



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 10:35 am BST

PDB ID : 4U1V
Title : Crystal structure of the E. coli ribosome bound to linopristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-07-16
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

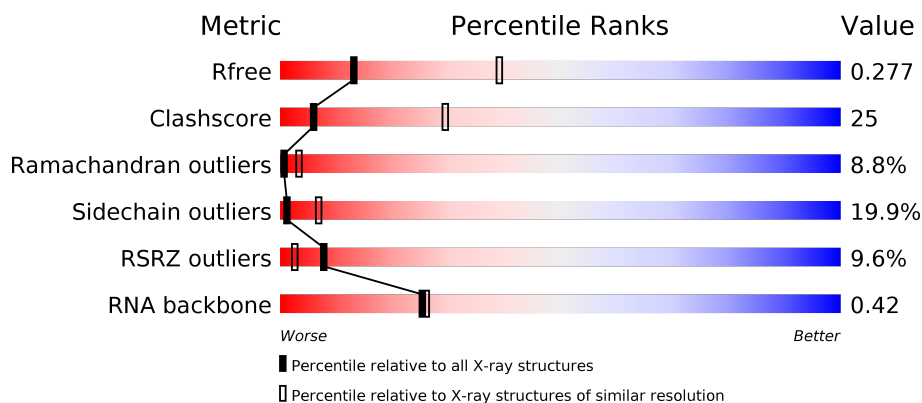
1 Overall quality at a glance

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	<div> <div>23%</div> <div>58%</div> <div>19%</div> <div>•</div> </div>
1	CA	1539	<div> <div>29%</div> <div>53%</div> <div>17%</div> </div>
2	AB	218	<div> <div>24%</div> <div>22%</div> <div>48%</div> <div>25%</div> <div>5%</div> </div>
2	CB	218	<div> <div>32%</div> <div>31%</div> <div>44%</div> <div>22%</div> <div>•</div> </div>

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



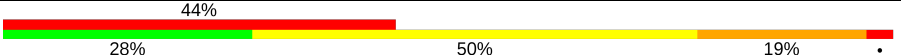
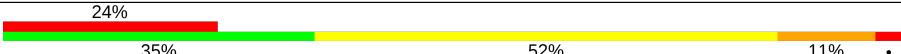
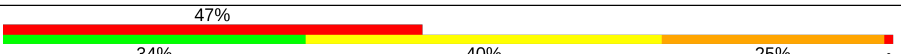

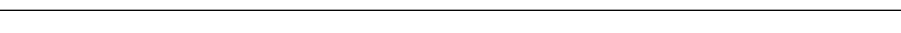
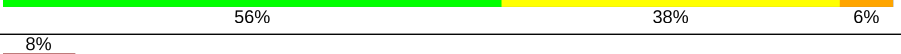




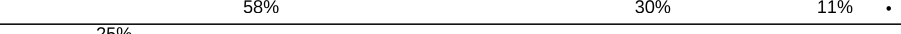


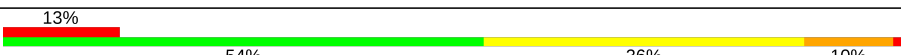
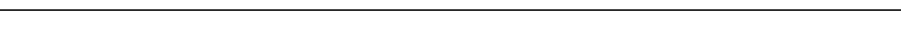





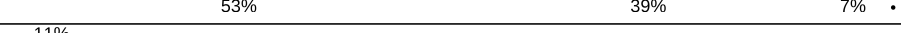

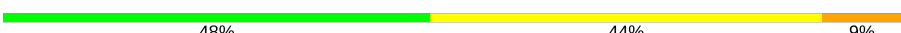
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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	119	
23	DB	119	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD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

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

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

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Mol	Chain	Length	Quality of chain
53	B5	228	
54	B6	7	
54	D6	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MHW	B6	1	-	X	-	-
54	MHW	D6	1	-	X	X	-
55	MG	AA	1627	-	-	-	X
55	MG	AA	1644	-	-	-	X
55	MG	AA	1665	-	-	-	X
55	MG	AA	1667	-	-	-	X
55	MG	AA	1670	-	-	-	X
55	MG	BA	3015	-	-	-	X
55	MG	BA	3098	-	-	-	X
55	MG	BA	3115	-	-	-	X
55	MG	BA	3190	-	-	-	X
55	MG	CA	1655	-	-	-	X
55	MG	DA	3002	-	-	-	X
55	MG	DA	3015	-	-	-	X
55	MG	DA	3016	-	-	-	X
55	MG	DA	3028	-	-	-	X
55	MG	DA	3041	-	-	-	X
55	MG	DA	3061	-	-	-	X
55	MG	DA	3062	-	-	-	X
55	MG	DA	3071	-	-	-	X
55	MG	DA	3072	-	-	-	X
55	MG	DA	3092	-	-	-	X
55	MG	DA	3120	-	-	-	X
55	MG	DA	3132	-	-	-	X
55	MG	DA	3134	-	-	-	X
55	MG	DA	3151	-	-	-	X
55	MG	DA	3158	-	-	-	X
55	MG	DA	3164	-	-	-	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	C	N	O	S	0	0	0
			509	313	99	95	2			
46	DY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a protein called Linopristin.

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

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

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

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

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	194	Total O 194 194	0	0
57	AL	1	Total O 1 1	0	0
57	AN	5	Total O 5 5	0	0
57	AT	2	Total O 2 2	0	0
57	AU	1	Total O 1 1	0	0
57	BA	615	Total O 615 615	0	0
57	BB	14	Total O 14 14	0	0
57	BC	10	Total O 10 10	0	0
57	BD	4	Total O 4 4	0	0
57	BE	4	Total O 4 4	0	0
57	BF	1	Total O 1 1	0	0
57	BG	1	Total O 1 1	0	0
57	BJ	1	Total O 1 1	0	0
57	BL	6	Total O 6 6	0	0
57	BN	2	Total O 2 2	0	0
57	BS	1	Total O 1 1	0	0
57	BU	1	Total O 1 1	0	0
57	B2	1	Total O 1 1	0	0
57	B3	3	Total O 3 3	0	0
57	B4	2	Total O 2 2	0	0
57	CA	189	Total O 189 189	0	0
57	CL	1	Total O 1 1	0	0

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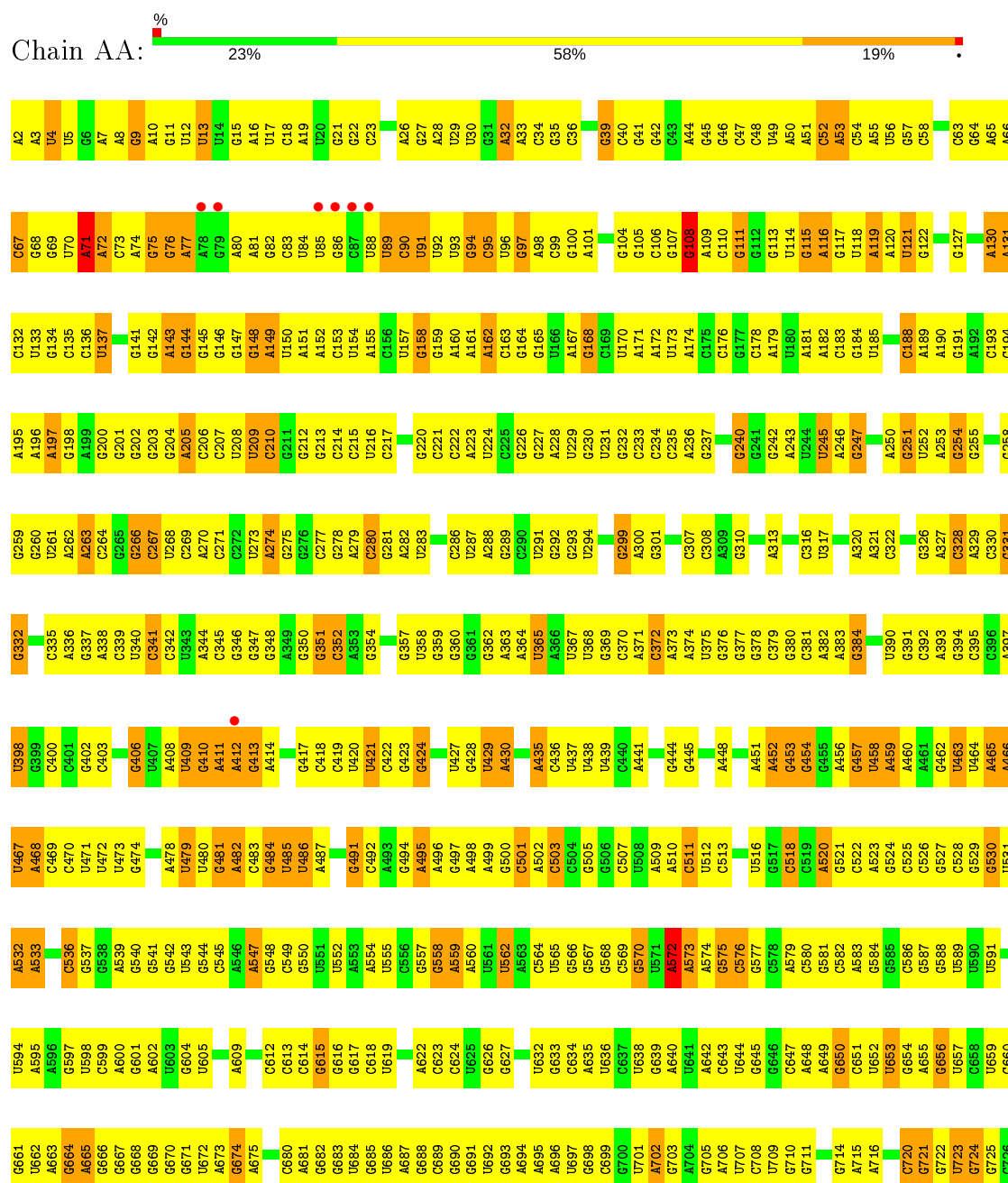
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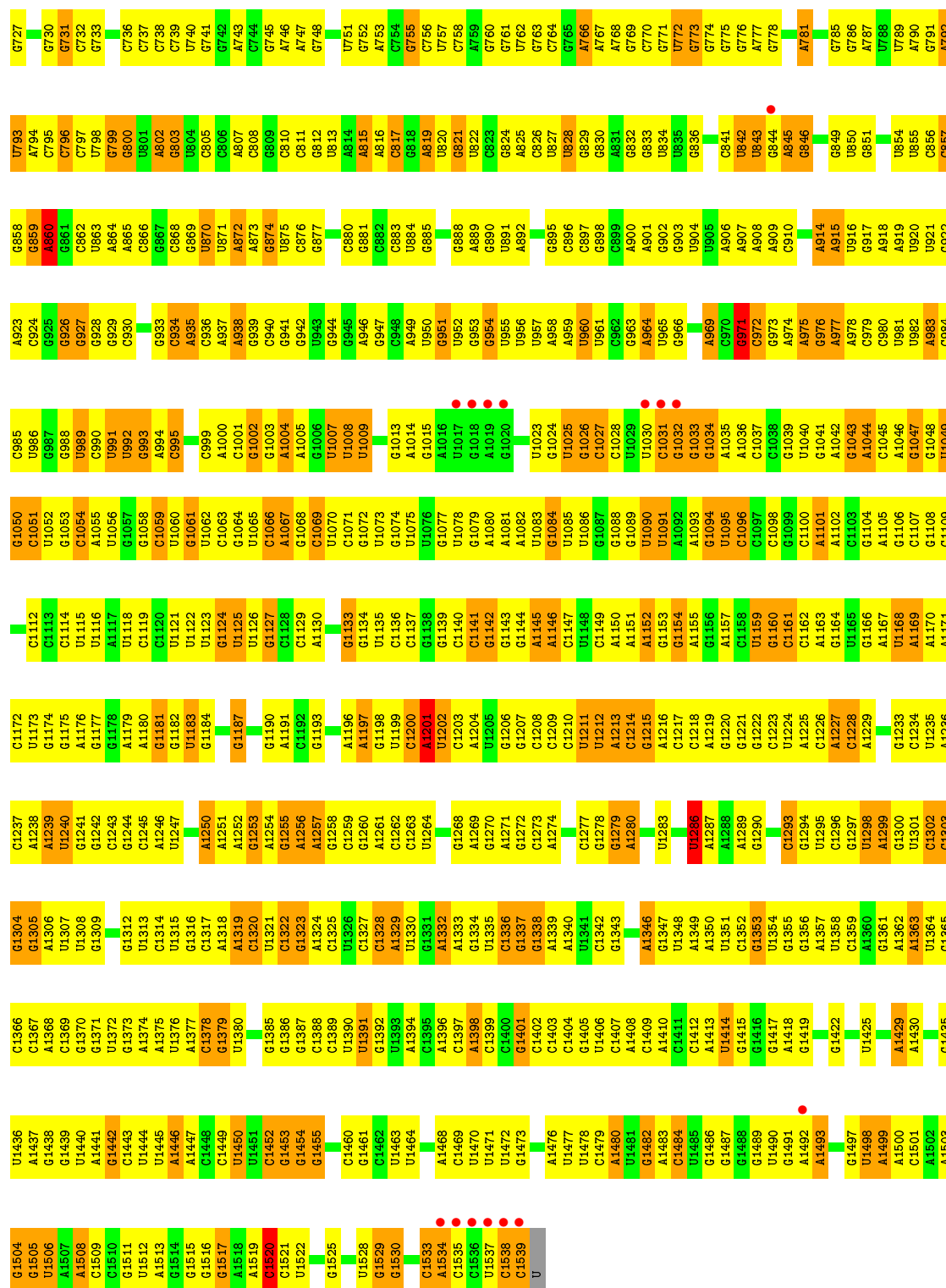
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57	CT	3	Total 3	O 3	0	0
57	CU	2	Total 2	O 2	0	0
57	DA	607	Total 607	O 607	0	0
57	DB	13	Total 13	O 13	0	0
57	DC	9	Total 9	O 9	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	6	Total 6	O 6	0	0
57	DL	5	Total 5	O 5	0	0
57	DN	2	Total 2	O 2	0	0
57	DT	2	Total 2	O 2	0	0
57	DU	1	Total 1	O 1	0	0
57	DV	1	Total 1	O 1	0	0
57	D0	1	Total 1	O 1	0	0
57	D2	2	Total 2	O 2	0	0
57	D3	2	Total 2	O 2	0	0
57	D4	1	Total 1	O 1	0	0

3 Residue-property plots

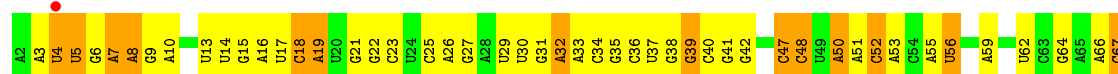
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S rRNA

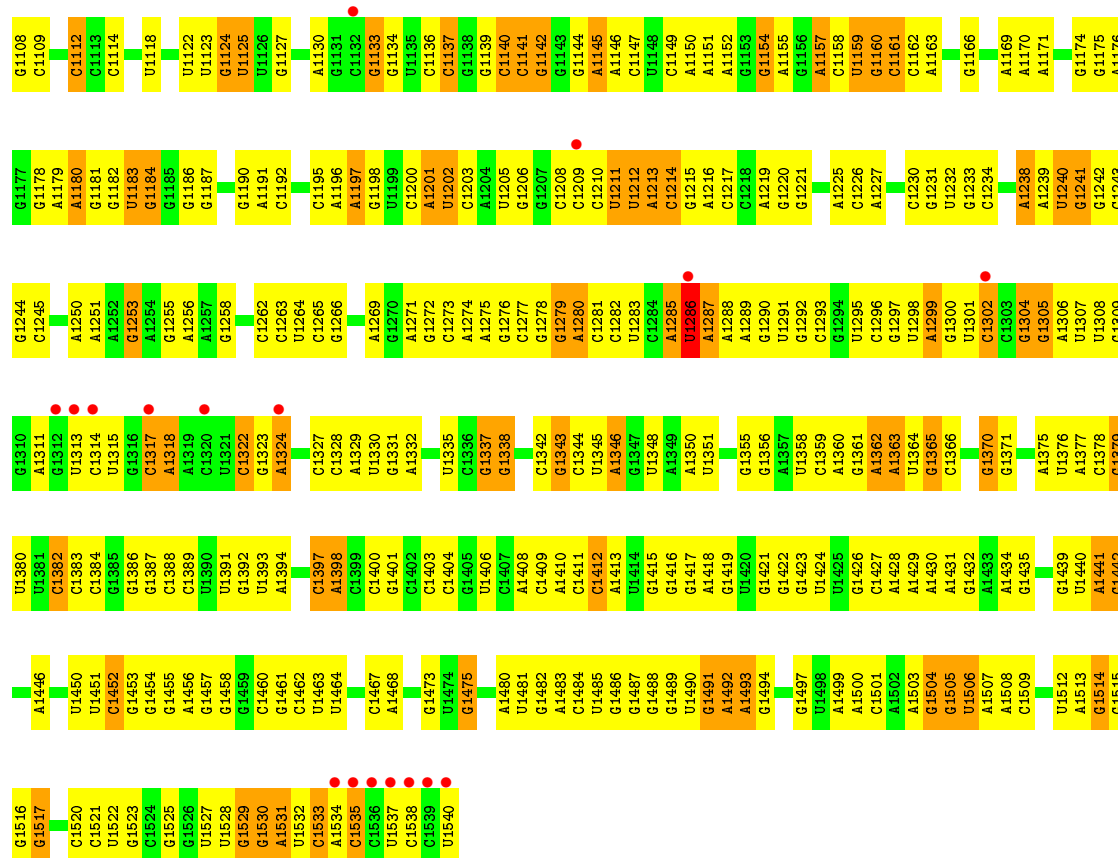




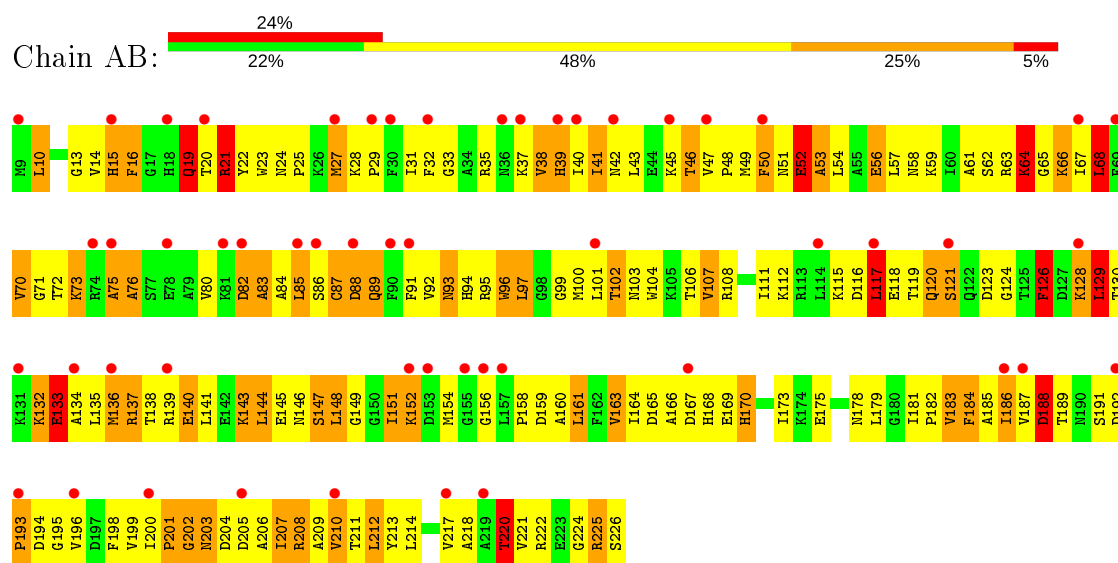
● Molecule 1: 16S rRNA



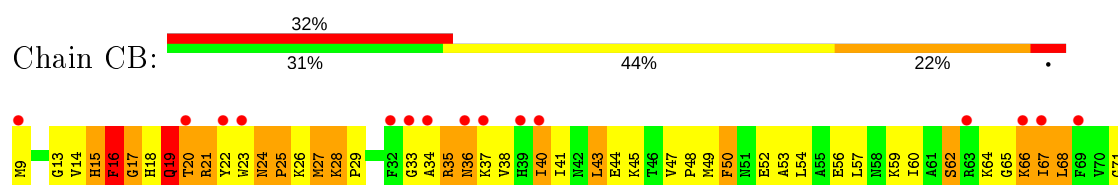
G1045	A877	C912	U842	G774	U707	C637	A559	U486	C418	A353	C280	C210	U137	G68
A1046	A978	A913	U843	G775	C708	U638	A560	G494	G418	G354	G281	G211	G143	G69
G1047	C979	A914	G844	G776	U709	G639	U861	G494	U421	A355	C285	G212	A142	A71
G1048	C980	G917	A845	G777	G710	U640	U862	U421	U421	A356	C286	G213	G143	A72
U1049	U981	G917	G846	G778	G711	U641	A563	G497	C422	G357	C286	G214	G144	A73
G1050	U982	A918	G847	G779	A712	G642	C564	G497	G423	U358	G289	G215	G145	C73
G1051	A983	A919	C948	A780	A715	C643	U655	A498	G424	G359	G289	U216	G146	A74
U1052	U920	U920	G851	A781	A716	U644	G566	A499	G425	G360	G293	U217	G75	G75
G1053	U921	U921	G852	A782	A717	G645	G567	G500	U426	G361	G293	U218	U150	G76
C1054	G922	G922	G853	A783	U717	G646	G568	G501	U427	G362	U294	U219	A151	A77
A1055	G923	G923	G854	A784	U718	G647	C569	A502	U428	U363	U295	C221	A152	A78
U1060	G926	G926	U854	A785	G719	G650	G570	C503	U429	U364	U296	C222	G153	G79
G1061	G927	G927	U855	A786	C720	C651	U571	C504	A430	A365	G297	A223	U154	A80
U1062	G928	G928	G856	A787	G721	U652	U572	G505	A431	U367	A298	U224	A155	A81
C1063	G929	G929	G857	A788	G722	U653	A573	G506	A432	U368	G299	G227	U156	G82
U1064	G930	G930	G858	A789	U723	U654	A574	G507	A433	U369	G300	G228	C188	C83
G1065	G931	G931	A860	A790	G724	U655	C575	A509	A435	C370	U304	A228	G158	U84
C1066	G932	G932	G861	A791	U725	U656	C576	A510	C436	A371	G305	A229	G159	U85
A1067	G933	G933	C862	A792	A728	C658	C577	C511	U437	C372	G306	A230	A160	G86
G1068	G934	G934	U863	A793	A729	U659	C578	U512	U438	A373	A306	A231	A161	G87
C1069	A935	A935	G864	A794	G730	C660	C579	C513	U439	A374	C307	G237	A162	U88
U1070	C936	C936	A865	A795	G731	U661	C580	C514	C440	U375	C308	A232	C163	
G1071	A937	A937	G866	A796	G732	U662	C581	C515	C441	G376	A309	U233	G164	U91
C1072	A938	A938	G867	A797	G733	G663	C582	C516	G442	G377	G310	G240	U92	U92
U1073	G939	G939	G868	A798	G734	U664	C583	C517	C443	G378	G311	G241	U93	U93
G1074	C940	C940	G869	A799	C735	A665	C584	A520	G444	C379	A313	G242	G188	G94
U1075	G941	G941	U870	A800	G736	G666	C585	G521	G445	C380	C314	U244	C189	C95
G1076	G942	G942	U871	A801	C737	U667	C586	C522	G446	G381	A315	U245	U170	U96
U1077	G943	G943	A872	A802	G738	G668	C587	C523	G447	C382	C316	A246	A171	G97
G1078	A944	A944	G874	A803	U740	A673	C588	U534	U458	C383	U317	G247	A172	A98
U1079	G945	G945	A878	A804	G741	G674	C589	A535	A459	G384	G318	G248	U173	C99
C1080	G946	G946	G879	A805	G742	A675	C590	C536	A460	C385	G319	C249	C176	U103
U1081	G947	G947	A880	A806	G743	A676	C591	G537	G461	U387	A321	U250	A179	G104
G1082	A949	A949	G881	A807	A744	U677	C592	A532	G462	U388	G320	U251	G105	G105
U1083	U952	U952	C882	A808	G745	U678	C593	A533	G463	U389	G321	U252	G106	G106
G1084	G953	G953	G883	A809	G746	C679	C594	U534	U464	U390	G322	U253	G107	G107
U1085	U954	U954	A884	A810	G747	C680	C595	A535	A465	U391	G323	G254	G108	G108
C1086	U955	U955	G885	A811	G748	A681	C596	A536	A466	C392	G324	G255	A109	A109
U1087	U956	U956	G886	A812	A749	G682	C597	C537	U467	A393	G325	G256	C110	C110
G1088	U957	U957	G887	A813	C750	U683	C598	G538	U468	C394	G326	G257	G111	G111
U1089	U958	U958	G888	A814	U751	U684	C599	A539	C469	C395	G327	G258	G112	G112
C1090	G959	G959	G889	A815	G754	G685	C600	A540	U469	C396	G328	G259	G115	G115
U1091	U960	U960	G890	A816	G755	U686	C601	A541	U470	C397	G329	G260	A116	A116
G1092	U961	U961	G891	A817	C756	A687	C602	G542	U471	U398	G330	G261	G117	G117
A1093	C962	C962	C892	A818	C757	G688	A621	U543	U472	G399	G331	U262	A189	A189
G1094	G963	G963	G893	A819	U757	C689	A622	C544	C469	G402	G332	G263	A196	A196
C1095	U964	U964	G894	A820	G758	G690	C623	C545	G474	C403	G333	G264	A197	A120
G1096	U965	U965	G895	A821	C759	G691	C624	A546	U475	G404	G334	G265	G198	U121
C1097	G966	G966	A900	A822	G760	U692	C625	A547	C476	U405	G335	G266	G199	A122
U1098	C967	C967	G901	A823	G761	G693	U626	G548	U477	G406	U340	G267	G200	G200
G1099	U968	U968	G902	A824	G765	A694	G627	C549	C477	U407	G345	G268	G201	G127
C1100	G969	G969	G903	A825	U766	G695	G628	G550	U478	A408	C346	G269	G202	G128
A1101	U970	U970	G904	A826	A767	G700	G629	U551	U479	U409	G347	A270	G203	G129
C1102	G971	G971	A906	A827	G768	U701	A630	U552	U480	G410	G348	C271	G204	A130
U1103	U972	U972	G907	A828	G769	U702	C631	U553	G481	A411	G349	C272	G205	A131
G1104	G973	G973	A908	U828	C770	G703	U632	A554	A482	A412	C350	A274	C206	A132
A1105	U974	U974	G909	A829	G771	A704	G633	C556	C483	A413	G351	G275	C207	G134
C1106	G975	G975	C910	A830	U772	G705	G634	G557	U484	A414	C352	G276	U208	C135
G1107	G976	G976	U911	A831	G773	A706	U636	G558	U485	A415			U209	C136

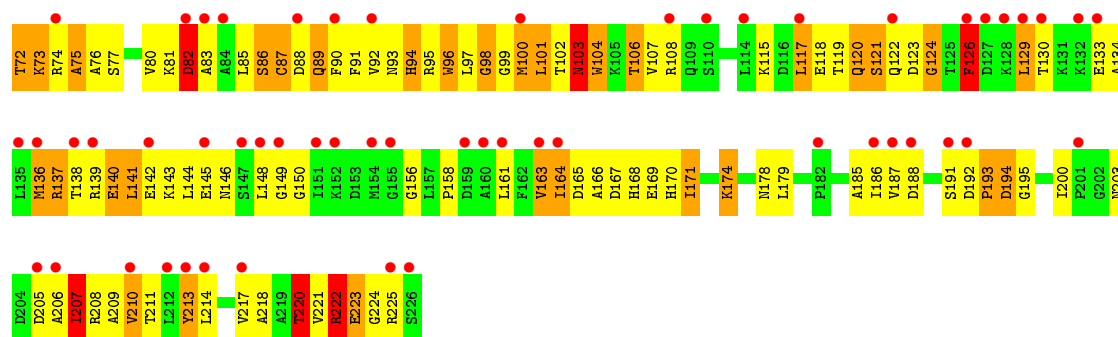


• Molecule 2: 30S ribosomal protein S2

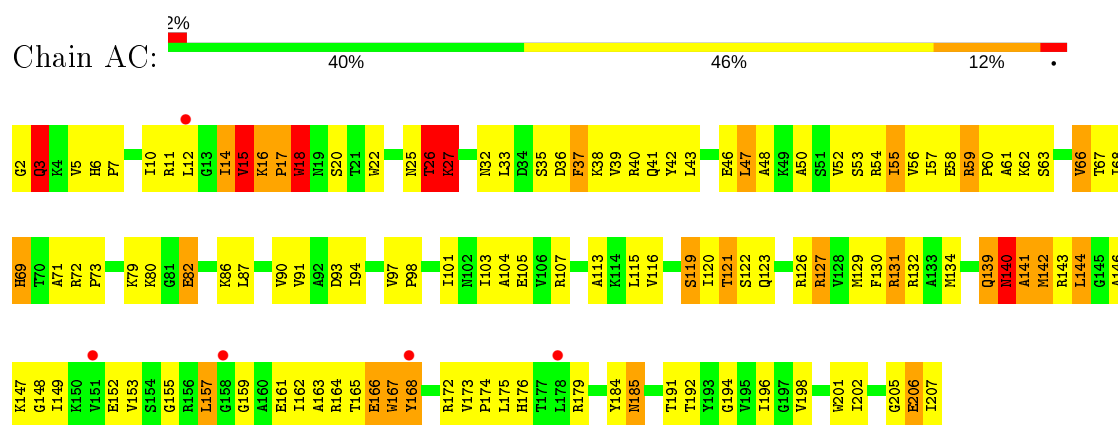


• Molecule 2: 30S ribosomal protein S2

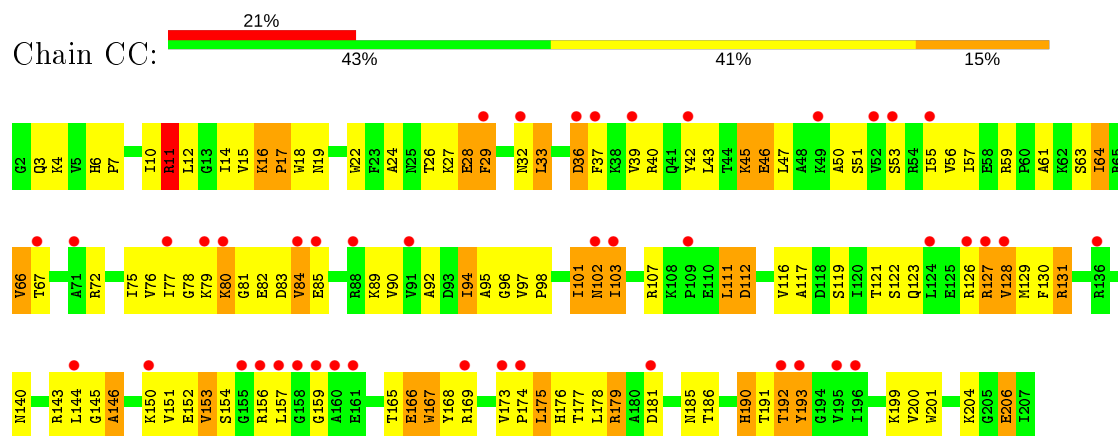




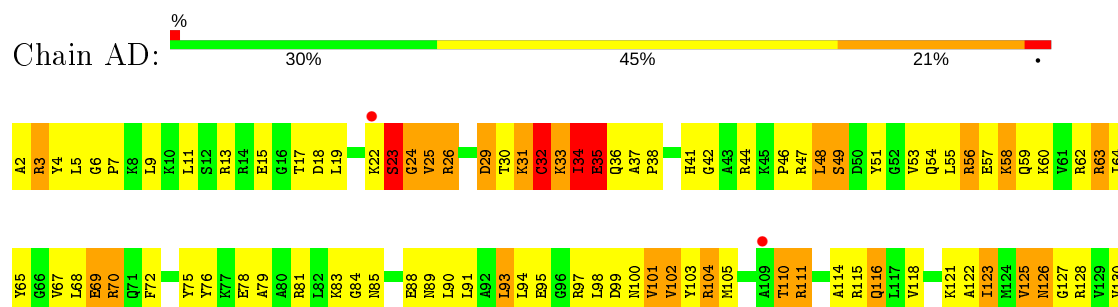
• Molecule 3: 30S ribosomal protein S3

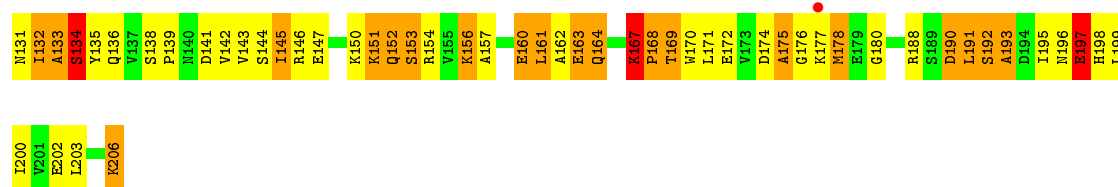


• Molecule 3: 30S ribosomal protein S3

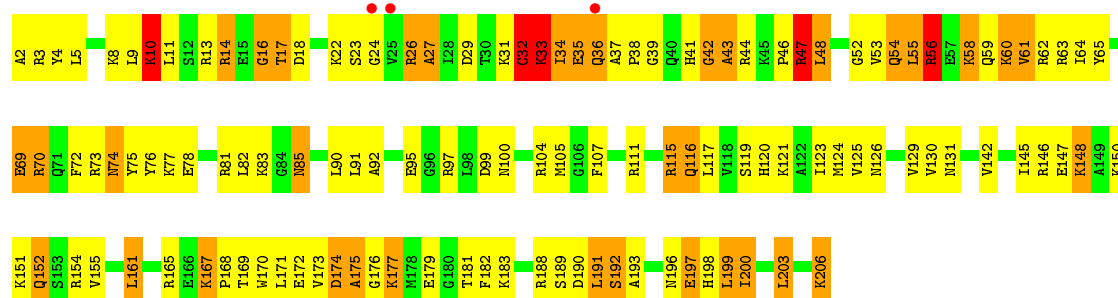
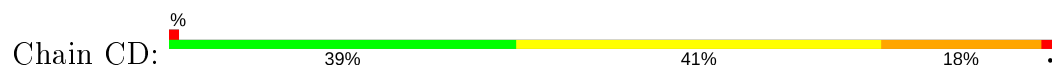


• Molecule 4: 30S ribosomal protein S4

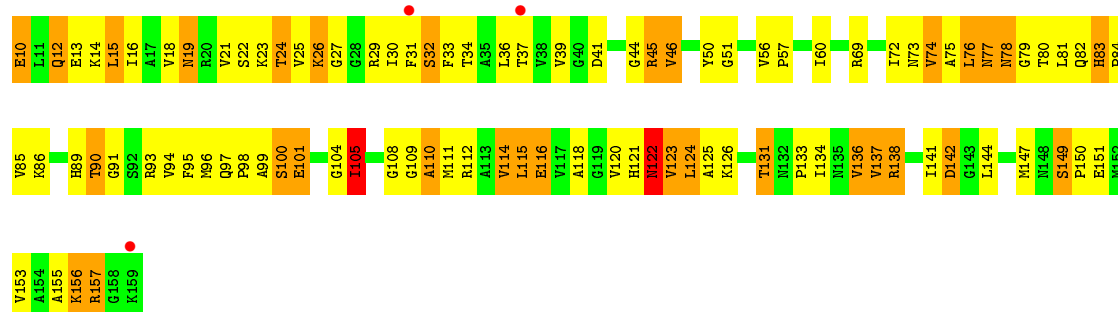




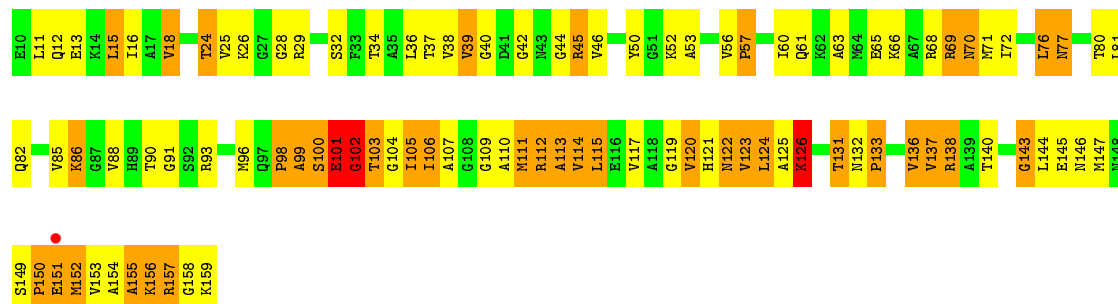
• Molecule 4: 30S ribosomal protein S4



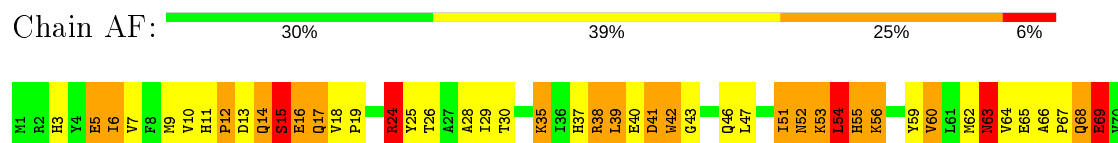
• Molecule 5: 30S ribosomal protein S5



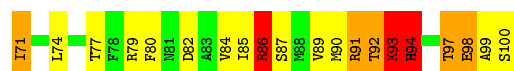
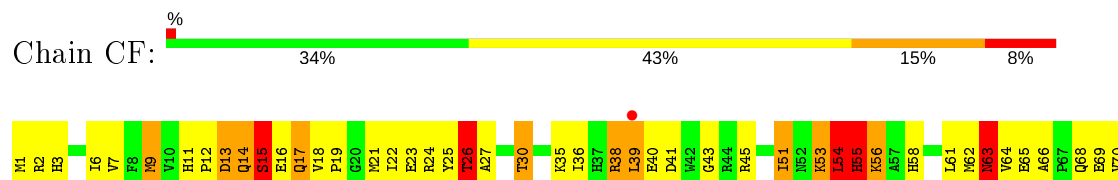
• Molecule 5: 30S ribosomal protein S5



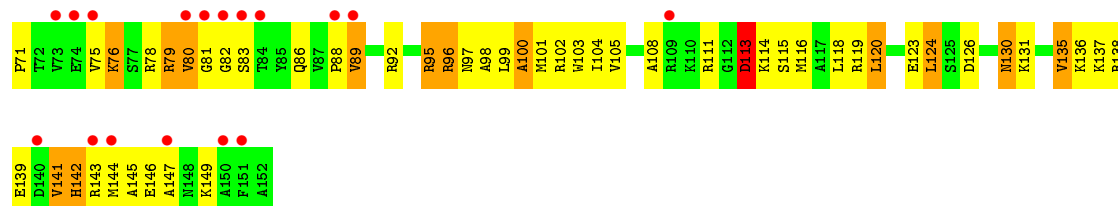
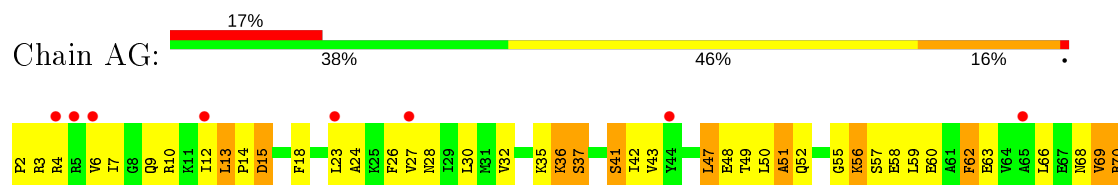
• Molecule 6: 30S ribosomal protein S6



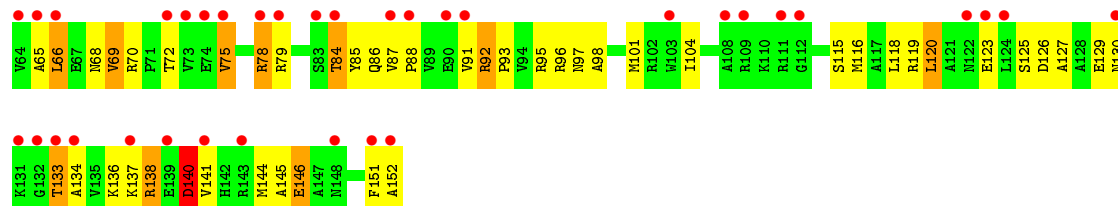
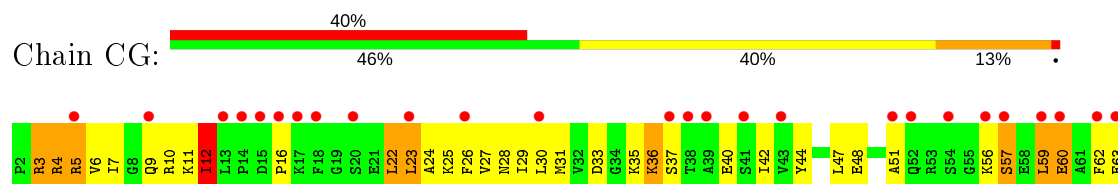
- Molecule 6: 30S ribosomal protein S6



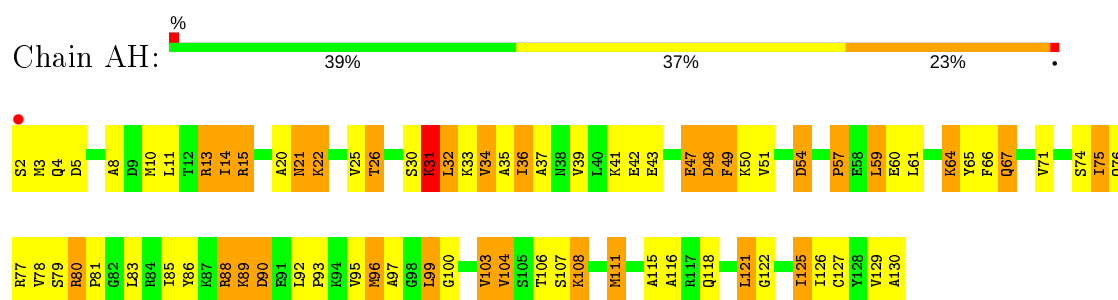
- Molecule 7: 30S ribosomal protein S7



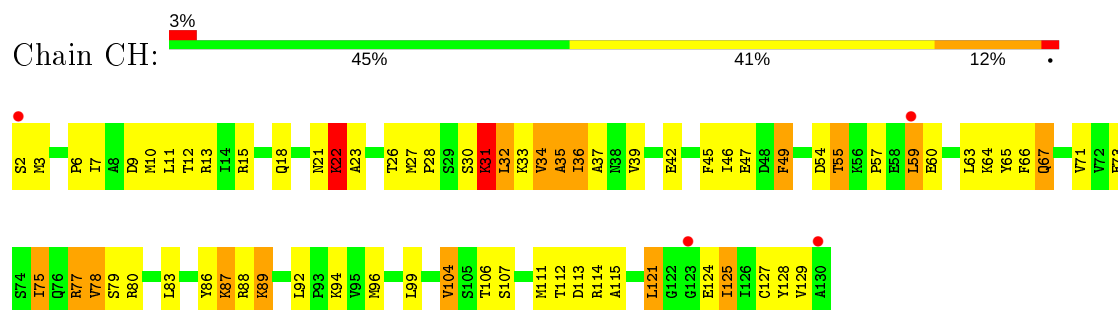
- Molecule 7: 30S ribosomal protein S7



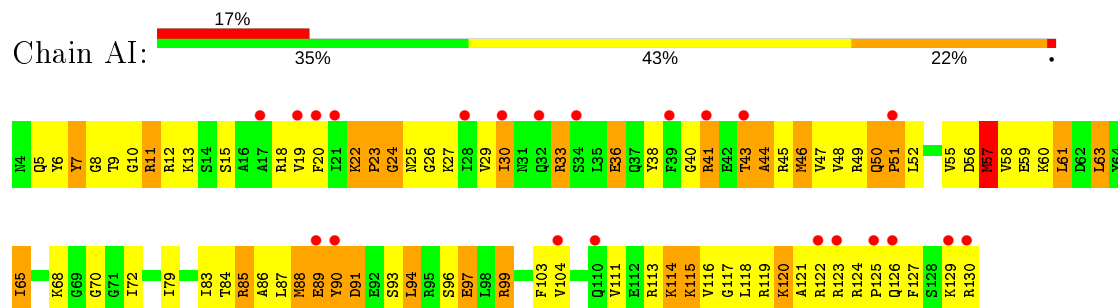
- Molecule 8: 30S ribosomal protein S8



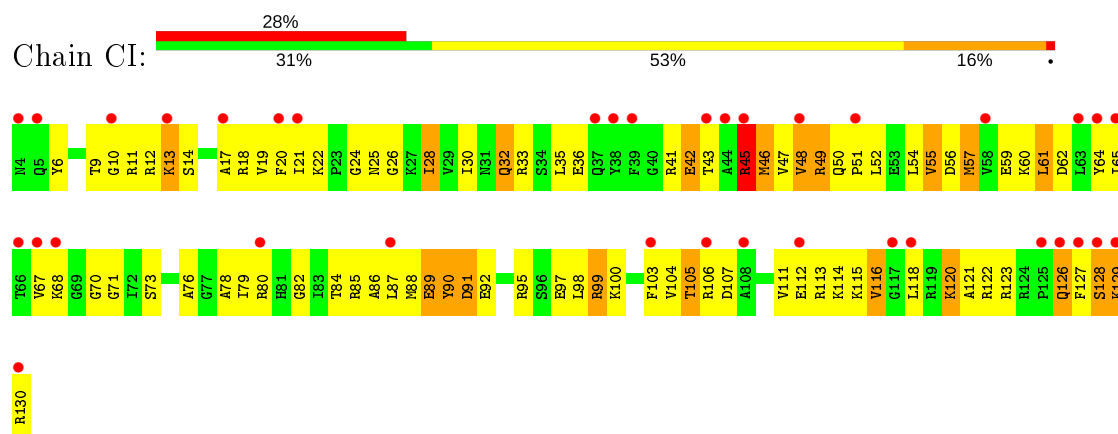
- Molecule 8: 30S ribosomal protein S8



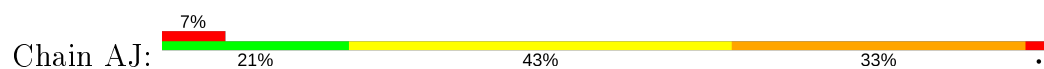
- Molecule 9: 30S ribosomal protein S9

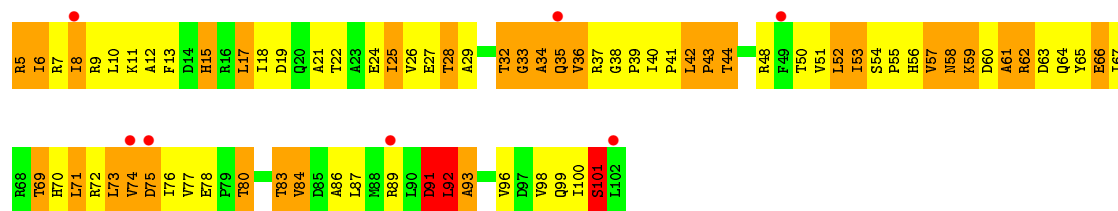


- Molecule 9: 30S ribosomal protein S9

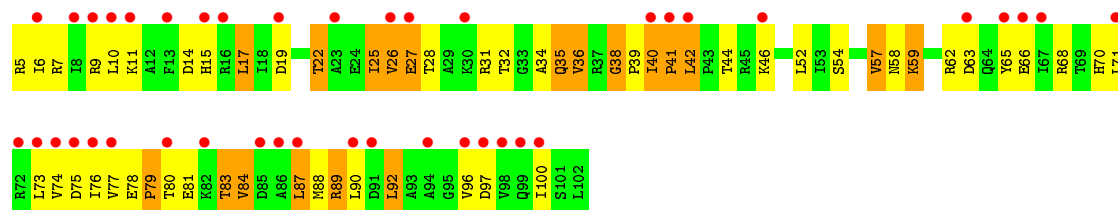
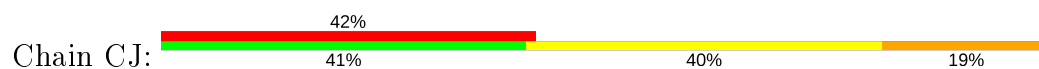


- Molecule 10: 30S ribosomal protein S10

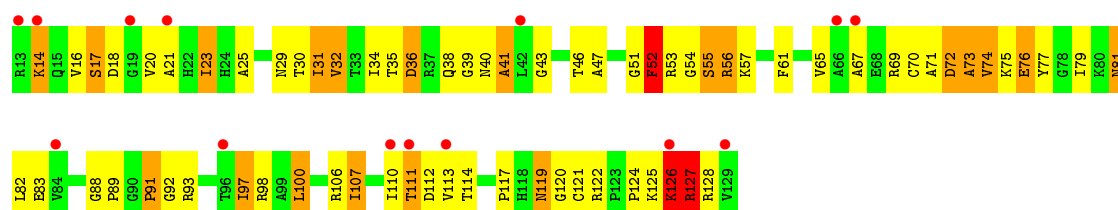




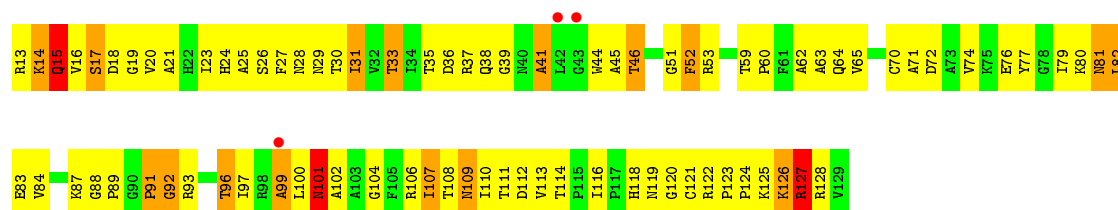
• Molecule 10: 30S ribosomal protein S10



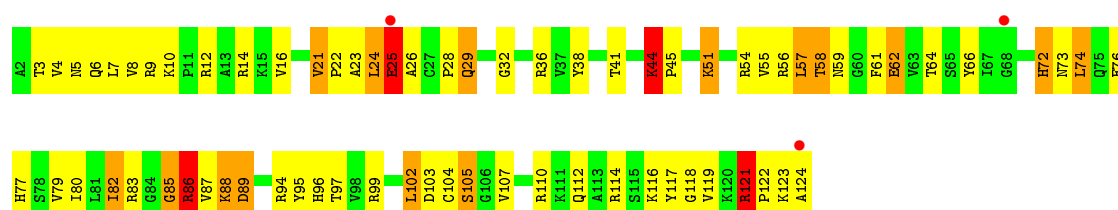
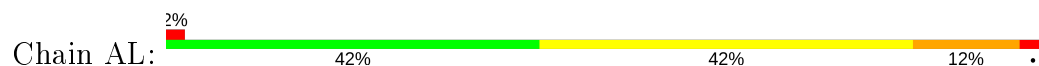
• Molecule 11: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S11

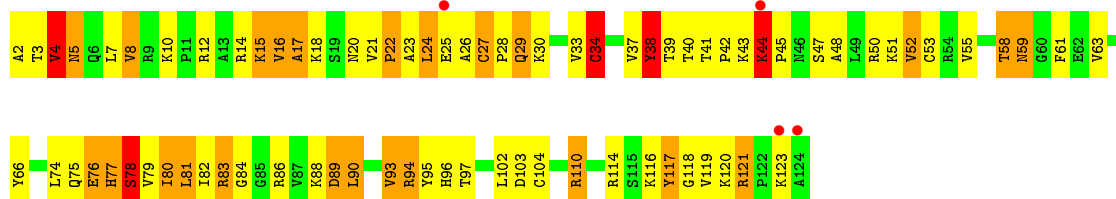


• Molecule 12: 30S ribosomal protein S12



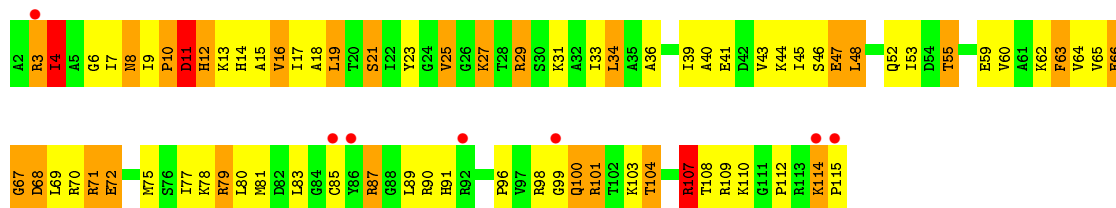
- Molecule 12: 30S ribosomal protein S12

Chain CL: 



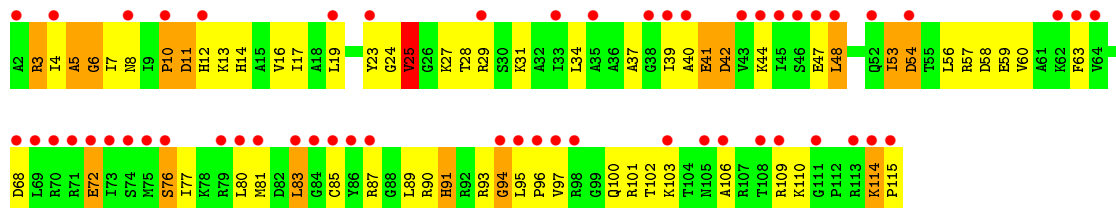
- Molecule 13: 30S ribosomal protein S13

Chain AM: 



- Molecule 13: 30S ribosomal protein S13

Chain CM: 

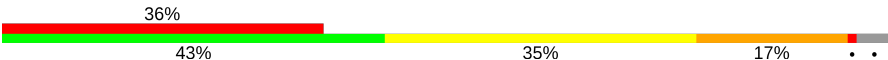


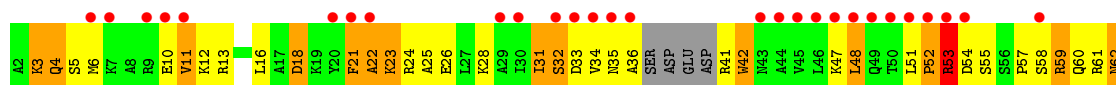
- Molecule 14: 30S ribosomal protein S14

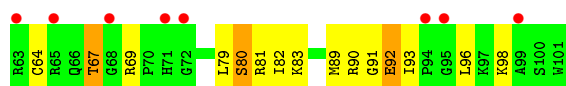
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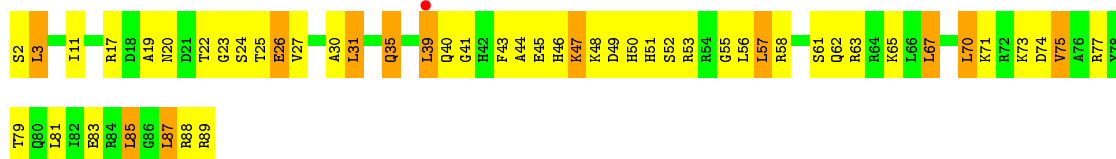
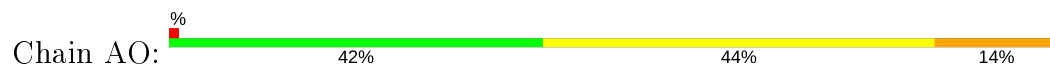
- Molecule 14: 30S ribosomal protein S14

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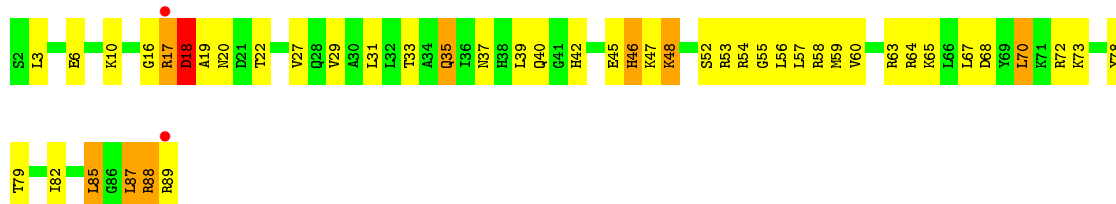




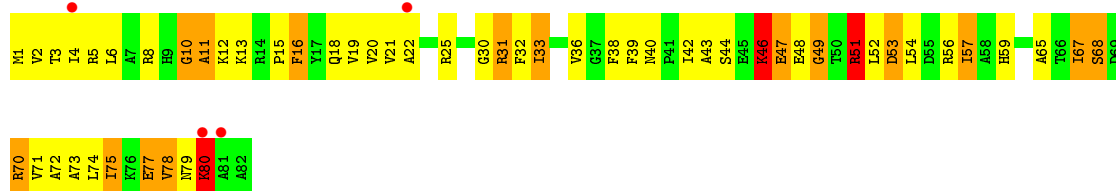
- Molecule 15: 30S ribosomal protein S15



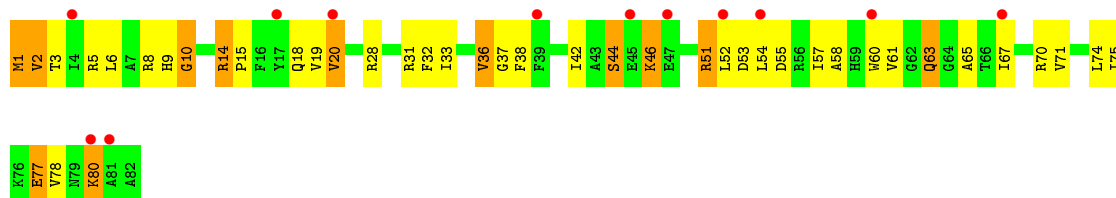
- Molecule 15: 30S ribosomal protein S15



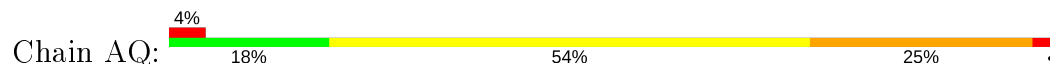
- Molecule 16: 30S ribosomal protein S16

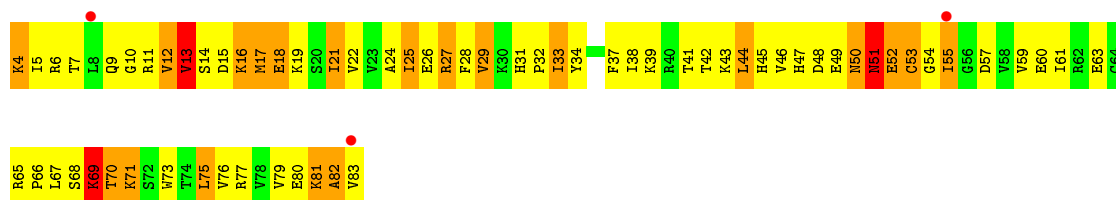


- Molecule 16: 30S ribosomal protein S16

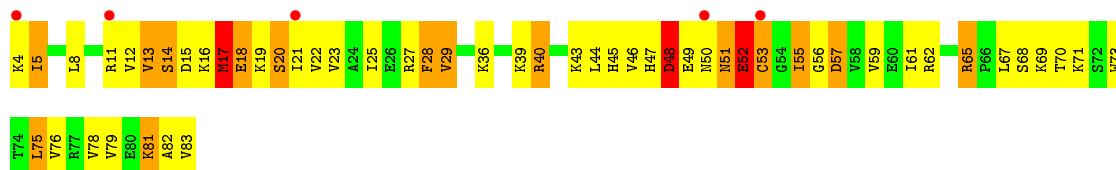


- Molecule 17: 30S ribosomal protein S17





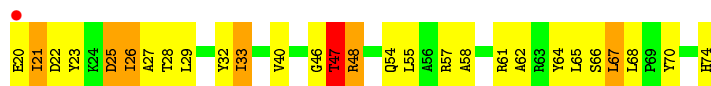
• Molecule 17: 30S ribosomal protein S17



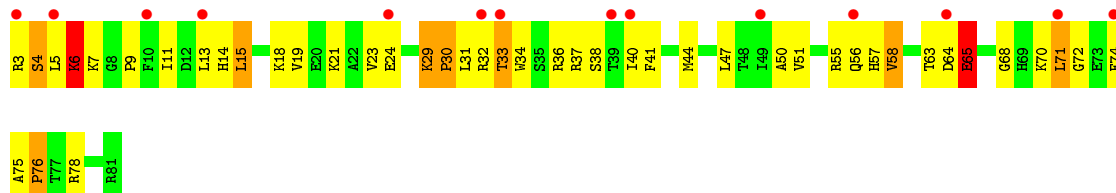
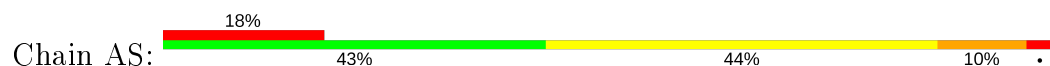
• Molecule 18: 30S ribosomal protein S18



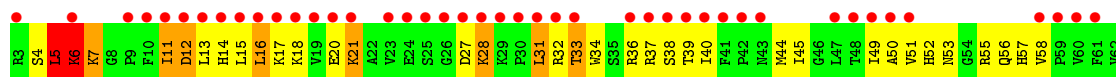
• Molecule 18: 30S ribosomal protein S18

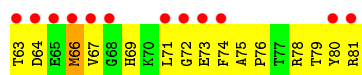


• Molecule 19: 30S ribosomal protein S19

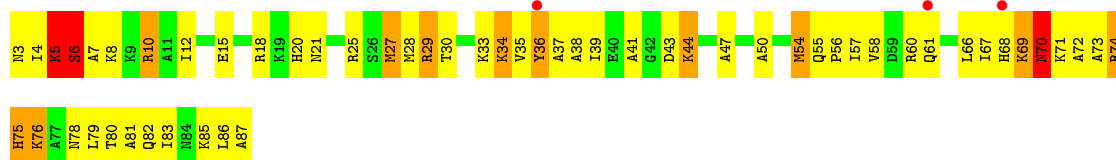


• Molecule 19: 30S ribosomal protein S19





• Molecule 20: 30S ribosomal protein S20



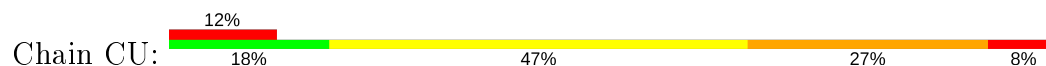
• Molecule 20: 30S ribosomal protein S20



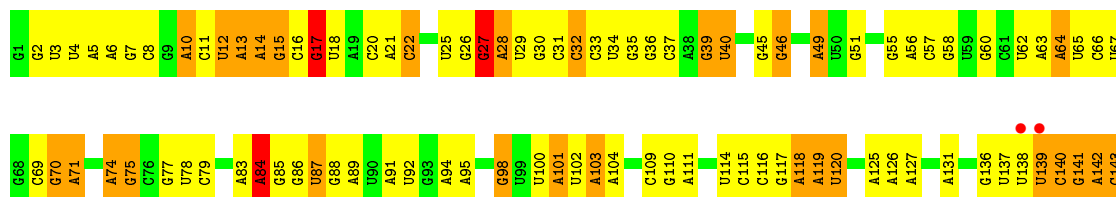
• Molecule 21: 30S ribosomal protein S21



• Molecule 21: 30S ribosomal protein S21

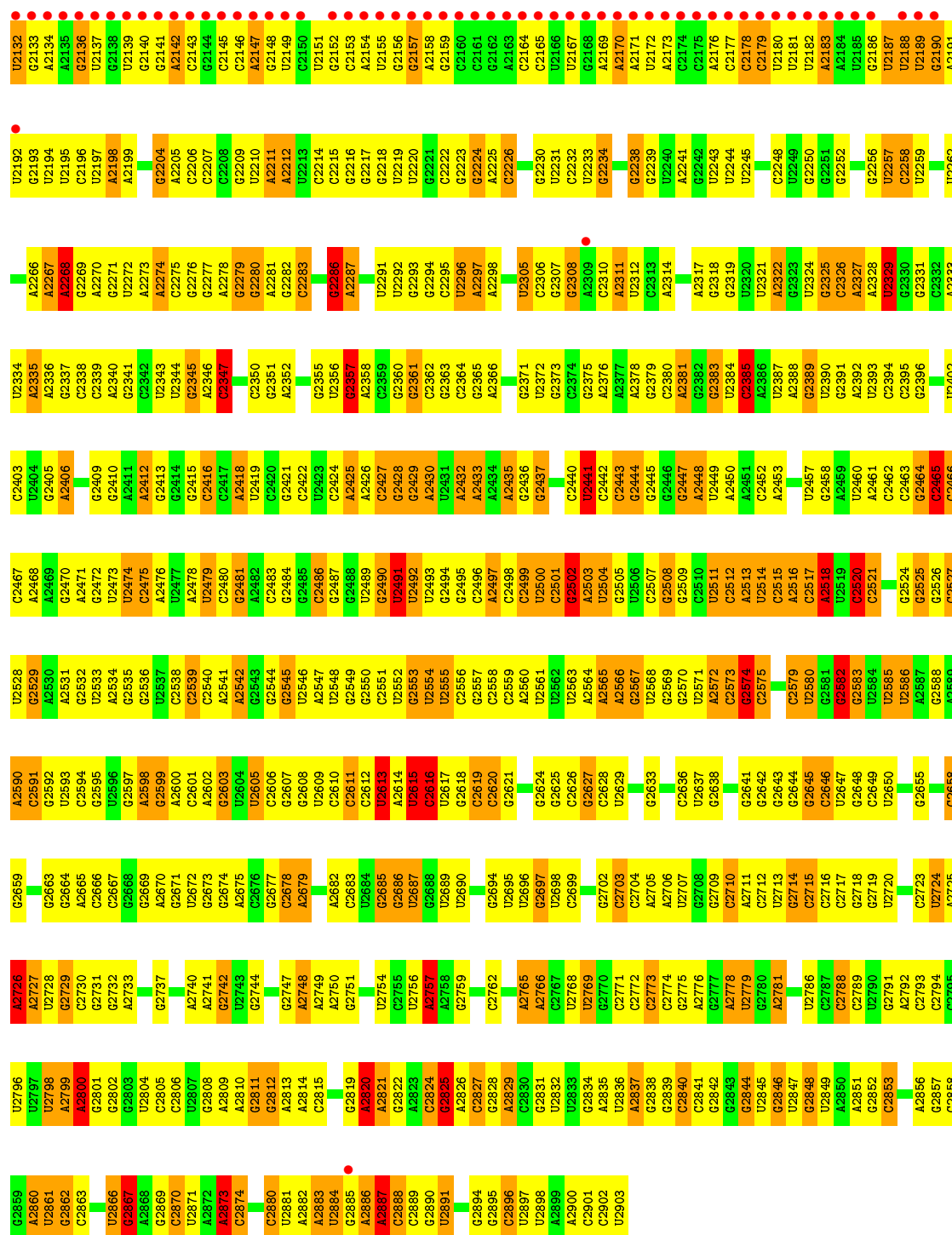


• Molecule 22: 23S rRNA



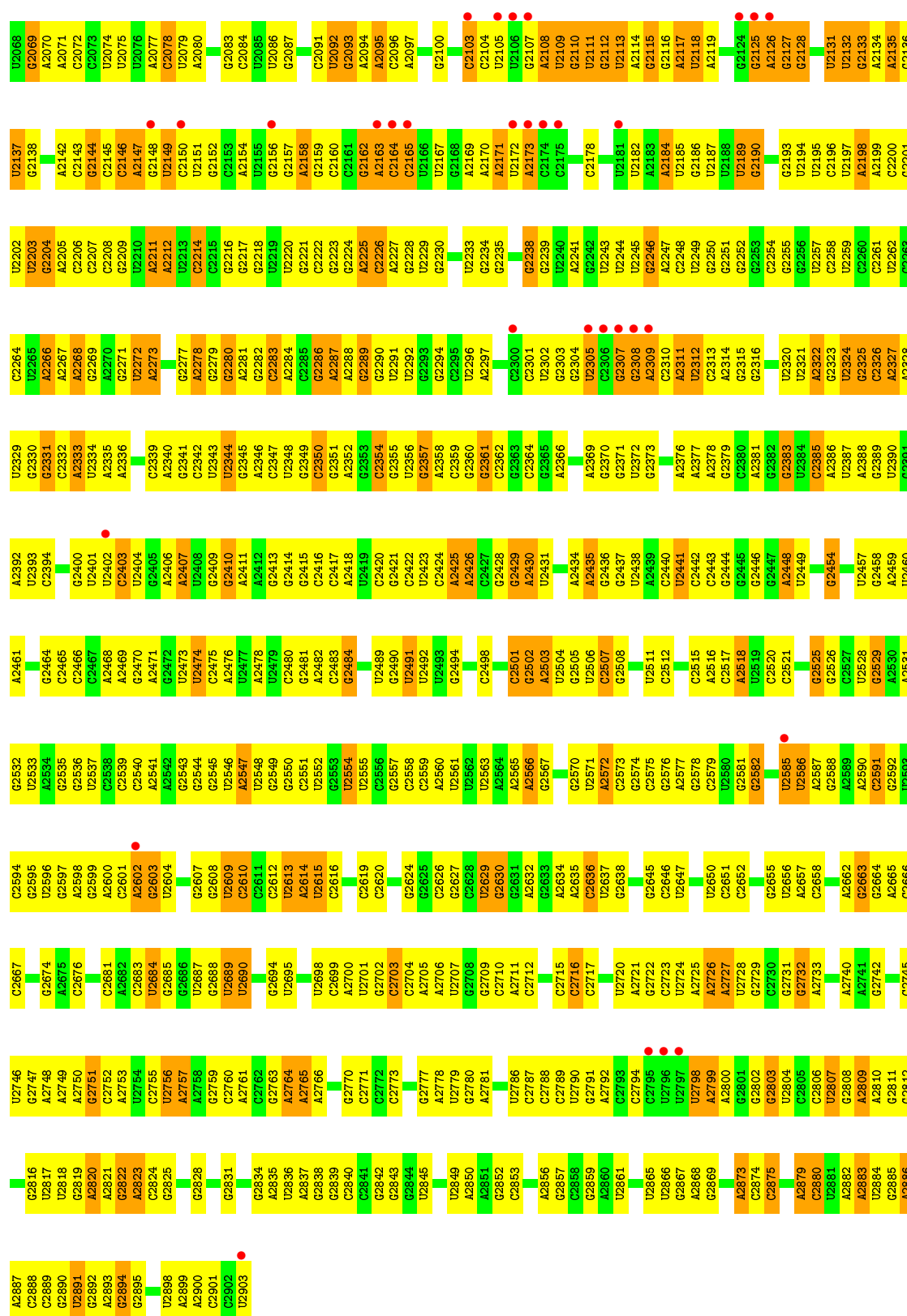
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C1134	A1073	U1004	A861	A861	A794	A734	C660	U596	C530	G468	G388	C316	G230	U150
C1135	G1074	C1005	G940	G864	C795	A735	A661	G597	C531	G469	G389	G317	G231	C151
G1136	C1075	C1006	A941	C865	C796	G736	G662	U598	A532	U350	G318	G319	U235	U158
G1137	G1076	C1007	G942	C866	C797	C737	G663	A599	A533	A391	U350	A320	C236	G159
G1138	A1077	A1008	A943	A866	G797	G738	G664	G600	U534	U397	G319	A321	C237	U160
G1139	U1078	A1009	C944	C867	A800	G739	U665	C601	G535	U397	G320	U322	G242	A161
C1140	C1079	A1010	A945	U868	G801	C740	A666	A602	U536	G400	G321	A322	U243	U162
U1141	A1080	G1011	G946	G869	A802	U741	U667	G603	G537	G476	G322	A323	U244	G163
A1142	U1081	U1012	A947	U870	A803	U742	G604	G604	A538	A477	G323	A324	G245	C164
A1143	U1082	C1013	C948	A877	A804	A743	G605	G606	C540	U403	G324	G325	G246	G165
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G1154	A1088	U1019	G959	C885	G812	U750	A677	G612	U546	C414	A334	G334	A256	G180
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G2116		C1985	A1916	G1849	U1779	U1637		C1499	A1433	A1365		
A2117	G2052	C1986	U1917	G1850	C1708	A1638	A1570	G1500	A1434	A1366	C1305	G1245
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A2119	A2054	C1990	A1919	U1852	U1713	G1639	A1572	A1502	A1436	A1368	A1307	A1247
G2120	C2055	U1991	A1920	U1853	G1715	A1640	G1573	A1503	G1437		A1308	G1248
	G2056	G1992	C1920	A1854	U1716	G1645	U1576	A1504	U1438	G1371	U1249	
G2121	G2057	U1993	G1921	U1855	U1717	C1646	C1577	A1505	A1439	U1372	G1250	
U2122	A2058	C1994	U1922	U1856	A1718	G1647	U1578	U1506	A1439	U1373	C1251	G1251
G2123	C2059	U1995	U1923	G1857	G1719	U1648	A1579	C1507	U1440	G1374	U1312	G1252
G2124	A2060	C1996	G1924	A1858	A1791	G1649	A1580	U1508	G1441	U1375	A1253	A1253
A2126	G2061	C1997	U1925	U1859	C1792	A1650	G1581	U1509	U1442	C1376	C1315	A1254
G2127	A2062	U1998	U1926	U1859	G1793	G1651	C1582	G1510	U1443	G1377	U1355	U1255
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G2128	C2064	C2000	A1928	U1864	U1795	A1652	U1584	C1512	G1445	U1379	U1318	G1257
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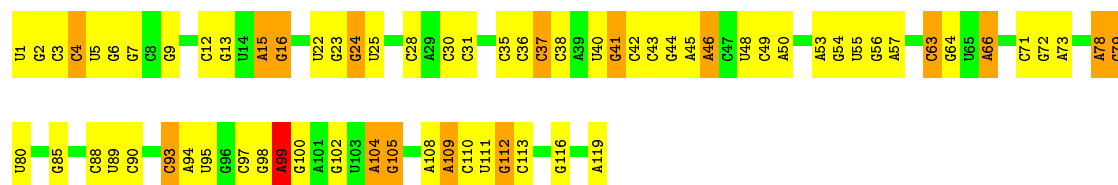


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C2006	G1935	U1865	G1721	U1648	C1582	G1500	G1432	G1368	A1302	G1227	A1155	U1082
C2008	A1936	G1866	U1722	G1649	A1583	U1504	A1433	G1369	G1303	C1229	A1156	U1084
A2009	G1937	G1867	C1726	G1651	U1584	A1509	A1434	G1370	A1304	A1230	G1157	A1084
G2010	A1938	C1868	G1727	A1652	C1585	G1510	G1435	G1371	C1305	U1231	G1162	A1085
U2011	U1939	G1869	C1728	G1653	G1587	U1513	C1437	U1372	A1308	G1236	G1163	A1086
A2012	C1940	A1870	U1729	A1654	G1588	G1514	A1438	A1373	G1309	G1237	G1164	G1087
A2013	U1941	A1871	G1730	C1655	U1589	U1515	A1439	G1374	G1310	A1238	G1165	A1088
A2014	A1942	A1872	A1731	A1656	U1590	A1515	A1440	U1375	G1311	G1239	G1166	A1089
A2015	G1943	G1873	G1732	G1660	A1591	U1519	G1441	G1376	G1312	G1240	G1170	A1090
U2016	U1944	A1804	G1733	G1661	C1592	U1520	U1442	G1377	U1312	U1241	G1171	G1091
U2017	C1945	C1806	U1734	U1662	U1593	G1519	U1443	A1378	U1313	U1242	G1172	C1092
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A2020	U1948	A1809	A1737	A1665	A1596	U1522	C1446	G1381	U1316	C1245	A1175	A1095
C2021	G1949	A1810	U1738	A1666	A1597	U1523	C1447	G1382	U1317	A1246	U1176	A1096
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G2046	G1970	G1831	G1766	C1694	A1619	A1548	U1474	G1408	U1340	U1267	U1201	A1127
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G2050	G1983	G1835	U1770	G1703	G1626	C1556	G1478	A1413	C1351	U1273	C1208	A1133
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A2062	C1998	U1857	A1787	U1716	C1644	U1578	A1494	G1429				
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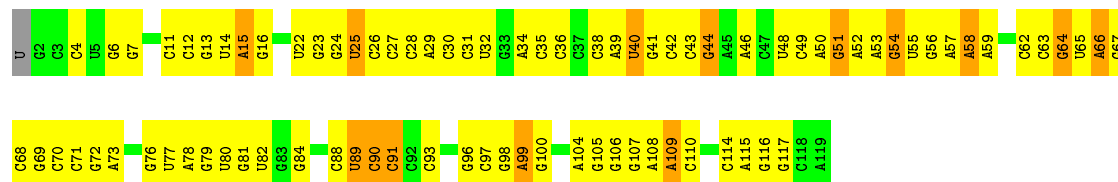
• Molecule 23: 5S rRNA

Chain BB: 42% 44% 13%



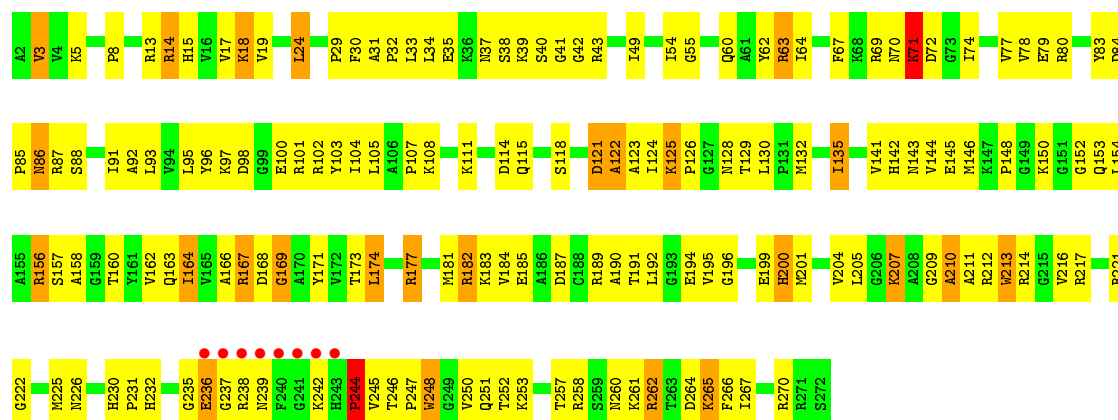
• Molecule 23: 5S rRNA

Chain DB: 29% 59% 12%



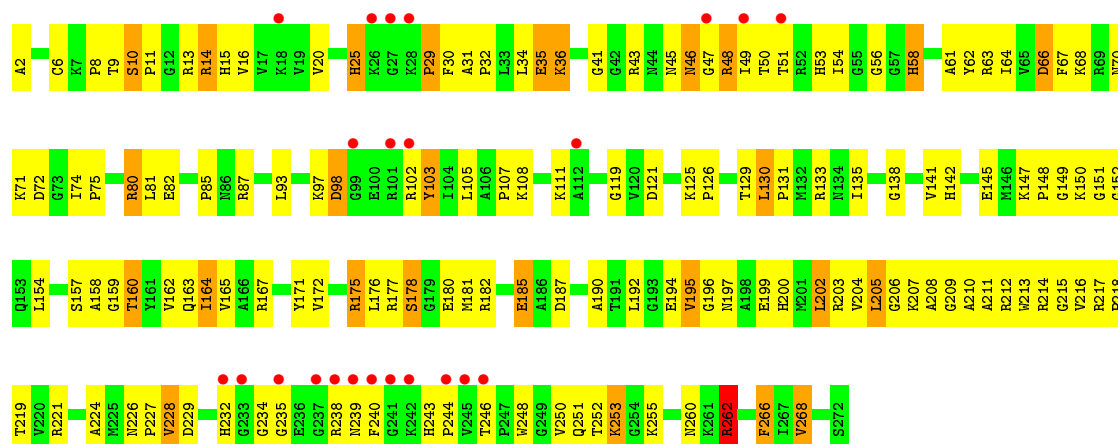
• Molecule 24: 50S ribosomal protein L2

Chain BC: 3% 40% 50% 9%

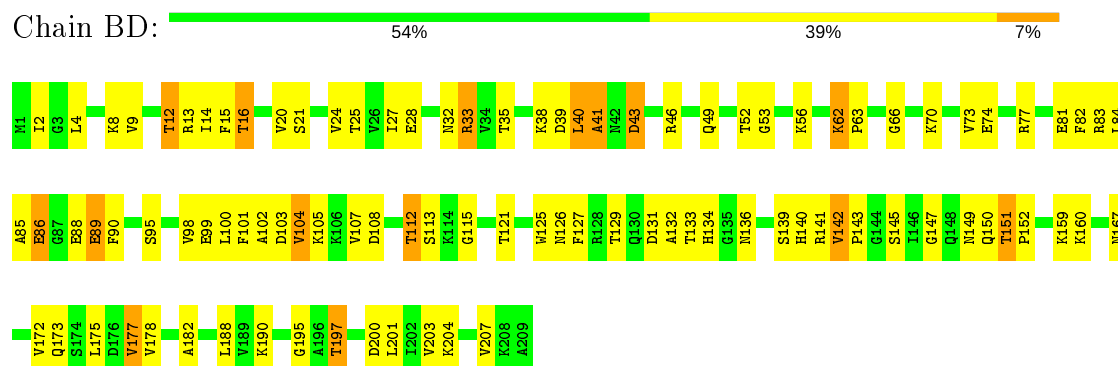


• Molecule 24: 50S ribosomal protein L2

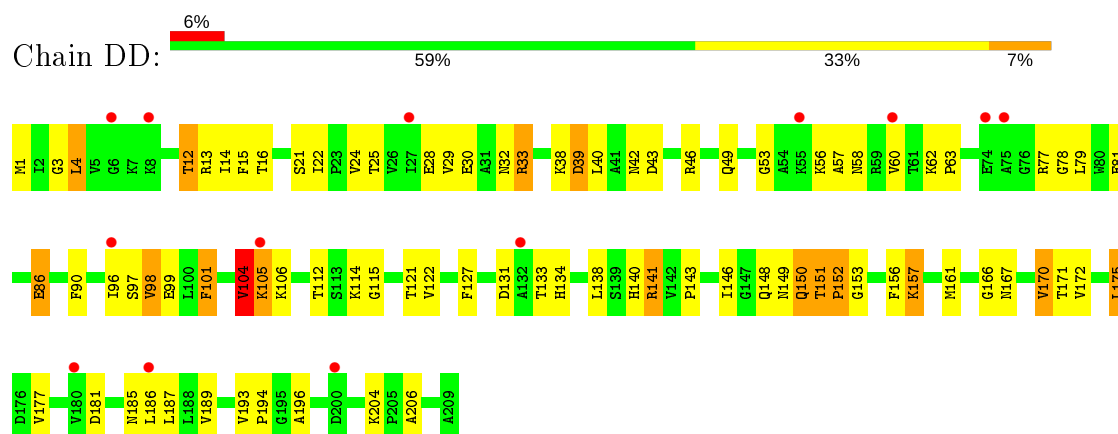
Chain DC: 8% 45% 45% 10%



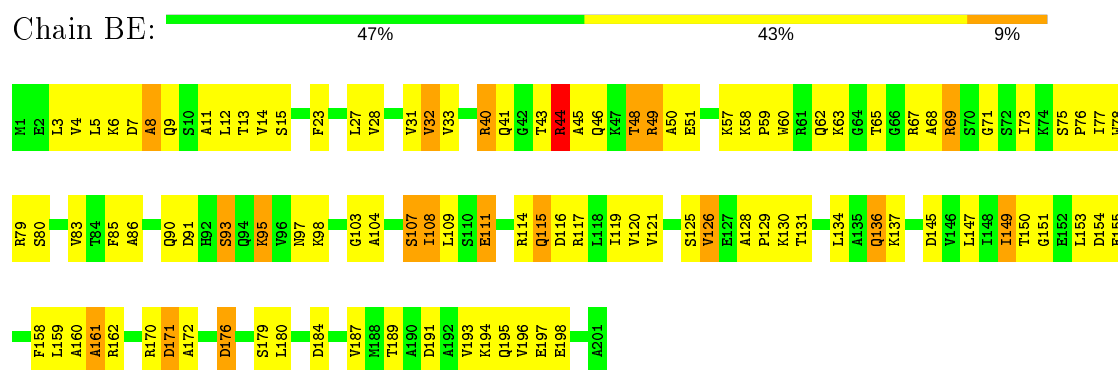
- Molecule 25: 50S ribosomal protein L3



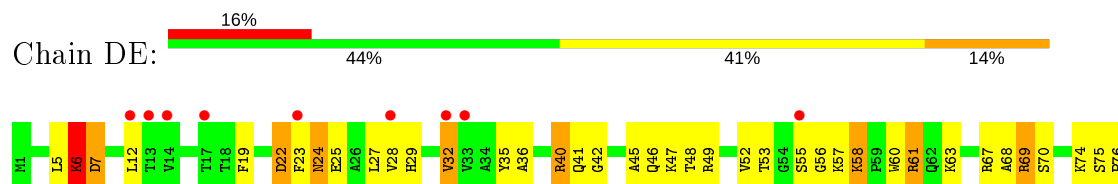
- Molecule 25: 50S ribosomal protein L3

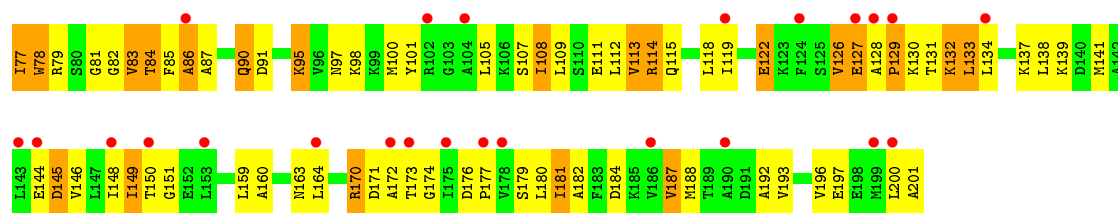


- Molecule 26: 50S ribosomal protein L4

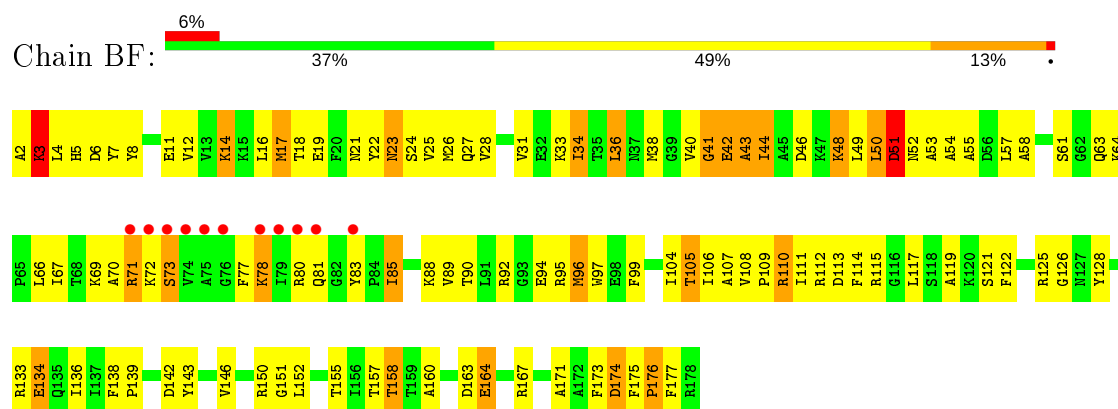


- Molecule 26: 50S ribosomal protein L4

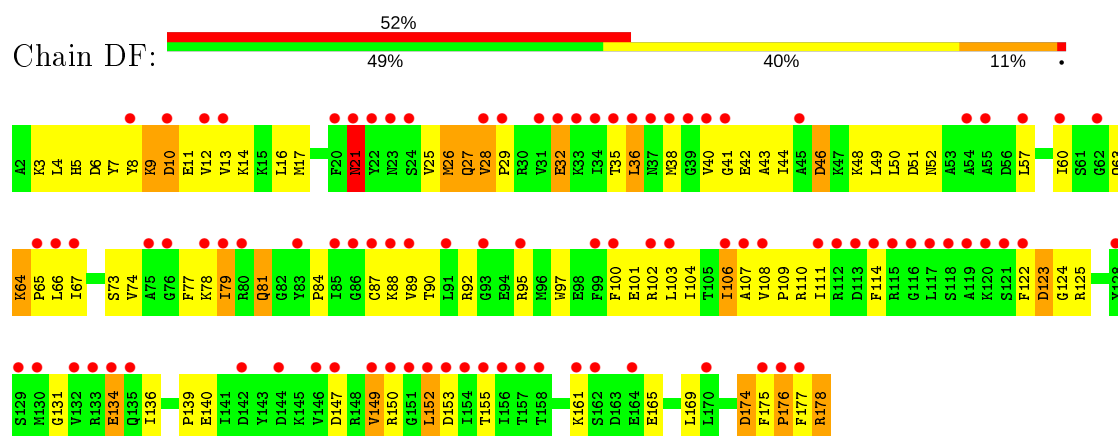




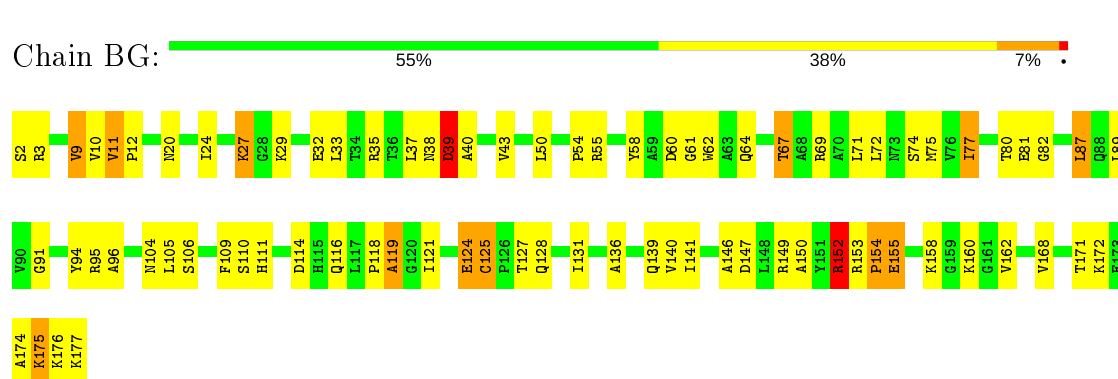
• Molecule 27: 50S ribosomal protein L5



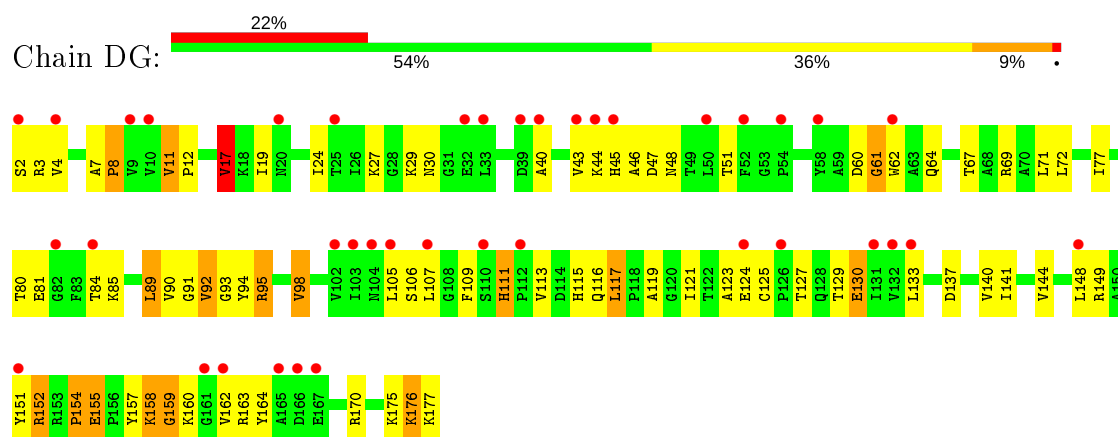
• Molecule 27: 50S ribosomal protein L5



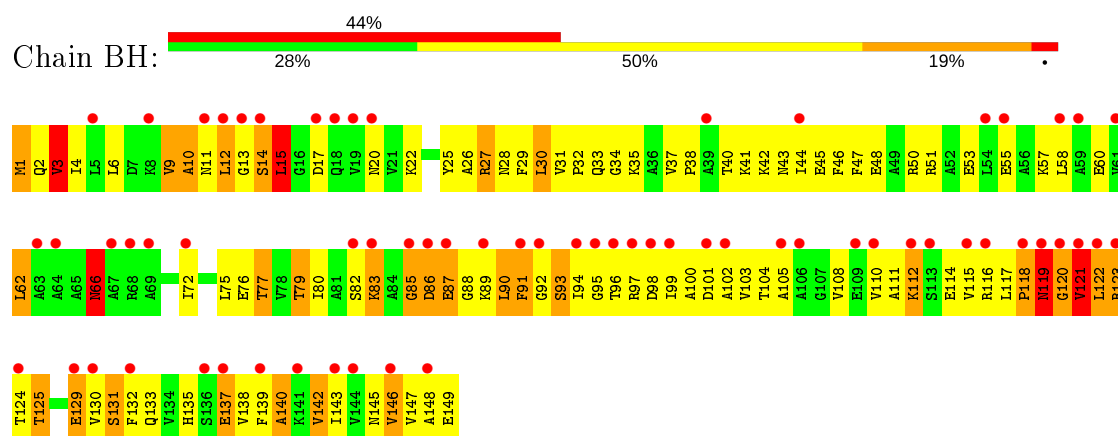
• Molecule 28: 50S ribosomal protein L6



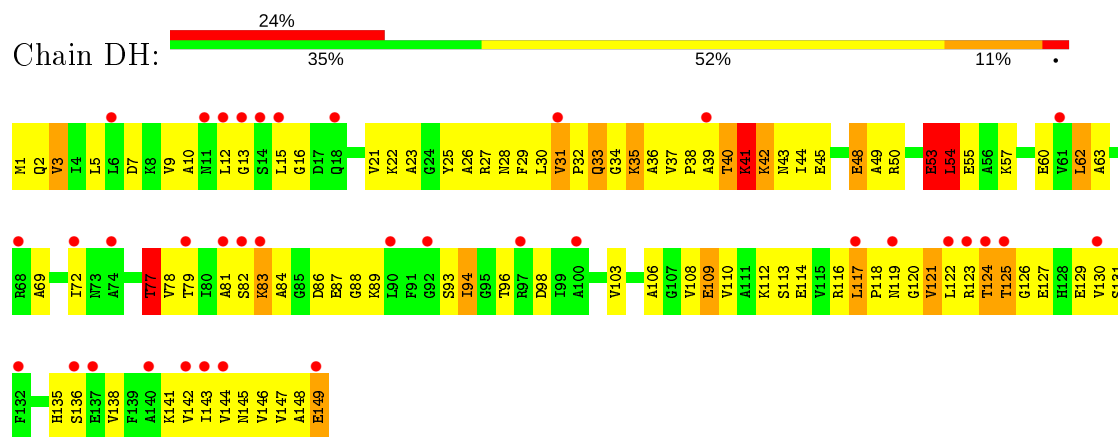
• Molecule 28: 50S ribosomal protein L6



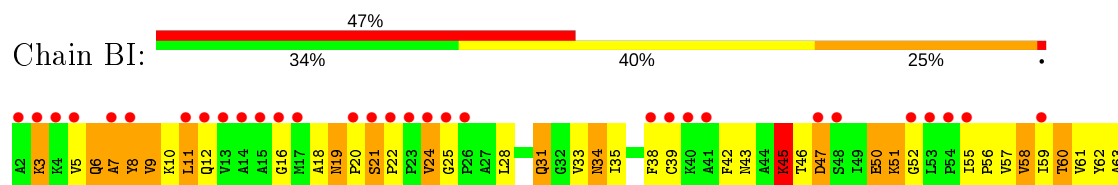
• Molecule 29: 50S ribosomal protein L9

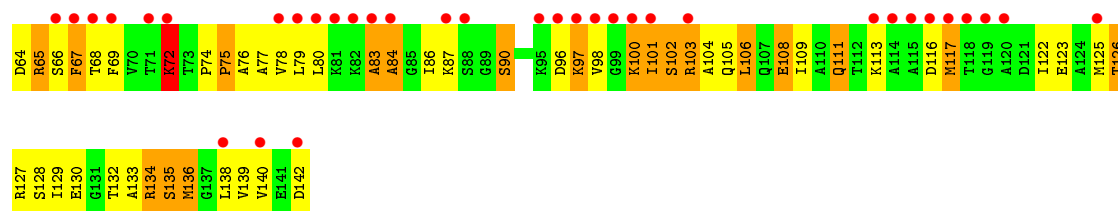


• Molecule 29: 50S ribosomal protein L9

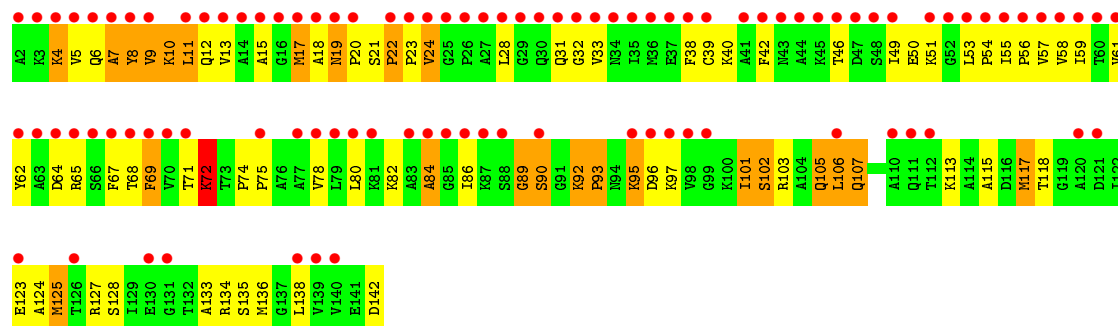
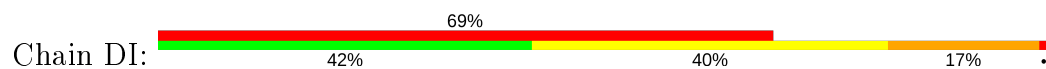


• Molecule 30: 50S ribosomal protein L11

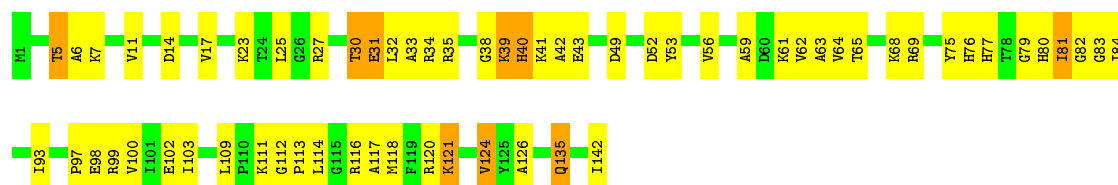




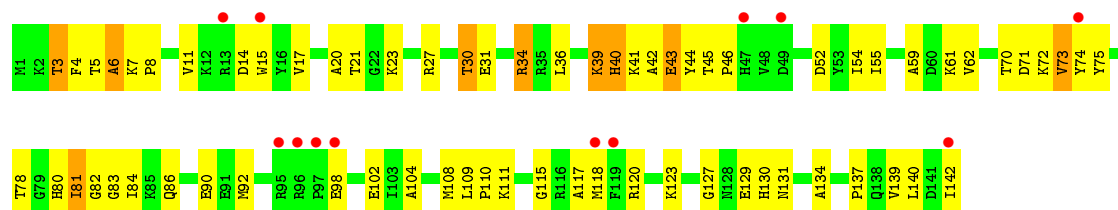
• Molecule 30: 50S ribosomal protein L11



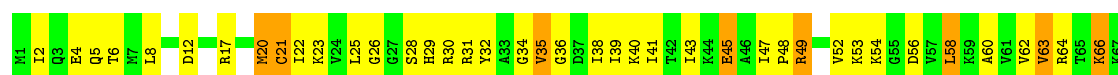
• Molecule 31: 50S ribosomal protein L13

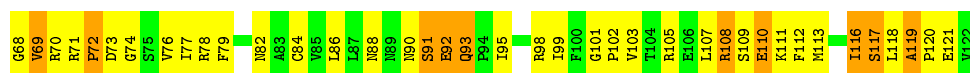


• Molecule 31: 50S ribosomal protein L13

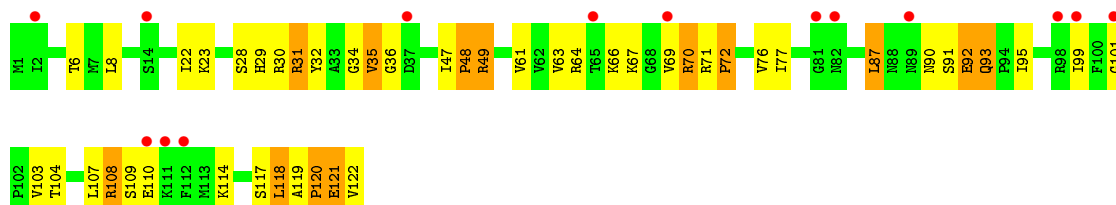


• Molecule 32: 50S ribosomal protein L14

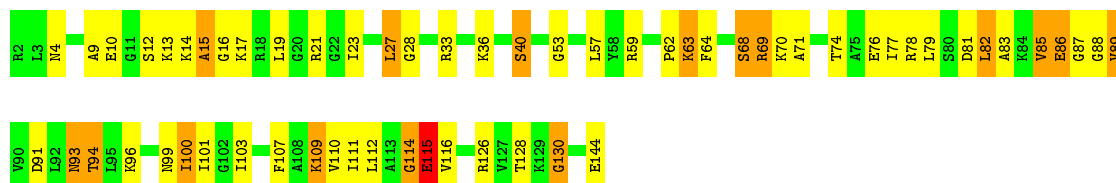




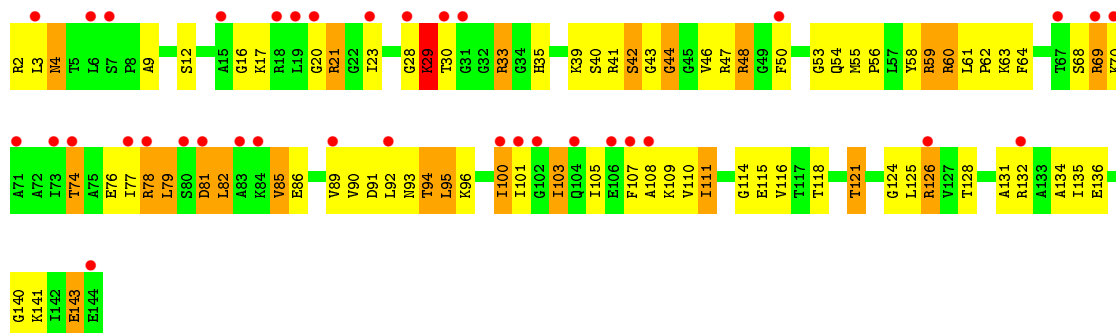
- Molecule 32: 50S ribosomal protein L14



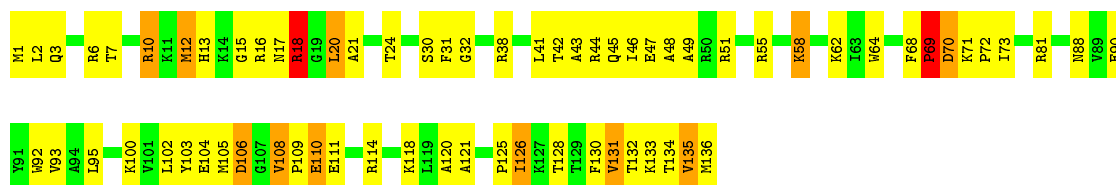
- Molecule 33: 50S ribosomal protein L15



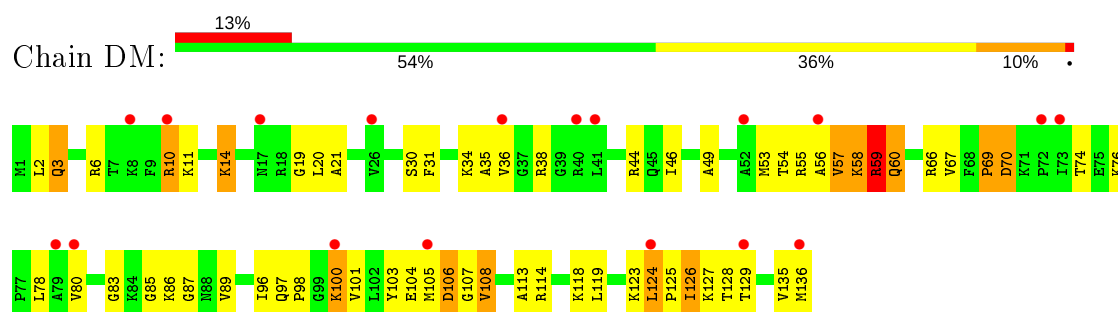
- Molecule 33: 50S ribosomal protein L15



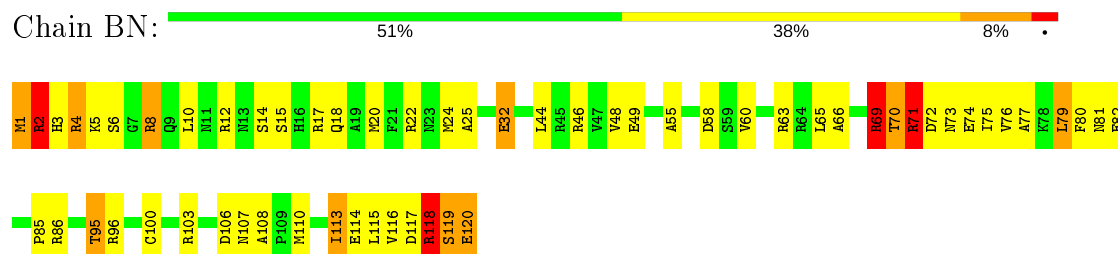
- Molecule 34: 50S ribosomal protein L16



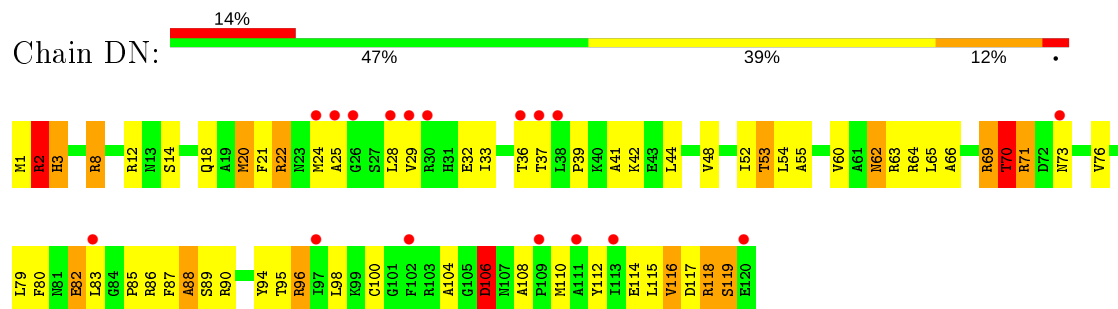
- Molecule 34: 50S ribosomal protein L16



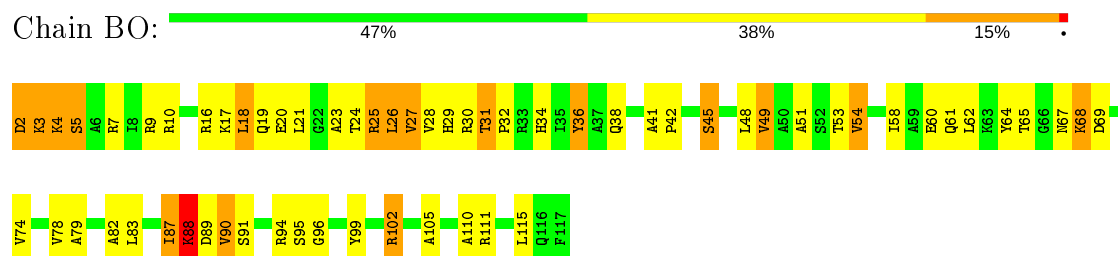
- Molecule 35: 50S ribosomal protein L17



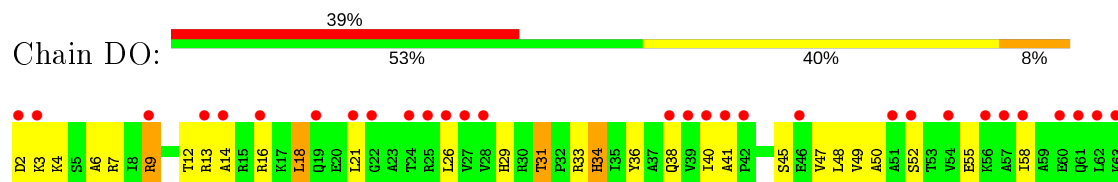
- Molecule 35: 50S ribosomal protein L17

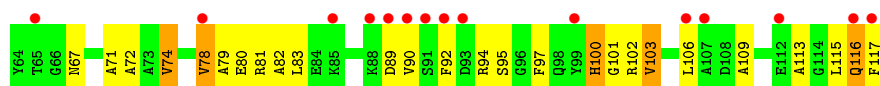


- Molecule 36: 50S ribosomal protein L18



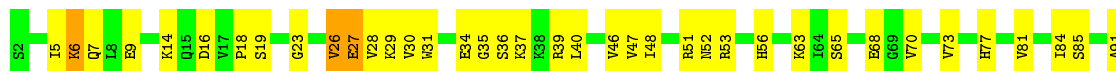
- Molecule 36: 50S ribosomal protein L18





- Molecule 37: 50S ribosomal protein L19

Chain BP: 53% 39% 7%



- Molecule 37: 50S ribosomal protein L19

Chain DP: 11% 54% 35% 11%



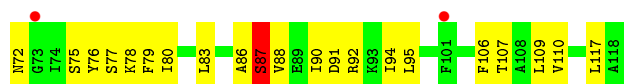
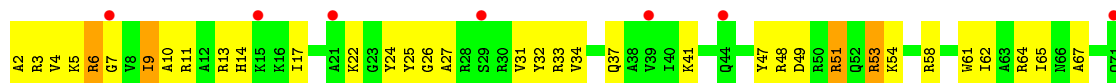
- Molecule 38: 50S ribosomal protein L20

Chain BQ: 48% 44% 9%



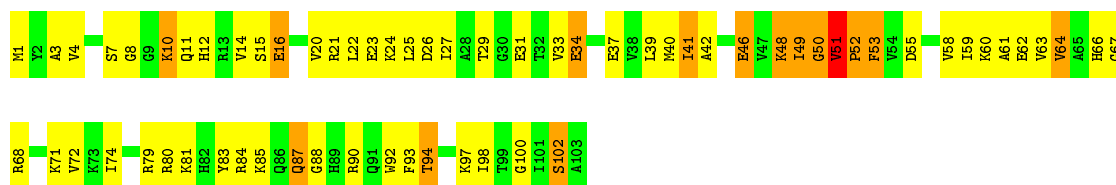
- Molecule 38: 50S ribosomal protein L20

Chain DQ: 8% 52% 44% 2%

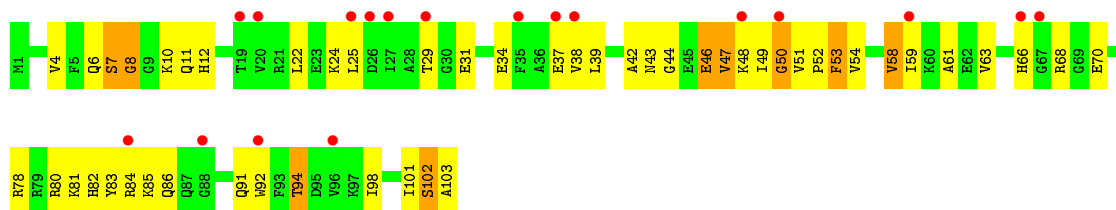


- Molecule 39: 50S ribosomal protein L21

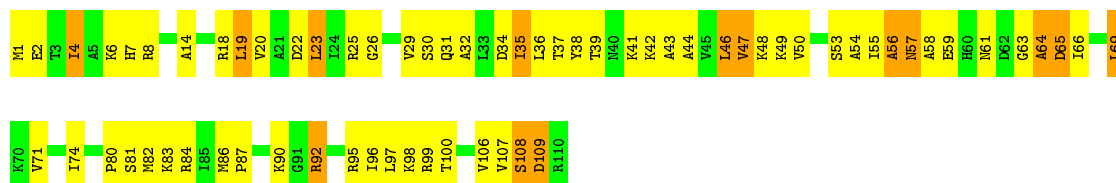
Chain BR: 37% 49% 14%



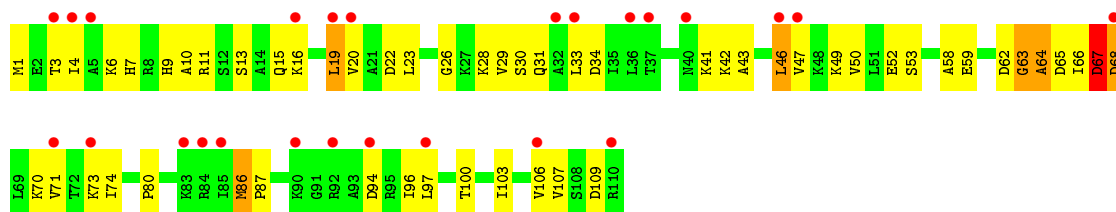
- Molecule 39: 50S ribosomal protein L21



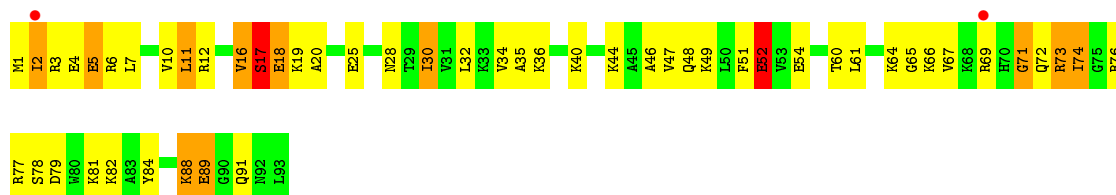
- Molecule 40: 50S ribosomal protein L22



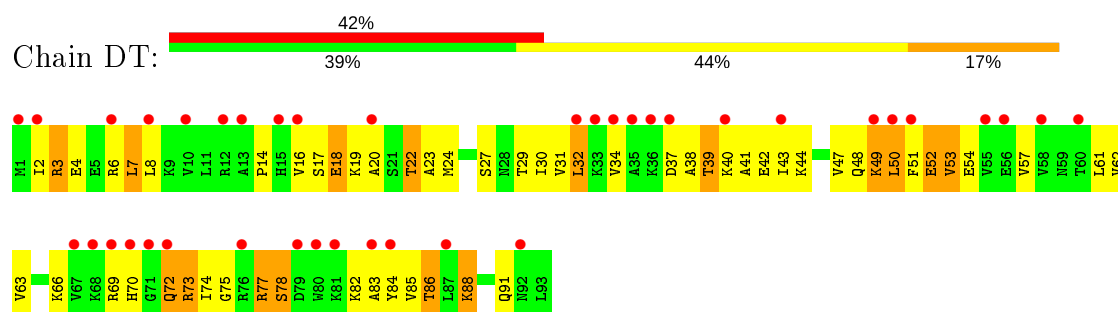
- Molecule 40: 50S ribosomal protein L22



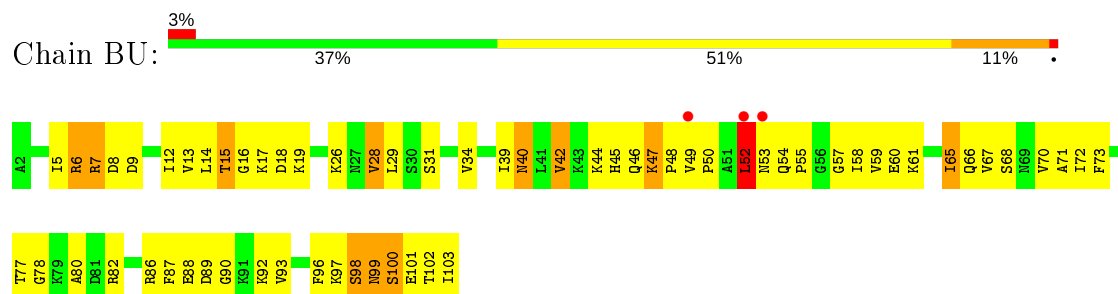
- Molecule 41: 50S ribosomal protein L23



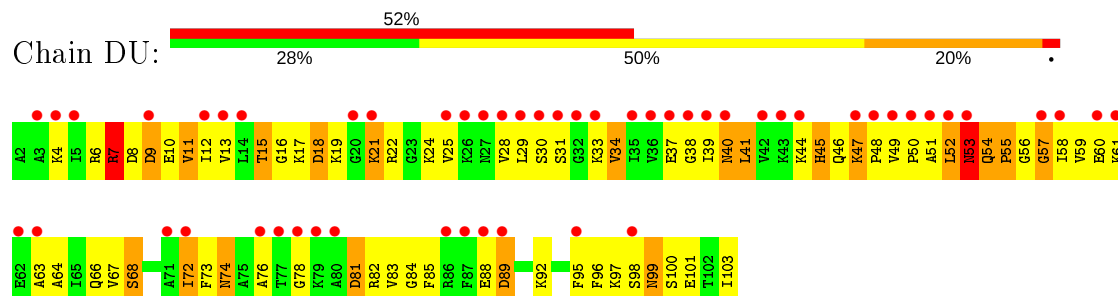
- Molecule 41: 50S ribosomal protein L23



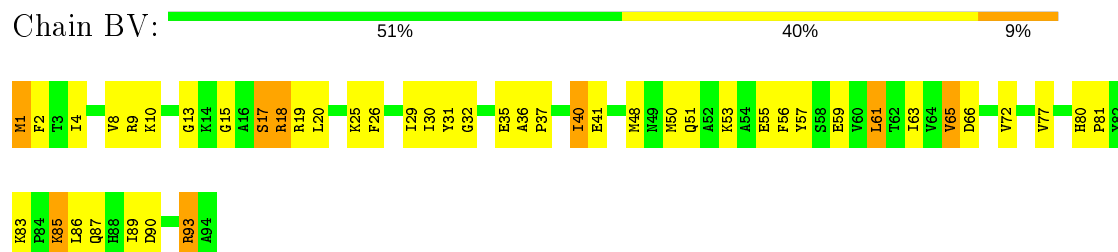
- Molecule 42: 50S ribosomal protein L24



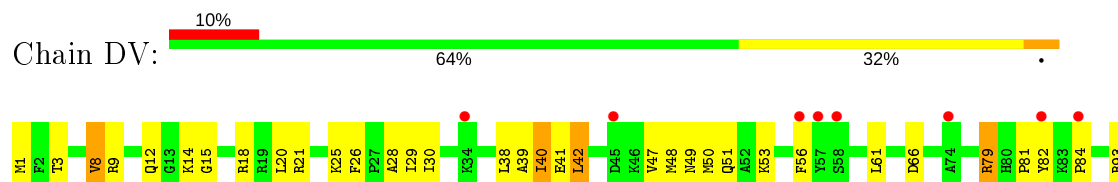
- Molecule 42: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L25



- Molecule 43: 50S ribosomal protein L25





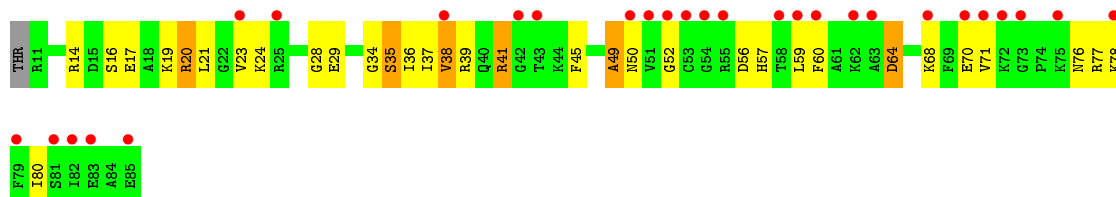
- Molecule 44: 50S ribosomal protein L27

Chain BW:



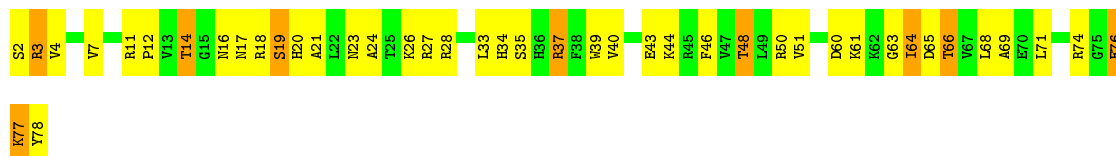
- Molecule 44: 50S ribosomal protein L27

Chain DW:



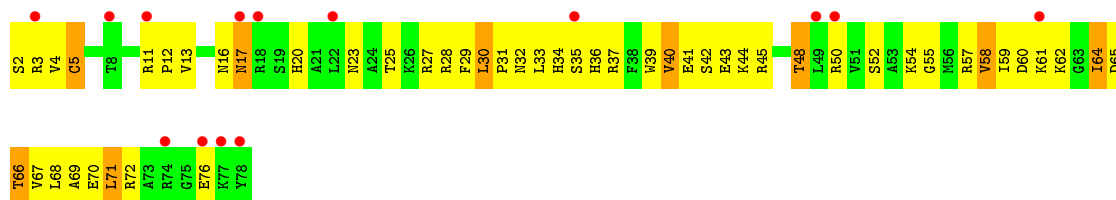
- Molecule 45: 50S ribosomal protein L28

Chain BX:



- Molecule 45: 50S ribosomal protein L28

Chain DX:

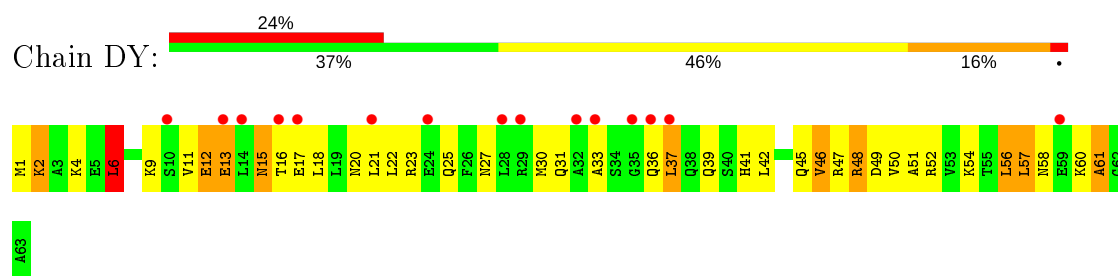


- Molecule 46: 50S ribosomal protein L29

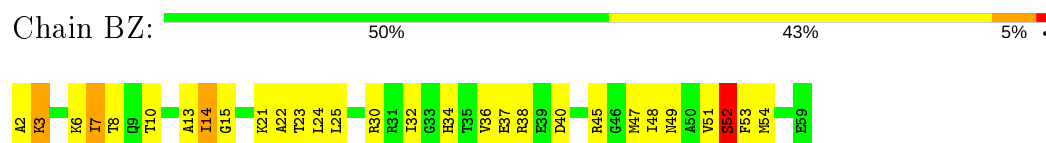
Chain BY:



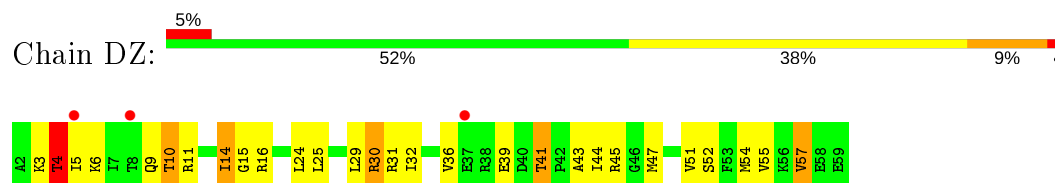
- Molecule 46: 50S ribosomal protein L29



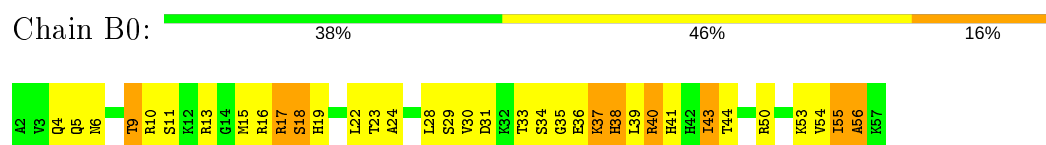
- Molecule 47: 50S ribosomal protein L30



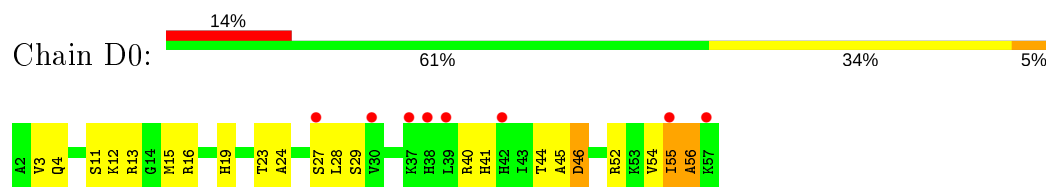
- Molecule 47: 50S ribosomal protein L30



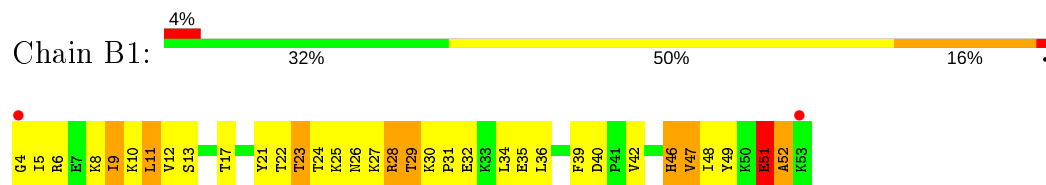
- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32

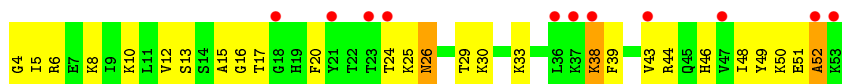


- Molecule 49: 50S ribosomal protein L33



- Molecule 49: 50S ribosomal protein L33





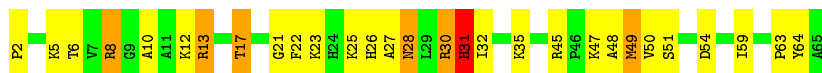
- Molecule 50: 50S ribosomal protein L34



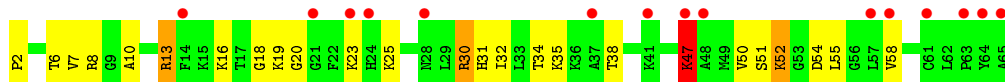
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



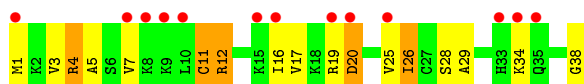
- Molecule 51: 50S ribosomal protein L35



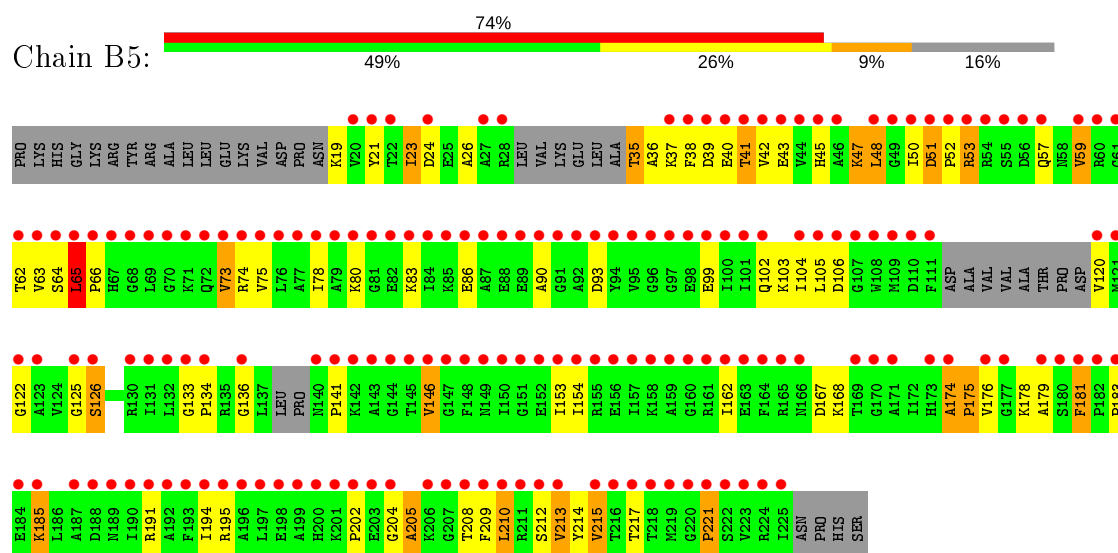
- Molecule 52: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L36



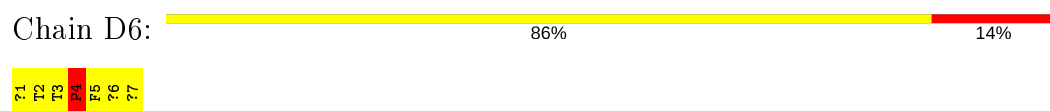
- Molecule 53: 50S ribosomal protein L1



- Molecule 54: Linopristin



- Molecule 54: Linopristin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, 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 0.228 , 0.277	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)	0.25 , 49.7	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: ZN, DBB, MG, 04X, 004, MHW, MHU

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

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	CE	0	1
6	CF	0	1

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

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

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

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

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

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
21	AU	39	GLU	Peptide
48	B0	24	ALA	Peptide
25	BD	151	THR	Peptide
33	BL	28	GLY	Peptide

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DU	780	0	831	65	0
43	BV	753	0	780	31	0
43	DV	753	0	780	25	0
44	BW	580	0	594	23	0
44	DW	569	0	581	26	0
45	BX	625	0	652	35	0
45	DX	625	0	652	55	0
46	BY	509	0	543	29	0
46	DY	509	0	543	38	0
47	BZ	449	0	488	19	0
47	DZ	449	0	488	14	0
48	B0	444	0	458	33	0
48	D0	444	0	458	18	0
49	B1	410	0	440	32	0
49	D1	410	0	440	19	0
50	B2	377	0	418	19	0
50	D2	377	0	418	34	0
51	B3	504	0	572	22	0
51	D3	504	0	572	29	0
52	B4	302	0	340	12	0
52	D4	302	0	342	17	0
53	B5	1142	0	865	49	0
54	B6	69	0	60	5	0
54	D6	69	0	60	14	0
55	AA	71	0	0	0	0
55	AM	1	0	0	0	0
55	BA	195	0	0	0	0
55	BB	4	0	0	0	0
55	CA	55	0	0	0	0
55	CM	1	0	0	0	0
55	DA	167	0	0	0	0
55	DB	3	0	0	0	0
55	DQ	1	0	0	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	194	0	0	23	0
57	AL	1	0	0	0	0
57	AN	5	0	0	1	0
57	AT	2	0	0	1	0
57	AU	1	0	0	1	0
57	B2	1	0	0	0	0
57	B3	3	0	0	0	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 11780 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1006:C:OP2	57:BA:3781:HOH:O	1.56	1.22

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

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:368:U:OP2	29:DH:123:ARG:NE[4_455]	1.78	0.42
1:AA:368:U:OP1	29:DH:93:SER:OG[4_455]	1.93	0.27
1:AA:368:U:OP2	29:DH:123:ARG:NH2[4_455]	2.03	0.17
1:AA:368:U:OP2	29:DH:123:ARG:CZ[4_455]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	135 (62%)	36 (17%)	45 (21%)	0	0
2	CB	216/218 (99%)	143 (66%)	36 (17%)	37 (17%)	0	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%)	1	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	2
5	CE	148/150 (99%)	96 (65%)	29 (20%)	23 (16%)	0	1
6	AF	98/100 (98%)	61 (62%)	19 (19%)	18 (18%)	0	0
6	CF	98/100 (98%)	64 (65%)	18 (18%)	16 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	110 (74%)	27 (18%)	12 (8%)	1	4
7	CG	149/151 (99%)	120 (80%)	21 (14%)	8 (5%)	2	11
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	7
9	AI	125/127 (98%)	90 (72%)	24 (19%)	11 (9%)	1	3
9	CI	125/127 (98%)	89 (71%)	27 (22%)	9 (7%)	1	5
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	3
11	AK	115/117 (98%)	83 (72%)	17 (15%)	15 (13%)	0	1
11	CK	115/117 (98%)	77 (67%)	28 (24%)	10 (9%)	1	3
12	AL	121/123 (98%)	92 (76%)	19 (16%)	10 (8%)	1	4
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	1
14	CN	92/100 (92%)	59 (64%)	20 (22%)	13 (14%)	0	1
15	AO	86/88 (98%)	60 (70%)	21 (24%)	5 (6%)	1	10
15	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	3	20
16	AP	80/82 (98%)	52 (65%)	16 (20%)	12 (15%)	0	1
16	CP	80/82 (98%)	54 (68%)	20 (25%)	6 (8%)	1	5
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%)	8	36
18	CR	53/55 (96%)	45 (85%)	4 (8%)	4 (8%)	1	5
19	AS	77/79 (98%)	52 (68%)	19 (25%)	6 (8%)	1	4
19	CS	77/79 (98%)	59 (77%)	14 (18%)	4 (5%)	2	12
20	AT	83/85 (98%)	51 (61%)	23 (28%)	9 (11%)	0	2
20	CT	83/85 (98%)	66 (80%)	11 (13%)	6 (7%)	1	5
21	AU	49/51 (96%)	23 (47%)	18 (37%)	8 (16%)	0	1
21	CU	49/51 (96%)	25 (51%)	10 (20%)	14 (29%)	0	0
24	BC	269/271 (99%)	208 (77%)	49 (18%)	12 (4%)	2	14

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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	15
25	DD	207/209 (99%)	175 (84%)	24 (12%)	8 (4%)	3	17
26	BE	199/201 (99%)	164 (82%)	26 (13%)	9 (4%)	2	14
26	DE	199/201 (99%)	160 (80%)	27 (14%)	12 (6%)	1	9
27	BF	175/177 (99%)	136 (78%)	24 (14%)	15 (9%)	1	3
27	DF	175/177 (99%)	141 (81%)	23 (13%)	11 (6%)	1	7
28	BG	174/176 (99%)	146 (84%)	20 (12%)	8 (5%)	2	14
28	DG	174/176 (99%)	132 (76%)	33 (19%)	9 (5%)	2	12
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%)	7	33
31	DJ	140/142 (99%)	116 (83%)	18 (13%)	6 (4%)	2	15
32	BK	120/122 (98%)	94 (78%)	15 (12%)	11 (9%)	1	3
32	DK	120/122 (98%)	96 (80%)	14 (12%)	10 (8%)	1	4
33	BL	141/143 (99%)	108 (77%)	23 (16%)	10 (7%)	1	5
33	DL	141/143 (99%)	104 (74%)	28 (20%)	9 (6%)	1	7
34	BM	134/136 (98%)	114 (85%)	16 (12%)	4 (3%)	4	24
34	DM	134/136 (98%)	115 (86%)	13 (10%)	6 (4%)	2	14
35	BN	118/120 (98%)	97 (82%)	18 (15%)	3 (2%)	5	28
35	DN	118/120 (98%)	94 (80%)	16 (14%)	8 (7%)	1	6
36	BO	114/116 (98%)	87 (76%)	22 (19%)	5 (4%)	2	15
36	DO	114/116 (98%)	97 (85%)	15 (13%)	2 (2%)	8	37
37	BP	112/114 (98%)	97 (87%)	10 (9%)	5 (4%)	2	14
37	DP	112/114 (98%)	86 (77%)	19 (17%)	7 (6%)	1	7
38	BQ	115/117 (98%)	96 (84%)	15 (13%)	4 (4%)	3	20
38	DQ	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	17	55
39	BR	101/103 (98%)	89 (88%)	5 (5%)	7 (7%)	1	6
39	DR	101/103 (98%)	77 (76%)	17 (17%)	7 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BS	108/110 (98%)	91 (84%)	11 (10%)	6 (6%)	2	10
40	DS	108/110 (98%)	87 (81%)	14 (13%)	7 (6%)	1	7
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	2
42	BU	100/102 (98%)	75 (75%)	17 (17%)	8 (8%)	1	4
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	15
44	BW	74/76 (97%)	65 (88%)	9 (12%)	0	100	100
44	DW	73/76 (96%)	58 (80%)	10 (14%)	5 (7%)	1	6
45	BX	75/77 (97%)	64 (85%)	7 (9%)	4 (5%)	2	11
45	DX	75/77 (97%)	56 (75%)	15 (20%)	4 (5%)	2	11
46	BY	61/63 (97%)	38 (62%)	13 (21%)	10 (16%)	0	1
46	DY	61/63 (97%)	44 (72%)	11 (18%)	6 (10%)	0	2
47	BZ	56/58 (97%)	49 (88%)	4 (7%)	3 (5%)	2	11
47	DZ	56/58 (97%)	48 (86%)	5 (9%)	3 (5%)	2	11
48	B0	54/56 (96%)	42 (78%)	7 (13%)	5 (9%)	0	3
48	D0	54/56 (96%)	42 (78%)	8 (15%)	4 (7%)	1	5
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	7
50	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	2	14
50	D2	44/46 (96%)	37 (84%)	4 (9%)	3 (7%)	1	6
51	B3	62/64 (97%)	51 (82%)	9 (14%)	2 (3%)	4	22
51	D3	62/64 (97%)	50 (81%)	9 (14%)	3 (5%)	2	13
52	B4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
52	D4	36/38 (95%)	29 (81%)	6 (17%)	1 (3%)	5	25
53	B5	183/228 (80%)	100 (55%)	53 (29%)	30 (16%)	0	1
54	B6	2/7 (29%)	2 (100%)	0	0	100	100
54	D6	2/7 (29%)	1 (50%)	0	1 (50%)	0	0
All	All	11422/11686 (98%)	8514 (74%)	1907 (17%)	1001 (9%)	1	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%)	125 (69%)	55 (31%)	0	1
2	CB	180/180 (100%)	126 (70%)	54 (30%)	0	1
3	AC	170/170 (100%)	137 (81%)	33 (19%)	1	7
3	CC	170/170 (100%)	130 (76%)	40 (24%)	1	3
4	AD	172/172 (100%)	128 (74%)	44 (26%)	0	3
4	CD	172/172 (100%)	140 (81%)	32 (19%)	1	8
5	AE	113/113 (100%)	85 (75%)	28 (25%)	0	3
5	CE	113/113 (100%)	83 (74%)	30 (26%)	0	2
6	AF	87/87 (100%)	63 (72%)	24 (28%)	0	2
6	CF	87/87 (100%)	58 (67%)	29 (33%)	0	1
7	AG	124/124 (100%)	88 (71%)	36 (29%)	0	2
7	CG	124/124 (100%)	92 (74%)	32 (26%)	0	2
8	AH	104/104 (100%)	80 (77%)	24 (23%)	1	4
8	CH	104/104 (100%)	79 (76%)	25 (24%)	0	3
9	AI	105/105 (100%)	73 (70%)	32 (30%)	0	1
9	CI	105/105 (100%)	73 (70%)	32 (30%)	0	1
10	AJ	86/86 (100%)	61 (71%)	25 (29%)	0	2
10	CJ	86/86 (100%)	70 (81%)	16 (19%)	1	8
11	AK	90/90 (100%)	70 (78%)	20 (22%)	1	4
11	CK	90/90 (100%)	67 (74%)	23 (26%)	0	3

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	4
30	BI	109/109 (100%)	80 (73%)	29 (27%)	0	2
30	DI	109/109 (100%)	85 (78%)	24 (22%)	1	4
31	BJ	116/116 (100%)	106 (91%)	10 (9%)	10	37
31	DJ	116/116 (100%)	103 (89%)	13 (11%)	6	24
32	BK	103/103 (100%)	90 (87%)	13 (13%)	4	20
32	DK	103/103 (100%)	93 (90%)	10 (10%)	8	31
33	BL	102/102 (100%)	86 (84%)	16 (16%)	2	13
33	DL	102/102 (100%)	80 (78%)	22 (22%)	1	5
34	BM	109/109 (100%)	92 (84%)	17 (16%)	2	13
34	DM	109/109 (100%)	93 (85%)	16 (15%)	3	15
35	BN	100/100 (100%)	83 (83%)	17 (17%)	2	10
35	DN	100/100 (100%)	77 (77%)	23 (23%)	1	4
36	BO	86/86 (100%)	63 (73%)	23 (27%)	0	2
36	DO	86/86 (100%)	71 (83%)	15 (17%)	2	10
37	BP	99/99 (100%)	84 (85%)	15 (15%)	3	14
37	DP	99/99 (100%)	83 (84%)	16 (16%)	2	12
38	BQ	89/89 (100%)	75 (84%)	14 (16%)	2	13
38	DQ	89/89 (100%)	76 (85%)	13 (15%)	3	15
39	BR	84/84 (100%)	69 (82%)	15 (18%)	2	9
39	DR	84/84 (100%)	73 (87%)	11 (13%)	4	18
40	BS	93/93 (100%)	75 (81%)	18 (19%)	1	7
40	DS	93/93 (100%)	80 (86%)	13 (14%)	3	16
41	BT	80/80 (100%)	68 (85%)	12 (15%)	3	14
41	DT	80/80 (100%)	64 (80%)	16 (20%)	1	7
42	BU	83/83 (100%)	66 (80%)	17 (20%)	1	6
42	DU	83/83 (100%)	60 (72%)	23 (28%)	0	2
43	BV	78/78 (100%)	62 (80%)	16 (20%)	1	6
43	DV	78/78 (100%)	67 (86%)	11 (14%)	3	16
44	BW	57/58 (98%)	50 (88%)	7 (12%)	4	21
44	DW	56/58 (97%)	51 (91%)	5 (9%)	9	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BX	67/67 (100%)	56 (84%)	11 (16%)	2	11
45	DX	67/67 (100%)	57 (85%)	10 (15%)	3	14
46	BY	55/55 (100%)	47 (86%)	8 (14%)	3	15
46	DY	55/55 (100%)	45 (82%)	10 (18%)	1	9
47	BZ	48/48 (100%)	42 (88%)	6 (12%)	4	20
47	DZ	48/48 (100%)	35 (73%)	13 (27%)	0	2
48	B0	47/47 (100%)	40 (85%)	7 (15%)	3	14
48	D0	47/47 (100%)	43 (92%)	4 (8%)	10	38
49	B1	45/45 (100%)	37 (82%)	8 (18%)	2	9
49	D1	45/45 (100%)	39 (87%)	6 (13%)	4	17
50	B2	38/38 (100%)	33 (87%)	5 (13%)	4	18
50	D2	38/38 (100%)	32 (84%)	6 (16%)	2	12
51	B3	51/51 (100%)	40 (78%)	11 (22%)	1	5
51	D3	51/51 (100%)	47 (92%)	4 (8%)	12	42
52	B4	34/34 (100%)	29 (85%)	5 (15%)	3	15
52	D4	34/34 (100%)	29 (85%)	5 (15%)	3	15
53	B5	61/180 (34%)	47 (77%)	14 (23%)	1	4
54	B6	2/2 (100%)	2 (100%)	0	100	100
54	D6	2/2 (100%)	2 (100%)	0	100	100
All	All	9390/9522 (99%)	7518 (80%)	1872 (20%)	1	7

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

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

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

Mol	Chain	Res	Type
37	BP	56	HIS

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

5.3.3 RNA ⓘ

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

5 of 2029 RNA backbone outliers are listed below:

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

5 of 103 RNA pucker outliers are listed below:

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

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	DBB	D6	3	54	4,5,6	0.76	0	1,5,7	0.74	0
54	004	D6	7	54	9,10,11	3.28	7 (77%)	9,12,14	2.38	2 (22%)
54	MHU	D6	5	54	14,15,16	2.80	6 (42%)	18,19,21	2.69	4 (22%)
54	DBB	B6	3	54	4,5,6	0.86	0	1,5,7	0.96	0
54	04X	B6	6	54	14,16,17	1.22	1 (7%)	11,20,22	4.65	6 (54%)
54	MHU	B6	5	54	14,15,16	2.87	7 (50%)	18,19,21	2.71	5 (27%)
54	MHW	B6	1	54	9,9,10	2.88	4 (44%)	10,11,13	3.44	8 (80%)
54	04X	D6	6	54	14,16,17	1.14	2 (14%)	11,20,22	5.43	7 (63%)
54	004	B6	7	54	9,10,11	3.36	6 (66%)	9,12,14	1.59	2 (22%)
54	MHW	D6	1	54	9,9,10	3.18	4 (44%)	10,11,13	2.22	7 (70%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	DBB	D6	3	54	-	2/3/4/6	-
54	004	D6	7	54	-	2/4/6/8	0/1/1/1
54	MHU	D6	5	54	-	3/9/12/14	0/1/1/1
54	DBB	B6	3	54	-	1/3/4/6	-
54	04X	B6	6	54	-	2/4/24/26	0/2/2/2
54	MHU	B6	5	54	-	2/9/12/14	0/1/1/1
54	MHW	B6	1	54	-	2/2/2/4	0/1/1/1
54	04X	D6	6	54	-	3/4/24/26	0/2/2/2
54	004	B6	7	54	-	3/4/6/8	0/1/1/1
54	MHW	D6	1	54	-	0/2/2/4	0/1/1/1

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	7	004	CB-CA	-6.34	1.45	1.52
54	D6	5	MHU	CE1-CD1	6.06	1.49	1.38
54	D6	7	004	CB-CA	-5.93	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D6	1	MHW	CG2-CB	-5.61	1.29	1.39
54	B6	1	MHW	CG2-CB	-5.54	1.29	1.39

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	04X	C0-N1-C1	15.71	135.46	111.09
54	B6	6	04X	C0-N1-C1	13.07	131.37	111.09
54	D6	5	MHU	CB-CA-N	7.71	122.60	110.65
54	B6	1	MHW	O-C-CA	-7.51	117.11	124.22
54	B6	5	MHU	CB-CA-N	7.43	122.16	110.65

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	D6	3	DBB	O-C-CA-CB
54	D6	3	DBB	C-CA-CB-CG
54	D6	5	MHU	O-C-CA-CB
54	B6	3	DBB	C-CA-CB-CG
54	B6	6	04X	CD-C0-N1-C1

There are no ring outliers.

8 monomers are involved in 18 short contacts:

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	-0.39	22 (1%) 75 49	14, 54, 137, 179	0
1	CA	1539/1539 (100%)	-0.19	35 (2%) 60 31	27, 72, 145, 177	0
2	AB	218/218 (100%)	1.16	53 (24%) 0 0	43, 76, 100, 125	0
2	CB	218/218 (100%)	1.54	69 (31%) 0 0	63, 86, 106, 126	0
3	AC	206/206 (100%)	0.10	5 (2%) 59 30	39, 61, 83, 96	0
3	CC	206/206 (100%)	1.24	44 (21%) 0 0	57, 79, 97, 109	0
4	AD	205/205 (100%)	0.04	3 (1%) 73 46	35, 58, 79, 106	0
4	CD	205/205 (100%)	-0.20	3 (1%) 73 46	21, 40, 71, 90	0
5	AE	150/150 (100%)	0.01	3 (2%) 65 36	27, 51, 82, 106	0
5	CE	150/150 (100%)	0.02	1 (0%) 87 69	34, 59, 87, 104	0
6	AF	100/100 (100%)	-0.31	0 100 100	38, 59, 76, 84	0
6	CF	100/100 (100%)	-0.14	1 (1%) 82 59	46, 74, 96, 104	0
7	AG	151/151 (100%)	0.82	25 (16%) 1 0	54, 78, 98, 108	0
7	CG	151/151 (100%)	1.77	61 (40%) 0 0	77, 97, 107, 113	0
8	AH	129/129 (100%)	-0.07	1 (0%) 86 65	30, 50, 73, 81	0
8	CH	129/129 (100%)	0.08	4 (3%) 49 21	45, 65, 81, 90	0
9	AI	127/127 (100%)	1.01	22 (17%) 1 0	51, 73, 97, 113	0
9	CI	127/127 (100%)	1.42	36 (28%) 0 0	71, 91, 109, 126	0
10	AJ	98/98 (100%)	0.44	7 (7%) 16 5	46, 68, 92, 122	0
10	CJ	98/98 (100%)	1.87	41 (41%) 0 0	71, 93, 110, 124	0
11	AK	117/117 (100%)	0.58	14 (11%) 4 1	32, 64, 91, 110	0
11	CK	117/117 (100%)	0.11	3 (2%) 56 27	44, 68, 82, 91	0
12	AL	123/123 (100%)	0.11	3 (2%) 59 30	23, 39, 68, 94	0
12	CL	123/123 (100%)	0.07	4 (3%) 46 20	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%)	0.42	7 (6%) 21 7	49, 71, 92, 105	0
13	CM	114/114 (100%)	1.96	55 (48%) 0 0	90, 103, 116, 120	0
14	AN	96/100 (96%)	0.83	16 (16%) 1 0	43, 63, 94, 106	0
14	CN	96/100 (96%)	1.89	36 (37%) 0 0	69, 91, 110, 118	0
15	AO	88/88 (100%)	-0.01	1 (1%) 80 56	31, 51, 68, 98	0
15	CO	88/88 (100%)	-0.02	2 (2%) 60 31	43, 63, 81, 105	0
16	AP	82/82 (100%)	0.48	4 (4%) 29 11	35, 49, 84, 100	0
16	CP	82/82 (100%)	0.66	12 (14%) 2 1	45, 62, 88, 106	0
17	AQ	80/80 (100%)	-0.03	3 (3%) 40 16	27, 54, 81, 124	0
17	CQ	80/80 (100%)	0.49	5 (6%) 20 6	44, 72, 96, 105	0
18	AR	55/55 (100%)	-0.14	3 (5%) 25 9	39, 53, 81, 112	0
18	CR	55/55 (100%)	0.01	1 (1%) 68 40	46, 56, 82, 111	0
19	AS	79/79 (100%)	1.00	14 (17%) 1 0	55, 72, 92, 101	0
19	CS	79/79 (100%)	3.08	55 (69%) 0 0	87, 103, 114, 123	0
20	AT	85/85 (100%)	0.10	3 (3%) 44 18	35, 51, 74, 111	0
20	CT	85/85 (100%)	1.25	20 (23%) 0 0	53, 72, 93, 96	0
21	AU	51/51 (100%)	1.69	21 (41%) 0 0	56, 76, 95, 108	0
21	CU	51/51 (100%)	0.40	6 (11%) 4 1	48, 72, 94, 108	0
22	BA	2897/2903 (99%)	-0.13	105 (3%) 42 17	0, 14, 130, 195	0
22	DA	2897/2903 (99%)	-0.07	71 (2%) 57 29	42, 83, 144, 183	0
23	BB	119/119 (100%)	-0.52	0 100 100	1, 24, 54, 90	0
23	DB	118/119 (99%)	-0.35	0 100 100	66, 111, 133, 141	0
24	BC	271/271 (100%)	-0.24	8 (2%) 50 22	3, 21, 43, 55	0
24	DC	271/271 (100%)	0.42	23 (8%) 10 3	42, 62, 76, 91	0
25	BD	209/209 (100%)	-0.45	0 100 100	0, 9, 38, 71	0
25	DD	209/209 (100%)	0.38	13 (6%) 20 7	46, 66, 81, 99	0
26	BE	201/201 (100%)	-0.43	0 100 100	0, 24, 56, 91	0
26	DE	201/201 (100%)	0.93	33 (16%) 1 0	45, 81, 98, 106	0
27	BF	177/177 (100%)	0.26	11 (6%) 20 7	15, 46, 88, 97	0
27	DF	177/177 (100%)	2.38	92 (51%) 0 0	85, 102, 117, 125	0
28	BG	176/176 (100%)	-0.16	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%)	1.19	39 (22%) 0 0	71, 90, 104, 117	0
29	BH	149/149 (100%)	2.29	65 (43%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.15	36 (24%) 0 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	2.43	66 (46%) 0 0	84, 108, 121, 136	0
30	DI	141/141 (100%)	3.62	97 (68%) 0 0	96, 114, 123, 127	0
31	BJ	142/142 (100%)	-0.46	0 100 100	1, 5, 23, 43	0
31	DJ	142/142 (100%)	0.41	12 (8%) 10 3	48, 64, 79, 96	0
32	BK	122/122 (100%)	-0.54	0 100 100	2, 11, 37, 67	0
32	DK	122/122 (100%)	0.64	14 (11%) 4 1	48, 61, 81, 96	0
33	BL	143/143 (100%)	-0.35	0 100 100	0, 21, 48, 76	0
33	DL	143/143 (100%)	1.25	36 (25%) 0 0	42, 77, 91, 113	0
34	BM	136/136 (100%)	-0.49	0 100 100	1, 9, 30, 87	0
34	DM	136/136 (100%)	0.80	18 (13%) 3 1	42, 67, 82, 108	0
35	BN	120/120 (100%)	-0.47	0 100 100	1, 6, 17, 62	0
35	DN	120/120 (100%)	0.58	17 (14%) 2 1	54, 74, 88, 110	0
36	BO	116/116 (100%)	-0.26	0 100 100	14, 27, 46, 52	0
36	DO	116/116 (100%)	1.68	45 (38%) 0 0	74, 91, 102, 114	0
37	BP	114/114 (100%)	-0.31	0 100 100	5, 19, 48, 70	0
37	DP	114/114 (100%)	0.58	13 (11%) 5 1	56, 68, 84, 93	0
38	BQ	117/117 (100%)	-0.45	0 100 100	0, 3, 11, 42	0
38	DQ	117/117 (100%)	0.40	9 (7%) 13 4	52, 66, 77, 84	0
39	BR	103/103 (100%)	-0.48	0 100 100	1, 9, 31, 63	0
39	DR	103/103 (100%)	0.87	18 (17%) 1 0	50, 75, 87, 97	0
40	BS	110/110 (100%)	-0.38	0 100 100	1, 3, 23, 84	0
40	DS	110/110 (100%)	1.07	25 (22%) 0 0	56, 73, 89, 96	0
41	BT	93/93 (100%)	-0.02	2 (2%) 62 33	10, 27, 80, 101	0
41	DT	93/93 (100%)	1.82	39 (41%) 0 0	63, 83, 103, 110	0
42	BU	102/102 (100%)	-0.10	3 (2%) 51 23	10, 30, 61, 92	0
42	DU	102/102 (100%)	2.61	53 (51%) 0 0	70, 88, 106, 112	0
43	BV	94/94 (100%)	-0.36	0 100 100	4, 22, 43, 54	0
43	DV	94/94 (100%)	0.46	9 (9%) 8 2	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%)	-0.42	0 100 100	3, 10, 27, 48	0
44	DW	75/76 (98%)	1.49	28 (37%) 0 0	54, 79, 88, 108	0
45	BX	77/77 (100%)	-0.36	0 100 100	6, 24, 52, 77	0
45	DX	77/77 (100%)	0.61	14 (18%) 1 0	49, 69, 86, 89	0
46	BY	63/63 (100%)	0.05	3 (4%) 30 11	22, 44, 74, 96	0
46	DY	63/63 (100%)	1.28	15 (23%) 0 0	71, 90, 99, 103	0
47	BZ	58/58 (100%)	-0.38	0 100 100	2, 7, 29, 41	0
47	DZ	58/58 (100%)	0.26	3 (5%) 27 10	52, 70, 84, 89	0
48	B0	56/56 (100%)	-0.53	0 100 100	0, 8, 35, 70	0
48	D0	56/56 (100%)	0.86	8 (14%) 2 1	53, 74, 91, 104	0
49	B1	50/50 (100%)	-0.28	2 (4%) 38 15	13, 31, 54, 87	0
49	D1	50/50 (100%)	1.17	11 (22%) 0 0	68, 84, 93, 105	0
50	B2	46/46 (100%)	-0.31	1 (2%) 62 33	3, 9, 17, 90	0
50	D2	46/46 (100%)	1.18	9 (19%) 1 0	53, 66, 79, 100	0
51	B3	64/64 (100%)	-0.32	0 100 100	4, 9, 18, 31	0
51	D3	64/64 (100%)	0.94	15 (23%) 0 0	58, 71, 79, 85	0
52	B4	38/38 (100%)	-0.08	0 100 100	11, 20, 35, 52	0
52	D4	38/38 (100%)	1.59	13 (34%) 0 0	63, 74, 85, 99	0
53	B5	191/228 (83%)	4.42	168 (87%) 0 0	85, 111, 123, 134	0
54	B6	2/7 (28%)	0.27	0 100 100	5, 5, 5, 9	0
54	D6	2/7 (28%)	0.74	0 100 100	53, 53, 53, 62	0
All	All	20738/20808 (99%)	0.28	1986 (9%) 8 2	0, 64, 119, 195	0

The worst 5 of 1986 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	DI	6	GLN	16.5
30	BI	53	LEU	16.3
22	BA	2100	G	15.9
30	DI	2	ALA	15.0
22	BA	2104	C	14.5

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

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	0.82	0.38	45,58,69,72	0
54	DBB	D6	3	6/7	0.88	0.50	45,50,65,70	0
54	04X	D6	6	15/16	0.90	0.27	47,59,67,73	0
54	MHU	B6	5	15/16	0.93	0.24	3,7,15,15	0
54	DBB	B6	3	6/7	0.94	0.28	8,14,20,33	0
54	MHW	D6	1	9/10	0.94	0.18	55,59,63,66	0
54	004	D6	7	10/11	0.95	0.23	47,52,61,64	0
54	04X	B6	6	15/16	0.97	0.19	6,11,15,20	0
54	004	B6	7	10/11	0.97	0.28	2,4,6,6	0
54	MHW	B6	1	9/10	0.97	0.20	8,13,21,30	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	AA	1627	1/1	0.17	0.55	76,76,76,76	0
55	MG	DA	3071	1/1	0.18	0.59	93,93,93,93	0
55	MG	DA	3072	1/1	0.23	0.50	89,89,89,89	0
55	MG	AA	1644	1/1	0.24	0.69	49,49,49,49	0
55	MG	DA	3061	1/1	0.25	1.80	97,97,97,97	0
55	MG	DA	3093	1/1	0.26	0.35	99,99,99,99	0
55	MG	CA	1631	1/1	0.35	0.26	98,98,98,98	0
55	MG	DA	3011	1/1	0.41	0.30	74,74,74,74	0
55	MG	DA	3057	1/1	0.41	0.29	82,82,82,82	0
55	MG	DA	3116	1/1	0.43	0.34	92,92,92,92	0
55	MG	DA	3005	1/1	0.44	0.12	90,90,90,90	0
55	MG	DA	3041	1/1	0.46	0.42	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1629	1/1	0.49	0.10	84,84,84,84	0
55	MG	CA	1621	1/1	0.51	0.09	67,67,67,67	0
55	MG	CA	1637	1/1	0.52	0.37	80,80,80,80	0
55	MG	DA	3132	1/1	0.53	0.79	85,85,85,85	0
55	MG	DA	3027	1/1	0.55	0.12	82,82,82,82	0
55	MG	DA	3104	1/1	0.56	0.18	76,76,76,76	0
55	MG	DA	3085	1/1	0.58	0.19	78,78,78,78	0
55	MG	DA	3120	1/1	0.58	0.56	95,95,95,95	0
55	MG	BA	3055	1/1	0.58	0.25	50,50,50,50	0
55	MG	DA	3134	1/1	0.58	0.58	87,87,87,87	0
55	MG	CA	1628	1/1	0.59	0.28	100,100,100,100	0
55	MG	DA	3070	1/1	0.60	0.11	93,93,93,93	0
55	MG	DA	3016	1/1	0.60	0.42	84,84,84,84	0
55	MG	CA	1627	1/1	0.61	0.29	88,88,88,88	0
55	MG	DA	3077	1/1	0.62	0.26	76,76,76,76	0
55	MG	AA	1665	1/1	0.63	0.74	53,53,53,53	0
55	MG	AA	1635	1/1	0.63	0.27	76,76,76,76	0
55	MG	BA	3119	1/1	0.64	0.36	49,49,49,49	0
55	MG	BA	3135	1/1	0.65	0.27	48,48,48,48	0
55	MG	CA	1609	1/1	0.67	0.09	78,78,78,78	0
55	MG	DA	3032	1/1	0.67	0.20	78,78,78,78	0
55	MG	DA	3079	1/1	0.68	0.08	94,94,94,94	0
55	MG	DA	3056	1/1	0.68	0.28	80,80,80,80	0
55	MG	DA	3062	1/1	0.68	0.77	70,70,70,70	0
55	MG	DA	3028	1/1	0.69	0.56	86,86,86,86	0
55	MG	DA	3111	1/1	0.69	0.12	81,81,81,81	0
55	MG	CA	1636	1/1	0.70	0.29	97,97,97,97	0
55	MG	DA	3008	1/1	0.70	0.16	80,80,80,80	0
55	MG	DA	3021	1/1	0.70	0.34	62,62,62,62	0
55	MG	BA	3016	1/1	0.70	0.22	31,31,31,31	0
55	MG	AA	1651	1/1	0.70	0.34	55,55,55,55	0
55	MG	DA	3137	1/1	0.70	0.27	84,84,84,84	0
55	MG	DA	3153	1/1	0.70	0.12	68,68,68,68	0
55	MG	DA	3078	1/1	0.71	0.20	95,95,95,95	0
55	MG	BA	3011	1/1	0.72	0.16	30,30,30,30	0
55	MG	DA	3082	1/1	0.72	0.11	65,65,65,65	0
55	MG	AA	1667	1/1	0.72	0.68	54,54,54,54	0
55	MG	BA	3090	1/1	0.73	0.20	33,33,33,33	0
55	MG	BA	3048	1/1	0.73	0.08	26,26,26,26	0
55	MG	BA	3115	1/1	0.73	0.51	76,76,76,76	0
55	MG	DA	3024	1/1	0.73	0.17	45,45,45,45	0
55	MG	BA	3098	1/1	0.73	0.59	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3047	1/1	0.74	0.11	40,40,40,40	0
55	MG	DA	3165	1/1	0.74	0.38	43,43,43,43	0
55	MG	DA	3155	1/1	0.74	0.28	37,37,37,37	0
55	MG	DA	3121	1/1	0.74	0.16	60,60,60,60	0
55	MG	DA	3122	1/1	0.74	0.08	64,64,64,64	0
55	MG	AA	1670	1/1	0.74	0.40	45,45,45,45	0
55	MG	DA	3094	1/1	0.75	0.20	83,83,83,83	0
55	MG	BA	3154	1/1	0.75	0.23	21,21,21,21	0
55	MG	AA	1634	1/1	0.75	0.09	49,49,49,49	0
55	MG	CA	1635	1/1	0.75	0.10	94,94,94,94	0
55	MG	DA	3151	1/1	0.75	0.47	40,40,40,40	0
55	MG	CA	1605	1/1	0.75	0.25	78,78,78,78	0
55	MG	DA	3150	1/1	0.75	0.21	50,50,50,50	0
55	MG	DA	3010	1/1	0.76	0.10	64,64,64,64	0
55	MG	DB	201	1/1	0.76	0.05	96,96,96,96	0
55	MG	AA	1601	1/1	0.76	0.11	61,61,61,61	0
55	MG	DA	3149	1/1	0.76	0.19	49,49,49,49	0
55	MG	CA	1655	1/1	0.76	1.02	67,67,67,67	0
55	MG	DA	3164	1/1	0.76	0.76	56,56,56,56	0
55	MG	DA	3145	1/1	0.76	0.09	68,68,68,68	0
55	MG	AA	1646	1/1	0.77	0.21	50,50,50,50	0
55	MG	DA	3029	1/1	0.77	0.37	66,66,66,66	0
55	MG	DA	3002	1/1	0.77	0.52	81,81,81,81	0
55	MG	DA	3019	1/1	0.77	0.15	84,84,84,84	0
55	MG	DA	3091	1/1	0.77	0.13	79,79,79,79	0
55	MG	AA	1648	1/1	0.77	0.26	39,39,39,39	0
55	MG	BA	3031	1/1	0.78	0.11	7,7,7,7	0
55	MG	CA	1626	1/1	0.78	0.26	66,66,66,66	0
55	MG	DA	3158	1/1	0.78	0.46	58,58,58,58	0
55	MG	CA	1602	1/1	0.78	0.12	69,69,69,69	0
55	MG	BA	3190	1/1	0.78	0.53	42,42,42,42	0
55	MG	DA	3048	1/1	0.78	0.22	93,93,93,93	0
55	MG	DA	3160	1/1	0.78	0.20	47,47,47,47	0
55	MG	DA	3084	1/1	0.78	0.15	75,75,75,75	0
55	MG	DA	3038	1/1	0.78	0.14	63,63,63,63	0
55	MG	DA	3106	1/1	0.78	0.31	70,70,70,70	0
55	MG	DA	3042	1/1	0.78	0.14	69,69,69,69	0
55	MG	DA	3161	1/1	0.79	0.33	48,48,48,48	0
55	MG	BA	3015	1/1	0.79	0.41	61,61,61,61	0
55	MG	DA	3014	1/1	0.79	0.36	73,73,73,73	0
55	MG	DA	3092	1/1	0.79	0.44	94,94,94,94	0
55	MG	AA	1623	1/1	0.79	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3025	1/1	0.79	0.18	40,40,40,40	0
55	MG	DA	3015	1/1	0.79	0.57	77,77,77,77	0
55	MG	DA	3126	1/1	0.80	0.17	61,61,61,61	0
55	MG	DA	3040	1/1	0.80	0.21	66,66,66,66	0
55	MG	DA	3044	1/1	0.81	0.21	83,83,83,83	0
55	MG	BA	3070	1/1	0.81	0.11	37,37,37,37	0
55	MG	DA	3133	1/1	0.81	0.19	55,55,55,55	0
55	MG	BA	3019	1/1	0.81	0.26	1,1,1,1	0
55	MG	BA	3004	1/1	0.81	0.14	52,52,52,52	0
55	MG	DA	3136	1/1	0.81	0.42	81,81,81,81	0
55	MG	CA	1652	1/1	0.81	0.11	62,62,62,62	0
55	MG	DA	3033	1/1	0.82	0.09	54,54,54,54	0
55	MG	BA	3029	1/1	0.82	0.12	35,35,35,35	0
55	MG	DA	3090	1/1	0.82	0.08	59,59,59,59	0
55	MG	DB	203	1/1	0.82	0.09	90,90,90,90	0
55	MG	DA	3098	1/1	0.82	0.08	50,50,50,50	0
55	MG	DA	3154	1/1	0.82	0.24	40,40,40,40	0
55	MG	AA	1630	1/1	0.83	0.15	67,67,67,67	0
55	MG	AA	1657	1/1	0.83	0.34	37,37,37,37	0
55	MG	CA	1638	1/1	0.83	0.16	74,74,74,74	0
55	MG	DA	3099	1/1	0.83	0.41	82,82,82,82	0
55	MG	DA	3166	1/1	0.83	0.19	44,44,44,44	0
55	MG	DA	3013	1/1	0.83	0.11	64,64,64,64	0
55	MG	AA	1662	1/1	0.83	0.27	49,49,49,49	0
55	MG	AA	1652	1/1	0.83	0.13	40,40,40,40	0
55	MG	BA	3157	1/1	0.83	0.34	34,34,34,34	0
55	MG	DA	3058	1/1	0.83	0.16	70,70,70,70	0
55	MG	BA	3161	1/1	0.84	0.17	15,15,15,15	0
55	MG	BA	3168	1/1	0.84	0.24	21,21,21,21	0
55	MG	DA	3055	1/1	0.84	0.07	57,57,57,57	0
55	MG	DA	3115	1/1	0.84	0.09	79,79,79,79	0
55	MG	DA	3006	1/1	0.84	0.22	98,98,98,98	0
55	MG	DA	3009	1/1	0.84	0.09	69,69,69,69	0
55	MG	CA	1611	1/1	0.84	0.17	69,69,69,69	0
55	MG	DA	3144	1/1	0.85	0.30	58,58,58,58	0
55	MG	DA	3046	1/1	0.85	0.11	62,62,62,62	0
55	MG	CA	1615	1/1	0.85	0.23	56,56,56,56	0
55	MG	DA	3127	1/1	0.85	0.13	88,88,88,88	0
55	MG	CM	201	1/1	0.85	0.38	50,50,50,50	0
55	MG	BA	3109	1/1	0.85	0.21	1,1,1,1	0
55	MG	CA	1604	1/1	0.85	0.07	78,78,78,78	0
55	MG	BA	3113	1/1	0.85	0.12	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3045	1/1	0.85	0.12	4,4,4,4	0
55	MG	AA	1617	1/1	0.85	0.11	62,62,62,62	0
55	MG	DA	3060	1/1	0.85	0.22	72,72,72,72	0
55	MG	AA	1659	1/1	0.85	0.48	32,32,32,32	0
55	MG	AA	1671	1/1	0.85	0.34	54,54,54,54	0
55	MG	DA	3100	1/1	0.85	0.31	73,73,73,73	0
55	MG	CA	1620	1/1	0.86	0.13	81,81,81,81	0
55	MG	DA	3112	1/1	0.86	0.13	64,64,64,64	0
55	MG	BA	3076	1/1	0.86	0.28	56,56,56,56	0
55	MG	BA	3129	1/1	0.86	0.13	0,0,0,0	0
55	MG	DA	3018	1/1	0.86	0.11	68,68,68,68	0
55	MG	DA	3102	1/1	0.86	0.31	72,72,72,72	0
55	MG	DA	3004	1/1	0.86	0.48	87,87,87,87	0
55	MG	BA	3150	1/1	0.87	0.20	37,37,37,37	0
55	MG	DA	3063	1/1	0.87	0.12	53,53,53,53	0
55	MG	BA	3093	1/1	0.87	0.10	26,26,26,26	0
55	MG	DA	3054	1/1	0.87	0.08	62,62,62,62	0
55	MG	DA	3135	1/1	0.87	0.08	46,46,46,46	0
55	MG	DA	3069	1/1	0.87	0.20	77,77,77,77	0
55	MG	DA	3073	1/1	0.87	0.10	35,35,35,35	0
55	MG	BA	3080	1/1	0.87	0.09	24,24,24,24	0
55	MG	AA	1624	1/1	0.87	0.10	50,50,50,50	0
55	MG	BA	3028	1/1	0.87	0.10	3,3,3,3	0
55	MG	DA	3081	1/1	0.88	0.12	62,62,62,62	0
55	MG	AA	1639	1/1	0.88	0.10	67,67,67,67	0
55	MG	BA	3002	1/1	0.88	0.09	18,18,18,18	0
55	MG	DA	3103	1/1	0.88	0.28	67,67,67,67	0
55	MG	CA	1606	1/1	0.88	0.25	76,76,76,76	0
55	MG	CA	1646	1/1	0.88	0.23	36,36,36,36	0
55	MG	DA	3118	1/1	0.88	0.11	73,73,73,73	0
55	MG	DA	3125	1/1	0.88	0.17	86,86,86,86	0
55	MG	BA	3180	1/1	0.88	0.62	25,25,25,25	0
55	MG	CA	1650	1/1	0.88	0.63	50,50,50,50	0
55	MG	DA	3088	1/1	0.88	0.08	69,69,69,69	0
55	MG	CA	1622	1/1	0.88	0.12	57,57,57,57	0
55	MG	DA	3152	1/1	0.88	0.32	55,55,55,55	0
55	MG	BA	3166	1/1	0.88	0.20	37,37,37,37	0
55	MG	BA	3003	1/1	0.88	0.10	29,29,29,29	0
55	MG	DA	3025	1/1	0.88	0.12	65,65,65,65	0
55	MG	BA	3160	1/1	0.88	0.20	5,5,5,5	0
55	MG	DQ	201	1/1	0.88	0.30	40,40,40,40	0
55	MG	BA	3124	1/1	0.88	0.09	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3089	1/1	0.88	0.62	91,91,91,91	0
55	MG	CA	1654	1/1	0.88	0.20	26,26,26,26	0
55	MG	AA	1607	1/1	0.88	0.12	48,48,48,48	0
55	MG	BA	3061	1/1	0.88	0.64	66,66,66,66	0
55	MG	BA	3167	1/1	0.88	0.17	22,22,22,22	0
55	MG	BA	3056	1/1	0.89	0.19	22,22,22,22	0
55	MG	BA	3020	1/1	0.89	0.13	5,5,5,5	0
55	MG	BB	202	1/1	0.89	0.10	4,4,4,4	0
55	MG	CA	1608	1/1	0.89	0.12	65,65,65,65	0
55	MG	DA	3113	1/1	0.89	0.46	75,75,75,75	0
55	MG	CA	1648	1/1	0.89	0.14	51,51,51,51	0
55	MG	DA	3045	1/1	0.89	0.21	61,61,61,61	0
55	MG	BA	3133	1/1	0.89	0.34	57,57,57,57	0
55	MG	DA	3157	1/1	0.89	0.14	29,29,29,29	0
55	MG	AA	1636	1/1	0.89	0.18	42,42,42,42	0
55	MG	CA	1633	1/1	0.89	0.80	82,82,82,82	0
55	MG	BA	3118	1/1	0.89	0.14	34,34,34,34	0
55	MG	AA	1614	1/1	0.89	0.19	66,66,66,66	0
55	MG	CA	1632	1/1	0.90	0.07	75,75,75,75	0
55	MG	BA	3007	1/1	0.90	0.09	32,32,32,32	0
55	MG	DA	3130	1/1	0.90	0.19	43,43,43,43	0
55	MG	CA	1624	1/1	0.90	0.07	52,52,52,52	0
55	MG	DA	3139	1/1	0.90	0.56	47,47,47,47	0
55	MG	BA	3099	1/1	0.90	0.16	21,21,21,21	0
55	MG	AA	1658	1/1	0.90	0.16	35,35,35,35	0
55	MG	DA	3047	1/1	0.90	0.14	71,71,71,71	0
55	MG	DA	3043	1/1	0.90	0.07	67,67,67,67	0
55	MG	DA	3049	1/1	0.90	0.10	69,69,69,69	0
55	MG	BA	3052	1/1	0.90	0.09	21,21,21,21	0
55	MG	BA	3077	1/1	0.90	0.07	38,38,38,38	0
55	MG	BA	3044	1/1	0.90	0.21	8,8,8,8	0
55	MG	AA	1643	1/1	0.90	0.15	23,23,23,23	0
55	MG	BA	3026	1/1	0.90	0.10	6,6,6,6	0
55	MG	CA	1630	1/1	0.90	0.65	102,102,102,102	0
55	MG	DA	3087	1/1	0.90	0.05	58,58,58,58	0
55	MG	BA	3088	1/1	0.90	0.08	29,29,29,29	0
55	MG	BA	3036	1/1	0.90	0.15	23,23,23,23	0
55	MG	DA	3083	1/1	0.90	0.24	65,65,65,65	0
55	MG	DA	3053	1/1	0.90	0.13	39,39,39,39	0
55	MG	DB	202	1/1	0.90	0.13	57,57,57,57	0
55	MG	DA	3138	1/1	0.90	0.36	37,37,37,37	0
55	MG	BA	3145	1/1	0.90	0.16	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3091	1/1	0.90	0.05	48,48,48,48	0
55	MG	BB	203	1/1	0.90	0.09	7,7,7,7	0
55	MG	BA	3075	1/1	0.91	0.14	6,6,6,6	0
55	MG	DA	3080	1/1	0.91	0.10	91,91,91,91	0
55	MG	CA	1618	1/1	0.91	0.21	35,35,35,35	0
55	MG	BA	3092	1/1	0.91	0.19	42,42,42,42	0
55	MG	DA	3163	1/1	0.91	0.21	47,47,47,47	0
55	MG	DA	3147	1/1	0.91	0.15	35,35,35,35	0
55	MG	DA	3065	1/1	0.91	0.07	41,41,41,41	0
55	MG	BA	3112	1/1	0.91	0.09	20,20,20,20	0
55	MG	CA	1645	1/1	0.91	0.12	32,32,32,32	0
55	MG	DA	3059	1/1	0.91	0.09	42,42,42,42	0
55	MG	BA	3054	1/1	0.91	0.08	7,7,7,7	0
55	MG	DA	3142	1/1	0.91	0.40	39,39,39,39	0
55	MG	BA	3073	1/1	0.91	0.15	9,9,9,9	0
55	MG	BA	3040	1/1	0.91	0.39	2,2,2,2	0
55	MG	DA	3128	1/1	0.91	0.07	74,74,74,74	0
55	MG	AA	1631	1/1	0.91	0.16	52,52,52,52	0
55	MG	BA	3173	1/1	0.91	0.29	30,30,30,30	0
55	MG	DA	3107	1/1	0.91	0.19	56,56,56,56	0
55	MG	BA	3050	1/1	0.91	0.07	7,7,7,7	0
55	MG	BA	3152	1/1	0.91	0.27	8,8,8,8	0
55	MG	DA	3101	1/1	0.91	0.08	63,63,63,63	0
55	MG	CA	1653	1/1	0.91	0.38	48,48,48,48	0
55	MG	DA	3035	1/1	0.91	0.13	71,71,71,71	0
55	MG	DA	3095	1/1	0.92	0.24	69,69,69,69	0
55	MG	BA	3034	1/1	0.92	0.13	5,5,5,5	0
55	MG	BA	3136	1/1	0.92	0.57	43,43,43,43	0
55	MG	CA	1601	1/1	0.92	0.17	52,52,52,52	0
55	MG	DA	3096	1/1	0.92	0.09	54,54,54,54	0
55	MG	DA	3064	1/1	0.92	0.19	48,48,48,48	0
55	MG	BA	3178	1/1	0.92	0.35	12,12,12,12	0
55	MG	DA	3148	1/1	0.92	0.22	51,51,51,51	0
55	MG	DA	3007	1/1	0.92	0.37	80,80,80,80	0
55	MG	BA	3066	1/1	0.92	0.14	2,2,2,2	0
55	MG	AA	1616	1/1	0.92	0.09	62,62,62,62	0
55	MG	BA	3095	1/1	0.92	0.08	14,14,14,14	0
55	MG	AA	1609	1/1	0.92	0.08	33,33,33,33	0
55	MG	AA	1610	1/1	0.92	0.15	51,51,51,51	0
55	MG	AA	1602	1/1	0.92	0.38	53,53,53,53	0
55	MG	DA	3129	1/1	0.92	0.13	70,70,70,70	0
55	MG	DA	3146	1/1	0.92	0.11	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1668	1/1	0.92	0.38	33,33,33,33	0
55	MG	DA	3108	1/1	0.92	0.14	55,55,55,55	0
55	MG	BA	3144	1/1	0.92	0.24	24,24,24,24	0
55	MG	AA	1604	1/1	0.92	0.08	48,48,48,48	0
55	MG	AA	1669	1/1	0.92	0.27	34,34,34,34	0
55	MG	BA	3059	1/1	0.92	0.12	5,5,5,5	0
55	MG	BA	3111	1/1	0.92	0.08	27,27,27,27	0
55	MG	DA	3031	1/1	0.92	0.14	59,59,59,59	0
55	MG	AA	1661	1/1	0.92	0.35	23,23,23,23	0
55	MG	AA	1663	1/1	0.92	0.23	49,49,49,49	0
55	MG	BA	3071	1/1	0.93	0.14	17,17,17,17	0
55	MG	AA	1619	1/1	0.93	0.15	65,65,65,65	0
55	MG	CA	1623	1/1	0.93	0.17	66,66,66,66	0
55	MG	AA	1606	1/1	0.93	0.06	58,58,58,58	0
55	MG	BA	3014	1/1	0.93	0.19	26,26,26,26	0
55	MG	BA	3120	1/1	0.93	0.12	11,11,11,11	0
55	MG	BA	3074	1/1	0.93	0.21	32,32,32,32	0
55	MG	BA	3102	1/1	0.93	0.18	17,17,17,17	0
55	MG	BA	3001	1/1	0.93	0.05	21,21,21,21	0
55	MG	BA	3151	1/1	0.93	0.14	23,23,23,23	0
55	MG	AA	1605	1/1	0.93	0.20	29,29,29,29	0
55	MG	CA	1619	1/1	0.93	0.12	27,27,27,27	0
55	MG	DA	3159	1/1	0.93	0.26	57,57,57,57	0
55	MG	BA	3123	1/1	0.93	0.13	11,11,11,11	0
55	MG	CA	1640	1/1	0.93	0.15	36,36,36,36	0
55	MG	CA	1639	1/1	0.93	0.13	43,43,43,43	0
55	MG	BA	3027	1/1	0.93	0.35	36,36,36,36	0
55	MG	BA	3179	1/1	0.93	0.34	30,30,30,30	0
55	MG	BA	3181	1/1	0.93	0.12	26,26,26,26	0
55	MG	BA	3032	1/1	0.93	0.12	2,2,2,2	0
55	MG	BA	3171	1/1	0.93	0.17	20,20,20,20	0
55	MG	AA	1655	1/1	0.93	0.14	20,20,20,20	0
55	MG	BA	3057	1/1	0.93	0.21	20,20,20,20	0
55	MG	BA	3023	1/1	0.93	0.17	0,0,0,0	0
55	MG	AA	1629	1/1	0.93	0.17	54,54,54,54	0
55	MG	DA	3036	1/1	0.93	0.12	57,57,57,57	0
55	MG	BA	3038	1/1	0.93	0.14	1,1,1,1	0
55	MG	AA	1625	1/1	0.94	0.09	51,51,51,51	0
55	MG	DA	3001	1/1	0.94	0.08	37,37,37,37	0
55	MG	AA	1615	1/1	0.94	0.13	63,63,63,63	0
55	MG	BA	3122	1/1	0.94	0.17	0,0,0,0	0
55	MG	DA	3167	1/1	0.94	0.13	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1610	1/1	0.94	0.07	58,58,58,58	0
55	MG	AM	201	1/1	0.94	0.61	50,50,50,50	0
55	MG	DA	3141	1/1	0.94	0.42	45,45,45,45	0
55	MG	BB	201	1/1	0.94	0.08	28,28,28,28	0
55	MG	AA	1608	1/1	0.94	0.15	20,20,20,20	0
55	MG	DA	3030	1/1	0.94	0.27	61,61,61,61	0
55	MG	BA	3138	1/1	0.94	0.30	0,0,0,0	0
55	MG	BA	3046	1/1	0.94	0.17	3,3,3,3	0
55	MG	AA	1640	1/1	0.94	0.10	57,57,57,57	0
55	MG	DA	3068	1/1	0.94	0.07	60,60,60,60	0
55	MG	AA	1613	1/1	0.94	0.07	23,23,23,23	0
55	MG	BA	3065	1/1	0.94	0.12	1,1,1,1	0
55	MG	AA	1620	1/1	0.94	0.06	55,55,55,55	0
55	MG	DA	3026	1/1	0.94	0.70	75,75,75,75	0
55	MG	CA	1616	1/1	0.94	0.10	38,38,38,38	0
55	MG	CA	1641	1/1	0.94	0.40	58,58,58,58	0
55	MG	BA	3140	1/1	0.94	0.15	7,7,7,7	0
55	MG	BA	3155	1/1	0.94	0.18	2,2,2,2	0
55	MG	DA	3119	1/1	0.94	0.07	58,58,58,58	0
55	MG	BA	3053	1/1	0.94	0.18	0,0,0,0	0
55	MG	AA	1638	1/1	0.94	0.11	63,63,63,63	0
55	MG	AA	1650	1/1	0.94	0.25	20,20,20,20	0
55	MG	BA	3177	1/1	0.94	0.10	9,9,9,9	0
55	MG	BA	3193	1/1	0.94	0.17	12,12,12,12	0
55	MG	BA	3108	1/1	0.94	0.16	5,5,5,5	0
55	MG	BA	3159	1/1	0.94	0.14	24,24,24,24	0
55	MG	CA	1614	1/1	0.94	0.05	52,52,52,52	0
55	MG	DA	3022	1/1	0.94	0.13	43,43,43,43	0
55	MG	BA	3087	1/1	0.94	0.09	27,27,27,27	0
55	MG	BA	3041	1/1	0.94	0.10	11,11,11,11	0
55	MG	BA	3174	1/1	0.94	0.14	5,5,5,5	0
55	MG	BA	3079	1/1	0.94	0.09	21,21,21,21	0
55	MG	BA	3089	1/1	0.94	0.14	1,1,1,1	0
55	MG	BA	3175	1/1	0.94	0.10	9,9,9,9	0
55	MG	BA	3183	1/1	0.94	0.26	22,22,22,22	0
55	MG	BA	3097	1/1	0.94	0.12	0,0,0,0	0
55	MG	AA	1618	1/1	0.95	0.09	34,34,34,34	0
55	MG	BA	3125	1/1	0.95	0.17	2,2,2,2	0
55	MG	DA	3012	1/1	0.95	0.14	39,39,39,39	0
55	MG	BA	3024	1/1	0.95	0.07	3,3,3,3	0
55	MG	AA	1660	1/1	0.95	0.09	41,41,41,41	0
55	MG	CA	1612	1/1	0.95	0.05	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3084	1/1	0.95	0.10	7,7,7,7	0
55	MG	CA	1642	1/1	0.95	0.20	25,25,25,25	0
55	MG	BA	3169	1/1	0.95	0.10	4,4,4,4	0
55	MG	AA	1666	1/1	0.95	0.25	32,32,32,32	0
55	MG	CA	1651	1/1	0.95	0.25	72,72,72,72	0
55	MG	BA	3096	1/1	0.95	0.18	2,2,2,2	0
55	MG	BA	3137	1/1	0.95	0.29	2,2,2,2	0
55	MG	BA	3176	1/1	0.95	0.27	24,24,24,24	0
55	MG	BA	3068	1/1	0.95	0.17	1,1,1,1	0
55	MG	DA	3037	1/1	0.95	0.08	76,76,76,76	0
55	MG	DA	3124	1/1	0.95	0.16	41,41,41,41	0
55	MG	BA	3105	1/1	0.95	0.22	0,0,0,0	0
55	MG	DA	3123	1/1	0.95	0.15	44,44,44,44	0
55	MG	DA	3034	1/1	0.95	0.20	58,58,58,58	0
55	MG	BA	3195	1/1	0.95	0.14	36,36,36,36	0
55	MG	BA	3194	1/1	0.95	0.19	22,22,22,22	0
55	MG	BA	3039	1/1	0.95	0.22	1,1,1,1	0
55	MG	BA	3064	1/1	0.95	0.15	0,0,0,0	0
55	MG	CA	1603	1/1	0.95	0.15	45,45,45,45	0
55	MG	DA	3051	1/1	0.95	0.05	33,33,33,33	0
55	MG	BA	3104	1/1	0.95	0.26	0,0,0,0	0
55	MG	DA	3097	1/1	0.95	0.15	67,67,67,67	0
55	MG	DA	3114	1/1	0.95	0.09	52,52,52,52	0
55	MG	DA	3039	1/1	0.95	0.10	53,53,53,53	0
55	MG	BA	3156	1/1	0.95	0.15	9,9,9,9	0
55	MG	BA	3101	1/1	0.95	0.09	11,11,11,11	0
55	MG	CA	1647	1/1	0.95	0.31	35,35,35,35	0
55	MG	DA	3052	1/1	0.95	0.06	47,47,47,47	0
55	MG	DA	3066	1/1	0.95	0.12	45,45,45,45	0
55	MG	BA	3184	1/1	0.95	0.13	8,8,8,8	0
55	MG	BA	3182	1/1	0.95	0.22	14,14,14,14	0
55	MG	DA	3143	1/1	0.95	0.18	35,35,35,35	0
55	MG	DA	3003	1/1	0.96	0.13	66,66,66,66	0
55	MG	BA	3170	1/1	0.96	0.26	22,22,22,22	0
55	MG	BA	3005	1/1	0.96	0.17	43,43,43,43	0
55	MG	BA	3085	1/1	0.96	0.17	11,11,11,11	0
55	MG	DA	3023	1/1	0.96	0.10	60,60,60,60	0
55	MG	DA	3117	1/1	0.96	0.12	55,55,55,55	0
55	MG	DA	3075	1/1	0.96	0.26	61,61,61,61	0
55	MG	BA	3146	1/1	0.96	0.21	22,22,22,22	0
55	MG	BA	3121	1/1	0.96	0.06	14,14,14,14	0
55	MG	DA	3076	1/1	0.96	0.13	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1637	1/1	0.96	0.14	16,16,16,16	0
55	MG	BA	3185	1/1	0.96	0.14	5,5,5,5	0
55	MG	DA	3105	1/1	0.96	0.12	52,52,52,52	0
55	MG	BA	3094	1/1	0.96	0.12	20,20,20,20	0
55	MG	BA	3022	1/1	0.96	0.15	0,0,0,0	0
55	MG	BA	3103	1/1	0.96	0.07	7,7,7,7	0
55	MG	AA	1633	1/1	0.96	0.08	35,35,35,35	0
55	MG	BA	3082	1/1	0.96	0.07	6,6,6,6	0
55	MG	CA	1634	1/1	0.96	0.06	58,58,58,58	0
55	MG	BA	3126	1/1	0.96	0.15	3,3,3,3	0
55	MG	BA	3013	1/1	0.96	0.17	0,0,0,0	0
55	MG	BA	3067	1/1	0.96	0.20	0,0,0,0	0
55	MG	BA	3191	1/1	0.96	0.18	26,26,26,26	0
55	MG	BA	3117	1/1	0.96	0.16	1,1,1,1	0
55	MG	BA	3188	1/1	0.96	0.10	35,35,35,35	0
55	MG	BA	3143	1/1	0.96	0.32	3,3,3,3	0
55	MG	AA	1626	1/1	0.96	0.21	26,26,26,26	0
55	MG	BA	3165	1/1	0.96	0.12	3,3,3,3	0
55	MG	BA	3172	1/1	0.96	0.12	16,16,16,16	0
55	MG	CA	1613	1/1	0.96	0.14	17,17,17,17	0
55	MG	BA	3049	1/1	0.96	0.14	3,3,3,3	0
55	MG	DA	3110	1/1	0.96	0.24	45,45,45,45	0
55	MG	BA	3012	1/1	0.96	0.16	0,0,0,0	0
55	MG	BA	3192	1/1	0.96	0.23	11,11,11,11	0
55	MG	DA	3156	1/1	0.96	0.13	58,58,58,58	0
55	MG	BA	3100	1/1	0.96	0.10	9,9,9,9	0
55	MG	BA	3163	1/1	0.96	0.14	27,27,27,27	0
55	MG	BA	3069	1/1	0.96	0.15	64,64,64,64	0
55	MG	CA	1644	1/1	0.96	0.38	36,36,36,36	0
55	MG	CA	1607	1/1	0.96	0.14	55,55,55,55	0
55	MG	BA	3083	1/1	0.96	0.22	34,34,34,34	0
55	MG	BA	3186	1/1	0.96	0.23	12,12,12,12	0
55	MG	BA	3110	1/1	0.96	0.11	26,26,26,26	0
55	MG	BA	3158	1/1	0.97	0.12	15,15,15,15	0
55	MG	AA	1649	1/1	0.97	0.12	28,28,28,28	0
55	MG	DA	3140	1/1	0.97	0.23	42,42,42,42	0
55	MG	AA	1611	1/1	0.97	0.07	21,21,21,21	0
55	MG	BA	3130	1/1	0.97	0.17	2,2,2,2	0
55	MG	BA	3006	1/1	0.97	0.07	13,13,13,13	0
55	MG	BA	3127	1/1	0.97	0.10	2,2,2,2	0
55	MG	BA	3162	1/1	0.97	0.14	23,23,23,23	0
55	MG	BA	3072	1/1	0.97	0.19	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1617	1/1	0.97	0.09	41,41,41,41	0
55	MG	AA	1628	1/1	0.97	0.04	39,39,39,39	0
55	MG	BA	3147	1/1	0.97	0.14	11,11,11,11	0
55	MG	BA	3062	1/1	0.97	0.11	4,4,4,4	0
55	MG	BA	3134	1/1	0.97	0.09	3,3,3,3	0
55	MG	AA	1632	1/1	0.97	0.13	40,40,40,40	0
55	MG	AA	1622	1/1	0.97	0.22	21,21,21,21	0
55	MG	BA	3058	1/1	0.97	0.07	15,15,15,15	0
55	MG	BA	3132	1/1	0.97	0.20	32,32,32,32	0
55	MG	AA	1664	1/1	0.97	0.13	51,51,51,51	0
55	MG	BA	3148	1/1	0.97	0.14	13,13,13,13	0
55	MG	DA	3162	1/1	0.97	0.11	48,48,48,48	0
55	MG	BA	3018	1/1	0.97	0.08	10,10,10,10	0
55	MG	AA	1603	1/1	0.97	0.21	57,57,57,57	0
55	MG	BA	3030	1/1	0.97	0.16	3,3,3,3	0
56	ZN	D4	101	1/1	0.97	0.07	74,74,74,74	0
55	MG	BA	3043	1/1	0.97	0.06	23,23,23,23	0
55	MG	DA	3020	1/1	0.97	0.19	44,44,44,44	0
55	MG	BA	3131	1/1	0.97	0.32	37,37,37,37	0
55	MG	BA	3189	1/1	0.97	0.20	0,0,0,0	0
55	MG	BA	3142	1/1	0.97	0.21	0,0,0,0	0
55	MG	AA	1653	1/1	0.97	0.18	34,34,34,34	0
55	MG	AA	1641	1/1	0.97	0.12	7,7,7,7	0
55	MG	DA	3109	1/1	0.97	0.19	30,30,30,30	0
55	MG	AA	1654	1/1	0.97	0.14	41,41,41,41	0
55	MG	BA	3153	1/1	0.97	0.16	2,2,2,2	0
55	MG	BB	204	1/1	0.97	0.36	0,0,0,0	0
55	MG	BA	3116	1/1	0.97	0.19	30,30,30,30	0
55	MG	BA	3042	1/1	0.97	0.14	1,1,1,1	0
55	MG	BA	3149	1/1	0.97	0.23	0,0,0,0	0
55	MG	BA	3009	1/1	0.97	0.08	2,2,2,2	0
55	MG	CA	1643	1/1	0.97	0.37	41,41,41,41	0
55	MG	BA	3164	1/1	0.98	0.30	6,6,6,6	0
55	MG	BA	3051	1/1	0.98	0.14	4,4,4,4	0
55	MG	CA	1649	1/1	0.98	0.22	24,24,24,24	0
55	MG	BA	3060	1/1	0.98	0.13	29,29,29,29	0
55	MG	AA	1612	1/1	0.98	0.13	38,38,38,38	0
55	MG	BA	3114	1/1	0.98	0.09	28,28,28,28	0
55	MG	DA	3131	1/1	0.98	0.13	50,50,50,50	0
55	MG	BA	3010	1/1	0.98	0.09	1,1,1,1	0
55	MG	BA	3017	1/1	0.98	0.16	0,0,0,0	0
55	MG	BA	3081	1/1	0.98	0.10	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3035	1/1	0.98	0.07	0,0,0,0	0
55	MG	BA	3021	1/1	0.98	0.15	2,2,2,2	0
55	MG	DA	3017	1/1	0.98	0.18	39,39,39,39	0
55	MG	BA	3037	1/1	0.98	0.19	0,0,0,0	0
55	MG	BA	3128	1/1	0.98	0.19	3,3,3,3	0
55	MG	BA	3139	1/1	0.98	0.27	0,0,0,0	0
55	MG	DA	3074	1/1	0.98	0.08	47,47,47,47	0
55	MG	BA	3008	1/1	0.98	0.13	0,0,0,0	0
55	MG	DA	3050	1/1	0.98	0.12	52,52,52,52	0
55	MG	CA	1625	1/1	0.98	0.17	18,18,18,18	0
55	MG	BA	3078	1/1	0.98	0.04	38,38,38,38	0
55	MG	BA	3187	1/1	0.98	0.21	3,3,3,3	0
55	MG	DA	3086	1/1	0.98	0.12	61,61,61,61	0
55	MG	BA	3106	1/1	0.98	0.24	0,0,0,0	0
55	MG	AA	1621	1/1	0.98	0.09	37,37,37,37	0
55	MG	BA	3086	1/1	0.99	0.20	0,0,0,0	0
55	MG	BA	3033	1/1	0.99	0.20	0,0,0,0	0
55	MG	BA	3063	1/1	0.99	0.13	2,2,2,2	0
55	MG	AA	1642	1/1	0.99	0.07	25,25,25,25	0
55	MG	AA	1647	1/1	0.99	0.17	44,44,44,44	0
55	MG	AA	1645	1/1	0.99	0.09	42,42,42,42	0
55	MG	DA	3067	1/1	0.99	0.18	43,43,43,43	0
55	MG	AA	1656	1/1	0.99	0.07	32,32,32,32	0
55	MG	BA	3141	1/1	0.99	0.40	0,0,0,0	0
55	MG	BA	3107	1/1	0.99	0.14	3,3,3,3	0
56	ZN	B4	101	1/1	1.00	0.08	76,76,76,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.