



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:18 PM GMT

PDB ID : 4U1V  
Title : Crystal structure of the E. coli ribosome bound to linopristin.  
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.  
Deposited on : 2014-06-06  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

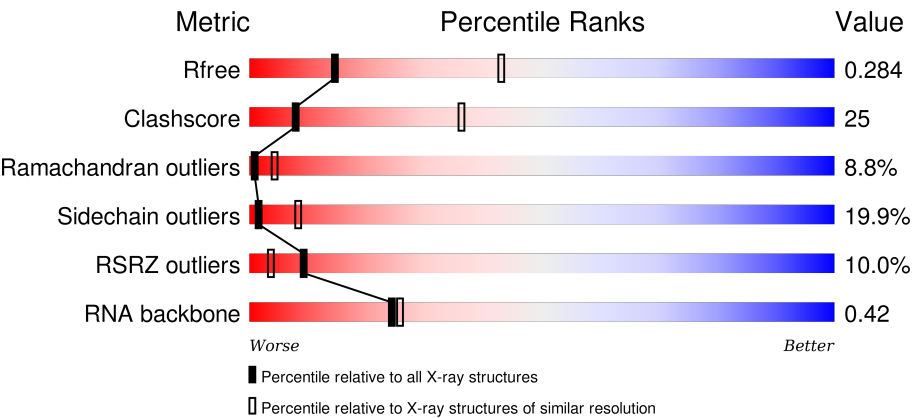
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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 <sub>free</sub>	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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

Mol	Chain	Length	Quality of chain
1	AA	1539	<div><div>23%58%19%</div><div>23%58%19%</div></div>
1	CA	1539	<div><div>29%53%17%</div><div>29%53%17%</div></div>
2	AB	218	<div><div>25%48%25%5%</div><div>22%48%25%5%</div></div>
2	CB	218	<div><div>33%44%22%</div><div>31%44%22%</div></div>

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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	



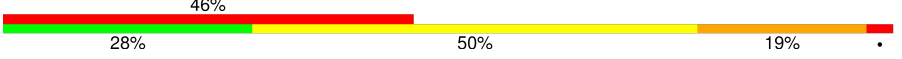

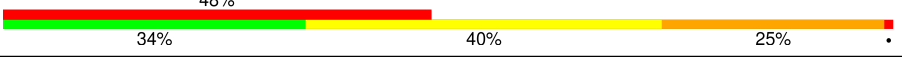



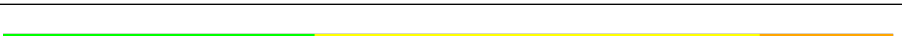
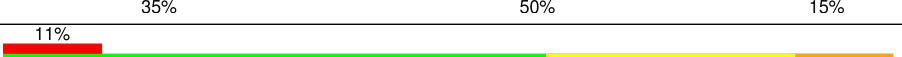
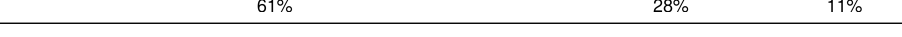

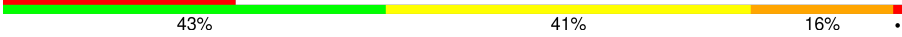


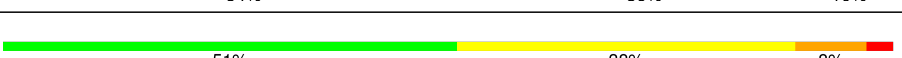
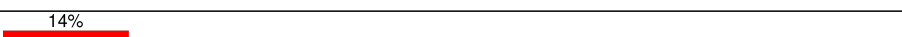


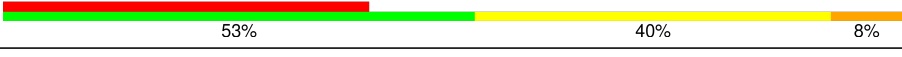





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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	119	
23	DB	119	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	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	7	
54	D6	7	

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	MHW	D6	1	-	-	X	-
55	MG	AA	1622	-	-	-	X
55	MG	AA	1669	-	-	-	X
55	MG	AA	1670	-	-	-	X
55	MG	AM	201	-	-	-	X
55	MG	BA	3005	-	-	-	X
55	MG	BA	3015	-	-	-	X
55	MG	BA	3027	-	-	-	X
55	MG	BA	3040	-	-	-	X
55	MG	BA	3055	-	-	-	X
55	MG	BA	3083	-	-	-	X
55	MG	BA	3104	-	-	-	X
55	MG	BA	3105	-	-	-	X
55	MG	BA	3109	-	-	-	X
55	MG	BA	3131	-	-	-	X
55	MG	BA	3136	-	-	-	X
55	MG	BA	3146	-	-	-	X
55	MG	BA	3152	-	-	-	X
55	MG	BA	3170	-	-	-	X
55	MG	BA	3178	-	-	-	X
55	MG	BA	3186	-	-	-	X
55	MG	CA	1615	-	-	-	X
55	MG	CA	1626	-	-	-	X
55	MG	DA	3002	-	-	-	X
55	MG	DA	3028	-	-	-	X
55	MG	DA	3032	-	-	-	X
55	MG	DA	3041	-	-	-	X
55	MG	DA	3071	-	-	-	X
55	MG	DA	3072	-	-	-	X
55	MG	DA	3106	-	-	-	X
55	MG	DA	3110	-	-	-	X
55	MG	DA	3113	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3154	-	-	-	X
55	MG	DA	3158	-	-	-	X



## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 288320 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	0	0	0
			780	492	146	142			

- 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	0	0	0
			753	479	137	134	3			
43	DV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- 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	0	0	0
			580	359	117	103	1			
44	DW	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			

- 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	0	0	0
			625	388	129	106	2			
45	DX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	B6	7	Total	C	N	O	0	0	0
			69	50	9	10			
54	D6	7	Total	C	N	O	0	0	0
			69	50	9	10			

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

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

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

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	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	615	Total O 615 615	0	0
57	BB	14	Total O 14 14	0	0
57	BC	10	Total O 10 10	0	0
57	BD	4	Total O 4 4	0	0
57	BE	4	Total O 4 4	0	0
57	BF	1	Total O 1 1	0	0
57	BG	1	Total O 1 1	0	0
57	BJ	1	Total O 1 1	0	0
57	BL	6	Total O 6 6	0	0
57	BN	2	Total O 2 2	0	0
57	BS	1	Total O 1 1	0	0
57	BU	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

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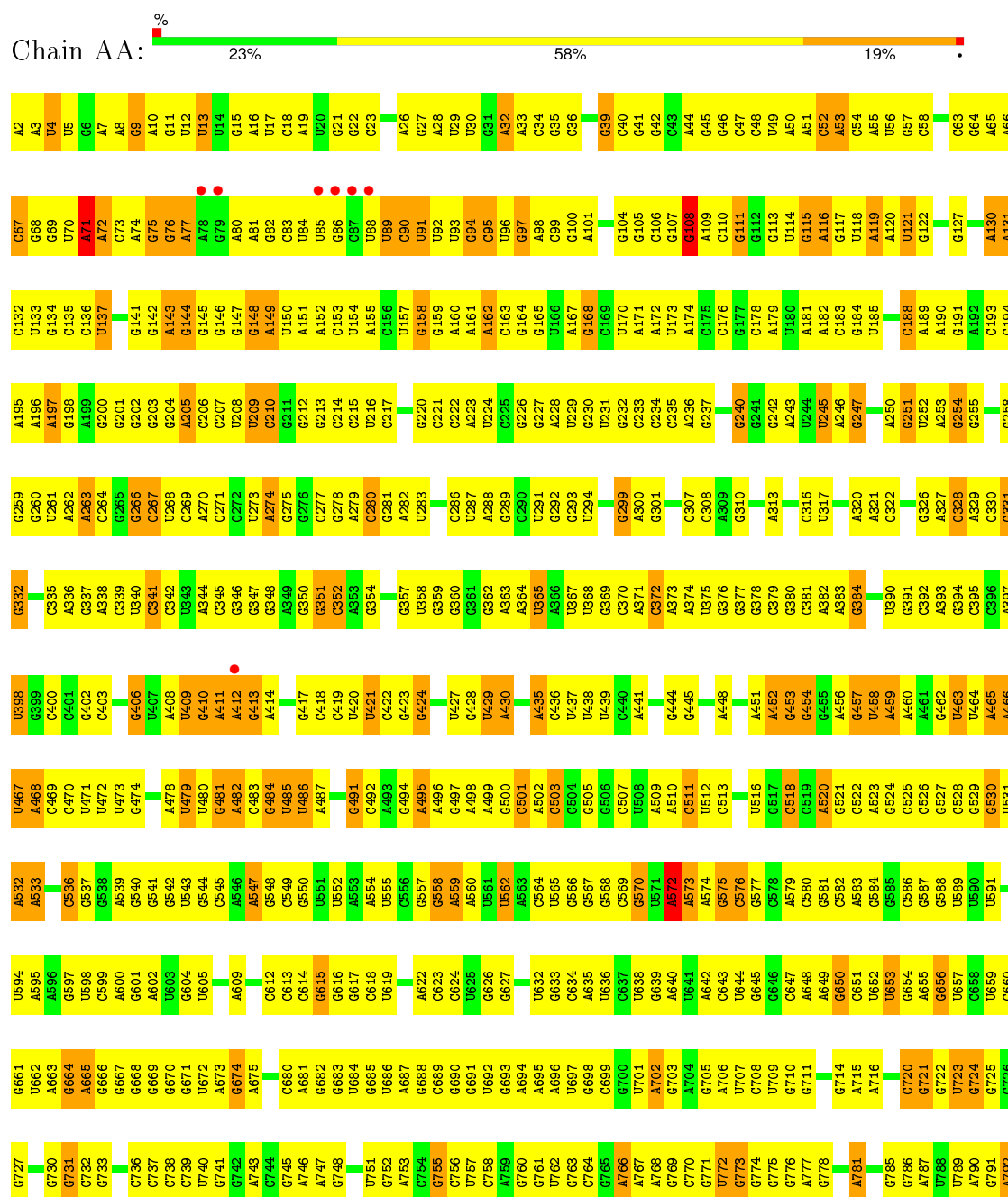
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CN	3	Total 3	O 3	0	0
57	CT	3	Total 3	O 3	0	0
57	CU	2	Total 2	O 2	0	0
57	DA	607	Total 607	O 607	0	0
57	DB	13	Total 13	O 13	0	0
57	DC	9	Total 9	O 9	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	6	Total 6	O 6	0	0
57	DL	5	Total 5	O 5	0	0
57	DN	2	Total 2	O 2	0	0
57	DT	2	Total 2	O 2	0	0
57	DU	1	Total 1	O 1	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	2	Total 2	O 2	0	0
57	D4	1	Total 1	O 1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

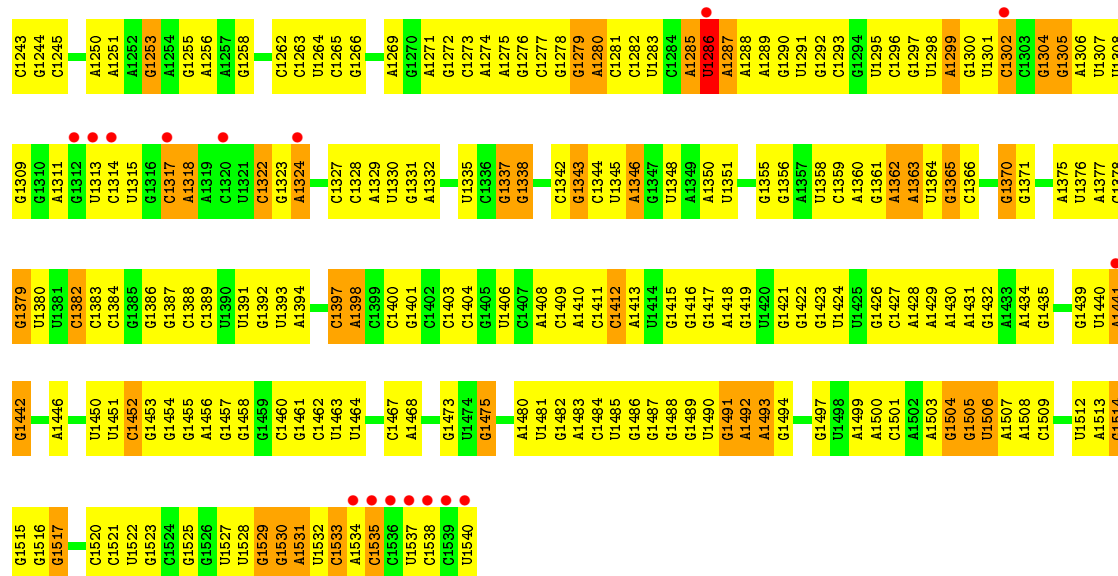
#### • Molecule 1: 16S rRNA



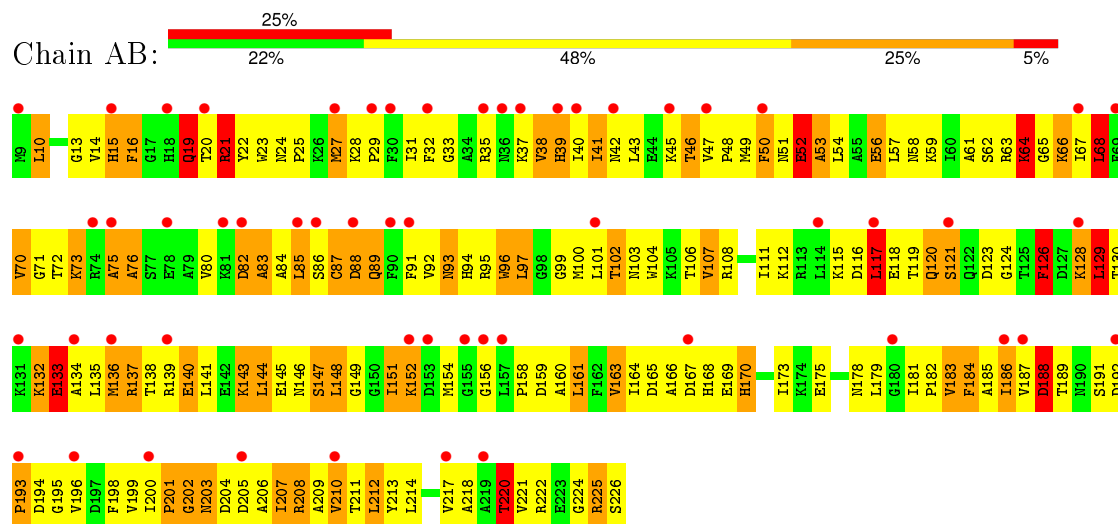


A1176	G1107	A1044	G976	G912	U911	C841	G773	A706	U636	G558	U485	A415	C352	A279	U209	G136
G1177	G1108	C1045	A977	C912	C912	U842	G774	U707	C637	A859	U486	C418	A353	C280	C210	U137
G1178	C1109	A1046	A978	A914	A914	G843	G775	G708	U638	U861			G354	G281	G211	
A1179	G1047	G979	C979	A914	A914	G844	G776	U709	U639	U861	G494		G355		G212	G142
A1180	G1112	G1048	C980	G917	G917	A845	A777	G710	A640	U862	A495	U421	A356	C285	G213	A143
G1181	G1113	U1049	U981	A918	A918	G846	A778	G711	U641	A563	A496	C422	G357	C286	G214	G144
G1182	C1114	G1050	U982	A919	A919	G847	C779	A712	A642	C564	A497	G423	U358		C215	G145
U1183		C1051	A983	A919	A919	C848	A780		U643	U865	A498	G424	C359	G289	U216	G146
G1184	U1118	U1052		U920	U920		A781	A715	U644	U866	A499	G424	G360		C217	
G1185	U1122	G1053	U986	U921	U921	G851	A782	A716	U645	G567	U500	U426	G361	G293	U218	U150
G1186	G1123	C1054	G987	G922	G922	G852	C783	U717	U645	G568	G501	U427	G362	U294	U151	A151
G1187	U1124		G988	G926	G926	G853	A784	A718	A649	C569	A502	G428	U365	C295	C221	A152
	U1125	U1060	C990	G927	G927	U855	G785	C719	G650	G570	C504	U429	A366	C296	C222	C183
	G1126	G1061	U991	G928	G928	U856	G786	C720	C651	U571		A430	U367	G297	A223	U154
	G1127	U1062	U992	G929	G929	U857	A787	G721	U652	A572	G505	A431	U368	A298	U224	C155
		C1063	G993	C930	C930	G858		G722	U653	A573	G506	A432	U369	G299		C156
		G1064	A994	C931	C931	A859	A790	U723	G656	A574			C370	A300	G227	U157
		U1065	A995	C932	C932	A860	G791	G724	U657	G575	A509	A435	C371	A301	A228	G158
		C1066	A996	G933	G933	G861	A792		U658	G576	A510	C436	A372	U304		G159
		U1067	U997	C934	C934	C862	U793	A728	U659	G577	C511	U437	A373	G305	C235	A160
		G1068	C998	A935	A935	A863	A794	G730	U660	A579	U512	U438	A374	A306	A236	A161
		C1069	C999	C936	C936	A864	C795	G731	G661	C580	C513	U439	A375	C307	G237	A162
		U1070	A1000	A937	A937	A865	C796	G732	U662	G581		A441	G376	C308	A238	C163
		C1071	C1001	A938	A938	C866	G797	G733	A663	C582	G517	A442	G377	A309	U239	G164
		U1072	G1002	G939	G939	C867	U798	G734	U664	A583	C519	C443	C378	G310		A167
		U1073	G1003	C940	C940	C868	G799	G735	G665	A584	A520	G444	C379	A313	G241	G168
		G1074	A1004	G941	G941	G869	U801	C736	U666	G585	G521	G445	G380	C314	A243	C169
		U1075	A1005	G942	G942	U870	A802	C737	U667	C586	C522	G446	U381	U244	U244	U170
		U1076	G1006			U871	G803						A382	C315	U245	A171
		G1077	U1007	G945	G945	A872	U804	U740	A673	A595	G527	A451	A383	C316	U246	A172
		U1078	A946	A946	A946	A873	U805	G741	C674	A596	G528	A452	A384	U317	G247	U173
		G1079	G947	C948	C948	G874	C806	G742	A675	A597	G529	A453	C385	G319	C248	
		U1080	A949	A949	A949	A878		A743	U677	U598	U531	G455	C386	A320	U249	C176
		A1081					G809	G744	U678	C599		A456	U387	A321		
		G1082	G1018			G881	C810	G745	U679	G604	A533	A457	G388	G324	G251	A179
		U1083	A1019			C882	C811	A746	C680	U605	A534	U458	U390	U252	A253	U180
		G1084	G1020	G953	G953	C883	G812	A747	U681	G606	U535	A459	G391	G254	G254	A181
		U1085	A1022				U813	G748	A682	A607	C536	A460	C392	A182		C183
		G1086	U1023	U955	U955	G886	A814	A749	U683	A608	G537		A393	G329	G257	G184
		U1087	G1024	U956	U956	G887	A815	C750	U684	A609	C538	U463	C396	G330	G258	U185
		G1088	U1025	U957	U957	G888	A816	U751	U685	A539	A539	U464	C397	G331	G259	C188
		U1089	A1026	A958	A958	G889	C817		U686	C618	G540	A465	A397	G332	G260	A189
		G1090	C1027	U959	U959	G890		C754	A687	U619	G541	A466	U398	U333	U261	
		U1091	C1028	U960	U960	U891	G821	G755	U688	C620	G542	U467	G399	C334	A262	
		A1092	U1029	U961	U961	A892	U822	C756	U689	A621	U543	A468	C395	C335	G263	A195
		U1093	U1030	C962	C962	C893	C823	U757	U690	A622	C544	C469	G402	G337	G264	A196
		G1094	C1031	G963	G963		G824	C758	U691	C623	G545		G403	G337	G265	A197
		U1095	G1032	A964	A964	G898		A759	G691	C624	A546	G474	G404	A338	G266	G198
		C1096	G1033	U965	U965	C899	U827	G760	U692	U625	A547	U475	U405	U340	U268	A199
		C1097	G1034	G966	G966	A900	U828	G761	U693	G626	G548	C476	G406	G339	G267	G200
		U1098	A1035	C967	C967	A901	G829		A694	U626	U548	U476	U407	U341	G269	G201
		G1099	A1036	U968	U968	G902	U829	G765	A695	G627	C549	C477	U407	G345	C269	G202
		C1100	C1037	A969	A969	G903	G833	A767	G700	G628	G550	A478	U409	G346	C271	G203
		A1101	U1038	G970	G970	A906	U834	U768	U701	A629	U551	U490	G410	G347	C272	G204
		U1102	G1039	G971	G971	A907	U835	A769	A702	A630	U552	U491	G411	G348	U273	A205
		C1103	U1040	C972	C972	A908	G836	G770	G703	C631	U553		A412	A349	A274	C206
		G1104	G1041	G973	G973	A909	U837	G771	A704	U632	C556	C482	G413	G350	G207	C207
		A1105	A1042	A974	A974	A910	C840	U772	G705	G633	G557	G484	A414	G351	G278	U208
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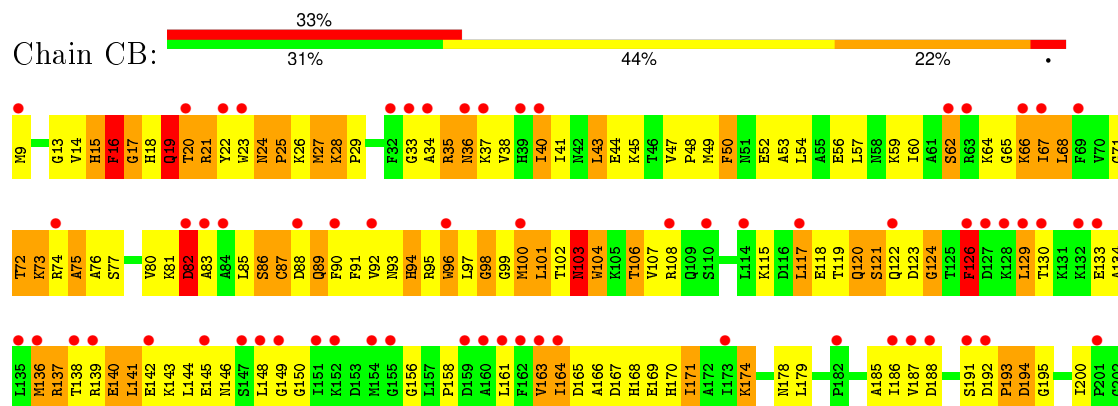


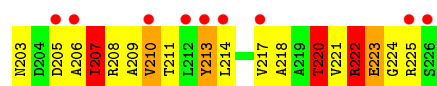


• Molecule 2: 30S ribosomal protein S2

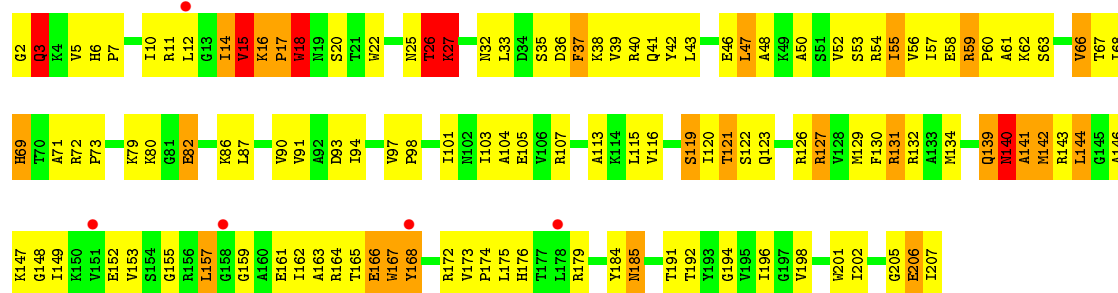
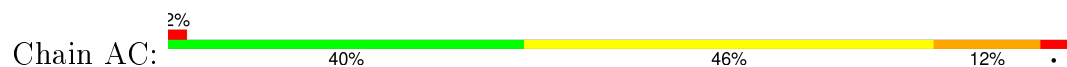


• Molecule 2: 30S ribosomal protein S2

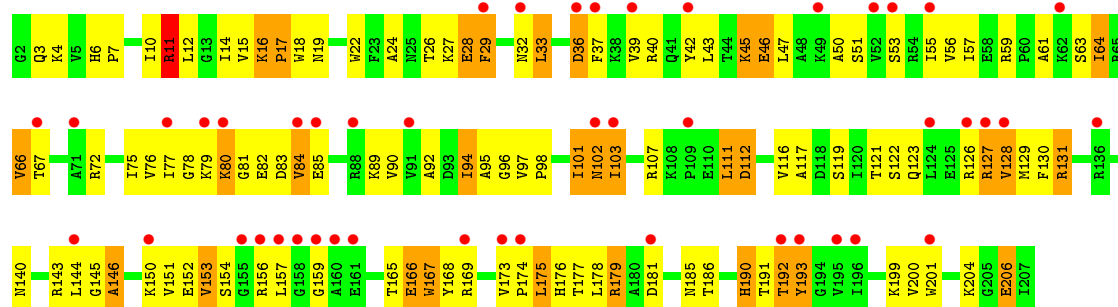
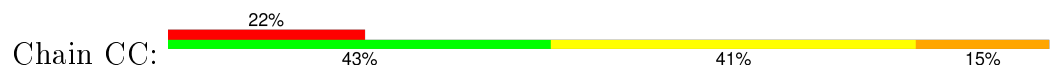




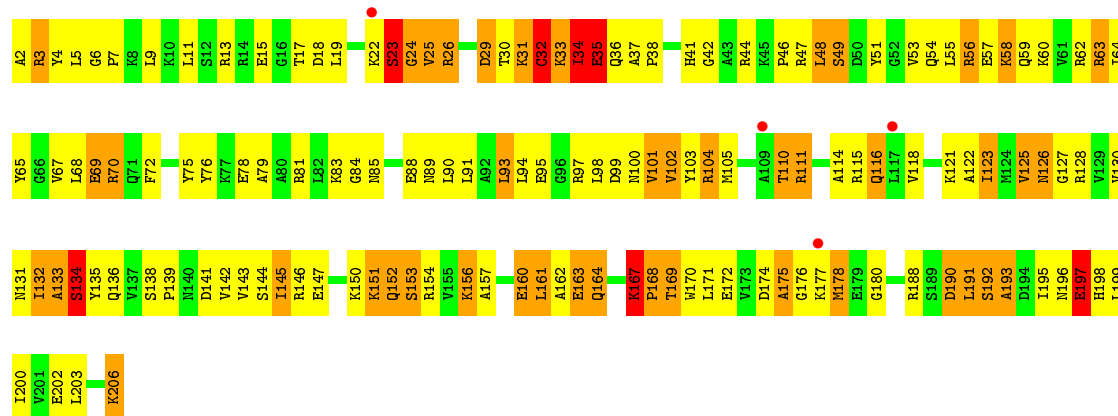
• Molecule 3: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S3

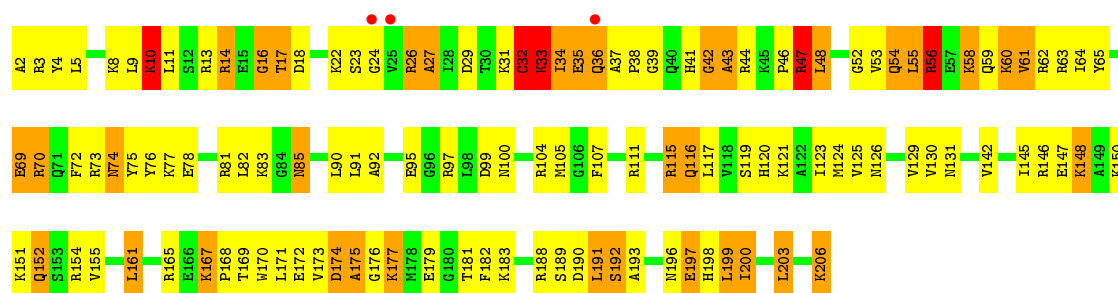


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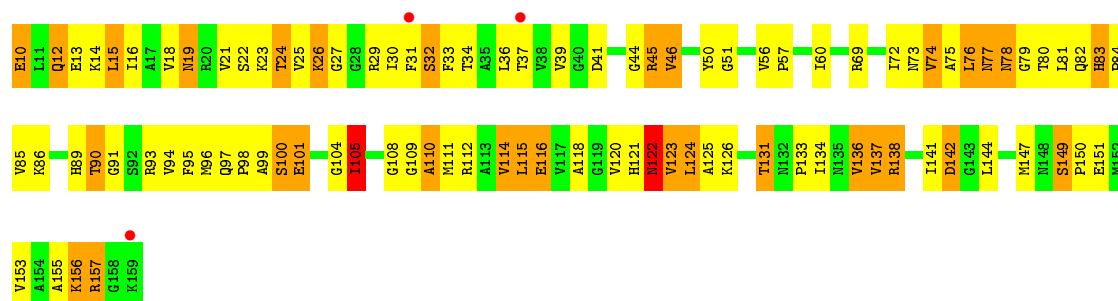


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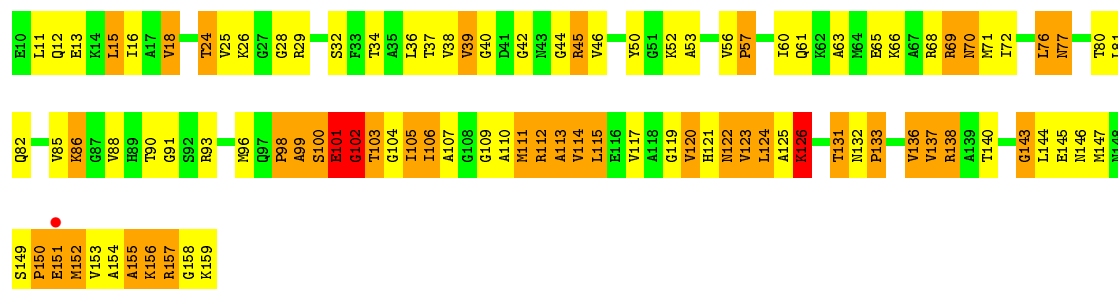




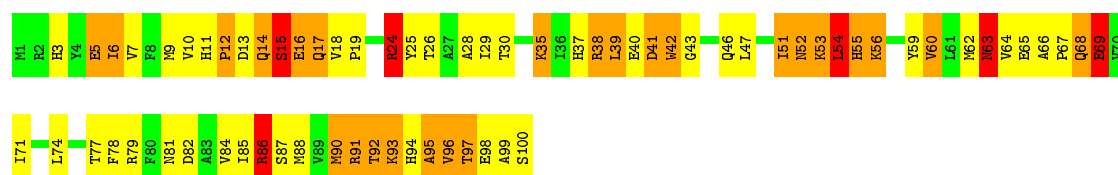
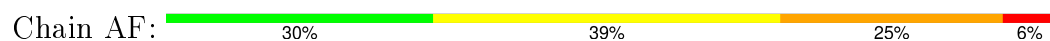
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

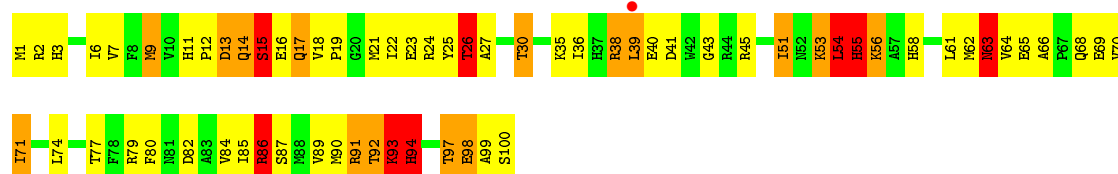


• Molecule 6: 30S ribosomal protein S6

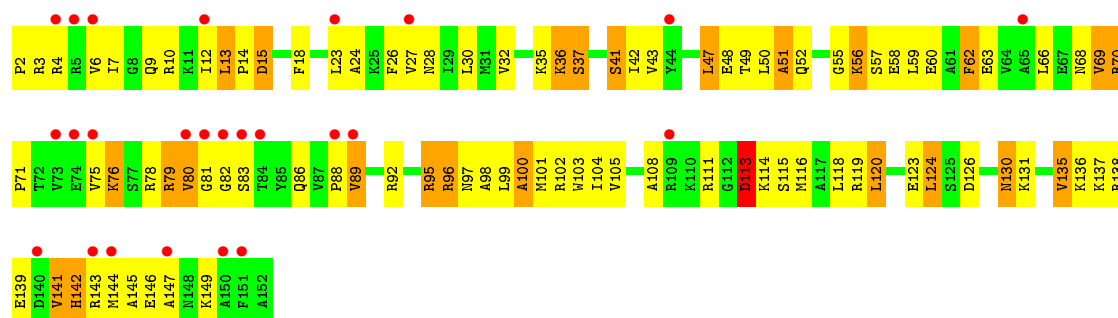


• Molecule 6: 30S ribosomal protein S6

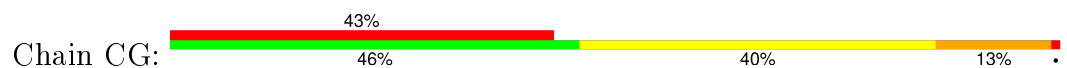




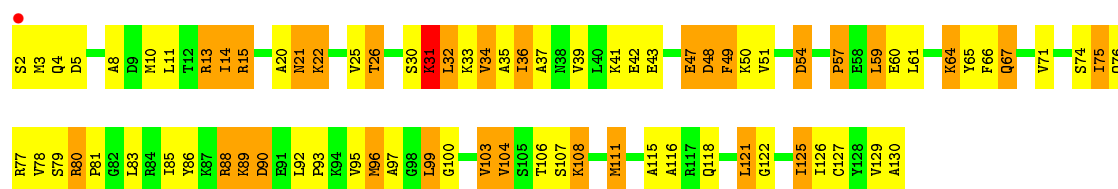
• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

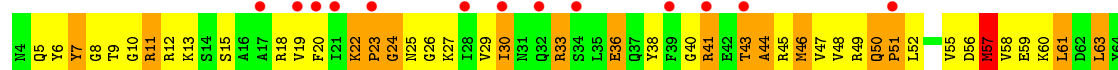


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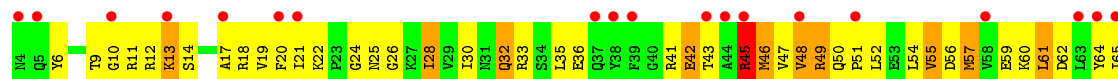




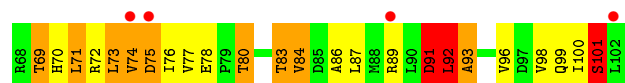
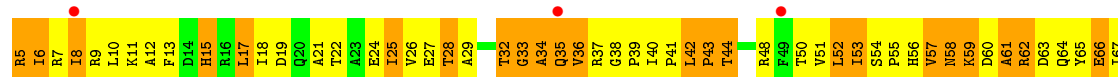
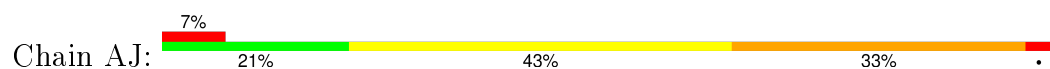
• Molecule 9: 30S ribosomal protein S9



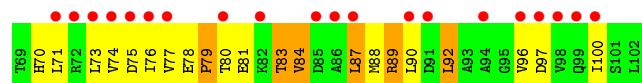
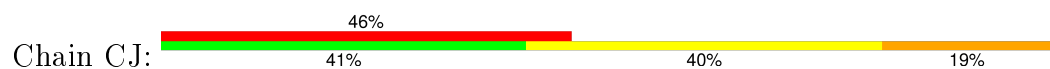
• Molecule 9: 30S ribosomal protein S9



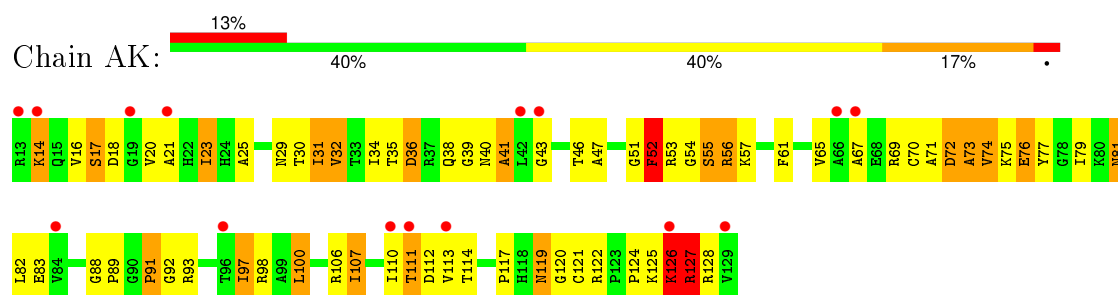
• Molecule 10: 30S ribosomal protein S10



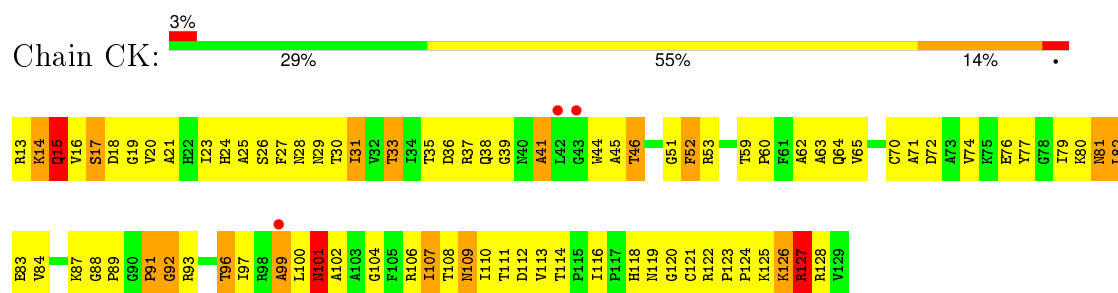
• Molecule 10: 30S ribosomal protein S10



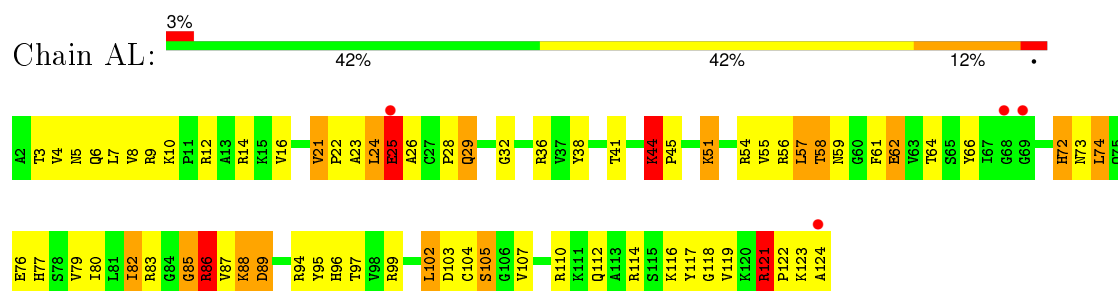
• Molecule 11: 30S ribosomal protein S11



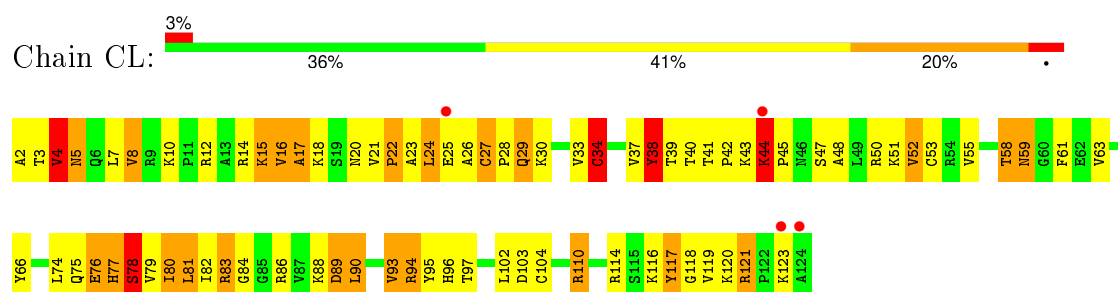
- Molecule 11: 30S ribosomal protein S11



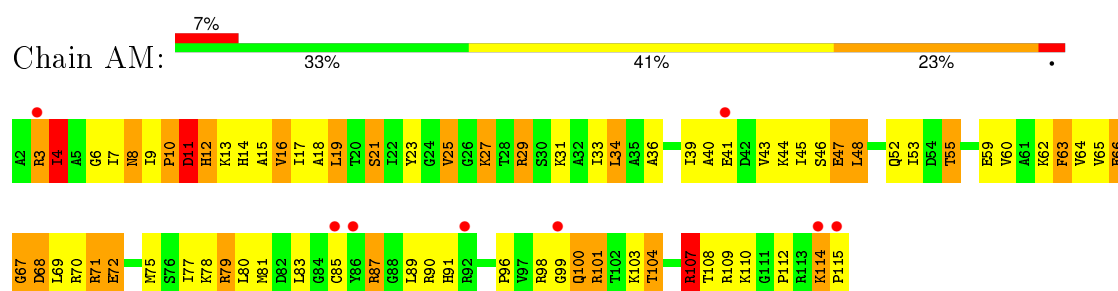
- Molecule 12: 30S ribosomal protein S12



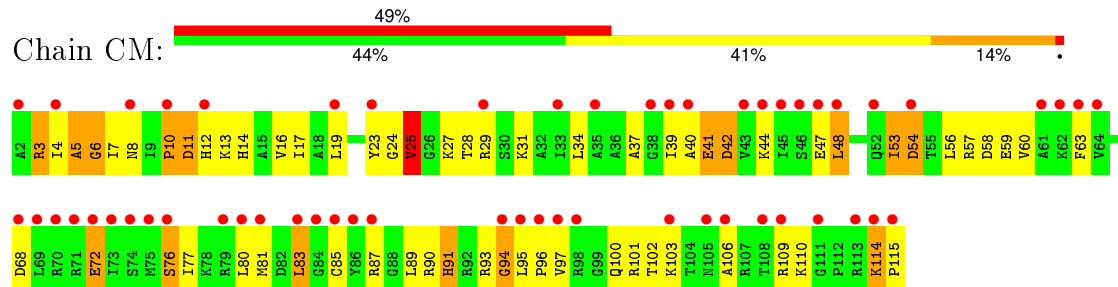
- Molecule 12: 30S ribosomal protein S12



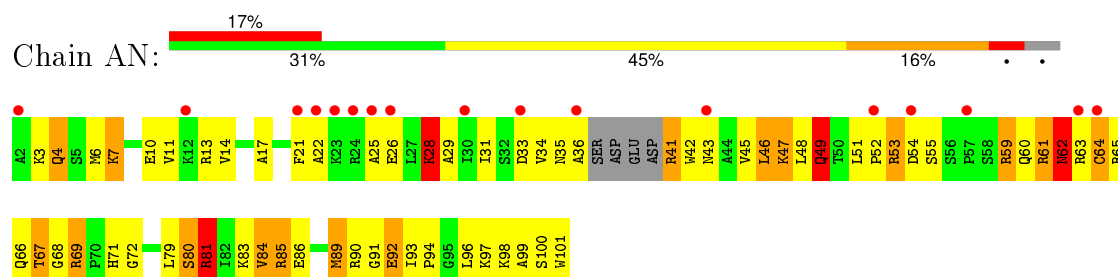
- Molecule 13: 30S ribosomal protein S13



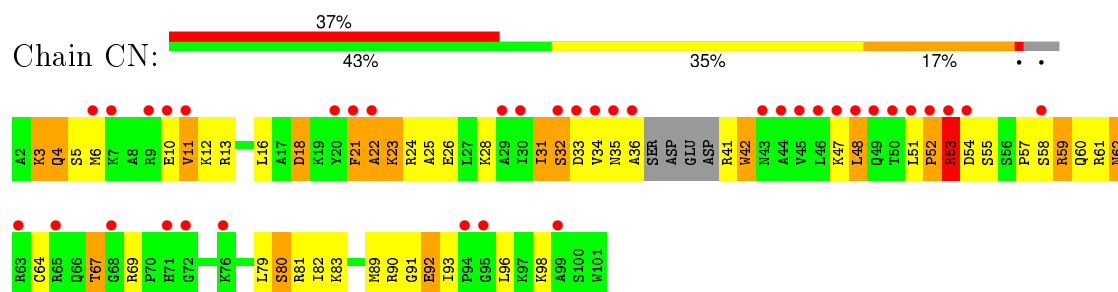
- Molecule 13: 30S ribosomal protein S13



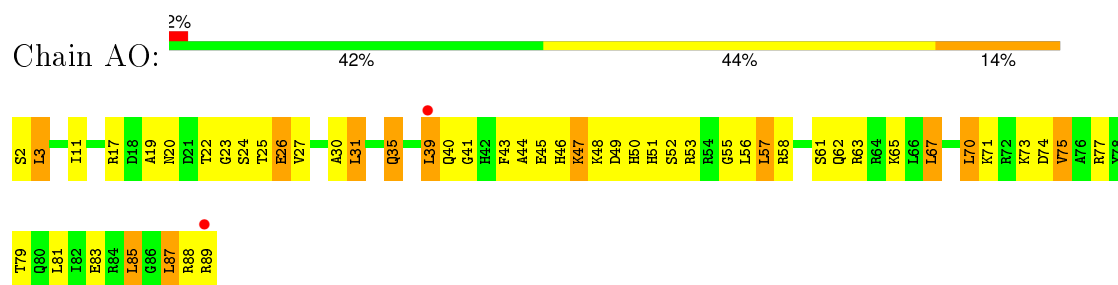
- Molecule 14: 30S ribosomal protein S14



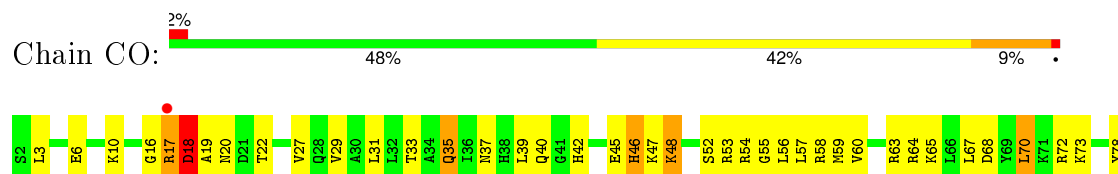
- Molecule 14: 30S ribosomal protein S14

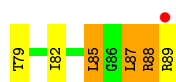


- Molecule 15: 30S ribosomal protein S15

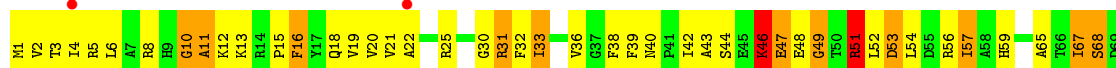


- Molecule 15: 30S ribosomal protein S15

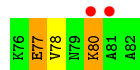
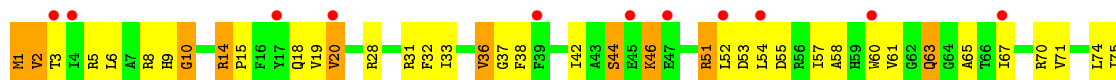




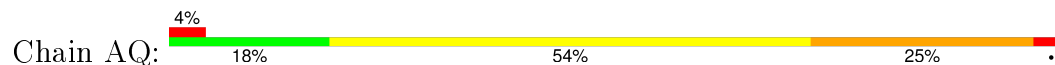
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

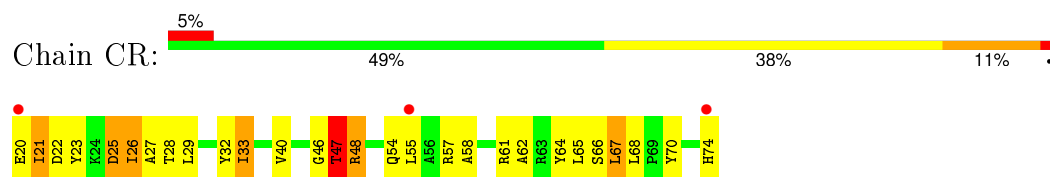


- Molecule 18: 30S ribosomal protein S18

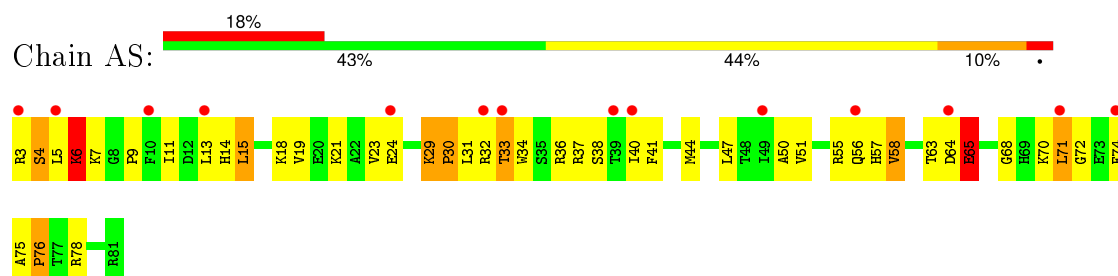




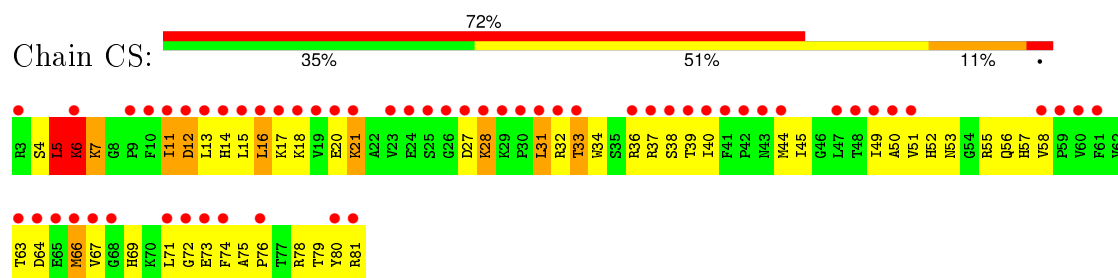
- Molecule 18: 30S ribosomal protein S18



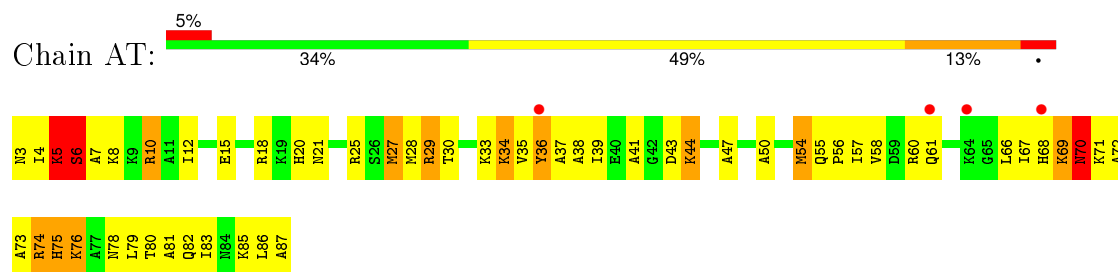
- Molecule 19: 30S ribosomal protein S19



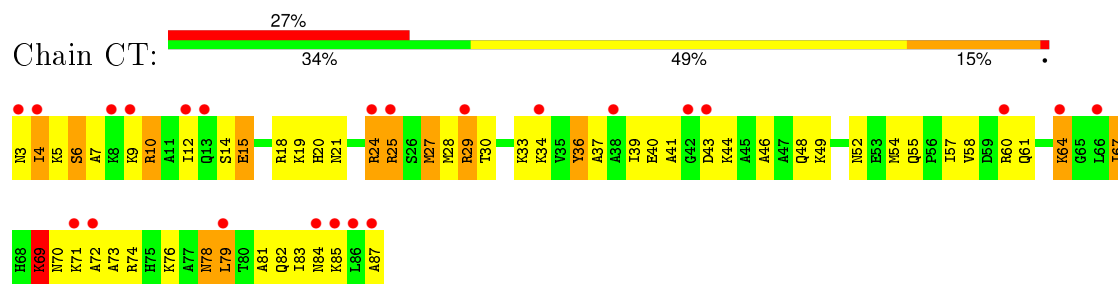
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

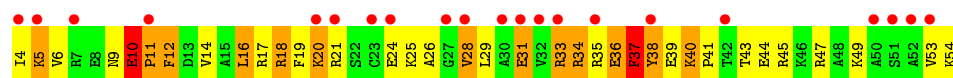


- Molecule 20: 30S ribosomal protein S20

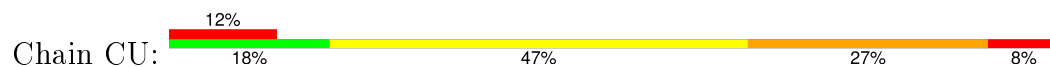


- Molecule 21: 30S ribosomal protein S21

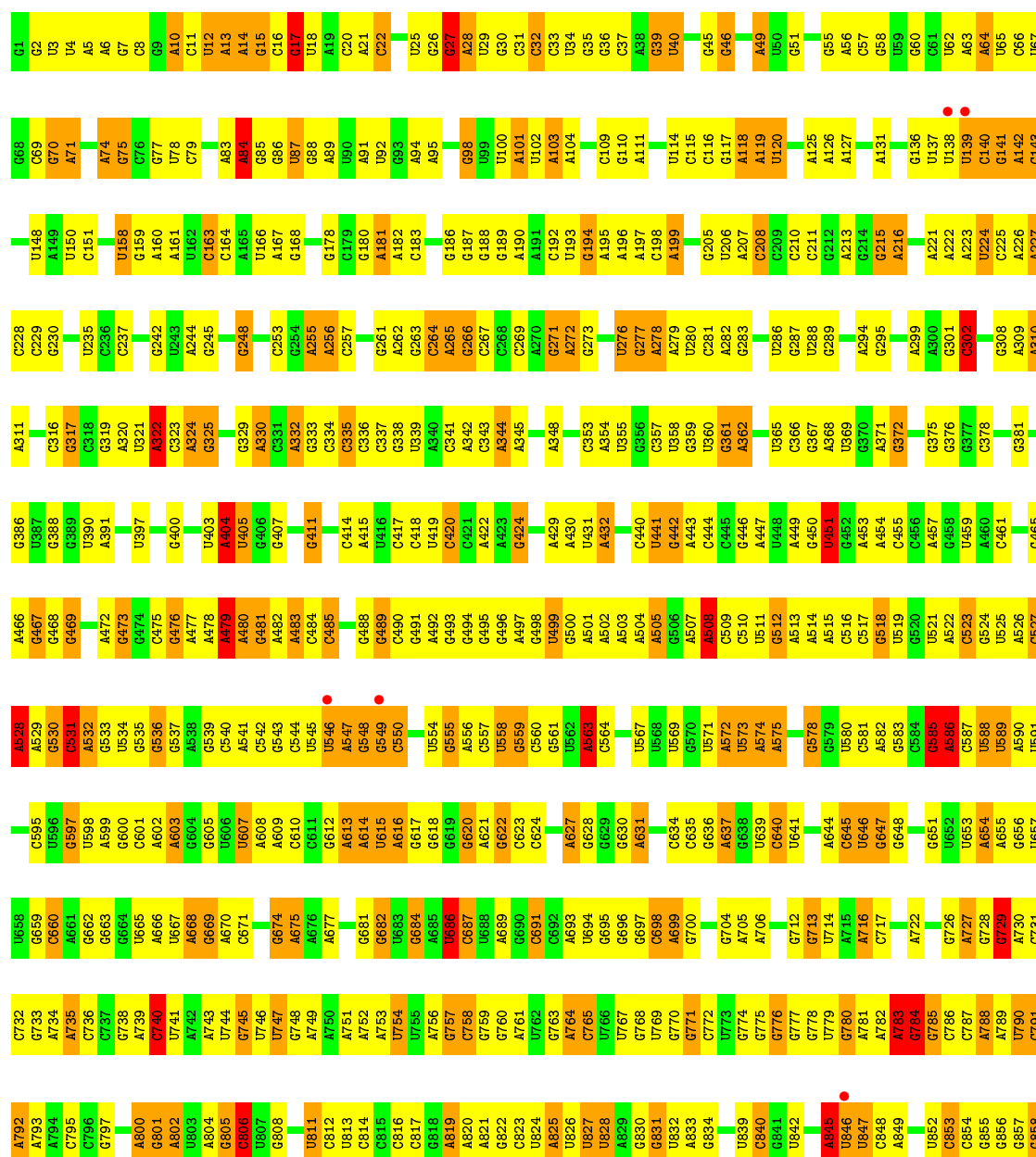
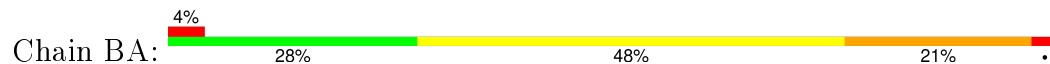




- Molecule 21: 30S ribosomal protein S21

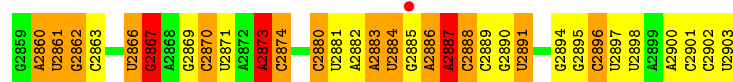


- Molecule 22: 23S rRNA

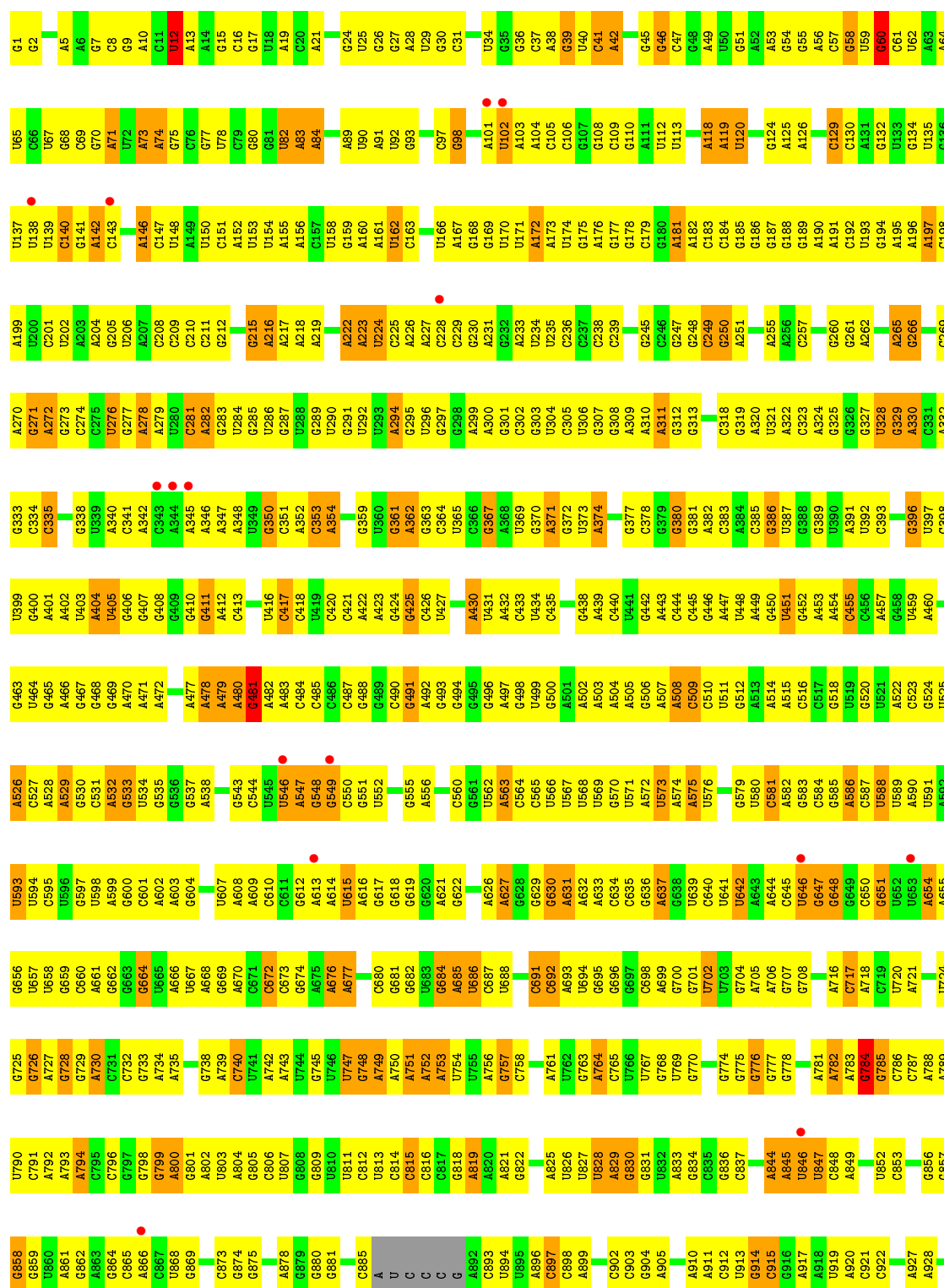


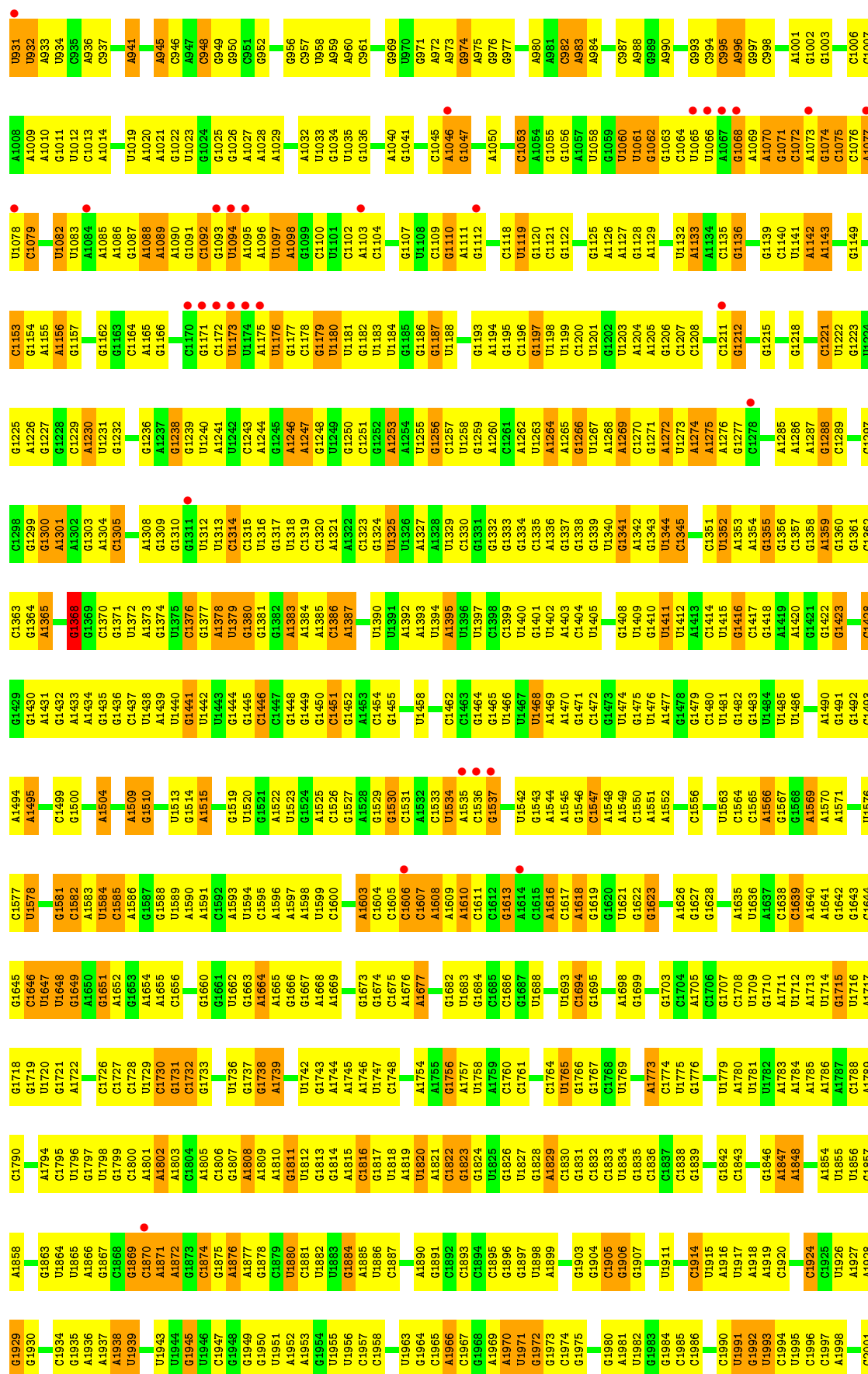
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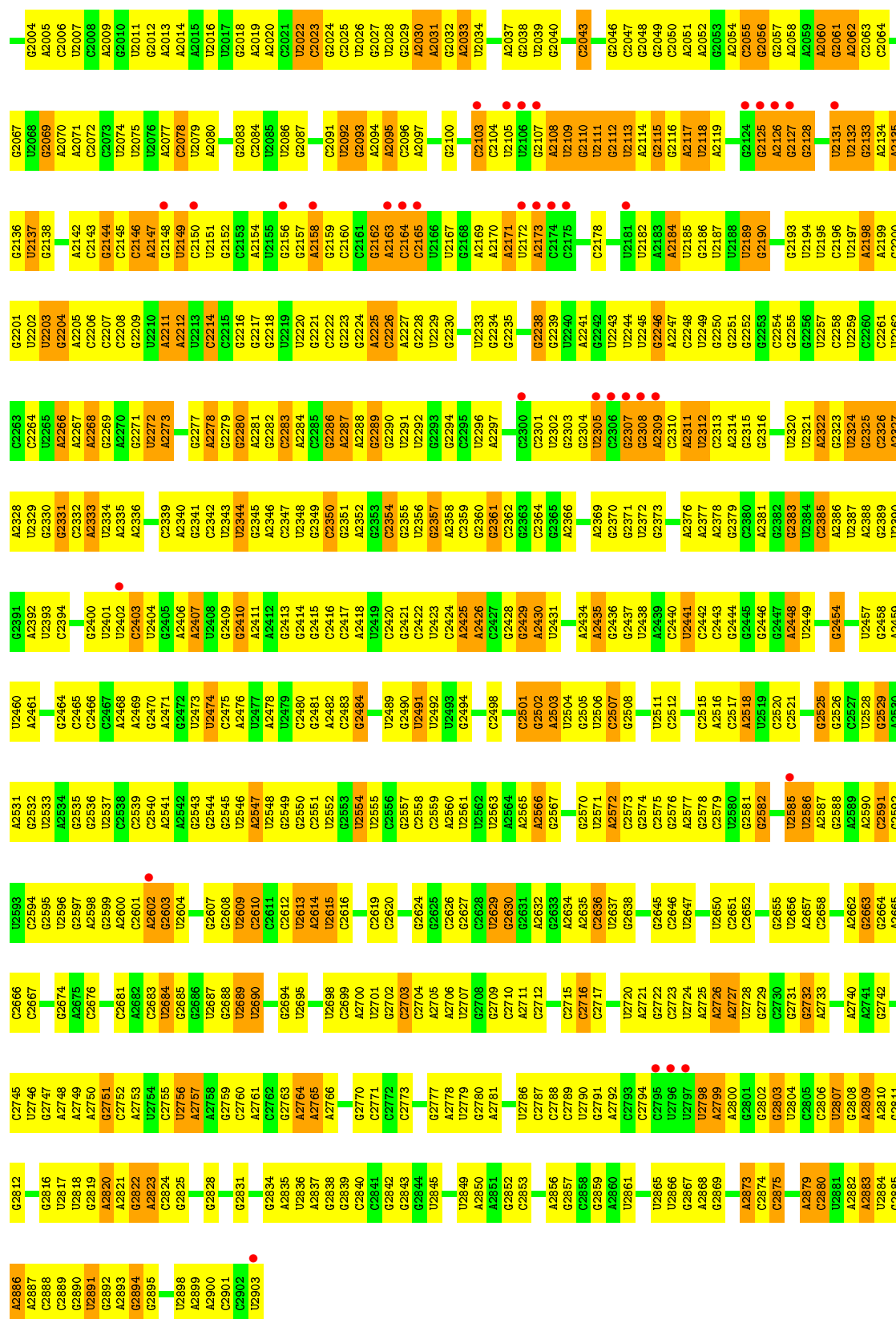
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C2771	C2703		G2567	U2506	G2444	A2377	A2311	G2239	U2171	G2110	C2043	G1973	C1909
G2772	G2704	U2633	U2568	C2507	G2445	G2379	C2313	U2244	U2172	G2112	C2044	G1974	U1911
A2773	A2705	G2633	U2569	G2508	G2446	C2380	A2314	U2245	U2173	U2113		G1975	A1912
G2774	G2706	G2636	G2570	U2509	G2447	A2381		G2246	C2174	A2114			A1913
U2775	U2707	U2637	U2571	G2510	A2448	G2382	A2317	G2247	G2175	G2115	C2050	G1983	C1914
A2776	G2708	U2638	U2572	U2511	U2449	G2383	G2318	U2248	A2176	G2116	A2051	C1984	U1915
G2777	G2709	G2638	A2573	C2512	A2450	U2384	G2319	U2249	C2177	A2117	A2052	C1985	U1916
A2778	C2710		C2574	U2513	A2451	G2385	U2320	U2245	C2178	U2118	G2053	A1917	U1917
G2779	A2711	G2641	G2574	G2514	C2452	A2386	U2321	U2246	C2179	A2119	A2054	A1918	U1918
U2780	C2712	G2642	C2575	U2515	A2453	A2387	G2322	G2248	U2180	G2120	C2055	C1990	A1919
G2781	U2713	G2643	C2575	C2516	A2453	U2388	A2322	U2249	U2181	G2121	G2056	G1991	A1919
U2782	C2714	G2644	C2579	U2517	U2457	U2388	U2323	G2249	U2182	U2122	G2057	G1992	C1920
	G2715	G2645	U2580	A2518	G2458	G2389	U2324	G2250	U2183	G2123		U1993	G1921
G2786	U2716	G2646	G2581	U2519	A2459	C2390	G2325	G2251	A2184	U2124	A2058	C1994	G1922
U2787	C2717	U2647	G2582	G2520	U2460	C2391	A2326	G2252	U2185	G2125	A2059	U1995	U1923
G2788	G2718	G2648	U2583	C2521	A2461	C2392	A2327	U2253	U2186	C2126	A2060	C1996	C1924
C2789	U2719	C2649	U2584	C2521	G2462	U2393	A2328	G2254	U2187	G2127	G2061	C1997	U1925
U2790	G2720	U2650	U2585	G2524	C2462	C2394	U2329	U2255	U2188	A2126		A1998	U1926
G2791			U2586	G2525	C2463	C2395	G2330	G2256	U2189	G2128	C2063	C1999	A1927
A2792	C2723	G2655	A2587	G2526	C2464	C2396	G2331	U2257	U2190	C2129	C2065	C2000	A1928
G2793	U2724	G2656	G2588	C2526	C2465	C2396	C2332	U2259	G2191	G2130		G2001	G1929
C2794			C2589	C2527	C2466		A2333	U2262	A2191	U2131	C2066	G2002	G1930

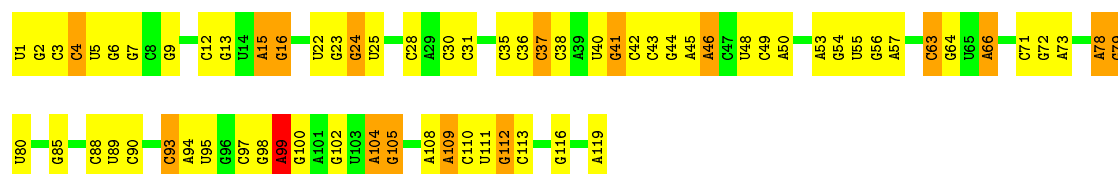


• Molecule 22: 23S rRNA



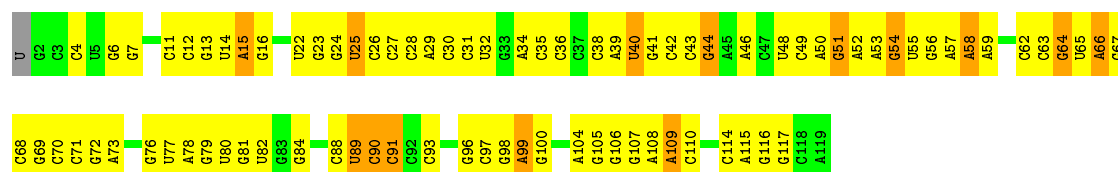






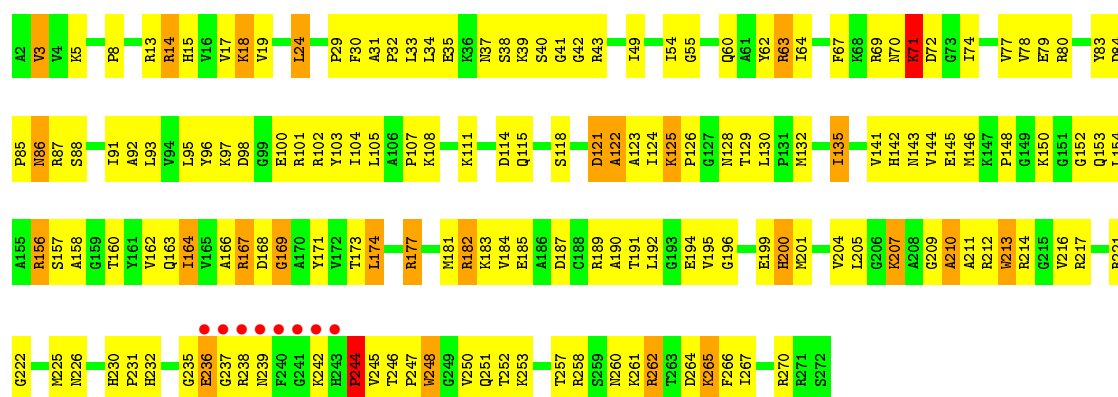
• Molecule 23: 5S rRNA

Chain DB: 29% 59% 12%



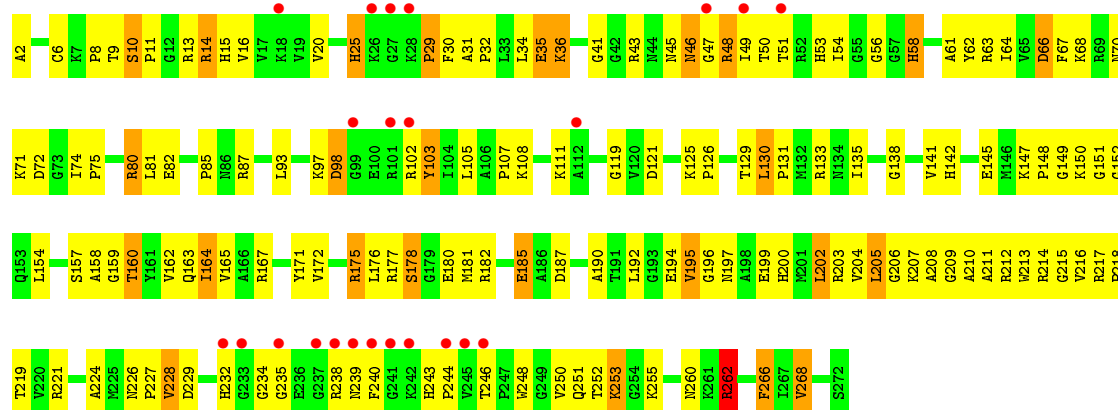
• Molecule 24: 50S ribosomal protein L2

Chain BC: 3% 40% 50% 9%



• Molecule 24: 50S ribosomal protein L2

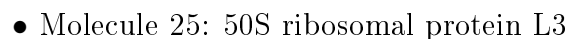
Chain DC: 8% 45% 45% 10%



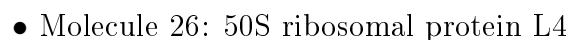
• Molecule 25: 50S ribosomal protein L3



Response	Percentage
Yes, the U.S. is a democracy	54%
No, the U.S. is not a democracy	39%
Don't know	7%



Frequency	Percentage
Daily	6%
Often	59%
Sometimes	33%
Never	7%



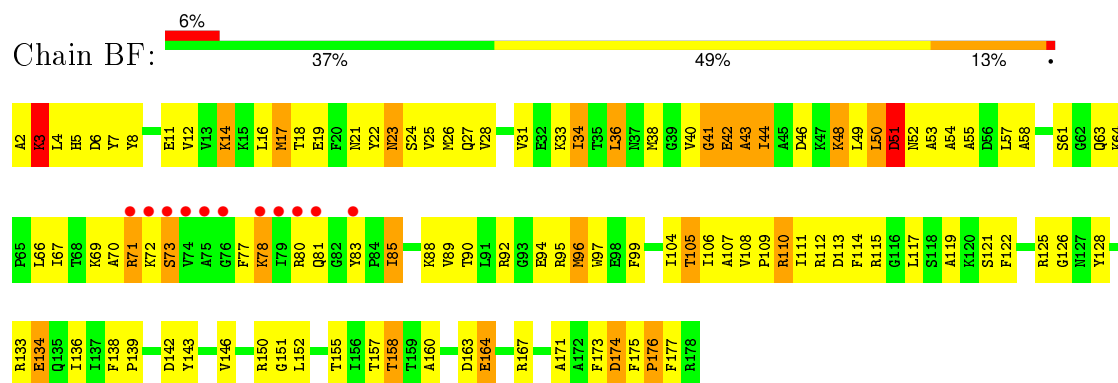
Response	Percentage
Yes	47%
No	43%
Don't know	9%



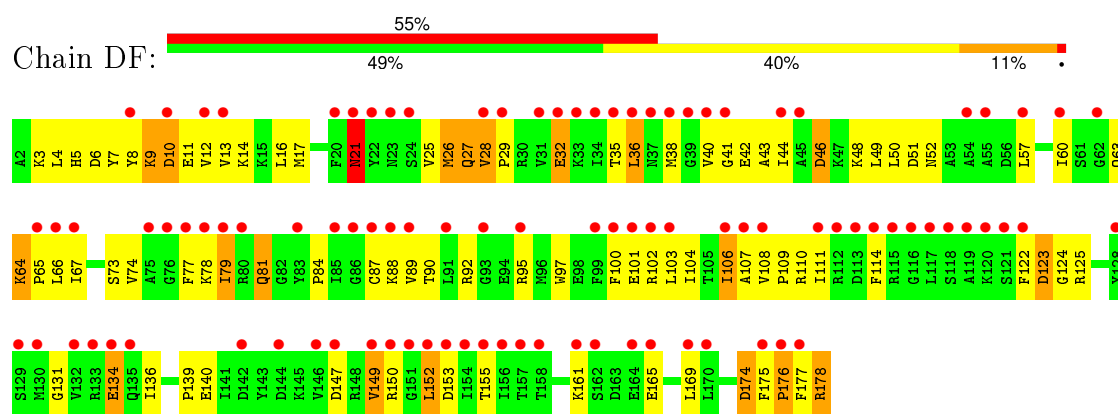
Government	Percentage
Current Government	18%
Opposition	44%
Current Government	41%
Opposition	14%



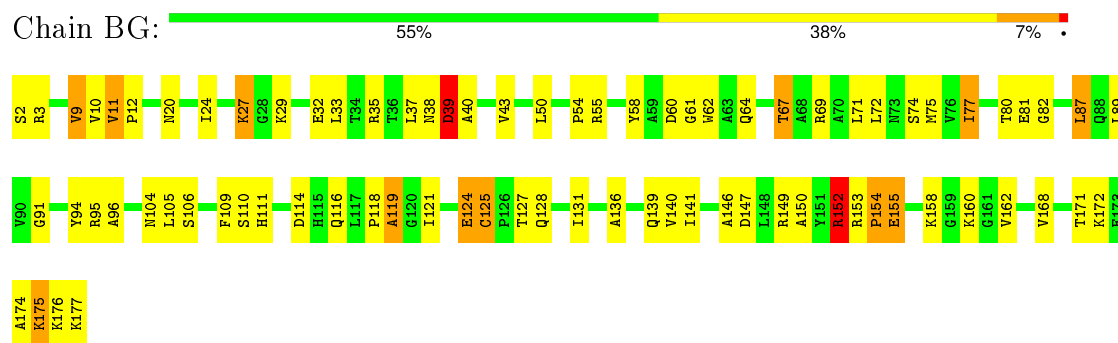
- Molecule 27: 50S ribosomal protein L5



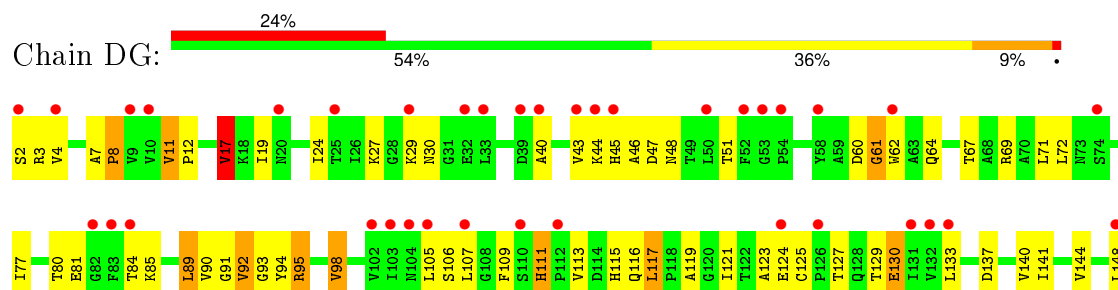
- Molecule 27: 50S ribosomal protein L5

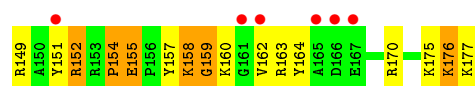


- Molecule 28: 50S ribosomal protein L6

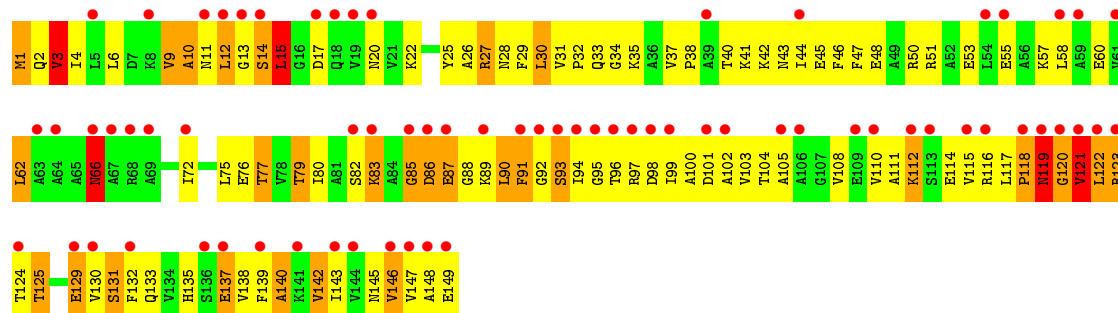


- Molecule 28: 50S ribosomal protein L6

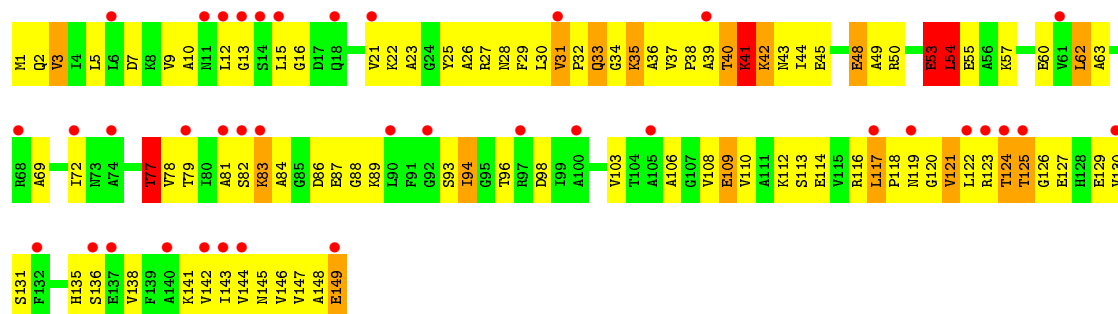




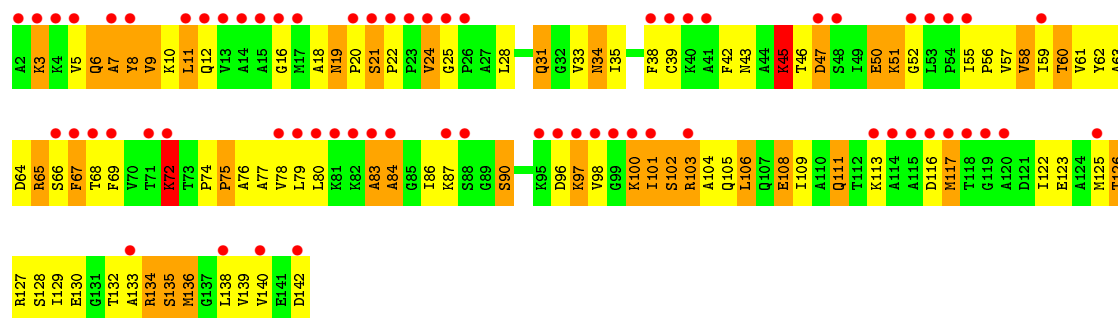
- Molecule 29: 50S ribosomal protein L9



- Molecule 29: 50S ribosomal protein L9

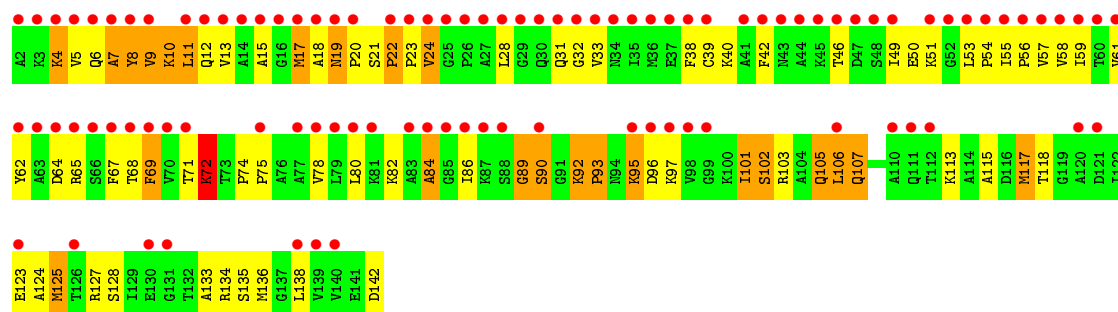


- Molecule 30: 50S ribosomal protein L11



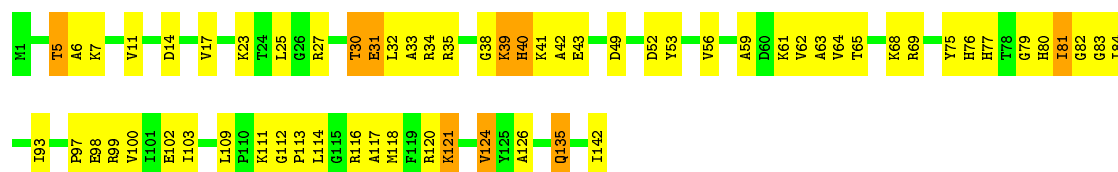
- Molecule 30: 50S ribosomal protein L11





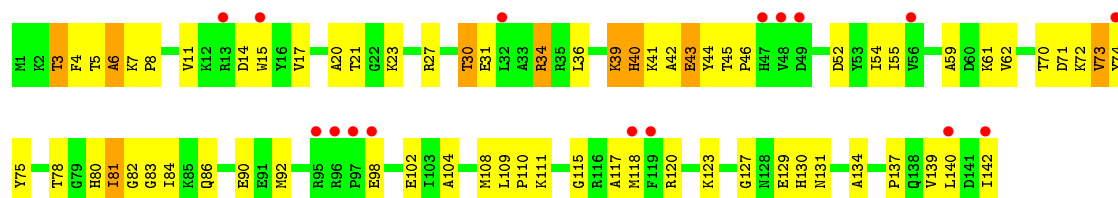
• Molecule 31: 50S ribosomal protein L13

Chain BJ: 56% 38% 6%



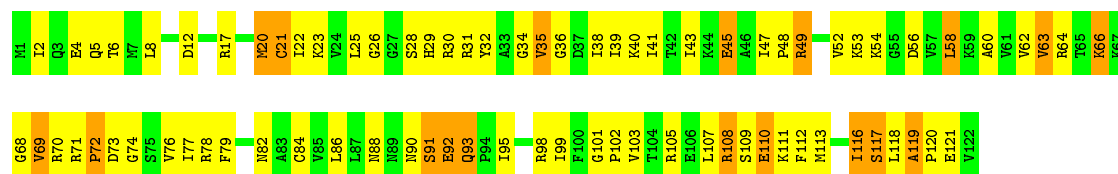
• Molecule 31: 50S ribosomal protein L13

Chain DJ: 11% 52% 42% 6%



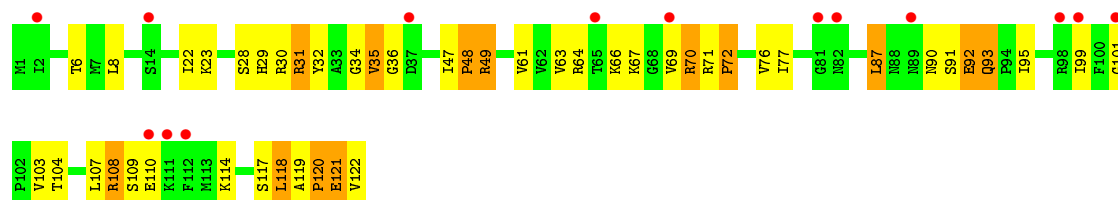
• Molecule 32: 50S ribosomal protein L14

Chain BK: 35% 50% 15%

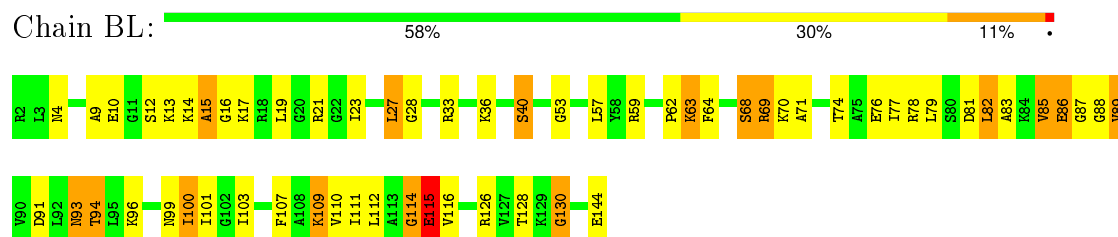


• Molecule 32: 50S ribosomal protein L14

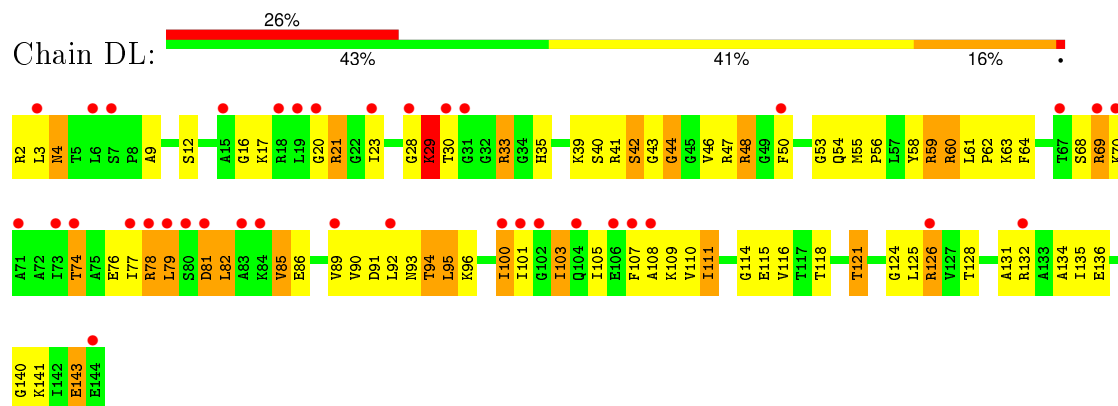
Chain DK: 11% 61% 28% 11%



- Molecule 33: 50S ribosomal protein L15



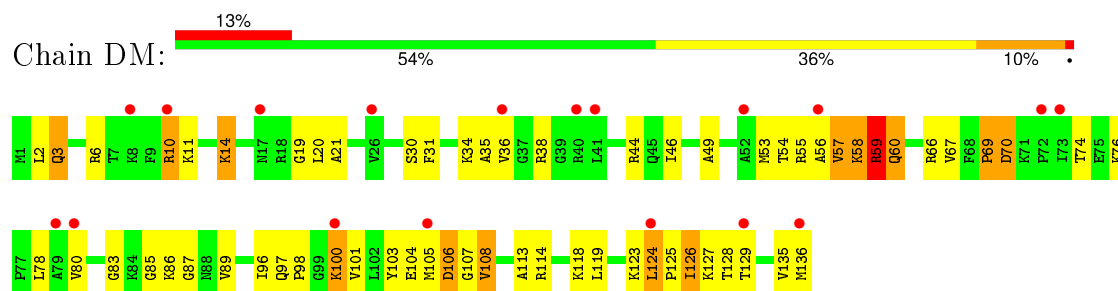
- Molecule 33: 50S ribosomal protein L15



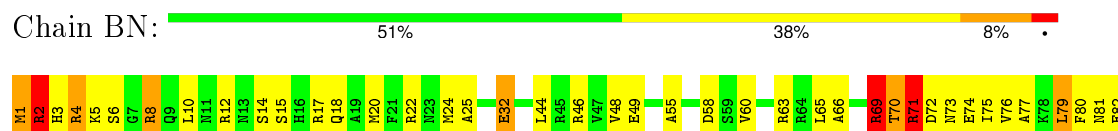
- Molecule 34: 50S ribosomal protein L16



- Molecule 34: 50S ribosomal protein L16

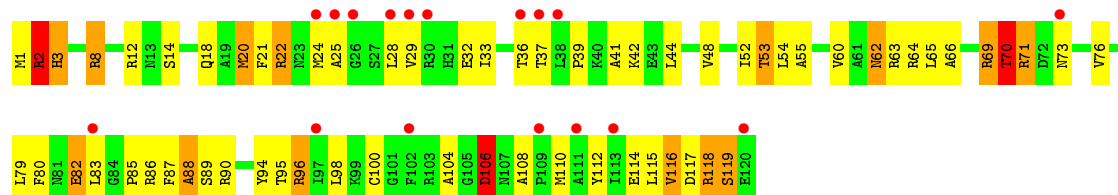


- Molecule 35: 50S ribosomal protein L17

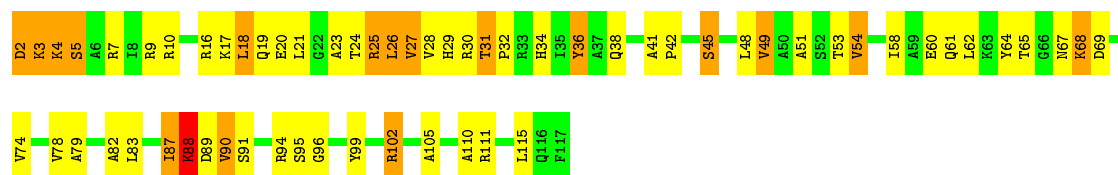




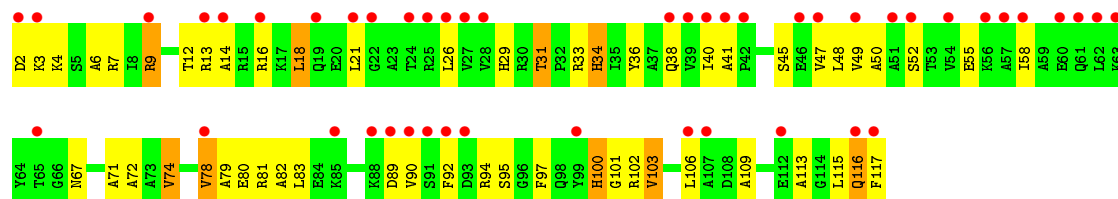
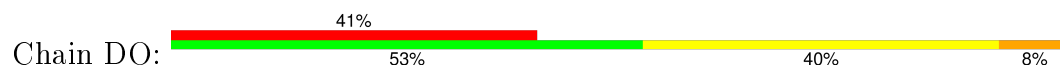
• Molecule 35: 50S ribosomal protein L17



• Molecule 36: 50S ribosomal protein L18



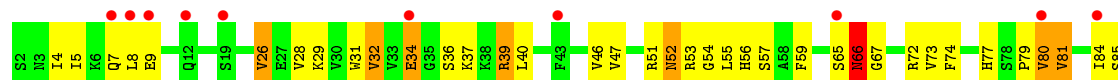
• Molecule 36: 50S ribosomal protein L18

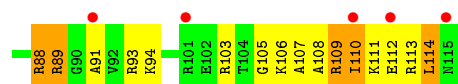


• Molecule 37: 50S ribosomal protein L19



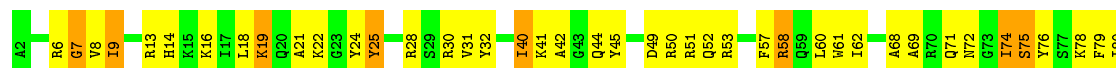
• Molecule 37: 50S ribosomal protein L19





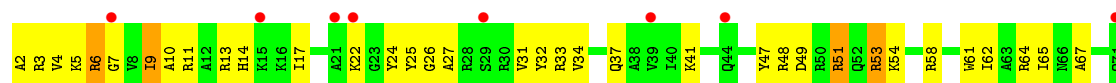
- Molecule 38: 50S ribosomal protein L20

Chain BQ: 48% 44% 9%



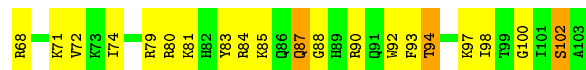
- Molecule 38: 50S ribosomal protein L20

Chain DQ: 9% 52% 44% . .



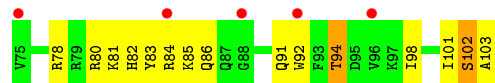
- Molecule 39: 50S ribosomal protein L21

Chain BR: 37% 49% 14% .



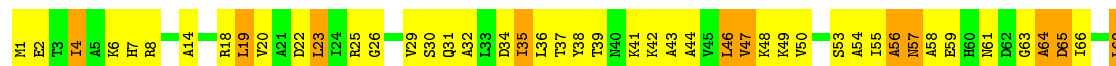
- Molecule 39: 50S ribosomal protein L21

Chain DR: 18% 51% 40% 9%



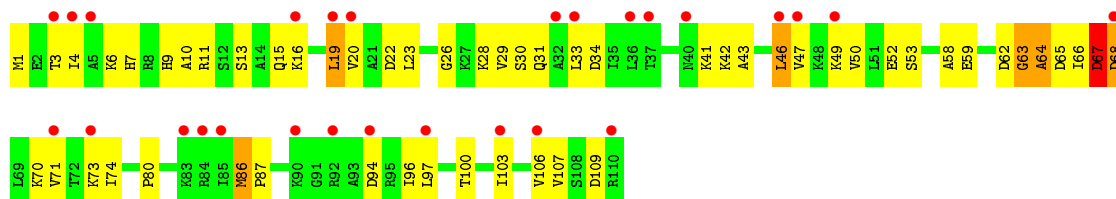
- Molecule 40: 50S ribosomal protein L22

Chain BS: 39% 48% 13%

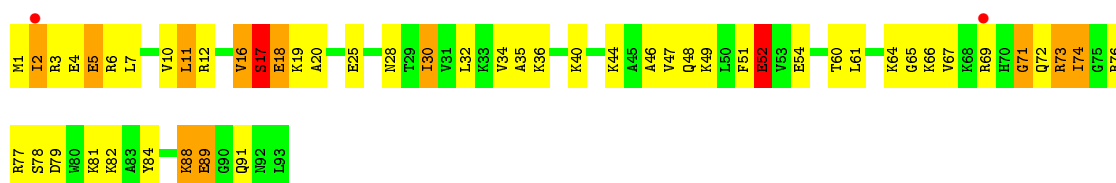
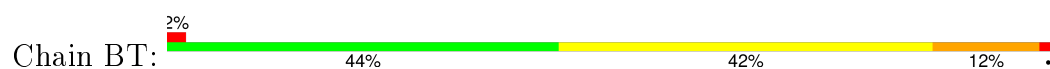




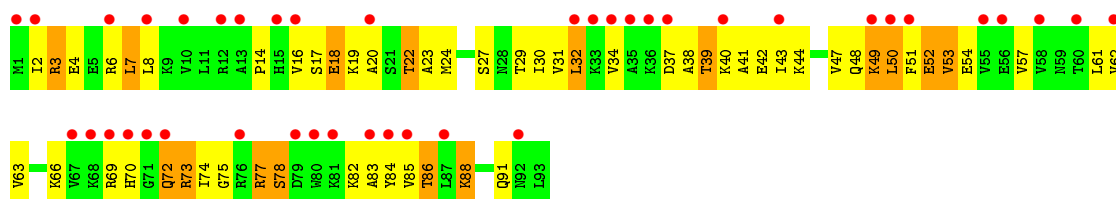
- Molecule 40: 50S ribosomal protein L22



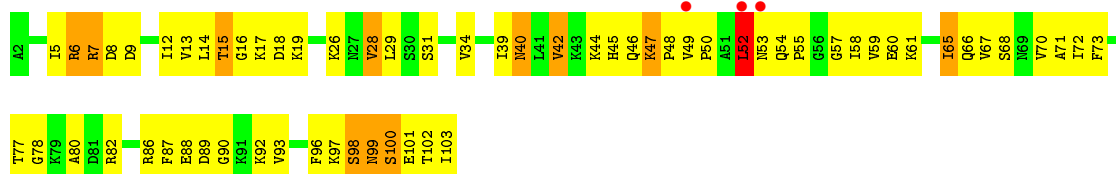
- Molecule 41: 50S ribosomal protein L23



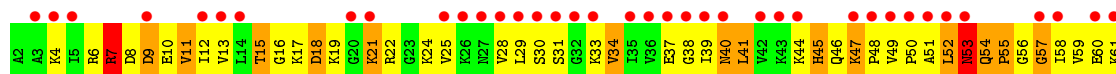
- Molecule 41: 50S ribosomal protein L23



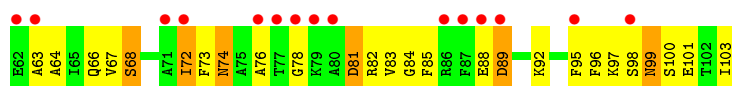
- Molecule 42: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L24

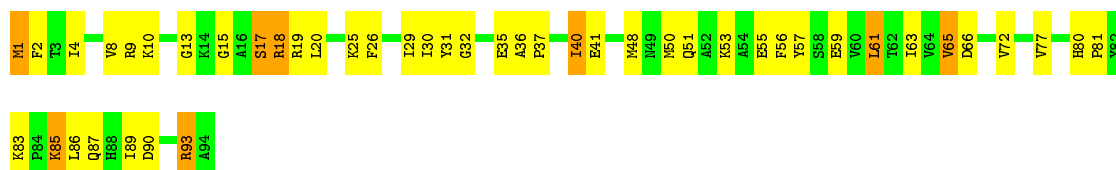






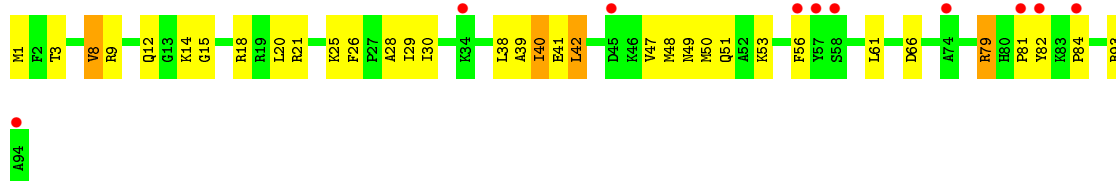
- Molecule 43: 50S ribosomal protein L25

Chain BV: 51% 40% 9%



- Molecule 43: 50S ribosomal protein L25

Chain DV: 11% 64% 32%



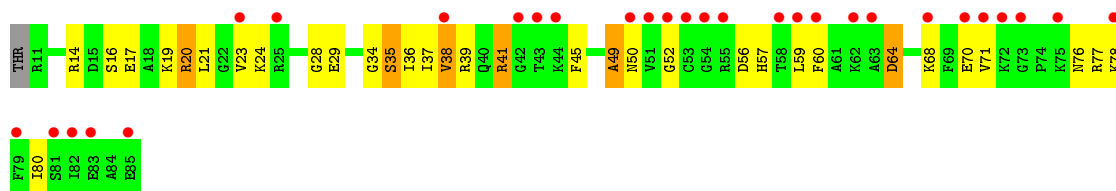
- Molecule 44: 50S ribosomal protein L27

Chain BW: 55% 39% 5%



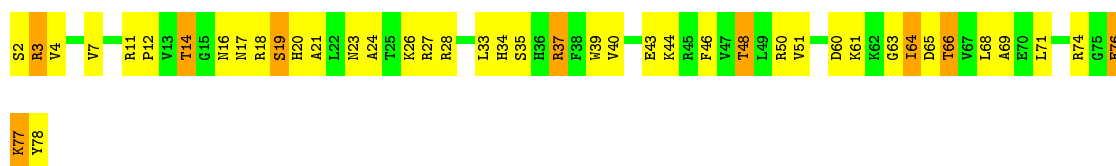
- Molecule 44: 50S ribosomal protein L27

Chain DW: 38% 55% 36% 8%

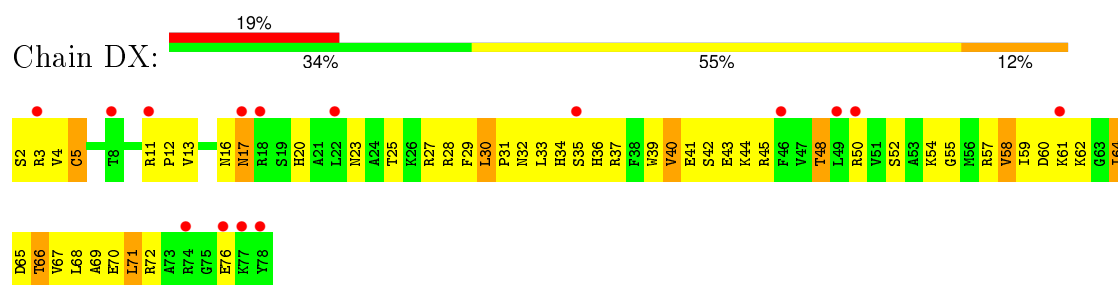


- Molecule 45: 50S ribosomal protein L28

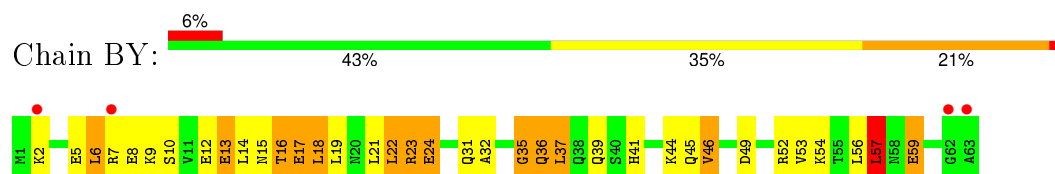
Chain BX: 44% 44% 12%



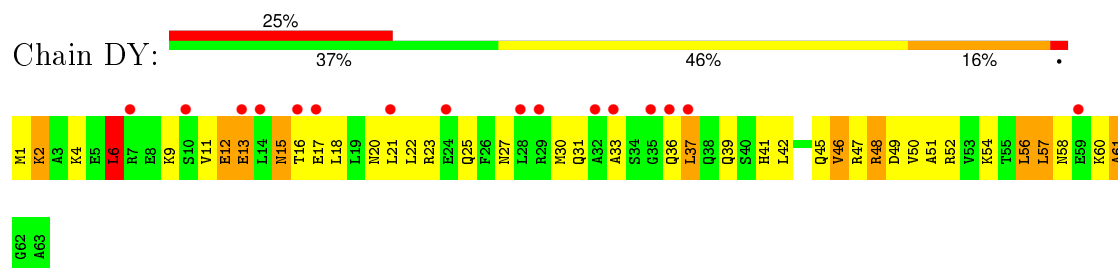
- Molecule 45: 50S ribosomal protein L28



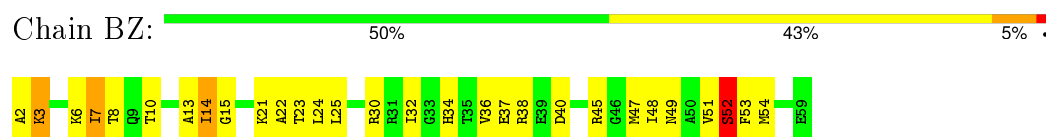
- Molecule 46: 50S ribosomal protein L29



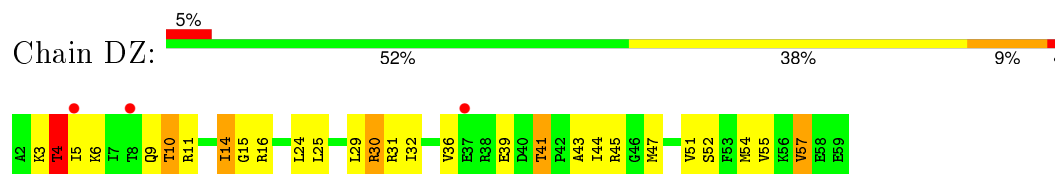
- Molecule 46: 50S ribosomal protein L29



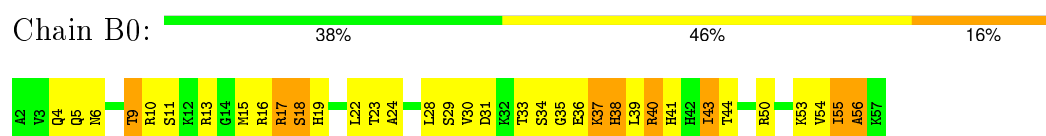
- Molecule 47: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L30



- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32

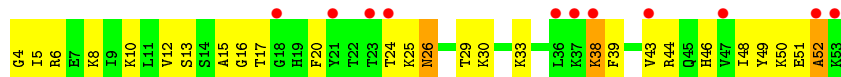




- Molecule 49: 50S ribosomal protein L33



- Molecule 49: 50S ribosomal protein L33



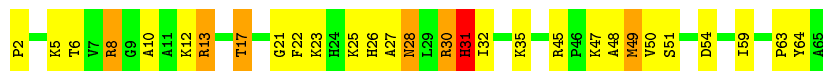
- Molecule 50: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L35

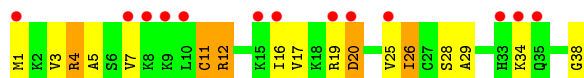


- Molecule 52: 50S ribosomal protein L36

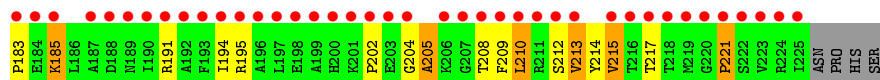
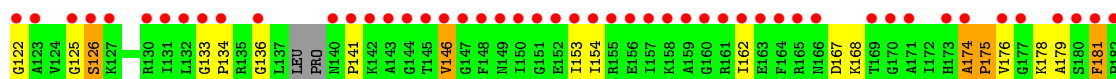
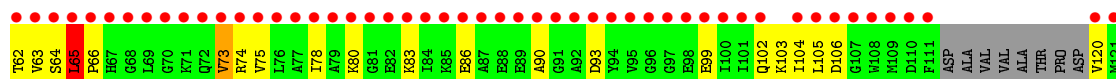
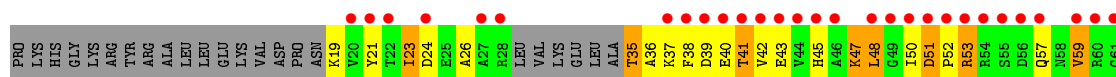
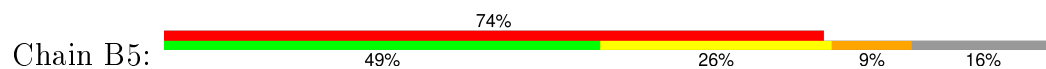




- Molecule 52: 50S ribosomal protein L36



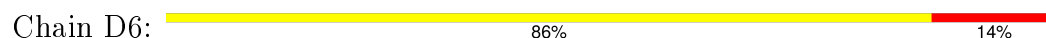
- Molecule 53: 50S ribosomal protein L1



- Molecule 54: Linopristin



- Molecule 54: Linopristin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.49Å 433.90Å 621.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.15 – 3.00 69.15 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (69.15-3.00) 90.2 (69.15-3.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.225 , 0.274 0.235 , 0.284	Depositor DCC
$R_{free}$ test set	4092 reflections (0.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.2	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1017015 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	288320	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DBB, MG, 04X, 004, MHW, MHU

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	0.52	0/36944	1.02	48/57632 (0.1%)
1	CA	0.45	0/36966	0.96	27/57666 (0.0%)
2	AB	0.44	0/1736	0.65	0/2338
2	CB	0.38	0/1736	0.59	0/2338
3	AC	0.39	0/1652	0.61	0/2225
3	CC	0.37	0/1652	0.58	1/2225 (0.0%)
4	AD	0.39	0/1665	0.64	0/2227
4	CD	0.43	0/1665	0.65	0/2227
5	AE	0.41	0/1119	0.75	0/1504
5	CE	0.41	0/1119	0.73	0/1504
6	AF	0.41	0/836	0.77	2/1128 (0.2%)
6	CF	0.35	0/836	0.64	1/1128 (0.1%)
7	AG	0.37	0/1196	0.60	0/1602
7	CG	0.38	0/1196	0.54	0/1602
8	AH	0.40	0/989	0.63	0/1326
8	CH	0.34	0/989	0.57	0/1326
9	AI	0.39	0/1034	0.65	0/1375
9	CI	0.36	0/1034	0.59	0/1375
10	AJ	0.37	0/797	0.62	0/1077
10	CJ	0.36	0/797	0.61	0/1077
11	AK	0.38	0/893	0.63	0/1205
11	CK	0.37	0/893	0.61	0/1205
12	AL	0.41	0/969	0.71	0/1300
12	CL	0.41	0/969	0.73	0/1300
13	AM	0.38	0/893	0.70	1/1193 (0.1%)
13	CM	0.39	0/893	0.62	0/1193
14	AN	0.38	0/785	0.61	0/1043
14	CN	0.34	0/785	0.52	0/1043
15	AO	0.34	0/718	0.59	0/959
15	CO	0.32	0/718	0.57	0/959
16	AP	0.40	0/659	0.70	1/884 (0.1%)
16	CP	0.36	0/659	0.60	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.37	0/658	0.66	0/881
17	CQ	0.39	0/658	0.61	0/881
18	AR	0.37	0/463	0.61	0/621
18	CR	0.37	0/463	0.58	0/621
19	AS	0.43	0/653	0.66	0/877
19	CS	0.38	0/653	0.58	0/877
20	AT	0.43	0/671	0.63	0/888
20	CT	0.35	0/671	0.56	0/888
21	AU	0.50	0/431	0.71	0/570
21	CU	0.44	0/431	0.66	0/570
22	BA	0.90	44/69659 (0.1%)	1.39	725/108672 (0.7%)
22	DA	0.45	0/69659	0.95	28/108672 (0.0%)
23	BB	0.78	2/2850 (0.1%)	1.29	20/4444 (0.5%)
23	DB	0.39	0/2828	0.89	0/4410
24	BC	0.56	1/2122 (0.0%)	0.75	1/2852 (0.0%)
24	DC	0.37	0/2122	0.61	0/2852
25	BD	0.62	0/1586	0.80	1/2134 (0.0%)
25	DD	0.34	0/1586	0.55	0/2134
26	BE	0.54	0/1571	0.70	0/2113
26	DE	0.38	0/1571	0.60	0/2113
27	BF	0.41	0/1435	0.62	0/1926
27	DF	0.37	0/1435	0.53	0/1926
28	BG	0.45	0/1343	0.67	0/1816
28	DG	0.34	0/1343	0.52	0/1816
29	BH	0.36	0/1121	0.66	1/1515 (0.1%)
29	DH	0.35	0/1121	0.56	0/1515
30	BI	0.44	0/1046	0.62	0/1410
30	DI	0.43	0/1046	0.59	0/1410
31	BJ	0.61	0/1152	0.75	1/1551 (0.1%)
31	DJ	0.35	0/1152	0.57	0/1551
32	BK	0.64	0/948	0.81	0/1268
32	DK	0.37	0/948	0.57	0/1268
33	BL	0.52	0/1054	0.75	0/1403
33	DL	0.38	0/1054	0.62	0/1403
34	BM	0.62	0/1093	0.80	1/1460 (0.1%)
34	DM	0.33	0/1093	0.56	0/1460
35	BN	0.61	0/974	0.88	3/1301 (0.2%)
35	DN	0.36	0/974	0.56	0/1301
36	BO	0.48	0/902	0.71	0/1209
36	DO	0.34	0/902	0.53	0/1209
37	BP	0.54	0/929	0.75	1/1242 (0.1%)
37	DP	0.37	0/929	0.58	0/1242
38	BQ	0.73	0/960	0.82	1/1278 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DQ	0.36	0/960	0.54	0/1278
39	BR	0.66	0/829	0.91	2/1107 (0.2%)
39	DR	0.36	0/829	0.59	0/1107
40	BS	0.72	0/864	0.81	0/1156
40	DS	0.36	0/864	0.63	0/1156
41	BT	0.49	0/745	0.68	0/994
41	DT	0.38	0/745	0.60	0/994
42	BU	0.48	0/788	0.72	0/1051
42	DU	0.43	0/788	0.61	0/1051
43	BV	0.52	0/766	0.70	0/1025
43	DV	0.32	0/766	0.48	0/1025
44	BW	0.64	0/587	0.79	0/776
44	DW	0.33	0/576	0.54	0/762
45	BX	0.45	0/635	0.73	0/848
45	DX	0.36	0/635	0.60	0/848
46	BY	0.46	0/510	0.71	0/677
46	DY	0.39	0/510	0.61	0/677
47	BZ	0.61	0/453	0.82	1/605 (0.2%)
47	DZ	0.32	0/453	0.58	0/605
48	B0	0.64	0/450	0.91	2/599 (0.3%)
48	D0	0.35	0/450	0.58	0/599
49	B1	0.46	0/417	0.67	0/554
49	D1	0.35	0/417	0.51	0/554
50	B2	0.55	0/380	0.83	0/498
50	D2	0.38	0/380	0.61	0/498
51	B3	0.58	0/513	0.75	0/676
51	D3	0.33	0/513	0.57	0/676
52	B4	0.60	0/303	0.71	0/397
52	D4	0.32	0/303	0.54	0/397
53	B5	0.39	0/1145	0.56	0/1556
54	B6	3.67	4/13 (30.8%)	4.12	3/15 (20.0%)
54	D6	3.86	3/13 (23.1%)	3.82	4/15 (26.7%)
All	All	0.59	54/310652 (0.0%)	1.02	876/464396 (0.2%)

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
5	CE	0	1
6	CF	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	AK	0	1
12	CL	0	2
21	AU	0	1
25	BD	0	1
25	DD	0	1
33	BL	0	1
48	B0	0	1
All	All	0	10

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	N9-C4	-12.83	1.30	1.37
22	BA	528	A	N9-C4	-10.27	1.31	1.37
22	BA	528	A	N3-C4	-8.70	1.29	1.34
22	BA	974	G	N9-C4	-8.12	1.31	1.38
22	BA	979	A	N9-C4	-7.80	1.33	1.37

The worst 5 of 876 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	974	G	C4-C5-N7	15.39	116.95	110.80
22	BA	974	G	C5-N7-C8	-15.02	96.79	104.30
22	BA	752	A	N1-C6-N6	14.90	127.54	118.60
22	BA	974	G	N1-C6-O6	14.51	128.61	119.90
22	BA	1779	U	N3-C4-O4	-13.09	110.24	119.40

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
21	AU	39	GLU	Peptide
48	B0	24	ALA	Peptide
25	BD	151	THR	Peptide
33	BL	28	GLY	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	1338	4
1	CA	33015	0	16617	1198	0
2	AB	1705	0	1732	164	0
2	CB	1705	0	1732	121	0
3	AC	1625	0	1696	89	0
3	CC	1625	0	1696	80	0
4	AD	1643	0	1707	133	0
4	CD	1643	0	1707	144	0
5	AE	1106	0	1148	83	0
5	CE	1106	0	1148	104	0
6	AF	818	0	808	62	0
6	CF	818	0	808	56	0
7	AG	1182	0	1238	65	0
7	CG	1182	0	1238	59	0
8	AH	979	0	1031	67	0
8	CH	979	0	1031	47	0
9	AI	1022	0	1070	77	0
9	CI	1022	0	1070	69	0
10	AJ	787	0	828	87	0
10	CJ	787	0	828	48	0
11	AK	877	0	887	79	0
11	CK	877	0	887	72	0
12	AL	955	0	1016	65	0
12	CL	955	0	1016	61	0
13	AM	884	0	941	80	0
13	CM	884	0	941	46	0
14	AN	774	0	824	66	0
14	CN	774	0	824	44	0
15	AO	710	0	728	35	0
15	CO	710	0	728	42	0
16	AP	649	0	666	53	0
16	CP	649	0	666	30	0
17	AQ	649	0	691	69	0
17	CQ	649	0	691	50	0
18	AR	456	0	478	22	0
18	CR	456	0	478	23	0
19	AS	638	0	665	48	0
19	CS	638	0	665	38	0
20	AT	665	0	714	54	0
20	CT	665	0	714	38	0
21	AU	426	0	449	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CU	426	0	449	37	0
22	BA	62195	0	31280	2134	0
22	DA	62195	0	31280	2174	0
23	BB	2549	0	1291	56	0
23	DB	2529	0	1281	72	0
24	BC	2083	0	2154	157	0
24	DC	2083	0	2154	123	0
25	BD	1565	0	1616	92	0
25	DD	1565	0	1616	81	0
26	BE	1552	0	1619	75	0
26	DE	1552	0	1619	103	0
27	BF	1411	0	1444	105	0
27	DF	1411	0	1444	63	0
28	BG	1323	0	1371	61	0
28	DG	1323	0	1371	56	0
29	BH	1110	0	1147	154	0
29	DH	1110	0	1148	90	4
30	BI	1032	0	1085	82	0
30	DI	1032	0	1085	72	0
31	BJ	1129	0	1162	64	0
31	DJ	1129	0	1162	55	0
32	BK	939	0	1012	75	0
32	DK	939	0	1012	38	0
33	BL	1045	0	1117	51	0
33	DL	1045	0	1117	81	0
34	BM	1074	0	1157	47	0
34	DM	1074	0	1157	43	0
35	BN	961	0	1000	51	0
35	DN	961	0	1000	55	0
36	BO	892	0	923	57	0
36	DO	892	0	923	50	0
37	BP	917	0	962	48	0
37	DP	917	0	962	47	0
38	BQ	947	0	1019	61	0
38	DQ	947	0	1019	55	0
39	BR	816	0	839	84	0
39	DR	816	0	839	47	0
40	BS	857	0	922	64	0
40	DS	857	0	922	39	0
41	BT	739	0	807	46	0
41	DT	739	0	807	44	0
42	BU	780	0	831	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DU	780	0	831	65	0
43	BV	753	0	780	31	0
43	DV	753	0	780	25	0
44	BW	580	0	594	23	0
44	DW	569	0	581	26	0
45	BX	625	0	652	35	0
45	DX	625	0	652	55	0
46	BY	509	0	543	29	0
46	DY	509	0	543	38	0
47	BZ	449	0	488	19	0
47	DZ	449	0	488	14	0
48	B0	444	0	458	33	0
48	D0	444	0	458	18	0
49	B1	410	0	440	32	0
49	D1	410	0	440	19	0
50	B2	377	0	418	19	0
50	D2	377	0	418	34	0
51	B3	504	0	572	22	0
51	D3	504	0	572	29	0
52	B4	302	0	340	12	0
52	D4	302	0	342	17	0
53	B5	1142	0	865	49	0
54	B6	69	0	60	5	0
54	D6	69	0	60	14	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	23	0
57	AL	1	0	0	0	0
57	AN	5	0	0	1	0
57	AT	2	0	0	1	0
57	AU	1	0	0	1	0
57	B2	1	0	0	0	0
57	B3	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B4	2	0	0	0	0
57	BA	615	0	0	101	0
57	BB	14	0	0	0	0
57	BC	10	0	0	0	0
57	BD	4	0	0	2	0
57	BE	4	0	0	0	0
57	BF	1	0	0	1	0
57	BG	1	0	0	0	0
57	BJ	1	0	0	0	0
57	BL	6	0	0	0	0
57	BN	2	0	0	0	0
57	BS	1	0	0	0	0
57	BU	1	0	0	0	0
57	CA	189	0	0	20	0
57	CL	1	0	0	0	0
57	CN	3	0	0	2	0
57	CT	3	0	0	0	0
57	CU	2	0	0	0	0
57	D0	1	0	0	0	0
57	D2	2	0	0	0	0
57	D3	2	0	0	0	0
57	D4	1	0	0	0	0
57	DA	607	0	0	82	0
57	DB	13	0	0	3	0
57	DC	9	0	0	1	0
57	DD	4	0	0	2	0
57	DE	6	0	0	1	0
57	DL	5	0	0	1	0
57	DN	2	0	0	0	0
57	DT	2	0	0	0	0
57	DU	1	0	0	1	0
57	DV	1	0	0	0	0
All	All	288320	0	192909	11780	4

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 25.

The worst 5 of 11780 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)
22:BA:1006:C:OP2	57:BA:3781:HOH:O	1.56	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
22:BA:2714:G:OP2	57:BA:3548:HOH:O	1.61	1.18
22:BA:1603:A:OP1	57:BA:3411:HOH:O	1.61	1.15
54:D6:4:PRO:HB2	54:D6:5:MHU:HM1	1.15	1.14

All (4) 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]	1.78	0.42
1:AA:368:U:OP1	29:DH:93:SER:OG[4_455]	1.93	0.27
1:AA:368:U:OP2	29:DH:123:ARG:NH2[4_455]	2.03	0.17
1:AA:368:U:OP2	29:DH:123:ARG:CZ[4_455]	2.07	0.13

## 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%)	135 (62%)	36 (17%)	45 (21%)	0	0
2	CB	216/218 (99%)	143 (66%)	36 (17%)	37 (17%)	0	1
3	AC	204/206 (99%)	142 (70%)	42 (21%)	20 (10%)	1	3
3	CC	204/206 (99%)	145 (71%)	41 (20%)	18 (9%)	1	4
4	AD	203/205 (99%)	133 (66%)	36 (18%)	34 (17%)	0	1
4	CD	203/205 (99%)	129 (64%)	48 (24%)	26 (13%)	0	1
5	AE	148/150 (99%)	98 (66%)	33 (22%)	17 (12%)	0	2
5	CE	148/150 (99%)	96 (65%)	29 (20%)	23 (16%)	0	1
6	AF	98/100 (98%)	61 (62%)	19 (19%)	18 (18%)	0	0
6	CF	98/100 (98%)	64 (65%)	18 (18%)	16 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	110 (74%)	27 (18%)	12 (8%)	1	5
7	CG	149/151 (99%)	120 (80%)	21 (14%)	8 (5%)	2	14
8	AH	127/129 (98%)	80 (63%)	29 (23%)	18 (14%)	0	1
8	CH	127/129 (98%)	100 (79%)	19 (15%)	8 (6%)	2	9
9	AI	125/127 (98%)	90 (72%)	24 (19%)	11 (9%)	1	4
9	CI	125/127 (98%)	89 (71%)	27 (22%)	9 (7%)	1	7
10	AJ	96/98 (98%)	68 (71%)	7 (7%)	21 (22%)	0	0
10	CJ	96/98 (98%)	69 (72%)	18 (19%)	9 (9%)	1	4
11	AK	115/117 (98%)	83 (72%)	17 (15%)	15 (13%)	0	1
11	CK	115/117 (98%)	77 (67%)	28 (24%)	10 (9%)	1	4
12	AL	121/123 (98%)	92 (76%)	19 (16%)	10 (8%)	1	5
12	CL	121/123 (98%)	89 (74%)	17 (14%)	15 (12%)	0	2
13	AM	112/114 (98%)	79 (70%)	22 (20%)	11 (10%)	1	3
13	CM	112/114 (98%)	86 (77%)	15 (13%)	11 (10%)	1	3
14	AN	92/100 (92%)	57 (62%)	20 (22%)	15 (16%)	0	1
14	CN	92/100 (92%)	59 (64%)	20 (22%)	13 (14%)	0	1
15	AO	86/88 (98%)	60 (70%)	21 (24%)	5 (6%)	2	12
15	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	4	24
16	AP	80/82 (98%)	52 (65%)	16 (20%)	12 (15%)	0	1
16	CP	80/82 (98%)	54 (68%)	20 (25%)	6 (8%)	1	6
17	AQ	78/80 (98%)	52 (67%)	16 (20%)	10 (13%)	0	1
17	CQ	78/80 (98%)	55 (70%)	13 (17%)	10 (13%)	0	1
18	AR	53/55 (96%)	40 (76%)	12 (23%)	1 (2%)	10	43
18	CR	53/55 (96%)	45 (85%)	4 (8%)	4 (8%)	1	6
19	AS	77/79 (98%)	52 (68%)	19 (25%)	6 (8%)	1	6
19	CS	77/79 (98%)	59 (77%)	14 (18%)	4 (5%)	2	15
20	AT	83/85 (98%)	51 (61%)	23 (28%)	9 (11%)	0	2
20	CT	83/85 (98%)	66 (80%)	11 (13%)	6 (7%)	1	7
21	AU	49/51 (96%)	23 (47%)	18 (37%)	8 (16%)	0	1
21	CU	49/51 (96%)	25 (51%)	10 (20%)	14 (29%)	0	0
24	BC	269/271 (99%)	208 (77%)	49 (18%)	12 (4%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	DC	269/271 (99%)	206 (77%)	42 (16%)	21 (8%)	1	6
25	BD	207/209 (99%)	176 (85%)	22 (11%)	9 (4%)	3	19
25	DD	207/209 (99%)	175 (84%)	24 (12%)	8 (4%)	4	21
26	BE	199/201 (99%)	164 (82%)	26 (13%)	9 (4%)	3	18
26	DE	199/201 (99%)	160 (80%)	27 (14%)	12 (6%)	2	11
27	BF	175/177 (99%)	136 (78%)	24 (14%)	15 (9%)	1	4
27	DF	175/177 (99%)	141 (81%)	23 (13%)	11 (6%)	2	9
28	BG	174/176 (99%)	146 (84%)	20 (12%)	8 (5%)	3	18
28	DG	174/176 (99%)	132 (76%)	33 (19%)	9 (5%)	2	15
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	1
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	1	3
30	BI	139/141 (99%)	79 (57%)	34 (24%)	26 (19%)	0	0
30	DI	139/141 (99%)	79 (57%)	42 (30%)	18 (13%)	0	1
31	BJ	140/142 (99%)	120 (86%)	17 (12%)	3 (2%)	9	40
31	DJ	140/142 (99%)	116 (83%)	18 (13%)	6 (4%)	3	19
32	BK	120/122 (98%)	94 (78%)	15 (12%)	11 (9%)	1	4
32	DK	120/122 (98%)	96 (80%)	14 (12%)	10 (8%)	1	5
33	BL	141/143 (99%)	108 (77%)	23 (16%)	10 (7%)	1	7
33	DL	141/143 (99%)	104 (74%)	28 (20%)	9 (6%)	2	9
34	BM	134/136 (98%)	114 (85%)	16 (12%)	4 (3%)	5	29
34	DM	134/136 (98%)	115 (86%)	13 (10%)	6 (4%)	3	18
35	BN	118/120 (98%)	97 (82%)	18 (15%)	3 (2%)	7	34
35	DN	118/120 (98%)	94 (80%)	16 (14%)	8 (7%)	1	7
36	BO	114/116 (98%)	87 (76%)	22 (19%)	5 (4%)	3	18
36	DO	114/116 (98%)	97 (85%)	15 (13%)	2 (2%)	11	45
37	BP	112/114 (98%)	97 (87%)	10 (9%)	5 (4%)	3	18
37	DP	112/114 (98%)	86 (77%)	19 (17%)	7 (6%)	2	9
38	BQ	115/117 (98%)	96 (84%)	15 (13%)	4 (4%)	4	24
38	DQ	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	21	64
39	BR	101/103 (98%)	89 (88%)	5 (5%)	7 (7%)	1	7
39	DR	101/103 (98%)	77 (76%)	17 (17%)	7 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BS	108/110 (98%)	91 (84%)	11 (10%)	6 (6%)	2	13
40	DS	108/110 (98%)	87 (81%)	14 (13%)	7 (6%)	1	8
41	BT	91/93 (98%)	69 (76%)	13 (14%)	9 (10%)	1	3
41	DT	91/93 (98%)	62 (68%)	19 (21%)	10 (11%)	0	2
42	BU	100/102 (98%)	75 (75%)	17 (17%)	8 (8%)	1	5
42	DU	100/102 (98%)	72 (72%)	15 (15%)	13 (13%)	0	1
43	BV	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
43	DV	92/94 (98%)	76 (83%)	12 (13%)	4 (4%)	3	19
44	BW	74/76 (97%)	65 (88%)	9 (12%)	0	100	100
44	DW	73/76 (96%)	58 (80%)	10 (14%)	5 (7%)	1	7
45	BX	75/77 (97%)	64 (85%)	7 (9%)	4 (5%)	2	14
45	DX	75/77 (97%)	56 (75%)	15 (20%)	4 (5%)	2	14
46	BY	61/63 (97%)	38 (62%)	13 (21%)	10 (16%)	0	1
46	DY	61/63 (97%)	44 (72%)	11 (18%)	6 (10%)	1	3
47	BZ	56/58 (97%)	49 (88%)	4 (7%)	3 (5%)	2	14
47	DZ	56/58 (97%)	48 (86%)	5 (9%)	3 (5%)	2	14
48	B0	54/56 (96%)	42 (78%)	7 (13%)	5 (9%)	1	4
48	D0	54/56 (96%)	42 (78%)	8 (15%)	4 (7%)	1	6
49	B1	48/50 (96%)	39 (81%)	4 (8%)	5 (10%)	1	3
49	D1	48/50 (96%)	39 (81%)	6 (12%)	3 (6%)	2	9
50	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	3	18
50	D2	44/46 (96%)	37 (84%)	4 (9%)	3 (7%)	1	7
51	B3	62/64 (97%)	51 (82%)	9 (14%)	2 (3%)	5	27
51	D3	62/64 (97%)	50 (81%)	9 (14%)	3 (5%)	3	17
52	B4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
52	D4	36/38 (95%)	29 (81%)	6 (17%)	1 (3%)	6	30
53	B5	183/228 (80%)	100 (55%)	53 (29%)	30 (16%)	0	1
54	B6	2/7 (29%)	2 (100%)	0	0	100	100
54	D6	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
All	All	11422/11686 (98%)	8514 (74%)	1907 (17%)	1001 (9%)	1	4

5 of 1001 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	22	TYR
2	AB	64	LYS
2	AB	68	LEU
2	AB	73	LYS
2	AB	75	ALA

### 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%)	125 (69%)	55 (31%)	0	2
2	CB	180/180 (100%)	126 (70%)	54 (30%)	0	2
3	AC	170/170 (100%)	137 (81%)	33 (19%)	2	9
3	CC	170/170 (100%)	130 (76%)	40 (24%)	1	4
4	AD	172/172 (100%)	128 (74%)	44 (26%)	0	3
4	CD	172/172 (100%)	140 (81%)	32 (19%)	2	10
5	AE	113/113 (100%)	85 (75%)	28 (25%)	1	3
5	CE	113/113 (100%)	83 (74%)	30 (26%)	0	3
6	AF	87/87 (100%)	63 (72%)	24 (28%)	0	2
6	CF	87/87 (100%)	58 (67%)	29 (33%)	0	1
7	AG	124/124 (100%)	88 (71%)	36 (29%)	0	2
7	CG	124/124 (100%)	92 (74%)	32 (26%)	0	3
8	AH	104/104 (100%)	80 (77%)	24 (23%)	1	5
8	CH	104/104 (100%)	79 (76%)	25 (24%)	1	4
9	AI	105/105 (100%)	73 (70%)	32 (30%)	0	2
9	CI	105/105 (100%)	73 (70%)	32 (30%)	0	2
10	AJ	86/86 (100%)	61 (71%)	25 (29%)	0	2
10	CJ	86/86 (100%)	70 (81%)	16 (19%)	2	10
11	AK	90/90 (100%)	70 (78%)	20 (22%)	1	5
11	CK	90/90 (100%)	67 (74%)	23 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	103/103 (100%)	78 (76%)	25 (24%)	1	4
12	CL	103/103 (100%)	78 (76%)	25 (24%)	1	4
13	AM	92/92 (100%)	65 (71%)	27 (29%)	0	2
13	CM	92/92 (100%)	69 (75%)	23 (25%)	1	3
14	AN	79/83 (95%)	63 (80%)	16 (20%)	1	7
14	CN	79/83 (95%)	69 (87%)	10 (13%)	5	23
15	AO	75/76 (99%)	61 (81%)	14 (19%)	2	10
15	CO	75/76 (99%)	64 (85%)	11 (15%)	4	18
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	5
16	CP	65/65 (100%)	52 (80%)	13 (20%)	1	8
17	AQ	74/74 (100%)	50 (68%)	24 (32%)	0	1
17	CQ	74/74 (100%)	54 (73%)	20 (27%)	0	3
18	AR	48/48 (100%)	40 (83%)	8 (17%)	3	13
18	CR	48/48 (100%)	43 (90%)	5 (10%)	9	32
19	AS	70/70 (100%)	59 (84%)	11 (16%)	3	15
19	CS	70/70 (100%)	53 (76%)	17 (24%)	1	4
20	AT	65/65 (100%)	49 (75%)	16 (25%)	1	4
20	CT	65/65 (100%)	49 (75%)	16 (25%)	1	4
21	AU	44/44 (100%)	29 (66%)	15 (34%)	0	1
21	CU	44/44 (100%)	29 (66%)	15 (34%)	0	1
24	BC	216/216 (100%)	182 (84%)	34 (16%)	3	15
24	DC	216/216 (100%)	189 (88%)	27 (12%)	6	24
25	BD	164/164 (100%)	145 (88%)	19 (12%)	7	27
25	DD	164/164 (100%)	145 (88%)	19 (12%)	7	27
26	BE	165/165 (100%)	137 (83%)	28 (17%)	2	13
26	DE	165/165 (100%)	131 (79%)	34 (21%)	1	7
27	BF	148/148 (100%)	121 (82%)	27 (18%)	2	11
27	DF	148/148 (100%)	116 (78%)	32 (22%)	1	6
28	BG	137/137 (100%)	118 (86%)	19 (14%)	4	19
28	DG	137/137 (100%)	119 (87%)	18 (13%)	5	22
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	5
30	BI	109/109 (100%)	80 (73%)	29 (27%)	0	3
30	DI	109/109 (100%)	85 (78%)	24 (22%)	1	6
31	BJ	116/116 (100%)	106 (91%)	10 (9%)	13	44
31	DJ	116/116 (100%)	103 (89%)	13 (11%)	7	29
32	BK	103/103 (100%)	90 (87%)	13 (13%)	5	24
32	DK	103/103 (100%)	93 (90%)	10 (10%)	10	37
33	BL	102/102 (100%)	86 (84%)	16 (16%)	3	15
33	DL	102/102 (100%)	80 (78%)	22 (22%)	1	6
34	BM	109/109 (100%)	92 (84%)	17 (16%)	3	16
34	DM	109/109 (100%)	93 (85%)	16 (15%)	4	18
35	BN	100/100 (100%)	83 (83%)	17 (17%)	2	13
35	DN	100/100 (100%)	77 (77%)	23 (23%)	1	5
36	BO	86/86 (100%)	63 (73%)	23 (27%)	0	3
36	DO	86/86 (100%)	71 (83%)	15 (17%)	2	12
37	BP	99/99 (100%)	84 (85%)	15 (15%)	3	16
37	DP	99/99 (100%)	83 (84%)	16 (16%)	3	14
38	BQ	89/89 (100%)	75 (84%)	14 (16%)	3	15
38	DQ	89/89 (100%)	76 (85%)	13 (15%)	4	18
39	BR	84/84 (100%)	69 (82%)	15 (18%)	2	11
39	DR	84/84 (100%)	73 (87%)	11 (13%)	5	22
40	BS	93/93 (100%)	75 (81%)	18 (19%)	2	9
40	DS	93/93 (100%)	80 (86%)	13 (14%)	4	19
41	BT	80/80 (100%)	68 (85%)	12 (15%)	3	17
41	DT	80/80 (100%)	64 (80%)	16 (20%)	1	8
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	7
42	DU	83/83 (100%)	60 (72%)	23 (28%)	0	2
43	BV	78/78 (100%)	62 (80%)	16 (20%)	1	7
43	DV	78/78 (100%)	67 (86%)	11 (14%)	4	19
44	BW	57/58 (98%)	50 (88%)	7 (12%)	6	25
44	DW	56/58 (97%)	51 (91%)	5 (9%)	12	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BX	67/67 (100%)	56 (84%)	11 (16%)	3	14
45	DX	67/67 (100%)	57 (85%)	10 (15%)	4	17
46	BY	55/55 (100%)	47 (86%)	8 (14%)	4	18
46	DY	55/55 (100%)	45 (82%)	10 (18%)	2	11
47	BZ	48/48 (100%)	42 (88%)	6 (12%)	6	24
47	DZ	48/48 (100%)	35 (73%)	13 (27%)	0	2
48	B0	47/47 (100%)	40 (85%)	7 (15%)	4	17
48	D0	47/47 (100%)	43 (92%)	4 (8%)	13	45
49	B1	45/45 (100%)	37 (82%)	8 (18%)	2	11
49	D1	45/45 (100%)	39 (87%)	6 (13%)	5	21
50	B2	38/38 (100%)	33 (87%)	5 (13%)	5	22
50	D2	38/38 (100%)	32 (84%)	6 (16%)	3	15
51	B3	51/51 (100%)	40 (78%)	11 (22%)	1	6
51	D3	51/51 (100%)	47 (92%)	4 (8%)	16	49
52	B4	34/34 (100%)	29 (85%)	5 (15%)	4	18
52	D4	34/34 (100%)	29 (85%)	5 (15%)	4	18
53	B5	61/180 (34%)	47 (77%)	14 (23%)	1	5
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%)	7518 (80%)	1872 (20%)	1	8

5 of 1872 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BU	15	THR
3	CC	185	ASN
38	DQ	51	ARG
43	BV	65	VAL
53	B5	39	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
37	BP	56	HIS

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Mol	Chain	Res	Type
51	B3	31	HIS
37	DP	41	GLN
48	B0	42	HIS
51	B3	43	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	361 (23%)	17 (1%)
1	CA	1538/1539 (99%)	335 (21%)	16 (1%)
22	BA	2895/2903 (99%)	672 (23%)	36 (1%)
22	DA	2895/2903 (99%)	609 (21%)	33 (1%)
23	BB	118/119 (99%)	27 (22%)	1 (0%)
23	DB	117/119 (98%)	25 (21%)	0
All	All	9100/9122 (99%)	2029 (22%)	103 (1%)

5 of 2029 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	13	U
1	AA	32	A

5 of 103 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2428	G
1	CA	209	U
22	DA	2286	G
22	BA	2430	A
22	BA	2873	A

## 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	MHW	B6	1	54	9,9,10	2.81	3 (33%)	8,11,13	2.60	6 (75%)
54	DBB	B6	3	54	4,5,6	0.84	0	3,5,7	4.30	1 (33%)
54	MHU	B6	5	54	13,15,16	2.96	7 (53%)	15,19,21	2.12	3 (20%)
54	04X	B6	6	54	12,16,17	1.48	2 (16%)	11,20,22	4.81	6 (54%)
54	004	B6	7	54	9,10,11	3.44	6 (66%)	10,12,14	1.88	2 (20%)
54	MHW	D6	1	54	9,9,10	3.01	4 (44%)	8,11,13	2.04	5 (62%)
54	DBB	D6	3	54	4,5,6	0.75	0	3,5,7	5.52	2 (66%)
54	MHU	D6	5	54	13,15,16	2.90	6 (46%)	15,19,21	2.11	3 (20%)
54	04X	D6	6	54	12,16,17	1.25	2 (16%)	11,20,22	5.59	6 (54%)
54	004	D6	7	54	9,10,11	3.34	6 (66%)	10,12,14	2.23	2 (20%)

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	MHW	B6	1	54	-	0/2/2/4	0/1/1/1
54	DBB	B6	3	54	-	0/2/4/6	0/0/0/0
54	MHU	B6	5	54	-	0/8/12/14	0/1/1/1
54	04X	B6	6	54	-	0/4/24/26	0/2/2/2
54	004	B6	7	54	-	0/4/6/8	0/1/1/1
54	MHW	D6	1	54	-	0/2/2/4	0/1/1/1
54	DBB	D6	3	54	-	0/2/4/6	0/0/0/0
54	MHU	D6	5	54	-	0/8/12/14	0/1/1/1
54	04X	D6	6	54	-	0/4/24/26	0/2/2/2
54	004	D6	7	54	-	0/4/6/8	0/1/1/1

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	7	004	CB-CA	-6.77	1.45	1.52
54	D6	7	004	CB-CA	-6.33	1.46	1.52
54	D6	1	MHW	CG2-CB	-5.43	1.29	1.39
54	B6	1	MHW	CG2-CB	-5.37	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D6	1	MHW	CA-N	-5.22	1.28	1.35

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	3	DBB	O-C-CA	-9.05	101.93	125.49
54	B6	3	DBB	O-C-CA	-7.15	106.86	125.49
54	D6	5	MHU	O-C-CA	-6.80	107.48	125.44
54	B6	5	MHU	O-C-CA	-6.35	108.66	125.44
54	D6	6	04X	C2-C1-N1	-4.83	102.81	110.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	B6	3	DBB	1	0
54	B6	5	MHU	2	0
54	B6	7	004	1	0
54	D6	1	MHW	4	0
54	D6	3	DBB	2	0
54	D6	5	MHU	5	0
54	D6	6	04X	1	0
54	D6	7	004	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
54	B6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B6	2:THR	C	3:DBB	N	1.61

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1538/1539 (99%)	-0.38	22 (1%) 78 51	14, 54, 137, 179	0
1	CA	1539/1539 (100%)	-0.18	38 (2%) 61 30	27, 72, 145, 177	0
2	AB	218/218 (100%)	1.21	55 (25%) 1 1	43, 76, 100, 125	0
2	CB	218/218 (100%)	1.60	73 (33%) 0 0	63, 86, 106, 126	0
3	AC	206/206 (100%)	0.12	5 (2%) 62 32	39, 61, 83, 96	0
3	CC	206/206 (100%)	1.28	46 (22%) 1 1	57, 79, 97, 109	0
4	AD	205/205 (100%)	0.06	4 (1%) 68 39	35, 58, 79, 106	0
4	CD	205/205 (100%)	-0.18	3 (1%) 76 49	21, 40, 71, 90	0
5	AE	150/150 (100%)	0.04	3 (2%) 68 39	27, 51, 82, 106	0
5	CE	150/150 (100%)	0.05	1 (0%) 89 70	34, 59, 87, 104	0
6	AF	100/100 (100%)	-0.29	0 100 100	38, 59, 76, 84	0
6	CF	100/100 (100%)	-0.12	1 (1%) 84 60	46, 74, 96, 104	0
7	AG	151/151 (100%)	0.86	25 (16%) 2 1	54, 78, 98, 108	0
7	CG	151/151 (100%)	1.84	65 (43%) 0 0	77, 97, 107, 113	0
8	AH	129/129 (100%)	-0.05	1 (0%) 87 67	30, 50, 73, 81	0
8	CH	129/129 (100%)	0.10	4 (3%) 52 24	45, 65, 81, 90	0
9	AI	127/127 (100%)	1.06	24 (18%) 2 1	51, 73, 97, 113	0
9	CI	127/127 (100%)	1.48	37 (29%) 1 0	71, 91, 109, 126	0
10	AJ	98/98 (100%)	0.47	7 (7%) 19 7	46, 68, 92, 122	0
10	CJ	98/98 (100%)	1.94	45 (45%) 0 0	71, 93, 110, 124	0
11	AK	117/117 (100%)	0.61	15 (12%) 5 2	32, 64, 91, 110	0
11	CK	117/117 (100%)	0.14	3 (2%) 59 29	44, 68, 82, 91	0
12	AL	123/123 (100%)	0.13	4 (3%) 50 22	23, 39, 68, 94	0
12	CL	123/123 (100%)	0.09	4 (3%) 50 22	39, 52, 79, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/114 (100%)	0.46	8 (7%) 19 7	49, 71, 92, 105	0
13	CM	114/114 (100%)	2.04	56 (49%) 0 0	90, 103, 116, 120	0
14	AN	96/100 (96%)	0.86	17 (17%) 2 1	43, 63, 94, 106	0
14	CN	96/100 (96%)	1.95	37 (38%) 0 0	69, 91, 110, 118	0
15	AO	88/88 (100%)	0.02	2 (2%) 64 33	31, 51, 68, 98	0
15	CO	88/88 (100%)	0.00	2 (2%) 64 33	43, 63, 81, 105	0
16	AP	82/82 (100%)	0.51	4 (4%) 33 13	35, 49, 84, 100	0
16	CP	82/82 (100%)	0.70	13 (15%) 3 1	45, 62, 88, 106	0
17	AQ	80/80 (100%)	-0.00	3 (3%) 44 18	27, 54, 81, 124	0
17	CQ	80/80 (100%)	0.53	5 (6%) 23 9	44, 72, 96, 105	0
18	AR	55/55 (100%)	-0.12	3 (5%) 29 11	39, 53, 81, 112	0
18	CR	55/55 (100%)	0.03	3 (5%) 29 11	46, 56, 82, 111	0
19	AS	79/79 (100%)	1.06	14 (17%) 2 1	55, 72, 92, 101	0
19	CS	79/79 (100%)	3.17	57 (72%) 0 0	87, 103, 114, 123	0
20	AT	85/85 (100%)	0.12	4 (4%) 35 14	35, 51, 74, 111	0
20	CT	85/85 (100%)	1.29	23 (27%) 1 0	53, 72, 93, 96	0
21	AU	51/51 (100%)	1.75	21 (41%) 0 0	56, 76, 95, 108	0
21	CU	51/51 (100%)	0.42	6 (11%) 6 2	48, 72, 94, 108	0
22	BA	2897/2903 (99%)	-0.12	106 (3%) 45 19	0, 14, 130, 195	0
22	DA	2897/2903 (99%)	-0.05	79 (2%) 58 28	42, 83, 144, 183	0
23	BB	119/119 (100%)	-0.51	0 100 100	1, 24, 54, 90	0
23	DB	118/119 (99%)	-0.34	0 100 100	66, 111, 133, 141	0
24	BC	271/271 (100%)	-0.22	8 (2%) 54 25	3, 21, 43, 55	0
24	DC	271/271 (100%)	0.46	23 (8%) 13 5	42, 62, 76, 91	0
25	BD	209/209 (100%)	-0.43	0 100 100	0, 9, 38, 71	0
25	DD	209/209 (100%)	0.41	13 (6%) 24 9	46, 66, 81, 99	0
26	BE	201/201 (100%)	-0.42	1 (0%) 91 76	0, 24, 56, 91	0
26	DE	201/201 (100%)	0.98	37 (18%) 2 1	45, 81, 98, 106	0
27	BF	177/177 (100%)	0.28	11 (6%) 24 9	15, 46, 88, 97	0
27	DF	177/177 (100%)	2.46	97 (54%) 0 0	85, 102, 117, 125	0
28	BG	176/176 (100%)	-0.14	0 100 100	15, 38, 64, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DG	176/176 (100%)	1.24	43 (24%) 1 1	71, 90, 104, 117	0
29	BH	149/149 (100%)	2.37	69 (46%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.21	38 (25%) 1 1	25, 92, 107, 115	0
30	BI	141/141 (100%)	2.51	67 (47%) 0 0	84, 108, 121, 136	0
30	DI	141/141 (100%)	3.72	97 (68%) 0 0	96, 114, 123, 127	0
31	BJ	142/142 (100%)	-0.45	0 100 100	1, 5, 23, 43	0
31	DJ	142/142 (100%)	0.44	16 (11%) 7 2	48, 64, 79, 96	0
32	BK	122/122 (100%)	-0.52	0 100 100	2, 11, 37, 67	0
32	DK	122/122 (100%)	0.69	14 (11%) 6 2	48, 61, 81, 96	0
33	BL	143/143 (100%)	-0.34	0 100 100	0, 21, 48, 76	0
33	DL	143/143 (100%)	1.31	37 (25%) 1 1	42, 77, 91, 113	0
34	BM	136/136 (100%)	-0.48	0 100 100	1, 9, 30, 87	0
34	DM	136/136 (100%)	0.84	18 (13%) 4 2	42, 67, 82, 108	0
35	BN	120/120 (100%)	-0.46	0 100 100	1, 6, 17, 62	0
35	DN	120/120 (100%)	0.63	17 (14%) 4 1	54, 74, 88, 110	0
36	BO	116/116 (100%)	-0.24	0 100 100	14, 27, 46, 52	0
36	DO	116/116 (100%)	1.75	47 (40%) 0 0	74, 91, 102, 114	0
37	BP	114/114 (100%)	-0.30	0 100 100	5, 19, 48, 70	0
37	DP	114/114 (100%)	0.61	15 (13%) 4 2	56, 68, 84, 93	0
38	BQ	117/117 (100%)	-0.43	0 100 100	0, 3, 11, 42	0
38	DQ	117/117 (100%)	0.44	11 (9%) 11 4	52, 66, 77, 84	0
39	BR	103/103 (100%)	-0.47	0 100 100	1, 9, 31, 63	0
39	DR	103/103 (100%)	0.91	19 (18%) 2 1	50, 75, 87, 97	0
40	BS	110/110 (100%)	-0.37	0 100 100	1, 3, 23, 84	0
40	DS	110/110 (100%)	1.11	27 (24%) 1 1	56, 73, 89, 96	0
41	BT	93/93 (100%)	0.01	2 (2%) 65 35	10, 27, 80, 101	0
41	DT	93/93 (100%)	1.89	41 (44%) 0 0	63, 83, 103, 110	0
42	BU	102/102 (100%)	-0.08	3 (2%) 55 26	10, 30, 61, 92	0
42	DU	102/102 (100%)	2.67	53 (51%) 0 0	70, 88, 106, 112	0
43	BV	94/94 (100%)	-0.34	0 100 100	4, 22, 43, 54	0
43	DV	94/94 (100%)	0.49	10 (10%) 8 3	65, 82, 94, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BW	76/76 (100%)	-0.41	0 100 100	3, 10, 27, 48	0
44	DW	75/76 (98%)	1.56	29 (38%) 0 0	54, 79, 88, 108	0
45	BX	77/77 (100%)	-0.35	0 100 100	6, 24, 52, 77	0
45	DX	77/77 (100%)	0.65	15 (19%) 1 1	49, 69, 86, 89	0
46	BY	63/63 (100%)	0.07	4 (6%) 23 9	22, 44, 74, 96	0
46	DY	63/63 (100%)	1.31	16 (25%) 1 1	71, 90, 99, 103	0
47	BZ	58/58 (100%)	-0.36	0 100 100	2, 7, 29, 41	0
47	DZ	58/58 (100%)	0.28	3 (5%) 31 12	52, 70, 84, 89	0
48	B0	56/56 (100%)	-0.52	0 100 100	0, 8, 35, 70	0
48	D0	56/56 (100%)	0.89	9 (16%) 3 1	53, 74, 91, 104	0
49	B1	50/50 (100%)	-0.26	2 (4%) 42 17	13, 31, 54, 87	0
49	D1	50/50 (100%)	1.22	11 (22%) 1 1	68, 84, 93, 105	0
50	B2	46/46 (100%)	-0.30	1 (2%) 65 35	3, 9, 17, 90	0
50	D2	46/46 (100%)	1.23	10 (21%) 1 1	53, 66, 79, 100	0
51	B3	64/64 (100%)	-0.31	0 100 100	4, 9, 18, 31	0
51	D3	64/64 (100%)	0.98	16 (25%) 1 1	58, 71, 79, 85	0
52	B4	38/38 (100%)	-0.06	0 100 100	11, 20, 35, 52	0
52	D4	38/38 (100%)	1.64	13 (34%) 0 0	63, 74, 85, 99	0
53	B5	191/228 (83%)	4.55	169 (88%) 0 0	85, 111, 123, 134	0
54	B6	2/7 (28%)	0.30	0 100 100	5, 5, 5, 9	0
54	D6	2/7 (28%)	0.79	0 100 100	53, 53, 53, 62	0
All	All	20738/20808 (99%)	0.30	2080 (10%) 9 4	0, 64, 119, 195	0

The worst 5 of 2080 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	BI	53	LEU	16.7
30	DI	6	GLN	16.5
22	BA	2100	G	16.3
30	DI	2	ALA	15.5
22	BA	2104	C	14.9

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
54	DBB	D6	3	6/7	0.88	0.50	-	45,50,65,70	0
54	004	D6	7	10/11	0.95	0.23	-	47,52,61,64	0
54	MHU	D6	5	15/16	0.82	0.38	-	45,58,69,72	0
54	DBB	B6	3	6/7	0.94	0.28	-	8,14,20,33	0
54	04X	B6	6	15/16	0.97	0.19	-	6,11,15,20	0
54	MHU	B6	5	15/16	0.93	0.24	-	3,7,15,15	0
54	MHW	B6	1	9/10	0.97	0.20	-	8,13,21,30	0
54	04X	D6	6	15/16	0.90	0.27	-	47,59,67,73	0
54	004	B6	7	10/11	0.97	0.28	-	2,4,6,6	0
54	MHW	D6	1	9/10	0.94	0.18	-	55,59,63,66	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	BA	3015	1/1	0.79	0.40	22.56	61,61,61,61	0
55	MG	BA	3186	1/1	0.96	0.23	20.31	12,12,12,12	0
55	MG	BA	3170	1/1	0.96	0.25	19.57	22,22,22,22	0
55	MG	DA	3113	1/1	0.89	0.45	17.52	75,75,75,75	0
55	MG	BA	3040	1/1	0.91	0.38	16.33	2,2,2,2	0
55	MG	DA	3002	1/1	0.77	0.52	15.16	81,81,81,81	0
55	MG	BA	3178	1/1	0.92	0.35	14.57	12,12,12,12	0
55	MG	AA	1670	1/1	0.74	0.40	13.74	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1615	1/1	0.85	0.23	13.71	56,56,56,56	0
55	MG	BA	3027	1/1	0.93	0.34	13.17	36,36,36,36	0
55	MG	DA	3072	1/1	0.23	0.51	12.25	89,89,89,89	0
55	MG	BA	3136	1/1	0.92	0.57	11.95	43,43,43,43	0
55	MG	DA	3071	1/1	0.19	0.59	11.68	93,93,93,93	0
55	MG	BA	3131	1/1	0.97	0.32	10.85	37,37,37,37	0
55	MG	DA	3041	1/1	0.46	0.42	10.25	66,66,66,66	0
55	MG	AM	201	1/1	0.94	0.62	8.94	50,50,50,50	0
55	MG	DA	3158	1/1	0.78	0.46	8.39	58,58,58,58	0
55	MG	BA	3146	1/1	0.96	0.21	5.57	22,22,22,22	0
55	MG	DA	3028	1/1	0.69	0.56	5.30	86,86,86,86	0
55	MG	DA	3106	1/1	0.78	0.31	4.98	70,70,70,70	0
55	MG	BA	3083	1/1	0.96	0.22	4.58	34,34,34,34	0
55	MG	CA	1626	1/1	0.78	0.26	4.56	66,66,66,66	0
55	MG	BA	3104	1/1	0.95	0.26	4.43	0,0,0,0	0
55	MG	BA	3055	1/1	0.58	0.25	4.05	50,50,50,50	0
55	MG	DA	3154	1/1	0.82	0.24	4.00	40,40,40,40	0
55	MG	DA	3110	1/1	0.96	0.24	3.67	45,45,45,45	0
55	MG	AA	1622	1/1	0.97	0.22	3.31	21,21,21,21	0
55	MG	BA	3005	1/1	0.96	0.17	2.52	43,43,43,43	0
55	MG	BA	3109	1/1	0.85	0.21	2.52	1,1,1,1	0
55	MG	DA	3032	1/1	0.67	0.20	2.32	78,78,78,78	0
55	MG	BA	3105	1/1	0.95	0.22	2.24	0,0,0,0	0
55	MG	AA	1669	1/1	0.92	0.27	2.20	34,34,34,34	0
55	MG	BA	3152	1/1	0.91	0.27	2.08	8,8,8,8	0
55	MG	AA	1662	1/1	0.83	0.27	1.81	49,49,49,49	0
55	MG	BA	3144	1/1	0.92	0.25	1.76	24,24,24,24	0
55	MG	BA	3053	1/1	0.94	0.18	1.69	0,0,0,0	0
55	MG	DA	3137	1/1	0.70	0.27	1.52	84,84,84,84	0
55	MG	DA	3140	1/1	0.97	0.22	1.50	42,42,42,42	0
55	MG	DA	3069	1/1	0.87	0.20	1.40	77,77,77,77	0
55	MG	DA	3060	1/1	0.85	0.22	1.09	72,72,72,72	0
55	MG	BA	3096	1/1	0.96	0.18	1.09	2,2,2,2	0
55	MG	DA	3058	1/1	0.83	0.17	0.97	70,70,70,70	0
55	MG	DA	3152	1/1	0.88	0.32	0.86	55,55,55,55	0
55	MG	BA	3187	1/1	0.98	0.21	0.85	3,3,3,3	0
55	MG	AA	1629	1/1	0.93	0.17	0.84	54,54,54,54	0
55	MG	DA	3064	1/1	0.92	0.19	0.83	48,48,48,48	0
55	MG	DA	3130	1/1	0.90	0.18	0.83	43,43,43,43	0
55	MG	DA	3048	1/1	0.78	0.22	0.67	93,93,93,93	0
55	MG	BA	3116	1/1	0.97	0.19	0.45	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1603	1/1	0.95	0.15	0.40	45,45,45,45	0
55	MG	DB	202	1/1	0.90	0.13	0.25	57,57,57,57	0
55	MG	DA	3109	1/1	0.97	0.19	0.06	30,30,30,30	0
55	MG	CA	1640	1/1	0.93	0.15	-0.05	36,36,36,36	0
55	MG	DA	3078	1/1	0.71	0.20	-0.32	95,95,95,95	0
55	MG	DA	3094	1/1	0.75	0.19	-0.41	83,83,83,83	0
55	MG	DA	3133	1/1	0.81	0.19	-0.44	55,55,55,55	0
55	MG	BA	3023	1/1	0.93	0.17	-0.45	0,0,0,0	0
55	MG	AA	1636	1/1	0.88	0.18	-0.55	42,42,42,42	0
55	MG	BA	3151	1/1	0.93	0.14	-0.58	23,23,23,23	0
55	MG	DA	3097	1/1	0.95	0.15	-0.61	67,67,67,67	0
55	MG	BA	3132	1/1	0.97	0.20	-0.65	32,32,32,32	0
55	MG	AA	1630	1/1	0.83	0.15	-0.70	67,67,67,67	0
55	MG	AA	1639	1/1	0.88	0.10	-0.74	67,67,67,67	0
55	MG	DA	3024	1/1	0.73	0.17	-0.78	45,45,45,45	0
55	MG	AA	1617	1/1	0.85	0.12	-0.82	62,62,62,62	0
55	MG	DA	3129	1/1	0.92	0.13	-0.84	70,70,70,70	0
55	MG	DA	3047	1/1	0.90	0.14	-0.84	71,71,71,71	0
55	MG	DA	3121	1/1	0.74	0.16	-0.85	60,60,60,60	0
55	MG	AA	1607	1/1	0.88	0.12	-0.99	48,48,48,48	0
55	MG	DA	3018	1/1	0.86	0.11	-1.10	68,68,68,68	0
55	MG	DA	3117	1/1	0.96	0.12	-1.22	55,55,55,55	0
55	MG	BA	3036	1/1	0.90	0.15	-1.25	23,23,23,23	0
55	MG	BA	3022	1/1	0.96	0.15	-1.30	0,0,0,0	0
55	MG	DA	3008	1/1	0.70	0.16	-1.30	80,80,80,80	0
56	ZN	D4	101	1/1	0.97	0.07	-1.32	74,74,74,74	0
55	MG	BA	3163	1/1	0.96	0.14	-1.35	27,27,27,27	0
55	MG	DA	3115	1/1	0.84	0.08	-1.35	79,79,79,79	0
55	MG	BA	3155	1/1	0.94	0.18	-1.35	2,2,2,2	0
55	MG	BA	3068	1/1	0.95	0.18	-1.43	1,1,1,1	0
55	MG	CA	1601	1/1	0.92	0.17	-1.49	52,52,52,52	0
56	ZN	B4	101	1/1	1.00	0.08	-1.49	76,76,76,76	0
55	MG	BA	3121	1/1	0.96	0.06	-1.52	14,14,14,14	0
55	MG	DA	3046	1/1	0.85	0.11	-1.60	62,62,62,62	0
55	MG	DA	3012	1/1	0.95	0.14	-1.63	39,39,39,39	0
55	MG	BA	3017	1/1	0.98	0.16	-1.66	0,0,0,0	0
55	MG	DA	3017	1/1	0.98	0.18	-1.70	39,39,39,39	0
55	MG	DA	3063	1/1	0.87	0.12	-1.70	53,53,53,53	0
55	MG	CA	1614	1/1	0.94	0.05	-1.72	52,52,52,52	0
55	MG	BA	3107	1/1	0.99	0.14	-1.76	3,3,3,3	0
55	MG	CA	1635	1/1	0.75	0.11	-1.78	94,94,94,94	0
55	MG	BA	3118	1/1	0.90	0.14	-1.80	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3037	1/1	0.95	0.08	-1.82	76,76,76,76	0
55	MG	DA	3135	1/1	0.87	0.08	-1.84	46,46,46,46	0
55	MG	DA	3050	1/1	0.98	0.12	-1.84	52,52,52,52	0
55	MG	DA	3005	1/1	0.43	0.12	-1.86	90,90,90,90	0
55	MG	BA	3063	1/1	0.99	0.13	-2.04	2,2,2,2	0
55	MG	DA	3023	1/1	0.96	0.11	-2.08	60,60,60,60	0
55	MG	DA	3025	1/1	0.88	0.12	-2.08	65,65,65,65	0
55	MG	CA	1607	1/1	0.96	0.14	-2.10	55,55,55,55	0
55	MG	AA	1618	1/1	0.95	0.09	-2.11	34,34,34,34	0
55	MG	BA	3161	1/1	0.85	0.16	-2.11	15,15,15,15	0
55	MG	DA	3098	1/1	0.82	0.08	-2.21	50,50,50,50	0
55	MG	BA	3013	1/1	0.96	0.17	-2.27	0,0,0,0	0
55	MG	BA	3159	1/1	0.94	0.14	-2.32	24,24,24,24	0
55	MG	BA	3077	1/1	0.90	0.07	-2.34	38,38,38,38	0
55	MG	DA	3079	1/1	0.67	0.08	-2.37	94,94,94,94	0
55	MG	BA	3108	1/1	0.94	0.16	-2.38	5,5,5,5	0
55	MG	CA	1622	1/1	0.88	0.13	-2.48	57,57,57,57	0
55	MG	BA	3049	1/1	0.96	0.14	-2.50	3,3,3,3	0
55	MG	BB	201	1/1	0.94	0.08	-2.52	28,28,28,28	0
55	MG	DA	3105	1/1	0.97	0.11	-2.64	52,52,52,52	0
55	MG	DA	3027	1/1	0.55	0.12	-2.69	82,82,82,82	0
55	MG	BA	3073	1/1	0.91	0.15	-2.71	9,9,9,9	0
55	MG	CA	1612	1/1	0.95	0.05	-2.72	43,43,43,43	0
55	MG	AA	1634	1/1	0.75	0.09	-2.75	49,49,49,49	0
55	MG	DA	3066	1/1	0.95	0.12	-2.79	45,45,45,45	0
55	MG	AA	1640	1/1	0.94	0.10	-2.88	57,57,57,57	0
55	MG	DA	3080	1/1	0.91	0.10	-2.95	91,91,91,91	0
55	MG	DA	3082	1/1	0.72	0.11	-3.11	65,65,65,65	0
55	MG	AA	1604	1/1	0.92	0.08	-3.16	48,48,48,48	0
55	MG	BA	3008	1/1	0.98	0.13	-3.18	0,0,0,0	0
55	MG	BA	3018	1/1	0.97	0.08	-3.33	10,10,10,10	0
55	MG	DA	3059	1/1	0.91	0.09	-3.34	42,42,42,42	0
55	MG	CA	1632	1/1	0.90	0.07	-3.42	75,75,75,75	0
55	MG	CA	1610	1/1	0.94	0.07	-3.46	58,58,58,58	0
55	MG	BA	3112	1/1	0.91	0.09	-3.47	20,20,20,20	0
55	MG	BA	3165	1/1	0.96	0.12	-3.59	3,3,3,3	0
55	MG	DA	3049	1/1	0.90	0.10	-3.61	69,69,69,69	0
55	MG	CA	1619	1/1	0.93	0.12	-3.65	27,27,27,27	0
55	MG	BA	3175	1/1	0.94	0.10	-3.68	9,9,9,9	0
55	MG	BA	3079	1/1	0.94	0.09	-3.68	21,21,21,21	0
55	MG	AA	1612	1/1	0.98	0.13	-3.72	38,38,38,38	0
55	MG	DA	3013	1/1	0.83	0.11	-3.72	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DB	201	1/1	0.76	0.05	-3.79	96,96,96,96	0
55	MG	BA	3065	1/1	0.94	0.12	-3.80	1,1,1,1	0
55	MG	BA	3097	1/1	0.94	0.12	-3.93	0,0,0,0	0
55	MG	DA	3096	1/1	0.92	0.09	-4.02	54,54,54,54	0
55	MG	BA	3101	1/1	0.95	0.09	-4.13	11,11,11,11	0
55	MG	DA	3022	1/1	0.94	0.13	-4.15	43,43,43,43	0
55	MG	CA	1616	1/1	0.94	0.10	-4.17	38,38,38,38	0
55	MG	AA	1616	1/1	0.92	0.09	-4.28	62,62,62,62	0
55	MG	DA	3054	1/1	0.87	0.08	-4.31	62,62,62,62	0
55	MG	BA	3012	1/1	0.96	0.16	-4.41	0,0,0,0	0
55	MG	AA	1625	1/1	0.94	0.09	-4.41	51,51,51,51	0
55	MG	BA	3093	1/1	0.87	0.10	-4.55	26,26,26,26	0
55	MG	BA	3032	1/1	0.93	0.12	-4.56	2,2,2,2	0
55	MG	AA	1641	1/1	0.97	0.12	-4.66	7,7,7,7	0
55	MG	BA	3110	1/1	0.96	0.11	-4.79	26,26,26,26	0
55	MG	AA	1609	1/1	0.92	0.08	-4.96	33,33,33,33	0
55	MG	BA	3002	1/1	0.88	0.09	-5.04	18,18,18,18	0
55	MG	BA	3028	1/1	0.87	0.10	-5.09	3,3,3,3	0
55	MG	BA	3021	1/1	0.99	0.15	-5.19	2,2,2,2	0
55	MG	CA	1617	1/1	0.97	0.09	-5.33	41,41,41,41	0
55	MG	AA	1633	1/1	0.96	0.08	-5.73	35,35,35,35	0
55	MG	BA	3130	1/1	0.97	0.16	-5.80	2,2,2,2	0
55	MG	BA	3024	1/1	0.95	0.07	-6.08	3,3,3,3	0
55	MG	BA	3058	1/1	0.97	0.07	-6.50	15,15,15,15	0
55	MG	BA	3050	1/1	0.92	0.07	-6.51	7,7,7,7	0
55	MG	AA	1642	1/1	0.99	0.07	-6.51	25,25,25,25	0
55	MG	AA	1613	1/1	0.94	0.07	-6.60	23,23,23,23	0
55	MG	DA	3043	1/1	0.90	0.07	-6.79	67,67,67,67	0
55	MG	BA	3120	1/1	0.93	0.12	-6.82	11,11,11,11	0
55	MG	BA	3071	1/1	0.93	0.15	-7.58	17,17,17,17	0
55	MG	BA	3134	1/1	0.97	0.09	-8.26	3,3,3,3	0
55	MG	AA	1606	1/1	0.93	0.06	-8.45	58,58,58,58	0
55	MG	BA	3129	1/1	0.86	0.13	-8.83	0,0,0,0	0
55	MG	DA	3039	1/1	0.95	0.10	-9.16	53,53,53,53	0
55	MG	BA	3009	1/1	0.97	0.08	-9.90	2,2,2,2	0
55	MG	AA	1611	1/1	0.97	0.07	-17.05	21,21,21,21	0
55	MG	BA	3177	1/1	0.94	0.10	-	9,9,9,9	0
55	MG	BA	3016	1/1	0.71	0.22	-	31,31,31,31	0
55	MG	BA	3169	1/1	0.95	0.10	-	4,4,4,4	0
55	MG	AA	1627	1/1	0.18	0.55	-	76,76,76,76	0
55	MG	DA	3124	1/1	0.95	0.16	-	41,41,41,41	0
55	MG	DA	3053	1/1	0.91	0.13	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1637	1/1	0.96	0.14	-	16,16,16,16	0
55	MG	BA	3173	1/1	0.91	0.29	-	30,30,30,30	0
55	MG	CA	1605	1/1	0.75	0.25	-	78,78,78,78	0
55	MG	BA	3067	1/1	0.96	0.20	-	0,0,0,0	0
55	MG	DA	3074	1/1	0.98	0.08	-	47,47,47,47	0
55	MG	DA	3139	1/1	0.90	0.56	-	47,47,47,47	0
55	MG	DA	3040	1/1	0.80	0.20	-	66,66,66,66	0
55	MG	AA	1628	1/1	0.97	0.04	-	39,39,39,39	0
55	MG	AA	1666	1/1	0.95	0.24	-	32,32,32,32	0
55	MG	DA	3011	1/1	0.41	0.31	-	74,74,74,74	0
55	MG	CA	1613	1/1	0.96	0.14	-	17,17,17,17	0
55	MG	BA	3047	1/1	0.74	0.11	-	40,40,40,40	0
55	MG	BA	3069	1/1	0.96	0.15	-	64,64,64,64	0
55	MG	DA	3116	1/1	0.44	0.33	-	92,92,92,92	0
55	MG	BA	3128	1/1	0.98	0.19	-	3,3,3,3	0
55	MG	CA	1642	1/1	0.95	0.19	-	25,25,25,25	0
55	MG	BA	3099	1/1	0.90	0.16	-	21,21,21,21	0
55	MG	AA	1653	1/1	0.97	0.18	-	34,34,34,34	0
55	MG	BA	3195	1/1	0.95	0.14	-	36,36,36,36	0
55	MG	BA	3038	1/1	0.93	0.14	-	1,1,1,1	0
55	MG	DA	3099	1/1	0.83	0.42	-	82,82,82,82	0
55	MG	BA	3106	1/1	0.98	0.24	-	0,0,0,0	0
55	MG	DA	3034	1/1	0.95	0.20	-	58,58,58,58	0
55	MG	BA	3194	1/1	0.95	0.18	-	22,22,22,22	0
55	MG	BA	3158	1/1	0.97	0.12	-	15,15,15,15	0
55	MG	DA	3091	1/1	0.77	0.13	-	79,79,79,79	0
55	MG	CA	1648	1/1	0.89	0.14	-	51,51,51,51	0
55	MG	BA	3034	1/1	0.92	0.13	-	5,5,5,5	0
55	MG	DA	3089	1/1	0.88	0.62	-	91,91,91,91	0
55	MG	DA	3162	1/1	0.97	0.11	-	48,48,48,48	0
55	MG	DA	3151	1/1	0.75	0.46	-	40,40,40,40	0
55	MG	DA	3153	1/1	0.70	0.12	-	68,68,68,68	0
55	MG	DA	3164	1/1	0.76	0.77	-	56,56,56,56	0
55	MG	BA	3191	1/1	0.96	0.17	-	26,26,26,26	0
55	MG	DA	3122	1/1	0.74	0.08	-	64,64,64,64	0
55	MG	BA	3154	1/1	0.75	0.24	-	21,21,21,21	0
55	MG	AA	1605	1/1	0.93	0.20	-	29,29,29,29	0
55	MG	BA	3189	1/1	0.97	0.20	-	0,0,0,0	0
55	MG	BA	3166	1/1	0.88	0.20	-	37,37,37,37	0
55	MG	BA	3171	1/1	0.93	0.17	-	20,20,20,20	0
55	MG	BA	3062	1/1	0.97	0.11	-	4,4,4,4	0
55	MG	BA	3137	1/1	0.95	0.29	-	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3192	1/1	0.96	0.23	-	11,11,11,11	0
55	MG	BA	3011	1/1	0.72	0.16	-	30,30,30,30	0
55	MG	AA	1621	1/1	0.98	0.09	-	37,37,37,37	0
55	MG	BA	3102	1/1	0.93	0.17	-	17,17,17,17	0
55	MG	DA	3001	1/1	0.95	0.08	-	37,37,37,37	0
55	MG	CA	1644	1/1	0.96	0.38	-	36,36,36,36	0
55	MG	BA	3037	1/1	0.98	0.19	-	0,0,0,0	0
55	MG	DA	3067	1/1	0.99	0.18	-	43,43,43,43	0
55	MG	BA	3162	1/1	0.97	0.13	-	23,23,23,23	0
55	MG	BA	3035	1/1	0.98	0.07	-	0,0,0,0	0
55	MG	BA	3089	1/1	0.94	0.14	-	1,1,1,1	0
55	MG	BA	3087	1/1	0.94	0.09	-	27,27,27,27	0
55	MG	CA	1638	1/1	0.84	0.16	-	74,74,74,74	0
55	MG	DA	3093	1/1	0.25	0.35	-	99,99,99,99	0
55	MG	BA	3113	1/1	0.85	0.12	-	2,2,2,2	0
55	MG	BA	3138	1/1	0.94	0.30	-	0,0,0,0	0
55	MG	AA	1664	1/1	0.97	0.13	-	51,51,51,51	0
55	MG	CA	1652	1/1	0.81	0.11	-	62,62,62,62	0
55	MG	AA	1610	1/1	0.92	0.15	-	51,51,51,51	0
55	MG	DA	3100	1/1	0.85	0.31	-	73,73,73,73	0
55	MG	CA	1649	1/1	0.97	0.21	-	24,24,24,24	0
55	MG	BA	3095	1/1	0.92	0.07	-	14,14,14,14	0
55	MG	AA	1658	1/1	0.90	0.17	-	35,35,35,35	0
55	MG	DA	3131	1/1	0.98	0.14	-	50,50,50,50	0
55	MG	DA	3029	1/1	0.77	0.36	-	66,66,66,66	0
55	MG	BA	3090	1/1	0.73	0.20	-	33,33,33,33	0
55	MG	DA	3021	1/1	0.70	0.33	-	62,62,62,62	0
55	MG	BA	3025	1/1	0.78	0.18	-	40,40,40,40	0
55	MG	BA	3020	1/1	0.88	0.13	-	5,5,5,5	0
55	MG	BA	3123	1/1	0.93	0.13	-	11,11,11,11	0
55	MG	DA	3163	1/1	0.91	0.21	-	47,47,47,47	0
55	MG	BA	3190	1/1	0.79	0.53	-	42,42,42,42	0
55	MG	AA	1649	1/1	0.97	0.12	-	28,28,28,28	0
55	MG	AA	1656	1/1	0.99	0.07	-	32,32,32,32	0
55	MG	DA	3015	1/1	0.79	0.57	-	77,77,77,77	0
55	MG	BA	3160	1/1	0.88	0.20	-	5,5,5,5	0
55	MG	DA	3149	1/1	0.76	0.19	-	49,49,49,49	0
55	MG	BA	3072	1/1	0.97	0.19	-	2,2,2,2	0
55	MG	BA	3133	1/1	0.88	0.34	-	57,57,57,57	0
55	MG	DA	3061	1/1	0.26	1.78	-	97,97,97,97	0
55	MG	BA	3075	1/1	0.91	0.14	-	6,6,6,6	0
55	MG	BA	3003	1/1	0.88	0.10	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3095	1/1	0.92	0.24	-	69,69,69,69	0
55	MG	AA	1614	1/1	0.89	0.19	-	66,66,66,66	0
55	MG	DA	3004	1/1	0.86	0.47	-	87,87,87,87	0
55	MG	BA	3046	1/1	0.94	0.17	-	3,3,3,3	0
55	MG	AA	1632	1/1	0.97	0.13	-	40,40,40,40	0
55	MG	BA	3111	1/1	0.92	0.07	-	27,27,27,27	0
55	MG	BA	3085	1/1	0.96	0.17	-	11,11,11,11	0
55	MG	BA	3078	1/1	0.98	0.04	-	38,38,38,38	0
55	MG	AA	1620	1/1	0.94	0.06	-	55,55,55,55	0
55	MG	DA	3118	1/1	0.88	0.11	-	73,73,73,73	0
55	MG	CA	1641	1/1	0.94	0.40	-	58,58,58,58	0
55	MG	DA	3077	1/1	0.62	0.26	-	76,76,76,76	0
55	MG	CA	1650	1/1	0.88	0.64	-	50,50,50,50	0
55	MG	DA	3134	1/1	0.58	0.57	-	87,87,87,87	0
55	MG	AA	1635	1/1	0.63	0.27	-	76,76,76,76	0
55	MG	BA	3149	1/1	0.97	0.23	-	0,0,0,0	0
55	MG	BA	3125	1/1	0.95	0.17	-	2,2,2,2	0
55	MG	AA	1602	1/1	0.92	0.37	-	53,53,53,53	0
55	MG	CA	1633	1/1	0.89	0.80	-	82,82,82,82	0
55	MG	BA	3091	1/1	0.90	0.05	-	48,48,48,48	0
55	MG	BB	203	1/1	0.90	0.09	-	7,7,7,7	0
55	MG	DA	3085	1/1	0.58	0.19	-	78,78,78,78	0
55	MG	CA	1623	1/1	0.93	0.17	-	66,66,66,66	0
55	MG	BA	3014	1/1	0.93	0.20	-	26,26,26,26	0
55	MG	CA	1624	1/1	0.90	0.07	-	52,52,52,52	0
55	MG	BA	3122	1/1	0.94	0.17	-	0,0,0,0	0
55	MG	BA	3064	1/1	0.95	0.15	-	0,0,0,0	0
55	MG	DA	3120	1/1	0.59	0.56	-	95,95,95,95	0
55	MG	DA	3086	1/1	0.98	0.12	-	61,61,61,61	0
55	MG	DA	3167	1/1	0.94	0.13	-	30,30,30,30	0
55	MG	BA	3056	1/1	0.89	0.19	-	22,22,22,22	0
55	MG	CA	1647	1/1	0.95	0.31	-	35,35,35,35	0
55	MG	BA	3019	1/1	0.81	0.26	-	1,1,1,1	0
55	MG	AA	1645	1/1	0.99	0.09	-	42,42,42,42	0
55	MG	CA	1620	1/1	0.86	0.13	-	81,81,81,81	0
55	MG	DA	3107	1/1	0.91	0.19	-	56,56,56,56	0
55	MG	DQ	201	1/1	0.89	0.29	-	40,40,40,40	0
55	MG	DA	3020	1/1	0.97	0.19	-	44,44,44,44	0
55	MG	AA	1660	1/1	0.95	0.09	-	41,41,41,41	0
55	MG	DA	3006	1/1	0.83	0.22	-	98,98,98,98	0
55	MG	BA	3029	1/1	0.82	0.12	-	35,35,35,35	0
55	MG	BA	3086	1/1	0.99	0.20	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3166	1/1	0.84	0.19	-	44,44,44,44	0
55	MG	BA	3080	1/1	0.87	0.09	-	24,24,24,24	0
55	MG	BA	3094	1/1	0.96	0.12	-	20,20,20,20	0
55	MG	BA	3103	1/1	0.96	0.07	-	7,7,7,7	0
55	MG	DA	3044	1/1	0.80	0.22	-	83,83,83,83	0
55	MG	DA	3030	1/1	0.94	0.26	-	61,61,61,61	0
55	MG	BA	3004	1/1	0.82	0.14	-	52,52,52,52	0
55	MG	BB	202	1/1	0.89	0.10	-	4,4,4,4	0
55	MG	CA	1645	1/1	0.91	0.13	-	32,32,32,32	0
55	MG	DA	3019	1/1	0.77	0.15	-	84,84,84,84	0
55	MG	AA	1651	1/1	0.70	0.34	-	55,55,55,55	0
55	MG	BA	3141	1/1	0.99	0.40	-	0,0,0,0	0
55	MG	DA	3142	1/1	0.91	0.39	-	39,39,39,39	0
55	MG	BA	3127	1/1	0.97	0.10	-	2,2,2,2	0
55	MG	DA	3155	1/1	0.74	0.28	-	37,37,37,37	0
55	MG	BA	3074	1/1	0.93	0.21	-	32,32,32,32	0
55	MG	DA	3003	1/1	0.96	0.13	-	66,66,66,66	0
55	MG	CA	1609	1/1	0.67	0.09	-	78,78,78,78	0
55	MG	AA	1644	1/1	0.23	0.69	-	49,49,49,49	0
55	MG	DA	3112	1/1	0.86	0.13	-	64,64,64,64	0
55	MG	BA	3033	1/1	0.99	0.20	-	0,0,0,0	0
55	MG	DA	3087	1/1	0.90	0.05	-	58,58,58,58	0
55	MG	BA	3088	1/1	0.90	0.08	-	29,29,29,29	0
55	MG	AA	1638	1/1	0.94	0.11	-	63,63,63,63	0
55	MG	BA	3031	1/1	0.78	0.11	-	7,7,7,7	0
55	MG	DA	3088	1/1	0.88	0.08	-	69,69,69,69	0
55	MG	DA	3132	1/1	0.53	0.79	-	85,85,85,85	0
55	MG	DA	3102	1/1	0.86	0.31	-	72,72,72,72	0
55	MG	BA	3172	1/1	0.96	0.12	-	16,16,16,16	0
55	MG	AA	1603	1/1	0.97	0.21	-	57,57,57,57	0
55	MG	DA	3045	1/1	0.89	0.21	-	61,61,61,61	0
55	MG	CM	201	1/1	0.85	0.38	-	50,50,50,50	0
55	MG	BA	3043	1/1	0.97	0.06	-	23,23,23,23	0
55	MG	DA	3157	1/1	0.89	0.14	-	29,29,29,29	0
55	MG	DA	3010	1/1	0.76	0.10	-	64,64,64,64	0
55	MG	AA	1643	1/1	0.90	0.15	-	23,23,23,23	0
55	MG	DA	3055	1/1	0.84	0.07	-	57,57,57,57	0
55	MG	DA	3108	1/1	0.92	0.14	-	55,55,55,55	0
55	MG	BA	3026	1/1	0.90	0.10	-	6,6,6,6	0
55	MG	AA	1647	1/1	0.99	0.17	-	44,44,44,44	0
55	MG	DA	3073	1/1	0.87	0.10	-	35,35,35,35	0
55	MG	AA	1657	1/1	0.83	0.34	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3066	1/1	0.92	0.14	-	2,2,2,2	0
55	MG	DA	3160	1/1	0.79	0.20	-	47,47,47,47	0
55	MG	BA	3082	1/1	0.96	0.07	-	6,6,6,6	0
55	MG	CA	1634	1/1	0.96	0.07	-	58,58,58,58	0
55	MG	BA	3098	1/1	0.73	0.59	-	73,73,73,73	0
55	MG	DA	3138	1/1	0.90	0.36	-	37,37,37,37	0
55	MG	DA	3081	1/1	0.88	0.12	-	62,62,62,62	0
55	MG	DA	3156	1/1	0.96	0.13	-	58,58,58,58	0
55	MG	BA	3156	1/1	0.95	0.15	-	9,9,9,9	0
55	MG	DA	3062	1/1	0.69	0.78	-	70,70,70,70	0
55	MG	AA	1626	1/1	0.96	0.21	-	26,26,26,26	0
55	MG	BA	3060	1/1	0.98	0.13	-	29,29,29,29	0
55	MG	BA	3147	1/1	0.97	0.14	-	11,11,11,11	0
55	MG	BA	3183	1/1	0.94	0.26	-	22,22,22,22	0
55	MG	AA	1650	1/1	0.94	0.25	-	20,20,20,20	0
55	MG	DA	3009	1/1	0.84	0.09	-	69,69,69,69	0
55	MG	CA	1611	1/1	0.84	0.17	-	69,69,69,69	0
55	MG	DA	3103	1/1	0.88	0.28	-	67,67,67,67	0
55	MG	CA	1627	1/1	0.61	0.29	-	88,88,88,88	0
55	MG	BA	3185	1/1	0.96	0.14	-	5,5,5,5	0
55	MG	BA	3114	1/1	0.98	0.09	-	28,28,28,28	0
55	MG	DA	3026	1/1	0.94	0.69	-	75,75,75,75	0
55	MG	DA	3065	1/1	0.91	0.07	-	41,41,41,41	0
55	MG	DA	3111	1/1	0.69	0.12	-	81,81,81,81	0
55	MG	BA	3153	1/1	0.97	0.16	-	2,2,2,2	0
55	MG	BA	3176	1/1	0.95	0.27	-	24,24,24,24	0
55	MG	BA	3042	1/1	0.97	0.14	-	1,1,1,1	0
55	MG	CA	1631	1/1	0.34	0.26	-	98,98,98,98	0
55	MG	CA	1625	1/1	0.98	0.17	-	18,18,18,18	0
55	MG	BA	3048	1/1	0.73	0.08	-	26,26,26,26	0
55	MG	DA	3161	1/1	0.79	0.33	-	48,48,48,48	0
55	MG	BA	3052	1/1	0.90	0.09	-	21,21,21,21	0
55	MG	DA	3075	1/1	0.96	0.26	-	61,61,61,61	0
55	MG	AA	1601	1/1	0.76	0.11	-	61,61,61,61	0
55	MG	BA	3044	1/1	0.90	0.21	-	8,8,8,8	0
55	MG	AA	1663	1/1	0.92	0.23	-	49,49,49,49	0
55	MG	BA	3100	1/1	0.96	0.10	-	9,9,9,9	0
55	MG	AA	1655	1/1	0.93	0.14	-	20,20,20,20	0
55	MG	DA	3127	1/1	0.85	0.13	-	88,88,88,88	0
55	MG	AA	1624	1/1	0.87	0.10	-	50,50,50,50	0
55	MG	DA	3144	1/1	0.85	0.30	-	58,58,58,58	0
55	MG	AA	1652	1/1	0.83	0.13	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3081	1/1	0.98	0.10	-	0,0,0,0	0
55	MG	BA	3184	1/1	0.95	0.13	-	8,8,8,8	0
55	MG	CA	1618	1/1	0.91	0.21	-	35,35,35,35	0
55	MG	BA	3054	1/1	0.91	0.08	-	7,7,7,7	0
55	MG	CA	1621	1/1	0.50	0.09	-	67,67,67,67	0
55	MG	DA	3038	1/1	0.78	0.14	-	63,63,63,63	0
55	MG	AA	1615	1/1	0.94	0.13	-	63,63,63,63	0
55	MG	BA	3039	1/1	0.96	0.22	-	1,1,1,1	0
55	MG	AA	1608	1/1	0.94	0.15	-	20,20,20,20	0
55	MG	DA	3068	1/1	0.94	0.07	-	60,60,60,60	0
55	MG	CA	1604	1/1	0.85	0.07	-	78,78,78,78	0
55	MG	CA	1651	1/1	0.95	0.25	-	72,72,72,72	0
55	MG	DA	3150	1/1	0.75	0.21	-	50,50,50,50	0
55	MG	BA	3007	1/1	0.90	0.09	-	32,32,32,32	0
55	MG	BA	3181	1/1	0.93	0.12	-	26,26,26,26	0
55	MG	BA	3124	1/1	0.88	0.09	-	9,9,9,9	0
55	MG	CA	1606	1/1	0.88	0.25	-	76,76,76,76	0
55	MG	DA	3123	1/1	0.95	0.15	-	44,44,44,44	0
55	MG	BA	3001	1/1	0.93	0.05	-	21,21,21,21	0
55	MG	DA	3128	1/1	0.92	0.07	-	74,74,74,74	0
55	MG	BA	3140	1/1	0.94	0.15	-	7,7,7,7	0
55	MG	AA	1631	1/1	0.91	0.16	-	52,52,52,52	0
55	MG	BA	3059	1/1	0.92	0.12	-	5,5,5,5	0
55	MG	AA	1623	1/1	0.79	0.17	-	49,49,49,49	0
55	MG	DA	3016	1/1	0.60	0.42	-	84,84,84,84	0
55	MG	DA	3090	1/1	0.82	0.08	-	59,59,59,59	0
55	MG	DA	3145	1/1	0.76	0.10	-	68,68,68,68	0
55	MG	DA	3035	1/1	0.91	0.14	-	71,71,71,71	0
55	MG	CA	1628	1/1	0.59	0.27	-	100,100,100,100	0
55	MG	BA	3119	1/1	0.64	0.36	-	49,49,49,49	0
55	MG	DA	3119	1/1	0.94	0.07	-	58,58,58,58	0
55	MG	BA	3157	1/1	0.83	0.33	-	34,34,34,34	0
55	MG	BA	3150	1/1	0.87	0.20	-	37,37,37,37	0
55	MG	DA	3092	1/1	0.79	0.44	-	94,94,94,94	0
55	MG	CA	1636	1/1	0.70	0.30	-	97,97,97,97	0
55	MG	BA	3070	1/1	0.80	0.11	-	37,37,37,37	0
55	MG	AA	1646	1/1	0.77	0.21	-	50,50,50,50	0
55	MG	BA	3045	1/1	0.85	0.12	-	4,4,4,4	0
55	MG	DA	3056	1/1	0.67	0.28	-	80,80,80,80	0
55	MG	BA	3030	1/1	0.97	0.16	-	3,3,3,3	0
55	MG	DA	3136	1/1	0.81	0.42	-	81,81,81,81	0
55	MG	BA	3061	1/1	0.89	0.64	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3174	1/1	0.94	0.14	-	5,5,5,5	0
55	MG	DB	203	1/1	0.82	0.09	-	90,90,90,90	0
55	MG	BA	3145	1/1	0.90	0.16	-	26,26,26,26	0
55	MG	DA	3146	1/1	0.93	0.10	-	41,41,41,41	0
55	MG	AA	1619	1/1	0.94	0.16	-	65,65,65,65	0
55	MG	BA	3092	1/1	0.91	0.19	-	42,42,42,42	0
55	MG	AA	1668	1/1	0.92	0.38	-	33,33,33,33	0
55	MG	BA	3143	1/1	0.96	0.32	-	3,3,3,3	0
55	MG	BA	3167	1/1	0.88	0.17	-	22,22,22,22	0
55	MG	BA	3164	1/1	0.98	0.30	-	6,6,6,6	0
55	MG	DA	3042	1/1	0.78	0.14	-	69,69,69,69	0
55	MG	BA	3148	1/1	0.97	0.14	-	13,13,13,13	0
55	MG	AA	1671	1/1	0.85	0.35	-	54,54,54,54	0
55	MG	BA	3051	1/1	0.98	0.14	-	4,4,4,4	0
55	MG	AA	1648	1/1	0.77	0.25	-	39,39,39,39	0
55	MG	CA	1643	1/1	0.97	0.37	-	41,41,41,41	0
55	MG	DA	3159	1/1	0.93	0.26	-	57,57,57,57	0
55	MG	BA	3041	1/1	0.94	0.10	-	11,11,11,11	0
55	MG	BA	3076	1/1	0.85	0.28	-	56,56,56,56	0
55	MG	DA	3101	1/1	0.91	0.08	-	63,63,63,63	0
55	MG	BA	3139	1/1	0.98	0.27	-	0,0,0,0	0
55	MG	CA	1602	1/1	0.78	0.12	-	69,69,69,69	0
55	MG	BA	3179	1/1	0.93	0.34	-	30,30,30,30	0
55	MG	AA	1654	1/1	0.96	0.14	-	41,41,41,41	0
55	MG	BA	3057	1/1	0.93	0.21	-	20,20,20,20	0
55	MG	BA	3182	1/1	0.95	0.22	-	14,14,14,14	0
55	MG	BA	3180	1/1	0.88	0.62	-	25,25,25,25	0
55	MG	CA	1646	1/1	0.88	0.23	-	36,36,36,36	0
55	MG	CA	1655	1/1	0.75	1.01	-	67,67,67,67	0
55	MG	DA	3125	1/1	0.88	0.17	-	86,86,86,86	0
55	MG	DA	3033	1/1	0.82	0.09	-	54,54,54,54	0
55	MG	DA	3057	1/1	0.42	0.29	-	82,82,82,82	0
55	MG	BA	3084	1/1	0.95	0.10	-	7,7,7,7	0
55	MG	BA	3126	1/1	0.96	0.15	-	3,3,3,3	0
55	MG	DA	3076	1/1	0.96	0.13	-	59,59,59,59	0
55	MG	DA	3007	1/1	0.92	0.37	-	80,80,80,80	0
55	MG	CA	1637	1/1	0.52	0.37	-	80,80,80,80	0
55	MG	BA	3006	1/1	0.97	0.07	-	13,13,13,13	0
55	MG	DA	3148	1/1	0.92	0.22	-	51,51,51,51	0
55	MG	CA	1629	1/1	0.50	0.10	-	84,84,84,84	0
55	MG	DA	3070	1/1	0.60	0.11	-	93,93,93,93	0
55	MG	BA	3188	1/1	0.96	0.11	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3104	1/1	0.57	0.18	-	76,76,76,76	0
55	MG	BA	3135	1/1	0.66	0.26	-	48,48,48,48	0
55	MG	BA	3117	1/1	0.96	0.16	-	1,1,1,1	0
55	MG	DA	3141	1/1	0.94	0.42	-	45,45,45,45	0
55	MG	BB	204	1/1	0.97	0.36	-	0,0,0,0	0
55	MG	CA	1630	1/1	0.90	0.65	-	102,102,102,102	0
55	MG	AA	1665	1/1	0.63	0.74	-	53,53,53,53	0
55	MG	DA	3014	1/1	0.79	0.35	-	73,73,73,73	0
55	MG	DA	3147	1/1	0.91	0.15	-	35,35,35,35	0
55	MG	BA	3168	1/1	0.84	0.24	-	21,21,21,21	0
55	MG	DA	3083	1/1	0.89	0.23	-	65,65,65,65	0
55	MG	CA	1639	1/1	0.93	0.13	-	43,43,43,43	0
55	MG	DA	3084	1/1	0.78	0.16	-	75,75,75,75	0
55	MG	BA	3115	1/1	0.73	0.51	-	76,76,76,76	0
55	MG	DA	3051	1/1	0.95	0.05	-	33,33,33,33	0
55	MG	CA	1654	1/1	0.88	0.21	-	26,26,26,26	0
55	MG	CA	1608	1/1	0.89	0.12	-	65,65,65,65	0
55	MG	DA	3165	1/1	0.74	0.39	-	43,43,43,43	0
55	MG	BA	3010	1/1	0.98	0.09	-	1,1,1,1	0
55	MG	BA	3142	1/1	0.97	0.21	-	0,0,0,0	0
55	MG	DA	3114	1/1	0.95	0.09	-	52,52,52,52	0
55	MG	AA	1659	1/1	0.85	0.47	-	32,32,32,32	0
55	MG	DA	3126	1/1	0.80	0.17	-	61,61,61,61	0
55	MG	AA	1667	1/1	0.73	0.69	-	54,54,54,54	0
55	MG	CA	1653	1/1	0.91	0.39	-	48,48,48,48	0
55	MG	DA	3031	1/1	0.92	0.14	-	59,59,59,59	0
55	MG	DA	3052	1/1	0.95	0.06	-	47,47,47,47	0
55	MG	AA	1661	1/1	0.92	0.36	-	23,23,23,23	0
55	MG	DA	3036	1/1	0.93	0.12	-	57,57,57,57	0
55	MG	BA	3193	1/1	0.94	0.16	-	12,12,12,12	0
55	MG	DA	3143	1/1	0.95	0.18	-	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.