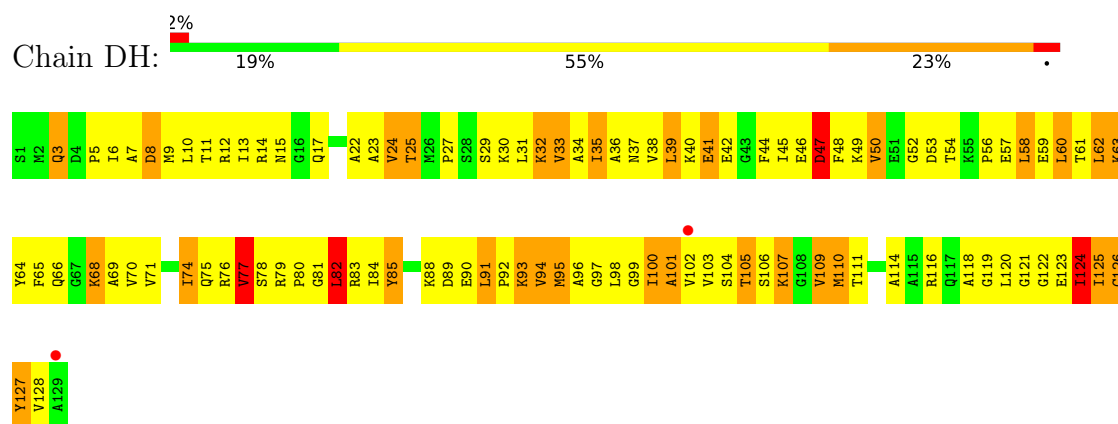
• Molecule 39: 30S RIBOSOMAL PROTEIN S7



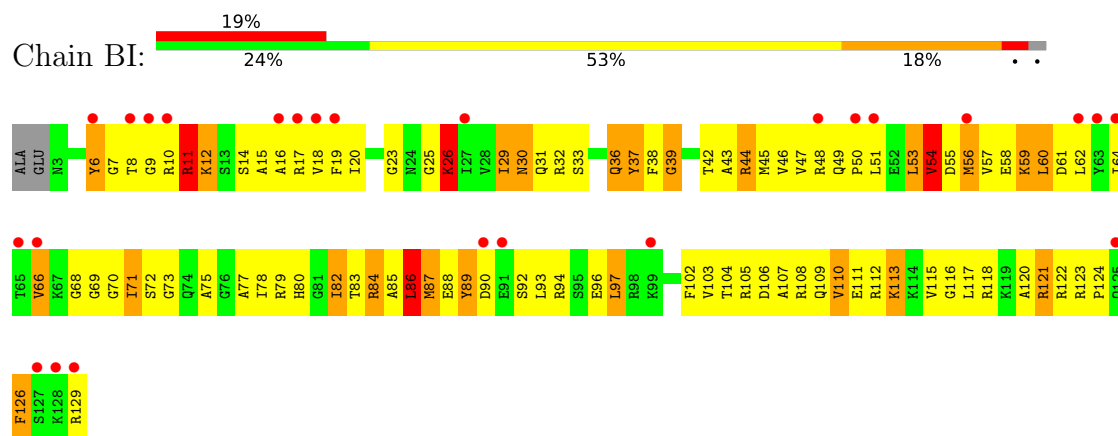
• Molecule 40: 30S RIBOSOMAL PROTEIN S8



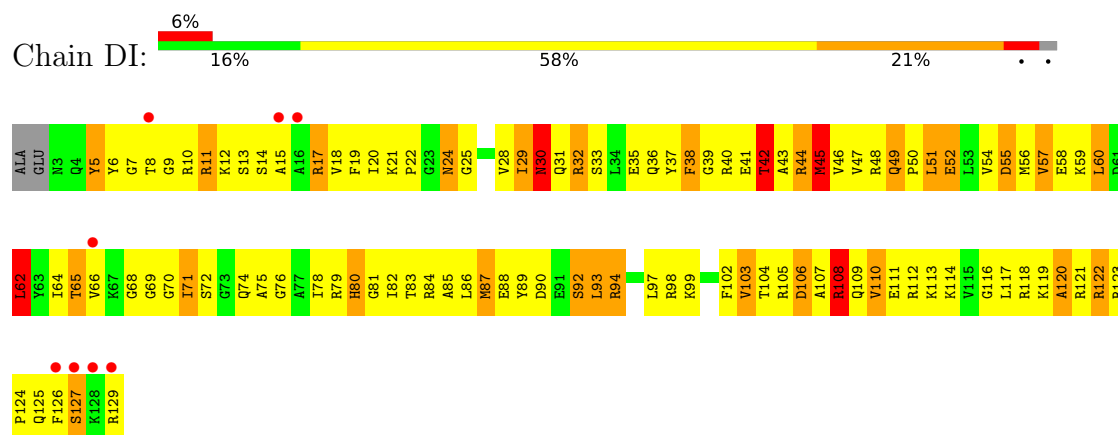
• Molecule 40: 30S RIBOSOMAL PROTEIN S8



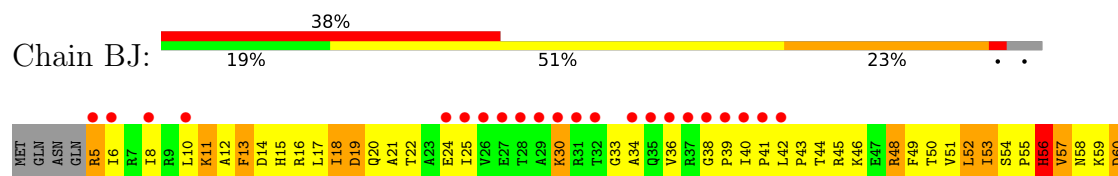
● Molecule 41: 30S RIBOSOMAL PROTEIN S9

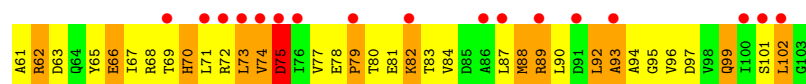


● Molecule 41: 30S RIBOSOMAL PROTEIN S9

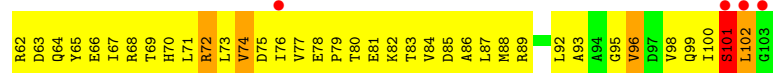
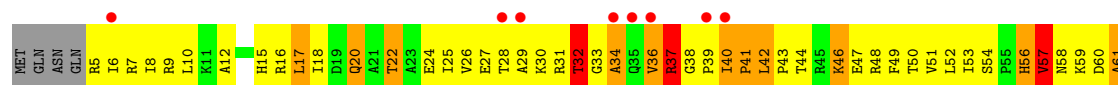
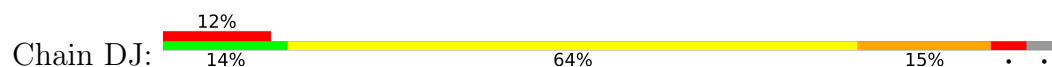


● Molecule 42: 30S RIBOSOMAL PROTEIN S10

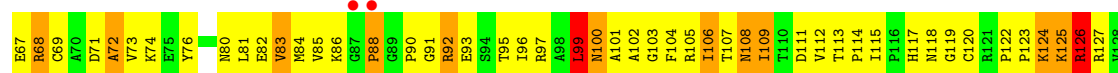
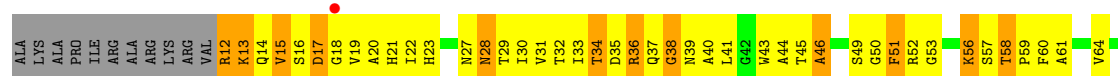




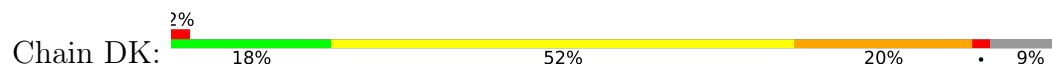
• Molecule 42: 30S RIBOSOMAL PROTEIN S10



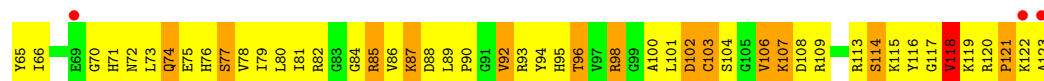
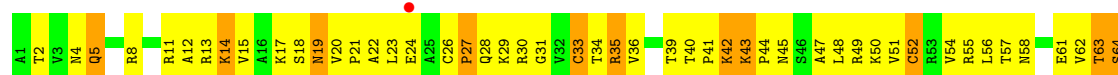
• Molecule 43: 30S RIBOSOMAL PROTEIN S11



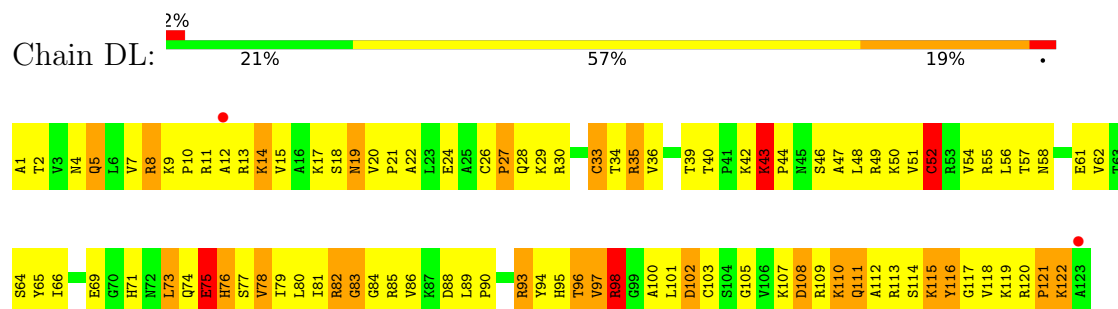
• Molecule 43: 30S RIBOSOMAL PROTEIN S11



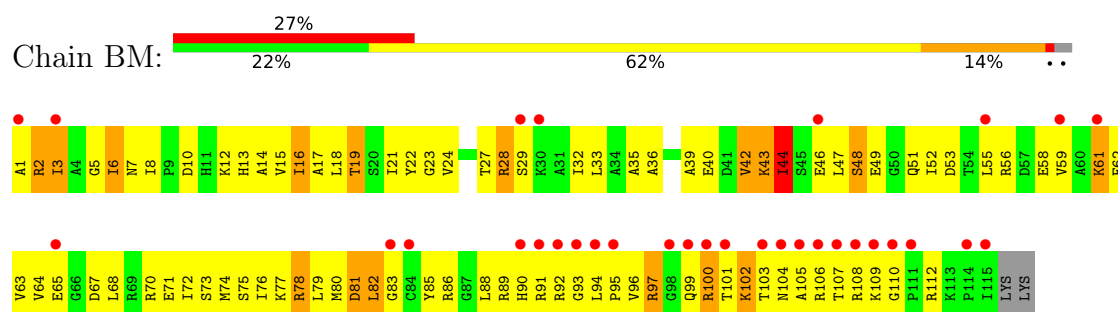
• Molecule 44: 30S RIBOSOMAL PROTEIN S12



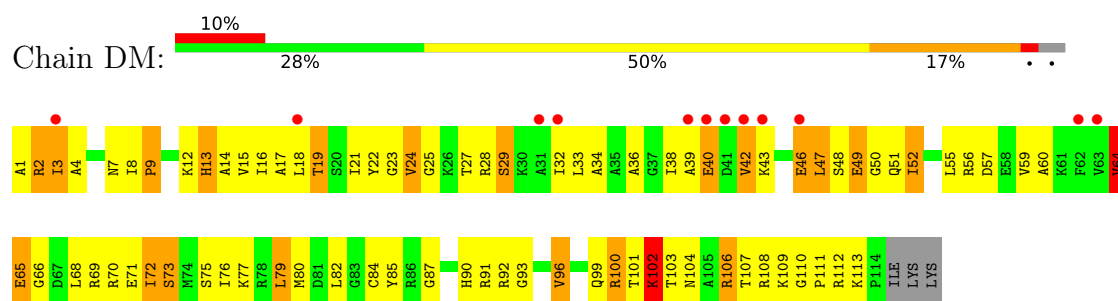
● Molecule 44: 30S RIBOSOMAL PROTEIN S12



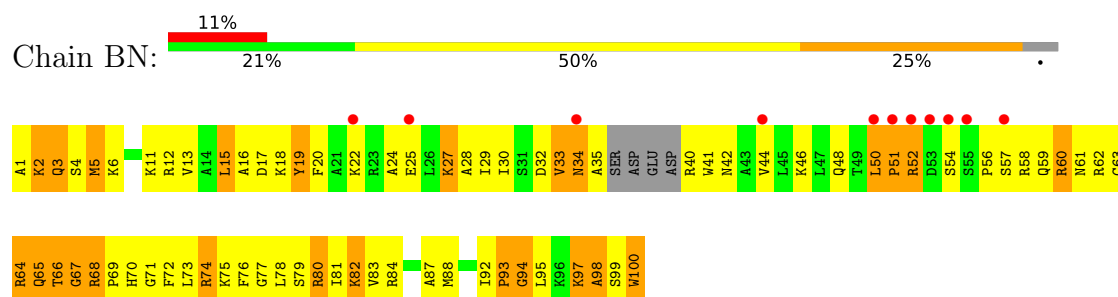
● Molecule 45: 30S RIBOSOMAL PROTEIN S13



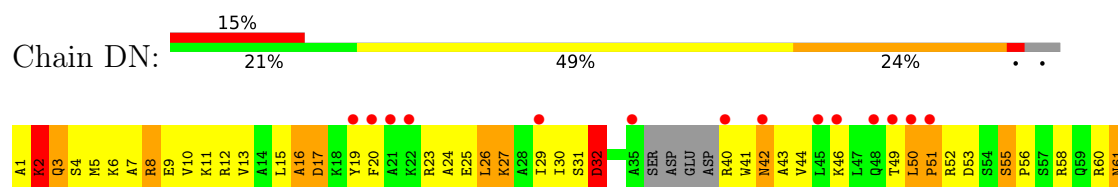
● Molecule 45: 30S RIBOSOMAL PROTEIN S13

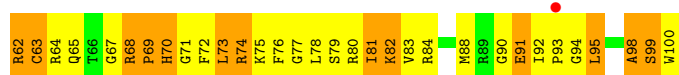


● Molecule 46: 30S RIBOSOMAL PROTEIN S14

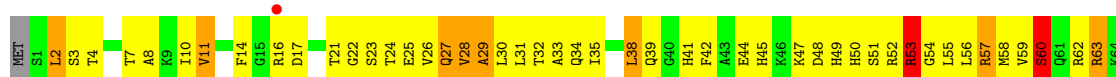


● Molecule 46: 30S RIBOSOMAL PROTEIN S14





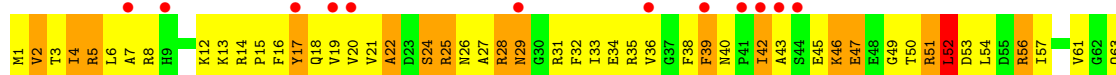
• Molecule 47: 30S RIBOSOMAL PROTEIN S15



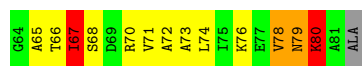
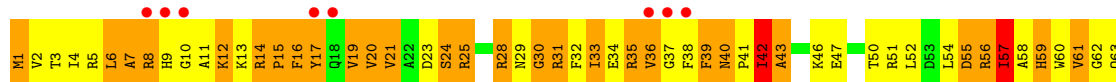
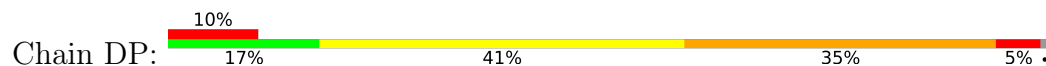
• Molecule 47: 30S RIBOSOMAL PROTEIN S15



• Molecule 48: 30S RIBOSOMAL PROTEIN S16

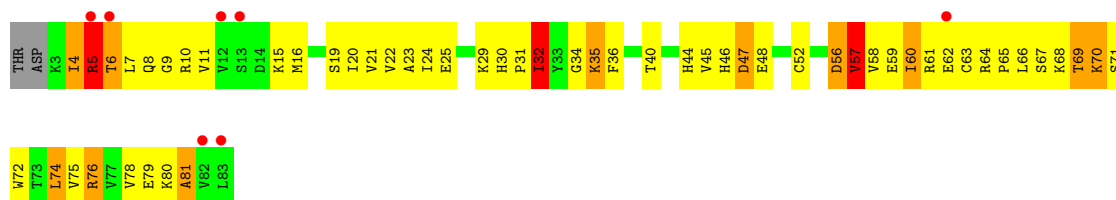


• Molecule 48: 30S RIBOSOMAL PROTEIN S16



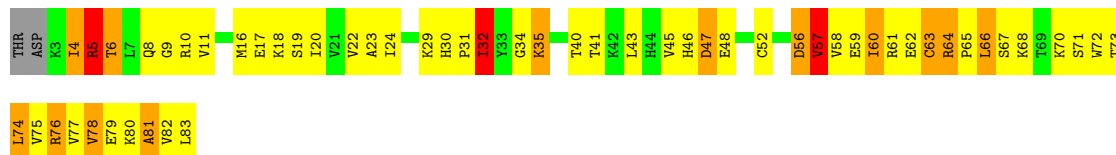
• Molecule 49: 30S RIBOSOMAL PROTEIN S17





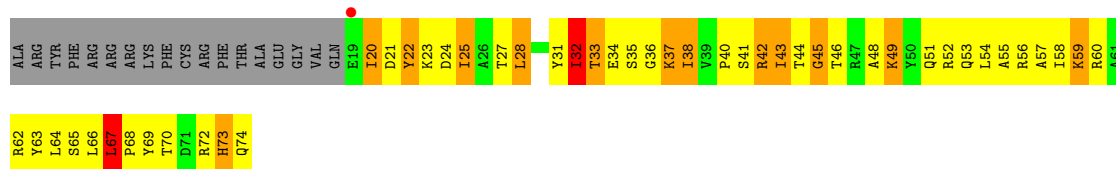
• Molecule 49: 30S RIBOSOMAL PROTEIN S17

Chain DQ: 30% 48% 16% . .



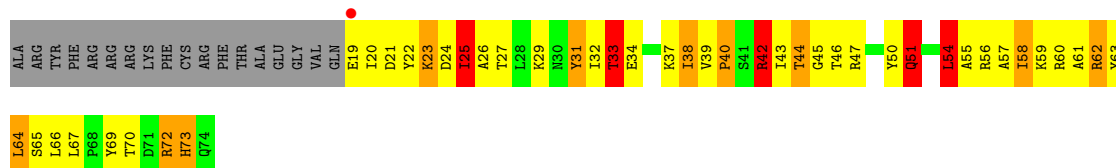
• Molecule 50: 30S RIBOSOMAL PROTEIN S18

Chain BR: 12% 43% 18% . 24%



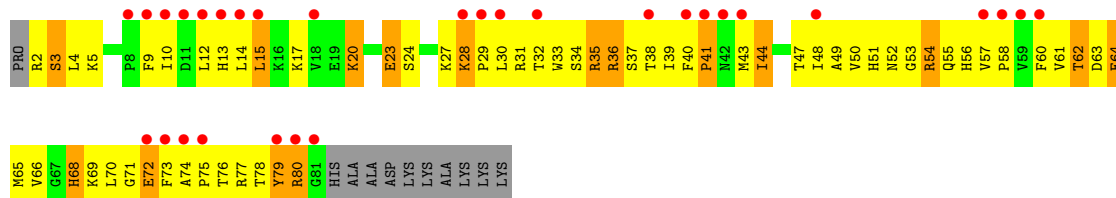
• Molecule 50: 30S RIBOSOMAL PROTEIN S18

Chain DR: 16% 39% 14% 7% 24%



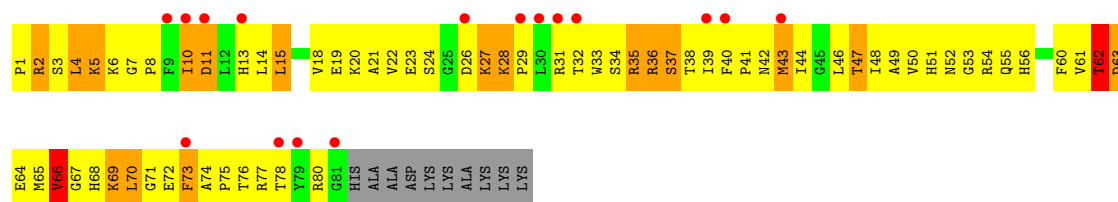
• Molecule 51: 30S RIBOSOMAL PROTEIN S19

Chain BS: 19% 33% 52% 18% 12%



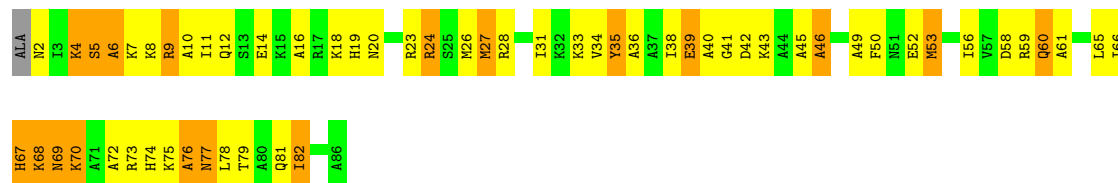
• Molecule 51: 30S RIBOSOMAL PROTEIN S19

Chain DS: 13% 18% 55% 19% . 11%



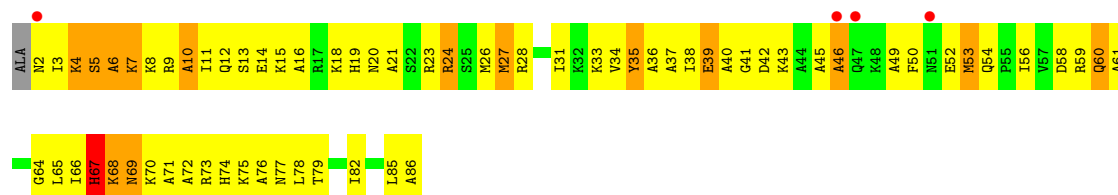
• Molecule 52: 30S RIBOSOMAL PROTEIN S20

Chain BT: 31% 47% 21%



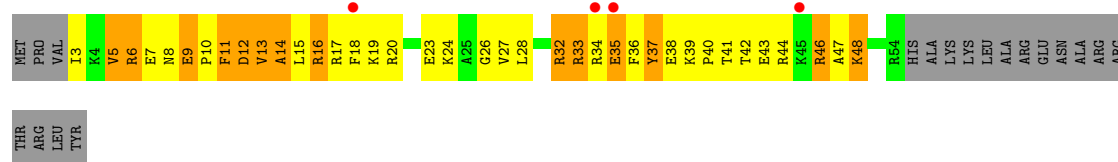
• Molecule 52: 30S RIBOSOMAL PROTEIN S20

Chain DT: 5% 21% 60% 16%



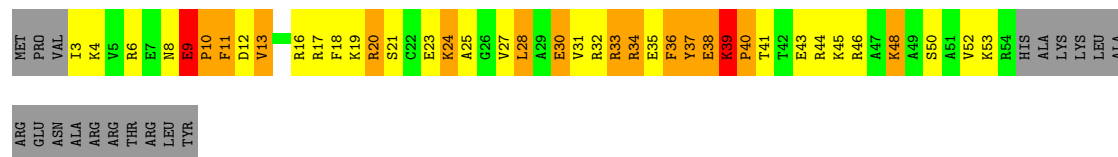
• Molecule 53: 30S RIBOSOMAL PROTEIN S21

Chain BU: 6% 20% 34% 20% 27%



• Molecule 53: 30S RIBOSOMAL PROTEIN S21

Chain DU: 17% 34% 20% 27%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.18Å 380.08Å 736.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.74 49.74 – 3.74	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-3.74) 91.5 (49.74-3.74)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.259 , 0.323 0.250 , 0.308	Depositor DCC
R_{free} test set	5544 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	90.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	284264	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A0	0.41	0/450	0.71	0/599
1	C0	0.48	0/450	0.78	0/599
2	A1	0.42	0/448	0.69	0/594
2	C1	0.46	0/448	0.73	0/594
3	A2	0.46	0/380	0.76	0/498
3	C2	0.46	0/380	0.83	1/498 (0.2%)
4	A3	0.52	0/513	0.79	0/676
4	C3	0.54	0/513	0.91	0/676
5	A4	0.43	0/303	0.69	0/397
5	C4	0.46	0/303	0.78	0/397
6	A5	0.64	0/134	0.72	0/176
7	AA	0.76	3/2803 (0.1%)	1.48	39/4371 (0.9%)
7	CA	0.79	2/2803 (0.1%)	1.52	47/4371 (1.1%)
8	AB	0.82	7/68314 (0.0%)	1.58	975/106569 (0.9%)
8	CB	0.90	15/68314 (0.0%)	1.64	1204/106569 (1.1%)
9	AC	0.51	0/2093	0.81	2/2815 (0.1%)
9	CC	0.55	0/2093	0.82	1/2815 (0.0%)
10	AD	0.45	0/1586	0.72	0/2134
10	CD	0.51	0/1586	0.77	0/2134
11	AE	0.47	0/1571	0.77	0/2113
11	CE	0.50	0/1571	0.75	0/2113
12	AF	0.30	0/1444	0.53	0/1937
12	CF	0.32	0/1444	0.54	0/1937
13	AG	0.38	0/1343	0.62	0/1816
13	CG	0.37	0/1343	0.62	0/1816
14	AH	0.34	0/1122	0.60	0/1515
14	CH	0.37	0/1122	0.64	0/1515
15	AI	0.29	0/1046	0.52	0/1410
15	CI	0.26	0/1045	0.52	0/1406
16	AJ	0.43	0/1136	0.71	0/1531
16	CJ	0.50	0/1136	0.75	0/1531
17	AK	0.50	0/940	0.71	0/1260

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	CK	0.54	0/940	0.72	0/1260
18	AL	0.46	0/1062	0.84	1/1413 (0.1%)
18	CL	0.44	0/1062	0.81	0/1413
19	AM	0.46	0/1093	0.73	0/1460
19	CM	0.48	0/1093	0.77	0/1460
20	AN	0.41	0/1021	0.66	0/1364
20	CN	0.49	0/1021	0.73	0/1364
21	AO	0.38	0/910	0.69	0/1219
21	CO	0.45	0/910	0.77	0/1219
22	AP	0.44	0/929	0.77	1/1242 (0.1%)
22	CP	0.51	0/929	0.81	1/1242 (0.1%)
23	AQ	0.45	0/960	0.71	0/1278
23	CQ	0.53	0/960	0.81	1/1278 (0.1%)
24	AR	0.41	0/829	0.72	0/1107
24	CR	0.46	0/829	0.75	0/1107
25	AS	0.43	0/864	0.74	0/1156
25	CS	0.44	0/864	0.82	0/1156
26	AT	0.45	0/785	0.68	0/1050
26	CT	0.43	0/785	0.69	0/1050
27	AU	0.48	0/788	0.72	0/1053
27	CU	0.42	0/788	0.69	0/1053
28	AV	0.34	0/766	0.52	0/1025
28	CV	0.36	0/766	0.52	0/1025
29	AW	0.42	0/642	0.76	0/848
29	CW	0.45	0/642	0.78	0/848
30	AX	0.47	0/510	0.76	0/677
30	CX	0.40	0/510	0.69	0/677
31	AY	0.36	0/453	0.66	0/605
31	CY	0.34	0/453	0.67	0/605
32	AZ	0.56	0/559	0.94	2/745 (0.3%)
32	CZ	0.68	0/559	0.97	0/745
33	BA	0.70	4/36761 (0.0%)	1.42	407/57346 (0.7%)
33	DA	0.82	4/36762 (0.0%)	1.58	674/57350 (1.2%)
34	BB	0.32	0/1736	0.54	0/2340
34	DB	0.36	0/1736	0.61	0/2340
35	BC	0.33	0/1652	0.53	0/2227
35	DC	0.39	0/1652	0.61	0/2227
36	BD	0.36	0/1665	0.62	0/2227
36	DD	0.46	0/1665	0.68	0/2227
37	BE	0.37	0/1119	0.56	0/1506
37	DE	0.43	0/1119	0.67	0/1506
38	BF	0.40	1/836 (0.1%)	0.57	0/1130
38	DF	0.41	1/836 (0.1%)	0.63	1/1130 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	BG	0.33	0/1188	0.52	0/1593
39	DG	0.38	0/1212	0.58	0/1626
40	BH	0.32	0/989	0.55	0/1326
40	DH	0.44	0/989	0.69	0/1326
41	BI	0.29	0/1034	0.51	0/1375
41	DI	0.33	0/1034	0.64	1/1375 (0.1%)
42	BJ	0.33	1/797 (0.1%)	0.53	0/1079
42	DJ	0.36	1/797 (0.1%)	0.57	0/1079
43	BK	0.35	0/893	0.61	0/1205
43	DK	0.43	0/893	0.70	0/1205
44	BL	0.33	0/969	0.58	0/1300
44	DL	0.42	0/969	0.67	0/1300
45	BM	0.29	0/893	0.50	0/1195
45	DM	0.37	1/885 (0.1%)	0.60	0/1183
46	BN	0.29	0/785	0.51	0/1043
46	DN	0.30	0/785	0.56	0/1043
47	BO	0.33	0/724	0.55	0/966
47	DO	0.38	0/724	0.63	0/966
48	BP	0.30	0/659	0.51	0/884
48	DP	0.49	0/649	0.69	0/872
49	BQ	0.37	0/658	0.59	0/883
49	DQ	0.39	0/666	0.65	0/892
50	BR	0.40	0/463	0.62	0/623
50	DR	0.49	0/463	0.70	0/623
51	BS	0.32	1/653 (0.2%)	0.50	0/879
51	DS	0.37	1/661 (0.2%)	0.62	0/890
52	BT	0.32	0/671	0.49	0/888
52	DT	0.39	0/671	0.58	0/888
53	BU	0.42	0/431	0.56	0/572
53	DU	0.55	0/431	0.73	0/572
All	All	0.73	42/306634 (0.0%)	1.39	3358/458333 (0.7%)

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	C0	0	2
4	C3	0	2
11	CE	0	3
13	AG	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
14	CH	0	1
16	AJ	0	1
16	CJ	0	1
18	AL	0	1
18	CL	0	1
19	AM	0	1
20	CN	0	2
22	AP	0	3
22	CP	0	4
24	CR	0	1
25	CS	0	2
26	CT	0	1
30	CX	0	1
32	AZ	0	1
32	CZ	0	1
All	All	0	30

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	DA	765	G	N9-C4	9.10	1.45	1.38
8	CB	301	G	C3'-O3'	7.66	1.52	1.42
7	CA	87	U	C1'-N1	7.10	1.59	1.48
7	AA	87	U	C1'-N1	6.70	1.58	1.48
33	DA	519	C	C1'-N1	6.38	1.58	1.48

The worst 5 of 3358 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AB	2288	A	C2-N3-C4	-70.19	75.50	110.60
8	CB	2288	A	C2-N3-C4	-69.49	75.85	110.60
8	CB	2288	A	N1-C2-N3	59.84	159.22	129.30
8	AB	2288	A	C6-N1-C2	-58.83	83.30	118.60
8	AB	2288	A	N1-C2-N3	58.75	158.67	129.30

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	AG	109	SER	Peptide
16	AJ	9	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
18	AL	53	GLY	Peptide
19	AM	88	ASN	Peptide
22	AP	46	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	444	0	461	86	0
1	C0	444	0	461	112	0
2	A1	441	0	485	104	0
2	C1	441	0	485	89	0
3	A2	377	0	418	106	0
3	C2	377	0	418	104	0
4	A3	504	0	574	171	0
4	C3	504	0	574	137	0
5	A4	302	0	340	104	0
5	C4	302	0	340	99	0
6	A5	134	0	153	17	0
7	AA	2507	0	1270	277	0
7	CA	2507	0	1270	303	0
8	AB	60995	0	30679	6966	0
8	CB	60995	0	30678	7146	0
9	AC	2054	0	2122	607	0
9	CC	2054	0	2122	625	0
10	AD	1565	0	1616	443	0
10	CD	1565	0	1616	508	0
11	AE	1552	0	1619	432	0
11	CE	1552	0	1619	401	0
12	AF	1420	0	1460	177	0
12	CF	1420	0	1460	216	0
13	AG	1323	0	1374	196	0
13	CG	1323	0	1374	226	0
14	AH	1111	0	1148	160	0
14	CH	1111	0	1148	191	0
15	AI	1032	0	1088	100	0
15	CI	1032	0	1088	131	0
16	AJ	1113	0	1147	293	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	CJ	1113	0	1147	307	0
17	AK	931	0	1000	161	0
17	CK	931	0	1000	159	0
18	AL	1053	0	1129	403	0
18	CL	1053	0	1129	336	0
19	AM	1074	0	1157	276	0
19	CM	1074	0	1157	294	0
20	AN	1008	0	1045	219	0
20	CN	1008	0	1045	248	0
21	AO	900	0	935	206	0
21	CO	900	0	935	247	0
22	AP	917	0	965	248	0
22	CP	917	0	965	243	0
23	AQ	947	0	1022	269	0
23	CQ	947	0	1022	284	0
24	AR	816	0	839	236	0
24	CR	816	0	839	308	0
25	AS	857	0	922	172	0
25	CS	857	0	922	200	0
26	AT	778	0	840	178	0
26	CT	778	0	840	173	0
27	AU	780	0	834	183	0
27	CU	780	0	834	172	0
28	AV	753	0	780	100	0
28	CV	753	0	780	90	0
29	AW	634	0	656	205	0
29	CW	634	0	656	226	0
30	AX	509	0	543	111	0
30	CX	509	0	543	123	0
31	AY	449	0	491	66	0
31	CY	449	0	491	84	0
32	AZ	549	0	552	174	0
32	CZ	549	0	552	152	0
33	BA	32831	0	16522	3630	0
33	DA	32831	0	16521	4106	0
34	BB	1705	0	1732	245	0
34	DB	1705	0	1732	220	0
35	BC	1625	0	1699	214	0
35	DC	1625	0	1699	274	0
36	BD	1643	0	1710	284	0
36	DD	1643	0	1710	280	0
37	BE	1106	0	1148	176	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	DE	1106	0	1148	200	0
38	BF	818	0	808	114	0
38	DF	818	0	808	143	0
39	BG	1175	0	1230	116	0
39	DG	1197	0	1246	145	0
40	BH	979	0	1034	141	0
40	DH	979	0	1034	156	0
41	BI	1022	0	1070	141	0
41	DI	1022	0	1070	158	0
42	BJ	787	0	828	99	0
42	DJ	787	0	828	129	0
43	BK	877	0	887	127	0
43	DK	877	0	887	134	0
44	BL	955	0	1019	145	0
44	DL	955	0	1019	149	0
45	BM	884	0	944	125	0
45	DM	877	0	937	107	0
46	BN	774	0	827	138	0
46	DN	774	0	827	127	0
47	BO	716	0	742	96	0
47	DO	716	0	742	106	0
48	BP	649	0	666	109	0
48	DP	639	0	656	121	0
49	BQ	649	0	691	70	0
49	DQ	657	0	702	91	0
50	BR	456	0	478	75	0
50	DR	456	0	478	100	0
51	BS	638	0	665	112	0
51	DS	645	0	675	97	0
52	BT	665	0	714	85	0
52	DT	665	0	714	91	0
53	BU	426	0	449	81	0
53	DU	426	0	449	67	0
54	AB	109	0	0	0	0
54	AE	1	0	0	0	0
54	BA	58	0	0	0	0
54	BN	1	0	0	0	0
54	BT	1	0	0	0	0
54	CB	109	0	0	0	0
54	CC	1	0	0	0	0
54	CL	1	0	0	0	0
54	DA	61	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	DN	1	0	0	0	0
55	A2	2	0	0	2	0
55	AB	489	0	0	65	0
55	AC	3	0	0	1	0
55	AD	1	0	0	0	0
55	AE	3	0	0	2	0
55	AJ	2	0	0	2	0
55	AL	3	0	0	1	0
55	BA	284	0	0	26	0
55	BE	3	0	0	0	0
55	BI	2	0	0	0	0
55	BK	1	0	0	0	0
55	BL	2	0	0	0	0
55	BN	3	0	0	0	0
55	BP	1	0	0	0	0
55	BT	2	0	0	0	0
55	C0	1	0	0	0	0
55	C2	2	0	0	0	0
55	CB	485	0	0	65	0
55	CC	3	0	0	0	0
55	CD	1	0	0	0	0
55	CE	1	0	0	0	0
55	CJ	2	0	0	0	0
55	CK	1	0	0	0	0
55	CL	5	0	0	1	0
55	CN	3	0	0	2	0
55	CP	1	0	0	0	0
55	CQ	1	0	0	0	0
55	CT	2	0	0	0	0
55	CU	1	0	0	2	0
55	DA	293	0	0	18	0
55	DD	1	0	0	0	0
55	DE	2	0	0	0	0
55	DG	1	0	0	0	0
55	DL	4	0	0	0	0
55	DN	2	0	0	1	0
55	DP	1	0	0	0	0
55	DT	3	0	0	2	0
All	All	284264	0	190919	37666	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 80.

The worst 5 of 37666 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)
8:CB:2822:G:OP2	20:CN:2:ARG:HB3	1.29	1.26
33:DA:585:G:H5'	33:DA:585:G:C8	1.76	1.21
33:DA:235:C:H2'	33:DA:236:A:C8	1.77	1.19
1:C0:27:LEU:HG	8:CB:2886:A:C6	1.77	1.19
23:CQ:49:ARG:HG3	24:CR:77:PHE:CZ	1.79	1.18

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	54/56 (96%)	26 (48%)	13 (24%)	15 (28%)	0	0
1	C0	54/56 (96%)	24 (44%)	12 (22%)	18 (33%)	0	0
2	A1	52/54 (96%)	18 (35%)	15 (29%)	19 (36%)	0	0
2	C1	52/54 (96%)	18 (35%)	12 (23%)	22 (42%)	0	0
3	A2	44/46 (96%)	15 (34%)	16 (36%)	13 (30%)	0	0
3	C2	44/46 (96%)	16 (36%)	16 (36%)	12 (27%)	0	0
4	A3	62/64 (97%)	24 (39%)	17 (27%)	21 (34%)	0	0
4	C3	62/64 (97%)	29 (47%)	20 (32%)	13 (21%)	0	1
5	A4	36/38 (95%)	14 (39%)	13 (36%)	9 (25%)	0	0
5	C4	36/38 (95%)	9 (25%)	16 (44%)	11 (31%)	0	0
6	A5	14/16 (88%)	6 (43%)	5 (36%)	3 (21%)	0	1
9	AC	266/273 (97%)	101 (38%)	67 (25%)	98 (37%)	0	0
9	CC	266/273 (97%)	101 (38%)	70 (26%)	95 (36%)	0	0
10	AD	207/209 (99%)	80 (39%)	56 (27%)	71 (34%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CD	207/209 (99%)	72 (35%)	65 (31%)	70 (34%)	0	0
11	AE	199/201 (99%)	76 (38%)	58 (29%)	65 (33%)	0	0
11	CE	199/201 (99%)	71 (36%)	63 (32%)	65 (33%)	0	0
12	AF	176/178 (99%)	95 (54%)	48 (27%)	33 (19%)	0	2
12	CF	176/178 (99%)	95 (54%)	45 (26%)	36 (20%)	0	1
13	AG	174/176 (99%)	98 (56%)	42 (24%)	34 (20%)	0	2
13	CG	174/176 (99%)	89 (51%)	52 (30%)	33 (19%)	0	2
14	AH	147/149 (99%)	94 (64%)	34 (23%)	19 (13%)	0	5
14	CH	147/149 (99%)	74 (50%)	39 (26%)	34 (23%)	0	0
15	AI	139/141 (99%)	92 (66%)	33 (24%)	14 (10%)	0	8
15	CI	137/141 (97%)	87 (64%)	32 (23%)	18 (13%)	0	4
16	AJ	139/142 (98%)	60 (43%)	34 (24%)	45 (32%)	0	0
16	CJ	139/142 (98%)	57 (41%)	37 (27%)	45 (32%)	0	0
17	AK	120/123 (98%)	67 (56%)	30 (25%)	23 (19%)	0	2
17	CK	120/123 (98%)	66 (55%)	29 (24%)	25 (21%)	0	1
18	AL	142/144 (99%)	53 (37%)	37 (26%)	52 (37%)	0	0
18	CL	142/144 (99%)	54 (38%)	39 (28%)	49 (34%)	0	0
19	AM	134/136 (98%)	51 (38%)	46 (34%)	37 (28%)	0	0
19	CM	134/136 (98%)	55 (41%)	45 (34%)	34 (25%)	0	0
20	AN	125/127 (98%)	55 (44%)	43 (34%)	27 (22%)	0	1
20	CN	125/127 (98%)	55 (44%)	44 (35%)	26 (21%)	0	1
21	AO	115/117 (98%)	49 (43%)	40 (35%)	26 (23%)	0	0
21	CO	115/117 (98%)	46 (40%)	41 (36%)	28 (24%)	0	0
22	AP	112/114 (98%)	48 (43%)	30 (27%)	34 (30%)	0	0
22	CP	112/114 (98%)	48 (43%)	31 (28%)	33 (30%)	0	0
23	AQ	115/117 (98%)	62 (54%)	26 (23%)	27 (24%)	0	0
23	CQ	115/117 (98%)	57 (50%)	30 (26%)	28 (24%)	0	0
24	AR	101/103 (98%)	31 (31%)	25 (25%)	45 (45%)	0	0
24	CR	101/103 (98%)	37 (37%)	23 (23%)	41 (41%)	0	0
25	AS	108/110 (98%)	58 (54%)	24 (22%)	26 (24%)	0	0
25	CS	108/110 (98%)	52 (48%)	29 (27%)	27 (25%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	AT	98/100 (98%)	42 (43%)	33 (34%)	23 (24%)	0	0
26	CT	98/100 (98%)	42 (43%)	33 (34%)	23 (24%)	0	0
27	AU	101/103 (98%)	40 (40%)	36 (36%)	25 (25%)	0	0
27	CU	101/103 (98%)	38 (38%)	31 (31%)	32 (32%)	0	0
28	AV	92/94 (98%)	58 (63%)	21 (23%)	13 (14%)	0	4
28	CV	92/94 (98%)	57 (62%)	21 (23%)	14 (15%)	0	3
29	AW	82/84 (98%)	20 (24%)	28 (34%)	34 (42%)	0	0
29	CW	82/84 (98%)	17 (21%)	29 (35%)	36 (44%)	0	0
30	AX	61/63 (97%)	17 (28%)	25 (41%)	19 (31%)	0	0
30	CX	61/63 (97%)	26 (43%)	22 (36%)	13 (21%)	0	1
31	AY	56/58 (97%)	25 (45%)	17 (30%)	14 (25%)	0	0
31	CY	56/58 (97%)	26 (46%)	19 (34%)	11 (20%)	0	2
32	AZ	68/70 (97%)	30 (44%)	19 (28%)	19 (28%)	0	0
32	CZ	68/70 (97%)	34 (50%)	21 (31%)	13 (19%)	0	2
34	BB	217/240 (90%)	128 (59%)	65 (30%)	24 (11%)	0	6
34	DB	217/240 (90%)	124 (57%)	59 (27%)	34 (16%)	0	3
35	BC	205/232 (88%)	116 (57%)	59 (29%)	30 (15%)	0	3
35	DC	205/232 (88%)	112 (55%)	67 (33%)	26 (13%)	0	5
36	BD	203/205 (99%)	120 (59%)	57 (28%)	26 (13%)	0	5
36	DD	203/205 (99%)	116 (57%)	50 (25%)	37 (18%)	0	2
37	BE	149/166 (90%)	94 (63%)	33 (22%)	22 (15%)	0	3
37	DE	149/166 (90%)	77 (52%)	49 (33%)	23 (15%)	0	3
38	BF	99/135 (73%)	62 (63%)	25 (25%)	12 (12%)	0	5
38	DF	99/135 (73%)	56 (57%)	22 (22%)	21 (21%)	0	1
39	BG	149/178 (84%)	100 (67%)	34 (23%)	15 (10%)	0	8
39	DG	151/178 (85%)	94 (62%)	43 (28%)	14 (9%)	0	10
40	BH	127/129 (98%)	73 (58%)	42 (33%)	12 (9%)	0	10
40	DH	127/129 (98%)	70 (55%)	34 (27%)	23 (18%)	0	2
41	BI	125/129 (97%)	78 (62%)	35 (28%)	12 (10%)	0	9
41	DI	125/129 (97%)	73 (58%)	32 (26%)	20 (16%)	0	3
42	BJ	97/103 (94%)	59 (61%)	23 (24%)	15 (16%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	DJ	97/103 (94%)	62 (64%)	24 (25%)	11 (11%)	0	6
43	BK	115/128 (90%)	69 (60%)	31 (27%)	15 (13%)	0	4
43	DK	115/128 (90%)	73 (64%)	30 (26%)	12 (10%)	0	8
44	BL	121/123 (98%)	67 (55%)	37 (31%)	17 (14%)	0	4
44	DL	121/123 (98%)	73 (60%)	32 (26%)	16 (13%)	0	4
45	BM	113/117 (97%)	70 (62%)	32 (28%)	11 (10%)	0	9
45	DM	112/117 (96%)	78 (70%)	20 (18%)	14 (12%)	0	5
46	BN	92/100 (92%)	58 (63%)	18 (20%)	16 (17%)	0	2
46	DN	92/100 (92%)	55 (60%)	18 (20%)	19 (21%)	0	1
47	BO	86/89 (97%)	51 (59%)	26 (30%)	9 (10%)	0	7
47	DO	86/89 (97%)	51 (59%)	26 (30%)	9 (10%)	0	7
48	BP	80/82 (98%)	43 (54%)	22 (28%)	15 (19%)	0	2
48	DP	79/82 (96%)	38 (48%)	24 (30%)	17 (22%)	0	1
49	BQ	79/83 (95%)	53 (67%)	15 (19%)	11 (14%)	0	4
49	DQ	79/83 (95%)	53 (67%)	16 (20%)	10 (13%)	0	5
50	BR	54/74 (73%)	25 (46%)	19 (35%)	10 (18%)	0	2
50	DR	54/74 (73%)	24 (44%)	19 (35%)	11 (20%)	0	1
51	BS	78/91 (86%)	52 (67%)	20 (26%)	6 (8%)	1	14
51	DS	79/91 (87%)	50 (63%)	20 (25%)	9 (11%)	0	6
52	BT	83/86 (96%)	51 (61%)	20 (24%)	12 (14%)	0	4
52	DT	83/86 (96%)	52 (63%)	20 (24%)	11 (13%)	0	4
53	BU	50/71 (70%)	26 (52%)	14 (28%)	10 (20%)	0	1
53	DU	50/71 (70%)	13 (26%)	27 (54%)	10 (20%)	0	1
All	All	11307/11918 (95%)	5696 (50%)	3156 (28%)	2455 (22%)	0	1

5 of 2455 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A0	19	ASP
1	A0	21	LEU
1	A0	25	THR
1	A0	29	VAL
1	A0	36	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	47/47 (100%)	34 (72%)	13 (28%)	0	2
1	C0	47/47 (100%)	39 (83%)	8 (17%)	2	13
2	A1	48/48 (100%)	40 (83%)	8 (17%)	2	14
2	C1	48/48 (100%)	36 (75%)	12 (25%)	0	4
3	A2	38/38 (100%)	18 (47%)	20 (53%)	0	0
3	C2	38/38 (100%)	20 (53%)	18 (47%)	0	0
4	A3	51/51 (100%)	34 (67%)	17 (33%)	0	1
4	C3	51/51 (100%)	30 (59%)	21 (41%)	0	0
5	A4	34/34 (100%)	21 (62%)	13 (38%)	0	0
5	C4	34/34 (100%)	19 (56%)	15 (44%)	0	0
6	A5	15/15 (100%)	12 (80%)	3 (20%)	1	8
9	AC	213/218 (98%)	150 (70%)	63 (30%)	0	2
9	CC	213/218 (98%)	147 (69%)	66 (31%)	0	2
10	AD	164/164 (100%)	112 (68%)	52 (32%)	0	1
10	CD	164/164 (100%)	111 (68%)	53 (32%)	0	1
11	AE	165/165 (100%)	120 (73%)	45 (27%)	0	3
11	CE	165/165 (100%)	118 (72%)	47 (28%)	0	2
12	AF	149/149 (100%)	129 (87%)	20 (13%)	4	22
12	CF	149/149 (100%)	131 (88%)	18 (12%)	5	25
13	AG	137/137 (100%)	103 (75%)	34 (25%)	0	4
13	CG	137/137 (100%)	106 (77%)	31 (23%)	1	6
14	AH	114/114 (100%)	87 (76%)	27 (24%)	1	5
14	CH	114/114 (100%)	85 (75%)	29 (25%)	0	4
15	AI	109/109 (100%)	93 (85%)	16 (15%)	3	19
15	CI	109/109 (100%)	98 (90%)	11 (10%)	7	32
16	AJ	114/116 (98%)	74 (65%)	40 (35%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
16	CJ	114/116 (98%)	76 (67%)	38 (33%)	0	1	
17	AK	102/104 (98%)	68 (67%)	34 (33%)	0	1	
17	CK	102/104 (98%)	65 (64%)	37 (36%)	0	0	
18	AL	103/103 (100%)	61 (59%)	42 (41%)	0	0	
18	CL	103/103 (100%)	63 (61%)	40 (39%)	0	0	
19	AM	109/109 (100%)	59 (54%)	50 (46%)	0	0	
19	CM	109/109 (100%)	66 (61%)	43 (39%)	0	0	
20	AN	103/103 (100%)	74 (72%)	29 (28%)	0	2	
20	CN	103/103 (100%)	69 (67%)	34 (33%)	0	1	
21	AO	87/87 (100%)	64 (74%)	23 (26%)	0	3	
21	CO	87/87 (100%)	69 (79%)	18 (21%)	1	7	
22	AP	99/99 (100%)	79 (80%)	20 (20%)	1	8	
22	CP	99/99 (100%)	81 (82%)	18 (18%)	1	10	
23	AQ	89/89 (100%)	58 (65%)	31 (35%)	0	1	
23	CQ	89/89 (100%)	55 (62%)	34 (38%)	0	0	
24	AR	84/84 (100%)	59 (70%)	25 (30%)	0	2	
24	CR	84/84 (100%)	52 (62%)	32 (38%)	0	0	
25	AS	93/93 (100%)	66 (71%)	27 (29%)	0	2	
25	CS	93/93 (100%)	66 (71%)	27 (29%)	0	2	
26	AT	83/84 (99%)	60 (72%)	23 (28%)	0	2	
26	CT	83/84 (99%)	59 (71%)	24 (29%)	0	2	
27	AU	83/84 (99%)	63 (76%)	20 (24%)	0	5	
27	CU	83/84 (99%)	63 (76%)	20 (24%)	0	5	
28	AV	78/78 (100%)	63 (81%)	15 (19%)	1	9	
28	CV	78/78 (100%)	62 (80%)	16 (20%)	1	7	
29	AW	62/62 (100%)	42 (68%)	20 (32%)	0	1	
29	CW	62/62 (100%)	39 (63%)	23 (37%)	0	0	
30	AX	55/55 (100%)	40 (73%)	15 (27%)	0	3	
30	CX	55/55 (100%)	38 (69%)	17 (31%)	0	2	
31	AY	48/48 (100%)	33 (69%)	15 (31%)	0	1	
31	CY	48/48 (100%)	32 (67%)	16 (33%)	0	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	AZ	62/62 (100%)	44 (71%)	18 (29%)	0	2
32	CZ	62/62 (100%)	43 (69%)	19 (31%)	0	2
34	BB	180/198 (91%)	143 (79%)	37 (21%)	1	7
34	DB	180/198 (91%)	140 (78%)	40 (22%)	1	6
35	BC	170/189 (90%)	142 (84%)	28 (16%)	2	14
35	DC	170/189 (90%)	130 (76%)	40 (24%)	1	5
36	BD	172/172 (100%)	137 (80%)	35 (20%)	1	8
36	DD	172/172 (100%)	126 (73%)	46 (27%)	0	3
37	BE	113/125 (90%)	86 (76%)	27 (24%)	0	5
37	DE	113/125 (90%)	82 (73%)	31 (27%)	0	3
38	BF	87/116 (75%)	71 (82%)	16 (18%)	1	10
38	DF	87/116 (75%)	67 (77%)	20 (23%)	1	6
39	BG	123/146 (84%)	105 (85%)	18 (15%)	3	19
39	DG	125/146 (86%)	95 (76%)	30 (24%)	0	5
40	BH	104/104 (100%)	78 (75%)	26 (25%)	0	4
40	DH	104/104 (100%)	78 (75%)	26 (25%)	0	4
41	BI	105/106 (99%)	81 (77%)	24 (23%)	1	6
41	DI	105/106 (99%)	82 (78%)	23 (22%)	1	6
42	BJ	86/90 (96%)	68 (79%)	18 (21%)	1	7
42	DJ	86/90 (96%)	71 (83%)	15 (17%)	2	12
43	BK	90/98 (92%)	68 (76%)	22 (24%)	0	5
43	DK	90/98 (92%)	61 (68%)	29 (32%)	0	1
44	BL	103/103 (100%)	82 (80%)	21 (20%)	1	7
44	DL	103/103 (100%)	79 (77%)	24 (23%)	1	5
45	BM	92/95 (97%)	76 (83%)	16 (17%)	2	12
45	DM	91/95 (96%)	74 (81%)	17 (19%)	1	10
46	BN	79/83 (95%)	66 (84%)	13 (16%)	2	14
46	DN	79/83 (95%)	64 (81%)	15 (19%)	1	9
47	BO	76/77 (99%)	63 (83%)	13 (17%)	2	13
47	DO	76/77 (99%)	60 (79%)	16 (21%)	1	7
48	BP	65/65 (100%)	54 (83%)	11 (17%)	2	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	DP	65/65 (100%)	42 (65%)	23 (35%)	0	0
49	BQ	74/77 (96%)	65 (88%)	9 (12%)	5	25
49	DQ	75/77 (97%)	63 (84%)	12 (16%)	2	16
50	BR	48/64 (75%)	39 (81%)	9 (19%)	1	10
50	DR	48/64 (75%)	35 (73%)	13 (27%)	0	3
51	BS	70/78 (90%)	59 (84%)	11 (16%)	2	17
51	DS	71/78 (91%)	53 (75%)	18 (25%)	0	4
52	BT	65/65 (100%)	55 (85%)	10 (15%)	2	17
52	DT	65/65 (100%)	57 (88%)	8 (12%)	4	25
53	BU	44/61 (72%)	39 (89%)	5 (11%)	5	28
53	DU	44/61 (72%)	31 (70%)	13 (30%)	0	2
All	All	9356/9707 (96%)	6965 (74%)	2391 (26%)	0	4

5 of 2391 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	CV	70	ILE
47	DO	17	ASP
31	CY	43	ILE
28	CV	60	VAL
37	DE	111	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 328 such sidechains are listed below:

Mol	Chain	Res	Type
22	CP	74	GLN
39	DG	8	GLN
24	CR	43	ASN
32	CZ	6	HIS
43	DK	28	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	BA	1528/1542 (99%)	618 (40%)	204 (13%)
33	DA	1529/1542 (99%)	663 (43%)	211 (13%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	AA	116/120 (96%)	40 (34%)	12 (10%)
7	CA	117/120 (97%)	48 (41%)	15 (12%)
8	AB	2839/2904 (97%)	1140 (40%)	396 (13%)
8	CB	2838/2904 (97%)	1137 (40%)	386 (13%)
All	All	8967/9132 (98%)	3646 (40%)	1224 (13%)

5 of 3646 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	AA	6	G
7	AA	7	G
7	AA	9	G
7	AA	12	C
7	AA	13	G

5 of 1224 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	CB	2223	G
33	DA	965	U
8	CB	2434	A
8	CB	2214	C
33	DA	238	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 343 ligands modelled in this entry, 343 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	BA	1
15	CI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1045:C	O3'	1046:A	P	4.69
1	CI	72:THR	C	73:PRO	N	4.33

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A0	56/56 (100%)	0.32	6 (10%) 6 5	109, 149, 271, 317	0
1	C0	56/56 (100%)	0.27	6 (10%) 6 5	97, 120, 190, 244	0
2	A1	54/54 (100%)	0.84	10 (18%) 1 1	124, 143, 239, 296	0
2	C1	54/54 (100%)	1.06	10 (18%) 1 1	92, 113, 223, 254	0
3	A2	46/46 (100%)	0.40	3 (6%) 18 14	74, 92, 165, 271	0
3	C2	46/46 (100%)	0.03	4 (8%) 10 8	68, 103, 198, 264	0
4	A3	64/64 (100%)	0.05	5 (7%) 13 11	80, 106, 228, 309	0
4	C3	64/64 (100%)	-0.10	2 (3%) 49 40	69, 99, 174, 229	0
5	A4	38/38 (100%)	1.03	9 (23%) 0 0	115, 135, 250, 284	0
5	C4	38/38 (100%)	0.87	7 (18%) 1 1	124, 144, 238, 298	0
6	A5	16/16 (100%)	-0.34	0 100 100	73, 108, 197, 216	0
7	AA	117/120 (97%)	-0.60	0 100 100	78, 127, 174, 316	0
7	CA	117/120 (97%)	-0.65	1 (0%) 84 81	71, 126, 170, 285	0
8	AB	2841/2904 (97%)	-0.46	34 (1%) 79 74	57, 105, 213, 373	0
8	CB	2841/2904 (97%)	-0.63	11 (0%) 92 91	41, 89, 202, 421	0
9	AC	268/273 (98%)	0.05	14 (5%) 27 24	71, 107, 196, 257	0
9	CC	268/273 (98%)	-0.09	11 (4%) 37 31	63, 91, 165, 248	0
10	AD	209/209 (100%)	0.18	9 (4%) 35 30	12, 127, 226, 325	0
10	CD	209/209 (100%)	-0.06	9 (4%) 35 30	11, 94, 186, 271	0
11	AE	201/201 (100%)	0.14	11 (5%) 25 21	92, 120, 206, 299	0
11	CE	201/201 (100%)	0.28	22 (10%) 5 5	88, 117, 224, 290	0
12	AF	178/178 (100%)	0.25	12 (6%) 17 14	121, 170, 253, 334	0
12	CF	178/178 (100%)	0.18	6 (3%) 45 38	92, 155, 224, 286	0
13	AG	176/176 (100%)	0.07	15 (8%) 10 9	100, 137, 207, 246	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	CG	176/176 (100%)	0.43	22 (12%) 3 4	88, 138, 222, 271	0
14	AH	149/149 (100%)	1.68	52 (34%) 0 0	71, 314, 427, 456	0
14	CH	149/149 (100%)	0.44	11 (7%) 14 12	107, 147, 233, 274	0
15	AI	141/141 (100%)	1.86	47 (33%) 0 0	155, 233, 307, 356	0
15	CI	141/141 (100%)	2.99	64 (45%) 0 0	219, 343, 422, 470	0
16	AJ	141/142 (99%)	0.06	6 (4%) 35 30	105, 130, 217, 267	0
16	CJ	141/142 (99%)	0.16	5 (3%) 44 37	104, 121, 207, 250	0
17	AK	122/123 (99%)	-0.18	1 (0%) 86 83	81, 109, 162, 234	0
17	CK	122/123 (99%)	-0.45	0 100 100	80, 94, 127, 208	0
18	AL	144/144 (100%)	1.07	21 (14%) 2 3	94, 138, 281, 363	0
18	CL	144/144 (100%)	0.63	23 (15%) 1 2	83, 128, 275, 315	0
19	AM	136/136 (100%)	0.06	12 (8%) 10 8	105, 126, 222, 268	0
19	CM	136/136 (100%)	-0.01	7 (5%) 28 24	77, 108, 223, 279	0
20	AN	127/127 (100%)	0.01	5 (3%) 39 33	96, 114, 200, 251	0
20	CN	127/127 (100%)	-0.13	6 (4%) 31 27	58, 78, 155, 257	0
21	AO	117/117 (100%)	0.21	7 (5%) 21 17	107, 162, 236, 299	0
21	CO	117/117 (100%)	0.39	14 (11%) 4 4	52, 118, 211, 255	0
22	AP	114/114 (100%)	-0.10	2 (1%) 68 63	85, 123, 219, 281	0
22	CP	114/114 (100%)	-0.24	1 (0%) 84 81	77, 96, 196, 257	0
23	AQ	117/117 (100%)	-0.30	0 100 100	70, 106, 152, 203	0
23	CQ	117/117 (100%)	-0.36	1 (0%) 84 81	70, 93, 148, 225	0
24	AR	103/103 (100%)	0.34	3 (2%) 51 43	105, 145, 250, 346	0
24	CR	103/103 (100%)	0.30	9 (8%) 10 8	87, 132, 229, 286	0
25	AS	110/110 (100%)	0.10	3 (2%) 54 46	77, 106, 167, 279	0
25	CS	110/110 (100%)	-0.09	3 (2%) 54 46	49, 85, 152, 211	0
26	AT	100/100 (100%)	0.04	4 (4%) 38 32	94, 130, 222, 250	0
26	CT	100/100 (100%)	0.39	8 (8%) 12 10	85, 120, 248, 278	0
27	AU	103/103 (100%)	1.05	23 (22%) 0 0	90, 140, 235, 264	0
27	CU	103/103 (100%)	0.92	23 (22%) 0 0	118, 162, 256, 281	0
28	AV	94/94 (100%)	-0.24	3 (3%) 47 39	86, 136, 209, 234	0
28	CV	94/94 (100%)	-0.20	3 (3%) 47 39	87, 124, 194, 215	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	AW	84/84 (100%)	1.16	16 (19%) 1 1	116, 147, 244, 330	0
29	CW	84/84 (100%)	0.69	12 (14%) 2 3	111, 136, 238, 275	0
30	AX	63/63 (100%)	-0.18	2 (3%) 47 39	84, 130, 208, 247	0
30	CX	63/63 (100%)	0.36	10 (15%) 1 2	86, 150, 233, 320	0
31	AY	58/58 (100%)	1.53	16 (27%) 0 0	116, 143, 272, 279	0
31	CY	58/58 (100%)	1.02	8 (13%) 2 3	126, 138, 240, 249	0
32	AZ	70/70 (100%)	0.17	5 (7%) 16 12	66, 104, 170, 258	0
32	CZ	70/70 (100%)	0.03	4 (5%) 23 19	70, 91, 169, 255	0
33	BA	1530/1542 (99%)	-0.36	19 (1%) 79 74	70, 137, 279, 497	0
33	DA	1530/1542 (99%)	-0.55	10 (0%) 87 85	45, 111, 224, 368	0
34	BB	219/240 (91%)	0.01	9 (4%) 37 31	94, 175, 269, 316	0
34	DB	219/240 (91%)	0.17	15 (6%) 17 13	108, 159, 243, 292	0
35	BC	207/232 (89%)	0.17	18 (8%) 10 8	87, 169, 255, 315	0
35	DC	207/232 (89%)	-0.03	12 (5%) 23 19	113, 140, 207, 226	0
36	BD	205/205 (100%)	-0.25	1 (0%) 91 89	61, 139, 230, 325	0
36	DD	205/205 (100%)	-0.27	2 (0%) 82 78	71, 102, 169, 227	0
37	BE	151/166 (90%)	0.28	14 (9%) 8 7	75, 156, 254, 336	0
37	DE	151/166 (90%)	-0.07	5 (3%) 46 39	56, 99, 174, 250	0
38	BF	101/135 (74%)	-0.05	6 (5%) 22 18	57, 140, 224, 279	0
38	DF	101/135 (74%)	-0.04	3 (2%) 50 41	110, 137, 200, 247	0
39	BG	151/178 (84%)	0.65	21 (13%) 2 3	94, 206, 288, 333	0
39	DG	153/178 (85%)	0.09	4 (2%) 56 48	44, 144, 206, 228	0
40	BH	129/129 (100%)	0.26	8 (6%) 20 16	76, 157, 231, 297	0
40	DH	129/129 (100%)	-0.27	2 (1%) 72 66	70, 98, 166, 216	0
41	BI	127/129 (98%)	0.86	25 (19%) 1 1	90, 194, 271, 307	0
41	DI	127/129 (98%)	0.34	8 (6%) 20 15	103, 165, 231, 281	0
42	BJ	99/103 (96%)	1.83	39 (39%) 0 0	131, 254, 373, 423	0
42	DJ	99/103 (96%)	0.52	12 (12%) 4 4	130, 173, 223, 237	0
43	BK	117/128 (91%)	-0.10	3 (2%) 56 48	54, 128, 245, 290	0
43	DK	117/128 (91%)	-0.08	2 (1%) 70 64	69, 100, 165, 222	0
44	BL	123/123 (100%)	-0.05	4 (3%) 46 39	50, 138, 215, 332	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DL	123/123 (100%)	-0.27	2 (1%) 72 66	64, 95, 150, 211	0
45	BM	115/117 (98%)	1.35	32 (27%) 0 0	144, 252, 315, 344	0
45	DM	114/117 (97%)	0.55	12 (10%) 6 5	113, 171, 221, 288	0
46	BN	96/100 (96%)	0.53	11 (11%) 4 5	85, 188, 308, 367	0
46	DN	96/100 (96%)	0.50	15 (15%) 2 2	105, 153, 250, 295	0
47	BO	88/89 (98%)	-0.12	1 (1%) 80 76	67, 133, 213, 255	0
47	DO	88/89 (98%)	-0.42	0 100 100	73, 105, 170, 201	0
48	BP	82/82 (100%)	0.98	15 (18%) 1 1	90, 168, 269, 347	0
48	DP	81/82 (98%)	0.48	8 (9%) 7 6	69, 93, 145, 202	0
49	BQ	81/83 (97%)	0.63	7 (8%) 10 9	101, 180, 266, 301	0
49	DQ	81/83 (97%)	-0.07	0 100 100	65, 109, 172, 212	0
50	BR	56/74 (75%)	-0.19	1 (1%) 68 63	66, 117, 216, 283	0
50	DR	56/74 (75%)	0.43	1 (1%) 68 63	74, 103, 172, 253	0
51	BS	80/91 (87%)	1.75	30 (37%) 0 0	152, 267, 315, 366	0
51	DS	81/91 (89%)	0.85	16 (19%) 1 1	122, 182, 230, 249	0
52	BT	85/86 (98%)	-0.11	0 100 100	76, 155, 224, 256	0
52	DT	85/86 (98%)	0.14	4 (4%) 31 27	79, 97, 185, 219	0
53	BU	52/71 (73%)	0.06	4 (7%) 13 11	91, 171, 256, 300	0
53	DU	52/71 (73%)	-0.41	0 100 100	95, 140, 201, 249	0
All	All	20487/21050 (97%)	-0.07	1080 (5%) 26 23	11, 121, 254, 497	0

The worst 5 of 1080 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	CI	98	GLY	29.4
15	CI	83	ALA	21.7
15	CI	137	LEU	18.5
15	AI	70	THR	16.5
18	AL	98	ALA	16.4

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(\AA^2)	Q<0.9
54	MG	BA	4056	1/1	0.70	0.28	81,81,81,81	0
54	MG	BA	4023	1/1	0.75	0.13	63,63,63,63	1
54	MG	BA	4053	1/1	0.76	0.48	109,109,109,109	0
54	MG	DA	1612	1/1	0.76	0.44	81,81,81,81	0
54	MG	BA	4054	1/1	0.79	1.05	90,90,90,90	0
54	MG	CB	3108	1/1	0.81	0.55	53,53,53,53	1
54	MG	DA	1610	1/1	0.82	0.17	48,48,48,48	0
54	MG	CB	3080	1/1	0.82	0.36	55,55,55,55	1
54	MG	CB	3038	1/1	0.83	0.15	58,58,58,58	0
54	MG	DA	1608	1/1	0.84	0.30	41,41,41,41	0
54	MG	AB	4050	1/1	0.85	0.33	49,49,49,49	0
54	MG	DA	1626	1/1	0.85	0.24	11,11,11,11	1
54	MG	BA	4028	1/1	0.86	0.20	61,61,61,61	0
54	MG	BA	4002	1/1	0.88	0.46	86,86,86,86	0
54	MG	CB	3094	1/1	0.89	0.14	16,16,16,16	0
54	MG	BT	101	1/1	0.89	0.19	27,27,27,27	0
54	MG	BA	4037	1/1	0.90	0.11	58,58,58,58	0
54	MG	AB	4096	1/1	0.90	0.31	46,46,46,46	0
54	MG	CB	3107	1/1	0.90	0.19	22,22,22,22	0
54	MG	AB	4013	1/1	0.90	0.15	46,46,46,46	0
54	MG	DA	1619	1/1	0.91	0.47	64,64,64,64	0
54	MG	BA	4013	1/1	0.91	0.25	73,73,73,73	0
54	MG	DA	1651	1/1	0.91	0.19	56,56,56,56	0
54	MG	AB	4069	1/1	0.92	0.16	51,51,51,51	0
54	MG	BA	4025	1/1	0.92	0.15	37,37,37,37	0
54	MG	AB	4047	1/1	0.92	0.19	48,48,48,48	0
54	MG	AB	4098	1/1	0.92	0.54	37,37,37,37	0
54	MG	AB	4042	1/1	0.92	0.10	90,90,90,90	0
54	MG	AB	4062	1/1	0.92	0.10	30,30,30,30	0
54	MG	BA	4014	1/1	0.92	0.11	44,44,44,44	0
54	MG	BA	4017	1/1	0.92	0.15	42,42,42,42	0
54	MG	BA	4021	1/1	0.92	0.28	28,28,28,28	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	1632	1/1	0.92	0.45	90,90,90,90	0
54	MG	DA	1634	1/1	0.92	0.32	110,110,110,110	0
54	MG	DA	1636	1/1	0.92	0.07	43,43,43,43	0
54	MG	CB	3050	1/1	0.92	0.08	45,45,45,45	0
54	MG	DA	1659	1/1	0.92	0.25	85,85,85,85	0
54	MG	CB	3076	1/1	0.93	0.28	15,15,15,15	0
54	MG	BA	4027	1/1	0.93	0.29	68,68,68,68	0
54	MG	DA	1624	1/1	0.93	0.38	57,57,57,57	0
54	MG	AB	4023	1/1	0.93	0.20	66,66,66,66	0
54	MG	DA	1628	1/1	0.93	0.27	33,33,33,33	1
54	MG	BA	4057	1/1	0.93	0.08	29,29,29,29	0
54	MG	AB	4036	1/1	0.93	0.09	12,12,12,12	0
54	MG	DA	1607	1/1	0.93	0.20	54,54,54,54	0
54	MG	BA	4043	1/1	0.93	0.59	25,25,25,25	0
54	MG	BA	4011	1/1	0.93	0.07	56,56,56,56	0
54	MG	BA	4036	1/1	0.94	0.09	5,5,5,5	0
54	MG	CB	3010	1/1	0.94	0.16	30,30,30,30	0
54	MG	CB	3029	1/1	0.94	0.15	39,39,39,39	0
54	MG	AB	4078	1/1	0.94	0.10	35,35,35,35	0
54	MG	DA	1613	1/1	0.94	0.20	62,62,62,62	0
54	MG	AB	4088	1/1	0.94	0.12	24,24,24,24	0
54	MG	BA	4046	1/1	0.94	0.26	62,62,62,62	0
54	MG	DA	1625	1/1	0.94	0.17	37,37,37,37	1
54	MG	CB	3079	1/1	0.94	0.16	54,54,54,54	0
54	MG	BA	4020	1/1	0.94	0.37	77,77,77,77	0
54	MG	AB	4109	1/1	0.94	0.16	34,34,34,34	0
54	MG	CB	3099	1/1	0.94	0.36	43,43,43,43	0
54	MG	BA	4029	1/1	0.94	0.10	44,44,44,44	0
54	MG	DA	1640	1/1	0.94	0.19	17,17,17,17	0
54	MG	DA	1644	1/1	0.94	0.34	53,53,53,53	0
54	MG	BA	4034	1/1	0.94	0.18	48,48,48,48	0
54	MG	CL	201	1/1	0.94	0.08	43,43,43,43	0
54	MG	CB	3100	1/1	0.95	0.12	43,43,43,43	0
54	MG	CB	3106	1/1	0.95	0.19	20,20,20,20	0
54	MG	AB	4092	1/1	0.95	0.64	27,27,27,27	1
54	MG	AB	4095	1/1	0.95	0.15	47,47,47,47	0
54	MG	AB	4045	1/1	0.95	0.08	51,51,51,51	0
54	MG	BA	4024	1/1	0.95	0.21	32,32,32,32	1
54	MG	AB	4022	1/1	0.95	0.27	11,11,11,11	0
54	MG	DA	1609	1/1	0.95	0.15	56,56,56,56	0
54	MG	CB	3009	1/1	0.95	0.11	13,13,13,13	0
54	MG	DA	1611	1/1	0.95	0.18	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	4026	1/1	0.95	0.15	75,75,75,75	0
54	MG	CB	3026	1/1	0.95	0.11	10,10,10,10	0
54	MG	AB	4107	1/1	0.95	0.10	6,6,6,6	0
54	MG	CB	3037	1/1	0.95	0.14	10,10,10,10	0
54	MG	AB	4007	1/1	0.95	0.11	37,37,37,37	0
54	MG	CB	3043	1/1	0.95	0.06	69,69,69,69	0
54	MG	CB	3049	1/1	0.95	0.17	30,30,30,30	1
54	MG	DA	1630	1/1	0.95	0.07	29,29,29,29	0
54	MG	AB	4031	1/1	0.95	0.19	56,56,56,56	0
54	MG	BA	4008	1/1	0.95	0.12	21,21,21,21	0
54	MG	AB	4034	1/1	0.95	0.25	51,51,51,51	0
54	MG	AB	4012	1/1	0.95	0.09	44,44,44,44	0
54	MG	CB	3092	1/1	0.95	0.12	7,7,7,7	0
54	MG	AB	4003	1/1	0.95	0.14	26,26,26,26	0
54	MG	DA	1653	1/1	0.95	0.15	21,21,21,21	0
54	MG	AB	4090	1/1	0.95	0.20	37,37,37,37	0
54	MG	CB	3095	1/1	0.96	0.15	22,22,22,22	0
54	MG	AB	4009	1/1	0.96	0.11	58,58,58,58	0
54	MG	AB	4061	1/1	0.96	0.15	35,35,35,35	0
54	MG	CB	3103	1/1	0.96	0.28	10,10,10,10	0
54	MG	AB	4046	1/1	0.96	0.07	26,26,26,26	0
54	MG	CB	3005	1/1	0.96	0.12	26,26,26,26	0
54	MG	CB	3006	1/1	0.96	0.09	19,19,19,19	0
54	MG	AB	4093	1/1	0.96	0.08	4,4,4,4	0
54	MG	BA	4012	1/1	0.96	0.20	54,54,54,54	0
54	MG	CB	3014	1/1	0.96	0.20	33,33,33,33	0
54	MG	BA	4033	1/1	0.96	0.22	90,90,90,90	0
54	MG	AB	4064	1/1	0.96	0.12	43,43,43,43	0
54	MG	BA	4035	1/1	0.96	0.45	30,30,30,30	0
54	MG	AB	4025	1/1	0.96	0.22	129,129,129,129	0
54	MG	CB	3040	1/1	0.96	0.27	46,46,46,46	0
54	MG	DA	1618	1/1	0.96	0.12	30,30,30,30	0
54	MG	AB	4097	1/1	0.96	0.21	17,17,17,17	0
54	MG	BA	4038	1/1	0.96	0.10	50,50,50,50	0
54	MG	BA	4039	1/1	0.96	0.23	31,31,31,31	0
54	MG	CB	3070	1/1	0.96	0.36	33,33,33,33	0
54	MG	CB	3071	1/1	0.96	0.23	52,52,52,52	0
54	MG	CB	3074	1/1	0.96	0.10	33,33,33,33	0
54	MG	AB	4077	1/1	0.96	0.28	28,28,28,28	0
54	MG	CB	3077	1/1	0.96	0.13	76,76,76,76	0
54	MG	CB	3078	1/1	0.96	0.12	57,57,57,57	0
54	MG	BA	4044	1/1	0.96	0.16	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	1641	1/1	0.96	0.06	63,63,63,63	0
54	MG	AB	4101	1/1	0.96	0.12	25,25,25,25	0
54	MG	CB	3087	1/1	0.96	0.28	25,25,25,25	0
54	MG	AB	4103	1/1	0.96	0.20	13,13,13,13	0
54	MG	AB	4048	1/1	0.96	0.19	22,22,22,22	0
54	MG	DN	201	1/1	0.96	0.12	48,48,48,48	0
54	MG	CB	3066	1/1	0.97	0.14	45,45,45,45	0
54	MG	CB	3068	1/1	0.97	0.11	59,59,59,59	0
54	MG	BA	4042	1/1	0.97	0.19	69,69,69,69	0
54	MG	AB	4057	1/1	0.97	0.23	49,49,49,49	0
54	MG	CB	3072	1/1	0.97	0.19	42,42,42,42	0
54	MG	AB	4021	1/1	0.97	0.12	33,33,33,33	0
54	MG	AB	4094	1/1	0.97	0.06	15,15,15,15	0
54	MG	BA	4048	1/1	0.97	0.05	73,73,73,73	0
54	MG	BA	4049	1/1	0.97	0.17	100,100,100,100	0
54	MG	BA	4050	1/1	0.97	0.11	51,51,51,51	0
54	MG	BA	4052	1/1	0.97	0.11	33,33,33,33	0
54	MG	CB	3081	1/1	0.97	0.15	10,10,10,10	0
54	MG	CB	3082	1/1	0.97	0.20	17,17,17,17	0
54	MG	BA	4018	1/1	0.97	0.09	64,64,64,64	0
54	MG	CB	3089	1/1	0.97	0.14	38,38,38,38	0
54	MG	AB	4027	1/1	0.97	0.15	22,22,22,22	0
54	MG	CB	3093	1/1	0.97	0.17	3,3,3,3	0
54	MG	AB	4029	1/1	0.97	0.19	55,55,55,55	0
54	MG	AB	4067	1/1	0.97	0.07	31,31,31,31	0
54	MG	BN	201	1/1	0.97	0.20	61,61,61,61	0
54	MG	AB	4008	1/1	0.97	0.08	38,38,38,38	0
54	MG	AB	4099	1/1	0.97	0.21	12,12,12,12	1
54	MG	CB	3104	1/1	0.97	0.39	6,6,6,6	0
54	MG	AB	4075	1/1	0.97	0.17	41,41,41,41	0
54	MG	AB	4001	1/1	0.97	0.07	5,5,5,5	0
54	MG	AB	4024	1/1	0.97	0.13	54,54,54,54	0
54	MG	AB	4108	1/1	0.97	0.14	9,9,9,9	0
54	MG	DA	1602	1/1	0.97	0.09	13,13,13,13	0
54	MG	DA	1605	1/1	0.97	0.13	76,76,76,76	0
54	MG	DA	1606	1/1	0.97	0.09	18,18,18,18	0
54	MG	CB	3020	1/1	0.97	0.16	8,8,8,8	0
54	MG	CB	3021	1/1	0.97	0.05	22,22,22,22	0
54	MG	CB	3022	1/1	0.97	0.07	21,21,21,21	0
54	MG	CB	3025	1/1	0.97	0.12	27,27,27,27	0
54	MG	BA	4030	1/1	0.97	0.41	34,34,34,34	0
54	MG	AB	4083	1/1	0.97	0.14	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CB	3030	1/1	0.97	0.19	17,17,17,17	0
54	MG	CB	3032	1/1	0.97	0.25	52,52,52,52	0
54	MG	CB	3033	1/1	0.97	0.12	33,33,33,33	0
54	MG	CB	3034	1/1	0.97	0.09	7,7,7,7	0
54	MG	BA	4001	1/1	0.97	0.14	69,69,69,69	0
54	MG	AB	4084	1/1	0.97	0.08	21,21,21,21	0
54	MG	DA	1627	1/1	0.97	0.16	51,51,51,51	0
54	MG	BA	4004	1/1	0.97	0.12	34,34,34,34	0
54	MG	DA	1629	1/1	0.97	0.29	52,52,52,52	0
54	MG	CB	3041	1/1	0.97	0.18	19,19,19,19	0
54	MG	AB	4053	1/1	0.97	0.11	14,14,14,14	0
54	MG	AB	4055	1/1	0.97	0.08	68,68,68,68	0
54	MG	AB	4091	1/1	0.97	0.31	34,34,34,34	0
54	MG	DA	1637	1/1	0.97	0.20	109,109,109,109	0
54	MG	CB	3052	1/1	0.97	0.22	43,43,43,43	0
54	MG	CB	3053	1/1	0.97	0.11	5,5,5,5	0
54	MG	CB	3059	1/1	0.97	0.10	12,12,12,12	0
54	MG	DA	1645	1/1	0.97	0.13	56,56,56,56	0
54	MG	DA	1647	1/1	0.97	0.15	30,30,30,30	0
54	MG	CB	3060	1/1	0.97	0.16	78,78,78,78	0
54	MG	CB	3061	1/1	0.97	0.09	31,31,31,31	0
54	MG	CB	3063	1/1	0.97	0.12	11,11,11,11	0
54	MG	DA	1660	1/1	0.97	0.23	14,14,14,14	0
54	MG	DA	1661	1/1	0.97	0.10	13,13,13,13	0
54	MG	CB	3065	1/1	0.97	0.08	26,26,26,26	0
54	MG	CB	3011	1/1	0.98	0.11	33,33,33,33	0
54	MG	CB	3012	1/1	0.98	0.08	10,10,10,10	0
54	MG	AB	4018	1/1	0.98	0.06	32,32,32,32	0
54	MG	CB	3015	1/1	0.98	0.17	9,9,9,9	0
54	MG	CB	3084	1/1	0.98	0.12	24,24,24,24	0
54	MG	CB	3018	1/1	0.98	0.16	25,25,25,25	0
54	MG	CB	3019	1/1	0.98	0.15	11,11,11,11	0
54	MG	CB	3090	1/1	0.98	0.09	67,67,67,67	0
54	MG	CB	3091	1/1	0.98	0.12	42,42,42,42	0
54	MG	BA	4032	1/1	0.98	0.13	27,27,27,27	0
54	MG	AB	4080	1/1	0.98	0.11	17,17,17,17	0
54	MG	AE	301	1/1	0.98	0.20	10,10,10,10	0
54	MG	CB	3023	1/1	0.98	0.14	7,7,7,7	0
54	MG	CB	3096	1/1	0.98	0.24	38,38,38,38	0
54	MG	CB	3097	1/1	0.98	0.06	9,9,9,9	0
54	MG	CB	3098	1/1	0.98	0.06	7,7,7,7	0
54	MG	CB	3024	1/1	0.98	0.07	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AB	4037	1/1	0.98	0.09	25,25,25,25	0
54	MG	CB	3102	1/1	0.98	0.12	17,17,17,17	0
54	MG	AB	4038	1/1	0.98	0.09	30,30,30,30	0
54	MG	AB	4085	1/1	0.98	0.24	53,53,53,53	0
54	MG	BA	4006	1/1	0.98	0.14	42,42,42,42	0
54	MG	BA	4007	1/1	0.98	0.52	81,81,81,81	0
54	MG	BA	4040	1/1	0.98	0.08	49,49,49,49	0
54	MG	CB	3109	1/1	0.98	0.08	16,16,16,16	0
54	MG	BA	4041	1/1	0.98	0.09	54,54,54,54	0
54	MG	DA	1601	1/1	0.98	0.07	28,28,28,28	0
54	MG	CB	3035	1/1	0.98	0.11	20,20,20,20	0
54	MG	DA	1604	1/1	0.98	0.15	35,35,35,35	0
54	MG	CB	3036	1/1	0.98	0.30	19,19,19,19	0
54	MG	AB	4087	1/1	0.98	0.14	38,38,38,38	0
54	MG	AB	4058	1/1	0.98	0.12	20,20,20,20	0
54	MG	CB	3039	1/1	0.98	0.13	27,27,27,27	0
54	MG	AB	4059	1/1	0.98	0.11	55,55,55,55	0
54	MG	AB	4005	1/1	0.98	0.16	11,11,11,11	0
54	MG	CB	3042	1/1	0.98	0.12	18,18,18,18	0
54	MG	BA	4047	1/1	0.98	0.09	29,29,29,29	0
54	MG	CB	3045	1/1	0.98	0.25	67,67,67,67	0
54	MG	DA	1614	1/1	0.98	0.13	25,25,25,25	0
54	MG	DA	1616	1/1	0.98	0.12	21,21,21,21	0
54	MG	AB	4044	1/1	0.98	0.04	17,17,17,17	0
54	MG	BA	4015	1/1	0.98	0.08	59,59,59,59	0
54	MG	DA	1620	1/1	0.98	0.10	19,19,19,19	0
54	MG	DA	1621	1/1	0.98	0.11	18,18,18,18	0
54	MG	CB	3051	1/1	0.98	0.23	12,12,12,12	0
54	MG	AB	4002	1/1	0.98	0.13	27,27,27,27	0
54	MG	AB	4032	1/1	0.98	0.09	35,35,35,35	0
54	MG	CB	3056	1/1	0.98	0.15	8,8,8,8	0
54	MG	CB	3057	1/1	0.98	0.14	7,7,7,7	0
54	MG	CB	3058	1/1	0.98	0.07	31,31,31,31	0
54	MG	BA	4019	1/1	0.98	0.26	11,11,11,11	0
54	MG	AB	4068	1/1	0.98	0.06	21,21,21,21	0
54	MG	AB	4033	1/1	0.98	0.12	52,52,52,52	0
54	MG	DA	1635	1/1	0.98	0.16	41,41,41,41	0
54	MG	AB	4071	1/1	0.98	0.18	29,29,29,29	0
54	MG	CB	3064	1/1	0.98	0.13	63,63,63,63	0
54	MG	DA	1639	1/1	0.98	0.08	79,79,79,79	0
54	MG	BA	4058	1/1	0.98	0.10	78,78,78,78	0
54	MG	AB	4072	1/1	0.98	0.10	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AB	4073	1/1	0.98	0.18	21,21,21,21	0
54	MG	CB	3001	1/1	0.98	0.05	9,9,9,9	0
54	MG	CB	3004	1/1	0.98	0.12	9,9,9,9	0
54	MG	DA	1648	1/1	0.98	0.09	43,43,43,43	0
54	MG	DA	1649	1/1	0.98	0.11	45,45,45,45	0
54	MG	DA	1650	1/1	0.98	0.09	48,48,48,48	0
54	MG	AB	4074	1/1	0.98	0.17	50,50,50,50	0
54	MG	AB	4026	1/1	0.98	0.12	78,78,78,78	0
54	MG	DA	1654	1/1	0.98	0.05	13,13,13,13	0
54	MG	DA	1657	1/1	0.98	0.52	63,63,63,63	0
54	MG	DA	1658	1/1	0.98	0.44	47,47,47,47	0
54	MG	CB	3075	1/1	0.98	0.12	61,61,61,61	0
54	MG	CB	3008	1/1	0.98	0.14	16,16,16,16	0
54	MG	AB	4105	1/1	0.98	0.11	33,33,33,33	0
54	MG	AB	4035	1/1	0.98	0.07	39,39,39,39	0
54	MG	BA	4031	1/1	0.99	0.26	40,40,40,40	0
54	MG	AB	4100	1/1	0.99	0.12	25,25,25,25	0
54	MG	AB	4028	1/1	0.99	0.13	16,16,16,16	0
54	MG	AB	4102	1/1	0.99	0.10	63,63,63,63	0
54	MG	AB	4070	1/1	0.99	0.09	20,20,20,20	0
54	MG	CB	3027	1/1	0.99	0.15	40,40,40,40	0
54	MG	CB	3028	1/1	0.99	0.27	46,46,46,46	0
54	MG	AB	4104	1/1	0.99	0.12	26,26,26,26	0
54	MG	AB	4010	1/1	0.99	0.11	32,32,32,32	0
54	MG	CB	3031	1/1	0.99	0.11	55,55,55,55	0
54	MG	AB	4106	1/1	0.99	0.06	9,9,9,9	0
54	MG	CB	3101	1/1	0.99	0.25	8,8,8,8	0
54	MG	AB	4030	1/1	0.99	0.04	34,34,34,34	0
54	MG	AB	4019	1/1	0.99	0.07	29,29,29,29	0
54	MG	AB	4020	1/1	0.99	0.47	67,67,67,67	0
54	MG	CB	3105	1/1	0.99	0.11	20,20,20,20	0
54	MG	AB	4049	1/1	0.99	0.21	21,21,21,21	0
54	MG	AB	4076	1/1	0.99	0.26	23,23,23,23	0
54	MG	AB	4011	1/1	0.99	0.20	45,45,45,45	0
54	MG	BA	4045	1/1	0.99	0.11	59,59,59,59	0
54	MG	CC	301	1/1	0.99	0.12	89,89,89,89	0
54	MG	BA	4003	1/1	0.99	0.21	29,29,29,29	0
54	MG	AB	4051	1/1	0.99	0.06	7,7,7,7	0
54	MG	BA	4005	1/1	0.99	0.23	59,59,59,59	0
54	MG	DA	1603	1/1	0.99	0.07	22,22,22,22	0
54	MG	AB	4079	1/1	0.99	0.18	43,43,43,43	0
54	MG	AB	4052	1/1	0.99	0.06	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CB	3046	1/1	0.99	0.11	29,29,29,29	0
54	MG	CB	3047	1/1	0.99	0.07	10,10,10,10	0
54	MG	CB	3048	1/1	0.99	0.13	4,4,4,4	0
54	MG	BA	4051	1/1	0.99	0.15	79,79,79,79	0
54	MG	AB	4081	1/1	0.99	0.11	60,60,60,60	0
54	MG	BA	4009	1/1	0.99	0.11	34,34,34,34	0
54	MG	BA	4010	1/1	0.99	0.04	17,17,17,17	0
54	MG	BA	4055	1/1	0.99	0.16	27,27,27,27	0
54	MG	CB	3054	1/1	0.99	0.21	13,13,13,13	0
54	MG	DA	1615	1/1	0.99	0.12	95,95,95,95	0
54	MG	CB	3055	1/1	0.99	0.10	5,5,5,5	0
54	MG	DA	1617	1/1	0.99	0.07	10,10,10,10	0
54	MG	AB	4082	1/1	0.99	0.25	50,50,50,50	0
54	MG	AB	4006	1/1	0.99	0.13	12,12,12,12	0
54	MG	AB	4004	1/1	0.99	0.07	41,41,41,41	0
54	MG	AB	4056	1/1	0.99	0.26	9,9,9,9	0
54	MG	DA	1622	1/1	0.99	0.25	27,27,27,27	0
54	MG	DA	1623	1/1	0.99	0.24	20,20,20,20	0
54	MG	AB	4086	1/1	0.99	0.12	39,39,39,39	0
54	MG	BA	4016	1/1	0.99	0.07	47,47,47,47	0
54	MG	CB	3062	1/1	0.99	0.07	7,7,7,7	0
54	MG	CB	3002	1/1	0.99	0.08	54,54,54,54	0
54	MG	CB	3003	1/1	0.99	0.07	8,8,8,8	0
54	MG	AB	4014	1/1	0.99	0.17	18,18,18,18	0
54	MG	AB	4015	1/1	0.99	0.06	3,3,3,3	0
54	MG	DA	1631	1/1	0.99	0.07	22,22,22,22	0
54	MG	CB	3067	1/1	0.99	0.21	9,9,9,9	0
54	MG	DA	1633	1/1	0.99	0.09	3,3,3,3	0
54	MG	AB	4089	1/1	0.99	0.08	31,31,31,31	0
54	MG	CB	3069	1/1	0.99	0.14	10,10,10,10	0
54	MG	CB	3007	1/1	0.99	0.13	25,25,25,25	0
54	MG	AB	4016	1/1	0.99	0.18	68,68,68,68	0
54	MG	DA	1638	1/1	0.99	0.16	12,12,12,12	0
54	MG	AB	4060	1/1	0.99	0.18	36,36,36,36	0
54	MG	CB	3073	1/1	0.99	0.17	14,14,14,14	0
54	MG	BA	4022	1/1	0.99	0.16	14,14,14,14	0
54	MG	DA	1643	1/1	0.99	0.09	70,70,70,70	0
54	MG	AB	4039	1/1	0.99	0.06	25,25,25,25	0
54	MG	AB	4040	1/1	0.99	0.13	77,77,77,77	0
54	MG	DA	1646	1/1	0.99	0.11	50,50,50,50	0
54	MG	CB	3013	1/1	0.99	0.07	14,14,14,14	0
54	MG	AB	4063	1/1	0.99	0.20	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AB	4041	1/1	0.99	0.07	11,11,11,11	0
54	MG	CB	3016	1/1	0.99	0.04	18,18,18,18	0
54	MG	CB	3017	1/1	0.99	0.07	13,13,13,13	0
54	MG	DA	1652	1/1	0.99	0.06	21,21,21,21	0
54	MG	AB	4065	1/1	0.99	0.15	20,20,20,20	0
54	MG	CB	3083	1/1	0.99	0.10	9,9,9,9	0
54	MG	DA	1655	1/1	0.99	0.04	12,12,12,12	0
54	MG	DA	1656	1/1	0.99	0.04	15,15,15,15	0
54	MG	AB	4066	1/1	0.99	0.14	33,33,33,33	0
54	MG	CB	3085	1/1	0.99	0.26	16,16,16,16	0
54	MG	CB	3086	1/1	0.99	0.13	17,17,17,17	0
54	MG	AB	4017	1/1	0.99	0.36	10,10,10,10	0
54	MG	CB	3088	1/1	0.99	0.07	52,52,52,52	0
54	MG	AB	4043	1/1	0.99	0.40	16,16,16,16	0
54	MG	DA	1642	1/1	1.00	0.04	31,31,31,31	0
54	MG	AB	4054	1/1	1.00	0.12	10,10,10,10	0
54	MG	CB	3044	1/1	1.00	0.31	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.