



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:26 AM UTC

PDB ID : 4U1U / pdb_00004u1u
Title : Crystal structure of the E. coli ribosome bound to quinupristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-07-16
Resolution : 2.95 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

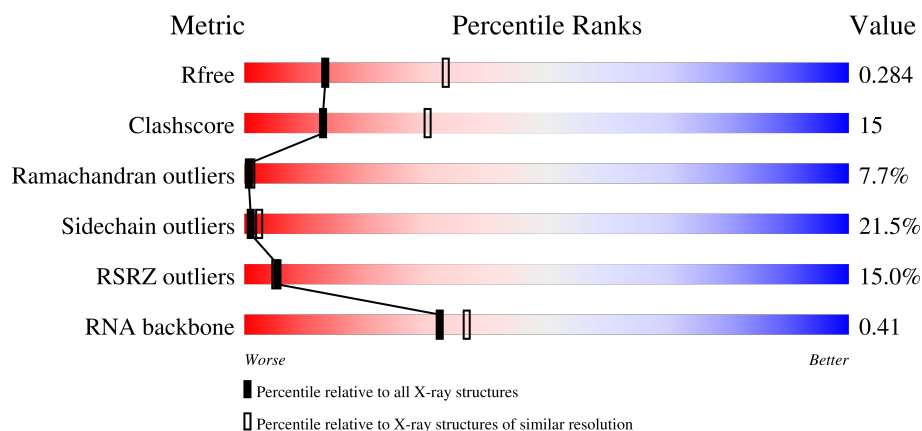
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)
RNA backbone	3983	1046 (3.16-2.76)

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	AA	1539	4% 43% 45% 12%
1	CA	1539	10% 43% 45% 12%
2	AB	218	10% 18% 47% 29% 6%
2	CB	218	26% 28% 44% 25% •

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	
6	CF	100	
7	AG	151	
7	CG	151	
8	AH	129	
8	CH	129	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	117	
11	CK	117	
12	AL	123	
12	CL	123	
13	AM	114	
13	CM	114	
14	AN	100	
14	CN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	119	
23	DB	119	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
27	DF	177	

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Mol	Chain	Length	Quality of chain
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
31	BJ	142	
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	

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Mol	Chain	Length	Quality of chain
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	76	
44	DW	76	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	
52	D4	38	

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Mol	Chain	Length	Quality of chain
53	B5	228	
54	B6	8	
54	D6	8	

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	004	D6	7	-	-	X	-
55	MG	DA	3060	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 288328 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	CA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	CB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	CC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			
5	CE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	CF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	CG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	CM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			
15	CO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	CP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	CQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	CR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	CS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
22	DA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			
23	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
24	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			
27	DF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 30 is a protein called 50S ribosomal protein L11.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
32	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			
35	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
41	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	102	Total	C	N	O	S	0	0	0
			780	492	146	142				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	DU	102	Total	C	N	O			
			780	492	146	142	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BW	76	Total	C	N	O	S		
			580	359	117	103	1	0	0
44	DW	75	Total	C	N	O	S		
			569	353	113	102	1	0	0

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	B5	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 54 is a protein called Quinupristin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B6	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			
54	D6	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	71	Total	Mg	0	0
			71	71		
55	AM	1	Total	Mg	0	0
			1	1		
55	BA	195	Total	Mg	0	0
			195	195		
55	BB	4	Total	Mg	0	0
			4	4		
55	CA	55	Total	Mg	0	0
			55	55		
55	CM	1	Total	Mg	0	0
			1	1		
55	DA	167	Total	Mg	0	0
			167	167		
55	DB	3	Total	Mg	0	0
			3	3		
55	DQ	1	Total	Mg	0	0
			1	1		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	194	Total O 194 194	0	0
57	AL	1	Total O 1 1	0	0
57	AN	5	Total O 5 5	0	0
57	AT	2	Total O 2 2	0	0
57	AU	1	Total O 1 1	0	0
57	BA	619	Total O 619 619	0	0
57	BB	13	Total O 13 13	0	0
57	BC	8	Total O 8 8	0	0
57	BD	3	Total O 3 3	0	0
57	BE	3	Total O 3 3	0	0
57	BF	1	Total O 1 1	0	0
57	BG	1	Total O 1 1	0	0
57	BL	5	Total O 5 5	0	0
57	BN	5	Total O 5 5	0	0
57	BS	1	Total O 1 1	0	0
57	BV	1	Total O 1 1	0	0
57	B2	1	Total O 1 1	0	0
57	B3	3	Total O 3 3	0	0
57	B4	2	Total O 2 2	0	0
57	CA	189	Total O 189 189	0	0
57	CL	1	Total O 1 1	0	0
57	CN	3	Total O 3 3	0	0

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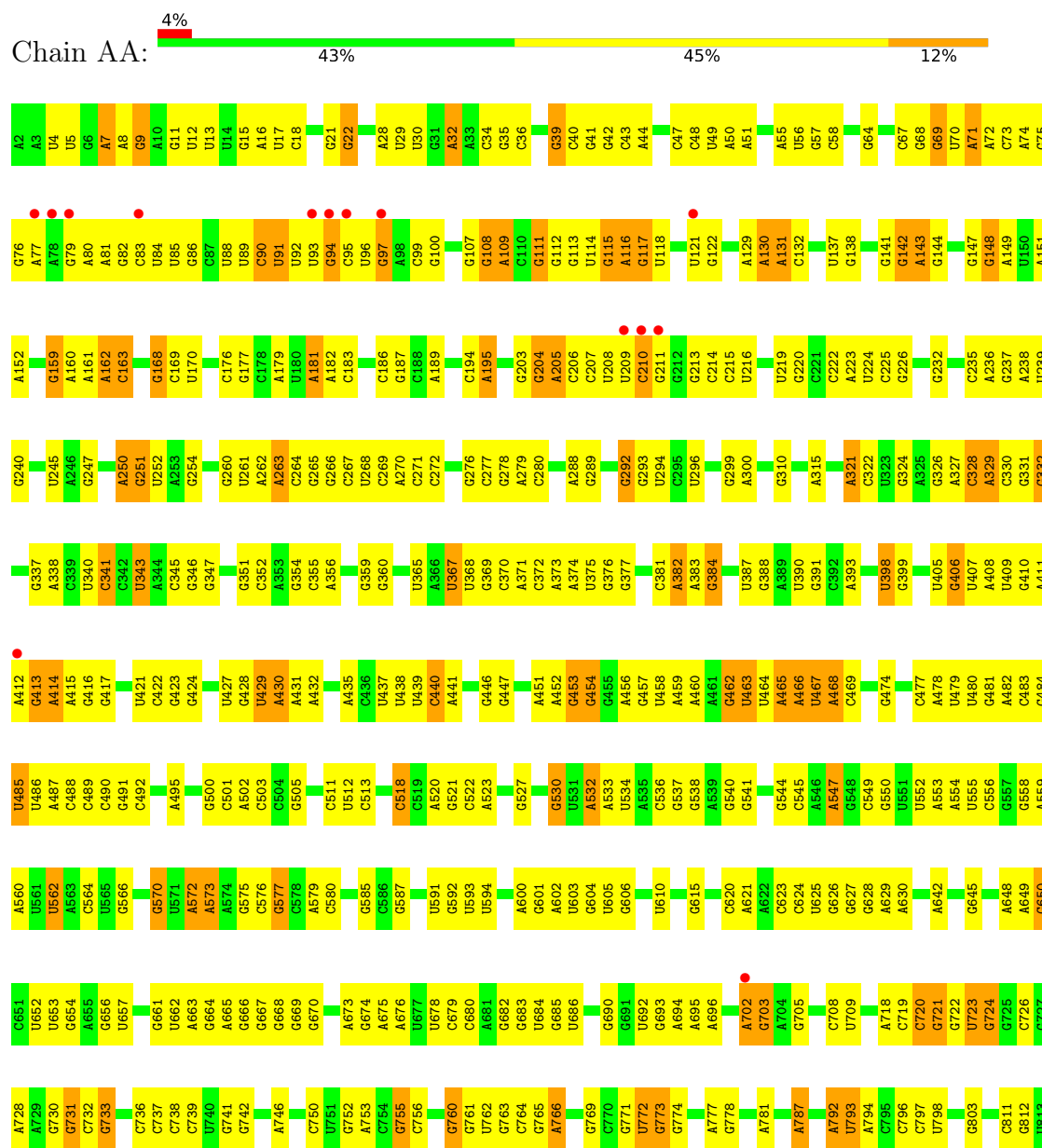
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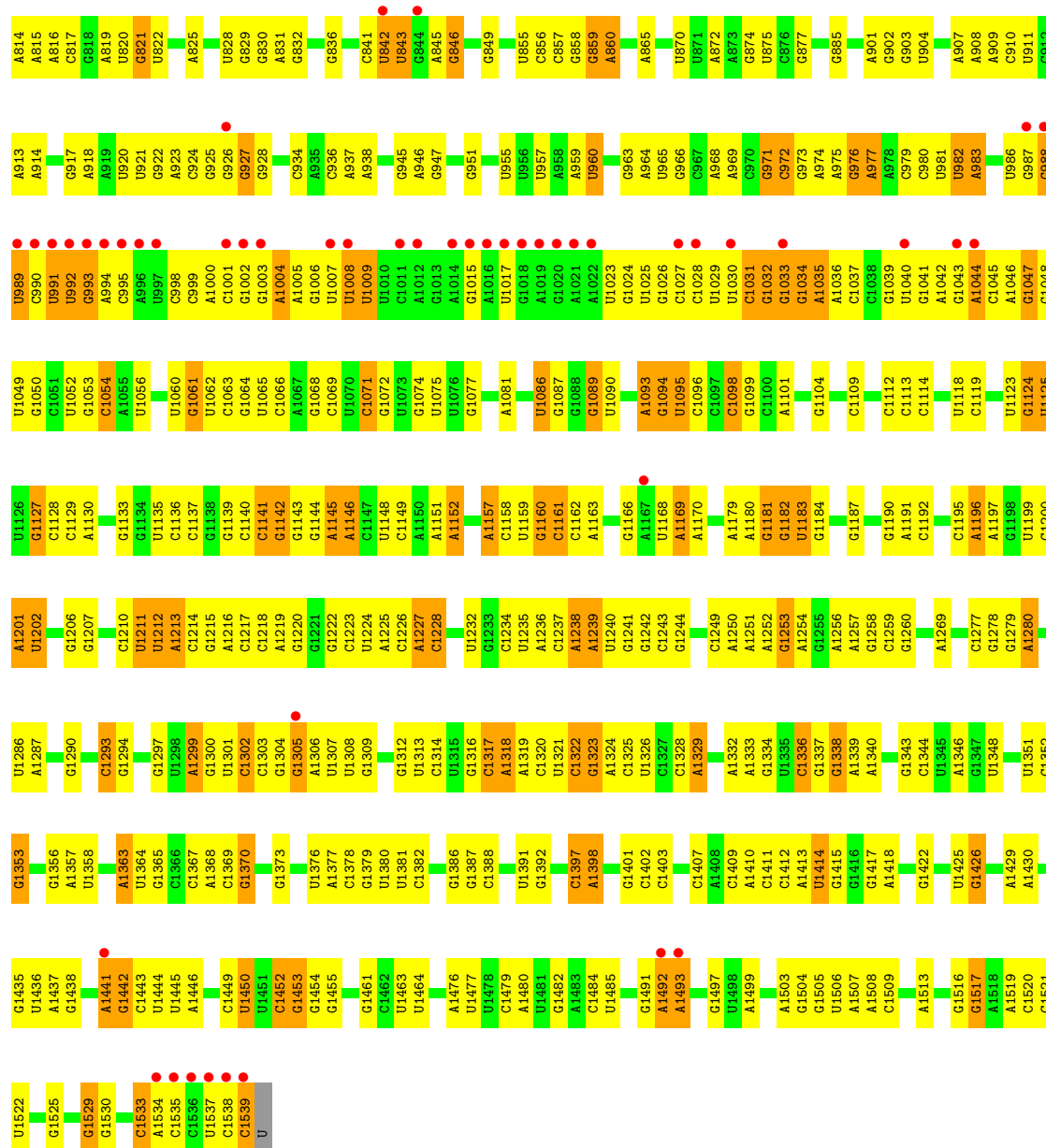
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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57	CU	1	Total 1	O 1	0	0
57	DA	612	Total 612	O 612	0	0
57	DB	13	Total 13	O 13	0	0
57	DC	7	Total 7	O 7	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	4	Total 4	O 4	0	0
57	DL	4	Total 4	O 4	0	0
57	DN	1	Total 1	O 1	0	0
57	DQ	2	Total 2	O 2	0	0
57	DT	3	Total 3	O 3	0	0
57	DV	1	Total 1	O 1	0	0
57	D0	1	Total 1	O 1	0	0
57	D2	2	Total 2	O 2	0	0
57	D3	1	Total 1	O 1	0	0
57	D4	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

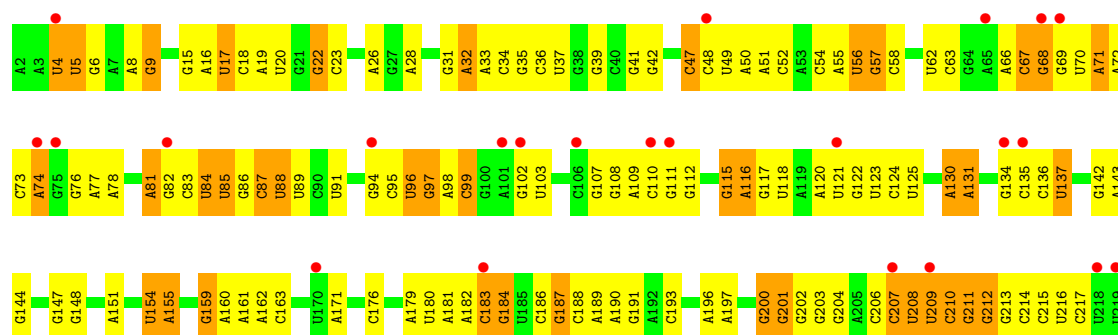
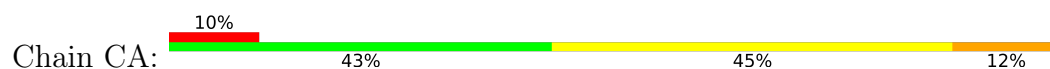
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

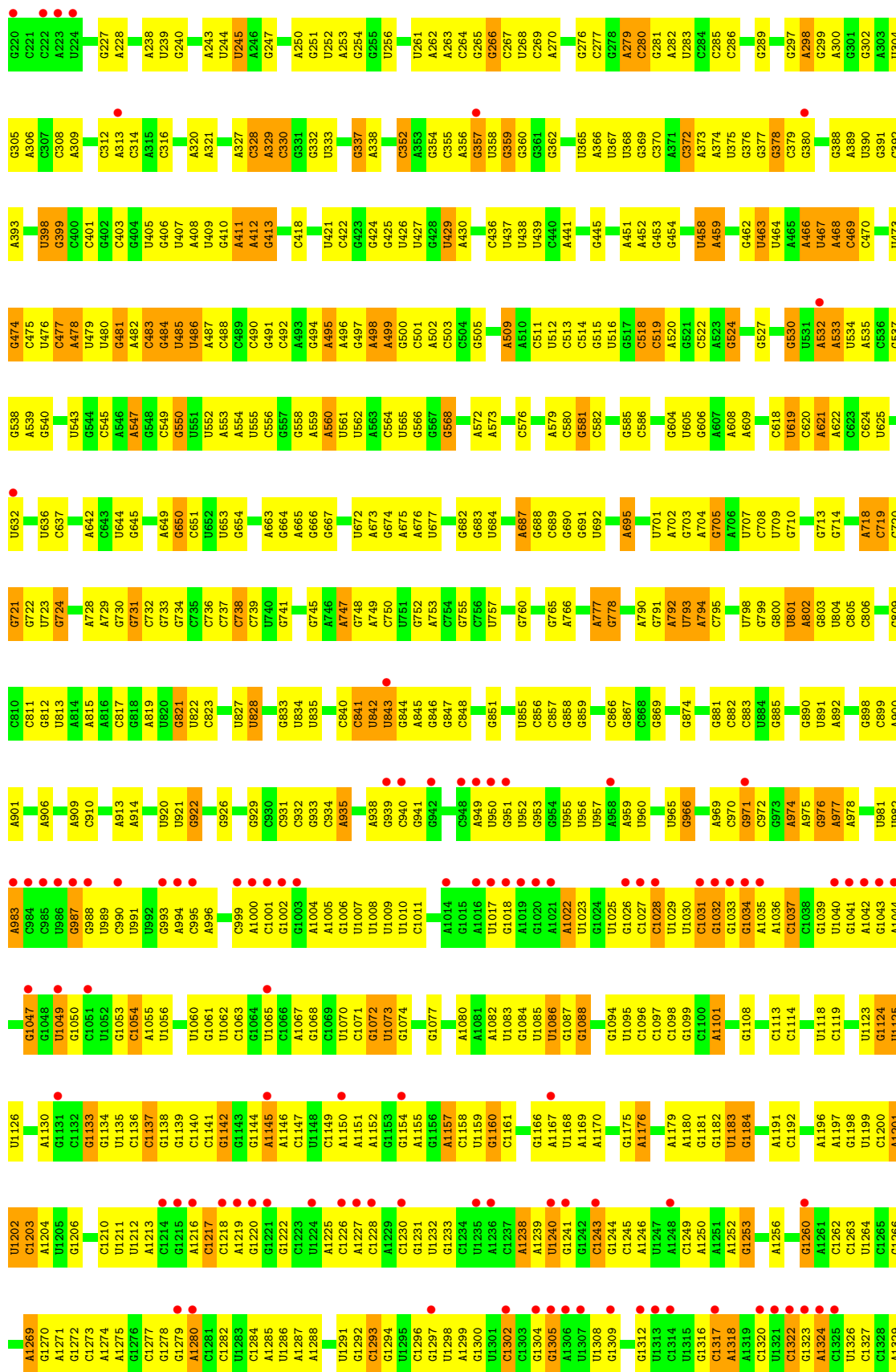
• Molecule 1: 16S rRNA

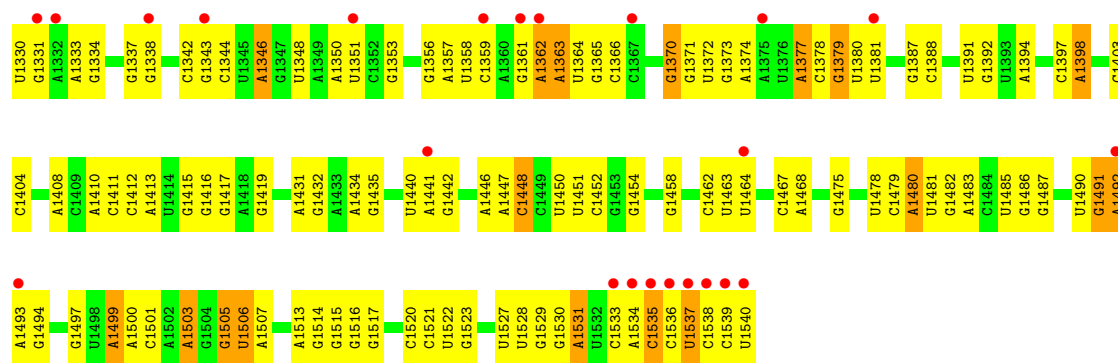




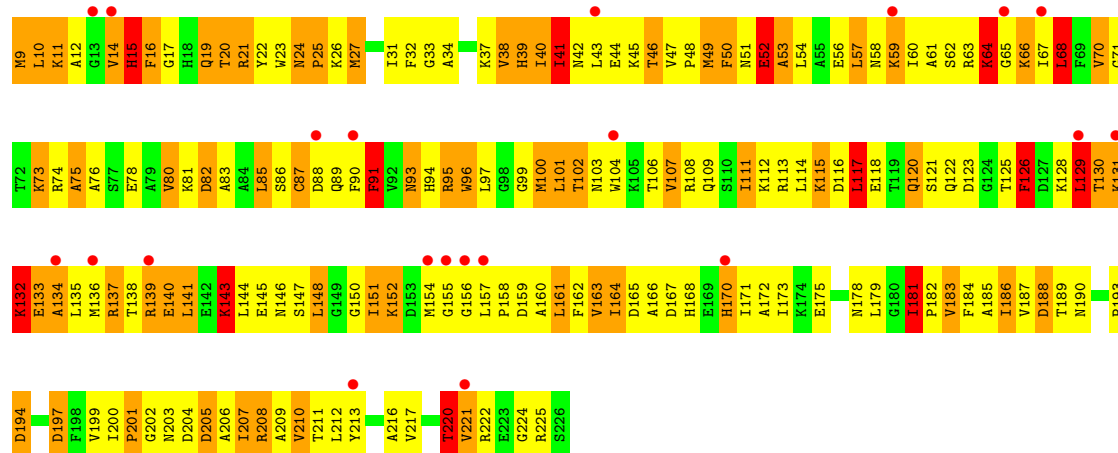
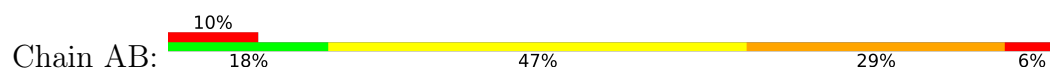
• Molecule 1: 16S rRNA



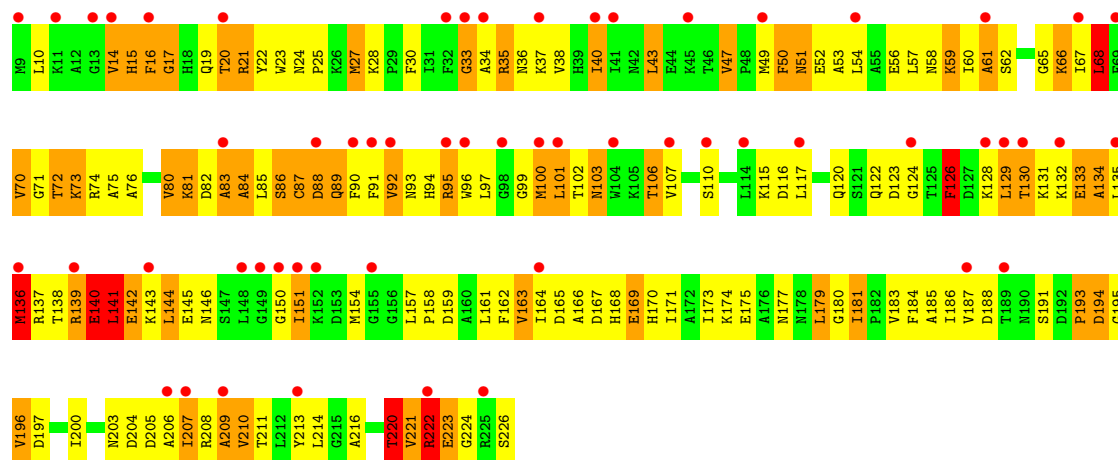




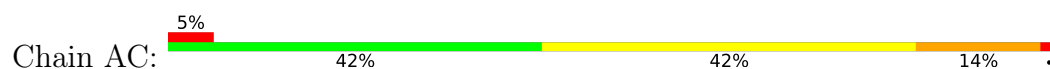
• Molecule 2: 30S ribosomal protein S2

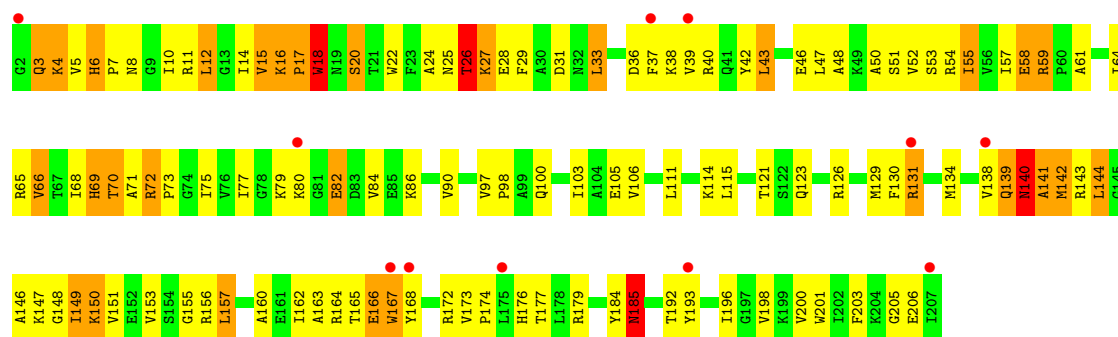


• Molecule 2: 30S ribosomal protein S2

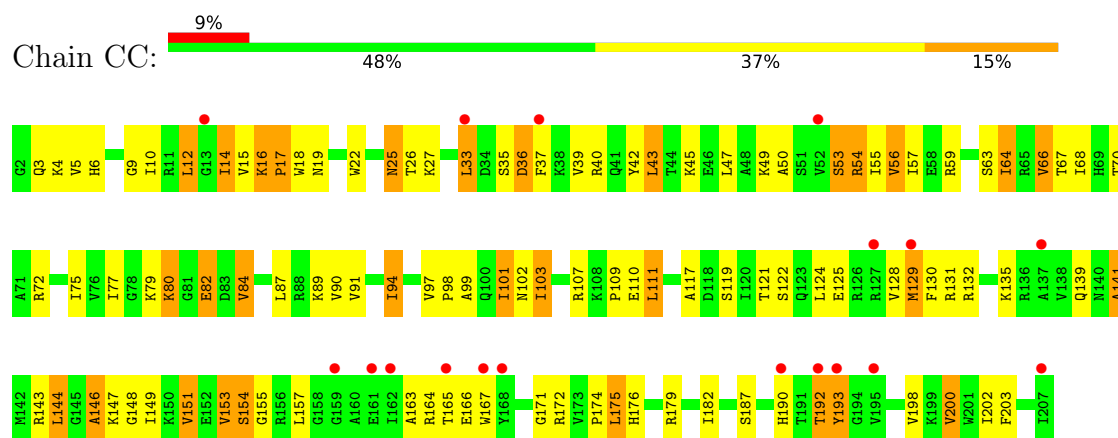


• Molecule 3: 30S ribosomal protein S3

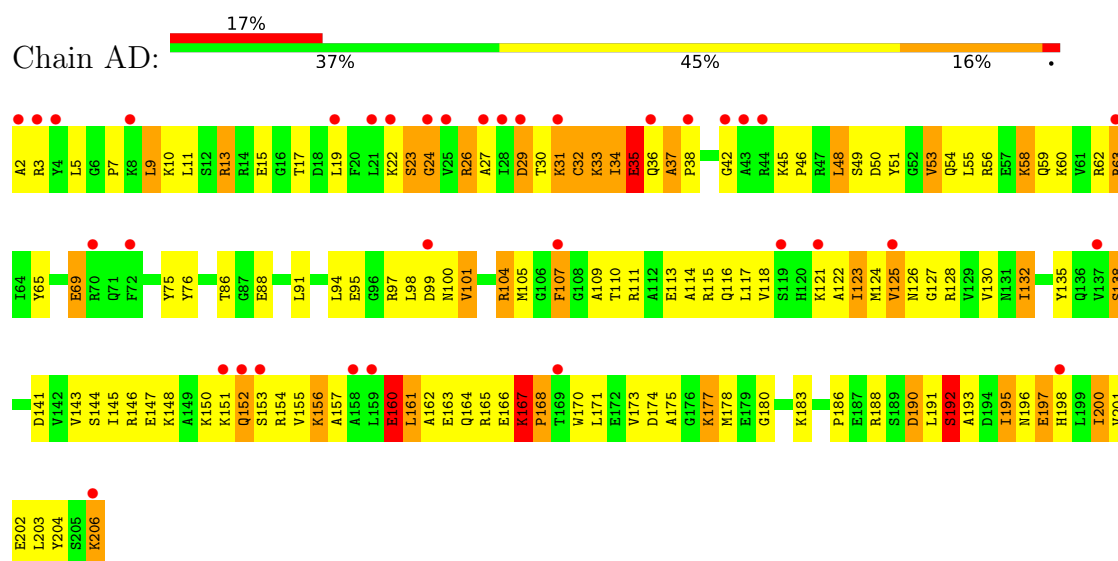




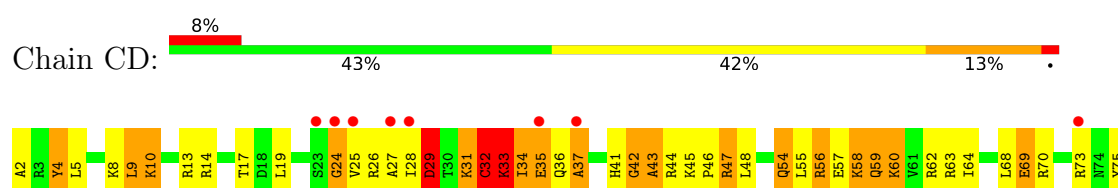
• Molecule 3: 30S ribosomal protein S3

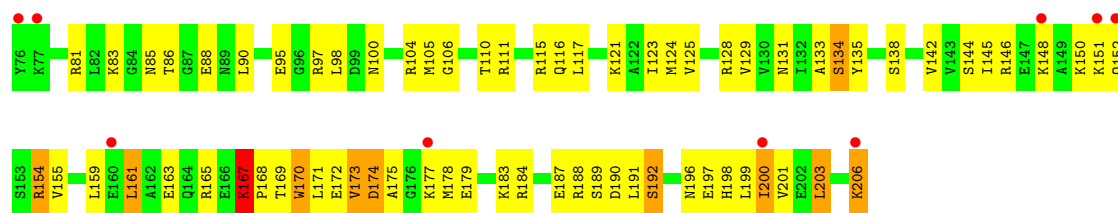


• Molecule 4: 30S ribosomal protein S4

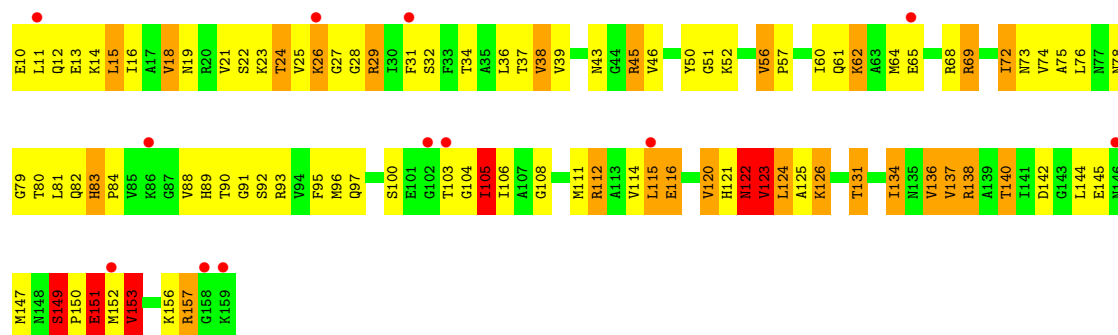


• Molecule 4: 30S ribosomal protein S4

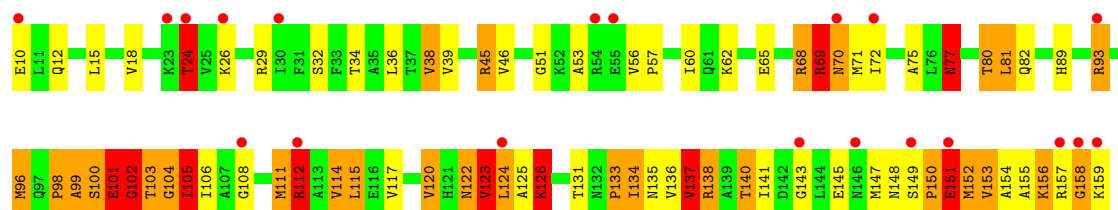




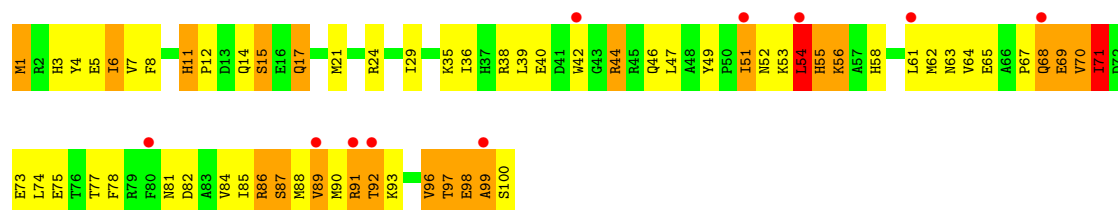
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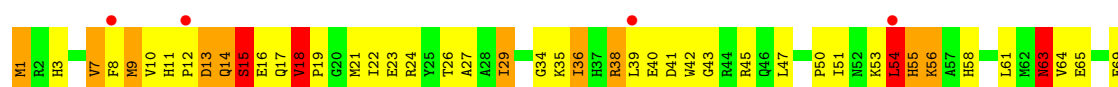
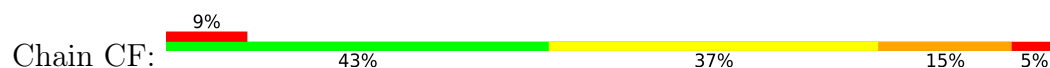
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

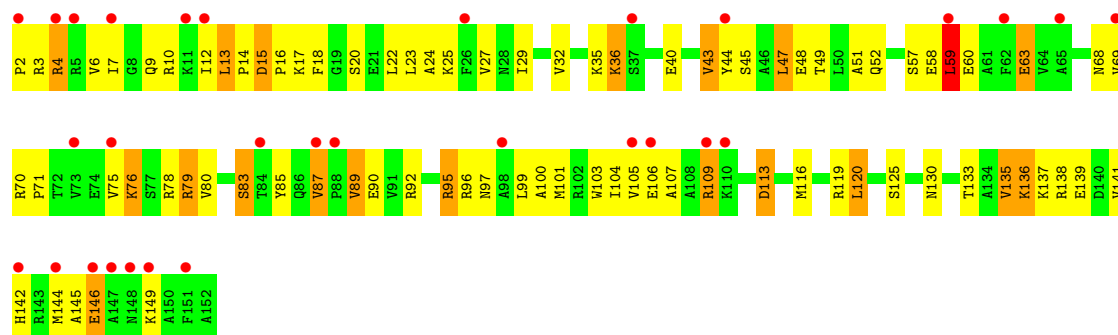


• Molecule 6: 30S ribosomal protein S6

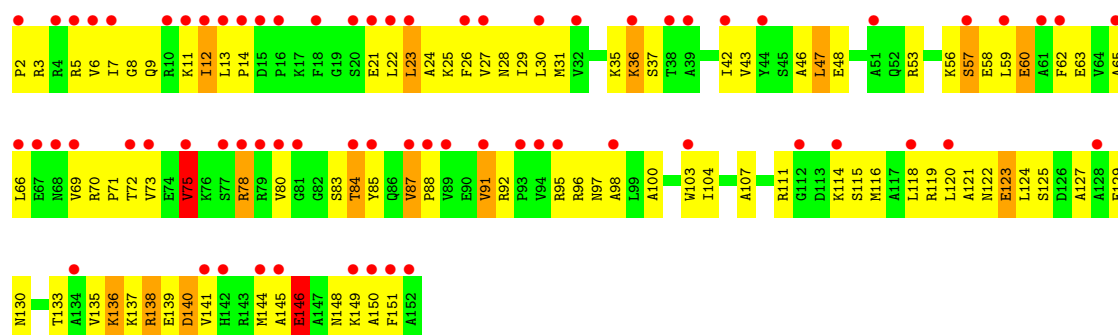




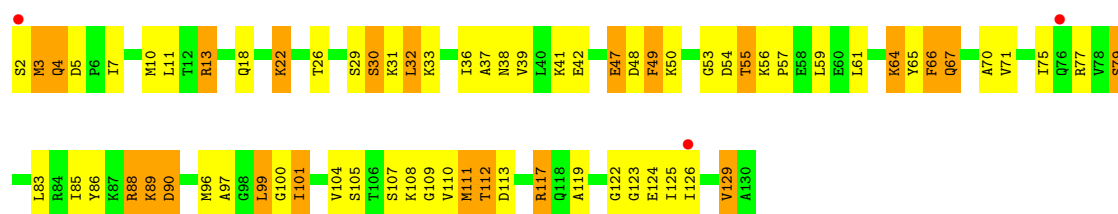
- Molecule 7: 30S ribosomal protein S7



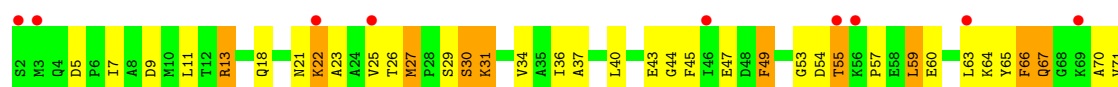
- Molecule 7: 30S ribosomal protein S7

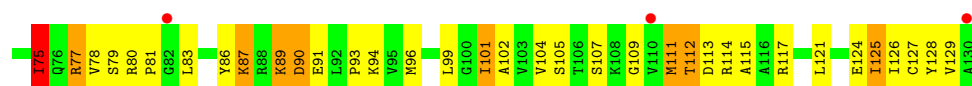


- Molecule 8: 30S ribosomal protein S8

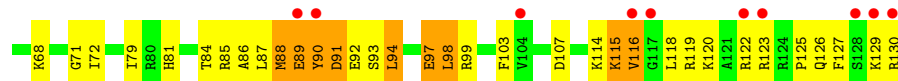
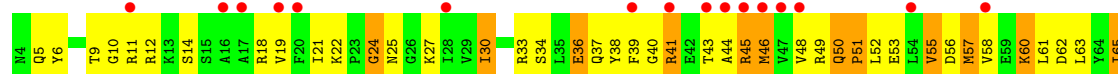


- Molecule 8: 30S ribosomal protein S8

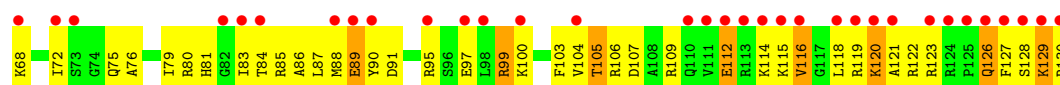
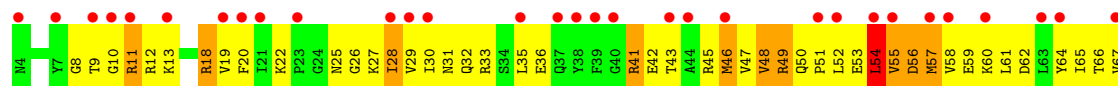




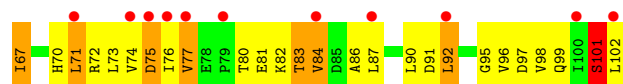
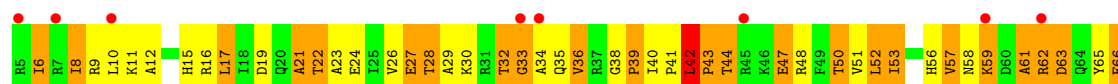
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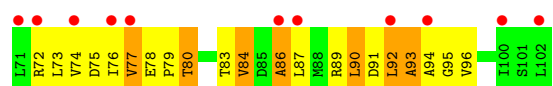
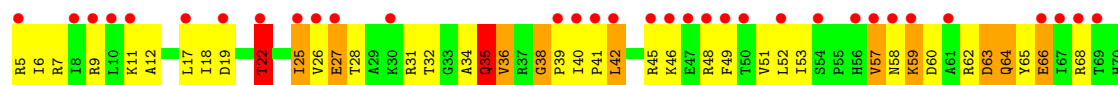
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10

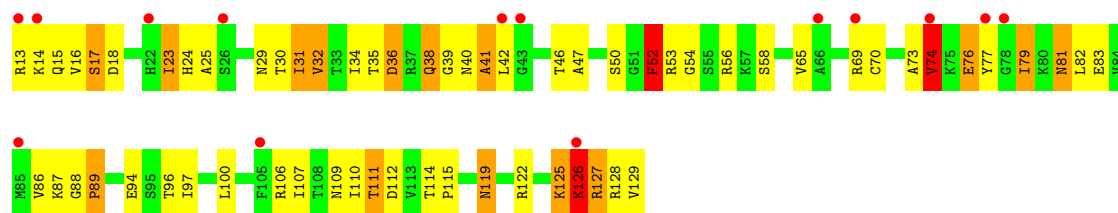


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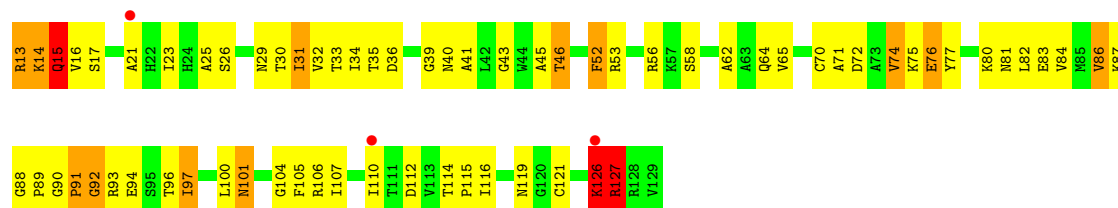


• Molecule 11: 30S ribosomal protein S11

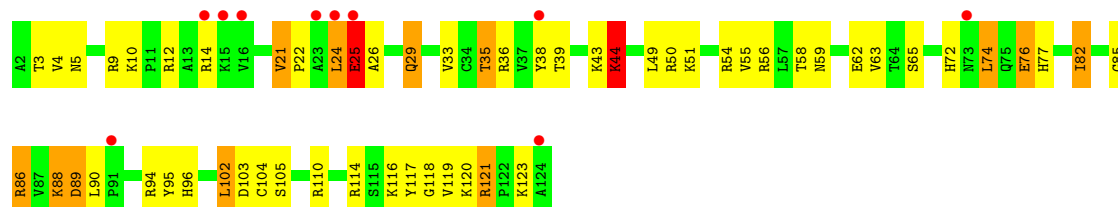




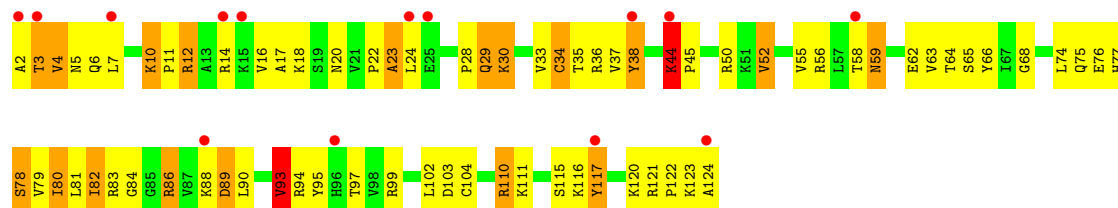
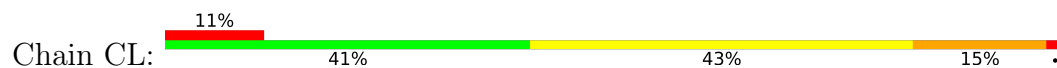
• Molecule 11: 30S ribosomal protein S11



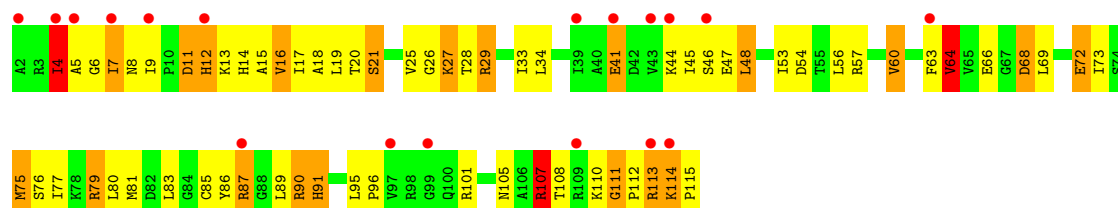
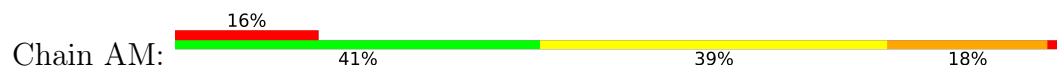
• Molecule 12: 30S ribosomal protein S12



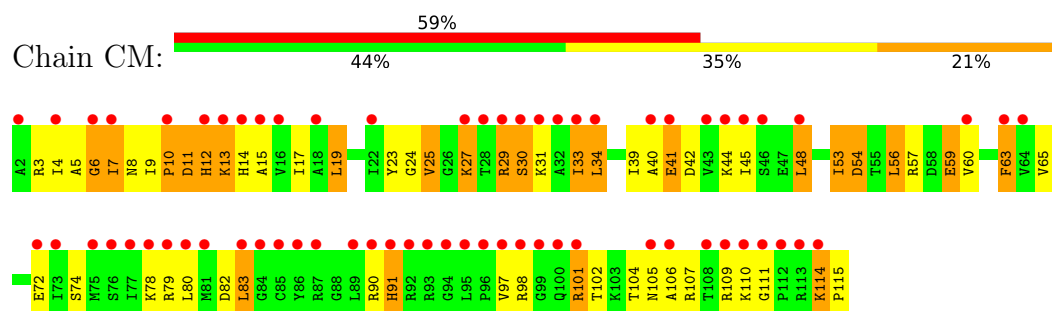
• Molecule 12: 30S ribosomal protein S12



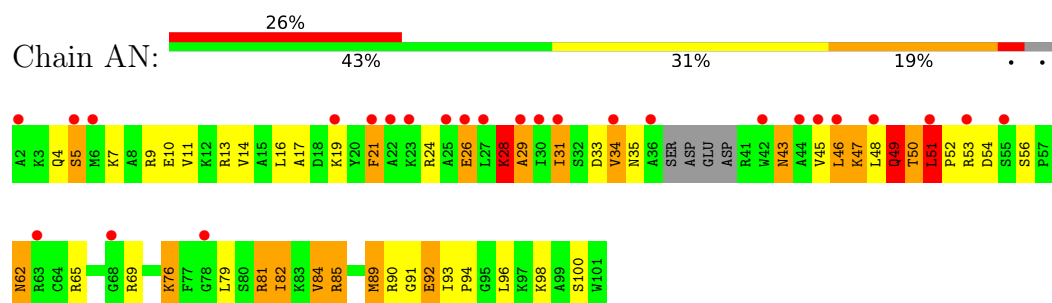
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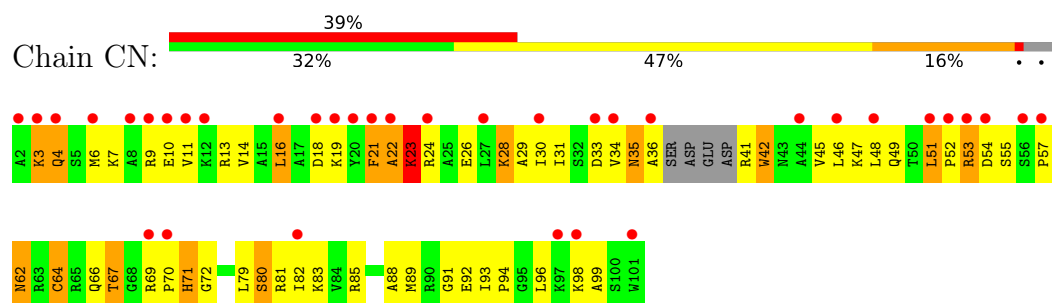
- Molecule 13: 30S ribosomal protein S13



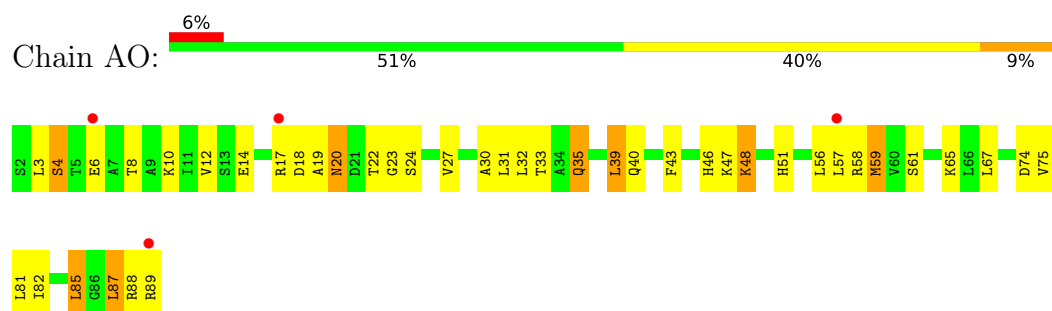
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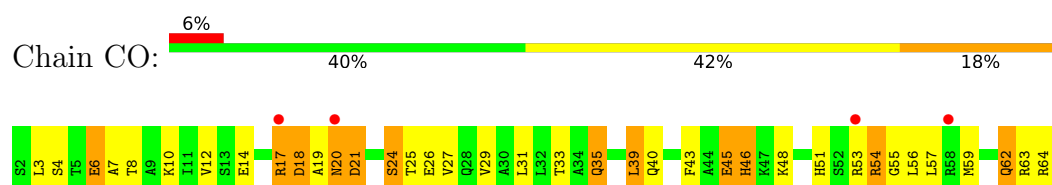
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

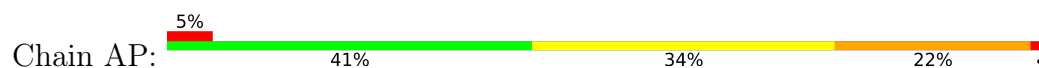


- Molecule 15: 30S ribosomal protein S15

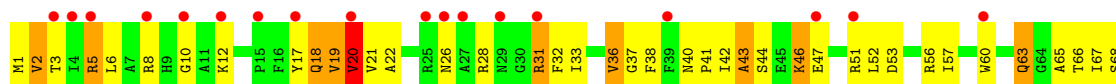




• Molecule 16: 30S ribosomal protein S16



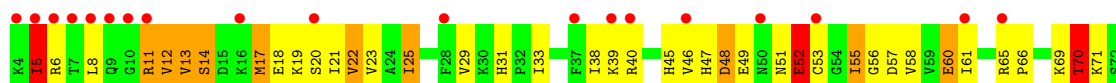
• Molecule 16: 30S ribosomal protein S16



• Molecule 17: 30S ribosomal protein S17



• Molecule 17: 30S ribosomal protein S17

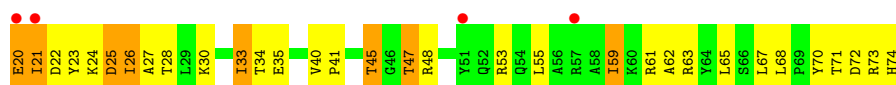


• Molecule 18: 30S ribosomal protein S18

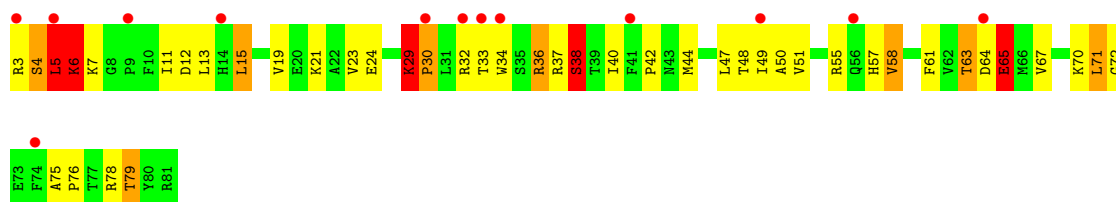




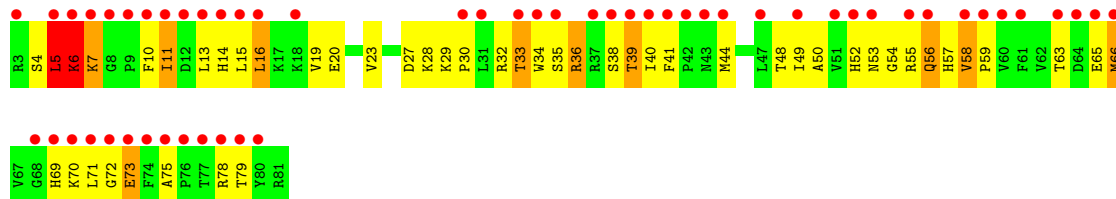
- Molecule 18: 30S ribosomal protein S18



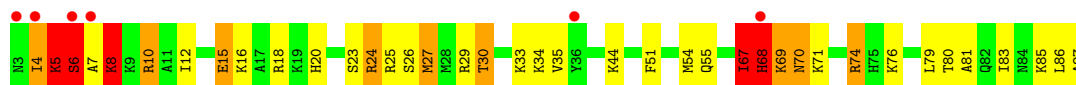
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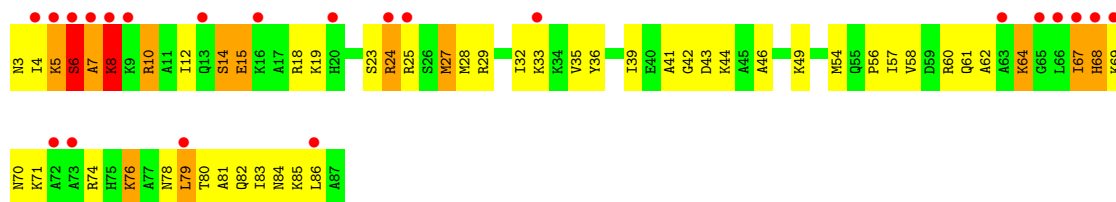
- Molecule 19: 30S ribosomal protein S19



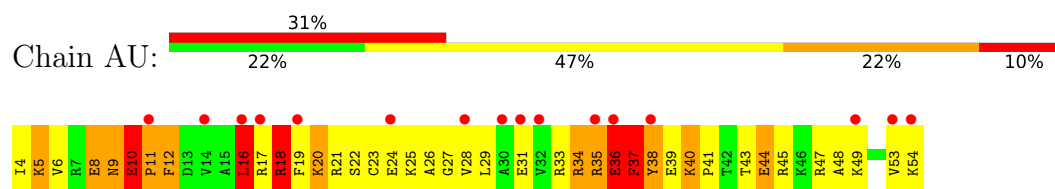
- Molecule 20: 30S ribosomal protein S20



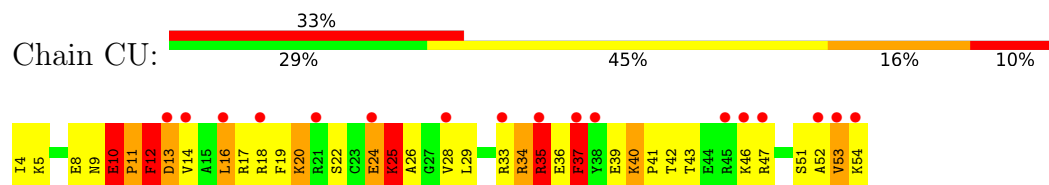
- Molecule 20: 30S ribosomal protein S20



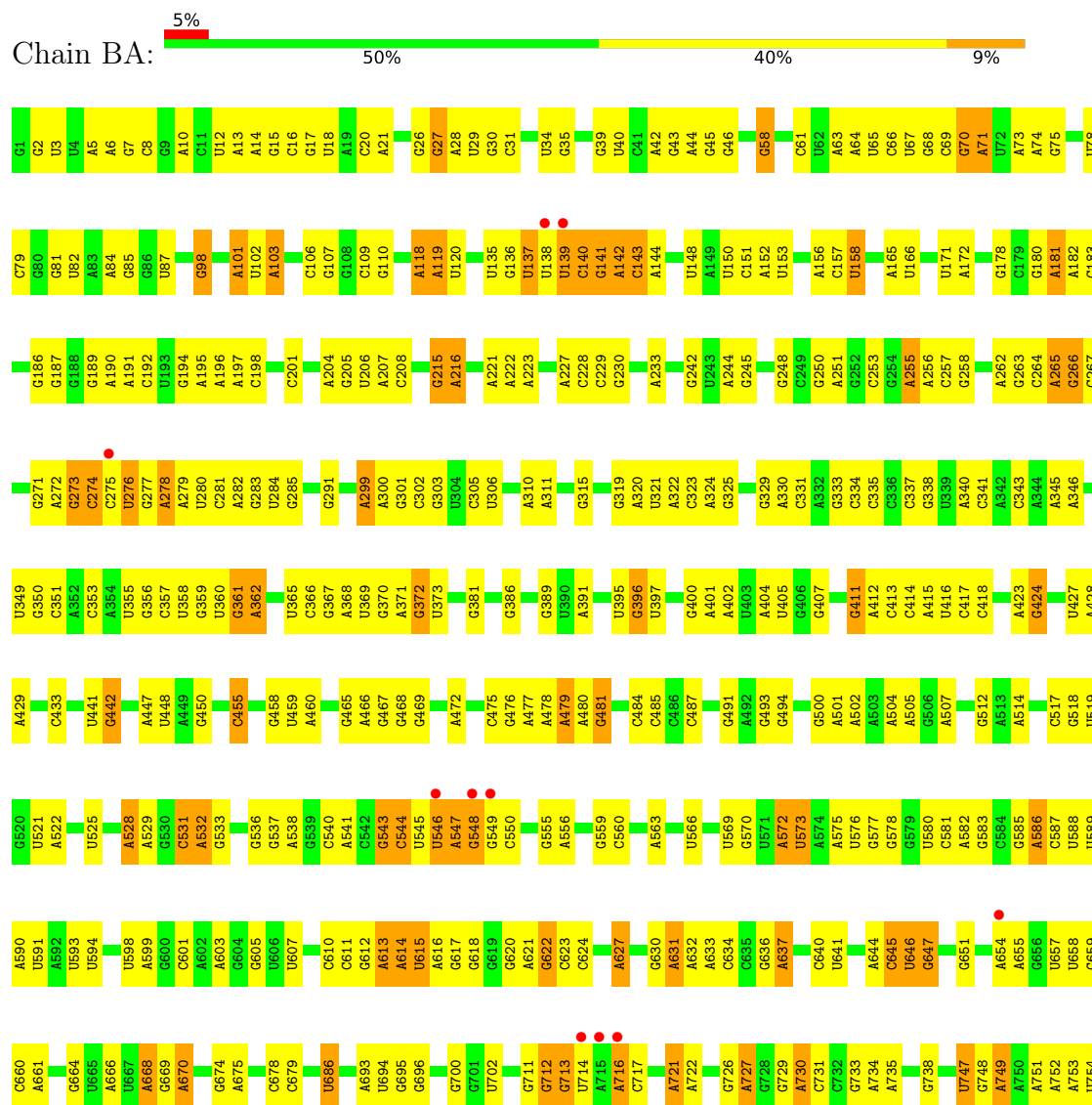
- Molecule 21: 30S ribosomal protein S21

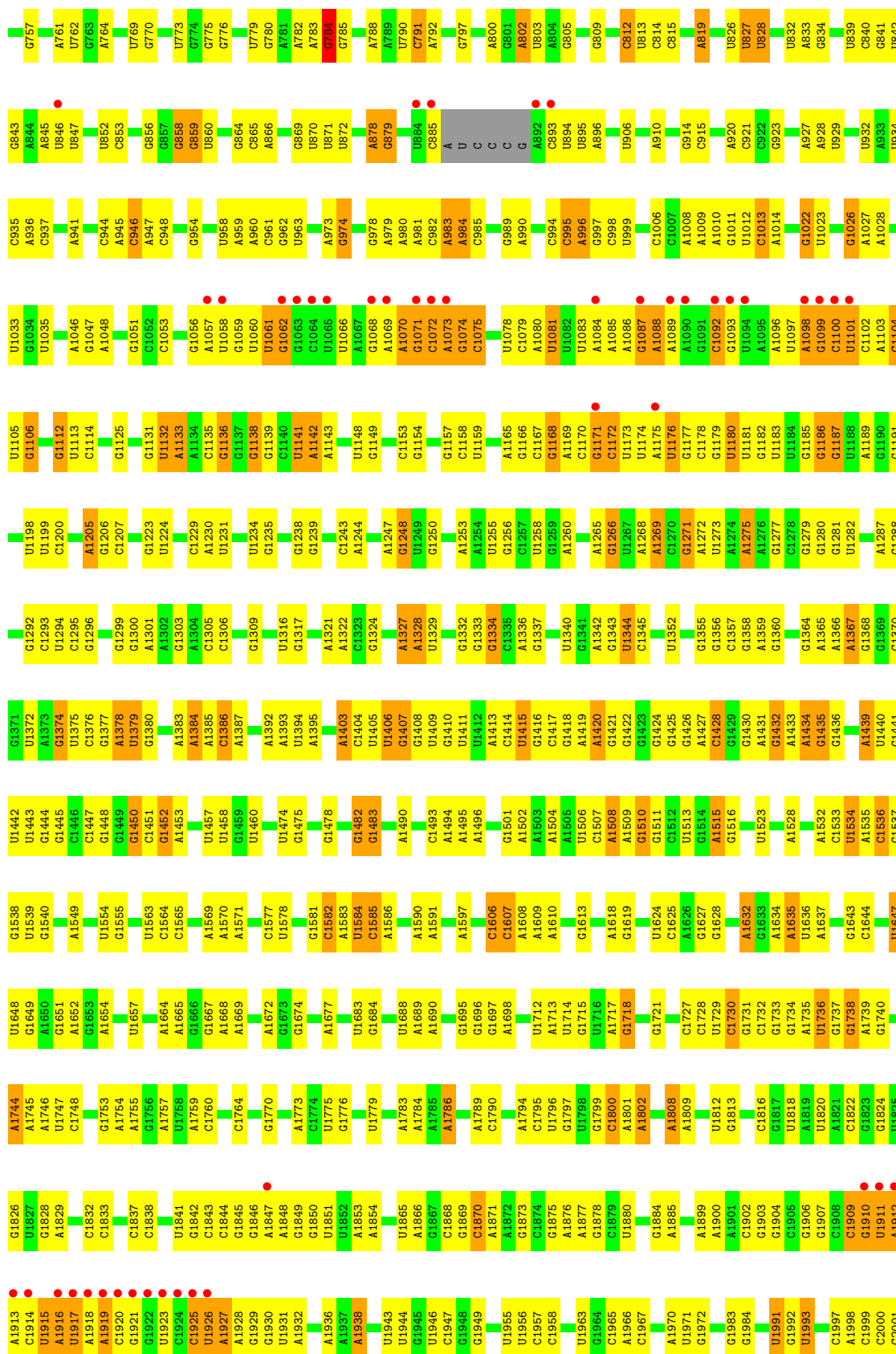


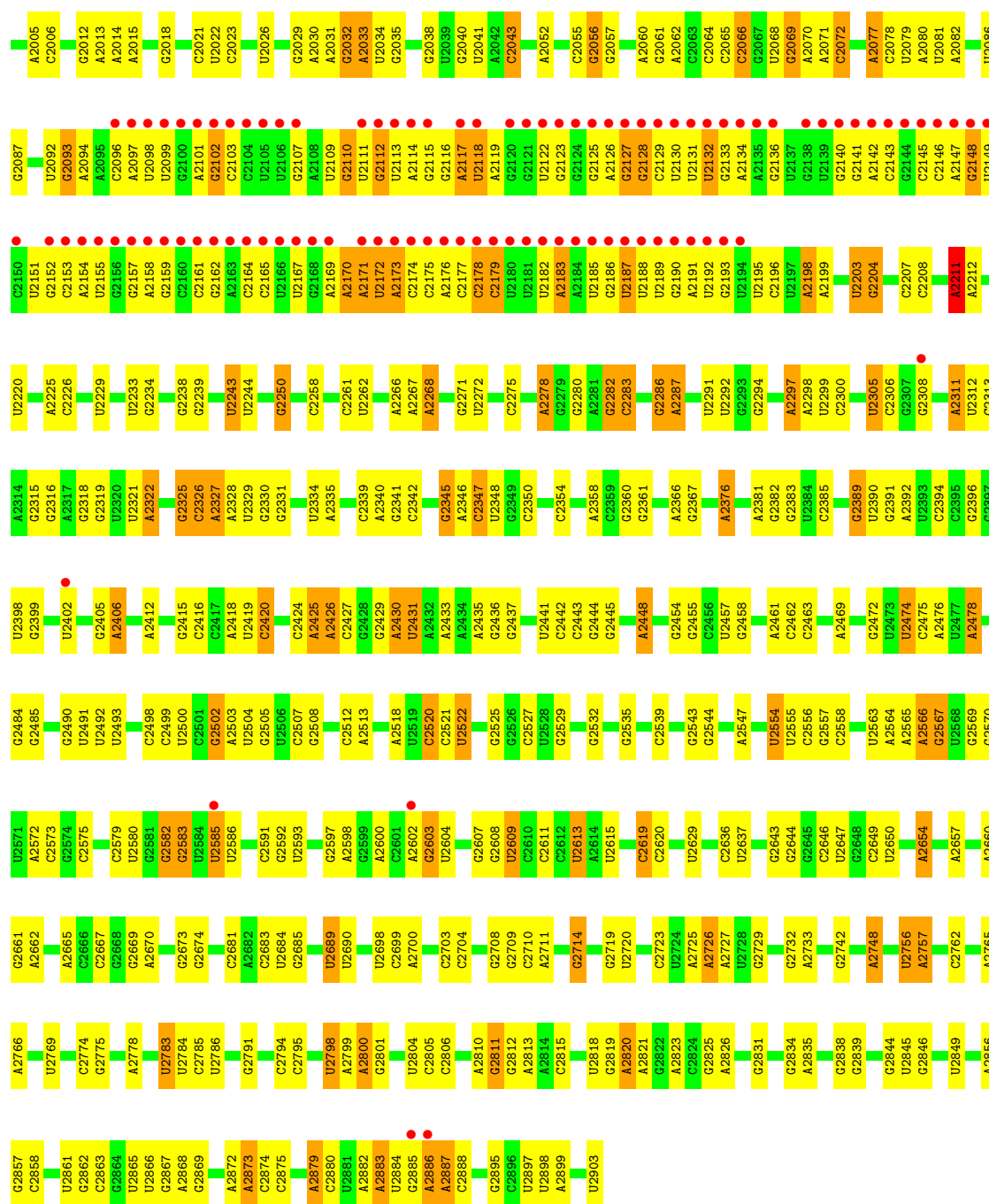
- Molecule 21: 30S ribosomal protein S21



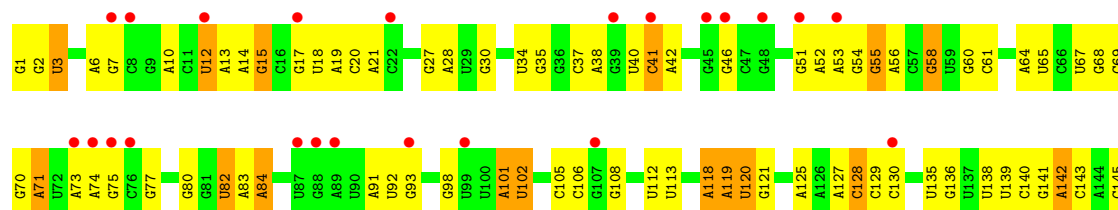
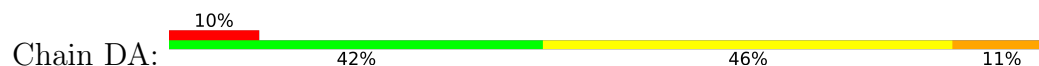
- Molecule 22: 23S rRNA

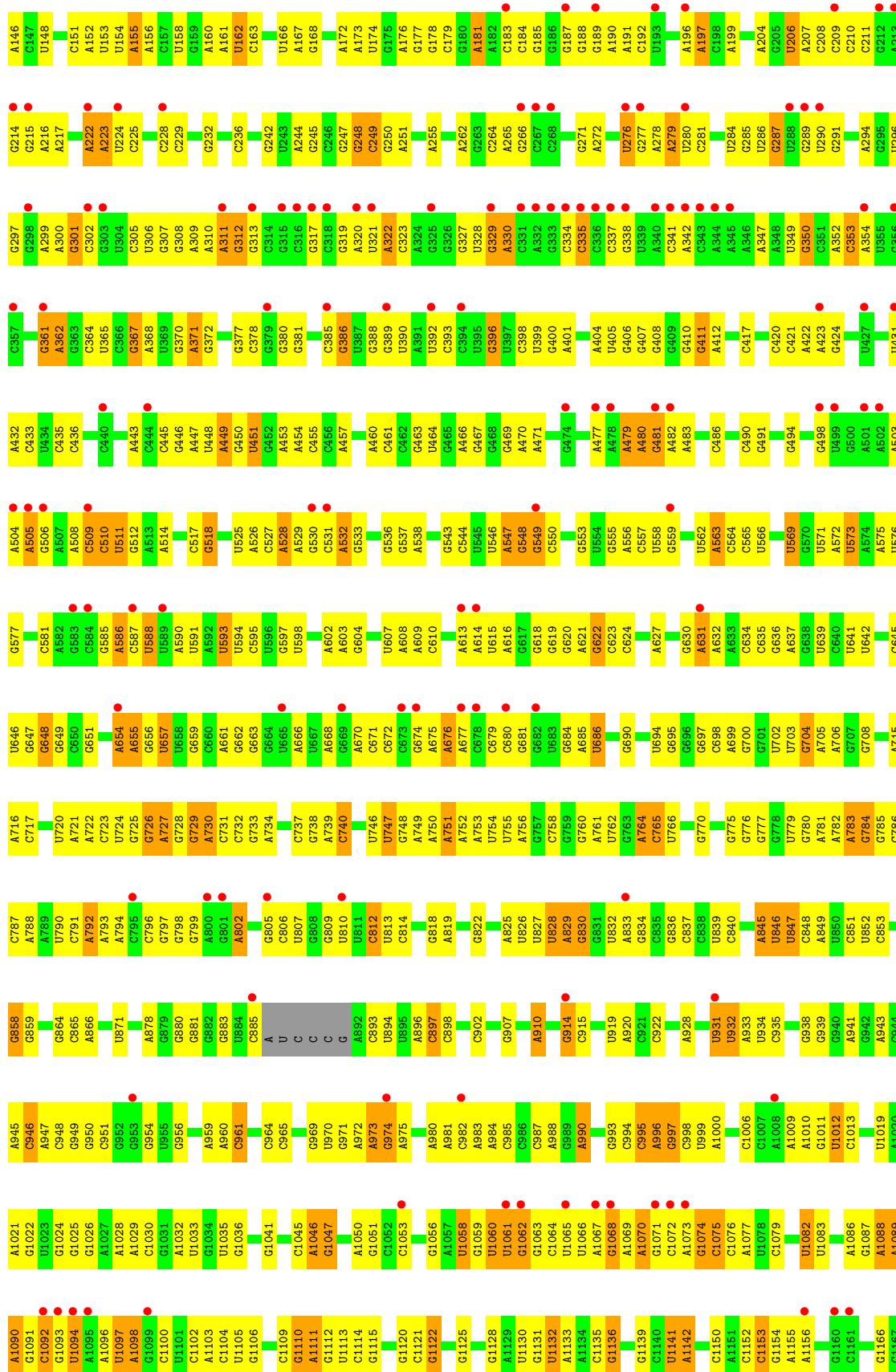




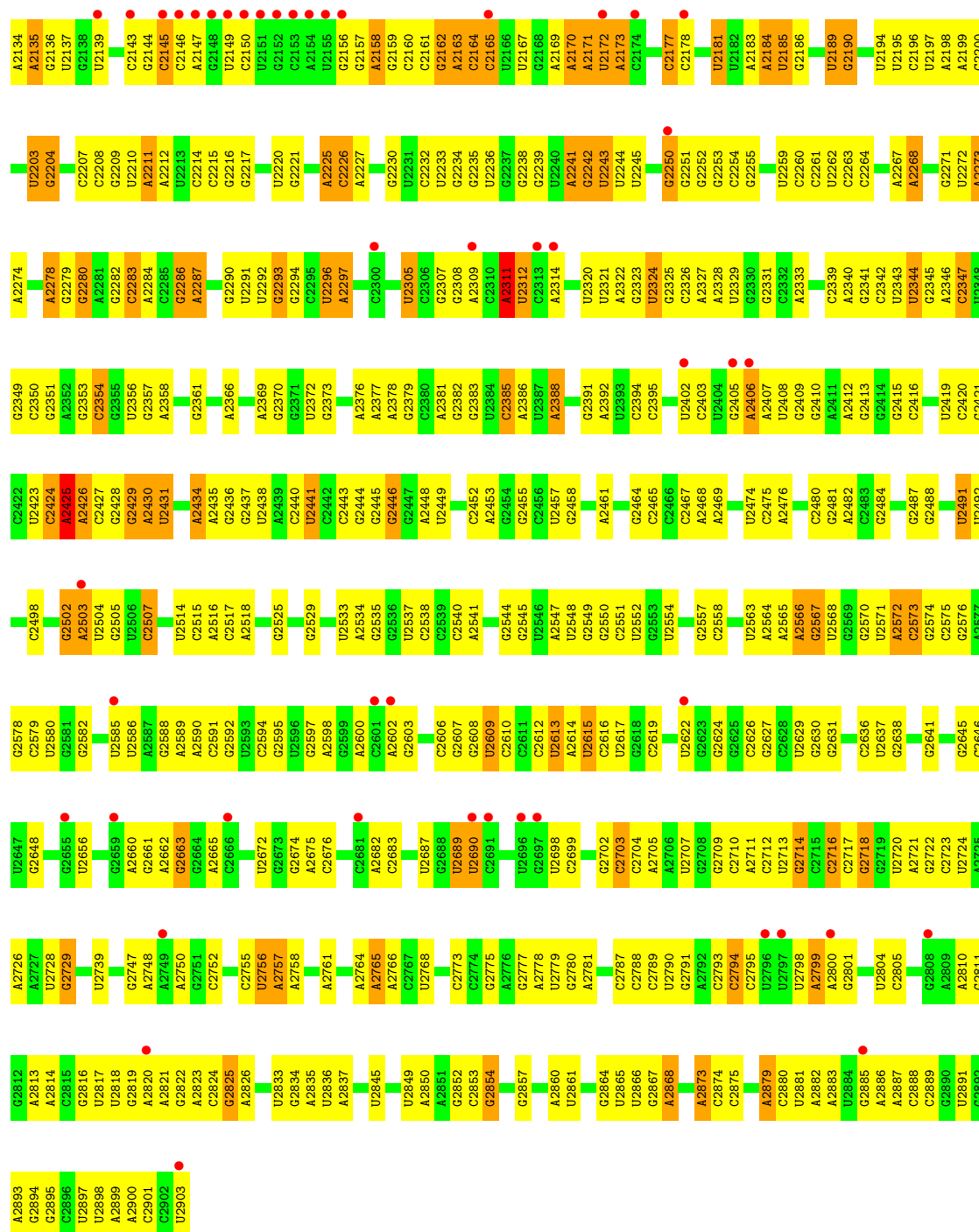


• Molecule 22: 23S rRNA

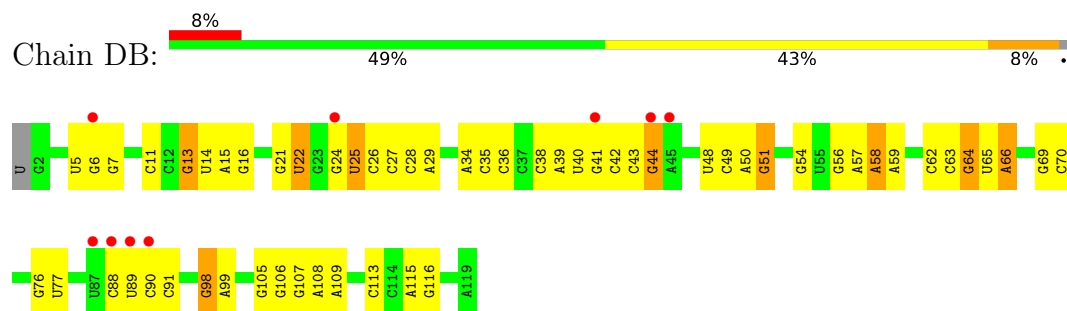




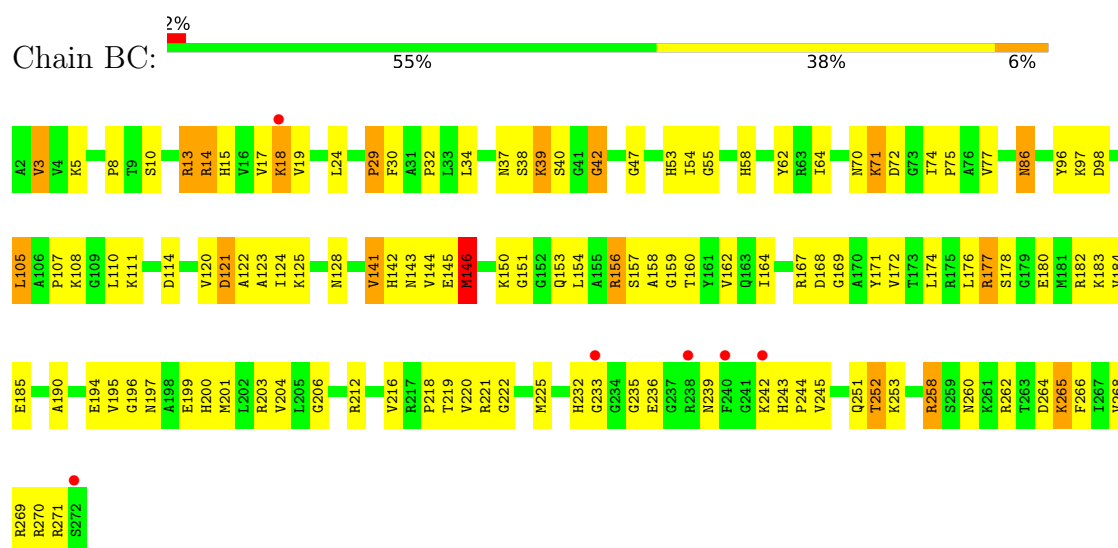
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C2063	U1993	A1821	C1748	A1674	U1599	G1526	G1452	U1379	G1311	G1239	C1172
C2064	C1994	G1822		G1674		G1527	A1453	G1380	U1312	U1240	U1173
C2065	U1995	G1823	U1751	C1675	U1603	A1528	C1454	G1381	U1313	U1241	U1174
C2066	C1996	U1827	C1752	A1676	A1602	G1529	G1455	G1382	U1314	U1242	A1175
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A2071	C2000	C1822	C1760	C1680	C1607	G1533	U1459	A1386	U1318	U1246	G1177
C2072	C2001	C1832	C1761	G1681	U1534	U1534	U1460	A1387	C1319	A1247	C1178
C2073			A1762	G1682	A1535	A1535	C1461		U1320	U1248	U1180
U2074	G2004	G1840	G1763	U1683	C1536	C1536	C1462	U1390	A1321	U1249	U1181
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	C2006	G1846		U1688	U1542		G1464	A1392	C1323	C1251	U1183
U2079	U2007	A1847	G1767	U1692			G1465	A1393	G1252	U1184	
A2080	C2008	A1848	C1768	U1693	A1545		U1468	A1394	A1253	G1195	
	A2009		U1769	C1694	A1469		A1469	U1395	U1254	G1196	
G2087	G2010	A1853	G1770	G1695	A1551		A1470	U1396	U1255	G1197	
	U2011	A1854			A1552		C1472	C1399	G1256	G1187	
C2091	G2012	U1855	A1773	G1696				U1400	U1257	U1188	
U2092	A2013	G1856	C1774		C1556				U1258	A1189	
G2093	A2014	G1857	U1775						G1259	G1190	
A2094		A1858		A1700					A1260		
A2095	U1943	A1859	U1779	C1706	U1559		G1475	C1404	G1335	G1195	
C2096	G1947	G1860	A1780	G1707			U1476	U1405	A1336	G1196	
A2097	G1948	G1861	U1781	C1708	U1563		A1477	U1406	G1337	G1197	
			U1782	U1709	C1564		G1478	G1407	G1338		
G2102	U1951	G1869	U1783	G1710	C1565		G1479	U1408	U1339	U1198	
C2103	C2023	C1870	A1784	G1711	C1566		U1480	U1409	U1340	U1199	
G2104	A1953	A1871	A1785		G1567		U1481	G1410	A1342	C1200	
C2105	G1954	A1872	A1786		G1568		G1482	U1411	A1268	U1201	
U2106	U1955	G1873	U1786		C1569		U1483	U1412	A1269		
U2107	U1956	C1874	U1715	U1716	A1569		U1484	A1413	G1270	A1205	
A2108	C1957	A1875	A1717	A1718	C1570		U1485	U1414	A1272	C1208	
U2109	C1958	G1876	G1718	C1639	A1571		U1486	U1415	U1273	U1209	
G2110		A1877	G1719	A1640	A1572			G1416	A1274	G1210	
U2111	C1961	G1878	U1720	A1641	G1573		A1490	G1417	A1275	G1211	
G2112	U1962	C1879	G1721		C1574		G1491	G1418	A1276	G1212	
U2113	C1963	A1880	C1726	G1642	U1575		G1492	A1419	G1277	A1213	
A2114	U1964	C1881	C1727	C1644	U1576		C1493	A1420	G1278	A1214	
G2115	C1965	U1882	C1728	G1645	C1577		A1494		G1281	G1215	
C2116	A1966	U1883	U1729	U1646	U1578		A1495	G1425	G1357	G1216	
U2117	G1967	G1888	U1730	U1647	A1579		A1496	A1427	G1358	U1217	
G2118	C1968		C1730	U1648	A1580		C1499	C1428	A1359	G1218	
A2119	A1969	C1895	G1731	G1649	G1581		G1500	G1429	G1360	U1219	
C2120	U1970	G1896	C1732	A1650	C1582		G1501	A1430	C1289	G1220	
U2121	U1971	G1897	A1903	G1651	U1584		A1502	A1431	G1296	U1222	
G2122	G1972	A1900	G1806	A1652	C1585		A1503	G1432	A1365	G1223	
C1973	C1974	A1901	G1807	G1653	A1586		A1504	A1433	A1366	U1224	
G1975	G1976	C1902	A1808	A1654	G1587		A1509	A1434	A1367	G1225	
U1977	A1977	G1903	G1738	A1655	U1588		G1510	G1435	G1368	A1226	
A2054	A1978	G1904	A1739	C1656	U1589		G1514	G1436	G1369	G1227	
C2055	G1905	C1905	G1740	G1661	A1590		A1515	C1437	A1301	G1228	
G1906	G1907		U1812		C1592		U1438	U1439	A1302	A1229	
A1981			U1741		C1593		A1516	A1439	G1372	A1230	
			U1742		A1594		G1516		A1373	U1231	
G1984			U1743		C1595		A1522		A1304	G1232	
			A1744		G1666				C1305		
			A1745		G1667				C1306		



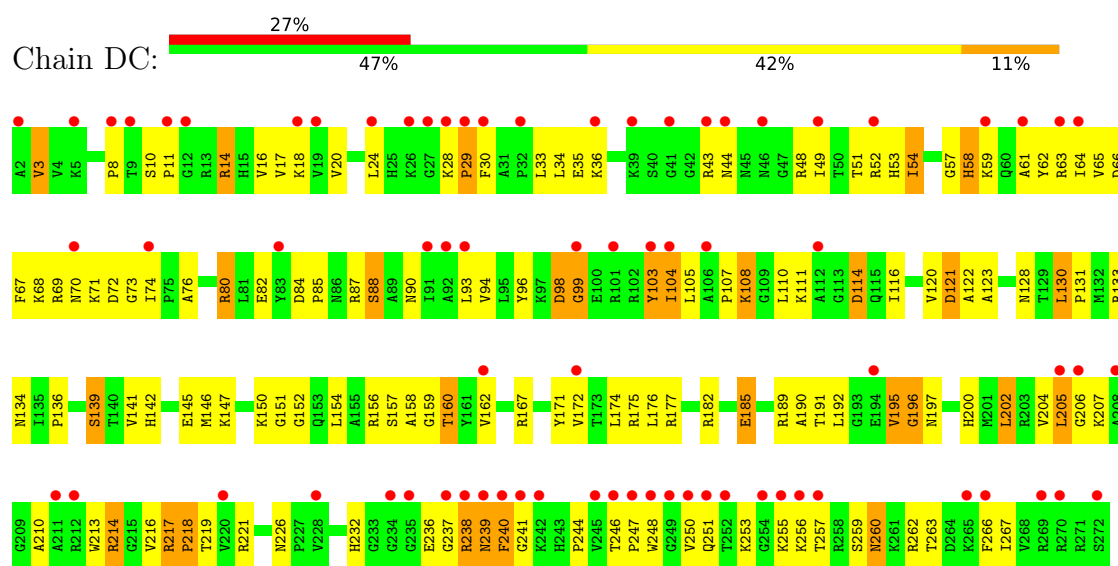
- Molecule 23: 5S rRNA



- Molecule 24: 50S ribosomal protein L2

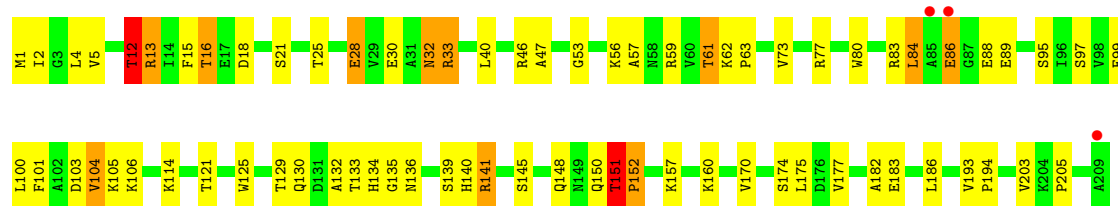


- Molecule 24: 50S ribosomal protein L2

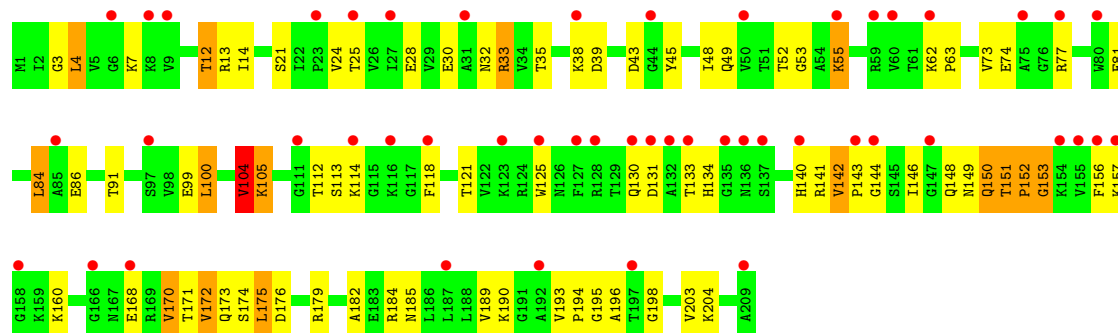


- Molecule 25: 50S ribosomal protein L3

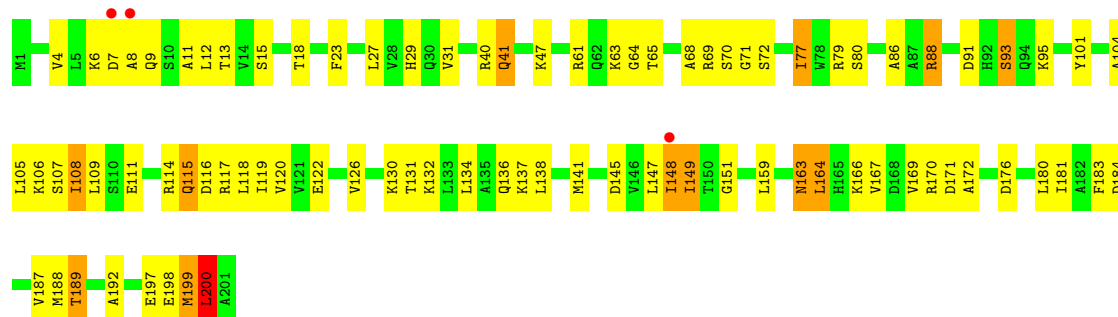




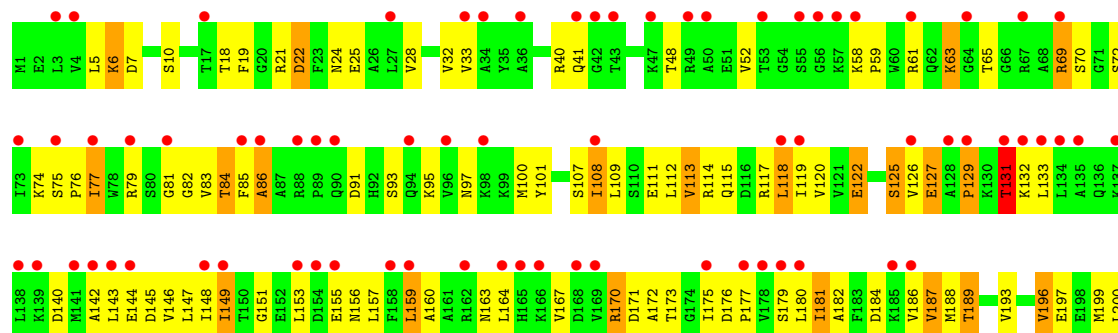
• Molecule 25: 50S ribosomal protein L3



• Molecule 26: 50S ribosomal protein L4

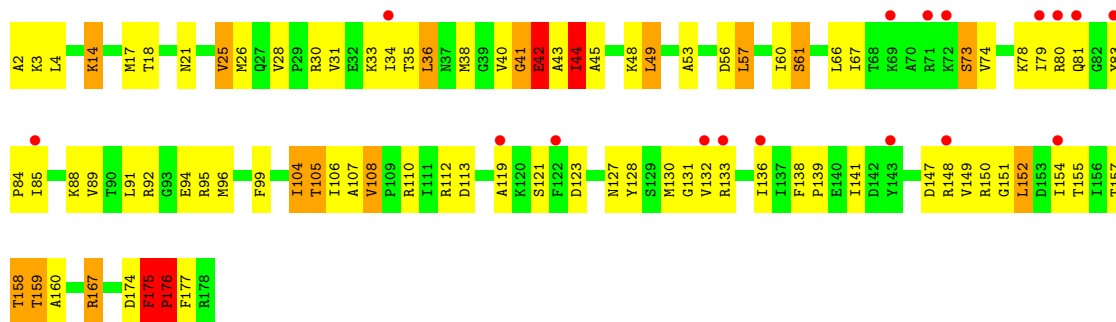


• Molecule 26: 50S ribosomal protein L4

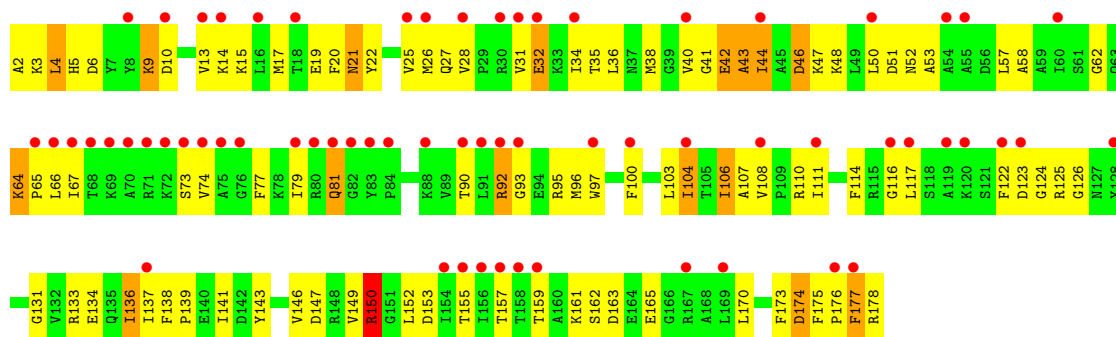
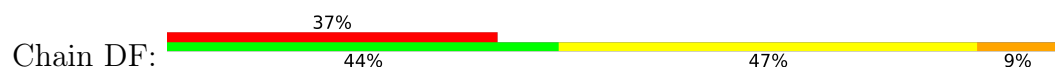


A201

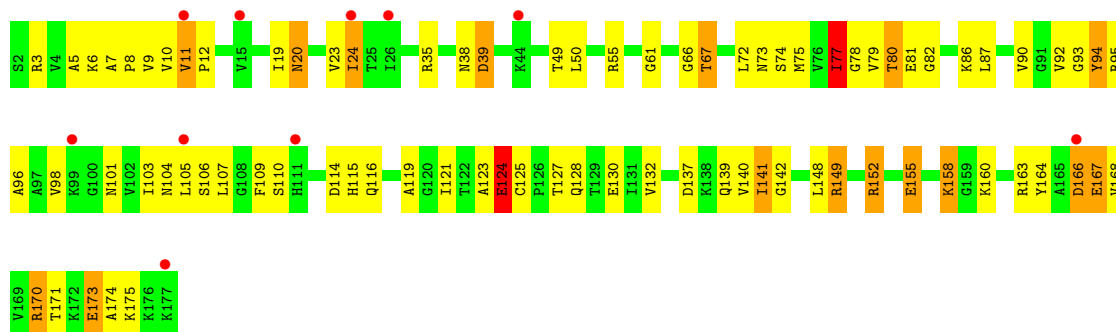
- Molecule 27: 50S ribosomal protein L5



- Molecule 27: 50S ribosomal protein L5

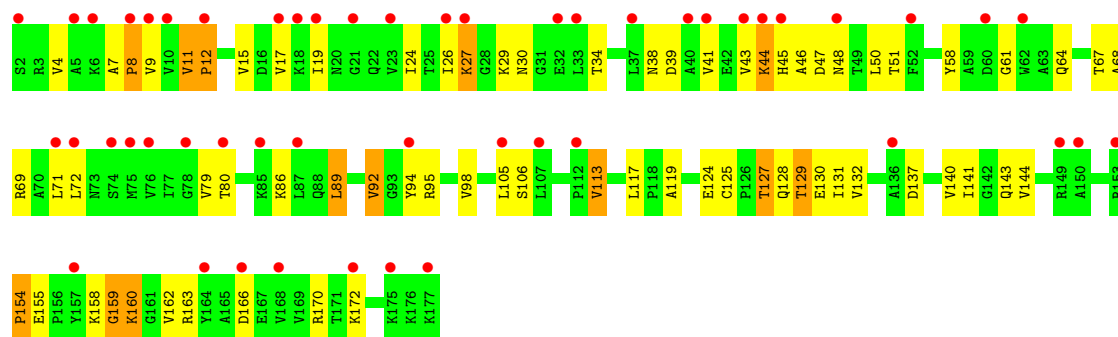


- Molecule 28: 50S ribosomal protein L6

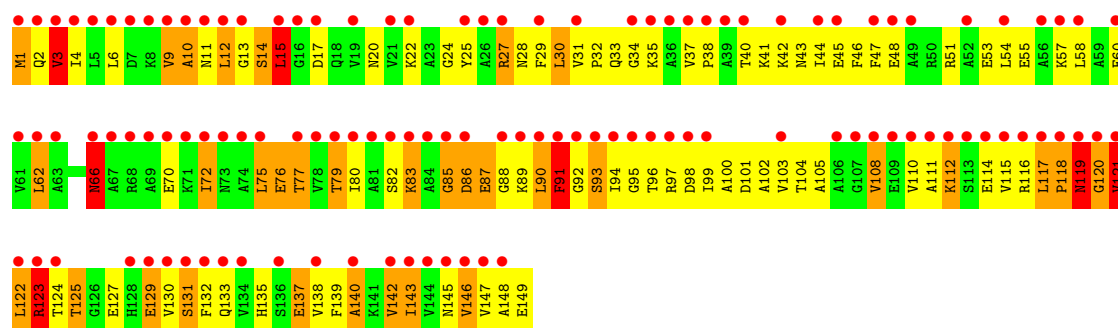
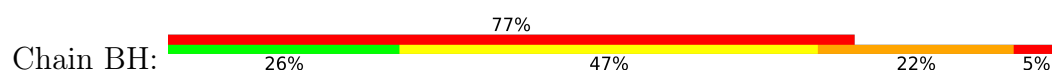


- Molecule 28: 50S ribosomal protein L6

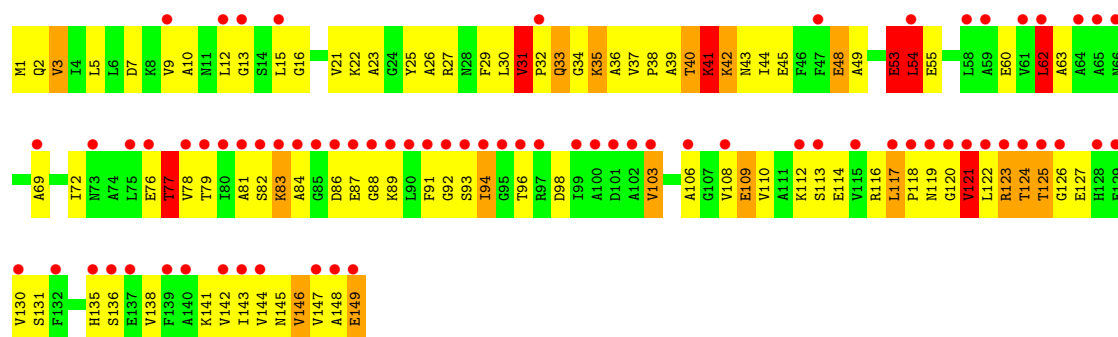




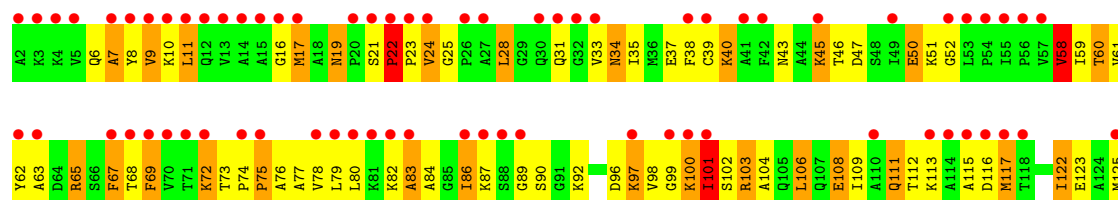
• Molecule 29: 50S ribosomal protein L9

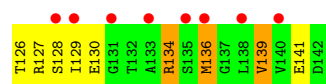


• Molecule 29: 50S ribosomal protein L9



• Molecule 30: 50S ribosomal protein L11

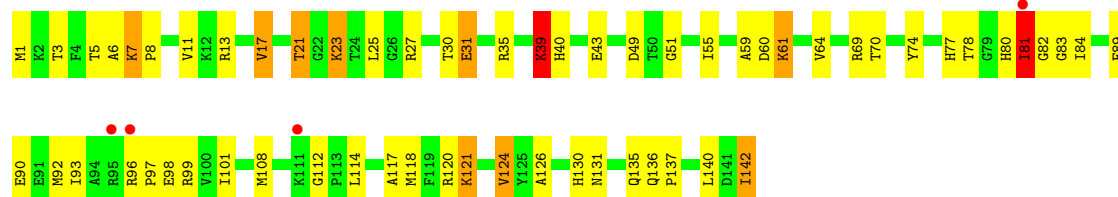




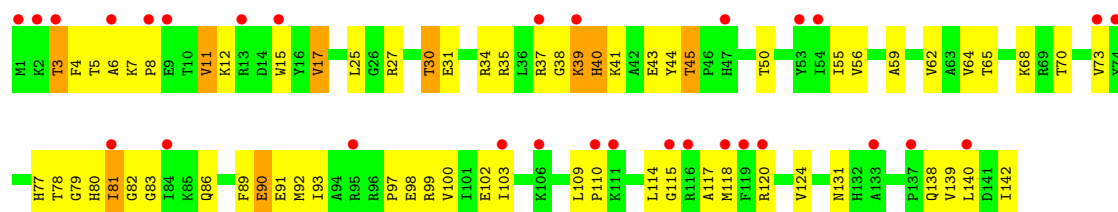
- Molecule 30: 50S ribosomal protein L11



- Molecule 31: 50S ribosomal protein L13



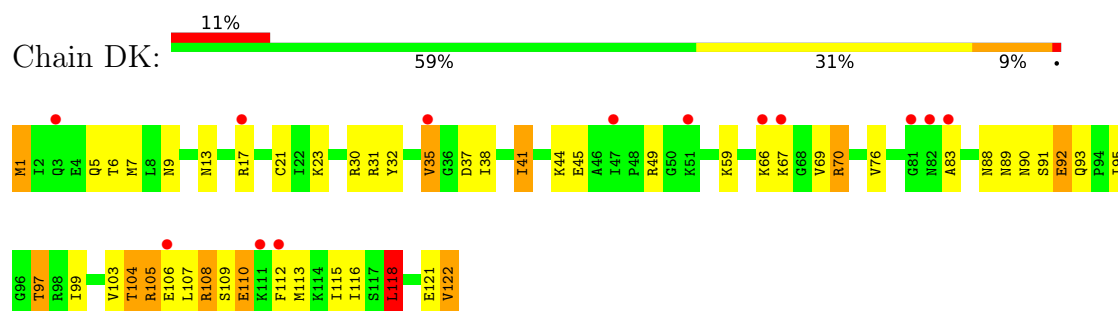
- Molecule 31: 50S ribosomal protein L13



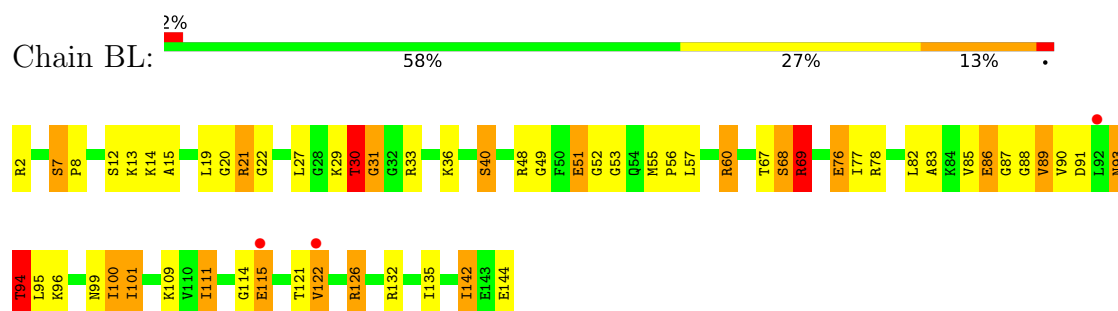
- Molecule 32: 50S ribosomal protein L14



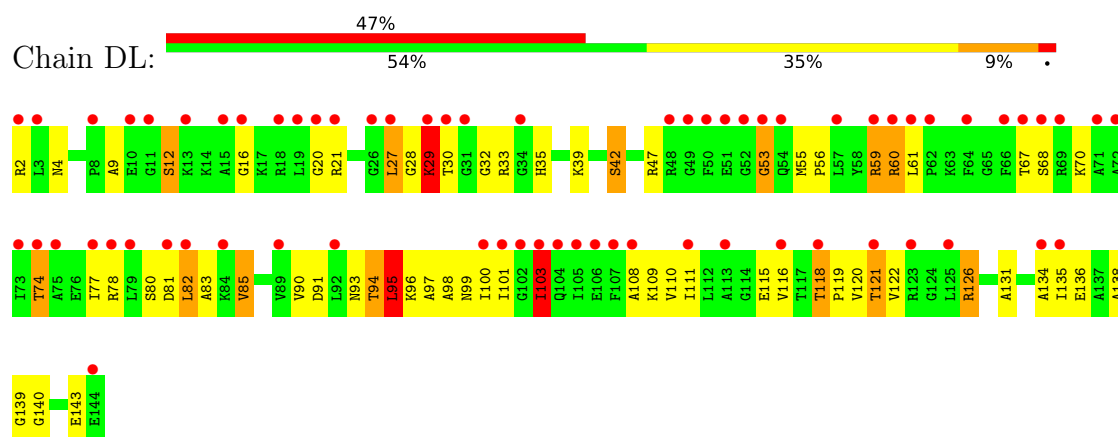
- Molecule 32: 50S ribosomal protein L14



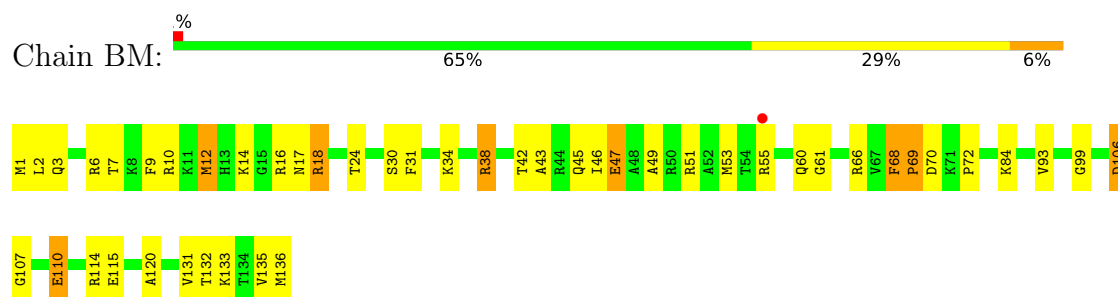
- Molecule 33: 50S ribosomal protein L15



- Molecule 33: 50S ribosomal protein L15

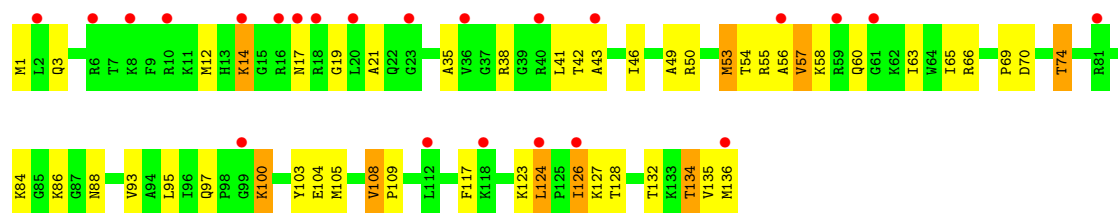


- Molecule 34: 50S ribosomal protein L16

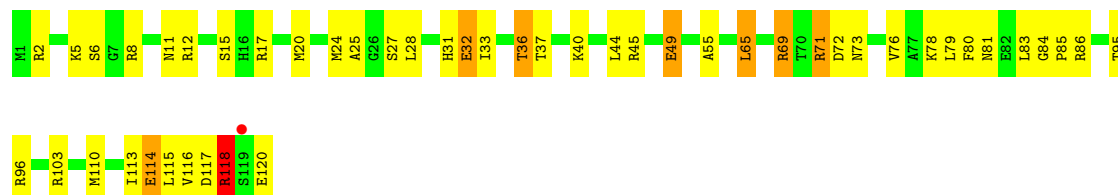


- Molecule 34: 50S ribosomal protein L16

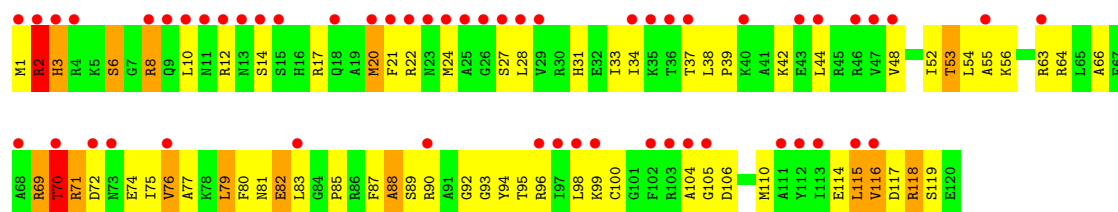




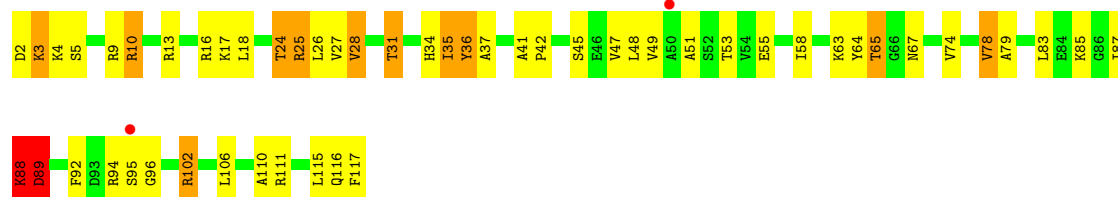
• Molecule 35: 50S ribosomal protein L17



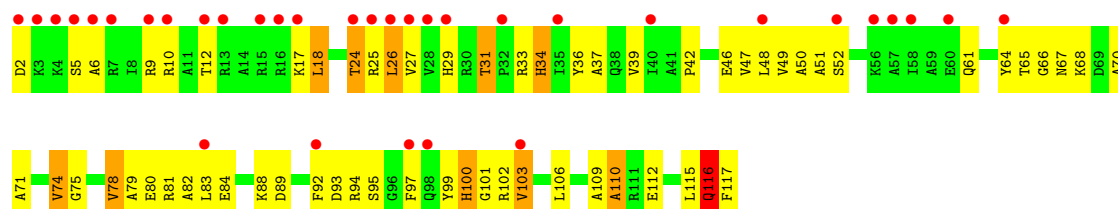
• Molecule 35: 50S ribosomal protein L17



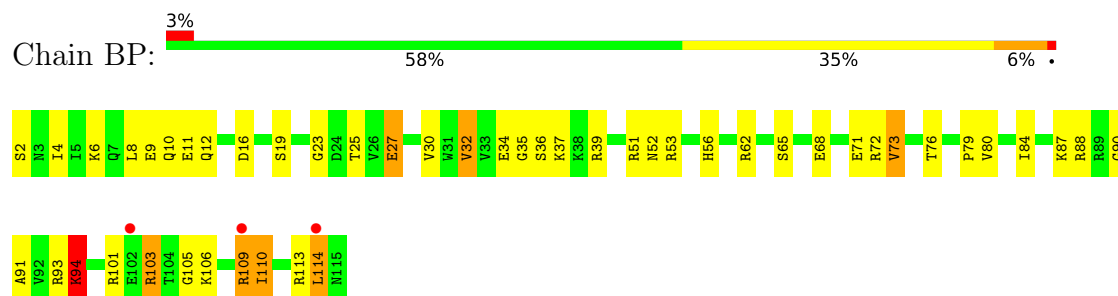
• Molecule 36: 50S ribosomal protein L18



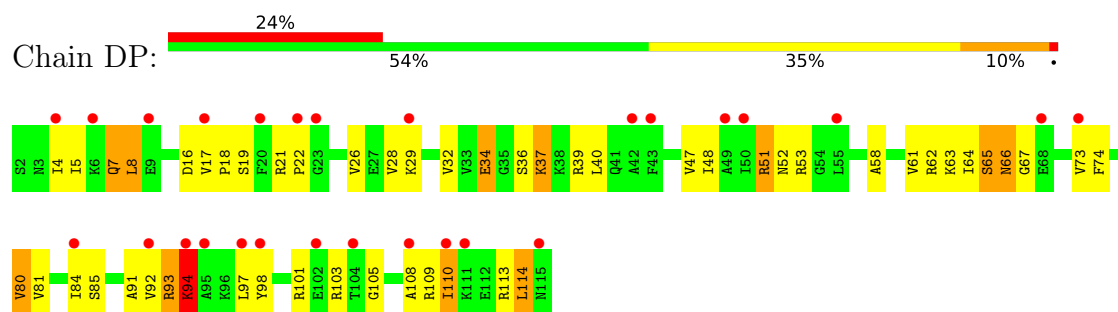
• Molecule 36: 50S ribosomal protein L18



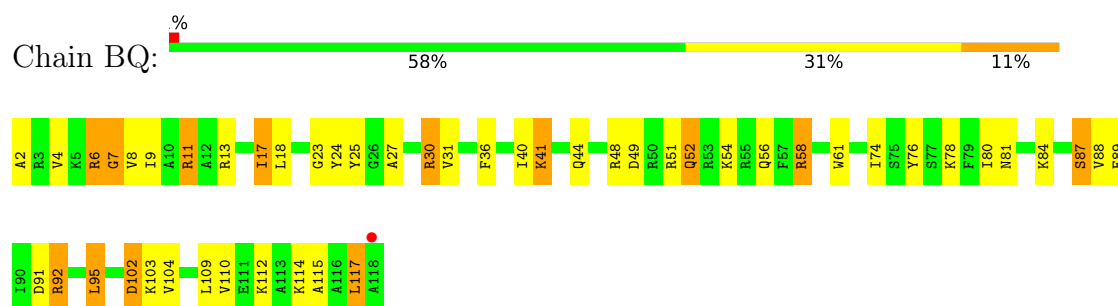
- Molecule 37: 50S ribosomal protein L19



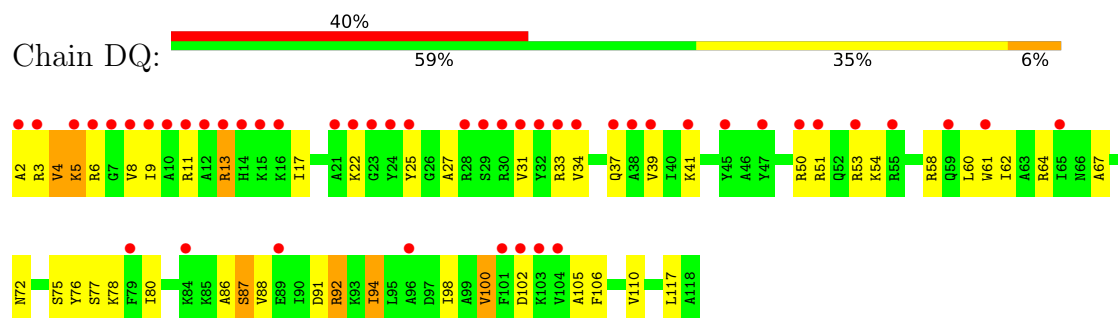
- Molecule 37: 50S ribosomal protein L19



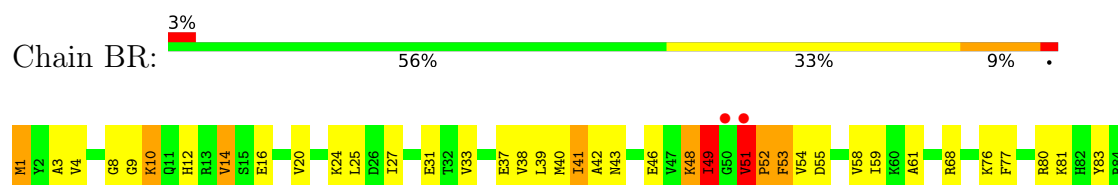
- Molecule 38: 50S ribosomal protein L20

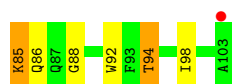


- Molecule 38: 50S ribosomal protein L20

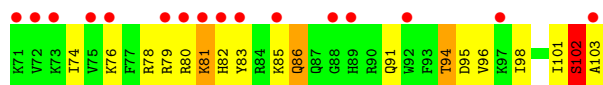
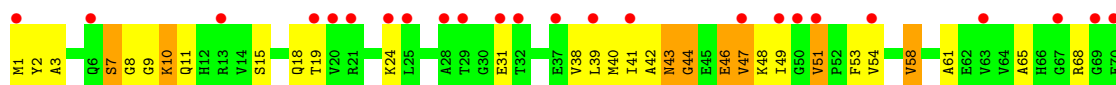
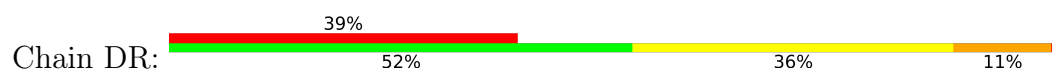


- Molecule 39: 50S ribosomal protein L21

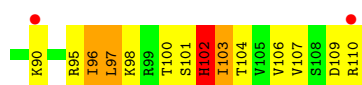




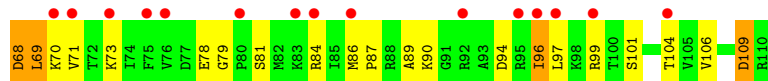
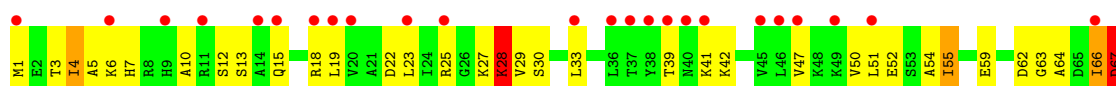
- Molecule 39: 50S ribosomal protein L21



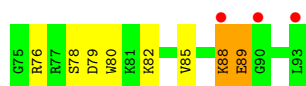
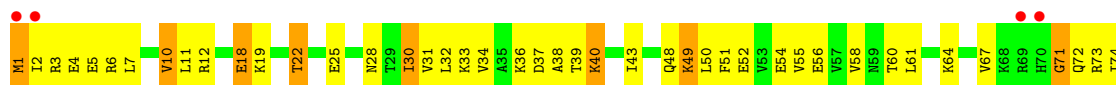
- Molecule 40: 50S ribosomal protein L22



- Molecule 40: 50S ribosomal protein L22

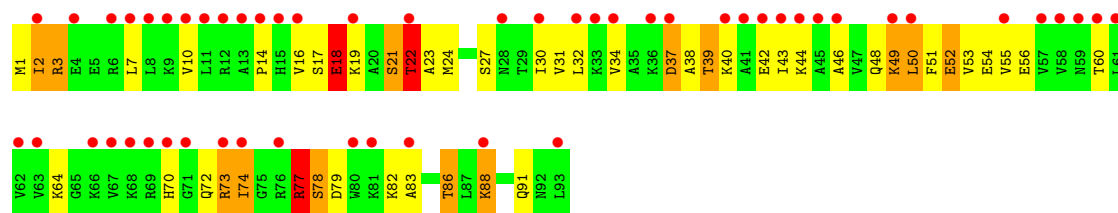


- Molecule 41: 50S ribosomal protein L23

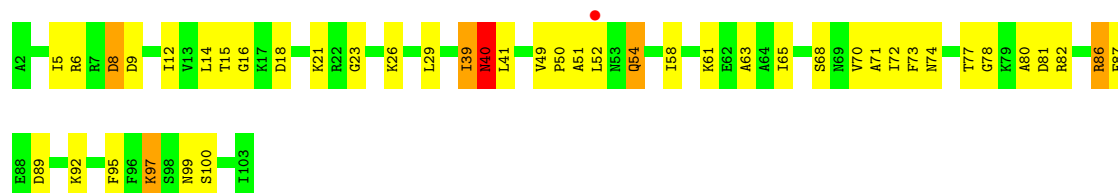


- Molecule 41: 50S ribosomal protein L23

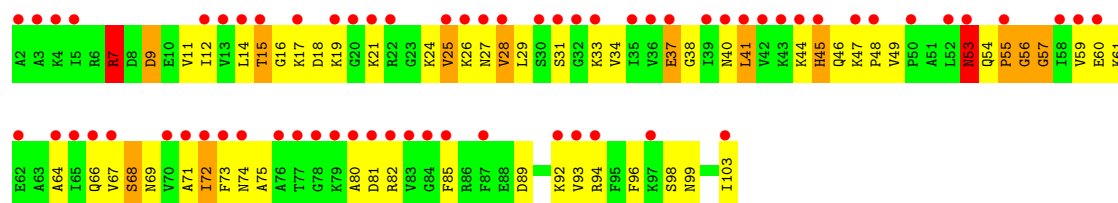




• Molecule 42: 50S ribosomal protein L24



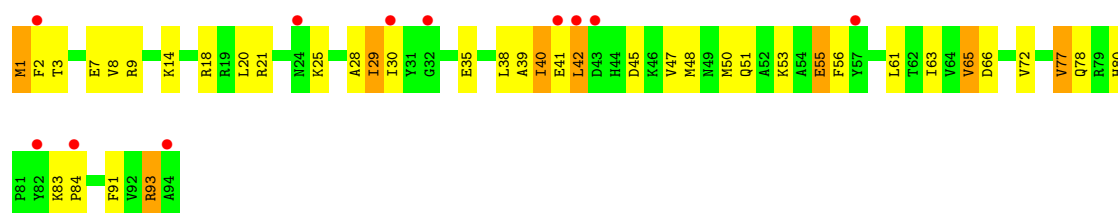
• Molecule 42: 50S ribosomal protein L24



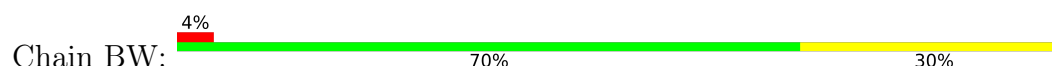
• Molecule 43: 50S ribosomal protein L25



• Molecule 43: 50S ribosomal protein L25

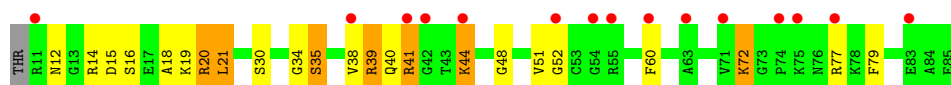
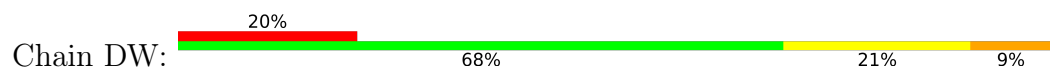


• Molecule 44: 50S ribosomal protein L27





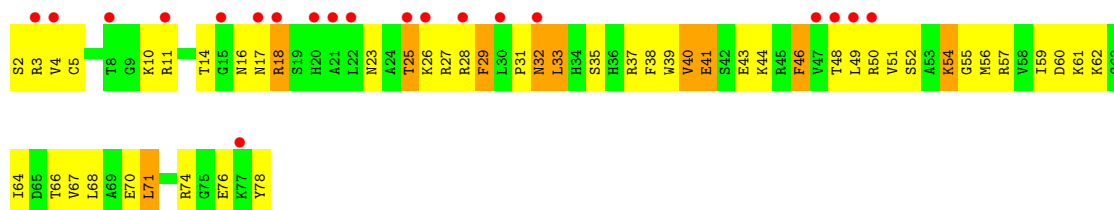
- Molecule 44: 50S ribosomal protein L27



- Molecule 45: 50S ribosomal protein L28



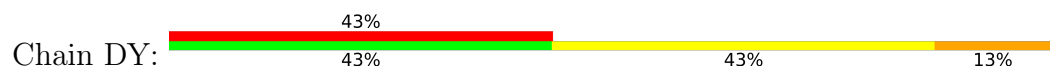
- Molecule 45: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L29



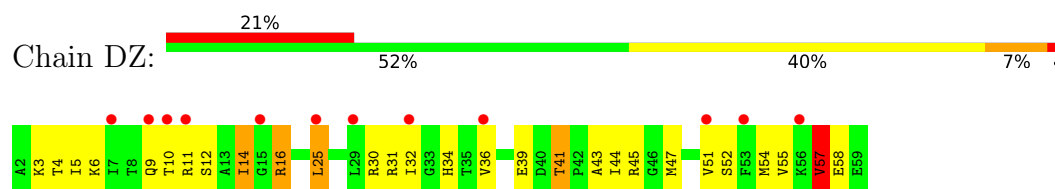
- Molecule 46: 50S ribosomal protein L29



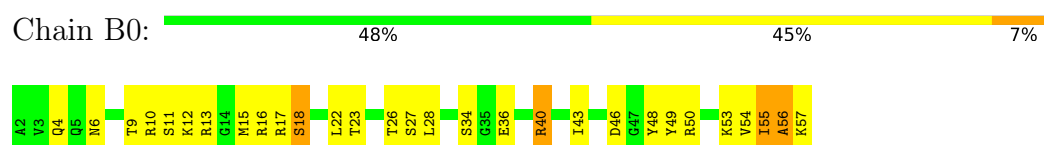
- Molecule 47: 50S ribosomal protein L30



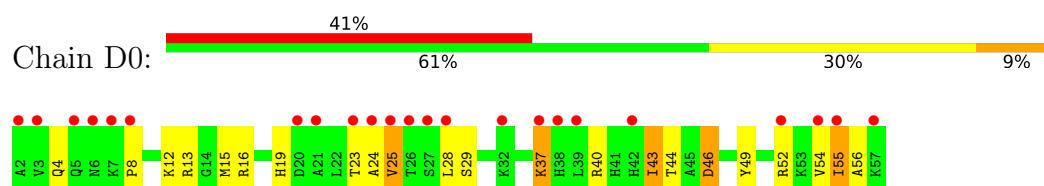
- Molecule 47: 50S ribosomal protein L30



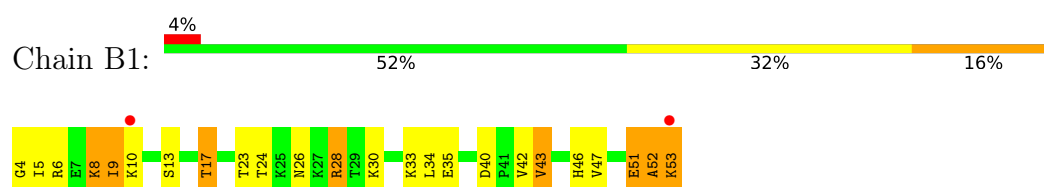
- Molecule 48: 50S ribosomal protein L32



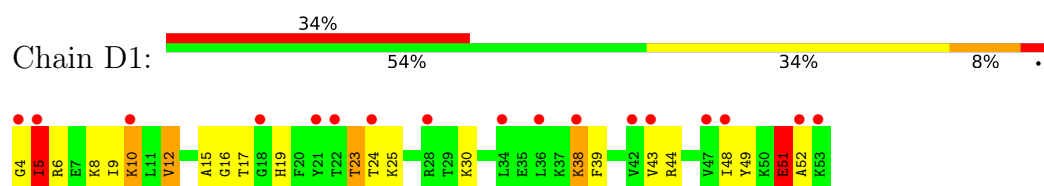
- Molecule 48: 50S ribosomal protein L32



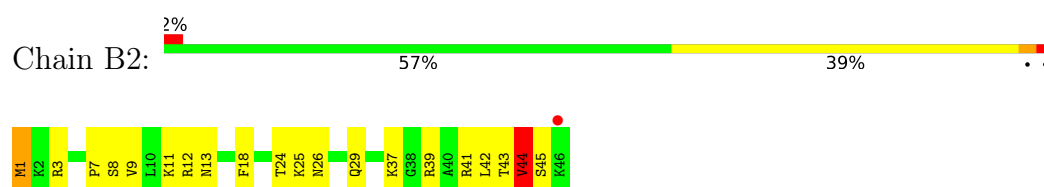
- Molecule 49: 50S ribosomal protein L33



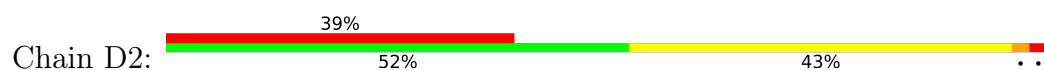
- Molecule 49: 50S ribosomal protein L33



- Molecule 50: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L34

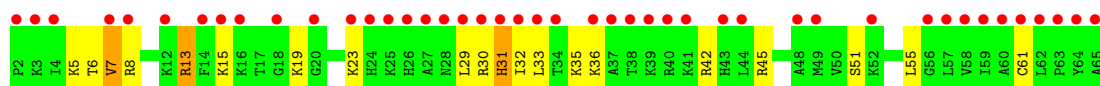




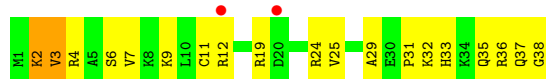
- Molecule 51: 50S ribosomal protein L35



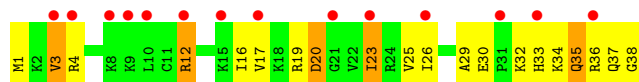
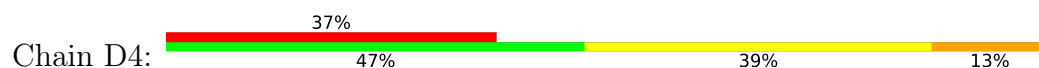
- Molecule 51: 50S ribosomal protein L35



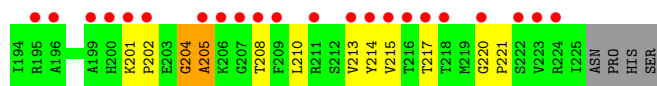
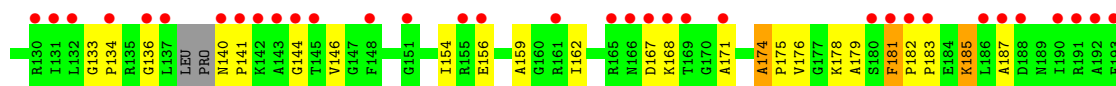
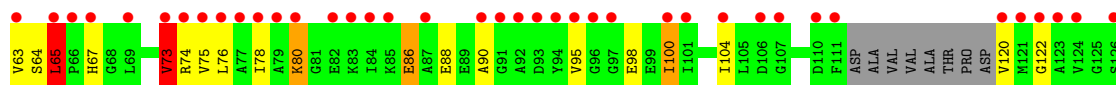
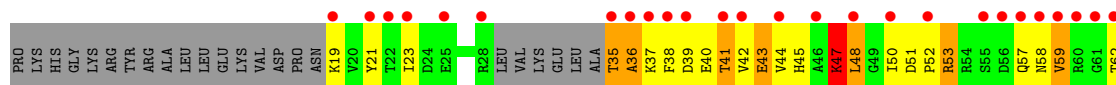
- Molecule 52: 50S ribosomal protein L36



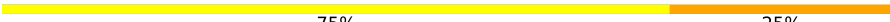
- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L1



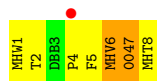
- Molecule 54: Quinupristin

Chain B6:  75% 25%



- Molecule 54: Quinupristin

Chain D6:  12% 12% 62% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.08Å 432.73Å 631.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.68 – 2.95 68.68 – 2.95	Depositor EDS
% Data completeness (in resolution range)	93.2 (68.68-2.95) 93.2 (68.68-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.248 , 0.282 0.249 , 0.284	Depositor DCC
R_{free} test set	4515 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	288328	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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, ZN, MHU, MHV, DBB, MHW, MHT, 004

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.24	0/36944	0.47	0/57632
1	CA	0.21	0/36966	0.44	1/57666 (0.0%)
2	AB	0.48	0/1736	1.12	10/2338 (0.4%)
2	CB	0.46	0/1736	1.04	8/2338 (0.3%)
3	AC	0.46	0/1652	1.01	8/2225 (0.4%)
3	CC	0.44	0/1652	0.93	0/2225
4	AD	0.44	0/1665	1.02	3/2227 (0.1%)
4	CD	0.51	0/1665	1.04	4/2227 (0.2%)
5	AE	0.55	0/1119	1.15	7/1504 (0.5%)
5	CE	0.52	0/1119	1.09	7/1504 (0.5%)
6	AF	0.53	0/836	1.05	6/1128 (0.5%)
6	CF	0.49	0/836	1.03	5/1128 (0.4%)
7	AG	0.43	0/1196	1.01	4/1602 (0.2%)
7	CG	0.42	0/1196	0.95	3/1602 (0.2%)
8	AH	0.47	0/989	1.04	4/1326 (0.3%)
8	CH	0.40	0/989	0.90	4/1326 (0.3%)
9	AI	0.41	0/1034	0.97	2/1375 (0.1%)
9	CI	0.43	0/1034	1.01	3/1375 (0.2%)
10	AJ	0.52	0/797	0.98	3/1077 (0.3%)
10	CJ	0.44	0/797	0.98	3/1077 (0.3%)
11	AK	0.51	0/893	0.99	2/1205 (0.2%)
11	CK	0.44	0/893	0.99	5/1205 (0.4%)
12	AL	0.50	0/969	0.98	0/1300
12	CL	0.45	0/969	1.07	4/1300 (0.3%)
13	AM	0.49	0/893	1.07	4/1193 (0.3%)
13	CM	0.48	0/893	1.03	3/1193 (0.3%)
14	AN	0.40	0/785	1.04	6/1043 (0.6%)
14	CN	0.38	0/785	0.95	2/1043 (0.2%)
15	AO	0.41	0/718	0.89	1/959 (0.1%)
15	CO	0.38	0/718	0.97	2/959 (0.2%)
16	AP	0.53	0/659	1.01	0/884
16	CP	0.41	0/659	0.89	1/884 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.50	0/658	0.99	1/881 (0.1%)
17	CQ	0.50	0/658	0.92	0/881
18	AR	0.37	0/463	0.93	0/621
18	CR	0.41	0/463	0.87	0/621
19	AS	0.41	0/653	1.13	7/877 (0.8%)
19	CS	0.46	0/653	0.98	2/877 (0.2%)
20	AT	0.49	0/671	0.99	2/888 (0.2%)
20	CT	0.44	0/671	1.02	1/888 (0.1%)
21	AU	0.57	0/431	1.14	3/570 (0.5%)
21	CU	0.54	0/431	1.07	1/570 (0.2%)
22	BA	0.37	0/69659	0.60	2/108672 (0.0%)
22	DA	0.21	0/69659	0.44	2/108672 (0.0%)
23	BB	0.33	0/2850	0.56	0/4444
23	DB	0.17	0/2828	0.37	0/4410
24	BC	0.57	0/2122	1.06	5/2852 (0.2%)
24	DC	0.44	0/2122	0.98	4/2852 (0.1%)
25	BD	0.66	0/1586	1.12	6/2134 (0.3%)
25	DD	0.44	0/1586	0.90	1/2134 (0.0%)
26	BE	0.57	0/1571	1.00	3/2113 (0.1%)
26	DE	0.44	0/1571	0.94	1/2113 (0.0%)
27	BF	0.51	0/1435	0.94	3/1926 (0.2%)
27	DF	0.40	0/1435	0.95	4/1926 (0.2%)
28	BG	0.51	0/1343	1.11	8/1816 (0.4%)
28	DG	0.42	0/1343	0.93	4/1816 (0.2%)
29	BH	0.48	0/1121	0.98	5/1515 (0.3%)
29	DH	0.47	0/1121	0.92	5/1515 (0.3%)
30	BI	0.59	0/1046	1.12	6/1410 (0.4%)
30	DI	0.54	0/1046	1.16	8/1410 (0.6%)
31	BJ	0.64	0/1152	1.07	8/1551 (0.5%)
31	DJ	0.40	0/1152	0.98	2/1551 (0.1%)
32	BK	0.62	0/948	1.06	2/1268 (0.2%)
32	DK	0.42	0/948	0.91	0/1268
33	BL	0.64	0/1054	1.18	9/1403 (0.6%)
33	DL	0.45	0/1054	1.05	5/1403 (0.4%)
34	BM	0.61	0/1093	1.00	3/1460 (0.2%)
34	DM	0.39	0/1093	0.87	0/1460
35	BN	0.64	0/974	1.06	5/1301 (0.4%)
35	DN	0.45	0/974	0.92	0/1301
36	BO	0.57	0/902	0.98	2/1209 (0.2%)
36	DO	0.38	0/902	0.93	3/1209 (0.2%)
37	BP	0.59	0/929	0.98	0/1242
37	DP	0.40	0/929	0.93	4/1242 (0.3%)
38	BQ	0.67	0/960	1.06	1/1278 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.40	0/960	0.91	2/1278 (0.2%)
39	BR	0.62	0/829	1.23	4/1107 (0.4%)
39	DR	0.45	0/829	1.03	3/1107 (0.3%)
40	BS	1.02	6/864 (0.7%)	1.22	7/1156 (0.6%)
40	DS	0.48	0/864	0.98	1/1156 (0.1%)
41	BT	0.58	0/745	1.06	3/994 (0.3%)
41	DT	0.44	0/745	0.92	0/994
42	BU	0.56	0/788	1.09	4/1051 (0.4%)
42	DU	0.50	0/788	0.97	0/1051
43	BV	0.54	0/766	0.95	0/1025
43	DV	0.37	0/766	0.92	3/1025 (0.3%)
44	BW	0.65	0/587	1.01	2/776 (0.3%)
44	DW	0.35	0/576	0.85	1/762 (0.1%)
45	BX	0.51	0/635	0.98	0/848
45	DX	0.42	0/635	0.96	2/848 (0.2%)
46	BY	0.53	0/510	1.12	4/677 (0.6%)
46	DY	0.41	0/510	0.95	1/677 (0.1%)
47	BZ	0.69	0/453	1.07	1/605 (0.2%)
47	DZ	0.43	0/453	0.96	1/605 (0.2%)
48	B0	0.68	0/450	1.05	0/599
48	D0	0.41	0/450	0.87	1/599 (0.2%)
49	B1	0.58	0/417	0.98	0/554
49	D1	0.44	0/417	0.81	1/554 (0.2%)
50	B2	0.65	0/380	1.06	0/498
50	D2	0.39	0/380	1.01	3/498 (0.6%)
51	B3	0.56	0/513	1.01	0/676
51	D3	0.38	0/513	0.83	0/676
52	B4	0.60	0/303	0.99	0/397
52	D4	0.65	1/303 (0.3%)	0.96	0/397
53	B5	0.50	0/1145	1.43	15/1556 (1.0%)
54	B6	1.90	0/13	2.90	1/15 (6.7%)
54	D6	1.61	0/13	3.28	2/15 (13.3%)
All	All	0.36	7/310652 (0.0%)	0.68	305/464396 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	CB	0	1
5	AE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	CE	0	2
6	CF	0	1
11	AK	0	1
11	CK	0	1
12	CL	0	2
21	AU	0	2
21	CU	0	1
25	BD	0	1
25	DD	0	1
26	BE	0	1
40	BS	0	1
All	All	0	16

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	BS	103	ILE	CA-CB	-10.16	1.42	1.54
40	BS	102	HIS	ND1-CE1	-8.61	1.24	1.32
40	BS	102	HIS	CB-CG	-8.36	1.38	1.50
52	D4	33	HIS	ND1-CE1	6.63	1.39	1.32
40	BS	102	HIS	CD2-NE2	-6.39	1.30	1.37

The worst 5 of 305 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	B5	220	GLY	CA-C-N	15.08	138.69	119.84
53	B5	220	GLY	C-N-CA	15.08	138.69	119.84
53	B5	174	ALA	CA-C-N	14.24	137.64	119.84
53	B5	174	ALA	C-N-CA	14.24	137.64	119.84
39	BR	51	VAL	CA-C-N	-14.12	102.19	119.84

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	123	VAL	Peptide
11	AK	126	LYS	Peptide
21	AU	39	GLU	Peptide
21	AU	8	GLU	Peptide
25	BD	151	THR	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	AA	32995	0	16607	609	14
1	CA	33015	0	16616	649	0
2	AB	1705	0	1732	138	0
2	CB	1705	0	1732	117	0
3	AC	1625	0	1696	77	0
3	CC	1625	0	1696	69	0
4	AD	1643	0	1707	98	0
4	CD	1643	0	1707	78	0
5	AE	1106	0	1148	64	0
5	CE	1106	0	1148	78	0
6	AF	818	0	808	38	0
6	CF	818	0	808	36	0
7	AG	1182	0	1238	50	0
7	CG	1182	0	1238	53	0
8	AH	979	0	1031	42	0
8	CH	979	0	1031	46	0
9	AI	1022	0	1070	56	0
9	CI	1022	0	1070	67	0
10	AJ	787	0	828	60	0
10	CJ	787	0	828	44	0
11	AK	877	0	887	56	0
11	CK	877	0	887	41	0
12	AL	955	0	1016	39	0
12	CL	955	0	1016	50	0
13	AM	884	0	941	48	0
13	CM	884	0	941	41	0
14	AN	774	0	824	43	0
14	CN	774	0	824	47	0
15	AO	710	0	728	23	0
15	CO	710	0	728	38	0
16	AP	649	0	666	36	0
16	CP	649	0	666	32	0
17	AQ	649	0	691	35	0
17	CQ	649	0	691	34	0
18	AR	456	0	478	13	0
18	CR	456	0	478	24	0
19	AS	638	0	665	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	638	0	665	31	0
20	AT	665	0	714	30	0
20	CT	665	0	714	35	0
21	AU	426	0	449	41	0
21	CU	426	0	449	28	0
22	BA	62195	0	31280	1058	0
22	DA	62195	0	31280	1204	1
23	BB	2549	0	1291	21	0
23	DB	2529	0	1281	44	0
24	BC	2083	0	2154	78	0
24	DC	2083	0	2154	97	0
25	BD	1565	0	1616	49	0
25	DD	1565	0	1616	58	0
26	BE	1552	0	1619	48	0
26	DE	1552	0	1619	65	0
27	BF	1411	0	1444	54	0
27	DF	1411	0	1444	52	0
28	BG	1323	0	1371	45	0
28	DG	1323	0	1371	39	0
29	BH	1110	0	1145	200	0
29	DH	1110	0	1148	96	13
30	BI	1032	0	1085	52	0
30	DI	1032	0	1085	59	0
31	BJ	1129	0	1162	31	0
31	DJ	1129	0	1162	50	0
32	BK	939	0	1012	36	0
32	DK	939	0	1012	29	0
33	BL	1045	0	1117	40	0
33	DL	1045	0	1117	46	0
34	BM	1074	0	1157	32	0
34	DM	1074	0	1157	28	0
35	BN	961	0	1000	39	0
35	DN	961	0	1000	49	0
36	BO	892	0	923	25	0
36	DO	892	0	923	42	0
37	BP	917	0	962	39	0
37	DP	917	0	962	35	0
38	BQ	947	0	1019	38	0
38	DQ	947	0	1019	46	0
39	BR	816	0	839	38	0
39	DR	816	0	839	37	0
40	BS	857	0	922	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DS	857	0	922	27	0
41	BT	739	0	807	27	0
41	DT	739	0	807	28	0
42	BU	780	0	831	17	0
42	DU	780	0	831	45	0
43	BV	753	0	780	16	0
43	DV	753	0	780	29	0
44	BW	580	0	594	14	0
44	DW	569	0	581	19	0
45	BX	625	0	652	29	0
45	DX	625	0	652	46	0
46	BY	509	0	543	25	0
46	DY	509	0	543	24	0
47	BZ	449	0	488	7	0
47	DZ	449	0	488	15	0
48	B0	444	0	458	20	0
48	D0	444	0	458	17	0
49	B1	410	0	440	15	0
49	D1	410	0	440	15	0
50	B2	377	0	418	13	0
50	D2	377	0	418	14	0
51	B3	504	0	572	18	0
51	D3	504	0	572	16	0
52	B4	302	0	341	15	0
52	D4	302	0	340	12	0
53	B5	1142	0	865	27	0
54	B6	73	0	64	5	0
54	D6	73	0	64	7	0
55	AA	71	0	0	0	0
55	AM	1	0	0	0	0
55	BA	195	0	0	0	0
55	BB	4	0	0	0	0
55	CA	55	0	0	0	0
55	CM	1	0	0	0	0
55	DA	167	0	0	0	0
55	DB	3	0	0	0	0
55	DQ	1	0	0	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	194	0	0	6	0
57	AL	1	0	0	0	0
57	AN	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AT	2	0	0	0	0
57	AU	1	0	0	1	0
57	B2	1	0	0	0	0
57	B3	3	0	0	0	0
57	B4	2	0	0	0	0
57	BA	619	0	0	59	0
57	BB	13	0	0	1	0
57	BC	8	0	0	1	0
57	BD	3	0	0	2	0
57	BE	3	0	0	0	0
57	BF	1	0	0	1	0
57	BG	1	0	0	0	0
57	BL	5	0	0	1	0
57	BN	5	0	0	1	0
57	BS	1	0	0	0	0
57	BV	1	0	0	0	0
57	CA	189	0	0	10	0
57	CL	1	0	0	0	0
57	CN	3	0	0	0	0
57	CT	4	0	0	0	0
57	CU	1	0	0	1	0
57	D0	1	0	0	0	0
57	D2	2	0	0	0	0
57	D3	1	0	0	0	0
57	D4	1	0	0	0	0
57	DA	612	0	0	63	0
57	DB	13	0	0	0	0
57	DC	7	0	0	1	0
57	DD	4	0	0	1	0
57	DE	4	0	0	0	0
57	DL	4	0	0	0	0
57	DN	1	0	0	0	0
57	DQ	2	0	0	0	0
57	DT	3	0	0	0	0
57	DV	1	0	0	0	0
All	All	288328	0	192913	6953	14

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 15.

The worst 5 of 6953 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)
29:BH:83:LYS:HD2	1:CA:55:A:O2'	1.21	1.29
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
29:BH:117:LEU:O	29:BH:121:VAL:CG2	1.95	1.14
29:BH:97:ARG:HD2	1:CA:369:G:O2'	1.51	1.09
29:BH:123:ARG:O	29:BH:124:THR:CG2	2.01	1.09

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:368:U:OP2	29:DH:123:ARG:NE[4_455]	1.50	0.70
1:AA:55:A:N1	29:DH:91:PHE:CE1[4_455]	1.60	0.60
1:AA:55:A:N3	29:DH:91:PHE:CZ[4_455]	1.66	0.54
1:AA:55:A:C2	29:DH:91:PHE:CE1[4_455]	1.70	0.50
1:AA:55:A:C2	29:DH:91:PHE:CZ[4_455]	1.71	0.49

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
2	AB	216/218 (99%)	130 (60%)	40 (18%)	46 (21%)	0	0
2	CB	216/218 (99%)	134 (62%)	47 (22%)	35 (16%)	0	0
3	AC	204/206 (99%)	158 (78%)	30 (15%)	16 (8%)	1	1
3	CC	204/206 (99%)	156 (76%)	33 (16%)	15 (7%)	1	1
4	AD	203/205 (99%)	150 (74%)	29 (14%)	24 (12%)	0	0
4	CD	203/205 (99%)	152 (75%)	29 (14%)	22 (11%)	0	0
5	AE	148/150 (99%)	112 (76%)	20 (14%)	16 (11%)	0	0
5	CE	148/150 (99%)	103 (70%)	20 (14%)	25 (17%)	0	0
6	AF	98/100 (98%)	72 (74%)	15 (15%)	11 (11%)	0	0
6	CF	98/100 (98%)	69 (70%)	14 (14%)	15 (15%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	110 (74%)	30 (20%)	9 (6%)	1	2
7	CG	149/151 (99%)	118 (79%)	22 (15%)	9 (6%)	1	2
8	AH	127/129 (98%)	94 (74%)	26 (20%)	7 (6%)	1	3
8	CH	127/129 (98%)	103 (81%)	17 (13%)	7 (6%)	1	3
9	AI	125/127 (98%)	96 (77%)	20 (16%)	9 (7%)	1	1
9	CI	125/127 (98%)	97 (78%)	20 (16%)	8 (6%)	1	2
10	AJ	96/98 (98%)	67 (70%)	12 (12%)	17 (18%)	0	0
10	CJ	96/98 (98%)	70 (73%)	14 (15%)	12 (12%)	0	0
11	AK	115/117 (98%)	90 (78%)	16 (14%)	9 (8%)	1	1
11	CK	115/117 (98%)	85 (74%)	21 (18%)	9 (8%)	1	1
12	AL	121/123 (98%)	96 (79%)	19 (16%)	6 (5%)	1	3
12	CL	121/123 (98%)	97 (80%)	13 (11%)	11 (9%)	0	1
13	AM	112/114 (98%)	85 (76%)	16 (14%)	11 (10%)	0	1
13	CM	112/114 (98%)	82 (73%)	19 (17%)	11 (10%)	0	1
14	AN	92/100 (92%)	61 (66%)	20 (22%)	11 (12%)	0	0
14	CN	92/100 (92%)	61 (66%)	15 (16%)	16 (17%)	0	0
15	AO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	3	7
15	CO	86/88 (98%)	68 (79%)	14 (16%)	4 (5%)	2	4
16	AP	80/82 (98%)	49 (61%)	15 (19%)	16 (20%)	0	0
16	CP	80/82 (98%)	59 (74%)	17 (21%)	4 (5%)	1	3
17	AQ	78/80 (98%)	57 (73%)	11 (14%)	10 (13%)	0	0
17	CQ	78/80 (98%)	53 (68%)	17 (22%)	8 (10%)	0	0
18	AR	53/55 (96%)	45 (85%)	4 (8%)	4 (8%)	1	1
18	CR	53/55 (96%)	40 (76%)	8 (15%)	5 (9%)	0	1
19	AS	77/79 (98%)	55 (71%)	14 (18%)	8 (10%)	0	0
19	CS	77/79 (98%)	61 (79%)	13 (17%)	3 (4%)	2	5
20	AT	83/85 (98%)	66 (80%)	12 (14%)	5 (6%)	1	2
20	CT	83/85 (98%)	68 (82%)	9 (11%)	6 (7%)	1	1
21	AU	49/51 (96%)	29 (59%)	9 (18%)	11 (22%)	0	0
21	CU	49/51 (96%)	29 (59%)	6 (12%)	14 (29%)	0	0
24	BC	269/271 (99%)	217 (81%)	41 (15%)	11 (4%)	2	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	DC	269/271 (99%)	209 (78%)	42 (16%)	18 (7%)	1	1
25	BD	207/209 (99%)	183 (88%)	19 (9%)	5 (2%)	4	13
25	DD	207/209 (99%)	173 (84%)	29 (14%)	5 (2%)	4	13
26	BE	199/201 (99%)	171 (86%)	22 (11%)	6 (3%)	3	9
26	DE	199/201 (99%)	157 (79%)	29 (15%)	13 (6%)	1	1
27	BF	175/177 (99%)	144 (82%)	23 (13%)	8 (5%)	2	4
27	DF	175/177 (99%)	146 (83%)	17 (10%)	12 (7%)	1	1
28	BG	174/176 (99%)	147 (84%)	15 (9%)	12 (7%)	1	1
28	DG	174/176 (99%)	138 (79%)	25 (14%)	11 (6%)	1	2
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	0
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	0	0
30	BI	139/141 (99%)	78 (56%)	37 (27%)	24 (17%)	0	0
30	DI	139/141 (99%)	80 (58%)	44 (32%)	15 (11%)	0	0
31	BJ	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	2	6
31	DJ	140/142 (99%)	123 (88%)	15 (11%)	2 (1%)	9	24
32	BK	120/122 (98%)	98 (82%)	13 (11%)	9 (8%)	1	1
32	DK	120/122 (98%)	100 (83%)	14 (12%)	6 (5%)	1	3
33	BL	141/143 (99%)	109 (77%)	20 (14%)	12 (8%)	0	1
33	DL	141/143 (99%)	105 (74%)	29 (21%)	7 (5%)	1	3
34	BM	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	8	23
34	DM	134/136 (98%)	112 (84%)	19 (14%)	3 (2%)	5	15
35	BN	118/120 (98%)	96 (81%)	21 (18%)	1 (1%)	16	37
35	DN	118/120 (98%)	97 (82%)	11 (9%)	10 (8%)	0	1
36	BO	114/116 (98%)	95 (83%)	15 (13%)	4 (4%)	3	7
36	DO	114/116 (98%)	96 (84%)	14 (12%)	4 (4%)	3	7
37	BP	112/114 (98%)	98 (88%)	9 (8%)	5 (4%)	2	4
37	DP	112/114 (98%)	91 (81%)	16 (14%)	5 (4%)	2	4
38	BQ	115/117 (98%)	107 (93%)	3 (3%)	5 (4%)	2	4
38	DQ	115/117 (98%)	108 (94%)	6 (5%)	1 (1%)	14	34
39	BR	101/103 (98%)	86 (85%)	8 (8%)	7 (7%)	1	1
39	DR	101/103 (98%)	77 (76%)	20 (20%)	4 (4%)	2	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BS	108/110 (98%)	100 (93%)	5 (5%)	3 (3%)	4	11
40	DS	108/110 (98%)	89 (82%)	14 (13%)	5 (5%)	2	4
41	BT	91/93 (98%)	70 (77%)	13 (14%)	8 (9%)	0	1
41	DT	91/93 (98%)	70 (77%)	9 (10%)	12 (13%)	0	0
42	BU	100/102 (98%)	80 (80%)	12 (12%)	8 (8%)	1	1
42	DU	100/102 (98%)	73 (73%)	17 (17%)	10 (10%)	0	0
43	BV	92/94 (98%)	85 (92%)	6 (6%)	1 (1%)	11	29
43	DV	92/94 (98%)	82 (89%)	8 (9%)	2 (2%)	5	15
44	BW	74/76 (97%)	67 (90%)	7 (10%)	0	100	100
44	DW	73/76 (96%)	65 (89%)	6 (8%)	2 (3%)	4	11
45	BX	75/77 (97%)	72 (96%)	1 (1%)	2 (3%)	4	11
45	DX	75/77 (97%)	64 (85%)	9 (12%)	2 (3%)	4	11
46	BY	61/63 (97%)	40 (66%)	12 (20%)	9 (15%)	0	0
46	DY	61/63 (97%)	49 (80%)	8 (13%)	4 (7%)	1	1
47	BZ	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
47	DZ	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	2	6
48	B0	54/56 (96%)	46 (85%)	5 (9%)	3 (6%)	1	2
48	D0	54/56 (96%)	41 (76%)	11 (20%)	2 (4%)	2	6
49	B1	48/50 (96%)	38 (79%)	6 (12%)	4 (8%)	0	1
49	D1	48/50 (96%)	37 (77%)	8 (17%)	3 (6%)	1	2
50	B2	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	2	4
50	D2	44/46 (96%)	38 (86%)	4 (9%)	2 (4%)	2	4
51	B3	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	7	21
51	D3	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	7	21
52	B4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
52	D4	36/38 (95%)	33 (92%)	1 (3%)	2 (6%)	1	2
53	B5	183/228 (80%)	94 (51%)	54 (30%)	35 (19%)	0	0
54	B6	2/8 (25%)	2 (100%)	0	0	100	100
54	D6	2/8 (25%)	2 (100%)	0	0	100	100
All	All	11422/11688 (98%)	8887 (78%)	1654 (14%)	881 (8%)	1	1

5 of 881 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	PHE
2	AB	22	TYR
2	AB	34	ALA
2	AB	64	LYS
2	AB	73	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	
2	AB	180/180 (100%)	113 (63%)	67 (37%)	0	0
2	CB	180/180 (100%)	127 (71%)	53 (29%)	0	0
3	AC	170/170 (100%)	131 (77%)	39 (23%)	1	2
3	CC	170/170 (100%)	134 (79%)	36 (21%)	1	2
4	AD	172/172 (100%)	129 (75%)	43 (25%)	0	1
4	CD	172/172 (100%)	136 (79%)	36 (21%)	1	2
5	AE	113/113 (100%)	79 (70%)	34 (30%)	0	0
5	CE	113/113 (100%)	84 (74%)	29 (26%)	0	1
6	AF	87/87 (100%)	60 (69%)	27 (31%)	0	0
6	CF	87/87 (100%)	60 (69%)	27 (31%)	0	0
7	AG	124/124 (100%)	89 (72%)	35 (28%)	0	0
7	CG	124/124 (100%)	92 (74%)	32 (26%)	0	1
8	AH	104/104 (100%)	75 (72%)	29 (28%)	0	0
8	CH	104/104 (100%)	80 (77%)	24 (23%)	1	2
9	AI	105/105 (100%)	77 (73%)	28 (27%)	0	0
9	CI	105/105 (100%)	75 (71%)	30 (29%)	0	0
10	AJ	86/86 (100%)	60 (70%)	26 (30%)	0	0
10	CJ	86/86 (100%)	63 (73%)	23 (27%)	0	0
11	AK	90/90 (100%)	68 (76%)	22 (24%)	1	1
11	CK	90/90 (100%)	66 (73%)	24 (27%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	103/103 (100%)	80 (78%)	23 (22%)	1	2
12	CL	103/103 (100%)	78 (76%)	25 (24%)	1	1
13	AM	92/92 (100%)	71 (77%)	21 (23%)	1	2
13	CM	92/92 (100%)	69 (75%)	23 (25%)	0	1
14	AN	79/83 (95%)	59 (75%)	20 (25%)	0	1
14	CN	79/83 (95%)	67 (85%)	12 (15%)	3	8
15	AO	75/76 (99%)	59 (79%)	16 (21%)	1	2
15	CO	75/76 (99%)	58 (77%)	17 (23%)	1	2
16	AP	65/65 (100%)	51 (78%)	14 (22%)	1	2
16	CP	65/65 (100%)	48 (74%)	17 (26%)	0	1
17	AQ	74/74 (100%)	52 (70%)	22 (30%)	0	0
17	CQ	74/74 (100%)	52 (70%)	22 (30%)	0	0
18	AR	48/48 (100%)	39 (81%)	9 (19%)	1	4
18	CR	48/48 (100%)	40 (83%)	8 (17%)	2	6
19	AS	70/70 (100%)	57 (81%)	13 (19%)	1	4
19	CS	70/70 (100%)	51 (73%)	19 (27%)	0	0
20	AT	65/65 (100%)	46 (71%)	19 (29%)	0	0
20	CT	65/65 (100%)	45 (69%)	20 (31%)	0	0
21	AU	44/44 (100%)	28 (64%)	16 (36%)	0	0
21	CU	44/44 (100%)	32 (73%)	12 (27%)	0	0
24	BC	216/216 (100%)	183 (85%)	33 (15%)	3	8
24	DC	216/216 (100%)	175 (81%)	41 (19%)	1	3
25	BD	164/164 (100%)	142 (87%)	22 (13%)	4	11
25	DD	164/164 (100%)	142 (87%)	22 (13%)	4	11
26	BE	165/165 (100%)	137 (83%)	28 (17%)	2	5
26	DE	165/165 (100%)	128 (78%)	37 (22%)	1	2
27	BF	148/148 (100%)	116 (78%)	32 (22%)	1	2
27	DF	148/148 (100%)	114 (77%)	34 (23%)	1	2
28	BG	137/137 (100%)	114 (83%)	23 (17%)	2	6
28	DG	137/137 (100%)	121 (88%)	16 (12%)	5	16
29	BH	114/114 (100%)	81 (71%)	33 (29%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DH	114/114 (100%)	89 (78%)	25 (22%)	1	2
30	BI	109/109 (100%)	78 (72%)	31 (28%)	0	0
30	DI	109/109 (100%)	83 (76%)	26 (24%)	1	1
31	BJ	116/116 (100%)	96 (83%)	20 (17%)	2	5
31	DJ	116/116 (100%)	99 (85%)	17 (15%)	3	9
32	BK	103/103 (100%)	90 (87%)	13 (13%)	4	13
32	DK	103/103 (100%)	88 (85%)	15 (15%)	3	9
33	BL	102/102 (100%)	79 (78%)	23 (22%)	1	2
33	DL	102/102 (100%)	80 (78%)	22 (22%)	1	2
34	BM	109/109 (100%)	95 (87%)	14 (13%)	4	13
34	DM	109/109 (100%)	96 (88%)	13 (12%)	5	15
35	BN	100/100 (100%)	87 (87%)	13 (13%)	4	12
35	DN	100/100 (100%)	83 (83%)	17 (17%)	2	5
36	BO	86/86 (100%)	57 (66%)	29 (34%)	0	0
36	DO	86/86 (100%)	69 (80%)	17 (20%)	1	3
37	BP	99/99 (100%)	86 (87%)	13 (13%)	4	12
37	DP	99/99 (100%)	77 (78%)	22 (22%)	1	2
38	BQ	89/89 (100%)	71 (80%)	18 (20%)	1	3
38	DQ	89/89 (100%)	75 (84%)	14 (16%)	2	8
39	BR	84/84 (100%)	70 (83%)	14 (17%)	2	6
39	DR	84/84 (100%)	69 (82%)	15 (18%)	2	4
40	BS	93/93 (100%)	75 (81%)	18 (19%)	1	3
40	DS	93/93 (100%)	72 (77%)	21 (23%)	1	2
41	BT	80/80 (100%)	67 (84%)	13 (16%)	2	7
41	DT	80/80 (100%)	64 (80%)	16 (20%)	1	3
42	BU	83/83 (100%)	67 (81%)	16 (19%)	1	3
42	DU	83/83 (100%)	61 (74%)	22 (26%)	0	1
43	BV	78/78 (100%)	65 (83%)	13 (17%)	2	6
43	DV	78/78 (100%)	64 (82%)	14 (18%)	2	4
44	BW	57/58 (98%)	51 (90%)	6 (10%)	6	19
44	DW	56/58 (97%)	48 (86%)	8 (14%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BX	67/67 (100%)	54 (81%)	13 (19%)	1	3
45	DX	67/67 (100%)	52 (78%)	15 (22%)	1	2
46	BY	55/55 (100%)	46 (84%)	9 (16%)	2	7
46	DY	55/55 (100%)	42 (76%)	13 (24%)	1	1
47	BZ	48/48 (100%)	39 (81%)	9 (19%)	1	4
47	DZ	48/48 (100%)	39 (81%)	9 (19%)	1	4
48	B0	47/47 (100%)	40 (85%)	7 (15%)	3	8
48	D0	47/47 (100%)	41 (87%)	6 (13%)	4	13
49	B1	45/45 (100%)	36 (80%)	9 (20%)	1	3
49	D1	45/45 (100%)	38 (84%)	7 (16%)	2	8
50	B2	38/38 (100%)	33 (87%)	5 (13%)	4	12
50	D2	38/38 (100%)	32 (84%)	6 (16%)	2	8
51	B3	51/51 (100%)	46 (90%)	5 (10%)	7	21
51	D3	51/51 (100%)	46 (90%)	5 (10%)	7	21
52	B4	34/34 (100%)	29 (85%)	5 (15%)	3	9
52	D4	34/34 (100%)	28 (82%)	6 (18%)	2	5
53	B5	61/180 (34%)	44 (72%)	17 (28%)	0	0
54	B6	2/2 (100%)	2 (100%)	0	100	100
54	D6	2/2 (100%)	2 (100%)	0	100	100
All	All	9390/9522 (99%)	7373 (78%)	2017 (22%)	1	2

5 of 2017 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BU	72	ILE
34	DM	57	VAL
4	CD	189	SER
33	DL	59	ARG
41	DT	7	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
10	CJ	58	ASN

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Mol	Chain	Res	Type
24	DC	251	GLN
46	DY	45	GLN
11	CK	15	GLN
18	CR	52	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	358 (23%)	16 (1%)
1	CA	1538/1539 (99%)	338 (21%)	9 (0%)
22	BA	2895/2903 (99%)	563 (19%)	28 (0%)
22	DA	2895/2903 (99%)	645 (22%)	34 (1%)
23	BB	118/119 (99%)	23 (19%)	0
23	DB	117/119 (98%)	25 (21%)	0
All	All	9100/9122 (99%)	1952 (21%)	87 (0%)

5 of 1952 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	7	A
1	AA	9	G
1	AA	13	U

5 of 87 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	DA	479	A
22	DA	1738	G
22	DA	529	A
22	DA	1089	A
22	DA	2146	C

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	DBB	B6	3	54	4,5,6	1.54	1 (25%)	1,5,7	0.12	0
54	004	D6	7	54	9,10,11	0.56	0	9,12,14	1.08	1 (11%)
54	MHW	D6	1	54	9,9,10	1.75	2 (22%)	10,11,13	3.23	3 (30%)
54	MHU	B6	5	54	14,15,16	1.76	3 (21%)	18,19,21	1.58	4 (22%)
54	MHW	B6	1	54	9,9,10	1.63	1 (11%)	10,11,13	2.57	4 (40%)
54	MHV	B6	6	54	7,9,10	1.45	1 (14%)	8,11,13	3.40	3 (37%)
54	DBB	D6	3	54	4,5,6	1.19	0	1,5,7	0.73	0
54	MHU	D6	5	54	14,15,16	1.98	3 (21%)	18,19,21	2.14	2 (11%)
54	MHV	D6	6	54	7,9,10	0.93	0	8,11,13	3.59	3 (37%)
54	004	B6	7	54	9,10,11	1.59	1 (11%)	9,12,14	2.23	3 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	DBB	B6	3	54	-	0/3/4/6	-
54	004	D6	7	54	-	0/4/6/8	0/1/1/1
54	MHW	D6	1	54	-	0/2/2/4	0/1/1/1
54	MHU	B6	5	54	-	0/9/12/14	0/1/1/1
54	MHW	B6	1	54	-	0/2/2/4	0/1/1/1
54	MHV	B6	6	54	-	0/1/12/14	0/1/1/1
54	DBB	D6	3	54	-	0/3/4/6	-
54	MHU	D6	5	54	-	0/9/12/14	0/1/1/1
54	MHV	D6	6	54	-	0/1/12/14	0/1/1/1
54	004	B6	7	54	-	0/4/6/8	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D6	5	MHU	CZ-NZ	5.63	1.50	1.37
54	B6	5	MHU	CZ-NZ	5.10	1.49	1.37
54	B6	7	004	CB-CA	-4.48	1.48	1.52
54	D6	1	MHW	CA-C	4.12	1.53	1.48
54	B6	1	MHW	CA-C	3.61	1.52	1.48

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	MHV	CD2-CE-N	-8.99	90.50	109.98
54	B6	6	MHV	CD2-CE-N	-8.20	92.22	109.98
54	D6	5	MHU	CG-CB-CA	8.03	124.94	113.51
54	D6	1	MHW	CD-CE-N	7.27	134.92	123.42
54	B6	1	MHW	CD-CE-N	5.16	131.58	123.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	B6	3	DBB	1	0
54	D6	7	004	6	0
54	B6	5	MHU	1	0
54	D6	6	MHV	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 500 ligands modelled in this entry, 500 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	AA	1538/1539 (99%)	0.13	62 (4%) 42 35	15, 50, 134, 177	0
1	CA	1539/1539 (100%)	0.66	147 (9%) 13 12	29, 70, 143, 176	0
2	AB	218/218 (100%)	0.87	21 (9%) 13 12	39, 71, 98, 131	0
2	CB	218/218 (100%)	1.53	57 (26%) 1 1	55, 80, 108, 126	0
3	AC	206/206 (100%)	0.48	11 (5%) 32 27	36, 56, 81, 95	0
3	CC	206/206 (100%)	0.98	18 (8%) 16 14	52, 73, 93, 114	0
4	AD	205/205 (100%)	1.03	35 (17%) 4 3	33, 55, 80, 109	0
4	CD	205/205 (100%)	0.53	17 (8%) 17 15	23, 40, 75, 93	0
5	AE	150/150 (100%)	0.70	12 (8%) 18 16	32, 49, 82, 111	0
5	CE	150/150 (100%)	0.89	20 (13%) 7 7	35, 56, 83, 105	0
6	AF	100/100 (100%)	0.83	10 (10%) 12 11	34, 55, 75, 85	0
6	CF	100/100 (100%)	0.85	9 (9%) 15 13	44, 72, 97, 105	0
7	AG	151/151 (100%)	1.40	30 (19%) 3 3	48, 73, 96, 107	0
7	CG	151/151 (100%)	1.98	69 (45%) 0 0	75, 92, 105, 113	0
8	AH	129/129 (100%)	0.31	3 (2%) 61 53	28, 47, 71, 80	0
8	CH	129/129 (100%)	0.95	12 (9%) 14 12	46, 63, 83, 90	0
9	AI	127/127 (100%)	1.24	26 (20%) 2 2	42, 68, 96, 115	0
9	CI	127/127 (100%)	2.15	64 (50%) 0 0	64, 87, 106, 131	0
10	AJ	98/98 (100%)	1.26	19 (19%) 3 3	42, 62, 93, 120	0
10	CJ	98/98 (100%)	2.14	44 (44%) 0 0	66, 89, 108, 122	0
11	AK	117/117 (100%)	1.08	14 (11%) 9 8	29, 61, 88, 106	0
11	CK	117/117 (100%)	0.48	3 (2%) 57 49	35, 63, 82, 90	0
12	AL	123/123 (100%)	0.58	10 (8%) 18 16	23, 36, 72, 102	0
12	CL	123/123 (100%)	0.93	14 (11%) 10 9	38, 50, 80, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.97	18 (15%) 5 4	43, 66, 91, 105	0
13	CM	114/114 (100%)	2.49	67 (58%) 0 0	80, 98, 113, 118	0
14	AN	96/100 (96%)	1.39	26 (27%) 1 1	39, 56, 93, 108	0
14	CN	96/100 (96%)	1.83	39 (40%) 0 0	60, 88, 106, 119	0
15	AO	88/88 (100%)	0.66	5 (5%) 29 24	31, 49, 66, 99	0
15	CO	88/88 (100%)	0.75	5 (5%) 29 24	42, 62, 84, 108	0
16	AP	82/82 (100%)	0.76	4 (4%) 35 29	35, 46, 80, 103	0
16	CP	82/82 (100%)	1.28	20 (24%) 2 2	43, 61, 87, 105	0
17	AQ	80/80 (100%)	0.92	11 (13%) 6 6	30, 55, 85, 123	0
17	CQ	80/80 (100%)	1.54	24 (30%) 1 1	42, 69, 97, 108	0
18	AR	55/55 (100%)	0.81	5 (9%) 15 13	38, 51, 76, 113	0
18	CR	55/55 (100%)	0.68	4 (7%) 21 18	40, 54, 83, 113	0
19	AS	79/79 (100%)	0.98	13 (16%) 4 4	45, 66, 92, 97	0
19	CS	79/79 (100%)	2.69	55 (69%) 0 0	79, 98, 113, 126	0
20	AT	85/85 (100%)	0.73	6 (7%) 22 19	35, 48, 74, 115	0
20	CT	85/85 (100%)	1.59	22 (25%) 1 1	52, 69, 91, 98	0
21	AU	51/51 (100%)	1.84	16 (31%) 1 1	49, 70, 92, 105	0
21	CU	51/51 (100%)	1.72	17 (33%) 1 1	43, 67, 92, 107	0
22	BA	2897/2903 (99%)	-0.33	153 (5%) 32 27	3, 18, 128, 196	0
22	DA	2897/2903 (99%)	1.03	286 (9%) 13 11	42, 82, 142, 182	0
23	BB	119/119 (100%)	-0.59	0 100 100	6, 26, 52, 94	0
23	DB	118/119 (99%)	0.94	9 (7%) 20 18	68, 109, 131, 143	0
24	BC	271/271 (100%)	0.01	6 (2%) 62 54	8, 24, 44, 65	0
24	DC	271/271 (100%)	1.43	74 (27%) 1 1	40, 60, 76, 84	0
25	BD	209/209 (100%)	-0.19	3 (1%) 73 67	4, 15, 42, 69	0
25	DD	209/209 (100%)	1.41	49 (23%) 2 2	47, 64, 83, 99	0
26	BE	201/201 (100%)	-0.01	3 (1%) 72 65	4, 27, 54, 95	0
26	DE	201/201 (100%)	1.81	73 (36%) 1 1	38, 76, 96, 108	0
27	BF	177/177 (100%)	0.53	17 (9%) 13 12	23, 44, 86, 104	0
27	DF	177/177 (100%)	1.83	65 (36%) 1 1	79, 97, 113, 125	0
28	BG	176/176 (100%)	0.44	10 (5%) 29 24	21, 39, 66, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	1.65	50 (28%) 1 1	66, 85, 103, 117	0
29	BH	149/149 (100%)	3.08	115 (77%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	2.31	73 (48%) 0 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	2.36	78 (55%) 0 0	80, 104, 120, 136	0
30	DI	141/141 (100%)	2.91	98 (69%) 0 0	91, 110, 121, 124	0
31	BJ	142/142 (100%)	-0.19	4 (2%) 55 47	5, 12, 32, 54	0
31	DJ	142/142 (100%)	1.32	30 (21%) 2 2	49, 64, 80, 96	0
32	BK	122/122 (100%)	-0.23	3 (2%) 58 50	7, 16, 40, 68	0
32	DK	122/122 (100%)	1.01	13 (10%) 11 10	47, 60, 81, 95	0
33	BL	143/143 (100%)	0.21	3 (2%) 63 55	4, 26, 49, 80	0
33	DL	143/143 (100%)	2.01	67 (46%) 0 0	45, 72, 90, 111	0
34	BM	136/136 (100%)	-0.28	1 (0%) 84 80	6, 16, 34, 93	0
34	DM	136/136 (100%)	1.11	23 (16%) 4 4	40, 64, 82, 110	0
35	BN	120/120 (100%)	-0.27	1 (0%) 82 78	7, 13, 25, 70	0
35	DN	120/120 (100%)	2.04	55 (45%) 0 0	50, 71, 88, 109	0
36	BO	116/116 (100%)	0.09	2 (1%) 69 62	18, 29, 52, 59	0
36	DO	116/116 (100%)	1.69	34 (29%) 1 1	64, 86, 100, 113	0
37	BP	114/114 (100%)	-0.04	3 (2%) 57 49	10, 22, 49, 73	0
37	DP	114/114 (100%)	1.37	27 (23%) 2 2	51, 66, 84, 91	0
38	BQ	117/117 (100%)	-0.37	1 (0%) 81 76	3, 8, 21, 57	0
38	DQ	117/117 (100%)	1.75	47 (40%) 0 0	46, 65, 79, 83	0
39	BR	103/103 (100%)	-0.13	3 (2%) 53 46	4, 15, 37, 64	0
39	DR	103/103 (100%)	1.89	40 (38%) 1 0	49, 72, 86, 96	0
40	BS	110/110 (100%)	-0.40	2 (1%) 67 59	4, 9, 27, 89	0
40	DS	110/110 (100%)	1.82	39 (35%) 1 1	53, 69, 89, 97	0
41	BT	93/93 (100%)	0.37	7 (7%) 20 18	15, 28, 83, 100	0
41	DT	93/93 (100%)	2.31	53 (56%) 0 0	60, 79, 102, 110	0
42	BU	102/102 (100%)	0.23	1 (0%) 79 74	15, 32, 62, 95	0
42	DU	102/102 (100%)	2.63	66 (64%) 0 0	61, 82, 103, 109	0
43	BV	94/94 (100%)	-0.15	1 (1%) 78 73	11, 24, 48, 59	0
43	DV	94/94 (100%)	1.08	11 (11%) 9 8	60, 78, 93, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.02	3 (3%) 43 35	10, 17, 37, 56	0
44	DW	75/76 (98%)	1.53	15 (20%) 3 3	49, 75, 86, 107	0
45	BX	77/77 (100%)	0.28	3 (3%) 43 35	11, 28, 53, 81	0
45	DX	77/77 (100%)	1.51	20 (25%) 1 1	49, 66, 84, 89	0
46	BY	63/63 (100%)	0.65	7 (11%) 10 9	21, 42, 71, 93	0
46	DY	63/63 (100%)	2.07	27 (42%) 0 0	63, 86, 95, 104	0
47	BZ	58/58 (100%)	-0.17	0 100 100	7, 11, 34, 40	0
47	DZ	58/58 (100%)	1.44	12 (20%) 2 2	50, 69, 82, 89	0
48	B0	56/56 (100%)	-0.33	0 100 100	4, 14, 38, 77	0
48	D0	56/56 (100%)	1.94	23 (41%) 0 0	49, 69, 90, 106	0
49	B1	50/50 (100%)	0.28	2 (4%) 42 35	19, 33, 61, 95	0
49	D1	50/50 (100%)	1.58	17 (34%) 1 1	63, 79, 91, 103	0
50	B2	46/46 (100%)	-0.05	1 (2%) 62 54	8, 14, 22, 97	0
50	D2	46/46 (100%)	1.91	18 (39%) 1 0	47, 64, 78, 100	0
51	B3	64/64 (100%)	-0.07	0 100 100	10, 16, 26, 37	0
51	D3	64/64 (100%)	2.49	44 (68%) 0 0	53, 67, 79, 83	0
52	B4	38/38 (100%)	0.30	2 (5%) 32 27	13, 23, 38, 60	0
52	D4	38/38 (100%)	1.70	14 (36%) 1 1	56, 71, 84, 96	0
53	B5	191/228 (83%)	2.44	121 (63%) 0 0	71, 107, 119, 133	0
54	B6	2/8 (25%)	-0.27	0 100 100	6, 6, 6, 8	0
54	D6	2/8 (25%)	1.55	1 (50%) 0 0	41, 41, 41, 44	0
All	All	20738/20810 (99%)	0.76	3113 (15%) 5 5	3, 61, 117, 196	0

The worst 5 of 3113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	BH	144	VAL	9.6
48	D0	27	SER	9.2
20	CT	4	ILE	8.4
10	AJ	102	LEU	8.2
4	CD	25	VAL	8.2

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
54	004	D6	7	10/11	0.82	0.17	38,42,48,48	0
54	DBB	D6	3	6/7	0.83	0.16	37,40,41,43	0
54	MHW	D6	1	9/10	0.83	0.19	49,54,56,59	0
54	MHU	D6	5	15/16	0.85	0.19	37,42,54,56	0
54	MHV	D6	6	9/10	0.89	0.10	39,40,42,43	0
54	MHU	B6	5	15/16	0.95	0.10	0,5,18,21	0
54	004	B6	7	10/11	0.95	0.11	3,6,7,10	0
54	MHW	B6	1	9/10	0.95	0.10	12,14,18,21	0
54	MHV	B6	6	9/10	0.96	0.07	2,6,13,14	0
54	DBB	B6	3	6/7	0.97	0.09	6,8,10,15	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
55	MG	AA	1648	1/1	0.45	0.10	38,38,38,38	0
55	MG	DA	3060	1/1	0.46	0.56	61,61,61,61	0
55	MG	CA	1636	1/1	0.53	0.21	79,79,79,79	0
55	MG	DA	3070	1/1	0.54	0.25	58,58,58,58	0
55	MG	DA	3119	1/1	0.61	0.36	68,68,68,68	0
55	MG	AA	1614	1/1	0.65	0.34	53,53,53,53	0
55	MG	DA	3158	1/1	0.65	0.14	55,55,55,55	0
55	MG	BA	3040	1/1	0.66	0.28	7,7,7,7	0
55	MG	DA	3155	1/1	0.66	0.31	44,44,44,44	0
55	MG	DA	3015	1/1	0.66	0.34	56,56,56,56	0
55	MG	AA	1657	1/1	0.67	0.24	40,40,40,40	0
55	MG	BA	3188	1/1	0.68	0.15	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3137	1/1	0.69	0.27	42,42,42,42	0
55	MG	DA	3041	1/1	0.70	0.25	53,53,53,53	0
55	MG	CA	1633	1/1	0.71	0.27	54,54,54,54	0
55	MG	BA	3098	1/1	0.71	0.37	58,58,58,58	0
55	MG	DA	3057	1/1	0.71	0.36	54,54,54,54	0
55	MG	AA	1615	1/1	0.72	0.13	46,46,46,46	0
55	MG	DA	3091	1/1	0.72	0.30	71,71,71,71	0
55	MG	DA	3076	1/1	0.73	0.24	48,48,48,48	0
55	MG	DA	3151	1/1	0.73	0.22	45,45,45,45	0
55	MG	DA	3161	1/1	0.73	0.11	42,42,42,42	0
55	MG	DA	3143	1/1	0.74	0.09	46,46,46,46	0
55	MG	CA	1652	1/1	0.75	0.12	39,39,39,39	0
55	MG	DA	3124	1/1	0.75	0.21	59,59,59,59	0
55	MG	DA	3131	1/1	0.75	0.36	71,71,71,71	0
55	MG	DA	3033	1/1	0.76	0.16	45,45,45,45	0
55	MG	BA	3060	1/1	0.76	0.37	33,33,33,33	0
55	MG	DA	3163	1/1	0.76	0.16	51,51,51,51	0
55	MG	BA	3061	1/1	0.77	0.32	55,55,55,55	0
55	MG	DA	3126	1/1	0.77	0.10	57,57,57,57	0
55	MG	DA	3090	1/1	0.77	0.16	58,58,58,58	0
55	MG	CA	1643	1/1	0.77	0.23	44,44,44,44	0
55	MG	BA	3179	1/1	0.77	0.21	39,39,39,39	0
55	MG	CM	201	1/1	0.78	0.13	46,46,46,46	0
55	MG	DA	3040	1/1	0.78	0.18	57,57,57,57	0
55	MG	DA	3115	1/1	0.79	0.13	58,58,58,58	0
55	MG	DA	3148	1/1	0.79	0.19	45,45,45,45	0
55	MG	CA	1609	1/1	0.79	0.17	58,58,58,58	0
55	MG	DA	3153	1/1	0.79	0.13	52,52,52,52	0
55	MG	CA	1628	1/1	0.79	0.26	64,64,64,64	0
55	MG	AA	1652	1/1	0.79	0.23	43,43,43,43	0
55	MG	DA	3046	1/1	0.79	0.18	53,53,53,53	0
55	MG	BA	3105	1/1	0.79	0.19	4,4,4,4	0
55	MG	CA	1635	1/1	0.80	0.14	76,76,76,76	0
55	MG	CA	1605	1/1	0.80	0.22	57,57,57,57	0
55	MG	BA	3157	1/1	0.80	0.23	26,26,26,26	0
55	MG	DA	3045	1/1	0.80	0.13	53,53,53,53	0
55	MG	DA	3016	1/1	0.80	0.26	53,53,53,53	0
55	MG	DA	3102	1/1	0.81	0.16	45,45,45,45	0
55	MG	BA	3015	1/1	0.81	0.24	52,52,52,52	0
55	MG	DA	3099	1/1	0.81	0.19	53,53,53,53	0
55	MG	DA	3034	1/1	0.82	0.26	56,56,56,56	0
55	MG	CA	1642	1/1	0.82	0.21	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1655	1/1	0.82	0.10	44,44,44,44	0
55	MG	DA	3092	1/1	0.82	0.24	62,62,62,62	0
55	MG	BA	3102	1/1	0.82	0.29	23,23,23,23	0
55	MG	DA	3047	1/1	0.83	0.20	66,66,66,66	0
55	MG	DA	3054	1/1	0.83	0.19	44,44,44,44	0
55	MG	DA	3055	1/1	0.83	0.34	53,53,53,53	0
55	MG	DA	3056	1/1	0.83	0.21	51,51,51,51	0
55	MG	DA	3039	1/1	0.83	0.08	53,53,53,53	0
55	MG	BA	3150	1/1	0.83	0.27	42,42,42,42	0
55	MG	BA	3116	1/1	0.83	0.15	11,11,11,11	0
55	MG	BA	3126	1/1	0.83	0.23	7,7,7,7	0
55	MG	DA	3006	1/1	0.83	0.19	64,64,64,64	0
55	MG	DA	3135	1/1	0.84	0.21	47,47,47,47	0
55	MG	DA	3093	1/1	0.84	0.10	65,65,65,65	0
55	MG	DA	3140	1/1	0.84	0.24	37,37,37,37	0
55	MG	BA	3191	1/1	0.84	0.14	35,35,35,35	0
55	MG	AA	1638	1/1	0.84	0.14	51,51,51,51	0
55	MG	DA	3106	1/1	0.84	0.08	56,56,56,56	0
55	MG	BA	3109	1/1	0.84	0.13	9,9,9,9	0
55	MG	BA	3173	1/1	0.84	0.10	20,20,20,20	0
55	MG	AA	1608	1/1	0.84	0.11	24,24,24,24	0
55	MG	AA	1671	1/1	0.84	0.13	35,35,35,35	0
55	MG	DA	3004	1/1	0.84	0.19	64,64,64,64	0
55	MG	DA	3098	1/1	0.85	0.28	63,63,63,63	0
55	MG	CA	1604	1/1	0.85	0.11	70,70,70,70	0
55	MG	DA	3013	1/1	0.85	0.24	45,45,45,45	0
55	MG	CA	1650	1/1	0.85	0.37	40,40,40,40	0
55	MG	DA	3111	1/1	0.85	0.09	42,42,42,42	0
55	MG	BA	3055	1/1	0.85	0.17	23,23,23,23	0
55	MG	DA	3026	1/1	0.85	0.10	53,53,53,53	0
55	MG	BA	3161	1/1	0.85	0.09	24,24,24,24	0
55	MG	DA	3125	1/1	0.85	0.09	51,51,51,51	0
55	MG	CA	1638	1/1	0.85	0.15	55,55,55,55	0
55	MG	AA	1620	1/1	0.85	0.09	44,44,44,44	0
55	MG	DA	3164	1/1	0.85	0.14	47,47,47,47	0
55	MG	DA	3031	1/1	0.86	0.19	50,50,50,50	0
55	MG	DA	3113	1/1	0.86	0.09	42,42,42,42	0
55	MG	DA	3147	1/1	0.86	0.10	49,49,49,49	0
55	MG	DA	3010	1/1	0.86	0.09	48,48,48,48	0
55	MG	AA	1664	1/1	0.86	0.10	36,36,36,36	0
55	MG	BA	3154	1/1	0.86	0.09	29,29,29,29	0
55	MG	BA	3143	1/1	0.86	0.17	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3025	1/1	0.86	0.34	49,49,49,49	0
55	MG	DA	3009	1/1	0.86	0.09	57,57,57,57	0
55	MG	DA	3104	1/1	0.86	0.12	54,54,54,54	0
55	MG	DA	3029	1/1	0.86	0.26	41,41,41,41	0
55	MG	AA	1605	1/1	0.87	0.10	32,32,32,32	0
55	MG	BA	3079	1/1	0.87	0.09	28,28,28,28	0
55	MG	BA	3146	1/1	0.87	0.19	23,23,23,23	0
55	MG	DA	3138	1/1	0.87	0.26	41,41,41,41	0
55	MG	BA	3087	1/1	0.87	0.12	18,18,18,18	0
55	MG	AA	1660	1/1	0.87	0.20	40,40,40,40	0
55	MG	CA	1611	1/1	0.87	0.17	55,55,55,55	0
55	MG	DA	3059	1/1	0.87	0.20	53,53,53,53	0
55	MG	BA	3034	1/1	0.87	0.29	18,18,18,18	0
55	MG	DA	3005	1/1	0.87	0.14	66,66,66,66	0
55	MG	DA	3116	1/1	0.87	0.11	51,51,51,51	0
55	MG	AA	1662	1/1	0.87	0.07	41,41,41,41	0
55	MG	DA	3160	1/1	0.87	0.10	35,35,35,35	0
55	MG	BA	3171	1/1	0.87	0.08	29,29,29,29	0
55	MG	AA	1646	1/1	0.87	0.09	44,44,44,44	0
55	MG	AA	1668	1/1	0.87	0.06	18,18,18,18	0
55	MG	BA	3117	1/1	0.88	0.04	4,4,4,4	0
55	MG	CA	1637	1/1	0.88	0.20	51,51,51,51	0
55	MG	BA	3119	1/1	0.88	0.28	21,21,21,21	0
55	MG	DA	3008	1/1	0.88	0.31	51,51,51,51	0
55	MG	BA	3036	1/1	0.88	0.18	19,19,19,19	0
55	MG	DA	3062	1/1	0.88	0.09	44,44,44,44	0
55	MG	DA	3112	1/1	0.88	0.11	52,52,52,52	0
55	MG	BA	3133	1/1	0.88	0.26	40,40,40,40	0
55	MG	CA	1647	1/1	0.88	0.16	24,24,24,24	0
55	MG	DA	3086	1/1	0.88	0.08	53,53,53,53	0
55	MG	DA	3087	1/1	0.88	0.11	51,51,51,51	0
55	MG	BA	3029	1/1	0.88	0.13	15,15,15,15	0
55	MG	BA	3111	1/1	0.88	0.10	23,23,23,23	0
55	MG	BA	3025	1/1	0.88	0.23	40,40,40,40	0
55	MG	BA	3190	1/1	0.88	0.13	33,33,33,33	0
55	MG	AM	201	1/1	0.89	0.07	29,29,29,29	0
55	MG	BA	3175	1/1	0.89	0.11	27,27,27,27	0
55	MG	BA	3077	1/1	0.89	0.07	26,26,26,26	0
55	MG	AA	1617	1/1	0.89	0.18	44,44,44,44	0
55	MG	BA	3023	1/1	0.89	0.11	15,15,15,15	0
55	MG	DA	3152	1/1	0.89	0.09	41,41,41,41	0
55	MG	AA	1669	1/1	0.89	0.17	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3036	1/1	0.89	0.13	61,61,61,61	0
55	MG	DA	3014	1/1	0.89	0.08	43,43,43,43	0
55	MG	DA	3061	1/1	0.89	0.40	53,53,53,53	0
55	MG	BA	3057	1/1	0.89	0.16	20,20,20,20	0
55	MG	AA	1654	1/1	0.89	0.31	40,40,40,40	0
55	MG	DA	3023	1/1	0.89	0.09	35,35,35,35	0
55	MG	DA	3165	1/1	0.89	0.29	34,34,34,34	0
55	MG	DA	3166	1/1	0.89	0.07	34,34,34,34	0
55	MG	DQ	201	1/1	0.89	0.19	32,32,32,32	0
55	MG	AA	1653	1/1	0.90	0.16	24,24,24,24	0
55	MG	BA	3004	1/1	0.90	0.14	33,33,33,33	0
55	MG	AA	1632	1/1	0.90	0.11	40,40,40,40	0
55	MG	DA	3139	1/1	0.90	0.24	31,31,31,31	0
55	MG	BA	3159	1/1	0.90	0.13	19,19,19,19	0
55	MG	DA	3142	1/1	0.90	0.26	38,38,38,38	0
55	MG	CA	1644	1/1	0.90	0.11	32,32,32,32	0
55	MG	BA	3160	1/1	0.90	0.20	7,7,7,7	0
55	MG	CA	1649	1/1	0.90	0.14	35,35,35,35	0
55	MG	BA	3045	1/1	0.90	0.10	13,13,13,13	0
55	MG	CA	1651	1/1	0.90	0.13	48,48,48,48	0
55	MG	BA	3170	1/1	0.90	0.09	35,35,35,35	0
55	MG	DA	3154	1/1	0.90	0.11	45,45,45,45	0
55	MG	DA	3114	1/1	0.90	0.18	64,64,64,64	0
55	MG	CA	1653	1/1	0.90	0.13	47,47,47,47	0
55	MG	CA	1614	1/1	0.90	0.07	44,44,44,44	0
55	MG	BA	3046	1/1	0.90	0.14	8,8,8,8	0
55	MG	DA	3123	1/1	0.90	0.09	47,47,47,47	0
55	MG	CA	1631	1/1	0.90	0.19	62,62,62,62	0
55	MG	AA	1637	1/1	0.90	0.10	18,18,18,18	0
55	MG	AA	1659	1/1	0.90	0.24	34,34,34,34	0
55	MG	AA	1630	1/1	0.90	0.11	49,49,49,49	0
55	MG	AA	1651	1/1	0.91	0.22	32,32,32,32	0
55	MG	CA	1621	1/1	0.91	0.08	53,53,53,53	0
55	MG	DA	3144	1/1	0.91	0.12	52,52,52,52	0
55	MG	DA	3145	1/1	0.91	0.10	37,37,37,37	0
55	MG	AA	1667	1/1	0.91	0.05	37,37,37,37	0
55	MG	DA	3084	1/1	0.91	0.20	56,56,56,56	0
55	MG	DA	3149	1/1	0.91	0.35	36,36,36,36	0
55	MG	DA	3011	1/1	0.91	0.25	46,46,46,46	0
55	MG	DA	3118	1/1	0.91	0.16	45,45,45,45	0
55	MG	BA	3125	1/1	0.91	0.10	8,8,8,8	0
55	MG	CA	1601	1/1	0.91	0.09	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3076	1/1	0.91	0.15	17,17,17,17	0
55	MG	BA	3174	1/1	0.91	0.08	20,20,20,20	0
55	MG	CA	1606	1/1	0.91	0.21	52,52,52,52	0
55	MG	CA	1608	1/1	0.91	0.18	50,50,50,50	0
55	MG	DA	3001	1/1	0.91	0.14	43,43,43,43	0
55	MG	DA	3028	1/1	0.91	0.10	50,50,50,50	0
55	MG	CA	1641	1/1	0.91	0.35	46,46,46,46	0
55	MG	BA	3113	1/1	0.91	0.15	10,10,10,10	0
55	MG	AA	1624	1/1	0.91	0.17	39,39,39,39	0
55	MG	DA	3127	1/1	0.92	0.10	47,47,47,47	0
55	MG	DA	3078	1/1	0.92	0.07	64,64,64,64	0
55	MG	CA	1602	1/1	0.92	0.07	61,61,61,61	0
55	MG	BA	3019	1/1	0.92	0.19	3,3,3,3	0
55	MG	AA	1665	1/1	0.92	0.11	34,34,34,34	0
55	MG	AA	1649	1/1	0.92	0.08	27,27,27,27	0
55	MG	AA	1643	1/1	0.92	0.10	19,19,19,19	0
55	MG	DA	3141	1/1	0.92	0.17	28,28,28,28	0
55	MG	DA	3044	1/1	0.92	0.08	61,61,61,61	0
55	MG	BA	3112	1/1	0.92	0.06	11,11,11,11	0
55	MG	CA	1646	1/1	0.92	0.07	40,40,40,40	0
55	MG	BA	3176	1/1	0.92	0.11	24,24,24,24	0
55	MG	DA	3146	1/1	0.92	0.04	35,35,35,35	0
55	MG	DA	3048	1/1	0.92	0.15	51,51,51,51	0
55	MG	DA	3051	1/1	0.92	0.06	35,35,35,35	0
55	MG	DA	3053	1/1	0.92	0.10	43,43,43,43	0
55	MG	DA	3109	1/1	0.92	0.15	37,37,37,37	0
55	MG	AA	1644	1/1	0.92	0.06	32,32,32,32	0
55	MG	BA	3182	1/1	0.92	0.14	22,22,22,22	0
55	MG	CA	1627	1/1	0.92	0.18	59,59,59,59	0
55	MG	DA	3024	1/1	0.92	0.12	45,45,45,45	0
55	MG	AA	1661	1/1	0.92	0.06	22,22,22,22	0
55	MG	CA	1630	1/1	0.92	0.19	66,66,66,66	0
55	MG	AA	1627	1/1	0.92	0.22	43,43,43,43	0
55	MG	AA	1663	1/1	0.92	0.08	35,35,35,35	0
55	MG	BB	201	1/1	0.92	0.07	28,28,28,28	0
55	MG	DA	3071	1/1	0.92	0.22	59,59,59,59	0
55	MG	DA	3074	1/1	0.92	0.10	41,41,41,41	0
55	MG	AA	1635	1/1	0.92	0.12	37,37,37,37	0
55	MG	DA	3133	1/1	0.93	0.38	57,57,57,57	0
55	MG	BA	3093	1/1	0.93	0.10	16,16,16,16	0
55	MG	BA	3194	1/1	0.93	0.07	28,28,28,28	0
55	MG	CA	1629	1/1	0.93	0.08	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3018	1/1	0.93	0.14	57,57,57,57	0
55	MG	AA	1634	1/1	0.93	0.07	36,36,36,36	0
55	MG	BA	3123	1/1	0.93	0.09	18,18,18,18	0
55	MG	DA	3101	1/1	0.93	0.07	40,40,40,40	0
55	MG	BA	3009	1/1	0.93	0.08	6,6,6,6	0
55	MG	BA	3090	1/1	0.93	0.06	17,17,17,17	0
55	MG	DA	3105	1/1	0.93	0.07	37,37,37,37	0
55	MG	BA	3128	1/1	0.93	0.15	9,9,9,9	0
55	MG	BA	3177	1/1	0.93	0.16	24,24,24,24	0
55	MG	DA	3002	1/1	0.93	0.25	52,52,52,52	0
55	MG	BA	3178	1/1	0.93	0.19	20,20,20,20	0
55	MG	DA	3066	1/1	0.93	0.06	39,39,39,39	0
55	MG	DA	3068	1/1	0.93	0.20	52,52,52,52	0
55	MG	CA	1639	1/1	0.93	0.07	34,34,34,34	0
55	MG	BA	3108	1/1	0.93	0.18	1,1,1,1	0
55	MG	DA	3073	1/1	0.93	0.10	37,37,37,37	0
55	MG	DA	3007	1/1	0.93	0.16	54,54,54,54	0
55	MG	BA	3136	1/1	0.93	0.21	24,24,24,24	0
55	MG	BA	3163	1/1	0.93	0.17	27,27,27,27	0
55	MG	DA	3080	1/1	0.93	0.10	39,39,39,39	0
55	MG	BA	3168	1/1	0.93	0.08	18,18,18,18	0
55	MG	CA	1645	1/1	0.93	0.13	41,41,41,41	0
55	MG	DA	3128	1/1	0.93	0.08	57,57,57,57	0
55	MG	CA	1624	1/1	0.93	0.09	33,33,33,33	0
55	MG	DA	3077	1/1	0.94	0.08	59,59,59,59	0
55	MG	AA	1650	1/1	0.94	0.08	35,35,35,35	0
55	MG	CA	1615	1/1	0.94	0.18	35,35,35,35	0
55	MG	CA	1618	1/1	0.94	0.08	28,28,28,28	0
55	MG	BA	3038	1/1	0.94	0.05	8,8,8,8	0
55	MG	AA	1655	1/1	0.94	0.07	34,34,34,34	0
55	MG	BA	3044	1/1	0.94	0.07	20,20,20,20	0
55	MG	AA	1622	1/1	0.94	0.18	21,21,21,21	0
55	MG	DA	3121	1/1	0.94	0.11	41,41,41,41	0
55	MG	DA	3150	1/1	0.94	0.07	42,42,42,42	0
55	MG	BA	3137	1/1	0.94	0.32	4,4,4,4	0
55	MG	BA	3082	1/1	0.94	0.20	15,15,15,15	0
55	MG	BA	3085	1/1	0.94	0.08	7,7,7,7	0
55	MG	BA	3115	1/1	0.94	0.15	35,35,35,35	0
55	MG	DA	3043	1/1	0.94	0.18	54,54,54,54	0
55	MG	CA	1634	1/1	0.94	0.08	49,49,49,49	0
55	MG	DA	3103	1/1	0.94	0.13	48,48,48,48	0
55	MG	BA	3030	1/1	0.94	0.15	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3047	1/1	0.94	0.10	34,34,34,34	0
55	MG	BA	3033	1/1	0.94	0.15	4,4,4,4	0
55	MG	DA	3107	1/1	0.94	0.08	49,49,49,49	0
55	MG	BA	3003	1/1	0.94	0.06	20,20,20,20	0
55	MG	DA	3110	1/1	0.94	0.24	57,57,57,57	0
55	MG	DA	3067	1/1	0.95	0.06	49,49,49,49	0
55	MG	BA	3181	1/1	0.95	0.09	14,14,14,14	0
55	MG	BA	3144	1/1	0.95	0.09	25,25,25,25	0
55	MG	BA	3114	1/1	0.95	0.07	19,19,19,19	0
55	MG	AA	1623	1/1	0.95	0.11	42,42,42,42	0
55	MG	BA	3152	1/1	0.95	0.07	11,11,11,11	0
55	MG	BA	3153	1/1	0.95	0.13	2,2,2,2	0
55	MG	BA	3195	1/1	0.95	0.07	20,20,20,20	0
55	MG	AA	1631	1/1	0.95	0.10	42,42,42,42	0
55	MG	BB	204	1/1	0.95	0.21	4,4,4,4	0
55	MG	DA	3081	1/1	0.95	0.12	43,43,43,43	0
55	MG	BA	3156	1/1	0.95	0.17	12,12,12,12	0
55	MG	AA	1656	1/1	0.95	0.10	37,37,37,37	0
55	MG	BA	3066	1/1	0.95	0.07	6,6,6,6	0
55	MG	BA	3120	1/1	0.95	0.07	7,7,7,7	0
55	MG	CA	1648	1/1	0.95	0.20	42,42,42,42	0
55	MG	DA	3038	1/1	0.95	0.05	42,42,42,42	0
55	MG	BA	3073	1/1	0.95	0.06	13,13,13,13	0
55	MG	BA	3162	1/1	0.95	0.17	21,21,21,21	0
55	MG	BA	3075	1/1	0.95	0.07	15,15,15,15	0
55	MG	BA	3166	1/1	0.95	0.15	25,25,25,25	0
55	MG	CA	1613	1/1	0.95	0.08	19,19,19,19	0
55	MG	CA	1654	1/1	0.95	0.04	26,26,26,26	0
55	MG	BA	3167	1/1	0.95	0.05	28,28,28,28	0
55	MG	AA	1603	1/1	0.95	0.09	34,34,34,34	0
55	MG	CA	1617	1/1	0.95	0.12	35,35,35,35	0
55	MG	AA	1658	1/1	0.95	0.04	33,33,33,33	0
55	MG	BA	3052	1/1	0.95	0.06	8,8,8,8	0
55	MG	BA	3135	1/1	0.95	0.15	17,17,17,17	0
55	MG	CA	1625	1/1	0.95	0.12	25,25,25,25	0
55	MG	DA	3159	1/1	0.95	0.12	39,39,39,39	0
55	MG	BA	3080	1/1	0.95	0.08	18,18,18,18	0
55	MG	AA	1602	1/1	0.95	0.11	33,33,33,33	0
55	MG	DA	3162	1/1	0.95	0.12	46,46,46,46	0
55	MG	BA	3138	1/1	0.95	0.17	4,4,4,4	0
55	MG	BA	3139	1/1	0.95	0.23	1,1,1,1	0
55	MG	BA	3140	1/1	0.95	0.13	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3012	1/1	0.95	0.06	40,40,40,40	0
55	MG	DA	3167	1/1	0.95	0.11	59,59,59,59	0
55	MG	BA	3084	1/1	0.95	0.17	12,12,12,12	0
55	MG	CA	1607	1/1	0.96	0.10	42,42,42,42	0
55	MG	DA	3069	1/1	0.96	0.05	63,63,63,63	0
55	MG	DA	3120	1/1	0.96	0.08	49,49,49,49	0
55	MG	AA	1639	1/1	0.96	0.06	51,51,51,51	0
55	MG	DA	3122	1/1	0.96	0.10	42,42,42,42	0
55	MG	BA	3172	1/1	0.96	0.11	23,23,23,23	0
55	MG	DA	3027	1/1	0.96	0.26	51,51,51,51	0
55	MG	AA	1666	1/1	0.96	0.07	30,30,30,30	0
55	MG	DA	3075	1/1	0.96	0.10	48,48,48,48	0
55	MG	BA	3145	1/1	0.96	0.09	15,15,15,15	0
55	MG	AA	1612	1/1	0.96	0.08	24,24,24,24	0
55	MG	BA	3149	1/1	0.96	0.05	1,1,1,1	0
55	MG	DA	3132	1/1	0.96	0.13	45,45,45,45	0
55	MG	DA	3079	1/1	0.96	0.05	62,62,62,62	0
55	MG	BA	3016	1/1	0.96	0.12	17,17,17,17	0
55	MG	DA	3136	1/1	0.96	0.16	57,57,57,57	0
55	MG	AA	1619	1/1	0.96	0.22	43,43,43,43	0
55	MG	BA	3121	1/1	0.96	0.08	22,22,22,22	0
55	MG	DA	3085	1/1	0.96	0.05	42,42,42,42	0
55	MG	BA	3101	1/1	0.96	0.07	2,2,2,2	0
55	MG	BA	3155	1/1	0.96	0.11	15,15,15,15	0
55	MG	DA	3088	1/1	0.96	0.18	51,51,51,51	0
55	MG	BA	3183	1/1	0.96	0.06	24,24,24,24	0
55	MG	BA	3187	1/1	0.96	0.13	28,28,28,28	0
55	MG	AA	1626	1/1	0.96	0.10	26,26,26,26	0
55	MG	BA	3103	1/1	0.96	0.06	9,9,9,9	0
55	MG	DA	3095	1/1	0.96	0.06	49,49,49,49	0
55	MG	DA	3097	1/1	0.96	0.04	44,44,44,44	0
55	MG	BA	3158	1/1	0.96	0.08	20,20,20,20	0
55	MG	CA	1632	1/1	0.96	0.09	54,54,54,54	0
55	MG	DA	3100	1/1	0.96	0.08	43,43,43,43	0
55	MG	BA	3193	1/1	0.96	0.04	12,12,12,12	0
55	MG	DA	3049	1/1	0.96	0.08	49,49,49,49	0
55	MG	AA	1606	1/1	0.96	0.06	31,31,31,31	0
55	MG	BA	3107	1/1	0.96	0.10	6,6,6,6	0
55	MG	DA	3157	1/1	0.96	0.07	47,47,47,47	0
55	MG	BA	3134	1/1	0.96	0.06	8,8,8,8	0
55	MG	BA	3028	1/1	0.96	0.06	4,4,4,4	0
55	MG	AA	1629	1/1	0.96	0.06	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3048	1/1	0.96	0.08	16,16,16,16	0
55	MG	CA	1603	1/1	0.96	0.09	44,44,44,44	0
55	MG	AA	1601	1/1	0.96	0.06	49,49,49,49	0
55	MG	BA	3083	1/1	0.96	0.15	32,32,32,32	0
55	MG	DA	3021	1/1	0.96	0.06	38,38,38,38	0
55	MG	DA	3063	1/1	0.96	0.11	41,41,41,41	0
55	MG	DA	3022	1/1	0.96	0.08	54,54,54,54	0
55	MG	DB	201	1/1	0.96	0.05	69,69,69,69	0
55	MG	BA	3031	1/1	0.96	0.07	8,8,8,8	0
55	MG	DA	3037	1/1	0.97	0.04	45,45,45,45	0
55	MG	DA	3083	1/1	0.97	0.12	61,61,61,61	0
55	MG	BA	3078	1/1	0.97	0.05	33,33,33,33	0
55	MG	CA	1619	1/1	0.97	0.07	26,26,26,26	0
55	MG	DA	3130	1/1	0.97	0.04	51,51,51,51	0
55	MG	AA	1613	1/1	0.97	0.04	20,20,20,20	0
55	MG	CA	1622	1/1	0.97	0.08	40,40,40,40	0
55	MG	CA	1623	1/1	0.97	0.19	40,40,40,40	0
55	MG	DA	3134	1/1	0.97	0.06	34,34,34,34	0
55	MG	DA	3089	1/1	0.97	0.19	58,58,58,58	0
55	MG	BA	3010	1/1	0.97	0.07	3,3,3,3	0
55	MG	DA	3003	1/1	0.97	0.05	52,52,52,52	0
55	MG	BA	3148	1/1	0.97	0.15	16,16,16,16	0
55	MG	CA	1626	1/1	0.97	0.05	42,42,42,42	0
55	MG	BA	3051	1/1	0.97	0.07	6,6,6,6	0
55	MG	DA	3096	1/1	0.97	0.15	52,52,52,52	0
55	MG	BA	3012	1/1	0.97	0.10	4,4,4,4	0
55	MG	BA	3151	1/1	0.97	0.12	31,31,31,31	0
55	MG	BA	3054	1/1	0.97	0.07	5,5,5,5	0
55	MG	AA	1616	1/1	0.97	0.06	42,42,42,42	0
55	MG	BA	3086	1/1	0.97	0.08	9,9,9,9	0
55	MG	AA	1645	1/1	0.97	0.08	39,39,39,39	0
55	MG	BA	3088	1/1	0.97	0.13	32,32,32,32	0
55	MG	BA	3059	1/1	0.97	0.16	16,16,16,16	0
55	MG	BA	3091	1/1	0.97	0.06	28,28,28,28	0
55	MG	BA	3092	1/1	0.97	0.11	20,20,20,20	0
55	MG	BA	3002	1/1	0.97	0.10	15,15,15,15	0
55	MG	DA	3020	1/1	0.97	0.20	42,42,42,42	0
55	MG	BA	3129	1/1	0.97	0.08	5,5,5,5	0
55	MG	BA	3132	1/1	0.97	0.12	27,27,27,27	0
55	MG	DA	3156	1/1	0.97	0.09	30,30,30,30	0
55	MG	BA	3020	1/1	0.97	0.06	7,7,7,7	0
55	MG	AA	1610	1/1	0.97	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3067	1/1	0.97	0.08	5,5,5,5	0
55	MG	BA	3071	1/1	0.97	0.10	11,11,11,11	0
55	MG	BA	3041	1/1	0.97	0.05	11,11,11,11	0
55	MG	DA	3117	1/1	0.97	0.05	49,49,49,49	0
55	MG	BA	3106	1/1	0.97	0.19	0,0,0,0	0
55	MG	AA	1618	1/1	0.97	0.05	35,35,35,35	0
55	MG	BA	3027	1/1	0.97	0.09	22,22,22,22	0
55	MG	DA	3032	1/1	0.97	0.10	49,49,49,49	0
55	MG	BA	3141	1/1	0.97	0.28	4,4,4,4	0
55	MG	BA	3142	1/1	0.97	0.28	15,15,15,15	0
55	MG	DB	203	1/1	0.97	0.04	56,56,56,56	0
55	MG	BA	3007	1/1	0.97	0.05	25,25,25,25	0
55	MG	BA	3169	1/1	0.98	0.14	24,24,24,24	0
55	MG	DA	3030	1/1	0.98	0.06	44,44,44,44	0
55	MG	AA	1636	1/1	0.98	0.13	26,26,26,26	0
55	MG	BA	3089	1/1	0.98	0.03	12,12,12,12	0
55	MG	BA	3021	1/1	0.98	0.06	1,1,1,1	0
55	MG	AA	1604	1/1	0.98	0.06	45,45,45,45	0
55	MG	DA	3035	1/1	0.98	0.06	38,38,38,38	0
55	MG	BA	3024	1/1	0.98	0.09	7,7,7,7	0
55	MG	BA	3074	1/1	0.98	0.08	20,20,20,20	0
55	MG	BA	3147	1/1	0.98	0.18	13,13,13,13	0
55	MG	CA	1616	1/1	0.98	0.04	29,29,29,29	0
55	MG	AA	1609	1/1	0.98	0.08	20,20,20,20	0
55	MG	BA	3100	1/1	0.98	0.06	6,6,6,6	0
55	MG	DA	3042	1/1	0.98	0.05	49,49,49,49	0
55	MG	BA	3124	1/1	0.98	0.18	21,21,21,21	0
55	MG	CA	1620	1/1	0.98	0.10	46,46,46,46	0
55	MG	DA	3094	1/1	0.98	0.14	59,59,59,59	0
55	MG	BA	3026	1/1	0.98	0.05	7,7,7,7	0
55	MG	BA	3008	1/1	0.98	0.04	9,9,9,9	0
55	MG	BA	3127	1/1	0.98	0.04	1,1,1,1	0
55	MG	BA	3184	1/1	0.98	0.12	23,23,23,23	0
55	MG	BA	3185	1/1	0.98	0.07	11,11,11,11	0
55	MG	BA	3186	1/1	0.98	0.24	18,18,18,18	0
55	MG	DA	3052	1/1	0.98	0.04	35,35,35,35	0
55	MG	AA	1621	1/1	0.98	0.07	33,33,33,33	0
55	MG	BA	3104	1/1	0.98	0.11	1,1,1,1	0
55	MG	BA	3189	1/1	0.98	0.09	3,3,3,3	0
55	MG	BA	3130	1/1	0.98	0.10	4,4,4,4	0
55	MG	BA	3131	1/1	0.98	0.16	35,35,35,35	0
55	MG	BA	3192	1/1	0.98	0.08	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3108	1/1	0.98	0.12	35,35,35,35	0
55	MG	AA	1670	1/1	0.98	0.20	26,26,26,26	0
55	MG	BA	3011	1/1	0.98	0.14	13,13,13,13	0
55	MG	DA	3017	1/1	0.98	0.03	40,40,40,40	0
55	MG	AA	1640	1/1	0.98	0.07	39,39,39,39	0
55	MG	DA	3019	1/1	0.98	0.09	47,47,47,47	0
55	MG	BA	3014	1/1	0.98	0.04	6,6,6,6	0
55	MG	BB	202	1/1	0.98	0.04	11,11,11,11	0
55	MG	BB	203	1/1	0.98	0.04	10,10,10,10	0
55	MG	BA	3058	1/1	0.98	0.04	13,13,13,13	0
55	MG	BA	3110	1/1	0.98	0.10	23,23,23,23	0
55	MG	DA	3072	1/1	0.98	0.17	42,42,42,42	0
55	MG	BA	3164	1/1	0.98	0.29	21,21,21,21	0
55	MG	AA	1641	1/1	0.98	0.05	20,20,20,20	0
55	MG	DB	202	1/1	0.98	0.03	42,42,42,42	0
55	MG	BA	3001	1/1	0.98	0.06	10,10,10,10	0
55	MG	AA	1625	1/1	0.98	0.06	31,31,31,31	0
56	ZN	B4	101	1/1	0.98	0.08	131,131,131,131	0
55	MG	BA	3070	1/1	0.99	0.13	9,9,9,9	0
55	MG	DA	3129	1/1	0.99	0.03	38,38,38,38	0
55	MG	AA	1647	1/1	0.99	0.04	39,39,39,39	0
55	MG	BA	3072	1/1	0.99	0.10	4,4,4,4	0
55	MG	BA	3017	1/1	0.99	0.04	6,6,6,6	0
55	MG	BA	3018	1/1	0.99	0.04	27,27,27,27	0
55	MG	BA	3180	1/1	0.99	0.12	25,25,25,25	0
55	MG	AA	1642	1/1	0.99	0.03	24,24,24,24	0
55	MG	AA	1611	1/1	0.99	0.04	18,18,18,18	0
55	MG	BA	3049	1/1	0.99	0.04	9,9,9,9	0
55	MG	BA	3050	1/1	0.99	0.03	11,11,11,11	0
55	MG	BA	3032	1/1	0.99	0.05	8,8,8,8	0
55	MG	DA	3050	1/1	0.99	0.05	29,29,29,29	0
55	MG	AA	1628	1/1	0.99	0.04	37,37,37,37	0
55	MG	BA	3081	1/1	0.99	0.07	1,1,1,1	0
55	MG	BA	3053	1/1	0.99	0.07	4,4,4,4	0
55	MG	BA	3022	1/1	0.99	0.07	3,3,3,3	0
55	MG	BA	3118	1/1	0.99	0.05	11,11,11,11	0
55	MG	BA	3035	1/1	0.99	0.04	2,2,2,2	0
55	MG	BA	3056	1/1	0.99	0.08	10,10,10,10	0
55	MG	DA	3058	1/1	0.99	0.04	37,37,37,37	0
55	MG	AA	1607	1/1	0.99	0.03	33,33,33,33	0
55	MG	BA	3122	1/1	0.99	0.14	2,2,2,2	0
55	MG	AA	1633	1/1	0.99	0.03	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3039	1/1	0.99	0.03	1,1,1,1	0
55	MG	BA	3005	1/1	0.99	0.04	31,31,31,31	0
55	MG	DA	3065	1/1	0.99	0.03	33,33,33,33	0
55	MG	BA	3006	1/1	0.99	0.04	20,20,20,20	0
55	MG	BA	3062	1/1	0.99	0.08	3,3,3,3	0
55	MG	CA	1640	1/1	0.99	0.14	23,23,23,23	0
55	MG	BA	3063	1/1	0.99	0.06	0,0,0,0	0
55	MG	BA	3064	1/1	0.99	0.05	2,2,2,2	0
55	MG	BA	3165	1/1	0.99	0.07	2,2,2,2	0
55	MG	BA	3094	1/1	0.99	0.04	17,17,17,17	0
55	MG	BA	3096	1/1	0.99	0.03	5,5,5,5	0
55	MG	BA	3097	1/1	0.99	0.03	6,6,6,6	0
55	MG	BA	3065	1/1	0.99	0.04	7,7,7,7	0
55	MG	BA	3099	1/1	0.99	0.04	3,3,3,3	0
55	MG	BA	3042	1/1	0.99	0.06	6,6,6,6	0
55	MG	CA	1610	1/1	0.99	0.03	47,47,47,47	0
55	MG	BA	3043	1/1	0.99	0.02	15,15,15,15	0
55	MG	CA	1612	1/1	0.99	0.04	30,30,30,30	0
55	MG	BA	3068	1/1	0.99	0.04	6,6,6,6	0
55	MG	DA	3082	1/1	0.99	0.10	50,50,50,50	0
55	MG	BA	3069	1/1	0.99	0.06	39,39,39,39	0
56	ZN	D4	101	1/1	0.99	0.07	79,79,79,79	0
55	MG	BA	3095	1/1	1.00	0.03	8,8,8,8	0
55	MG	BA	3037	1/1	1.00	0.08	2,2,2,2	0
55	MG	DA	3064	1/1	1.00	0.02	38,38,38,38	0
55	MG	BA	3013	1/1	1.00	0.07	0,0,0,0	0

6.5 Other polymers [i](#)

There are no such residues in this entry.