



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:19 PM UTC

PDB ID : 4U1V / pdb_00004u1v
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 : 2014-07-16
Resolution : 3.00 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

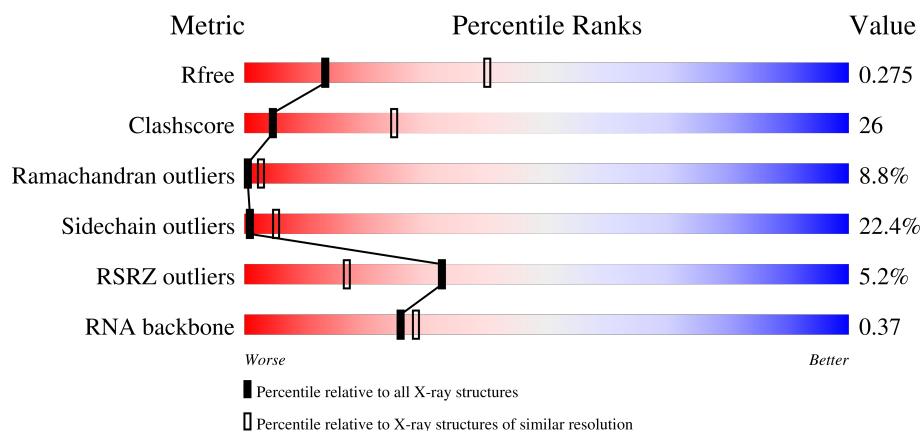
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	AA	1539	2% 23% 60% 18%
1	CA	1539	3% 29% 54% 17%
2	AB	218	5% 21% 47% 26% 6%
2	CB	218	6% 27% 49% 20% 5%

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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	

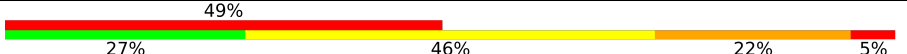
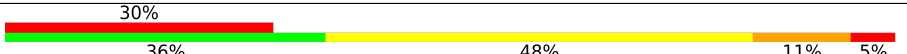
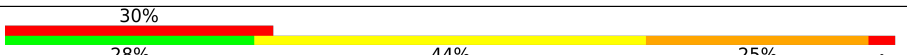
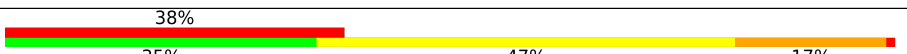
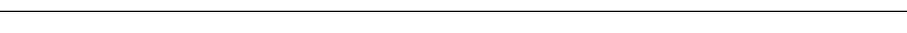
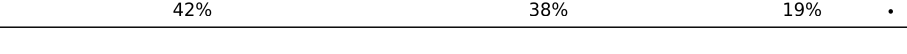
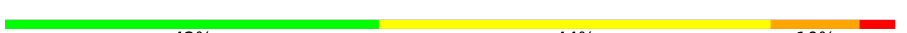
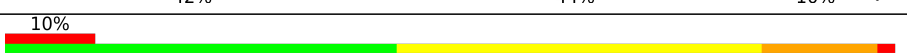
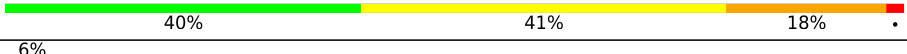
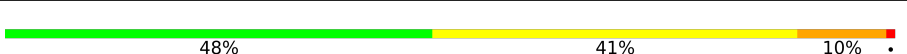
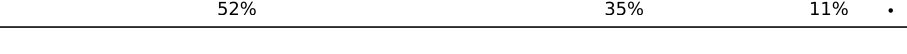
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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	119	
23	DB	119	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	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	B6	1	-	X	-	-
54	MHW	D6	1	-	X	X	-
55	MG	BA	3135	-	-	-	X
55	MG	DA	3026	-	-	-	X
55	MG	DA	3061	-	-	-	X
55	MG	DA	3132	-	-	-	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 (CCD ID: MG) (formula: Mg).

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

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

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	194	Total O 194 194	0	0
57	AL	1	Total O 1 1	0	0
57	AN	5	Total O 5 5	0	0
57	AT	2	Total O 2 2	0	0
57	AU	1	Total O 1 1	0	0
57	BA	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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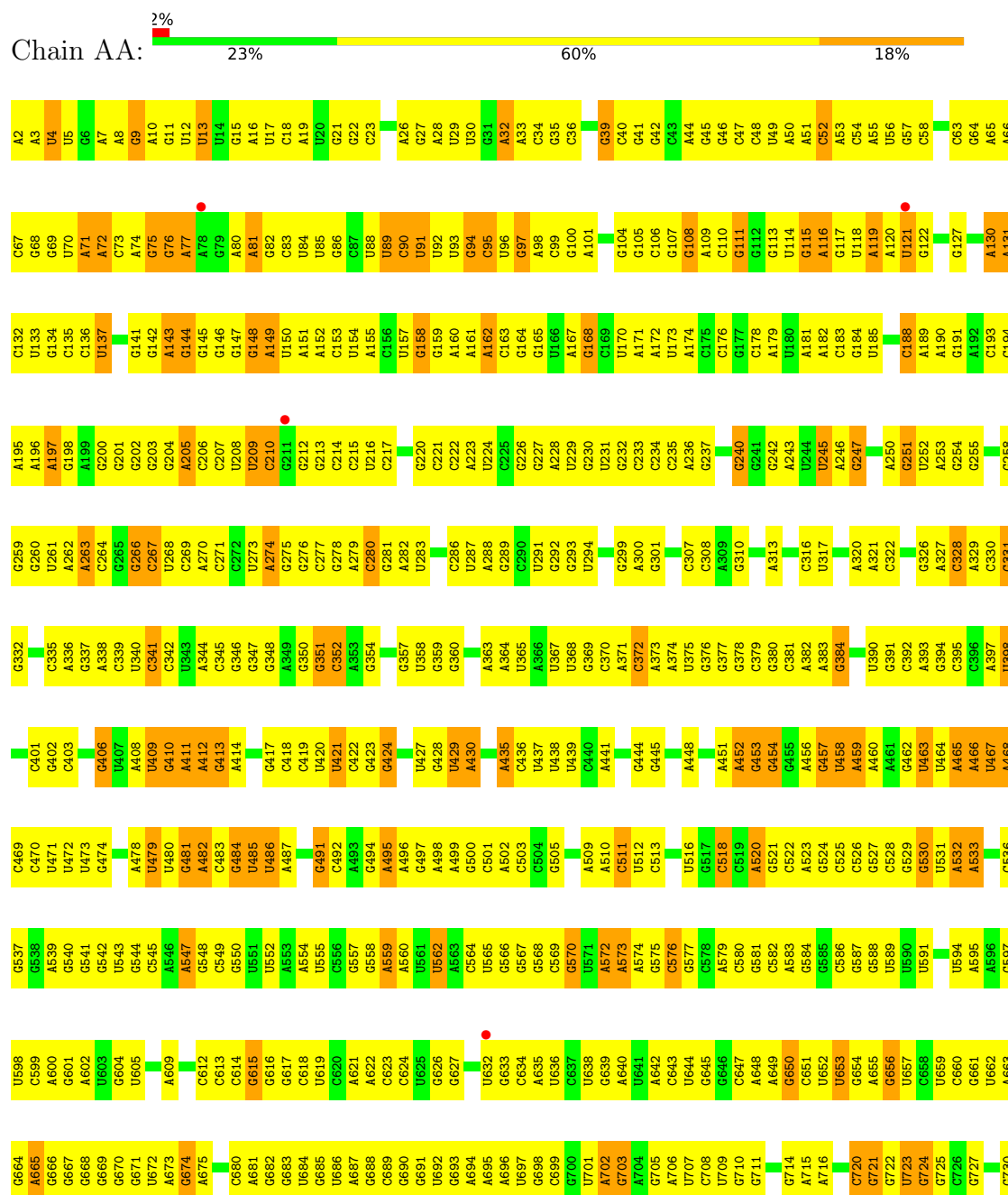
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CN	3	Total 3	O 3	0	0
57	CT	3	Total 3	O 3	0	0
57	CU	2	Total 2	O 2	0	0
57	DA	607	Total 607	O 607	0	0
57	DB	13	Total 13	O 13	0	0
57	DC	9	Total 9	O 9	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	6	Total 6	O 6	0	0
57	DL	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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S rRNA

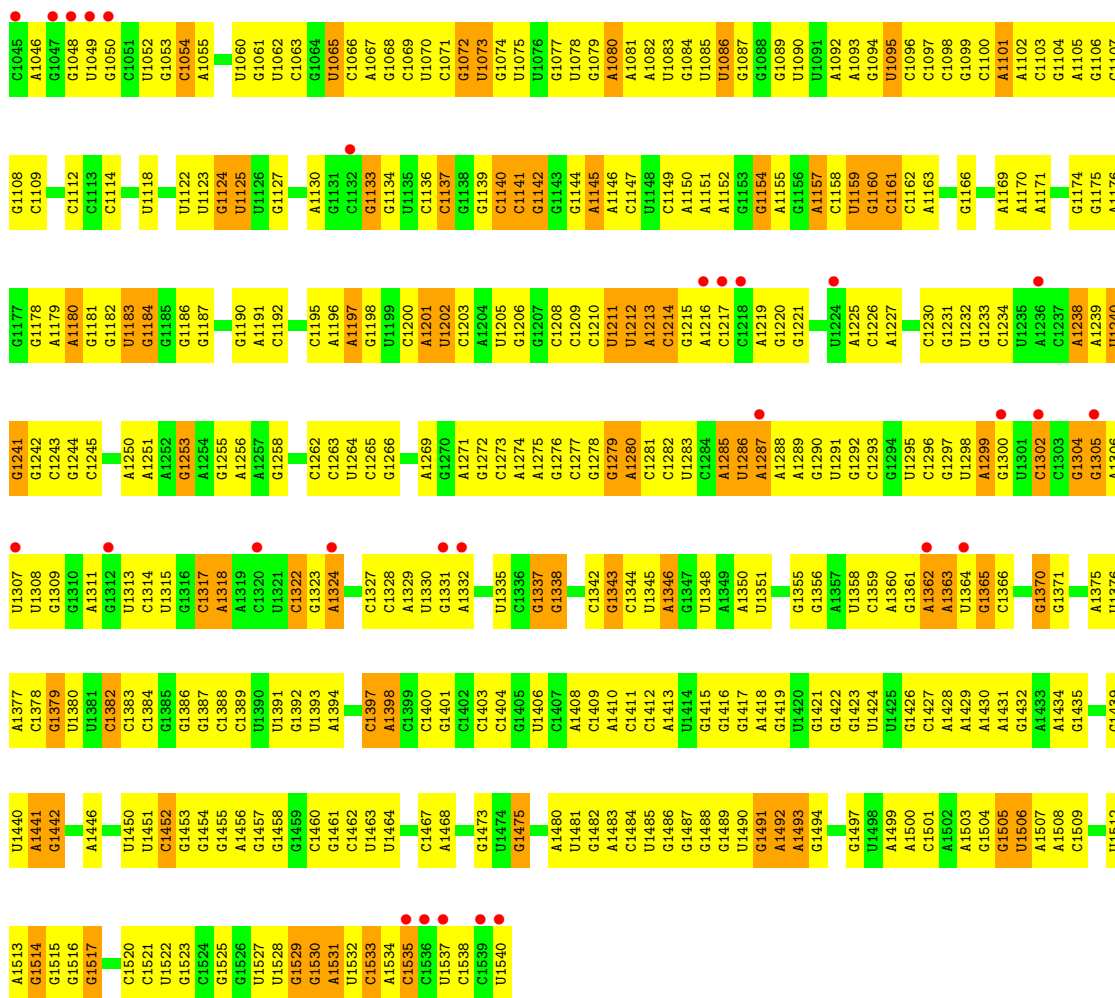


A1508	G1370	U1308	G1241	A1176	U1115	C1054	U989	G927	G861	C796	G731
C1509	G1371	G1309	G1242	G1177	U1116	A1055	C990	G928	C862	C797	C732
C1510	G1372	G1312	G1243	G1178	A1117	G1056	U991	G929	U863	C798	G733
C1443	G1373	G1443	G1244	G1179	U1117	G1057	U992	G930	U864	C799	
U1444	A1374	A1313	A1245	A1180	C1119	G1058	G993		A865	U800	C736
A1445	A1375	C1314	A1246	G1181	C1120	C1059	A994		C866	A802	C737
A1446	U1376	U1315	U1247	G1182	U1121	U1060	C995		C867	U803	C738
A1447	C1377	G1316	U1247	U1183	U1122	G1061	C996		C868	U804	C739
C1378	C1378	C1317	A1250	G1184	U1123	U1062	C997		C869	U805	U740
C1448	G1379	A1318	A1251	U1189	G1124	C1063	A998		U870	C806	G741
U1450	U1380	A1319	A1252	G1190	U1125	G1064	A999		U871	C807	G742
U1451	G1385	C1320	G1253	G1187	U1126	U1065	C999		A872	U808	A743
G1386	G1386	U1321	A1254	G1190	G1127	C1066	U1002		A873	C809	A744
G1387	G1387	C1322	G1255	A1191	C1128	A1067	A1004		C874	G809	G745
G1388	C1388	G1323	A1256	C1192	G1129	G1068	A1005		U875	C810	A746
A1394	C1389	A1324	A1257	G1193	A1130	U1069	U1007		C876	C811	A747
C1395	C1395	C1325	G1258	C1194	U1131	U1070	U1008		G877	U812	G748
A1396	U1390	U1326	C1259	A1196	G1133	C1071	U1009		C880	U813	
C1397	U1391	C1327	G1260	A1197	G1134	G1072	U1010		C881	A814	U751
A1468	G1392	C1328	A1261	G1198	U1135	U1073	G1013		C882	A815	G752
C1399	U1393	A1329	C1262	U1199	C1136	G1074	A1014		C883	A816	A753
C1400	C1394	U1330	C1263	C1200	U1137	U1075	U884		U884	C817	C754
G1401	C1395	G1331	U1264	A1201	C1138	U1076	U885		C885	C818	G755
A1402	A1396	A1332	G1268	U1202	G1139	G1077	G951		A889	U819	C756
C1403	C1397	A1333	A1269	C1203	C1140	U1078	U852		C890	U820	U757
C1404	A1400	G1334	A1270	A1204	C1141	G1079	G953		U891	C821	C758
C1405	U1478	U1341	G1277	U1210	G1142	A1080	G954		C892	U822	A759
U1406	C1342	G1342	G1278	U1212	G1143	A1081	U955		U893	C823	G760
C1407	G1343	G1343	G1279	A1213	A1150	U1082	U956		A894	G824	G761
A1408	A1408	A1346	A1280	C1214	A1151	U1083	U957		C895	U825	U762
C1409	A1409	G1347	U1283	G1215	A1152	G1084	U958		A900	C826	G763
A1410	A1410	G1348	U1284	A1216	G1153	U1085	C896		U901	U827	C764
C1411	C1411	U1348	U1285	C1217	G1154	U1086	C897		U902	U828	G765
A1412	C1412	A1349	U1286	C1218	A1155	G1087	C898		U903	G829	A766
A1413	A1413	A1350	A1287	G1219	G1156	U1088	U961		C899	G830	A767
U1414	U1414	U1351	A1288	G1220	A1157	G1089	G962		A901	A831	A768
G1415	G1415	C1352	A1289	G1221	C1158	C1096	G963		U904	G832	G769
G1416	C1353	G1353	G1290	G1222	U1159	C1097	A964		U905	G833	C770
G1417	U1354	U1354	C1293	C1223	G1160	C1098	U965		A906	U834	G771
A1418	G1355	G1356	G1294	U1224	C1161	G1099	G966		U907	U835	U772
A1419	A1492	A1357	U1295	A1225	C1162	C1100	A969		A908	C841	G773
G1422	G1422	C1359	C1296	A1227	A1163	A1101	G971		U909	U842	G774
U1425	U1425	A1360	U1297	C1228	G1164	A1102	C972		A843	G844	G775
A1429	A1429	G1361	U1298	A1229	U1165	C1103	A973		A845	U845	A776
A1430	A1430	A1362	A1299	G1233	G1166	G1104	G974		A914	G846	G777
A1431	A1431	A1363	A1300	C1234	A1167	A1105	A975		A915	G849	A781
U1435	G1435	U1364	U1301	U1235	U1168	G1106	A976		U916	U850	G785
G1436	U1436	G1365	C1302	A1236	A1169	C1107	G977		G917	G851	G786
A1437	A1437	C1366	C1303	C1237	U1170	C1108	U978		A918	U854	A787
U1438	U1438	C1367	G1304	C1237	A1171	G1109	U981		U919	U855	U788
A1507	G1439	C1369	A1305	A1238	C1172	C1112	U982		U920	U856	U789
			A1306	A1239	U1173	C1113	C984		U921	C857	G790
			U1307	U1240	G1175	C1114	C985		U922	G858	A791
							C986		G923	C859	A792
							U987		G924	U793	U793
							G988		G925	A794	G794
									G926	C795	C795

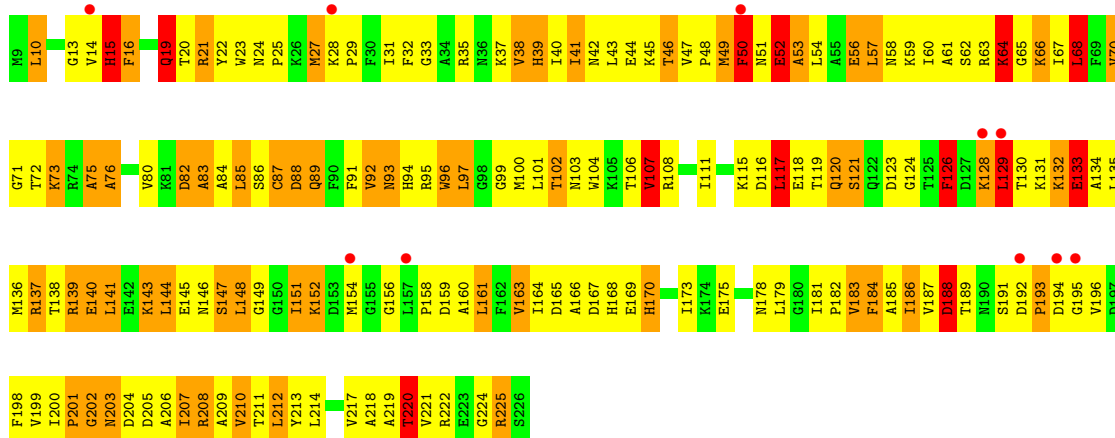
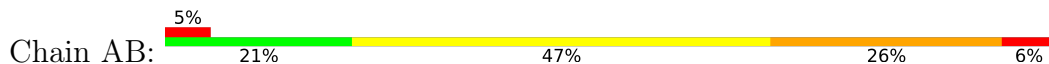
• Molecule 1: 16S rRNA



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U911	C912	A913	A914	G917	A918	A919	U920	U921	G922	G851	G852	C853	U854	U855	G858	G859	A860	G861	C862	U863	A864	A865	C866	G867	C868	G869	U870	U871	A872	A873	G874	A878	G881	C882	C883	G886	G887	G888	A889	G890	U891	C962	G963	A964	U965	G966	C967	A968	A969	C970	G971	C972	G973	A974	A975									
U772	G773	G774	G775	G776	G777	G778	G779	A780	A781	A782	C783	A784	G785	G786	A787	U788	C789	A790	G791	A792	U793	A794	C795	C796	C797	U798	G799	G800	U801	A802	G803	U804	C805	C806	G809	C810	C811	G812	U813	A814	A815	A816	C817	G821	U822	C823	G824	U827	U828	G829	G833	U834	U835	G836	U837									
G705	A706	G707	C708	U709	G710	G711	A712	A715	A716	A717	A718	C719	G720	G721	U722	U723	A724	A725	C726	A727	C728	C729	C730	C731	C732	G733	G734	C735	C736	C737	U740	G741	G742	A743	C744	G745	A746	A747	A748	A749	C750	U751	C754	G755	C756	U757	C758	A759	G760	G761	G765	A766	A767	A768	G769	C770	G771							
G557	G558	A559	A560	U561	U562	A563	A564	A565	A566	A567	C568	C569	C570	C571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	A583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	G604	U605	G606	A607	A608	A609	C618	U619	C620	G621	G622	G623	C624	C625	U626	G627	G628	A629	A630	C631	U632	G633
G484	U485	U486	C418	U421	C422	G423	G424	G425	U426	U427	G428	U429	A430	A431	A432	A433	A434	A435	C436	U437	U438	U439	C440	A441	G442	G443	G444	G445	G446	A451	A452	G453	G454	G455	A456	G457	U458	A459	A460	U463	U464	A465	A466	U467	A468	C469	G474	C475	U476	C477	A478	U479	U480	G481	A482	C483								
G351	C352	A353	C354	C355	A356	C357	U358	C359	G360	C361	G362	U365	A366	U367	U368	C369	C370	A371	C372	A373	U374	C375	C376	G377	C378	C379	C380	C381	A382	A383	C384	C385	C386	U387	C388	A389	U390	C391	C392	A393	C396	A397	U398	C399	G402	C403	G404	U405	A406	U407	A408	U409	G410	A411	A412	C413								
C210	G211	G212	G213	C214	C215	U216	C217	U218	C221	C222	C223	A224	G227	U228	A229	A230	U231	U232	U233	U234	U235	U236	U237	U238	U239	U240	U241	U242	U243	U244	U245	U246	U247	U248	U249	U250	U251	U252	A253	C254	G257	U258	C259	G260	U261	U262	A263	C264	C265	G266	C267	U268	C269	G270	A271	C272	U273	U274						
G278	A279	C280	C281	C285	C286	G289	G293	U294	C295	U296	G297	A298	G299	A300	U304	G305	A306	C307	C308	A309	G310	A313	C314	A315	C316	U317	C318	C319	A320	A321	G324	A327	C328	A329	C330	C331	G332	U333	C334	C335	A336	C337	A338	C339	U340	C345	G346	G347	G348	A349	G350													
U137	G142	A143	G144	G145	G146	U150	A151	A152	C153	U154	A155	U157	G158	G159	A160	A161	A162	C163	G164	U167	G168	C169	U170	A171	A172	U173	C176	G179	U180	A181	A182	C183	G184	U185	C188	A189	G115	A116	G117	A195	A196	A197	G198	A199	G200	G201	G202	C203	G204	A205	C206	C207	U208	U209										
G68	G69	U70	A71	A72	C73	A74	G75	G76	A77	A78	G79	A80	A81	G82	C83	U84	U85	G86	C87	U88	U91	U92	U93	G94	C95	U96	G97	A98	C99	U103	G104	G105	C106	G107	G108	A109	C110	G111	G112	G115	A116	G117	A120	U121	G122	G127	G128	A129	A130	A131	G134	A135	A136	C136										
A2	A3	U4	U5	G6	A7	A8	G9	A10	U13	U14	G15	A16	U17	C18	A19	U20	G21	C22	C23	U24	C25	A26	G27	A28	U29	U30	G31	A32	A33	C34	G35	C36	U37	G38	G39	C40	G41	G42	C47	C48	U49	A50	A51	C52	A53	C54	A55	U56	A59	G62	C63	G64	A65	A66	C67									

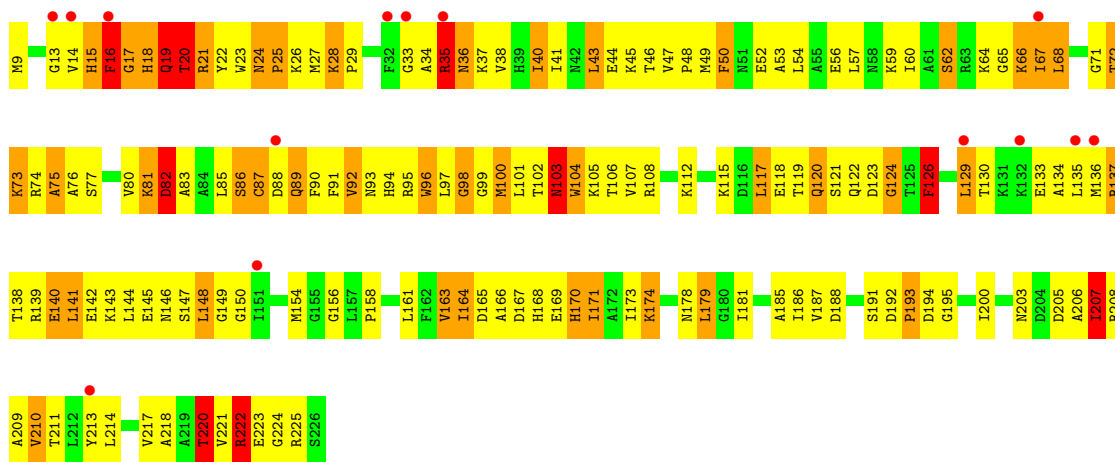


• Molecule 2: 30S ribosomal protein S2

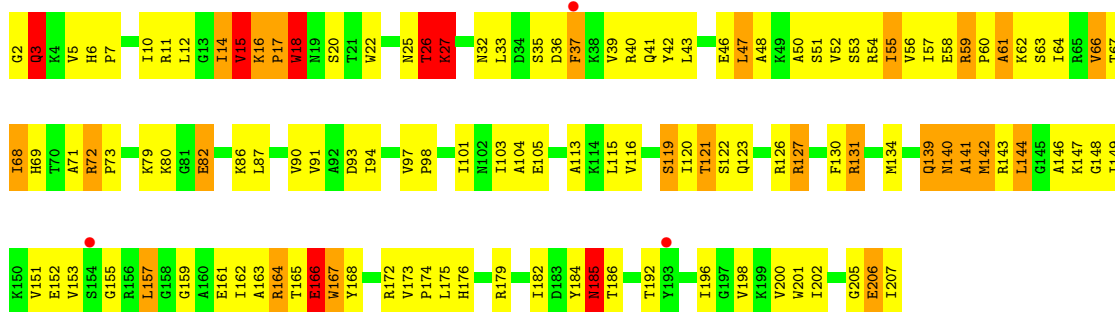


• Molecule 2: 30S ribosomal protein S2

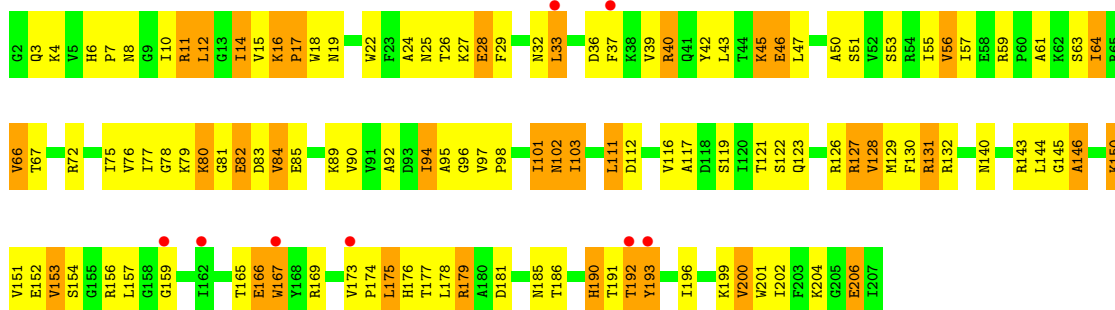
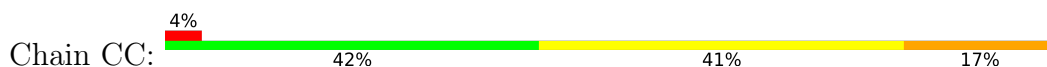




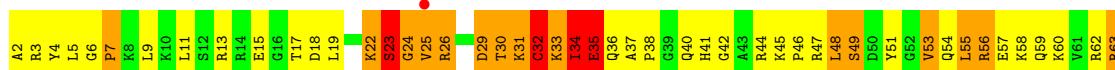
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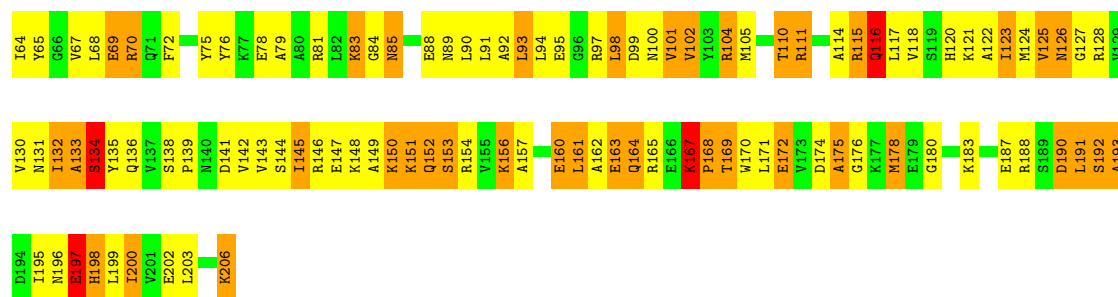


• Molecule 3: 30S ribosomal protein S3

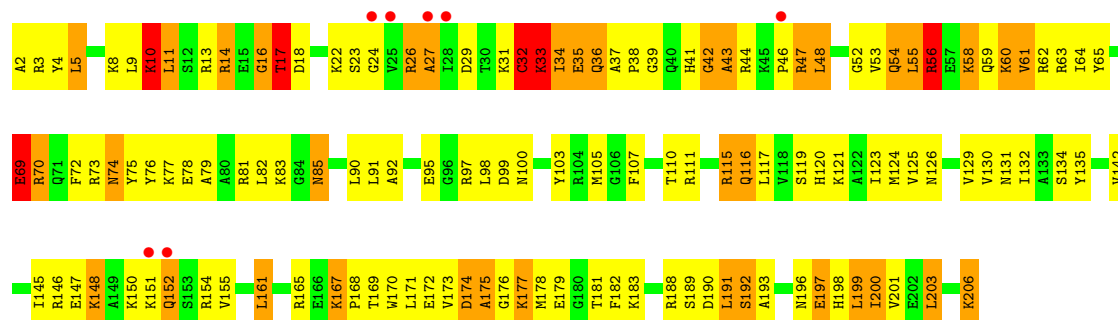


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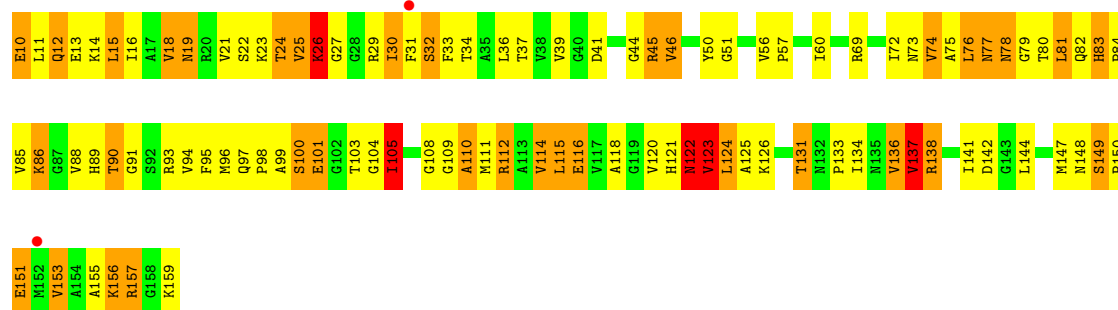




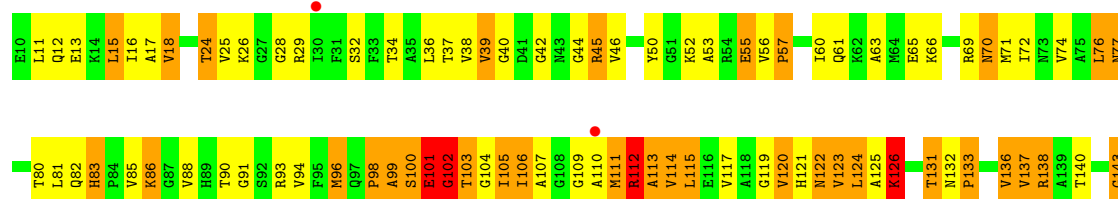
• Molecule 4: 30S ribosomal protein S4

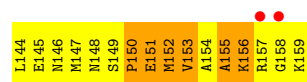


• Molecule 5: 30S ribosomal protein S5

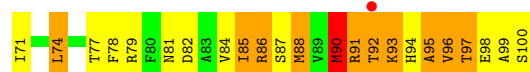
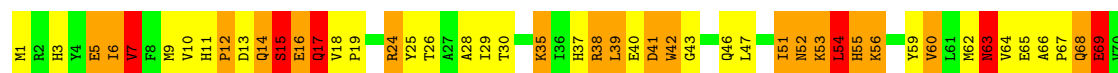


• Molecule 5: 30S ribosomal protein S5

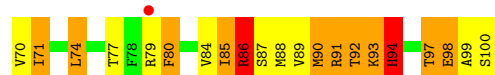




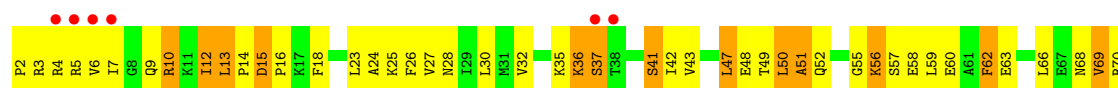
• Molecule 6: 30S ribosomal protein S6



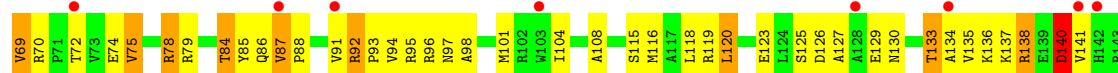
• Molecule 6: 30S ribosomal protein S6

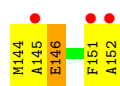


• Molecule 7: 30S ribosomal protein S7

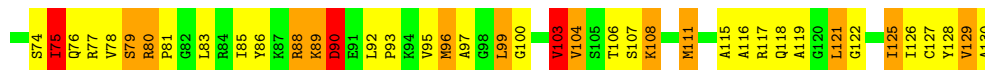
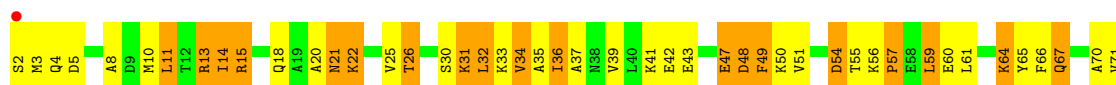


• Molecule 7: 30S ribosomal protein S7

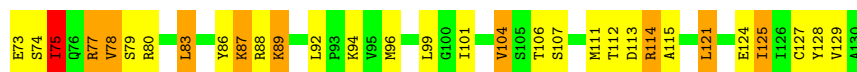
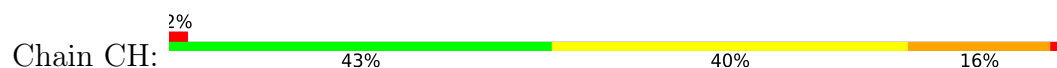




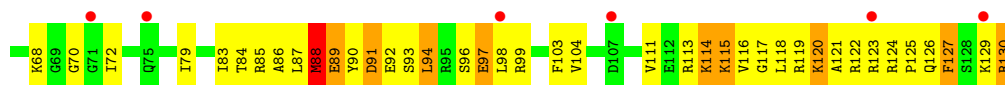
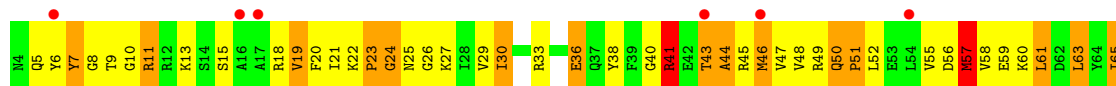
• Molecule 8: 30S ribosomal protein S8



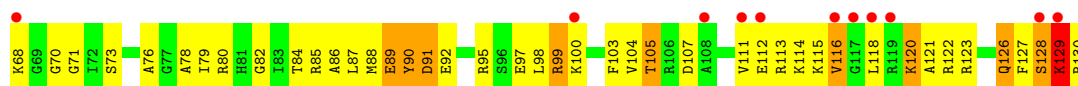
• Molecule 8: 30S ribosomal protein S8



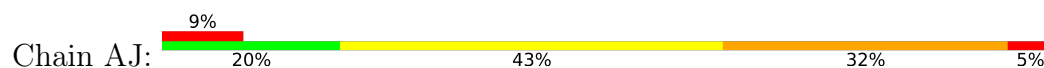
• Molecule 9: 30S ribosomal protein S9

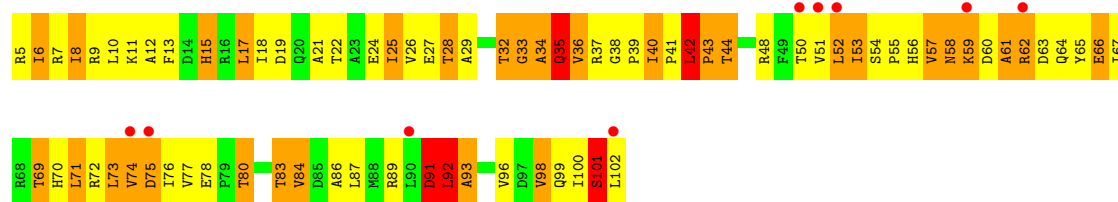


• Molecule 9: 30S ribosomal protein S9

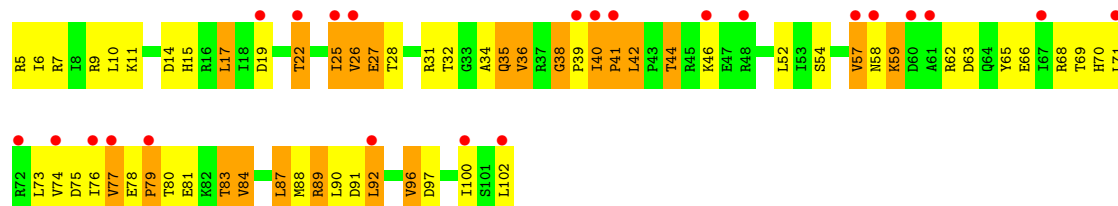


• Molecule 10: 30S ribosomal protein S10

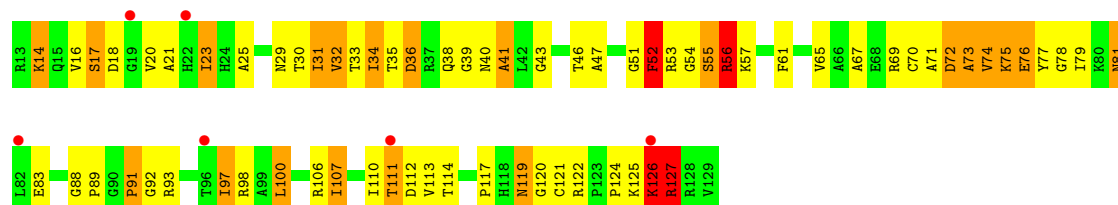
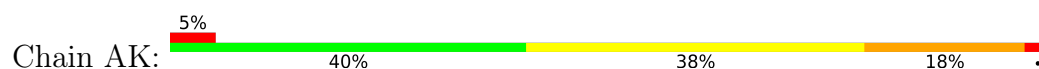




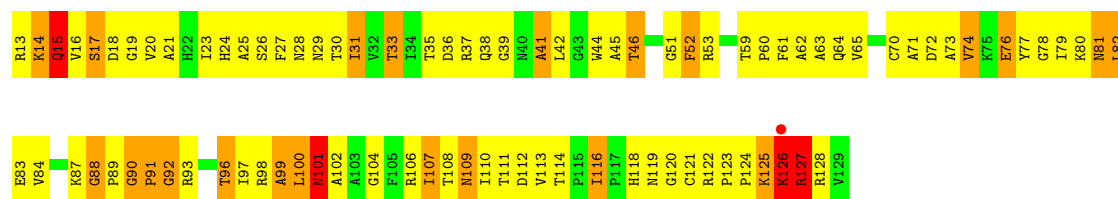
• Molecule 10: 30S ribosomal protein S10



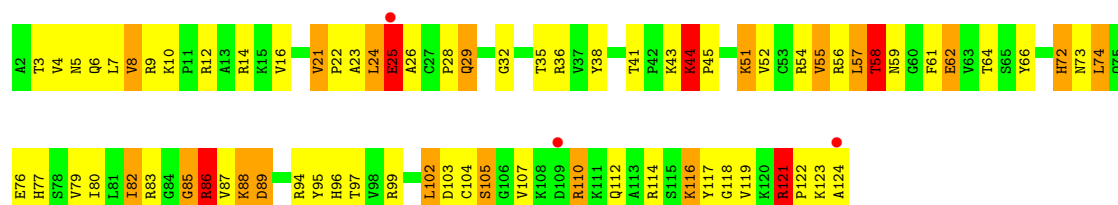
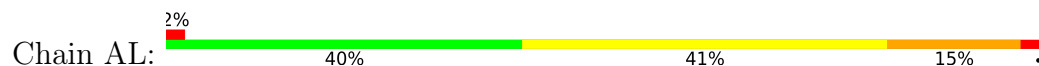
• Molecule 11: 30S ribosomal protein S11



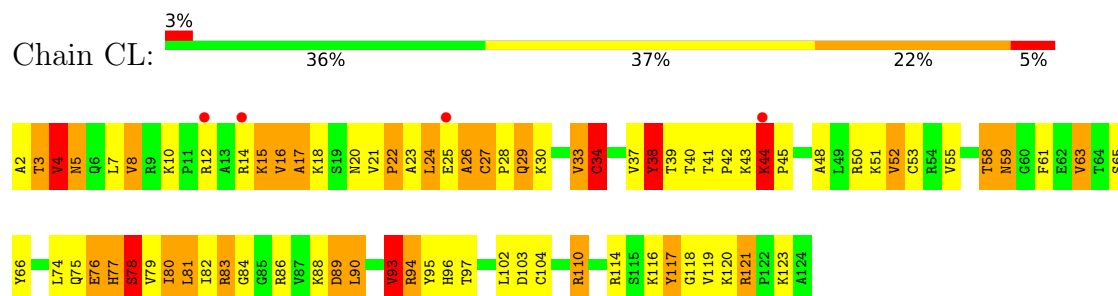
• Molecule 11: 30S ribosomal protein S11



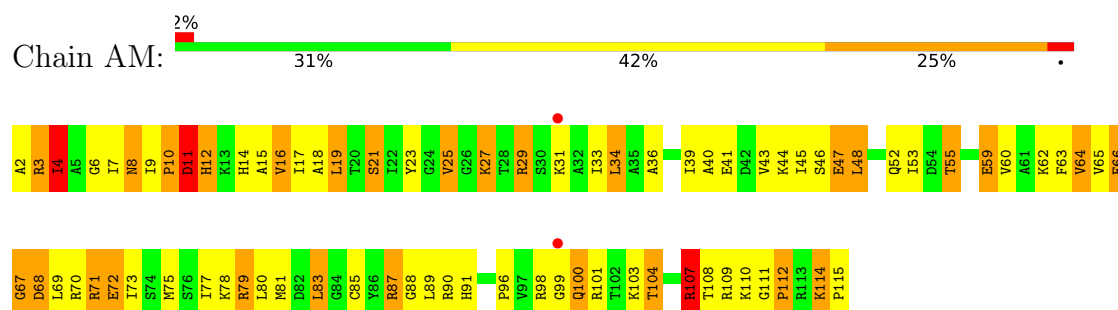
• Molecule 12: 30S ribosomal protein S12



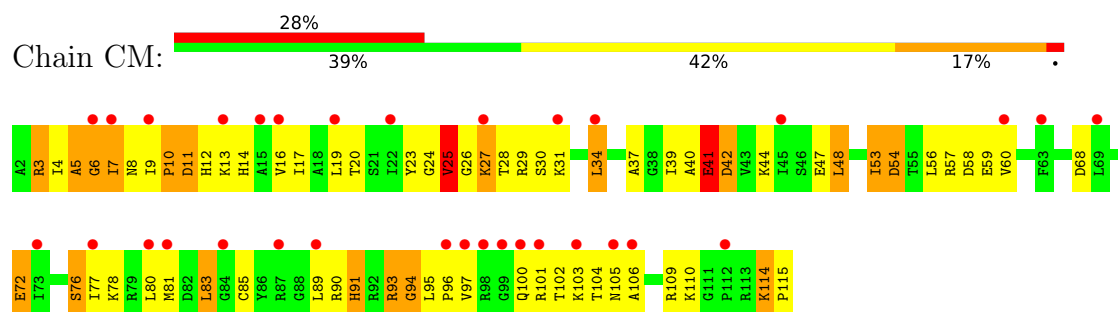
- Molecule 12: 30S ribosomal protein S12



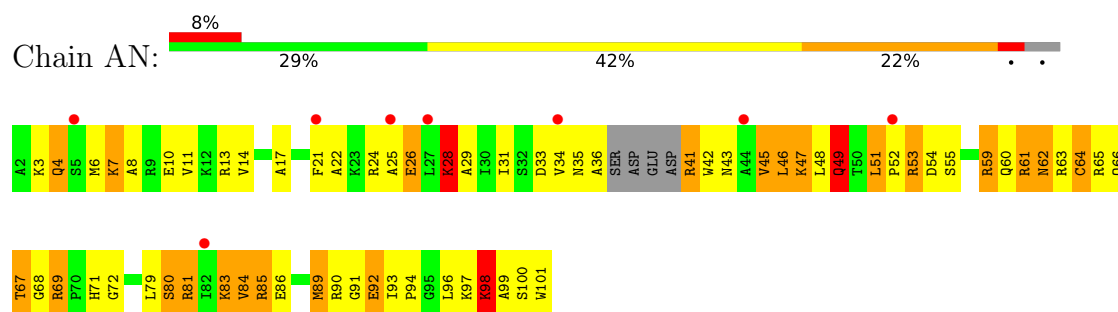
- Molecule 13: 30S ribosomal protein S13



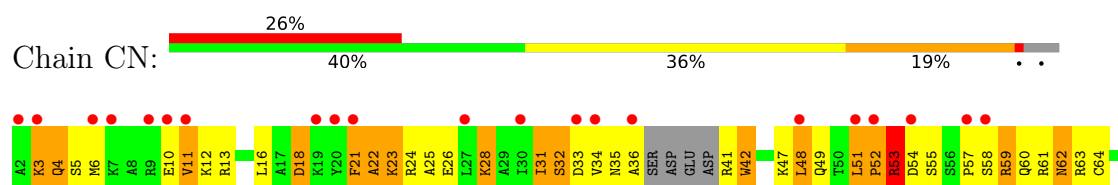
- Molecule 13: 30S ribosomal protein S13

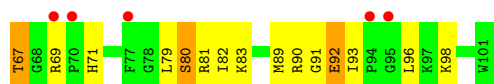


- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14

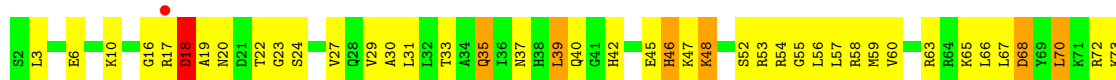
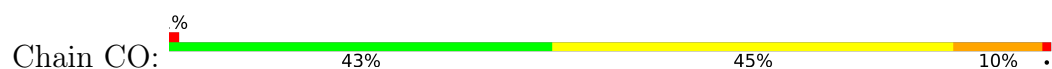




- Molecule 15: 30S ribosomal protein S15



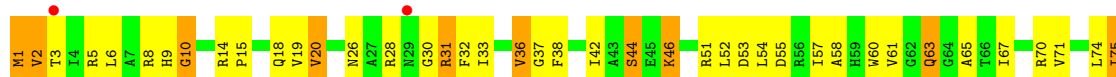
- Molecule 15: 30S ribosomal protein S15



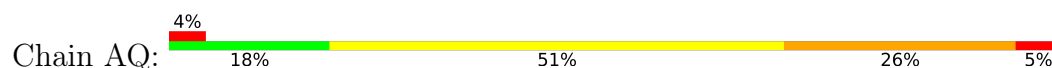
- Molecule 16: 30S ribosomal protein S16

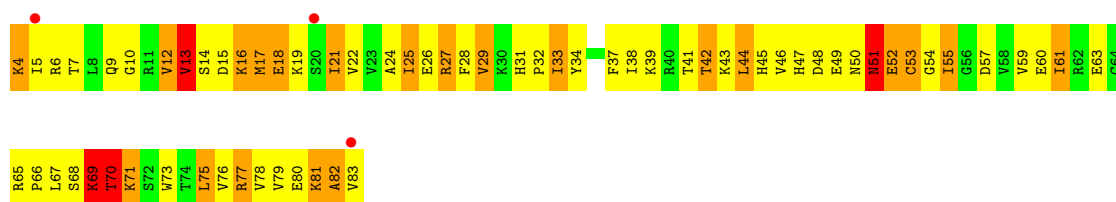


- Molecule 16: 30S ribosomal protein S16

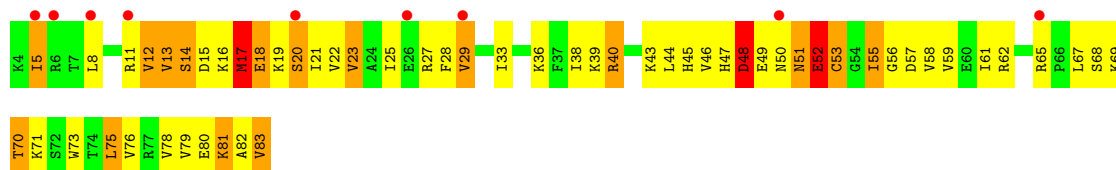


- Molecule 17: 30S ribosomal protein S17

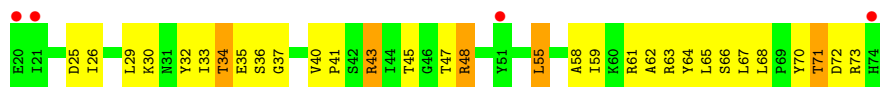




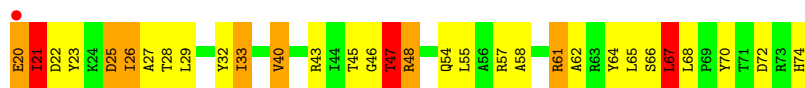
• Molecule 17: 30S ribosomal protein S17



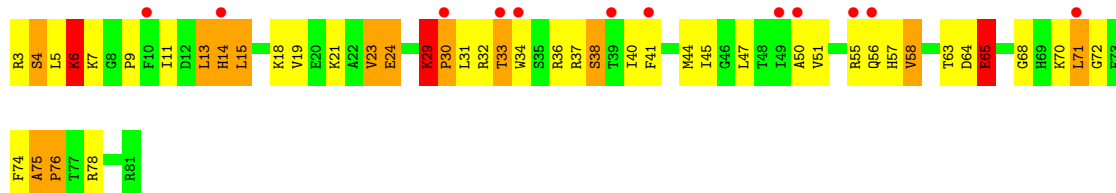
• Molecule 18: 30S ribosomal protein S18



• Molecule 18: 30S ribosomal protein S18

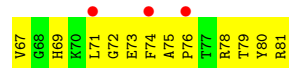


• Molecule 19: 30S ribosomal protein S19

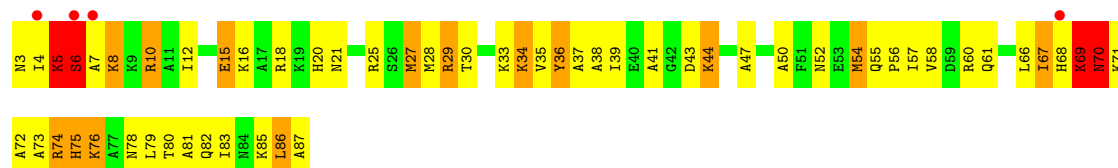


• Molecule 19: 30S ribosomal protein S19





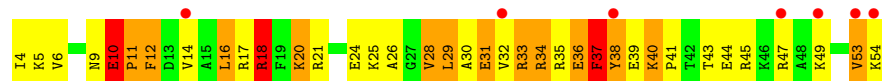
• Molecule 20: 30S ribosomal protein S20



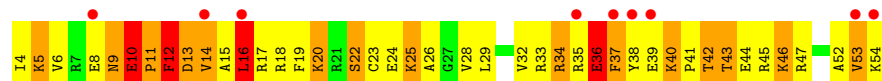
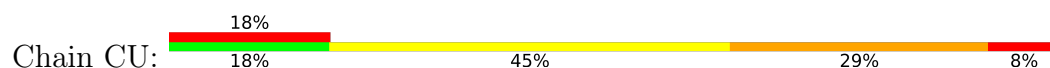
• Molecule 20: 30S ribosomal protein S20



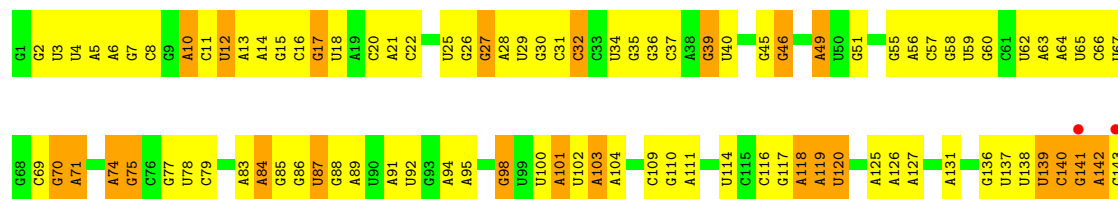
• Molecule 21: 30S ribosomal protein S21



• Molecule 21: 30S ribosomal protein S21

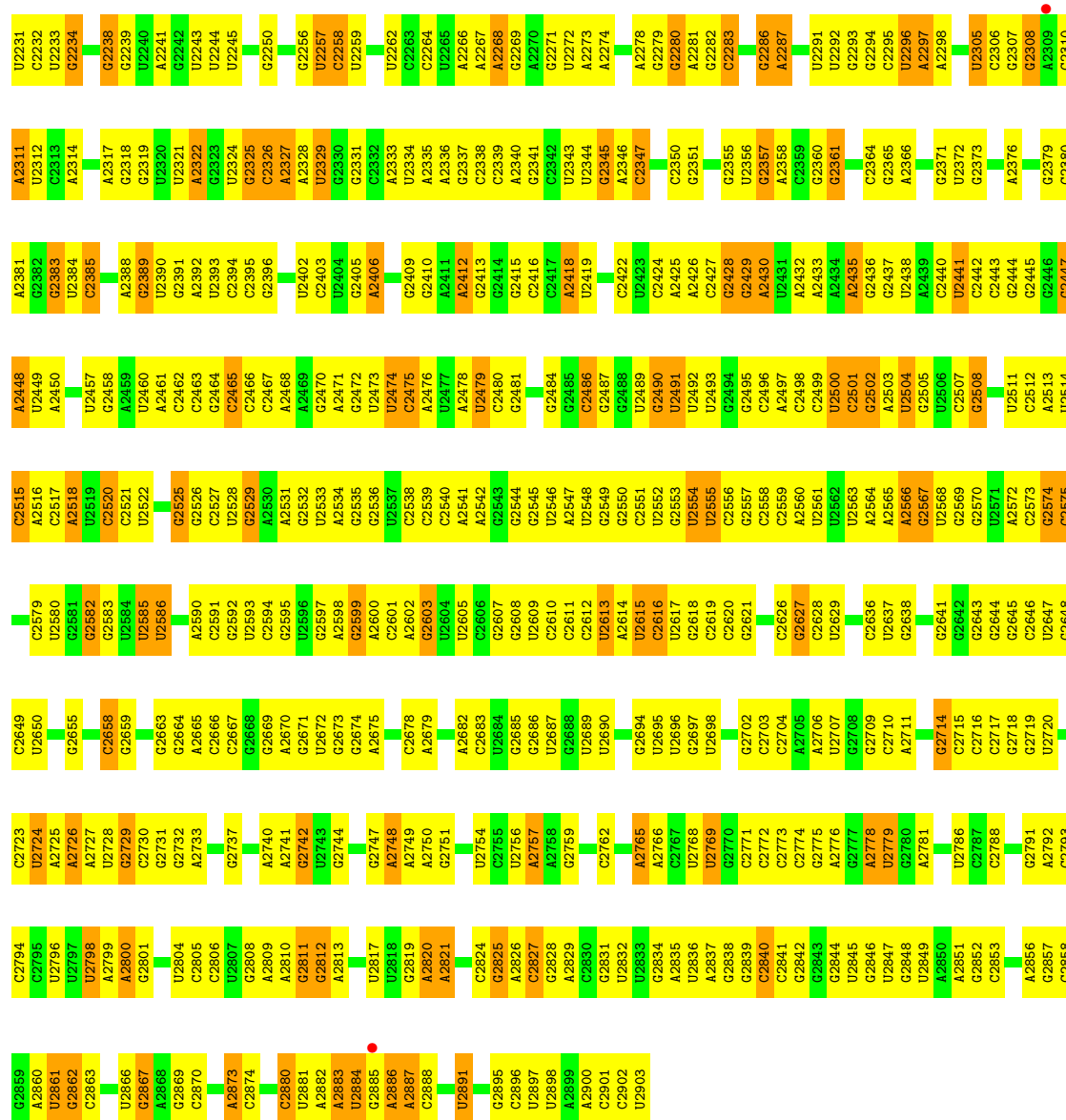


• Molecule 22: 23S rRNA

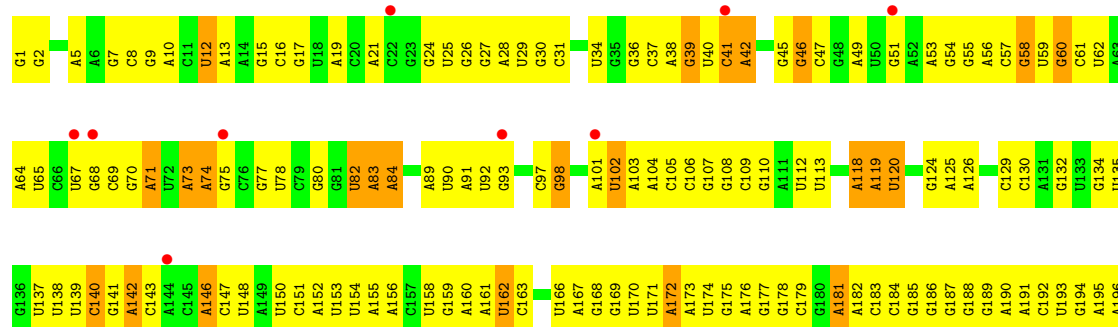


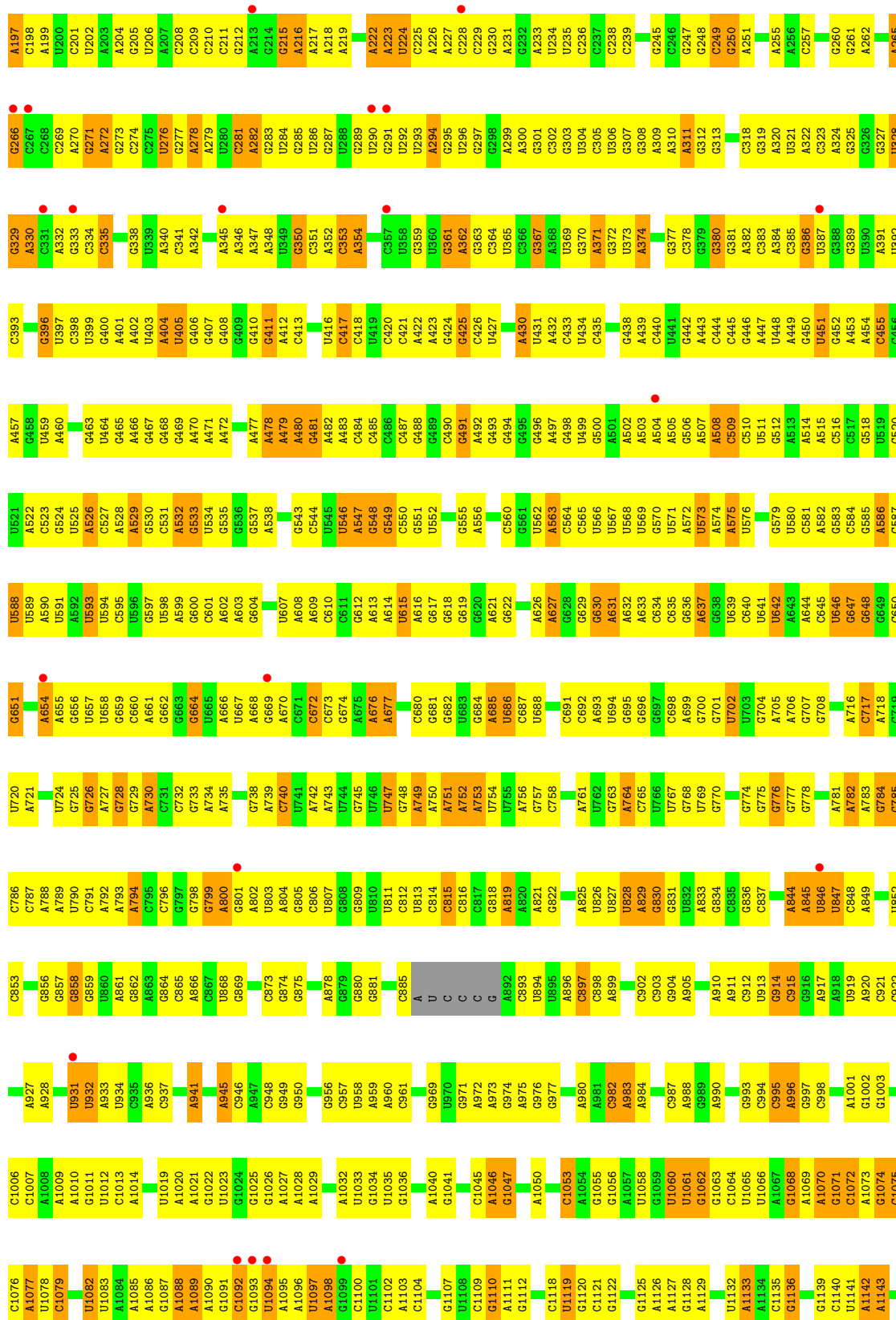
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G1187	U1188	U1119	A988	G989	C915	U839	U762	U683	G612	A541	G481	U403	A322	G242	U158
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U1188	U1188	C1121	A990	A990	A917	G841	A765	A686	U615	C543	A483	U405	A324	A244	A160
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G1192	G1192	A1126	U1065	C994	C921	U846	G769	C692	G619	A548	G487	A330	C164		C164
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G1195	G1195		C998	C997	G924	A849		G695	G622			A415	G333	A255	A167
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G1197	G1197		A1000		A928	C853	G776	G697	C624	A556	A492	C417	C335	C257	
U1198	U1198	A1134	A1001			C854	G778	C698		A557	G493	C418	C336		G178
U1199	U1199	G1135	G1002		U831	G855	G779	A699	A627	C557	G494	U419	C337	G261	
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C1208	C1208	A1142	A1080			A861	G785	A716	C635		G500		A345	G187	G188
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G1238	G1238	C1170	U1033		A973			G745	A661		G525		G375	A299	
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A1244	A1244	U1176			A979	U906	U826	A753	U667		C531			A309	A226
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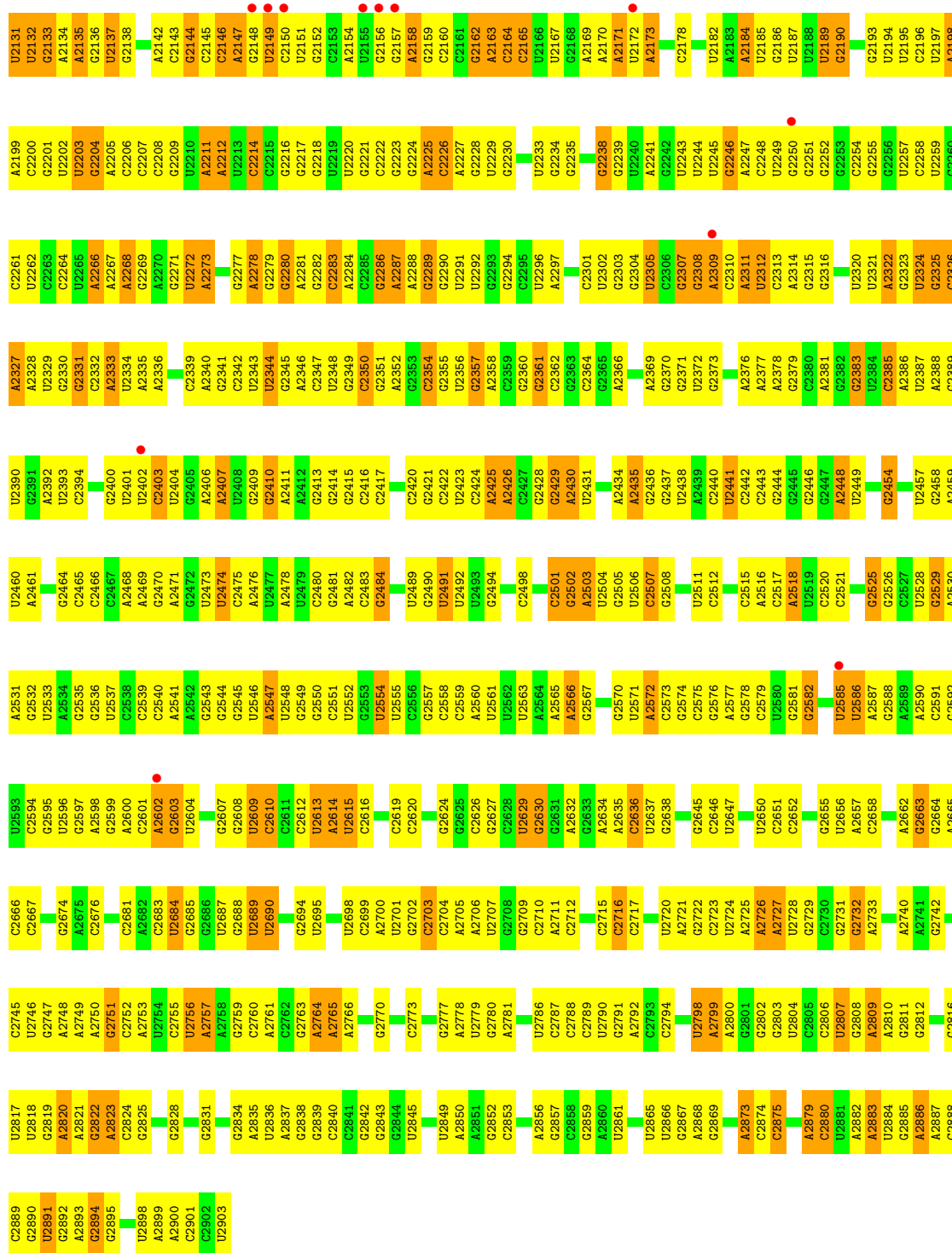


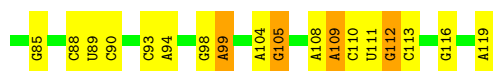
• Molecule 22: 23S rRNA



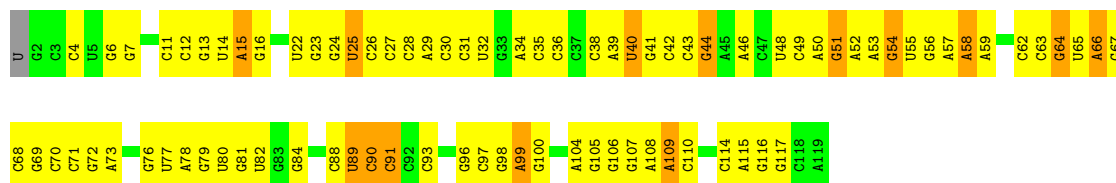


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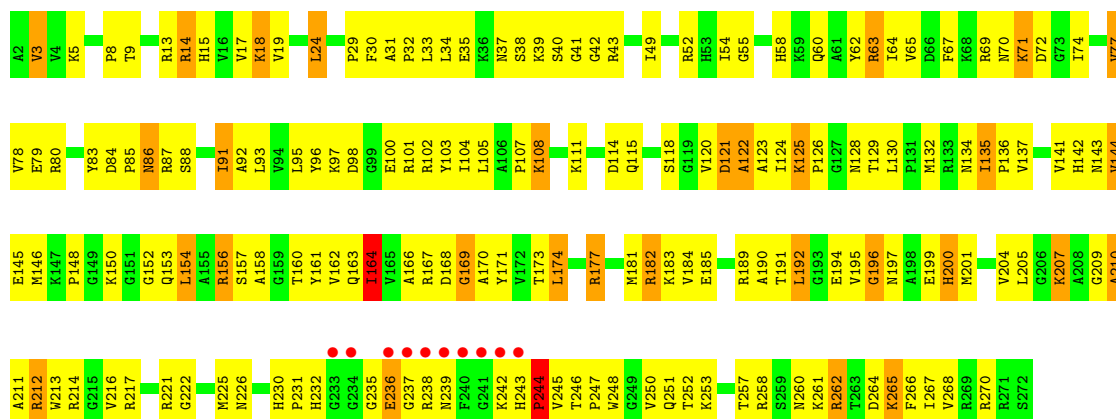




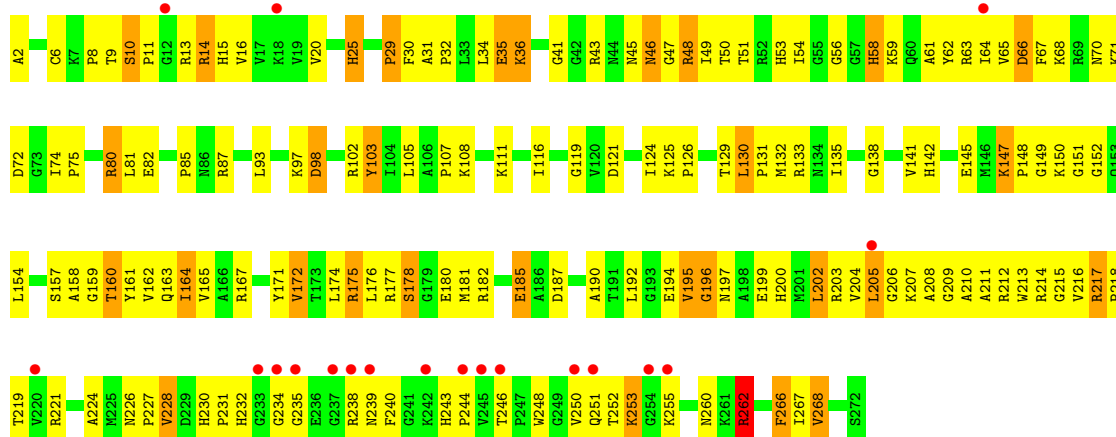
• Molecule 23: 5S rRNA



• Molecule 24: 50S ribosomal protein L2



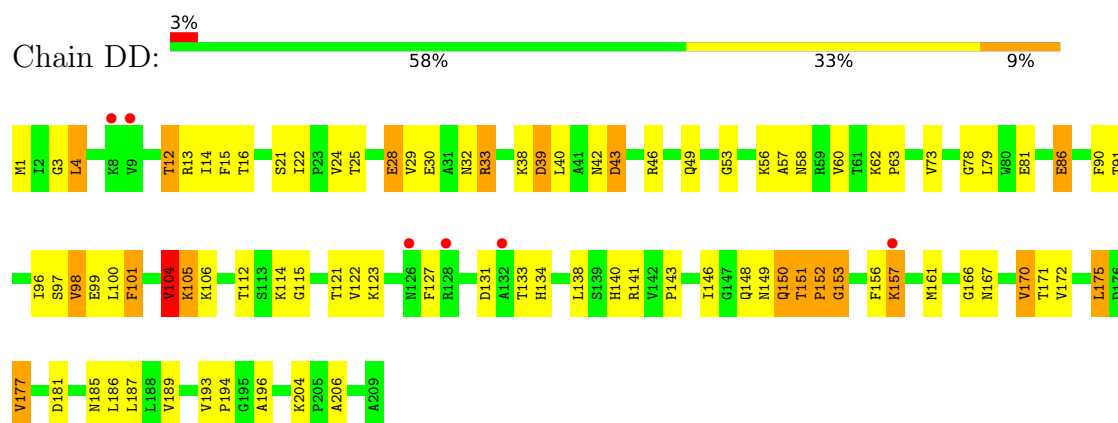
• Molecule 24: 50S ribosomal protein L2



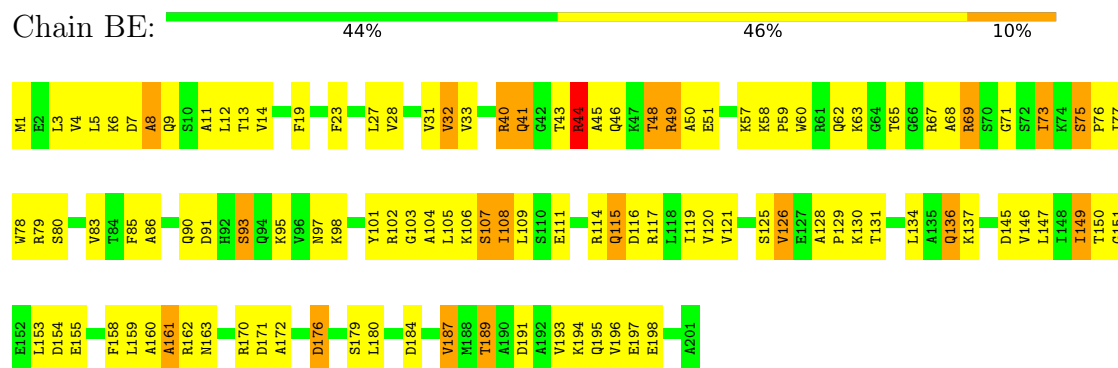
• Molecule 25: 50S ribosomal protein L3



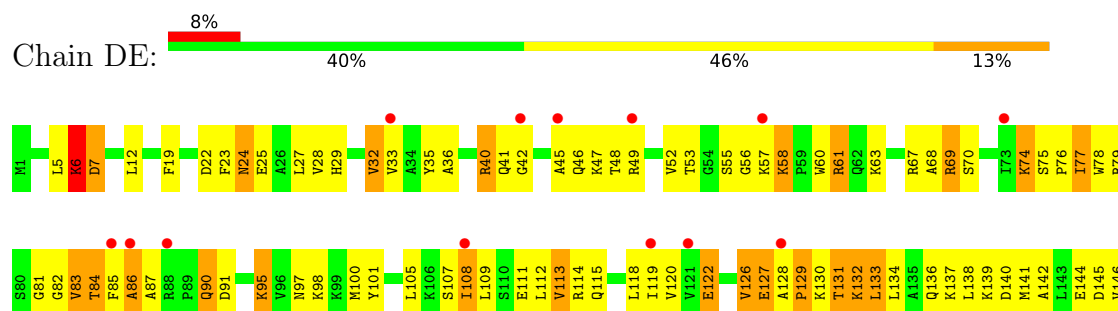
• Molecule 25: 50S ribosomal protein L3

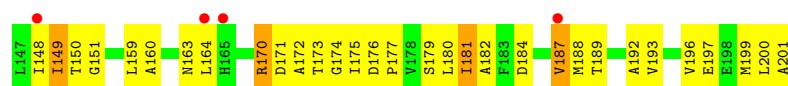


• Molecule 26: 50S ribosomal protein L4

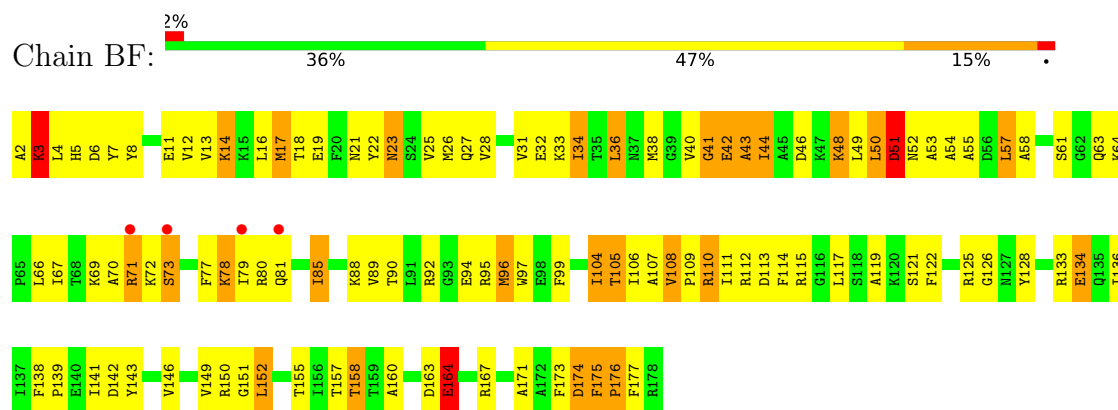


• Molecule 26: 50S ribosomal protein L4

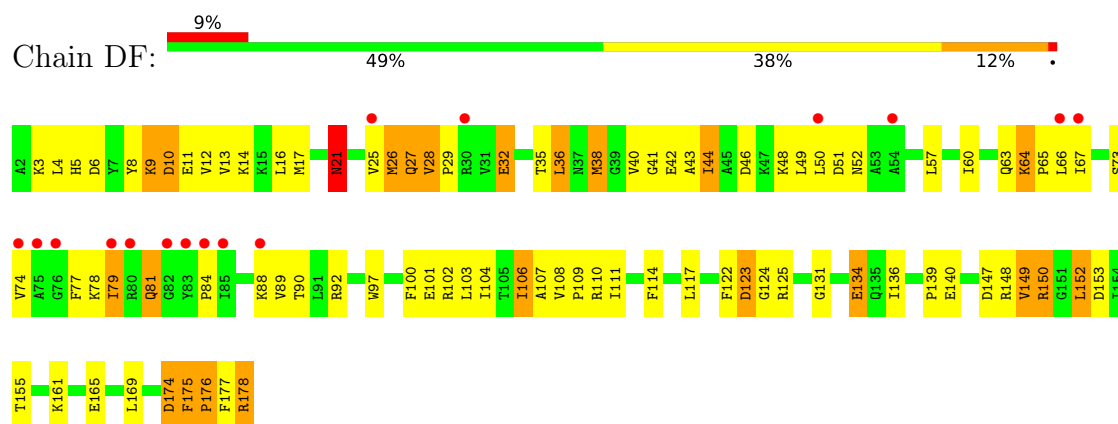




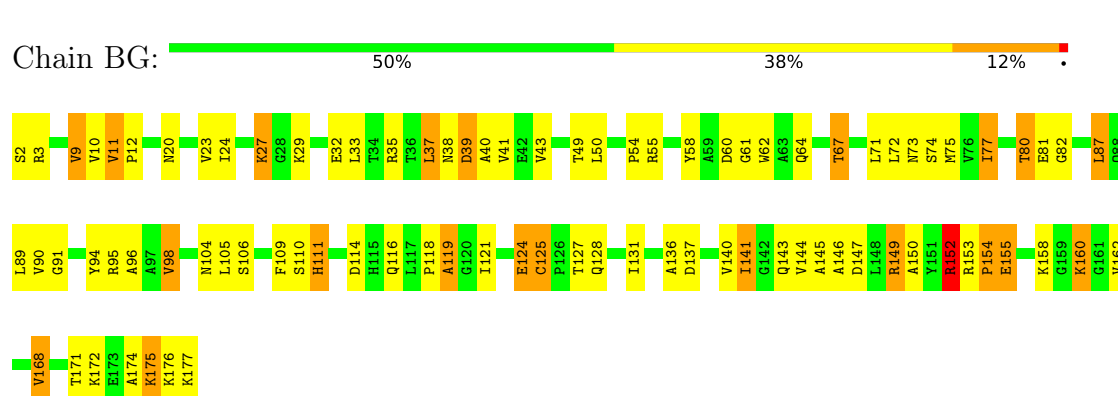
- Molecule 27: 50S ribosomal protein L5



- Molecule 27: 50S ribosomal protein L5

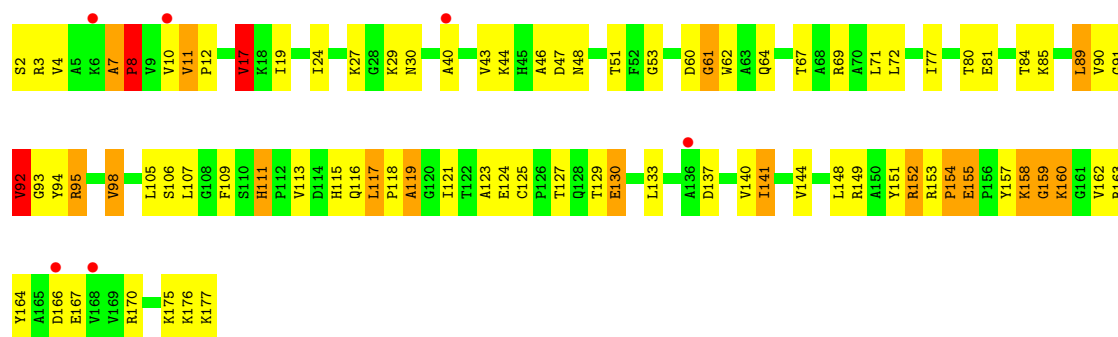


- Molecule 28: 50S ribosomal protein L6

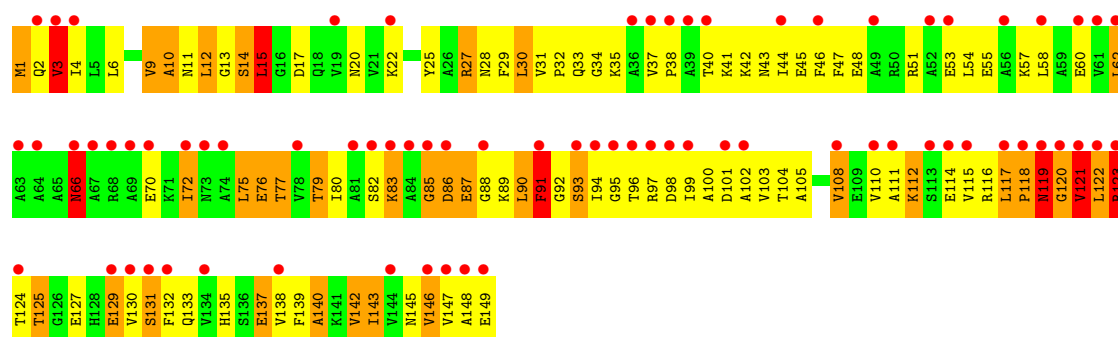


- Molecule 28: 50S ribosomal protein L6

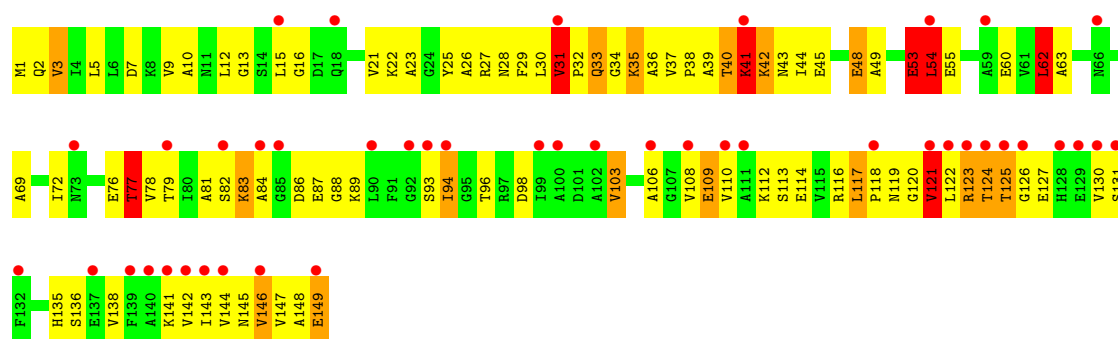




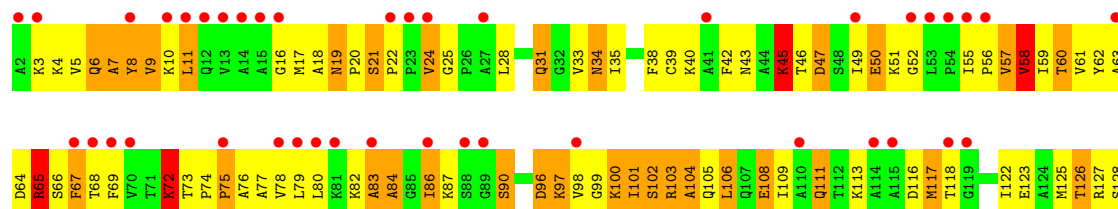
• Molecule 29: 50S ribosomal protein L9



• Molecule 29: 50S ribosomal protein L9

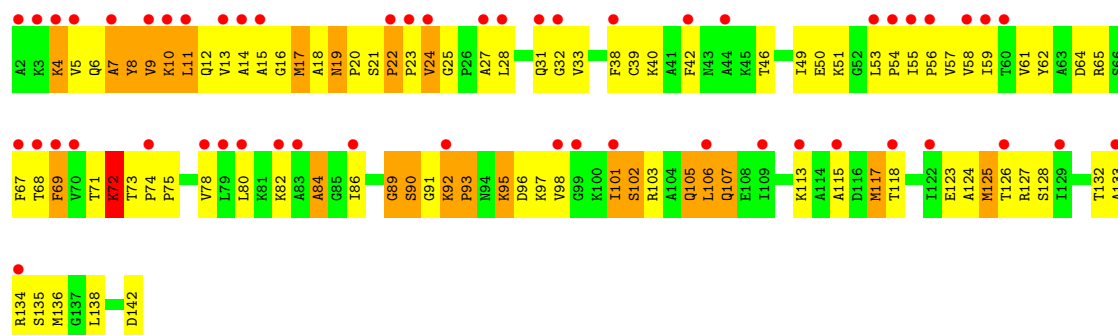


• Molecule 30: 50S ribosomal protein L11

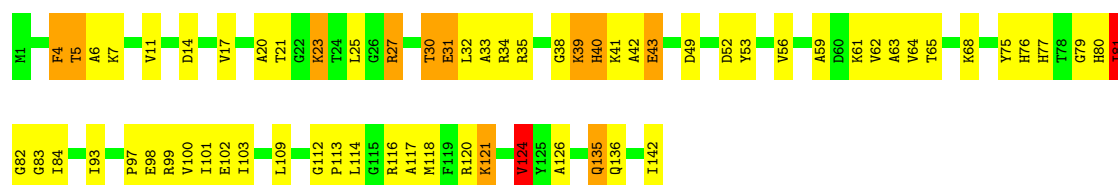




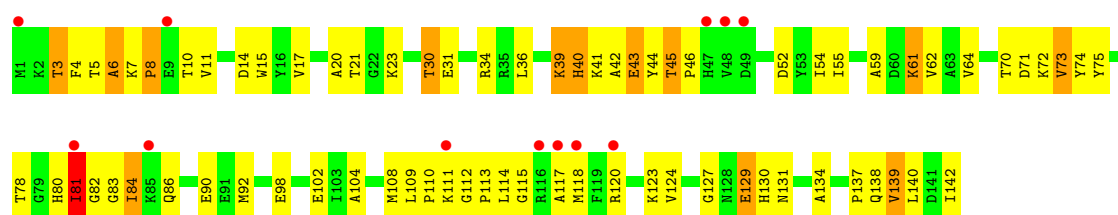
• Molecule 30: 50S ribosomal protein L11



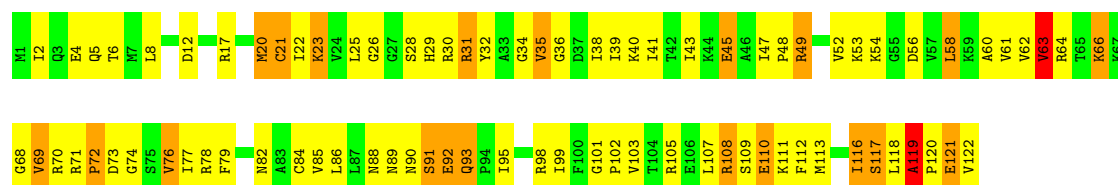
• Molecule 31: 50S ribosomal protein L13



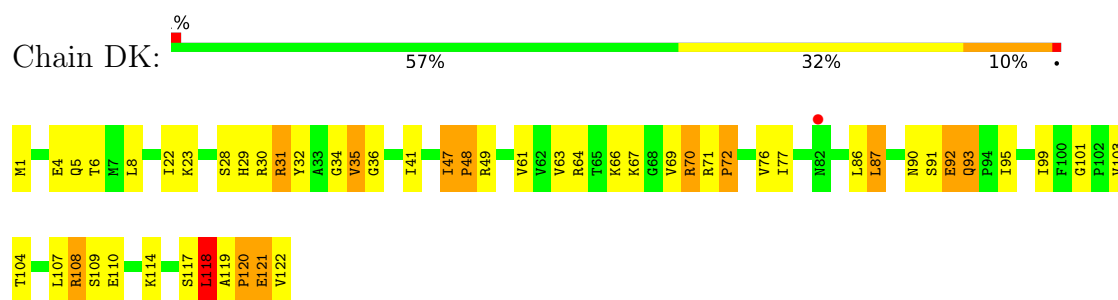
• Molecule 31: 50S ribosomal protein L13



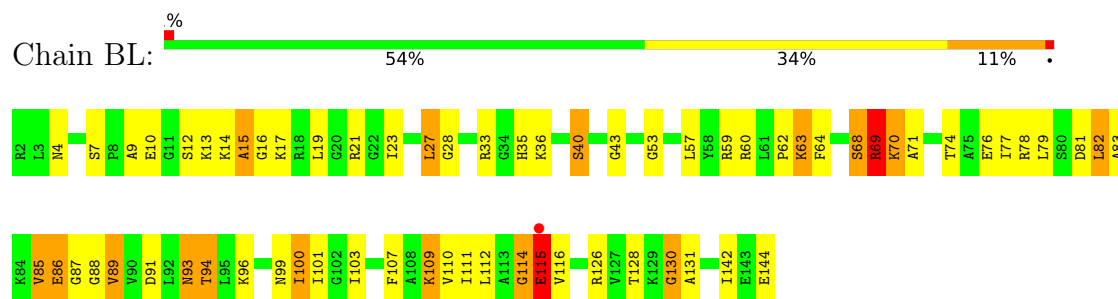
• Molecule 32: 50S ribosomal protein L14



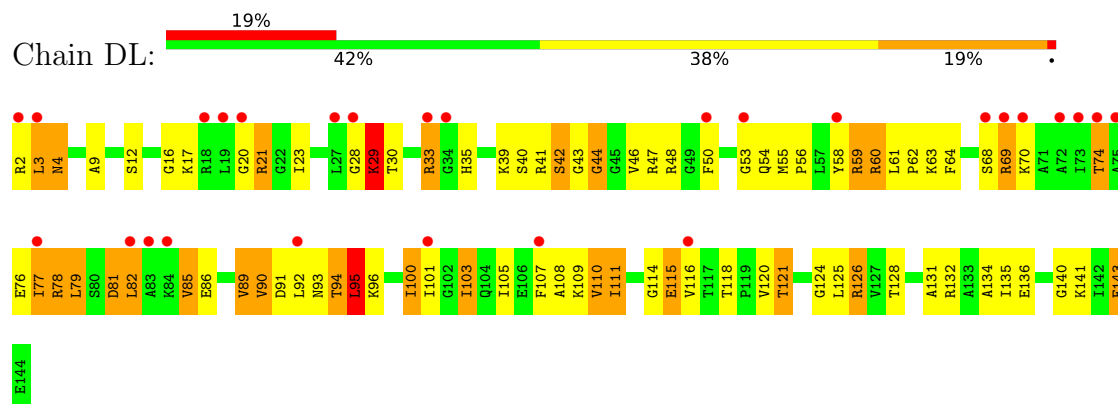
• Molecule 32: 50S ribosomal protein L14



- Molecule 33: 50S ribosomal protein L15



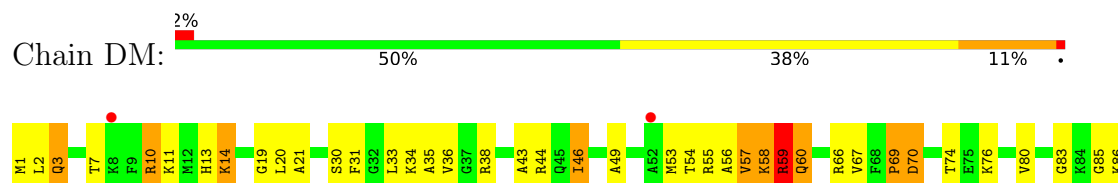
- Molecule 33: 50S ribosomal protein L15

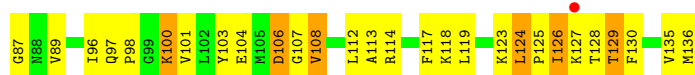


- Molecule 34: 50S ribosomal protein L16

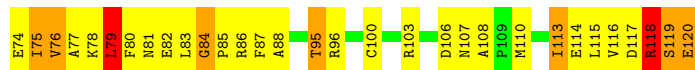


- Molecule 34: 50S ribosomal protein L16

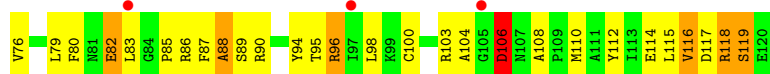
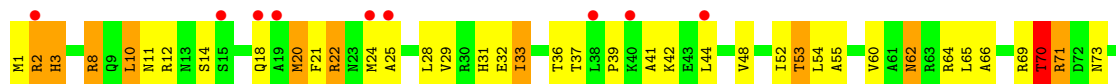




- Molecule 35: 50S ribosomal protein L17



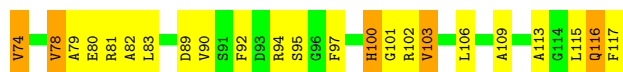
- Molecule 35: 50S ribosomal protein L17



- Molecule 36: 50S ribosomal protein L18

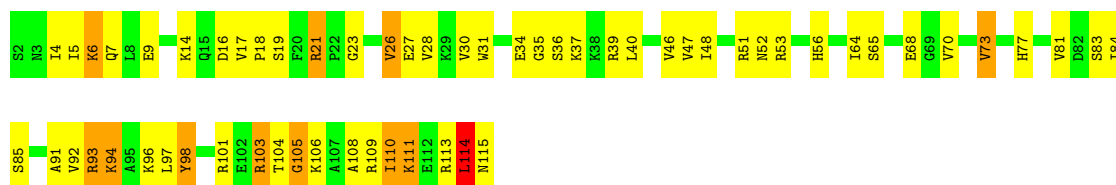


- Molecule 36: 50S ribosomal protein L18



- Molecule 37: 50S ribosomal protein L19

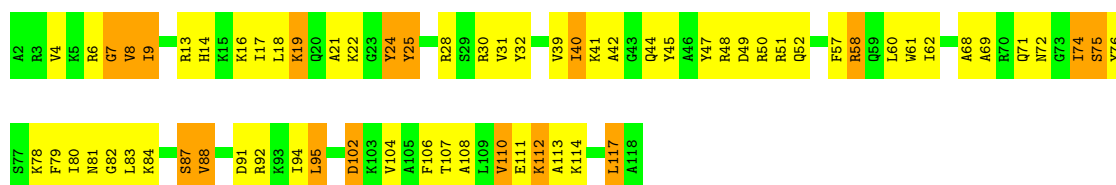




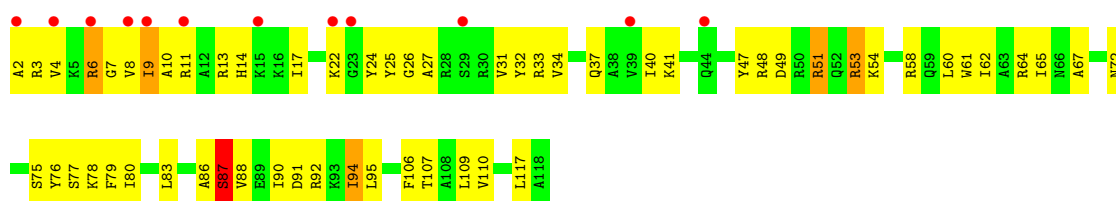
- Molecule 37: 50S ribosomal protein L19



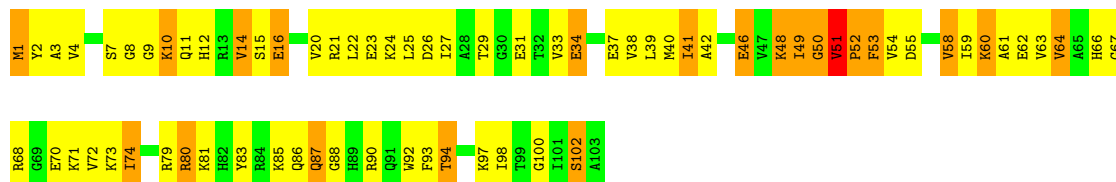
- Molecule 38: 50S ribosomal protein L20



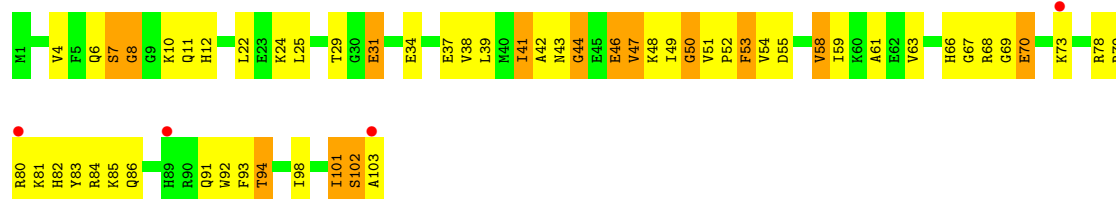
- Molecule 38: 50S ribosomal protein L20



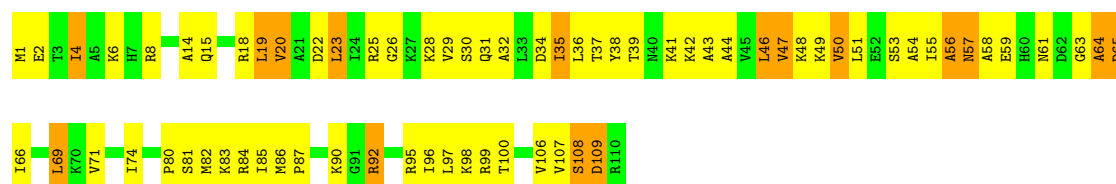
- Molecule 39: 50S ribosomal protein L21



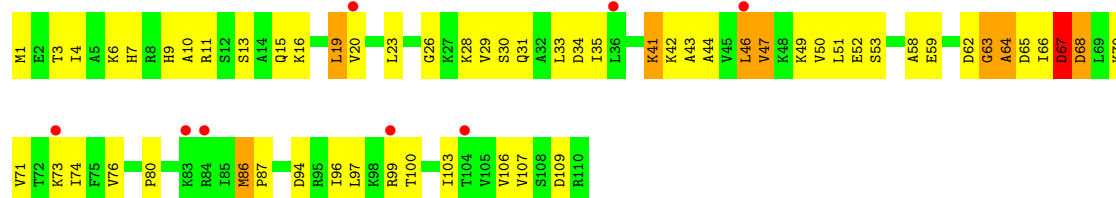
- Molecule 39: 50S ribosomal protein L21



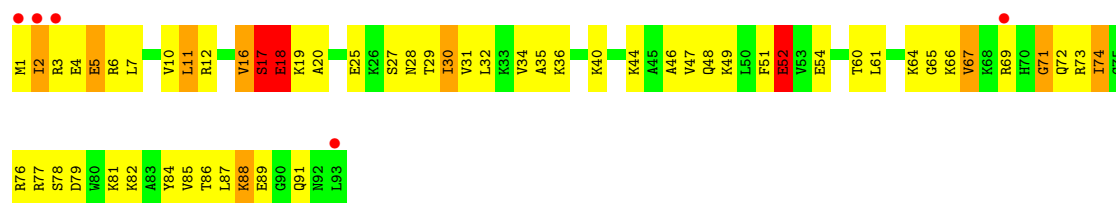
- Molecule 40: 50S ribosomal protein L22



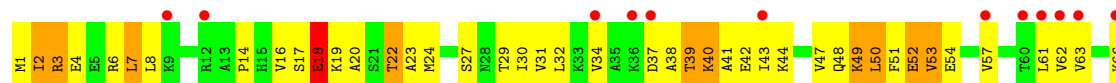
- Molecule 40: 50S ribosomal protein L22



- Molecule 41: 50S ribosomal protein L23

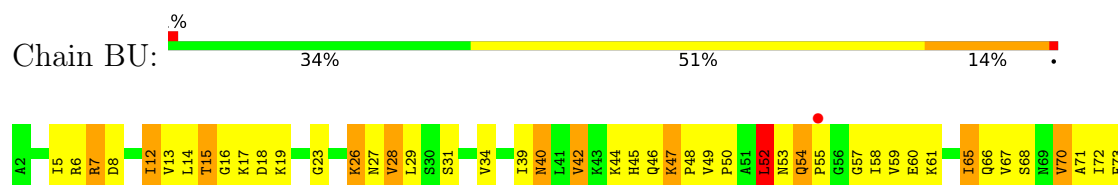


- Molecule 41: 50S ribosomal protein L23

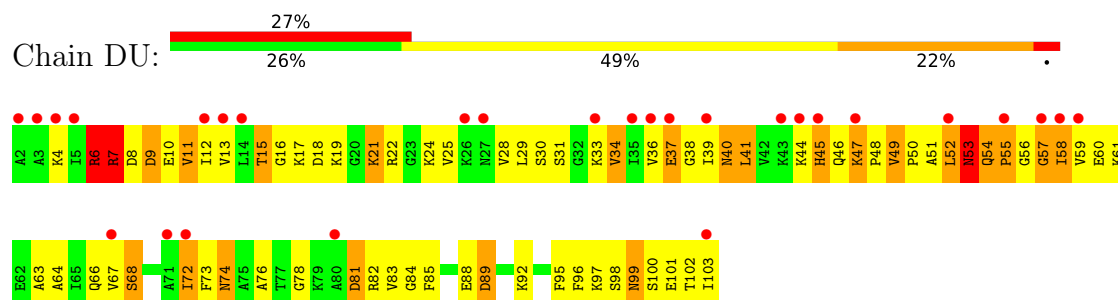




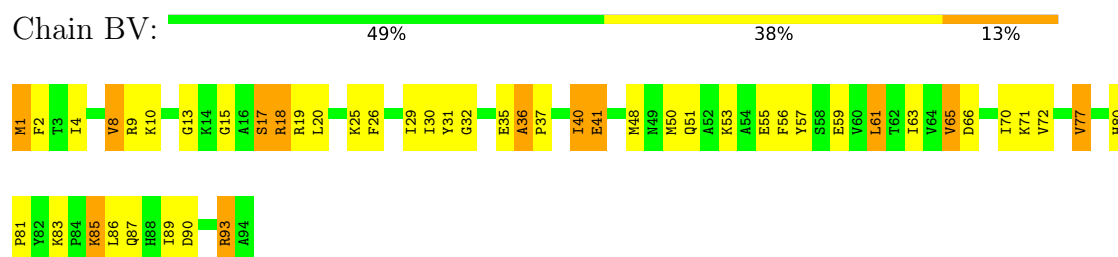
- Molecule 42: 50S ribosomal protein L24



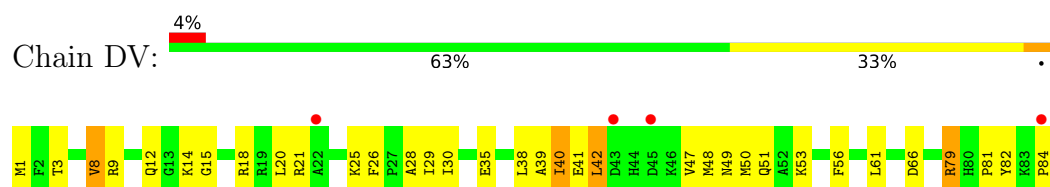
- Molecule 42: 50S ribosomal protein L24



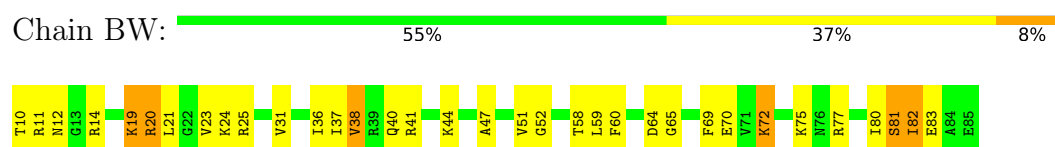
- Molecule 43: 50S ribosomal protein L25



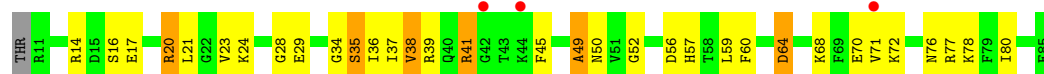
- Molecule 43: 50S ribosomal protein L25



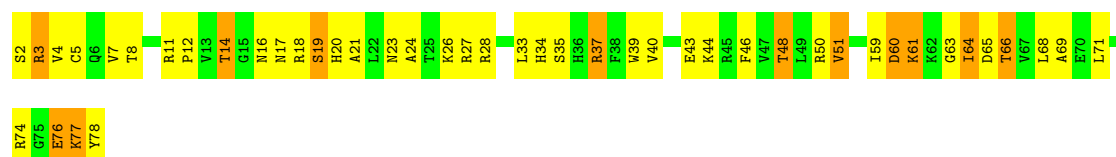
- Molecule 44: 50S ribosomal protein L27



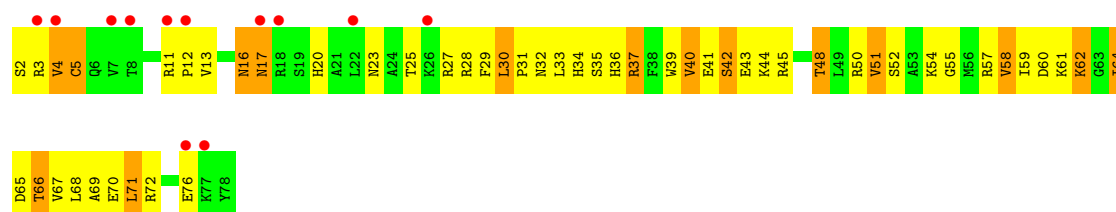
- Molecule 44: 50S ribosomal protein L27



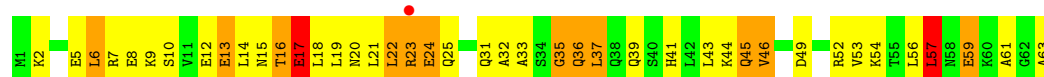
- Molecule 45: 50S ribosomal protein L28



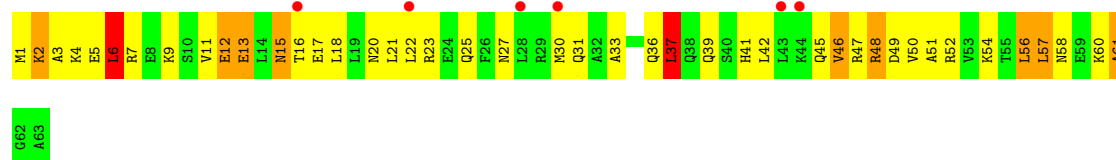
- Molecule 45: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L29



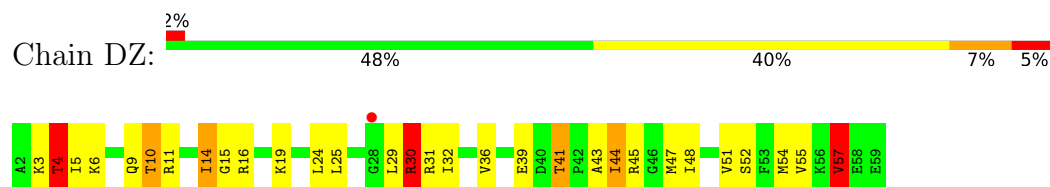
- Molecule 46: 50S ribosomal protein L29



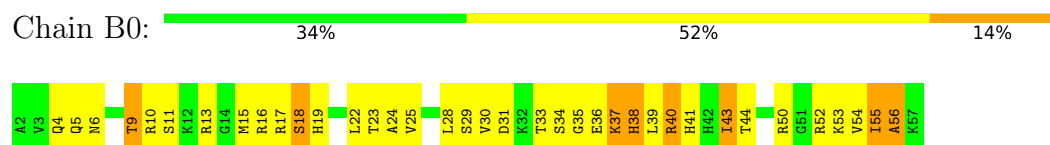
- Molecule 47: 50S ribosomal protein L30



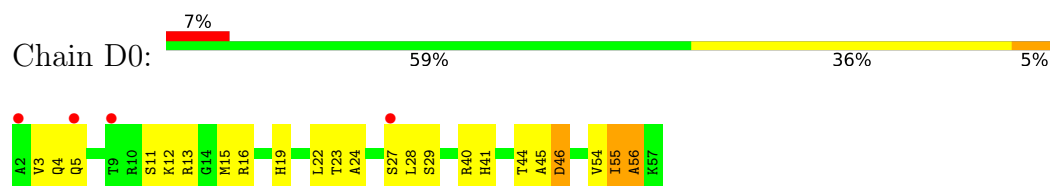
• Molecule 47: 50S ribosomal protein L30



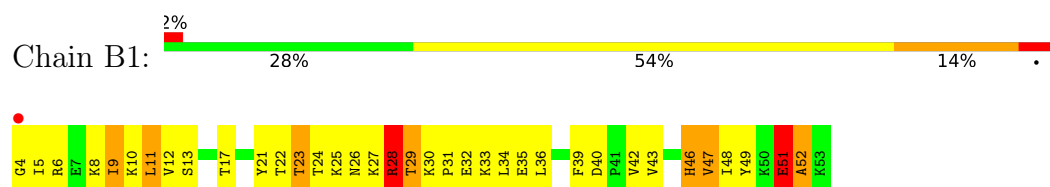
• Molecule 48: 50S ribosomal protein L32



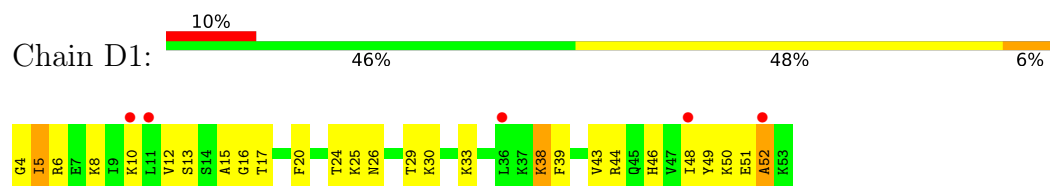
• Molecule 48: 50S ribosomal protein L32



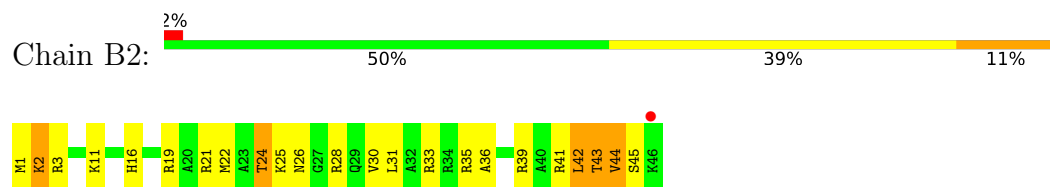
• Molecule 49: 50S ribosomal protein L33



• Molecule 49: 50S ribosomal protein L33

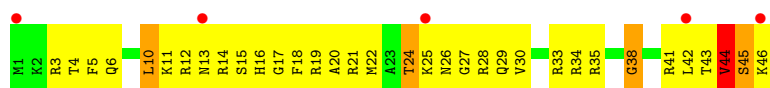


• Molecule 50: 50S ribosomal protein L34



• Molecule 50: 50S ribosomal protein L34





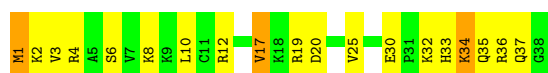
- Molecule 51: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L35



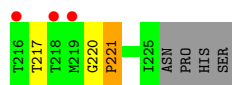
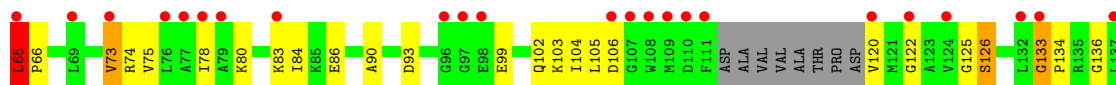
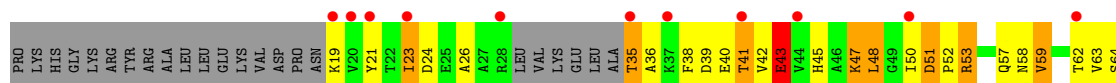
- Molecule 52: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L1



- Molecule 54: Linopristin

Chain B6:  43% 57%



- Molecule 54: Linopristin

Chain D6:  14% 71% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.225 , 0.274 0.226 , 0.275	Depositor DCC
R_{free} test set	4092 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	288320	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DBB, 04X, MHW, MG, 004, ZN, 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	0.29	0/36944	0.51	0/57632
1	CA	0.25	0/36966	0.46	0/57666
2	AB	0.57	0/1736	0.95	3/2338 (0.1%)
2	CB	0.55	1/1736 (0.1%)	0.93	3/2338 (0.1%)
3	AC	0.51	0/1652	0.91	3/2225 (0.1%)
3	CC	0.49	0/1652	0.84	1/2225 (0.0%)
4	AD	0.45	0/1665	0.91	4/2227 (0.2%)
4	CD	0.55	0/1665	0.93	2/2227 (0.1%)
5	AE	0.54	0/1119	1.00	5/1504 (0.3%)
5	CE	0.54	0/1119	1.06	6/1504 (0.4%)
6	AF	0.55	0/836	0.97	2/1128 (0.2%)
6	CF	0.48	0/836	0.89	1/1128 (0.1%)
7	AG	0.48	0/1196	0.94	4/1602 (0.2%)
7	CG	0.52	0/1196	0.87	2/1602 (0.1%)
8	AH	0.51	0/989	0.96	4/1326 (0.3%)
8	CH	0.41	0/989	0.87	1/1326 (0.1%)
9	AI	0.48	0/1034	0.90	1/1375 (0.1%)
9	CI	0.47	0/1034	0.85	1/1375 (0.1%)
10	AJ	0.53	0/797	0.86	0/1077
10	CJ	0.54	0/797	0.88	1/1077 (0.1%)
11	AK	0.53	0/893	0.92	1/1205 (0.1%)
11	CK	0.47	0/893	0.98	8/1205 (0.7%)
12	AL	0.52	0/969	0.97	2/1300 (0.2%)
12	CL	0.52	0/969	1.01	4/1300 (0.3%)
13	AM	0.54	0/893	0.93	0/1193
13	CM	0.57	0/893	0.92	2/1193 (0.2%)
14	AN	0.49	0/785	0.94	3/1043 (0.3%)
14	CN	0.43	0/785	0.85	2/1043 (0.2%)
15	AO	0.43	0/718	0.84	1/959 (0.1%)
15	CO	0.40	0/718	0.86	1/959 (0.1%)
16	AP	0.53	0/659	0.92	2/884 (0.2%)
16	CP	0.44	0/659	0.80	1/884 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.50	0/658	0.89	0/881
17	CQ	0.51	0/658	0.84	0/881
18	AR	0.47	0/463	0.91	0/621
18	CR	0.50	0/463	0.91	3/621 (0.5%)
19	AS	0.58	0/653	1.05	5/877 (0.6%)
19	CS	0.56	0/653	0.94	5/877 (0.6%)
20	AT	0.54	0/671	0.95	2/888 (0.2%)
20	CT	0.44	0/671	0.91	2/888 (0.2%)
21	AU	0.61	0/431	0.98	3/570 (0.5%)
21	CU	0.55	0/431	0.88	0/570
22	BA	0.48	0/69659	0.67	1/108672 (0.0%)
22	DA	0.25	0/69659	0.44	0/108672
23	BB	0.42	0/2850	0.63	0/4444
23	DB	0.21	0/2828	0.37	0/4410
24	BC	0.69	0/2122	1.09	11/2852 (0.4%)
24	DC	0.46	0/2122	0.89	3/2852 (0.1%)
25	BD	0.81	0/1586	1.12	4/2134 (0.2%)
25	DD	0.46	0/1586	0.81	1/2134 (0.0%)
26	BE	0.72	0/1571	1.02	4/2113 (0.2%)
26	DE	0.52	0/1571	0.88	0/2113
27	BF	0.55	0/1435	0.92	2/1926 (0.1%)
27	DF	0.51	0/1435	0.87	2/1926 (0.1%)
28	BG	0.57	0/1343	1.03	4/1816 (0.2%)
28	DG	0.47	0/1343	0.87	5/1816 (0.3%)
29	BH	0.48	0/1121	0.99	5/1515 (0.3%)
29	DH	0.47	0/1121	0.92	5/1515 (0.3%)
30	BI	0.66	0/1046	0.99	6/1410 (0.4%)
30	DI	0.66	0/1046	0.98	4/1410 (0.3%)
31	BJ	0.85	0/1152	1.15	6/1551 (0.4%)
31	DJ	0.46	0/1152	0.89	2/1551 (0.1%)
32	BK	0.75	0/948	1.14	6/1268 (0.5%)
32	DK	0.45	0/948	0.88	2/1268 (0.2%)
33	BL	0.69	0/1054	1.12	6/1403 (0.4%)
33	DL	0.51	0/1054	0.96	2/1403 (0.1%)
34	BM	0.78	0/1093	1.07	5/1460 (0.3%)
34	DM	0.42	0/1093	0.86	0/1460
35	BN	0.81	0/974	1.19	6/1301 (0.5%)
35	DN	0.44	0/974	0.83	0/1301
36	BO	0.66	0/902	0.99	3/1209 (0.2%)
36	DO	0.45	0/902	0.87	1/1209 (0.1%)
37	BP	0.67	0/929	1.04	4/1242 (0.3%)
37	DP	0.45	0/929	0.83	1/1242 (0.1%)
38	BQ	0.87	0/960	1.13	3/1278 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.45	0/960	0.84	1/1278 (0.1%)
39	BR	0.83	0/829	1.26	5/1107 (0.5%)
39	DR	0.44	0/829	0.84	1/1107 (0.1%)
40	BS	0.95	0/864	1.01	1/1156 (0.1%)
40	DS	0.50	0/864	0.87	0/1156
41	BT	0.61	0/745	0.95	1/994 (0.1%)
41	DT	0.50	0/745	0.82	0/994
42	BU	0.62	0/788	1.07	4/1051 (0.4%)
42	DU	0.64	0/788	0.97	2/1051 (0.2%)
43	BV	0.63	0/766	1.01	2/1025 (0.2%)
43	DV	0.40	0/766	0.78	0/1025
44	BW	0.78	0/587	1.05	0/776
44	DW	0.41	0/576	0.79	0/762
45	BX	0.60	0/635	1.02	1/848 (0.1%)
45	DX	0.46	0/635	0.88	2/848 (0.2%)
46	BY	0.58	0/510	0.97	2/677 (0.3%)
46	DY	0.48	0/510	0.86	0/677
47	BZ	0.86	0/453	1.09	2/605 (0.3%)
47	DZ	0.43	0/453	0.84	1/605 (0.2%)
48	B0	0.85	0/450	1.13	2/599 (0.3%)
48	D0	0.47	0/450	0.80	1/599 (0.2%)
49	B1	0.56	0/417	0.94	0/554
49	D1	0.47	0/417	0.71	0/554
50	B2	0.76	0/380	1.11	2/498 (0.4%)
50	D2	0.46	0/380	0.85	0/498
51	B3	0.74	0/513	1.03	0/676
51	D3	0.42	0/513	0.81	0/676
52	B4	0.74	0/303	0.98	0/397
52	D4	0.41	0/303	0.82	0/397
53	B5	0.63	0/1145	1.18	13/1556 (0.8%)
54	B6	3.99	4/13 (30.8%)	4.63	7/15 (46.7%)
54	D6	4.18	3/13 (23.1%)	4.30	5/15 (33.3%)
All	All	0.43	8/310652 (0.0%)	0.68	250/464396 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D6	2	THR	CB-OG1	-7.98	1.30	1.43
54	D6	4	PRO	N-CD	-7.02	1.38	1.47
54	B6	4	PRO	N-CA	-6.83	1.36	1.47
54	B6	2	THR	CB-OG1	-6.81	1.32	1.43
2	CB	20	THR	CA-C	6.50	1.55	1.52

The worst 5 of 250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	BR	51	VAL	CA-C-N	-10.92	106.19	119.84
39	BR	51	VAL	C-N-CA	-10.92	106.19	119.84
53	B5	220	GLY	CA-C-N	10.40	132.84	119.84
53	B5	220	GLY	C-N-CA	10.40	132.84	119.84
53	B5	182	PRO	CA-C-N	10.02	132.36	119.84

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	1349	4
1	CA	33015	0	16617	1202	0
2	AB	1705	0	1732	181	0
2	CB	1705	0	1732	130	0
3	AC	1625	0	1696	92	0
3	CC	1625	0	1696	84	0
4	AD	1643	0	1707	151	0
4	CD	1643	0	1707	156	0
5	AE	1106	0	1148	88	0
5	CE	1106	0	1148	115	0
6	AF	818	0	808	69	0
6	CF	818	0	808	61	0
7	AG	1182	0	1238	77	0
7	CG	1182	0	1238	62	0
8	AH	979	0	1031	75	0
8	CH	979	0	1031	59	0
9	AI	1022	0	1070	85	0
9	CI	1022	0	1070	75	0
10	AJ	787	0	828	88	0
10	CJ	787	0	828	48	0
11	AK	877	0	887	82	0
11	CK	877	0	887	80	0
12	AL	955	0	1016	67	0
12	CL	955	0	1016	63	0
13	AM	884	0	941	85	0
13	CM	884	0	941	52	0
14	AN	774	0	824	72	0
14	CN	774	0	824	46	0
15	AO	710	0	728	39	0
15	CO	710	0	728	46	0
16	AP	649	0	666	56	0
16	CP	649	0	666	33	0
17	AQ	649	0	691	75	0
17	CQ	649	0	691	51	0
18	AR	456	0	478	24	0
18	CR	456	0	478	25	0
19	AS	638	0	665	49	0
19	CS	638	0	665	39	0
20	AT	665	0	714	57	0
20	CT	665	0	714	41	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	38	0
22	BA	62195	0	31280	2148	0
22	DA	62195	0	31280	2172	0
23	BB	2549	0	1291	56	0
23	DB	2529	0	1281	73	0
24	BC	2083	0	2154	166	0
24	DC	2083	0	2154	128	0
25	BD	1565	0	1616	103	0
25	DD	1565	0	1616	84	0
26	BE	1552	0	1619	80	0
26	DE	1552	0	1619	108	0
27	BF	1411	0	1444	111	0
27	DF	1411	0	1444	65	0
28	BG	1323	0	1371	69	0
28	DG	1323	0	1371	58	0
29	BH	1110	0	1147	161	0
29	DH	1110	0	1148	96	4
30	BI	1032	0	1085	94	0
30	DI	1032	0	1085	74	0
31	BJ	1129	0	1162	68	0
31	DJ	1129	0	1162	61	0
32	BK	939	0	1012	80	0
32	DK	939	0	1012	41	0
33	BL	1045	0	1117	52	0
33	DL	1045	0	1117	84	0
34	BM	1074	0	1157	56	0
34	DM	1074	0	1157	50	0
35	BN	961	0	1000	63	0
35	DN	961	0	1000	59	0
36	BO	892	0	923	61	0
36	DO	892	0	923	50	0
37	BP	917	0	962	49	0
37	DP	917	0	962	49	0
38	BQ	947	0	1019	69	0
38	DQ	947	0	1019	55	0
39	BR	816	0	839	89	0
39	DR	816	0	839	52	0
40	BS	857	0	922	71	0
40	DS	857	0	922	42	0
41	BT	739	0	807	48	0
41	DT	739	0	807	45	0
42	BU	780	0	831	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DU	780	0	831	69	0
43	BV	753	0	780	35	0
43	DV	753	0	780	28	0
44	BW	580	0	594	23	0
44	DW	569	0	581	25	0
45	BX	625	0	652	38	0
45	DX	625	0	652	60	0
46	BY	509	0	543	35	0
46	DY	509	0	543	42	0
47	BZ	449	0	488	20	0
47	DZ	449	0	488	15	0
48	B0	444	0	458	33	0
48	D0	444	0	458	18	0
49	B1	410	0	440	33	0
49	D1	410	0	440	20	0
50	B2	377	0	418	21	0
50	D2	377	0	418	35	0
51	B3	504	0	572	22	0
51	D3	504	0	572	29	0
52	B4	302	0	340	13	0
52	D4	302	0	342	16	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	1	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	12207	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 26.

The worst 5 of 12207 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	0
3	AC	204/206 (99%)	142 (70%)	42 (21%)	20 (10%)	0	2
3	CC	204/206 (99%)	145 (71%)	41 (20%)	18 (9%)	0	3
4	AD	203/205 (99%)	133 (66%)	36 (18%)	34 (17%)	0	0
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	1
5	CE	148/150 (99%)	96 (65%)	29 (20%)	23 (16%)	0	0
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	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	110 (74%)	27 (18%)	12 (8%)	1	3
7	CG	149/151 (99%)	120 (80%)	21 (14%)	8 (5%)	1	9
8	AH	127/129 (98%)	80 (63%)	29 (23%)	18 (14%)	0	1
8	CH	127/129 (98%)	100 (79%)	19 (15%)	8 (6%)	1	6
9	AI	125/127 (98%)	90 (72%)	24 (19%)	11 (9%)	0	3
9	CI	125/127 (98%)	89 (71%)	27 (22%)	9 (7%)	1	4
10	AJ	96/98 (98%)	68 (71%)	7 (7%)	21 (22%)	0	0
10	CJ	96/98 (98%)	69 (72%)	18 (19%)	9 (9%)	0	2
11	AK	115/117 (98%)	83 (72%)	17 (15%)	15 (13%)	0	1
11	CK	115/117 (98%)	77 (67%)	28 (24%)	10 (9%)	0	3
12	AL	121/123 (98%)	92 (76%)	19 (16%)	10 (8%)	0	3
12	CL	121/123 (98%)	89 (74%)	17 (14%)	15 (12%)	0	1
13	AM	112/114 (98%)	79 (70%)	22 (20%)	11 (10%)	0	2
13	CM	112/114 (98%)	86 (77%)	15 (13%)	11 (10%)	0	2
14	AN	92/100 (92%)	57 (62%)	20 (22%)	15 (16%)	0	0
14	CN	92/100 (92%)	59 (64%)	20 (22%)	13 (14%)	0	1
15	AO	86/88 (98%)	60 (70%)	21 (24%)	5 (6%)	1	8
15	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	3	16
16	AP	80/82 (98%)	52 (65%)	16 (20%)	12 (15%)	0	0
16	CP	80/82 (98%)	54 (68%)	20 (25%)	6 (8%)	1	4
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%)	6	30
18	CR	53/55 (96%)	45 (85%)	4 (8%)	4 (8%)	1	4
19	AS	77/79 (98%)	52 (68%)	19 (25%)	6 (8%)	1	4
19	CS	77/79 (98%)	59 (77%)	14 (18%)	4 (5%)	1	9
20	AT	83/85 (98%)	51 (61%)	23 (28%)	9 (11%)	0	1
20	CT	83/85 (98%)	66 (80%)	11 (13%)	6 (7%)	1	4
21	AU	49/51 (96%)	23 (47%)	18 (37%)	8 (16%)	0	0
21	CU	49/51 (96%)	25 (51%)	10 (20%)	14 (29%)	0	0
24	BC	269/271 (99%)	208 (77%)	49 (18%)	12 (4%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	DC	269/271 (99%)	206 (77%)	42 (16%)	21 (8%)	1	4
25	BD	207/209 (99%)	176 (85%)	22 (11%)	9 (4%)	2	12
25	DD	207/209 (99%)	175 (84%)	24 (12%)	8 (4%)	2	14
26	BE	199/201 (99%)	164 (82%)	26 (13%)	9 (4%)	2	12
26	DE	199/201 (99%)	160 (80%)	27 (14%)	12 (6%)	1	7
27	BF	175/177 (99%)	136 (78%)	24 (14%)	15 (9%)	0	3
27	DF	175/177 (99%)	141 (81%)	23 (13%)	11 (6%)	1	6
28	BG	174/176 (99%)	146 (84%)	20 (12%)	8 (5%)	2	11
28	DG	174/176 (99%)	132 (76%)	33 (19%)	9 (5%)	1	9
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	1
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	0	2
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%)	5	27
31	DJ	140/142 (99%)	116 (83%)	18 (13%)	6 (4%)	2	12
32	BK	120/122 (98%)	94 (78%)	15 (12%)	11 (9%)	0	2
32	DK	120/122 (98%)	96 (80%)	14 (12%)	10 (8%)	0	3
33	BL	141/143 (99%)	108 (77%)	23 (16%)	10 (7%)	1	4
33	DL	141/143 (99%)	104 (74%)	28 (20%)	9 (6%)	1	6
34	BM	134/136 (98%)	114 (85%)	16 (12%)	4 (3%)	3	19
34	DM	134/136 (98%)	115 (86%)	13 (10%)	6 (4%)	2	12
35	BN	118/120 (98%)	97 (82%)	18 (15%)	3 (2%)	4	23
35	DN	118/120 (98%)	94 (80%)	16 (14%)	8 (7%)	1	5
36	BO	114/116 (98%)	87 (76%)	22 (19%)	5 (4%)	2	12
36	DO	114/116 (98%)	97 (85%)	15 (13%)	2 (2%)	6	31
37	BP	112/114 (98%)	97 (87%)	10 (9%)	5 (4%)	2	12
37	DP	112/114 (98%)	86 (77%)	19 (17%)	7 (6%)	1	6
38	BQ	115/117 (98%)	96 (84%)	15 (13%)	4 (4%)	3	16
38	DQ	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	14	48
39	BR	101/103 (98%)	89 (88%)	5 (5%)	7 (7%)	1	5
39	DR	101/103 (98%)	77 (76%)	17 (17%)	7 (7%)	1	5

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

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%)	121 (67%)	59 (33%)	0	1
2	CB	180/180 (100%)	128 (71%)	52 (29%)	0	2
3	AC	170/170 (100%)	134 (79%)	36 (21%)	1	6
3	CC	170/170 (100%)	127 (75%)	43 (25%)	0	3
4	AD	172/172 (100%)	123 (72%)	49 (28%)	0	2
4	CD	172/172 (100%)	138 (80%)	34 (20%)	1	8
5	AE	113/113 (100%)	77 (68%)	36 (32%)	0	1
5	CE	113/113 (100%)	82 (73%)	31 (27%)	0	2
6	AF	87/87 (100%)	59 (68%)	28 (32%)	0	1
6	CF	87/87 (100%)	58 (67%)	29 (33%)	0	1
7	AG	124/124 (100%)	85 (68%)	39 (32%)	0	1
7	CG	124/124 (100%)	88 (71%)	36 (29%)	0	2
8	AH	104/104 (100%)	77 (74%)	27 (26%)	0	3
8	CH	104/104 (100%)	73 (70%)	31 (30%)	0	2
9	AI	105/105 (100%)	74 (70%)	31 (30%)	0	2
9	CI	105/105 (100%)	71 (68%)	34 (32%)	0	1
10	AJ	86/86 (100%)	57 (66%)	29 (34%)	0	1
10	CJ	86/86 (100%)	65 (76%)	21 (24%)	1	4
11	AK	90/90 (100%)	69 (77%)	21 (23%)	1	4
11	CK	90/90 (100%)	65 (72%)	25 (28%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	103/103 (100%)	74 (72%)	29 (28%)	0	2
12	CL	103/103 (100%)	77 (75%)	26 (25%)	0	3
13	AM	92/92 (100%)	65 (71%)	27 (29%)	0	2
13	CM	92/92 (100%)	67 (73%)	25 (27%)	0	2
14	AN	79/83 (95%)	63 (80%)	16 (20%)	1	7
14	CN	79/83 (95%)	66 (84%)	13 (16%)	2	12
15	AO	75/76 (99%)	61 (81%)	14 (19%)	1	9
15	CO	75/76 (99%)	64 (85%)	11 (15%)	3	15
16	AP	65/65 (100%)	47 (72%)	18 (28%)	0	2
16	CP	65/65 (100%)	54 (83%)	11 (17%)	2	11
17	AQ	74/74 (100%)	47 (64%)	27 (36%)	0	1
17	CQ	74/74 (100%)	50 (68%)	24 (32%)	0	1
18	AR	48/48 (100%)	39 (81%)	9 (19%)	1	9
18	CR	48/48 (100%)	38 (79%)	10 (21%)	1	7
19	AS	70/70 (100%)	55 (79%)	15 (21%)	1	6
19	CS	70/70 (100%)	49 (70%)	21 (30%)	0	1
20	AT	65/65 (100%)	46 (71%)	19 (29%)	0	2
20	CT	65/65 (100%)	47 (72%)	18 (28%)	0	2
21	AU	44/44 (100%)	29 (66%)	15 (34%)	0	1
21	CU	44/44 (100%)	28 (64%)	16 (36%)	0	1
24	BC	216/216 (100%)	180 (83%)	36 (17%)	2	12
24	DC	216/216 (100%)	183 (85%)	33 (15%)	3	14
25	BD	164/164 (100%)	140 (85%)	24 (15%)	3	15
25	DD	164/164 (100%)	141 (86%)	23 (14%)	3	16
26	BE	165/165 (100%)	136 (82%)	29 (18%)	2	10
26	DE	165/165 (100%)	129 (78%)	36 (22%)	1	6
27	BF	148/148 (100%)	117 (79%)	31 (21%)	1	7
27	DF	148/148 (100%)	117 (79%)	31 (21%)	1	7
28	BG	137/137 (100%)	113 (82%)	24 (18%)	2	10
28	DG	137/137 (100%)	115 (84%)	22 (16%)	2	12
29	BH	114/114 (100%)	81 (71%)	33 (29%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DH	114/114 (100%)	89 (78%)	25 (22%)	1	5
30	BI	109/109 (100%)	77 (71%)	32 (29%)	0	2
30	DI	109/109 (100%)	84 (77%)	25 (23%)	1	5
31	BJ	116/116 (100%)	104 (90%)	12 (10%)	7	28
31	DJ	116/116 (100%)	98 (84%)	18 (16%)	2	13
32	BK	103/103 (100%)	86 (84%)	17 (16%)	2	12
32	DK	103/103 (100%)	91 (88%)	12 (12%)	5	23
33	BL	102/102 (100%)	84 (82%)	18 (18%)	2	10
33	DL	102/102 (100%)	76 (74%)	26 (26%)	0	3
34	BM	109/109 (100%)	90 (83%)	19 (17%)	2	10
34	DM	109/109 (100%)	90 (83%)	19 (17%)	2	10
35	BN	100/100 (100%)	81 (81%)	19 (19%)	1	8
35	DN	100/100 (100%)	79 (79%)	21 (21%)	1	6
36	BO	86/86 (100%)	58 (67%)	28 (33%)	0	1
36	DO	86/86 (100%)	67 (78%)	19 (22%)	1	5
37	BP	99/99 (100%)	83 (84%)	16 (16%)	2	12
37	DP	99/99 (100%)	80 (81%)	19 (19%)	1	8
38	BQ	89/89 (100%)	70 (79%)	19 (21%)	1	6
38	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	11
39	BR	84/84 (100%)	62 (74%)	22 (26%)	0	3
39	DR	84/84 (100%)	68 (81%)	16 (19%)	1	8
40	BS	93/93 (100%)	74 (80%)	19 (20%)	1	7
40	DS	93/93 (100%)	77 (83%)	16 (17%)	2	11
41	BT	80/80 (100%)	67 (84%)	13 (16%)	2	12
41	DT	80/80 (100%)	64 (80%)	16 (20%)	1	7
42	BU	83/83 (100%)	65 (78%)	18 (22%)	1	6
42	DU	83/83 (100%)	58 (70%)	25 (30%)	0	1
43	BV	78/78 (100%)	58 (74%)	20 (26%)	0	3
43	DV	78/78 (100%)	68 (87%)	10 (13%)	4	19
44	BW	57/58 (98%)	48 (84%)	9 (16%)	2	13
44	DW	56/58 (97%)	50 (89%)	6 (11%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BX	67/67 (100%)	55 (82%)	12 (18%)	2	10
45	DX	67/67 (100%)	54 (81%)	13 (19%)	1	8
46	BY	55/55 (100%)	47 (86%)	8 (14%)	3	15
46	DY	55/55 (100%)	44 (80%)	11 (20%)	1	7
47	BZ	48/48 (100%)	39 (81%)	9 (19%)	1	9
47	DZ	48/48 (100%)	31 (65%)	17 (35%)	0	1
48	B0	47/47 (100%)	40 (85%)	7 (15%)	3	15
48	D0	47/47 (100%)	43 (92%)	4 (8%)	10	36
49	B1	45/45 (100%)	34 (76%)	11 (24%)	1	4
49	D1	45/45 (100%)	39 (87%)	6 (13%)	4	18
50	B2	38/38 (100%)	34 (90%)	4 (10%)	6	27
50	D2	38/38 (100%)	32 (84%)	6 (16%)	2	13
51	B3	51/51 (100%)	39 (76%)	12 (24%)	1	4
51	D3	51/51 (100%)	46 (90%)	5 (10%)	7	30
52	B4	34/34 (100%)	27 (79%)	7 (21%)	1	7
52	D4	34/34 (100%)	26 (76%)	8 (24%)	1	4
53	B5	61/180 (34%)	45 (74%)	16 (26%)	0	3
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%)	7288 (78%)	2102 (22%)	1	5

5 of 2102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	DM	14	LYS
36	DO	103	VAL
34	DM	7	THR
49	D1	38	LYS
32	BK	88	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
3	CC	140	ASN

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Mol	Chain	Res	Type
15	CO	46	HIS
41	DT	28	ASN
4	CD	116	GLN
7	CG	130	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	362 (23%)	17 (1%)
1	CA	1538/1539 (99%)	337 (21%)	16 (1%)
22	BA	2895/2903 (99%)	673 (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%)	2033 (22%)	103 (1%)

5 of 2033 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
1	CA	209	U
22	DA	83	A
22	DA	2501	C
1	CA	429	U
1	CA	873	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	004	D6	7	54	9,10,11	3.70	7 (77%)	9,12,14	1.77	3 (33%)
54	DBB	B6	3	54	4,5,6	0.94	0	1,5,7	1.35	0
54	MHU	B6	5	54	14,15,16	3.11	7 (50%)	18,19,21	2.81	5 (27%)
54	004	B6	7	54	9,10,11	3.78	7 (77%)	9,12,14	1.56	3 (33%)
54	04X	B6	6	54	14,16,17	1.23	1 (7%)	11,20,22	4.66	6 (54%)
54	MHW	D6	1	54	9,9,10	3.42	5 (55%)	10,11,13	2.58	7 (70%)
54	MHU	D6	5	54	14,15,16	3.04	7 (50%)	18,19,21	2.80	4 (22%)
54	MHW	B6	1	54	9,9,10	3.08	5 (55%)	10,11,13	3.22	8 (80%)
54	DBB	D6	3	54	4,5,6	0.81	0	1,5,7	2.19	1 (100%)
54	04X	D6	6	54	14,16,17	1.13	1 (7%)	11,20,22	5.43	7 (63%)

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	004	D6	7	54	-	0/4/6/8	0/1/1/1
54	DBB	B6	3	54	-	1/3/4/6	-
54	MHU	B6	5	54	-	2/9/12/14	0/1/1/1
54	004	B6	7	54	-	0/4/6/8	0/1/1/1
54	04X	B6	6	54	-	2/5/24/26	0/2/2/2
54	MHW	D6	1	54	-	0/2/2/4	0/1/1/1
54	MHU	D6	5	54	-	3/9/12/14	0/1/1/1
54	MHW	B6	1	54	-	2/2/2/4	0/1/1/1
54	DBB	D6	3	54	-	2/3/4/6	-
54	04X	D6	6	54	-	3/5/24/26	0/2/2/2

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D6	5	MHU	CE1-CD1	6.79	1.49	1.38
54	B6	7	004	CB-CA	-6.72	1.45	1.52
54	D6	7	004	CB-CA	-6.29	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	5	MHU	CE1-CD1	6.20	1.48	1.38
54	D6	1	MHW	CA-N	-6.18	1.28	1.35

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	04X	C0-N1-C1	15.63	135.46	111.14
54	B6	6	04X	C0-N1-C1	13.01	131.37	111.14
54	D6	5	MHU	CB-CA-N	8.23	122.60	110.48
54	B6	5	MHU	CB-CA-N	7.93	122.16	110.48
54	D6	5	MHU	O-C-CA	-6.72	107.48	124.77

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	B6	1	MHW	O-C-CA-N
54	B6	3	DBB	C-CA-CB-CG
54	D6	3	DBB	O-C-CA-CB
54	D6	3	DBB	C-CA-CB-CG
54	D6	5	MHU	O-C-CA-CB

There are no ring outliers.

8 monomers are involved in 18 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	-0.27	25 (1%) 70 47	14, 54, 137, 179	0
1	CA	1539/1539 (100%)	0.03	45 (2%) 53 31	27, 72, 145, 177	0
2	AB	218/218 (100%)	0.51	10 (4%) 37 20	43, 76, 100, 125	0
2	CB	218/218 (100%)	0.67	14 (6%) 25 13	63, 86, 106, 126	0
3	AC	206/206 (100%)	0.10	3 (1%) 72 49	39, 61, 83, 96	0
3	CC	206/206 (100%)	0.44	8 (3%) 43 24	57, 79, 97, 109	0
4	AD	205/205 (100%)	0.04	1 (0%) 87 72	35, 58, 79, 106	0
4	CD	205/205 (100%)	-0.16	7 (3%) 48 27	21, 40, 71, 90	0
5	AE	150/150 (100%)	0.13	2 (1%) 75 53	27, 51, 82, 106	0
5	CE	150/150 (100%)	0.25	4 (2%) 56 33	34, 59, 87, 104	0
6	AF	100/100 (100%)	0.15	1 (1%) 79 59	38, 59, 76, 84	0
6	CF	100/100 (100%)	0.11	2 (2%) 65 41	46, 74, 96, 104	0
7	AG	151/151 (100%)	0.65	7 (4%) 37 20	54, 78, 98, 108	0
7	CG	151/151 (100%)	1.20	28 (18%) 3 2	77, 97, 107, 113	0
8	AH	129/129 (100%)	-0.13	1 (0%) 82 64	30, 50, 73, 81	0
8	CH	129/129 (100%)	0.09	2 (1%) 70 47	45, 65, 81, 90	0
9	AI	127/127 (100%)	0.93	12 (9%) 14 7	51, 73, 97, 113	0
9	CI	127/127 (100%)	1.01	18 (14%) 6 4	71, 91, 109, 126	0
10	AJ	98/98 (100%)	0.68	9 (9%) 14 8	46, 68, 92, 122	0
10	CJ	98/98 (100%)	1.40	23 (23%) 2 1	71, 93, 110, 124	0
11	AK	117/117 (100%)	0.38	6 (5%) 33 17	32, 64, 91, 110	0
11	CK	117/117 (100%)	0.07	1 (0%) 81 61	44, 68, 82, 91	0
12	AL	123/123 (100%)	0.05	3 (2%) 59 36	23, 39, 68, 94	0
12	CL	123/123 (100%)	0.17	4 (3%) 49 28	39, 52, 79, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.52	2 (1%) 67 44	49, 71, 92, 105	0
13	CM	114/114 (100%)	1.52	32 (28%) 1 1	90, 103, 116, 120	0
14	AN	96/100 (96%)	0.75	8 (8%) 17 9	43, 63, 94, 106	0
14	CN	96/100 (96%)	1.42	26 (27%) 1 1	69, 91, 110, 118	0
15	AO	88/88 (100%)	0.15	2 (2%) 61 38	31, 51, 68, 98	0
15	CO	88/88 (100%)	0.01	1 (1%) 78 57	43, 63, 81, 105	0
16	AP	82/82 (100%)	0.24	3 (3%) 45 25	35, 49, 84, 100	0
16	CP	82/82 (100%)	0.45	2 (2%) 59 36	45, 62, 88, 106	0
17	AQ	80/80 (100%)	0.18	3 (3%) 44 24	27, 54, 81, 124	0
17	CQ	80/80 (100%)	0.75	9 (11%) 10 6	44, 72, 96, 105	0
18	AR	55/55 (100%)	0.10	4 (7%) 21 11	39, 53, 81, 112	0
18	CR	55/55 (100%)	0.16	1 (1%) 67 44	46, 56, 82, 111	0
19	AS	79/79 (100%)	0.97	12 (15%) 5 3	55, 72, 92, 101	0
19	CS	79/79 (100%)	1.35	15 (18%) 3 2	87, 103, 114, 123	0
20	AT	85/85 (100%)	0.07	4 (4%) 36 19	35, 51, 74, 111	0
20	CT	85/85 (100%)	0.69	10 (11%) 9 5	53, 72, 93, 96	0
21	AU	51/51 (100%)	1.20	7 (13%) 6 4	56, 76, 95, 108	0
21	CU	51/51 (100%)	0.84	9 (17%) 4 3	48, 72, 94, 108	0
22	BA	2897/2903 (99%)	-0.66	89 (3%) 51 30	0, 14, 130, 195	0
22	DA	2897/2903 (99%)	0.26	57 (1%) 65 41	42, 83, 144, 183	0
23	BB	119/119 (100%)	-0.84	0 100 100	1, 24, 54, 90	0
23	DB	118/119 (99%)	0.14	0 100 100	66, 111, 133, 141	0
24	BC	271/271 (100%)	-0.26	10 (3%) 45 25	3, 21, 43, 55	0
24	DC	271/271 (100%)	0.55	19 (7%) 22 12	42, 62, 76, 91	0
25	BD	209/209 (100%)	-0.64	0 100 100	0, 9, 38, 71	0
25	DD	209/209 (100%)	0.39	6 (2%) 53 31	46, 66, 81, 99	0
26	BE	201/201 (100%)	-0.51	0 100 100	0, 24, 56, 91	0
26	DE	201/201 (100%)	0.90	17 (8%) 16 8	45, 81, 98, 106	0
27	BF	177/177 (100%)	-0.02	4 (2%) 61 38	15, 46, 88, 97	0
27	DF	177/177 (100%)	0.95	16 (9%) 15 8	85, 102, 117, 125	0
28	BG	176/176 (100%)	-0.38	0 100 100	15, 38, 64, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	0.57	6 (3%) 48 27	71, 90, 104, 117	0
29	BH	149/149 (100%)	2.00	73 (48%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.46	44 (29%) 1 1	25, 92, 107, 115	0
30	BI	141/141 (100%)	1.61	42 (29%) 1 1	84, 108, 121, 136	0
30	DI	141/141 (100%)	1.82	53 (37%) 1 1	96, 114, 123, 127	0
31	BJ	142/142 (100%)	-0.63	0 100 100	1, 5, 23, 43	0
31	DJ	142/142 (100%)	0.43	12 (8%) 16 8	48, 64, 79, 96	0
32	BK	122/122 (100%)	-0.61	0 100 100	2, 11, 37, 67	0
32	DK	122/122 (100%)	0.13	1 (0%) 82 64	48, 61, 81, 96	0
33	BL	143/143 (100%)	-0.39	1 (0%) 84 66	0, 21, 48, 76	0
33	DL	143/143 (100%)	1.11	27 (18%) 3 2	42, 77, 91, 113	0
34	BM	136/136 (100%)	-0.67	0 100 100	1, 9, 30, 87	0
34	DM	136/136 (100%)	0.25	3 (2%) 62 39	42, 67, 82, 108	0
35	BN	120/120 (100%)	-0.57	0 100 100	1, 6, 17, 62	0
35	DN	120/120 (100%)	0.79	12 (10%) 12 7	54, 74, 88, 110	0
36	BO	116/116 (100%)	-0.44	0 100 100	14, 27, 46, 52	0
36	DO	116/116 (100%)	0.74	7 (6%) 27 14	74, 91, 102, 114	0
37	BP	114/114 (100%)	-0.49	0 100 100	5, 19, 48, 70	0
37	DP	114/114 (100%)	0.50	2 (1%) 67 44	56, 68, 84, 93	0
38	BQ	117/117 (100%)	-0.64	0 100 100	0, 3, 11, 42	0
38	DQ	117/117 (100%)	0.55	12 (10%) 12 6	52, 66, 77, 84	0
39	BR	103/103 (100%)	-0.50	0 100 100	0, 9, 31, 63	0
39	DR	103/103 (100%)	0.54	4 (3%) 43 24	50, 75, 87, 97	0
40	BS	110/110 (100%)	-0.64	0 100 100	1, 3, 23, 84	0
40	DS	110/110 (100%)	0.72	8 (7%) 21 11	56, 73, 89, 96	0
41	BT	93/93 (100%)	-0.12	5 (5%) 31 16	10, 27, 80, 101	0
41	DT	93/93 (100%)	1.23	17 (18%) 3 2	63, 83, 103, 110	0
42	BU	102/102 (100%)	-0.21	1 (0%) 79 59	10, 30, 61, 92	0
42	DU	102/102 (100%)	1.63	28 (27%) 1 1	70, 88, 106, 112	0
43	BV	94/94 (100%)	-0.49	0 100 100	4, 22, 43, 54	0
43	DV	94/94 (100%)	0.50	4 (4%) 40 21	65, 82, 94, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.52	0 100 100	3, 10, 27, 48	0
44	DW	75/76 (98%)	0.80	3 (4%) 42 23	54, 79, 88, 108	0
45	BX	77/77 (100%)	-0.33	0 100 100	6, 24, 52, 77	0
45	DX	77/77 (100%)	0.89	12 (15%) 5 3	49, 69, 86, 89	0
46	BY	63/63 (100%)	0.01	1 (1%) 70 47	22, 44, 74, 96	0
46	DY	63/63 (100%)	0.99	6 (9%) 14 7	71, 90, 99, 103	0
47	BZ	58/58 (100%)	-0.47	0 100 100	2, 7, 29, 41	0
47	DZ	58/58 (100%)	0.42	1 (1%) 69 45	52, 70, 84, 89	0
48	B0	56/56 (100%)	-0.70	0 100 100	0, 8, 35, 70	0
48	D0	56/56 (100%)	0.81	4 (7%) 22 11	53, 74, 91, 104	0
49	B1	50/50 (100%)	-0.36	1 (2%) 65 41	13, 31, 54, 87	0
49	D1	50/50 (100%)	0.83	5 (10%) 12 7	68, 84, 93, 105	0
50	B2	46/46 (100%)	-0.43	1 (2%) 62 39	3, 9, 17, 90	0
50	D2	46/46 (100%)	0.95	5 (10%) 10 6	53, 66, 79, 100	0
51	B3	64/64 (100%)	-0.53	0 100 100	4, 9, 18, 31	0
51	D3	64/64 (100%)	1.50	20 (31%) 1 1	58, 71, 79, 85	0
52	B4	38/38 (100%)	-0.42	0 100 100	11, 20, 35, 52	0
52	D4	38/38 (100%)	1.22	8 (21%) 2 1	63, 74, 85, 99	0
53	B5	191/228 (83%)	1.53	55 (28%) 1 1	85, 111, 123, 134	0
54	B6	2/7 (28%)	0.00	0 100 100	5, 5, 5, 9	0
54	D6	2/7 (28%)	0.69	0 100 100	53, 53, 53, 62	0
All	All	20738/20808 (99%)	0.13	1088 (5%) 33 17	0, 64, 119, 195	0

The worst 5 of 1088 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	BI	53	LEU	10.7
22	BA	2104	C	7.9
33	DL	92	LEU	7.6
50	D2	46	LYS	7.5
7	CG	62	PHE	7.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MHU	D6	5	15/16	0.70	0.22	45,58,69,72	0
54	04X	D6	6	15/16	0.71	0.19	47,59,67,73	0
54	DBB	D6	3	6/7	0.85	0.27	45,50,65,70	0
54	MHW	D6	1	9/10	0.88	0.11	55,59,63,66	0
54	004	D6	7	10/11	0.88	0.12	47,52,61,64	0
54	MHW	B6	1	9/10	0.92	0.11	8,13,21,30	0
54	04X	B6	6	15/16	0.93	0.11	6,11,15,20	0
54	DBB	B6	3	6/7	0.94	0.12	8,14,20,33	0
54	MHU	B6	5	15/16	0.94	0.11	3,7,15,15	0
54	004	B6	7	10/11	0.98	0.07	2,4,6,6	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	DA	3072	1/1	0.12	0.35	89,89,89,89	0
55	MG	CA	1655	1/1	0.18	0.12	67,67,67,67	0
55	MG	DA	3061	1/1	0.30	0.61	97,97,97,97	0
55	MG	CA	1630	1/1	0.37	0.26	102,102,102,102	0
55	MG	DA	3093	1/1	0.37	0.23	99,99,99,99	0
55	MG	DA	3071	1/1	0.39	0.27	93,93,93,93	0
55	MG	DA	3040	1/1	0.41	0.17	66,66,66,66	0
55	MG	DA	3127	1/1	0.48	0.11	88,88,88,88	0
55	MG	DA	3102	1/1	0.49	0.15	72,72,72,72	0
55	MG	DA	3041	1/1	0.49	0.25	66,66,66,66	0
55	MG	CA	1652	1/1	0.50	0.19	62,62,62,62	0
55	MG	CA	1633	1/1	0.57	0.35	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3028	1/1	0.57	0.32	86,86,86,86	0
55	MG	BA	3135	1/1	0.59	0.41	48,48,48,48	0
55	MG	AA	1627	1/1	0.60	0.33	76,76,76,76	0
55	MG	DA	3134	1/1	0.60	0.27	87,87,87,87	0
55	MG	DA	3026	1/1	0.61	0.40	75,75,75,75	0
55	MG	DA	3153	1/1	0.64	0.16	68,68,68,68	0
55	MG	AA	1644	1/1	0.65	0.12	49,49,49,49	0
55	MG	CA	1628	1/1	0.66	0.19	100,100,100,100	0
55	MG	DA	3032	1/1	0.66	0.37	78,78,78,78	0
55	MG	AA	1667	1/1	0.67	0.12	54,54,54,54	0
55	MG	CA	1631	1/1	0.67	0.16	98,98,98,98	0
55	MG	AA	1635	1/1	0.69	0.20	76,76,76,76	0
55	MG	DA	3159	1/1	0.69	0.14	57,57,57,57	0
55	MG	CA	1627	1/1	0.72	0.21	88,88,88,88	0
55	MG	CA	1636	1/1	0.73	0.18	97,97,97,97	0
55	MG	DA	3132	1/1	0.74	0.42	85,85,85,85	0
55	MG	CA	1637	1/1	0.74	0.25	80,80,80,80	0
55	MG	DA	3113	1/1	0.74	0.12	75,75,75,75	0
55	MG	AA	1648	1/1	0.74	0.11	39,39,39,39	0
55	MG	BA	3015	1/1	0.75	0.27	61,61,61,61	0
55	MG	BA	3055	1/1	0.75	0.22	50,50,50,50	0
55	MG	DA	3165	1/1	0.75	0.24	43,43,43,43	0
55	MG	DA	3019	1/1	0.76	0.15	84,84,84,84	0
55	MG	AA	1662	1/1	0.77	0.25	49,49,49,49	0
55	MG	DA	3011	1/1	0.77	0.25	74,74,74,74	0
55	MG	DA	3112	1/1	0.78	0.14	64,64,64,64	0
55	MG	BA	3016	1/1	0.78	0.20	31,31,31,31	0
55	MG	DA	3029	1/1	0.78	0.27	66,66,66,66	0
55	MG	DA	3164	1/1	0.78	0.11	56,56,56,56	0
55	MG	DA	3103	1/1	0.78	0.24	67,67,67,67	0
55	MG	DA	3042	1/1	0.79	0.11	69,69,69,69	0
55	MG	DA	3152	1/1	0.79	0.18	55,55,55,55	0
55	MG	DA	3106	1/1	0.79	0.14	70,70,70,70	0
55	MG	DA	3015	1/1	0.80	0.29	77,77,77,77	0
55	MG	DA	3002	1/1	0.80	0.20	81,81,81,81	0
55	MG	CM	201	1/1	0.80	0.10	50,50,50,50	0
55	MG	DA	3120	1/1	0.80	0.28	95,95,95,95	0
55	MG	BA	3025	1/1	0.81	0.20	40,40,40,40	0
55	MG	BA	3160	1/1	0.81	0.14	5,5,5,5	0
55	MG	AA	1659	1/1	0.81	0.20	32,32,32,32	0
55	MG	DA	3133	1/1	0.81	0.30	55,55,55,55	0
55	MG	BA	3098	1/1	0.81	0.28	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3190	1/1	0.82	0.09	42,42,42,42	0
55	MG	AA	1665	1/1	0.82	0.27	53,53,53,53	0
55	MG	DA	3027	1/1	0.82	0.10	82,82,82,82	0
55	MG	DA	3077	1/1	0.82	0.16	76,76,76,76	0
55	MG	CA	1645	1/1	0.83	0.10	32,32,32,32	0
55	MG	CA	1647	1/1	0.83	0.23	35,35,35,35	0
55	MG	DA	3136	1/1	0.83	0.22	81,81,81,81	0
55	MG	DA	3138	1/1	0.83	0.17	37,37,37,37	0
55	MG	CA	1650	1/1	0.83	0.15	50,50,50,50	0
55	MG	BA	3115	1/1	0.83	0.16	76,76,76,76	0
55	MG	DA	3085	1/1	0.83	0.15	78,78,78,78	0
55	MG	BA	3004	1/1	0.83	0.16	52,52,52,52	0
55	MG	BA	3154	1/1	0.83	0.18	21,21,21,21	0
55	MG	DA	3166	1/1	0.83	0.18	44,44,44,44	0
55	MG	DA	3141	1/1	0.84	0.20	45,45,45,45	0
55	MG	DA	3016	1/1	0.84	0.20	84,84,84,84	0
55	MG	DA	3034	1/1	0.84	0.09	58,58,58,58	0
55	MG	DA	3048	1/1	0.84	0.10	93,93,93,93	0
55	MG	DA	3060	1/1	0.84	0.24	72,72,72,72	0
55	MG	DA	3091	1/1	0.84	0.11	79,79,79,79	0
55	MG	CA	1629	1/1	0.84	0.09	84,84,84,84	0
55	MG	BA	3111	1/1	0.85	0.09	27,27,27,27	0
55	MG	BA	3090	1/1	0.85	0.08	33,33,33,33	0
55	MG	DA	3047	1/1	0.85	0.11	71,71,71,71	0
55	MG	DA	3155	1/1	0.85	0.17	37,37,37,37	0
55	MG	DA	3157	1/1	0.85	0.06	29,29,29,29	0
55	MG	BA	3061	1/1	0.85	0.26	66,66,66,66	0
55	MG	DA	3004	1/1	0.85	0.18	87,87,87,87	0
55	MG	DA	3137	1/1	0.85	0.23	84,84,84,84	0
55	MG	CA	1653	1/1	0.85	0.11	48,48,48,48	0
55	MG	DA	3167	1/1	0.85	0.06	30,30,30,30	0
55	MG	AA	1664	1/1	0.86	0.11	51,51,51,51	0
55	MG	CA	1638	1/1	0.86	0.10	74,74,74,74	0
55	MG	DA	3161	1/1	0.86	0.19	48,48,48,48	0
55	MG	DA	3149	1/1	0.86	0.12	49,49,49,49	0
55	MG	DA	3099	1/1	0.86	0.23	82,82,82,82	0
55	MG	DA	3010	1/1	0.86	0.10	64,64,64,64	0
55	MG	AA	1619	1/1	0.86	0.18	65,65,65,65	0
55	MG	BA	3099	1/1	0.87	0.22	21,21,21,21	0
55	MG	BA	3040	1/1	0.87	0.24	2,2,2,2	0
55	MG	BA	3047	1/1	0.87	0.10	40,40,40,40	0
55	MG	CA	1654	1/1	0.87	0.05	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3070	1/1	0.87	0.05	93,93,93,93	0
55	MG	BA	3119	1/1	0.87	0.27	49,49,49,49	0
55	MG	DA	3121	1/1	0.87	0.09	60,60,60,60	0
55	MG	AA	1646	1/1	0.87	0.17	50,50,50,50	0
55	MG	BA	3060	1/1	0.87	0.15	29,29,29,29	0
55	MG	AA	1602	1/1	0.87	0.23	53,53,53,53	0
55	MG	BA	3179	1/1	0.87	0.17	30,30,30,30	0
55	MG	AA	1630	1/1	0.87	0.13	67,67,67,67	0
55	MG	AA	1660	1/1	0.87	0.11	41,41,41,41	0
55	MG	DA	3056	1/1	0.88	0.29	80,80,80,80	0
55	MG	DA	3092	1/1	0.88	0.16	94,94,94,94	0
55	MG	BA	3176	1/1	0.88	0.17	24,24,24,24	0
55	MG	BA	3087	1/1	0.88	0.15	27,27,27,27	0
55	MG	BA	3014	1/1	0.88	0.18	26,26,26,26	0
55	MG	AA	1669	1/1	0.88	0.08	34,34,34,34	0
55	MG	DA	3104	1/1	0.88	0.15	76,76,76,76	0
55	MG	AA	1657	1/1	0.88	0.07	37,37,37,37	0
55	MG	BA	3070	1/1	0.88	0.14	37,37,37,37	0
55	MG	DA	3014	1/1	0.88	0.20	73,73,73,73	0
55	MG	DA	3145	1/1	0.88	0.11	68,68,68,68	0
55	MG	BA	3188	1/1	0.89	0.11	35,35,35,35	0
55	MG	DA	3107	1/1	0.89	0.10	56,56,56,56	0
55	MG	DA	3094	1/1	0.89	0.09	83,83,83,83	0
55	MG	DA	3084	1/1	0.89	0.08	75,75,75,75	0
55	MG	DA	3100	1/1	0.89	0.17	73,73,73,73	0
55	MG	DA	3160	1/1	0.89	0.11	47,47,47,47	0
55	MG	BA	3076	1/1	0.89	0.16	56,56,56,56	0
55	MG	BA	3148	1/1	0.89	0.06	13,13,13,13	0
55	MG	DA	3146	1/1	0.89	0.06	41,41,41,41	0
55	MG	AA	1636	1/1	0.89	0.15	42,42,42,42	0
55	MG	DA	3150	1/1	0.89	0.17	50,50,50,50	0
55	MG	BA	3011	1/1	0.90	0.19	30,30,30,30	0
55	MG	CA	1607	1/1	0.90	0.18	55,55,55,55	0
55	MG	DA	3151	1/1	0.90	0.13	40,40,40,40	0
55	MG	DA	3025	1/1	0.90	0.08	65,65,65,65	0
55	MG	CA	1615	1/1	0.90	0.17	56,56,56,56	0
55	MG	CA	1620	1/1	0.90	0.13	81,81,81,81	0
55	MG	AA	1651	1/1	0.90	0.32	55,55,55,55	0
55	MG	DA	3069	1/1	0.90	0.16	77,77,77,77	0
55	MG	DA	3006	1/1	0.90	0.12	98,98,98,98	0
55	MG	BA	3173	1/1	0.90	0.05	30,30,30,30	0
55	MG	BA	3029	1/1	0.90	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3036	1/1	0.90	0.15	23,23,23,23	0
55	MG	DA	3078	1/1	0.90	0.12	95,95,95,95	0
55	MG	AA	1614	1/1	0.90	0.23	66,66,66,66	0
55	MG	BA	3143	1/1	0.91	0.14	3,3,3,3	0
55	MG	AA	1652	1/1	0.91	0.15	40,40,40,40	0
55	MG	DA	3054	1/1	0.91	0.12	62,62,62,62	0
55	MG	DA	3007	1/1	0.91	0.18	80,80,80,80	0
55	MG	AA	1661	1/1	0.91	0.16	23,23,23,23	0
55	MG	CA	1611	1/1	0.91	0.10	69,69,69,69	0
55	MG	DA	3156	1/1	0.91	0.10	58,58,58,58	0
55	MG	AA	1650	1/1	0.91	0.12	20,20,20,20	0
55	MG	DA	3158	1/1	0.91	0.24	58,58,58,58	0
55	MG	BA	3084	1/1	0.91	0.14	7,7,7,7	0
55	MG	DA	3035	1/1	0.91	0.14	71,71,71,71	0
55	MG	AA	1663	1/1	0.91	0.15	49,49,49,49	0
55	MG	AA	1639	1/1	0.91	0.06	67,67,67,67	0
55	MG	DA	3021	1/1	0.91	0.16	62,62,62,62	0
55	MG	DA	3081	1/1	0.91	0.13	62,62,62,62	0
55	MG	DA	3108	1/1	0.91	0.10	55,55,55,55	0
55	MG	DQ	201	1/1	0.91	0.12	40,40,40,40	0
55	MG	CA	1635	1/1	0.92	0.07	94,94,94,94	0
55	MG	DA	3148	1/1	0.92	0.06	51,51,51,51	0
55	MG	DA	3024	1/1	0.92	0.10	45,45,45,45	0
55	MG	DA	3089	1/1	0.92	0.23	91,91,91,91	0
55	MG	DA	3116	1/1	0.92	0.14	92,92,92,92	0
55	MG	BA	3057	1/1	0.92	0.26	20,20,20,20	0
55	MG	AM	201	1/1	0.92	0.10	50,50,50,50	0
55	MG	DA	3154	1/1	0.92	0.17	40,40,40,40	0
55	MG	DA	3125	1/1	0.92	0.09	86,86,86,86	0
55	MG	BA	3165	1/1	0.92	0.08	3,3,3,3	0
55	MG	BA	3136	1/1	0.92	0.36	43,43,43,43	0
55	MG	AA	1649	1/1	0.92	0.05	28,28,28,28	0
55	MG	BA	3146	1/1	0.92	0.17	22,22,22,22	0
55	MG	DA	3013	1/1	0.92	0.09	64,64,64,64	0
55	MG	AA	1643	1/1	0.92	0.10	23,23,23,23	0
55	MG	BA	3152	1/1	0.92	0.12	8,8,8,8	0
55	MG	CA	1601	1/1	0.92	0.13	52,52,52,52	0
55	MG	DA	3142	1/1	0.92	0.20	39,39,39,39	0
55	MG	DA	3143	1/1	0.92	0.17	35,35,35,35	0
55	MG	CA	1605	1/1	0.92	0.13	78,78,78,78	0
55	MG	AA	1654	1/1	0.93	0.16	41,41,41,41	0
55	MG	DA	3005	1/1	0.93	0.07	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3102	1/1	0.93	0.19	17,17,17,17	0
55	MG	DA	3090	1/1	0.93	0.11	59,59,59,59	0
55	MG	DA	3139	1/1	0.93	0.32	47,47,47,47	0
55	MG	DA	3038	1/1	0.93	0.07	63,63,63,63	0
55	MG	BA	3178	1/1	0.93	0.17	12,12,12,12	0
55	MG	DA	3008	1/1	0.93	0.12	80,80,80,80	0
55	MG	BA	3144	1/1	0.93	0.12	24,24,24,24	0
55	MG	AA	1615	1/1	0.93	0.11	63,63,63,63	0
55	MG	AA	1670	1/1	0.93	0.20	45,45,45,45	0
55	MG	BA	3195	1/1	0.93	0.11	36,36,36,36	0
55	MG	BA	3118	1/1	0.93	0.12	34,34,34,34	0
55	MG	DA	3057	1/1	0.93	0.17	82,82,82,82	0
55	MG	DA	3058	1/1	0.93	0.15	70,70,70,70	0
55	MG	AA	1671	1/1	0.93	0.17	54,54,54,54	0
55	MG	BA	3159	1/1	0.93	0.10	24,24,24,24	0
55	MG	CA	1609	1/1	0.93	0.08	78,78,78,78	0
55	MG	BA	3133	1/1	0.93	0.23	57,57,57,57	0
55	MG	AA	1629	1/1	0.93	0.10	54,54,54,54	0
55	MG	DA	3117	1/1	0.93	0.09	55,55,55,55	0
55	MG	BA	3166	1/1	0.93	0.12	37,37,37,37	0
55	MG	DA	3075	1/1	0.93	0.16	61,61,61,61	0
55	MG	CA	1621	1/1	0.93	0.08	67,67,67,67	0
55	MG	DA	3126	1/1	0.93	0.08	61,61,61,61	0
55	MG	BA	3167	1/1	0.93	0.07	22,22,22,22	0
55	MG	DA	3129	1/1	0.93	0.08	70,70,70,70	0
55	MG	DA	3080	1/1	0.93	0.06	91,91,91,91	0
55	MG	BA	3172	1/1	0.93	0.05	16,16,16,16	0
55	MG	BA	3112	1/1	0.94	0.06	20,20,20,20	0
55	MG	DA	3110	1/1	0.94	0.09	45,45,45,45	0
55	MG	DA	3111	1/1	0.94	0.09	81,81,81,81	0
55	MG	DA	3147	1/1	0.94	0.04	35,35,35,35	0
55	MG	AA	1658	1/1	0.94	0.04	35,35,35,35	0
55	MG	CA	1643	1/1	0.94	0.27	41,41,41,41	0
55	MG	BA	3059	1/1	0.94	0.15	5,5,5,5	0
55	MG	CA	1646	1/1	0.94	0.07	36,36,36,36	0
55	MG	CA	1618	1/1	0.94	0.12	35,35,35,35	0
55	MG	DA	3046	1/1	0.94	0.06	62,62,62,62	0
55	MG	AA	1647	1/1	0.94	0.08	44,44,44,44	0
55	MG	CA	1651	1/1	0.94	0.08	72,72,72,72	0
55	MG	BA	3048	1/1	0.94	0.08	26,26,26,26	0
55	MG	BA	3180	1/1	0.94	0.24	25,25,25,25	0
55	MG	BA	3182	1/1	0.94	0.12	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1601	1/1	0.94	0.12	61,61,61,61	0
55	MG	BA	3074	1/1	0.94	0.26	32,32,32,32	0
55	MG	BA	3104	1/1	0.94	0.17	0,0,0,0	0
55	MG	DA	3162	1/1	0.94	0.04	48,48,48,48	0
55	MG	DA	3068	1/1	0.94	0.06	60,60,60,60	0
55	MG	BA	3056	1/1	0.94	0.16	22,22,22,22	0
55	MG	BA	3168	1/1	0.94	0.07	21,21,21,21	0
55	MG	DA	3030	1/1	0.94	0.18	61,61,61,61	0
55	MG	BA	3171	1/1	0.94	0.08	20,20,20,20	0
55	MG	DA	3033	1/1	0.95	0.07	54,54,54,54	0
55	MG	BA	3142	1/1	0.95	0.13	0,0,0,0	0
55	MG	AA	1603	1/1	0.95	0.16	57,57,57,57	0
55	MG	DA	3037	1/1	0.95	0.06	76,76,76,76	0
55	MG	DA	3088	1/1	0.95	0.07	69,69,69,69	0
55	MG	BA	3031	1/1	0.95	0.10	7,7,7,7	0
55	MG	BA	3009	1/1	0.95	0.03	2,2,2,2	0
55	MG	DA	3140	1/1	0.95	0.09	42,42,42,42	0
55	MG	AA	1653	1/1	0.95	0.10	34,34,34,34	0
55	MG	BA	3181	1/1	0.95	0.09	26,26,26,26	0
55	MG	DA	3043	1/1	0.95	0.05	67,67,67,67	0
55	MG	DA	3044	1/1	0.95	0.12	83,83,83,83	0
55	MG	DA	3095	1/1	0.95	0.11	69,69,69,69	0
55	MG	DA	3045	1/1	0.95	0.10	61,61,61,61	0
55	MG	BA	3105	1/1	0.95	0.10	0,0,0,0	0
55	MG	AA	1617	1/1	0.95	0.11	62,62,62,62	0
55	MG	BA	3189	1/1	0.95	0.12	0,0,0,0	0
55	MG	BA	3156	1/1	0.95	0.06	9,9,9,9	0
55	MG	AA	1638	1/1	0.95	0.08	63,63,63,63	0
55	MG	CA	1642	1/1	0.95	0.15	25,25,25,25	0
55	MG	BA	3080	1/1	0.95	0.12	24,24,24,24	0
55	MG	CA	1602	1/1	0.95	0.06	69,69,69,69	0
55	MG	BA	3162	1/1	0.95	0.10	23,23,23,23	0
55	MG	DA	3062	1/1	0.95	0.28	70,70,70,70	0
55	MG	AA	1666	1/1	0.95	0.10	32,32,32,32	0
55	MG	DA	3115	1/1	0.95	0.08	79,79,79,79	0
55	MG	CA	1648	1/1	0.95	0.13	51,51,51,51	0
55	MG	CA	1608	1/1	0.95	0.09	65,65,65,65	0
55	MG	BA	3002	1/1	0.95	0.18	18,18,18,18	0
55	MG	BA	3131	1/1	0.95	0.24	37,37,37,37	0
55	MG	BA	3027	1/1	0.95	0.24	36,36,36,36	0
55	MG	BA	3093	1/1	0.95	0.06	26,26,26,26	0
55	MG	BA	3095	1/1	0.95	0.13	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DB	203	1/1	0.95	0.07	90,90,90,90	0
55	MG	DA	3079	1/1	0.95	0.06	94,94,94,94	0
55	MG	CA	1606	1/1	0.96	0.16	76,76,76,76	0
55	MG	CA	1649	1/1	0.96	0.14	24,24,24,24	0
55	MG	DA	3128	1/1	0.96	0.07	74,74,74,74	0
55	MG	BA	3073	1/1	0.96	0.07	9,9,9,9	0
55	MG	BA	3034	1/1	0.96	0.17	5,5,5,5	0
55	MG	DA	3082	1/1	0.96	0.07	65,65,65,65	0
55	MG	DA	3083	1/1	0.96	0.13	65,65,65,65	0
55	MG	BA	3075	1/1	0.96	0.06	6,6,6,6	0
55	MG	CA	1610	1/1	0.96	0.05	58,58,58,58	0
55	MG	DA	3086	1/1	0.96	0.06	61,61,61,61	0
55	MG	BA	3170	1/1	0.96	0.08	22,22,22,22	0
55	MG	CA	1614	1/1	0.96	0.05	52,52,52,52	0
55	MG	AA	1606	1/1	0.96	0.06	58,58,58,58	0
55	MG	BA	3079	1/1	0.96	0.06	21,21,21,21	0
55	MG	AA	1634	1/1	0.96	0.07	49,49,49,49	0
55	MG	DA	3144	1/1	0.96	0.12	58,58,58,58	0
55	MG	BA	3174	1/1	0.96	0.09	5,5,5,5	0
55	MG	CA	1626	1/1	0.96	0.14	66,66,66,66	0
55	MG	BA	3108	1/1	0.96	0.05	5,5,5,5	0
55	MG	DA	3097	1/1	0.96	0.06	67,67,67,67	0
55	MG	BA	3110	1/1	0.96	0.07	26,26,26,26	0
55	MG	BA	3149	1/1	0.96	0.09	0,0,0,0	0
55	MG	DA	3052	1/1	0.96	0.05	47,47,47,47	0
55	MG	BA	3083	1/1	0.96	0.15	34,34,34,34	0
55	MG	BA	3045	1/1	0.96	0.07	4,4,4,4	0
55	MG	BA	3046	1/1	0.96	0.08	3,3,3,3	0
55	MG	BA	3157	1/1	0.96	0.30	34,34,34,34	0
55	MG	BA	3158	1/1	0.96	0.05	15,15,15,15	0
55	MG	DA	3018	1/1	0.96	0.07	68,68,68,68	0
55	MG	AA	1608	1/1	0.96	0.06	20,20,20,20	0
55	MG	BA	3193	1/1	0.96	0.07	12,12,12,12	0
55	MG	CA	1641	1/1	0.96	0.22	58,58,58,58	0
55	MG	BA	3092	1/1	0.96	0.18	42,42,42,42	0
55	MG	BA	3128	1/1	0.96	0.09	3,3,3,3	0
55	MG	BA	3163	1/1	0.96	0.12	27,27,27,27	0
55	MG	DA	3119	1/1	0.96	0.09	58,58,58,58	0
55	MG	DA	3073	1/1	0.96	0.07	35,35,35,35	0
55	MG	CA	1604	1/1	0.96	0.04	78,78,78,78	0
55	MG	DB	201	1/1	0.96	0.04	96,96,96,96	0
55	MG	DA	3124	1/1	0.96	0.05	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3020	1/1	0.96	0.12	5,5,5,5	0
55	MG	DA	3118	1/1	0.97	0.04	73,73,73,73	0
55	MG	BA	3077	1/1	0.97	0.05	38,38,38,38	0
55	MG	DA	3064	1/1	0.97	0.09	48,48,48,48	0
55	MG	CA	1616	1/1	0.97	0.04	38,38,38,38	0
55	MG	DA	3122	1/1	0.97	0.06	64,64,64,64	0
55	MG	AA	1640	1/1	0.97	0.09	57,57,57,57	0
55	MG	CA	1619	1/1	0.97	0.05	27,27,27,27	0
55	MG	AA	1631	1/1	0.97	0.13	52,52,52,52	0
55	MG	BA	3169	1/1	0.97	0.03	4,4,4,4	0
55	MG	BA	3120	1/1	0.97	0.08	11,11,11,11	0
55	MG	AA	1632	1/1	0.97	0.06	40,40,40,40	0
55	MG	DA	3076	1/1	0.97	0.09	59,59,59,59	0
55	MG	BA	3052	1/1	0.97	0.08	21,21,21,21	0
55	MG	BA	3086	1/1	0.97	0.06	0,0,0,0	0
55	MG	BA	3053	1/1	0.97	0.09	0,0,0,0	0
55	MG	BA	3175	1/1	0.97	0.04	9,9,9,9	0
55	MG	CA	1632	1/1	0.97	0.07	75,75,75,75	0
55	MG	BA	3054	1/1	0.97	0.07	7,7,7,7	0
55	MG	BA	3177	1/1	0.97	0.03	9,9,9,9	0
55	MG	BA	3138	1/1	0.97	0.16	0,0,0,0	0
55	MG	BA	3140	1/1	0.97	0.10	7,7,7,7	0
55	MG	BA	3091	1/1	0.97	0.05	48,48,48,48	0
55	MG	CA	1639	1/1	0.97	0.05	43,43,43,43	0
55	MG	BA	3023	1/1	0.97	0.07	0,0,0,0	0
55	MG	AA	1620	1/1	0.97	0.04	55,55,55,55	0
55	MG	BA	3183	1/1	0.97	0.12	22,22,22,22	0
55	MG	BA	3026	1/1	0.97	0.09	6,6,6,6	0
55	MG	DA	3039	1/1	0.97	0.04	53,53,53,53	0
55	MG	AA	1616	1/1	0.97	0.05	62,62,62,62	0
55	MG	BA	3005	1/1	0.97	0.10	43,43,43,43	0
55	MG	BA	3191	1/1	0.97	0.09	26,26,26,26	0
55	MG	DA	3098	1/1	0.97	0.08	50,50,50,50	0
55	MG	BA	3150	1/1	0.97	0.21	37,37,37,37	0
55	MG	BA	3101	1/1	0.97	0.07	11,11,11,11	0
55	MG	BA	3007	1/1	0.97	0.07	32,32,32,32	0
55	MG	BA	3155	1/1	0.97	0.05	2,2,2,2	0
55	MG	BA	3032	1/1	0.97	0.07	2,2,2,2	0
55	MG	DA	3105	1/1	0.97	0.06	52,52,52,52	0
55	MG	BA	3071	1/1	0.97	0.17	17,17,17,17	0
55	MG	DA	3049	1/1	0.97	0.09	69,69,69,69	0
55	MG	AA	1628	1/1	0.97	0.07	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3163	1/1	0.97	0.14	47,47,47,47	0
55	MG	BA	3109	1/1	0.97	0.12	1,1,1,1	0
55	MG	DA	3055	1/1	0.97	0.08	57,57,57,57	0
55	MG	BA	3010	1/1	0.97	0.05	1,1,1,1	0
55	MG	BA	3161	1/1	0.97	0.04	15,15,15,15	0
55	MG	AA	1605	1/1	0.97	0.07	29,29,29,29	0
55	MG	AA	1609	1/1	0.97	0.09	33,33,33,33	0
55	MG	BA	3114	1/1	0.97	0.04	28,28,28,28	0
55	MG	BA	3147	1/1	0.98	0.05	11,11,11,11	0
55	MG	BA	3116	1/1	0.98	0.12	30,30,30,30	0
55	MG	BA	3003	1/1	0.98	0.04	29,29,29,29	0
55	MG	CA	1644	1/1	0.98	0.18	36,36,36,36	0
55	MG	DA	3031	1/1	0.98	0.04	59,59,59,59	0
55	MG	AA	1621	1/1	0.98	0.09	37,37,37,37	0
55	MG	BA	3151	1/1	0.98	0.07	23,23,23,23	0
55	MG	AA	1623	1/1	0.98	0.11	49,49,49,49	0
55	MG	DA	3130	1/1	0.98	0.06	43,43,43,43	0
55	MG	DA	3131	1/1	0.98	0.04	50,50,50,50	0
55	MG	BA	3153	1/1	0.98	0.03	2,2,2,2	0
55	MG	DA	3036	1/1	0.98	0.05	57,57,57,57	0
55	MG	BA	3126	1/1	0.98	0.05	3,3,3,3	0
55	MG	DA	3135	1/1	0.98	0.06	46,46,46,46	0
55	MG	CA	1612	1/1	0.98	0.04	43,43,43,43	0
55	MG	AA	1645	1/1	0.98	0.08	42,42,42,42	0
55	MG	DA	3087	1/1	0.98	0.04	58,58,58,58	0
55	MG	AA	1668	1/1	0.98	0.06	33,33,33,33	0
55	MG	AA	1624	1/1	0.98	0.09	50,50,50,50	0
55	MG	CA	1617	1/1	0.98	0.12	41,41,41,41	0
55	MG	AA	1604	1/1	0.98	0.07	48,48,48,48	0
55	MG	AA	1607	1/1	0.98	0.04	48,48,48,48	0
55	MG	DA	3001	1/1	0.98	0.04	37,37,37,37	0
55	MG	BA	3137	1/1	0.98	0.14	2,2,2,2	0
55	MG	BA	3184	1/1	0.98	0.07	8,8,8,8	0
55	MG	DA	3096	1/1	0.98	0.04	54,54,54,54	0
55	MG	CA	1622	1/1	0.98	0.10	57,57,57,57	0
55	MG	CA	1623	1/1	0.98	0.09	66,66,66,66	0
55	MG	DA	3051	1/1	0.98	0.03	33,33,33,33	0
55	MG	CA	1624	1/1	0.98	0.06	52,52,52,52	0
55	MG	DA	3101	1/1	0.98	0.03	63,63,63,63	0
55	MG	BA	3185	1/1	0.98	0.04	5,5,5,5	0
55	MG	BA	3187	1/1	0.98	0.10	3,3,3,3	0
55	MG	AA	1655	1/1	0.98	0.08	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3139	1/1	0.98	0.10	0,0,0,0	0
55	MG	BA	3038	1/1	0.98	0.04	1,1,1,1	0
55	MG	DA	3059	1/1	0.98	0.04	42,42,42,42	0
55	MG	BA	3001	1/1	0.98	0.07	21,21,21,21	0
55	MG	DA	3109	1/1	0.98	0.11	30,30,30,30	0
55	MG	BA	3043	1/1	0.98	0.08	23,23,23,23	0
55	MG	BA	3194	1/1	0.98	0.20	22,22,22,22	0
55	MG	DA	3063	1/1	0.98	0.04	53,53,53,53	0
55	MG	BA	3019	1/1	0.98	0.14	1,1,1,1	0
55	MG	DA	3067	1/1	0.98	0.05	43,43,43,43	0
55	MG	DA	3020	1/1	0.98	0.10	44,44,44,44	0
55	MG	BB	204	1/1	0.98	0.21	0,0,0,0	0
55	MG	BA	3145	1/1	0.98	0.07	26,26,26,26	0
55	MG	DB	202	1/1	0.98	0.06	57,57,57,57	0
55	MG	AA	1656	1/1	0.98	0.03	32,32,32,32	0
55	MG	CA	1603	1/1	0.98	0.06	45,45,45,45	0
56	ZN	B4	101	1/1	0.98	0.09	76,76,76,76	0
55	MG	AA	1637	1/1	0.99	0.04	16,16,16,16	0
55	MG	BA	3117	1/1	0.99	0.05	1,1,1,1	0
55	MG	AA	1611	1/1	0.99	0.04	21,21,21,21	0
55	MG	AA	1612	1/1	0.99	0.02	38,38,38,38	0
55	MG	BA	3078	1/1	0.99	0.04	38,38,38,38	0
55	MG	BA	3121	1/1	0.99	0.07	14,14,14,14	0
55	MG	BA	3123	1/1	0.99	0.03	11,11,11,11	0
55	MG	BA	3125	1/1	0.99	0.04	2,2,2,2	0
55	MG	CA	1634	1/1	0.99	0.05	58,58,58,58	0
55	MG	AA	1622	1/1	0.99	0.11	21,21,21,21	0
55	MG	AA	1642	1/1	0.99	0.06	25,25,25,25	0
55	MG	DA	3114	1/1	0.99	0.03	52,52,52,52	0
55	MG	BA	3129	1/1	0.99	0.08	0,0,0,0	0
55	MG	BA	3081	1/1	0.99	0.04	0,0,0,0	0
55	MG	BA	3132	1/1	0.99	0.15	32,32,32,32	0
55	MG	CA	1640	1/1	0.99	0.09	36,36,36,36	0
55	MG	BA	3082	1/1	0.99	0.10	6,6,6,6	0
55	MG	BA	3134	1/1	0.99	0.04	3,3,3,3	0
55	MG	AA	1613	1/1	0.99	0.06	23,23,23,23	0
55	MG	DA	3053	1/1	0.99	0.03	39,39,39,39	0
55	MG	DA	3123	1/1	0.99	0.04	44,44,44,44	0
55	MG	BA	3049	1/1	0.99	0.03	3,3,3,3	0
55	MG	BA	3186	1/1	0.99	0.19	12,12,12,12	0
55	MG	BA	3085	1/1	0.99	0.04	11,11,11,11	0
55	MG	BA	3050	1/1	0.99	0.07	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3024	1/1	0.99	0.04	3,3,3,3	0
55	MG	BA	3088	1/1	0.99	0.11	29,29,29,29	0
55	MG	BA	3141	1/1	0.99	0.27	0,0,0,0	0
55	MG	BA	3192	1/1	0.99	0.16	11,11,11,11	0
55	MG	AA	1618	1/1	0.99	0.03	34,34,34,34	0
55	MG	BA	3006	1/1	0.99	0.04	13,13,13,13	0
55	MG	AA	1633	1/1	0.99	0.02	35,35,35,35	0
55	MG	DA	3065	1/1	0.99	0.03	41,41,41,41	0
55	MG	DA	3066	1/1	0.99	0.06	45,45,45,45	0
55	MG	BB	201	1/1	0.99	0.03	28,28,28,28	0
55	MG	BB	202	1/1	0.99	0.04	4,4,4,4	0
55	MG	BB	203	1/1	0.99	0.06	7,7,7,7	0
55	MG	BA	3028	1/1	0.99	0.10	3,3,3,3	0
55	MG	DA	3003	1/1	0.99	0.04	66,66,66,66	0
55	MG	BA	3094	1/1	0.99	0.06	20,20,20,20	0
55	MG	BA	3008	1/1	0.99	0.04	0,0,0,0	0
55	MG	DA	3074	1/1	0.99	0.06	47,47,47,47	0
55	MG	BA	3096	1/1	0.99	0.05	2,2,2,2	0
55	MG	BA	3097	1/1	0.99	0.06	0,0,0,0	0
55	MG	BA	3058	1/1	0.99	0.04	15,15,15,15	0
55	MG	DA	3009	1/1	0.99	0.03	69,69,69,69	0
55	MG	AA	1625	1/1	0.99	0.04	51,51,51,51	0
55	MG	BA	3100	1/1	0.99	0.04	9,9,9,9	0
55	MG	DA	3012	1/1	0.99	0.05	39,39,39,39	0
55	MG	AA	1626	1/1	0.99	0.10	26,26,26,26	0
55	MG	BA	3033	1/1	0.99	0.15	0,0,0,0	0
55	MG	BA	3103	1/1	0.99	0.05	7,7,7,7	0
55	MG	BA	3064	1/1	0.99	0.03	0,0,0,0	0
55	MG	DA	3017	1/1	0.99	0.07	39,39,39,39	0
55	MG	BA	3065	1/1	0.99	0.05	1,1,1,1	0
55	MG	CA	1613	1/1	0.99	0.03	17,17,17,17	0
55	MG	BA	3106	1/1	0.99	0.15	0,0,0,0	0
55	MG	BA	3107	1/1	0.99	0.05	3,3,3,3	0
55	MG	DA	3022	1/1	0.99	0.07	43,43,43,43	0
55	MG	DA	3023	1/1	0.99	0.03	60,60,60,60	0
55	MG	BA	3067	1/1	0.99	0.07	0,0,0,0	0
55	MG	BA	3068	1/1	0.99	0.03	1,1,1,1	0
55	MG	BA	3069	1/1	0.99	0.11	64,64,64,64	0
55	MG	AA	1610	1/1	0.99	0.08	51,51,51,51	0
55	MG	BA	3164	1/1	0.99	0.19	6,6,6,6	0
55	MG	BA	3012	1/1	0.99	0.03	0,0,0,0	0
55	MG	BA	3113	1/1	0.99	0.04	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3013	1/1	0.99	0.08	0,0,0,0	0
55	MG	BA	3039	1/1	0.99	0.05	1,1,1,1	0
55	MG	CA	1625	1/1	0.99	0.07	18,18,18,18	0
56	ZN	D4	101	1/1	0.99	0.04	74,74,74,74	0
55	MG	AA	1641	1/1	1.00	0.03	7,7,7,7	0
55	MG	BA	3130	1/1	1.00	0.02	2,2,2,2	0
55	MG	BA	3037	1/1	1.00	0.05	0,0,0,0	0
55	MG	BA	3030	1/1	1.00	0.04	3,3,3,3	0
55	MG	BA	3062	1/1	1.00	0.04	4,4,4,4	0
55	MG	BA	3063	1/1	1.00	0.02	2,2,2,2	0
55	MG	BA	3017	1/1	1.00	0.04	0,0,0,0	0
55	MG	BA	3051	1/1	1.00	0.03	4,4,4,4	0
55	MG	DA	3050	1/1	1.00	0.02	52,52,52,52	0
55	MG	BA	3066	1/1	1.00	0.03	2,2,2,2	0
55	MG	BA	3021	1/1	1.00	0.03	2,2,2,2	0
55	MG	BA	3041	1/1	1.00	0.02	11,11,11,11	0
55	MG	BA	3042	1/1	1.00	0.02	1,1,1,1	0
55	MG	BA	3022	1/1	1.00	0.03	0,0,0,0	0
55	MG	BA	3044	1/1	1.00	0.06	8,8,8,8	0
55	MG	BA	3122	1/1	1.00	0.03	0,0,0,0	0
55	MG	BA	3072	1/1	1.00	0.06	2,2,2,2	0
55	MG	BA	3124	1/1	1.00	0.12	9,9,9,9	0
55	MG	BA	3089	1/1	1.00	0.03	1,1,1,1	0
55	MG	BA	3018	1/1	1.00	0.01	10,10,10,10	0
55	MG	BA	3127	1/1	1.00	0.03	2,2,2,2	0
55	MG	BA	3035	1/1	1.00	0.03	0,0,0,0	0

6.5 Other polymers [i](#)

There are no such residues in this entry.