



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:11 PM GMT

PDB ID : 4U1U
Title : Crystal structure of the E. coli ribosome bound to quinupristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-04-23
Resolution : 2.95 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

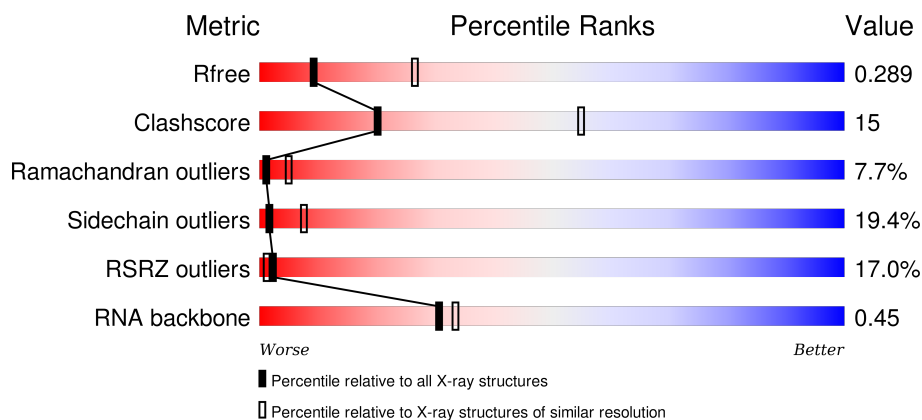
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)
RNA backbone	2183	1010 (3.36-2.56)

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. 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>3%</div> <div>42%</div> <div>44%</div> <div>12%</div> <div>.</div> </div>
1	CA	1539	<div> <div>7%</div> <div>43%</div> <div>44%</div> <div>12%</div> <div>.</div> </div>
2	AB	218	<div> <div>19%</div> <div>20%</div> <div>47%</div> <div>28%</div> <div>6%</div> </div>
2	CB	218	<div> <div>36%</div> <div>30%</div> <div>47%</div> <div>20%</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	

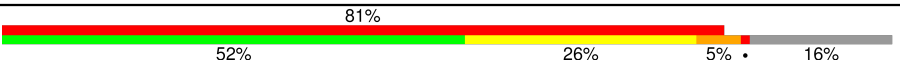


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Mol	Chain	Length	Quality of chain
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	76	
44	DW	76	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	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	8	
54	D6	8	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	004	D6	7	-	-	X	-
55	MG	AA	1622	-	-	-	X
55	MG	AA	1669	-	-	-	X
55	MG	BA	3040	-	-	-	X
55	MG	BA	3070	-	-	-	X
55	MG	BA	3108	-	-	-	X
55	MG	BA	3113	-	-	-	X
55	MG	BA	3116	-	-	-	X
55	MG	BA	3130	-	-	-	X
55	MG	BA	3152	-	-	-	X
55	MG	BA	3153	-	-	-	X
55	MG	BA	3161	-	-	-	X
55	MG	BA	3163	-	-	-	X
55	MG	BA	3168	-	-	-	X
55	MG	BA	3170	-	-	-	X
55	MG	BA	3178	-	-	-	X
55	MG	BA	3186	-	-	-	X
55	MG	BA	3188	-	-	-	X
55	MG	DA	3002	-	-	-	X
55	MG	DA	3005	-	-	-	X
55	MG	DA	3008	-	-	-	X
55	MG	DA	3013	-	-	-	X
55	MG	DA	3027	-	-	-	X
55	MG	DA	3057	-	-	-	X
55	MG	DA	3070	-	-	-	X
55	MG	DA	3071	-	-	-	X
55	MG	DA	3109	-	-	-	X
55	MG	DA	3124	-	-	-	X
55	MG	DA	3153	-	-	-	X
55	MG	DA	3157	-	-	-	X
55	MG	DA	3162	-	-	-	X
55	MG	DA	3165	-	-	-	X

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a protein called Quinupristin.

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

- Molecule 55 is MAGNESIUM ION (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	619	Total O 619 619	0	0
57	BB	13	Total O 13 13	0	0
57	BC	8	Total O 8 8	0	0
57	BD	3	Total O 3 3	0	0
57	BE	3	Total O 3 3	0	0
57	BF	1	Total O 1 1	0	0
57	BG	1	Total O 1 1	0	0
57	BL	5	Total O 5 5	0	0
57	BN	5	Total O 5 5	0	0
57	BS	1	Total O 1 1	0	0
57	BV	1	Total O 1 1	0	0
57	B2	1	Total O 1 1	0	0
57	B3	3	Total O 3 3	0	0
57	B4	2	Total O 2 2	0	0
57	CA	189	Total O 189 189	0	0
57	CL	1	Total O 1 1	0	0
57	CN	3	Total O 3 3	0	0

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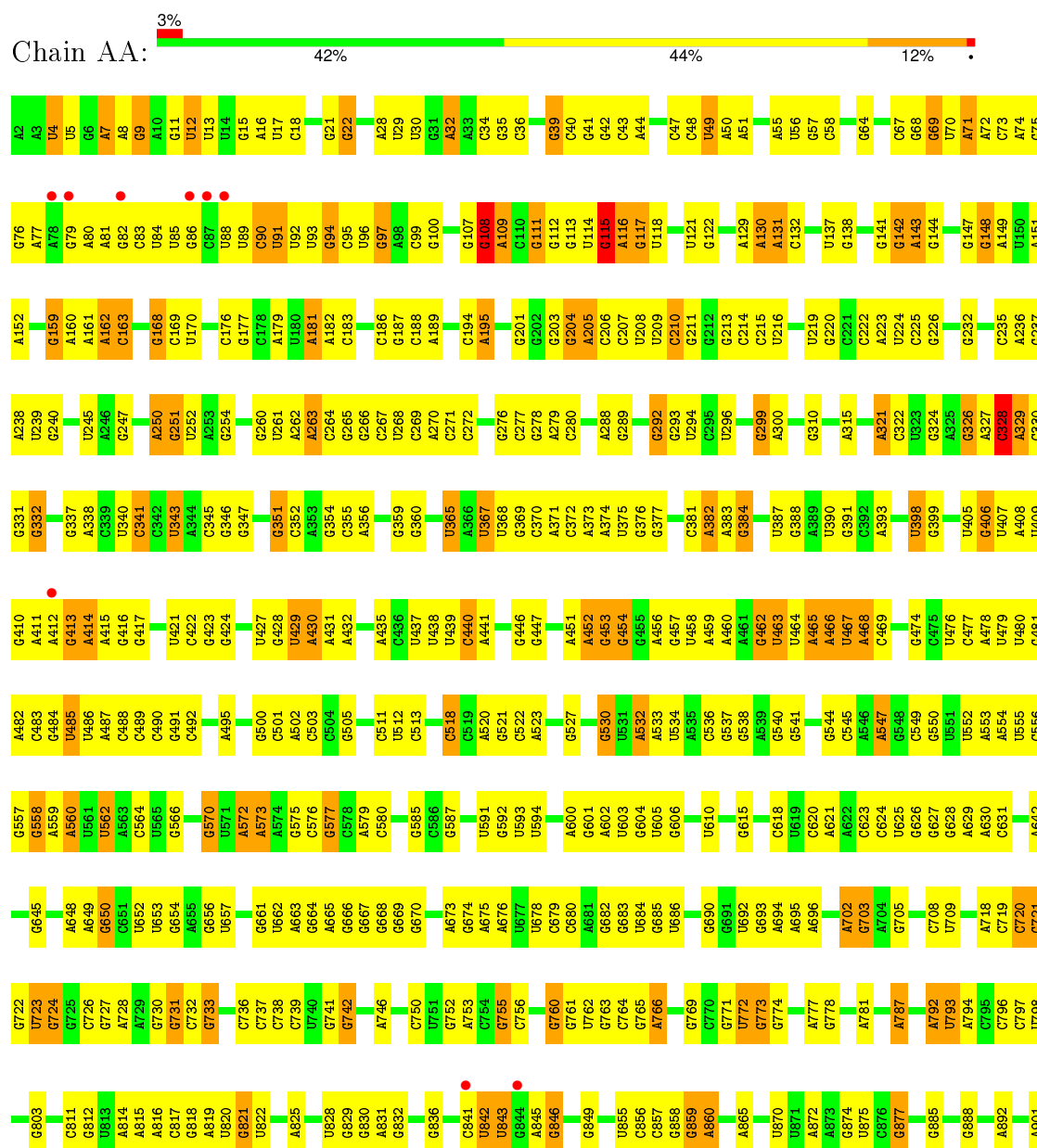
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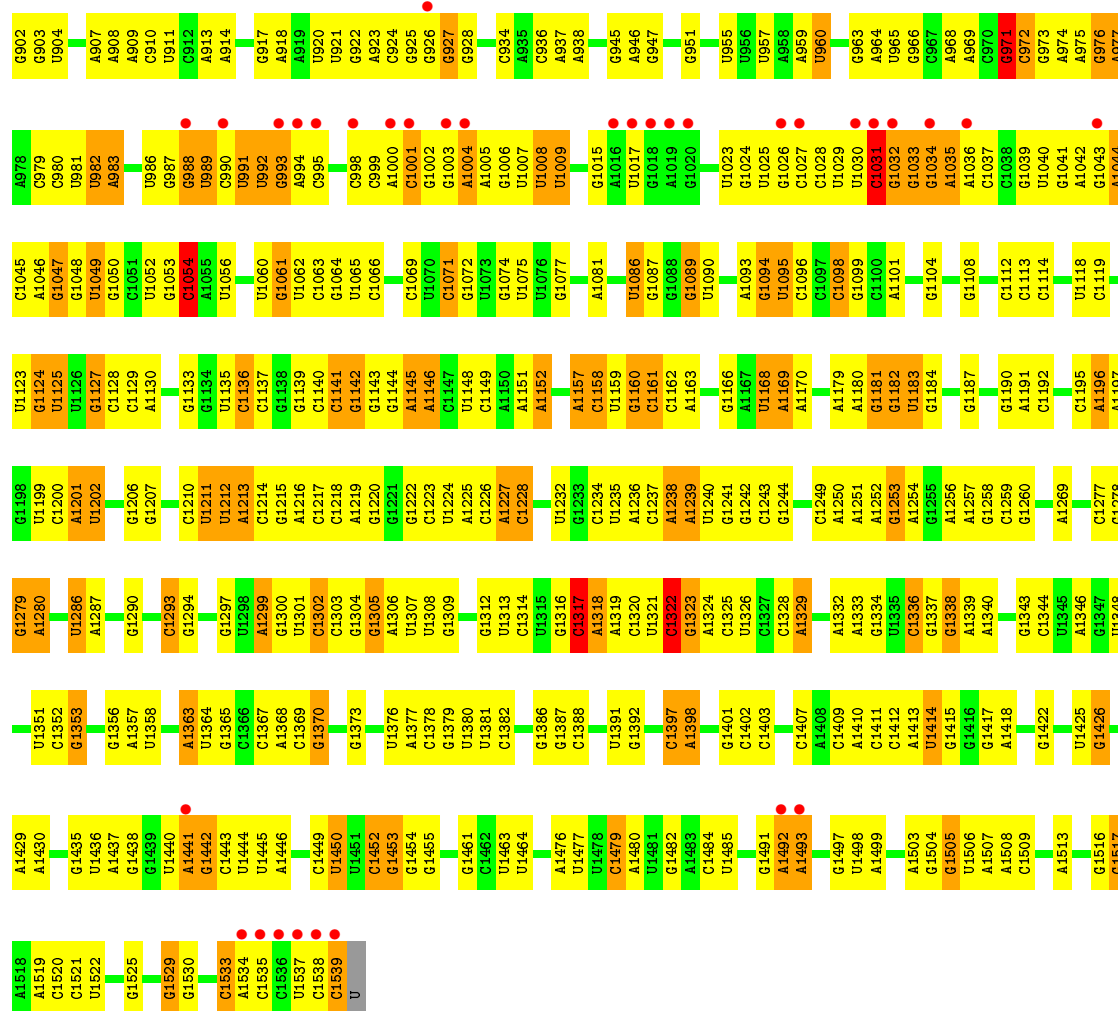
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57	DB	13	Total 13	O 13	0	0
57	DC	7	Total 7	O 7	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	4	Total 4	O 4	0	0
57	DL	4	Total 4	O 4	0	0
57	DN	1	Total 1	O 1	0	0
57	DQ	2	Total 2	O 2	0	0
57	DT	3	Total 3	O 3	0	0
57	DV	1	Total 1	O 1	0	0
57	D0	1	Total 1	O 1	0	0
57	D2	2	Total 2	O 2	0	0
57	D3	1	Total 1	O 1	0	0
57	D4	1	Total 1	O 1	0	0

3 Residue-property plots

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

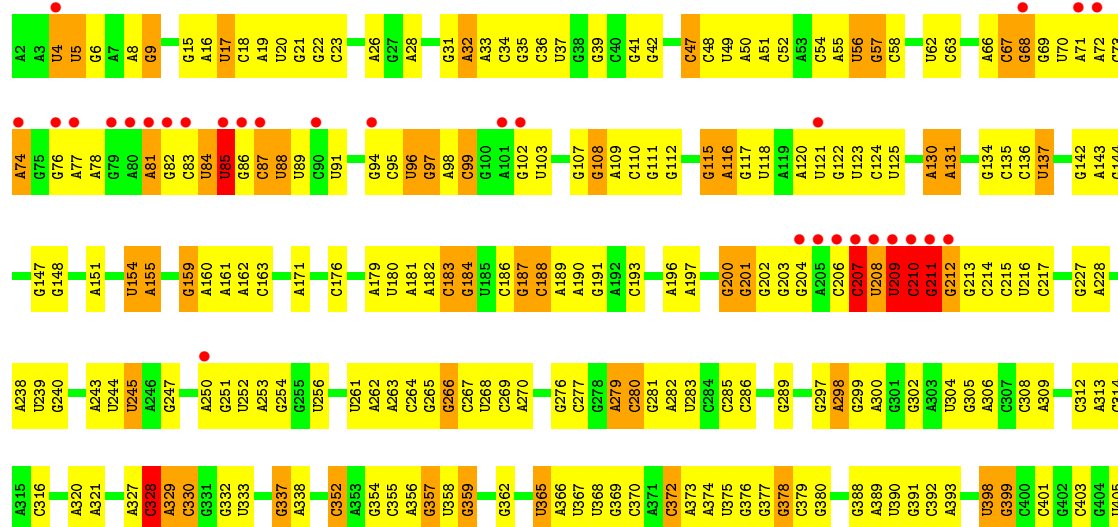
• Molecule 1: 16S rRNA





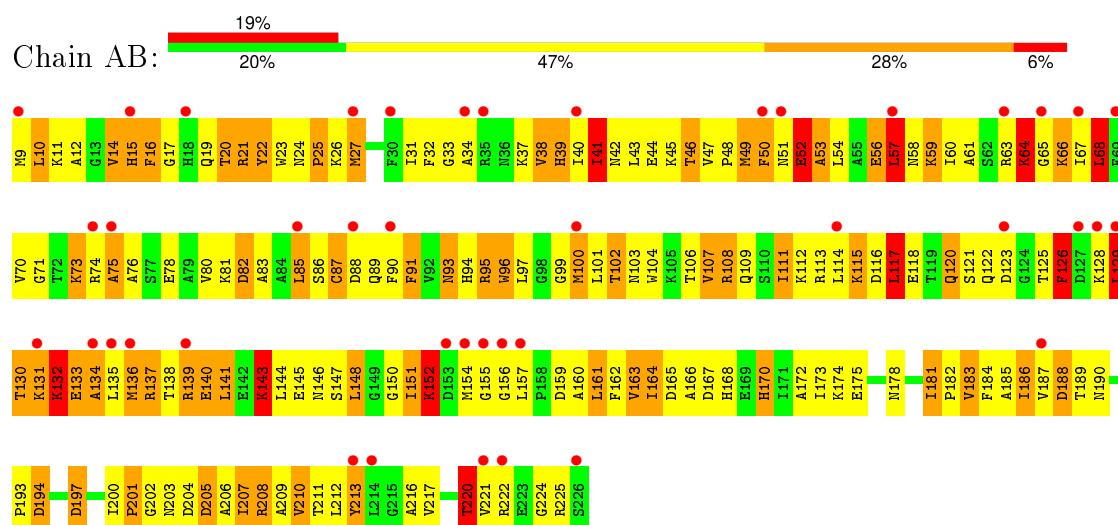
• Molecule 1: 16S rRNA

Chain CA: 7% 43% 44% 12%

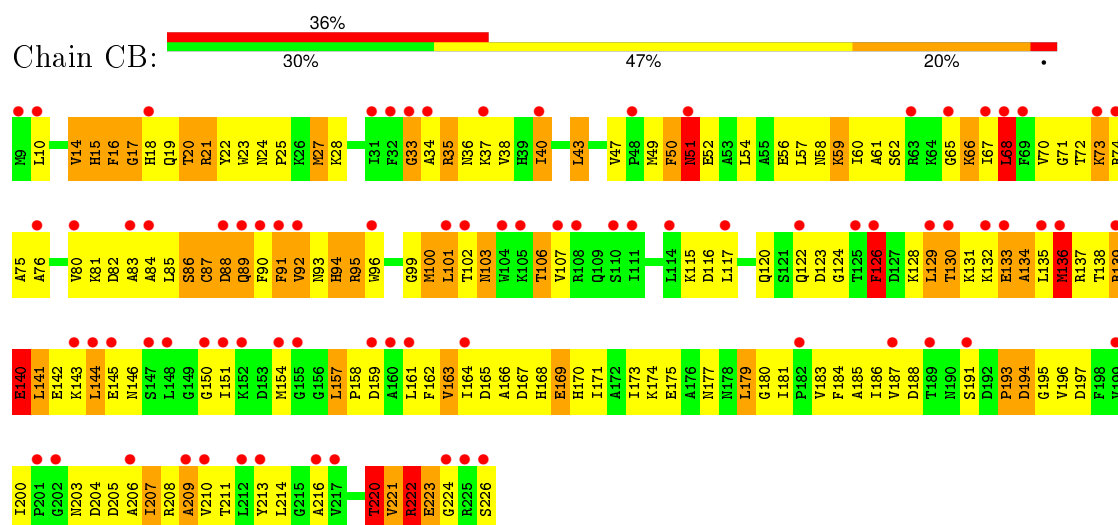


C1509	A1433	C1284	G1218	U062	U997	U921	U820	G733	A649	C549	G484	G406
A1434	A1350	A1285	A1219	C1063	C998	G922	G821	G734	G650	G950	U485	U407
G1435	U1351	U1286	G1220	G1064	C999	G926	U822	C735	G651	U551	U486	A408
C1352	C1352	A1287	G1221	U1065	A1000	G926	C823	C736	U652	U552	A487	U409
G1353	U1353	A1288	G1222	C1066	C1001	G929	U827	C737	U653	A553	C488	G410
U1354	U1354	C1296	A1225	A1067	G1002	G930	U828	C738	G654	U555	C489	A411
G1355	G1355	U1291	A1226	C1068	G1003	C931	U833	C739	A663	C556	C490	A412
C1356	A1292	G1292	C1226	G1069	A1004	C932	G833	U740	A664	G557	C491	G413
A1357	C1293	A1227	A1227	U1070	A1005	C931	U841	U741	G665	U561	C492	C418
U1358	C1294	A1228	C1228	C1071	A1006	C933	U842	G745	A665	A558	A493	U421
C1359	U1295	A1229	A1229	G1072	U1007	C934	U843	U751	A666	A559	A494	G424
A1360	C1296	A1230	G1230	U1073	U1008	A935	U844	U752	G667	A560	A495	U422
G1361	G1297	G1231	G1231	G1074	U1009	A935	G846	A753	U672	U562	A496	G423
A1362	U1298	U1232	U1232	G1077	U1010	A938	U847	C754	A673	C563	C497	G424
A1363	A1299	G1233	G1233	G1077	C1011	G939	U848	U757	A674	U564	A498	G425
U1364	A1300	A1299	G1233	G1077	A1012	C940	U849	C758	A675	C565	A499	G426
G1365	U1301	A1301	A1299	G1077	C1012	C941	U850	U759	A676	C566	C501	U427
C1366	C1302	A1298	A1238	U1080	G1013	G942	U851	U760	U677	G568	C502	U428
U1367	U1303	A1299	A1239	A1081	A1014	A949	U855	G765	G682	A572	C503	A430
G1368	C1304	G1304	G1241	U1082	A1015	A950	U856	U766	A687	A574	G504	C436
A1370	G1242	G1242	G1242	U1083	U1017	A951	C857	U767	G688	A575	G505	U437
U1370	G1243	C1243	C1243	U1084	U1018	G952	C858	U768	G689	C576	C511	U438
G1371	A1167	A1167	A1167	U1085	A1019	G953	C859	U769	A689	C577	C512	U439
A1372	U1244	A1167	A1167	U1086	G1020	G954	C860	U770	G690	C578	C513	U440
C1373	G1245	U1168	U1168	G1087	A1021	G955	C861	U771	G691	C579	C514	A441
A1374	A1246	U1169	A1246	G1088	A1022	G956	C862	U772	G692	C580	C515	G445
U1377	U1247	A1170	U1247	U1094	U1023	U960	C863	U773	A695	C582	C516	G446
G1378	A1248	A1248	A1248	U1095	G1024	U965	C864	U774	G695	C583	C517	A451
C1379	C1249	A1249	C1249	U1096	U1025	U966	C865	U775	G696	C584	C518	A452
U1380	A1250	A1176	A1176	C1096	G1026	G966	C866	U776	G697	C585	C519	A453
G1381	U1251	A1177	A1177	C1097	U1027	G967	C867	U777	G698	C586	C520	G454
U1382	A1252	A1178	A1252	U1098	G1028	U968	C868	U778	G699	C587	C521	U458
C1383	C1317	A1180	A1253	U1099	U1029	U969	C869	U779	G700	C588	C522	A459
A1384	A1254	G1181	A1254	C1100	U1030	U970	C870	U780	G701	C589	C523	U463
U1385	G1255	U1182	G1255	A1101	C1031	G971	C871	U781	G702	C590	C524	U464
G1386	A1256	G1183	A1256	C1102	G1032	G972	C872	U782	G703	C591	C525	U465
C1387	A1257	U1184	A1257	G1108	G1033	C973	C873	U783	G704	C592	C526	U466
U1388	U1260	A1191	A1260	C1113	A1034	G974	C874	U784	G705	C593	C527	U467
G1389	A1261	C1192	A1261	G1114	A1035	G975	C875	U785	G706	C594	C528	U468
C1390	C1262	A1196	C1262	C1115	A1036	G976	C876	U786	G707	C595	C529	U469
U1391	U1263	A1197	U1263	U1118	C1037	G977	C877	U787	G708	C596	C530	U473
G1392	U1264	A1198	U1264	C1119	G1038	A974	C878	U788	G709	C597	C531	U474
A1393	G1265	U1199	G1265	U1123	U1039	A975	C879	U789	G710	C598	C532	U475
C1394	U1266	C1200	U1266	G1124	U1040	A976	C880	U790	G711	C599	C533	U476
U1395	A1269	A1201	A1269	U1125	U1041	A977	C881	U791	G712	C600	C534	U477
G1396	G1270	U1202	G1270	U1126	A1042	A978	C882	U792	G713	C601	C535	U478
A1400	A1271	C1203	A1271	U1127	U1043	U981	C883	U793	G714	C602	C536	U479
C1401	C1272	A1204	C1272	U1128	A1044	A982	C884	U794	G715	C603	C537	U480
U1402	U1273	U1205	U1273	U1129	G1045	A983	C885	U795	G716	C604	C538	U481
G1403	A1274	G1206	A1274	A1130	U1046	G987	C886	U796	G717	C605	C539	U482
A1404	U1275	C1209	U1275	G1131	G1047	G988	C887	U797	G718	C606	C540	U483
C1405	G1276	A1276	G1276	G1132	U1048	G989	C888	U798	G719	C607	C541	U484
U1406	C1277	C1210	C1277	G1133	U1049	G990	C889	U799	G720	C608	C542	U485
G1407	G1278	U1211	G1278	U1134	G1050	G991	C890	U800	G721	C609	C543	U486
A1408	U1279	A1212	U1279	U1135	U1051	G992	C891	U801	G722	C610	C544	U487
C1409	C1280	A1213	C1280	U1136	A1052	G993	C892	U802	G723	C611	C545	U488
U1410	G1281	U1214	G1281	C1137	U1053	A994	C893	U803	G724	C612	C546	U489
C1411	U1282	C1282	U1282	U1138	U1054	A995	C894	U804	G725	C613	C547	U490
U1412	U1283	A1216	U1283	U1139	A1055	A996	C895	U805	G726	C614	C548	U491
A1413	G1337	G1337	G1337	C1140	U1056	A997	C896	U806	G727	C615	C549	U492
C1414	U1338	U1338	U1338	U1141	U1060	A998	C897	U807	G728	C616	C550	U493
U1415	G1342	C1276	G1342	G1142	G1061	A999	C898	U808	G729	C617	C551	U494
G1416	U1343	U1210	U1343	U1143	U1062	A999	C899	U809	G730	C618	C552	U495
A1417	C1344	U1212	C1344	U1144	U1063	A999	C900	U810	G731	C619	C553	U496
U1418	U1345	A1213	U1345	U1145	U1064	A999	C901	U811	G732	C620	C554	U497
G1419	G1346	C1281	G1346	U1146	U1065	A999	C902	U812	G733	C621	C555	U498
A1431	A1347	U1282	A1347	U1147	U1066	A999	C903	U813	G734	C622	C556	U499
G1432	U1348	U1283	U1348	U1148	U1067	A999	C904	U814	G735	C623	C557	U500

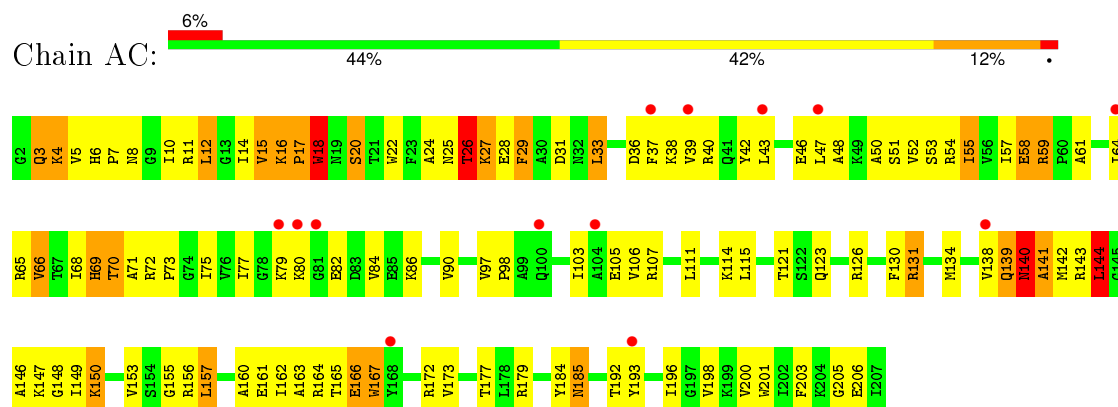
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• Molecule 2: 30S ribosomal protein S2

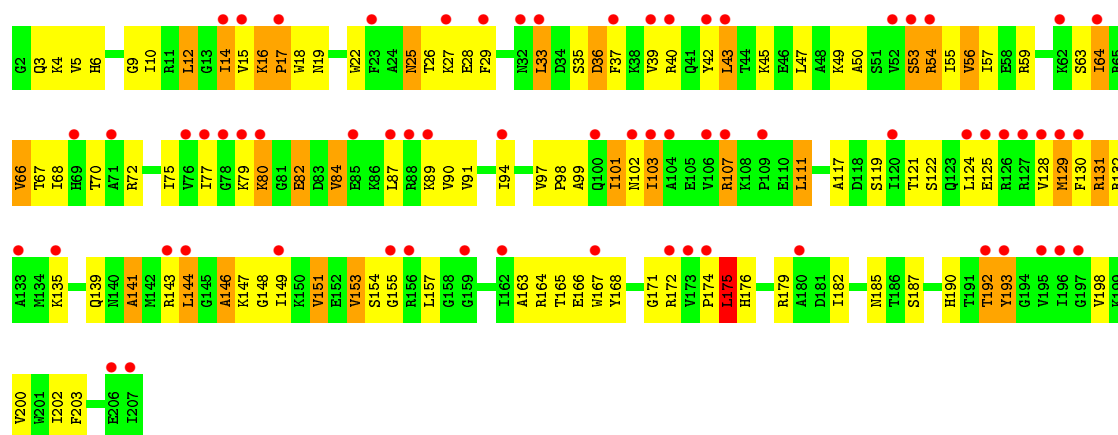


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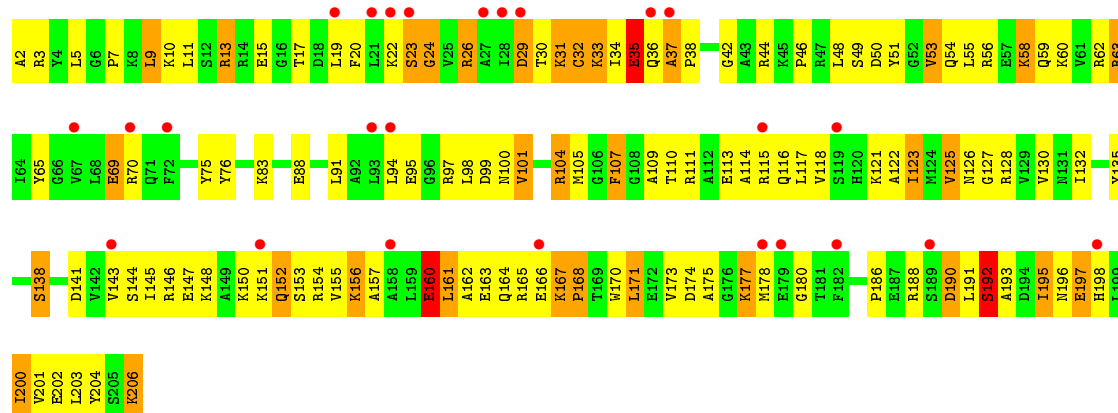
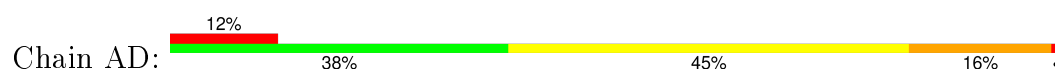


• Molecule 3: 30S ribosomal protein S3

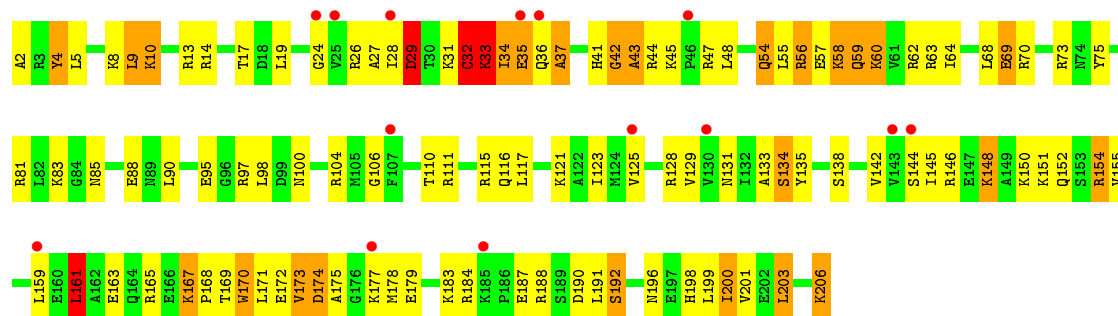




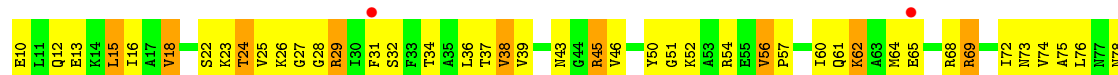
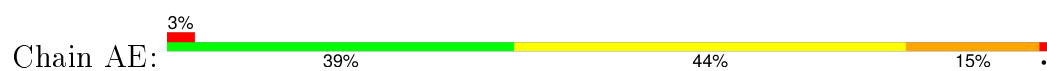
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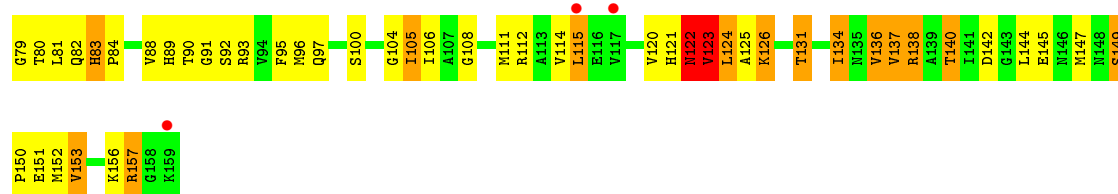


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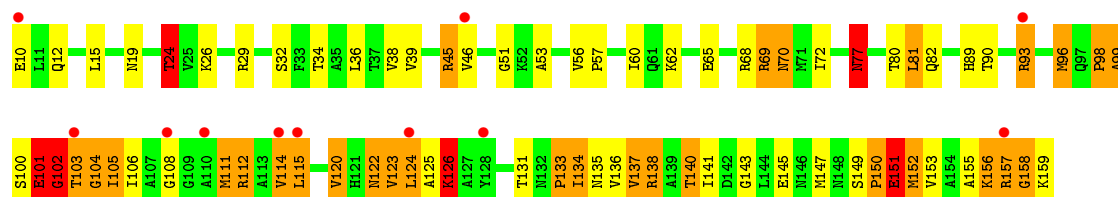


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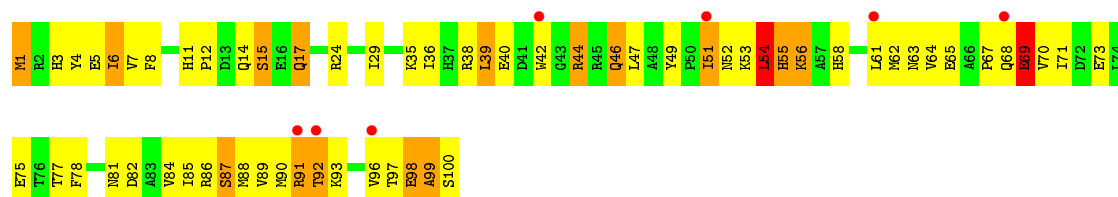




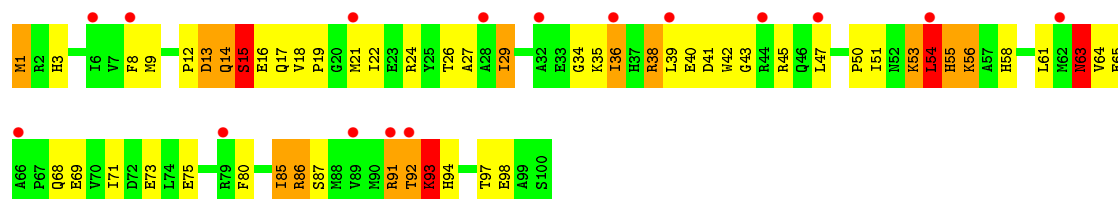
• Molecule 5: 30S ribosomal protein S5



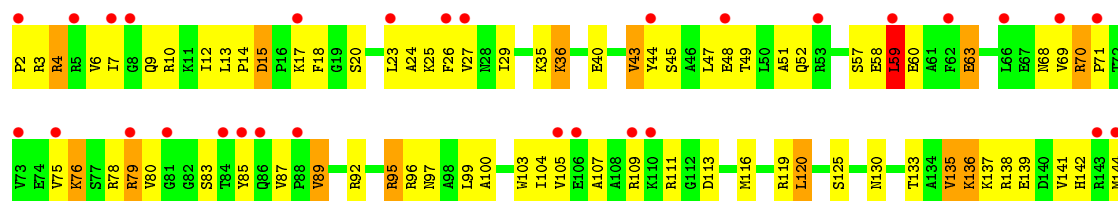
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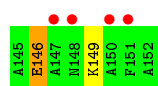


• Molecule 6: 30S ribosomal protein S6

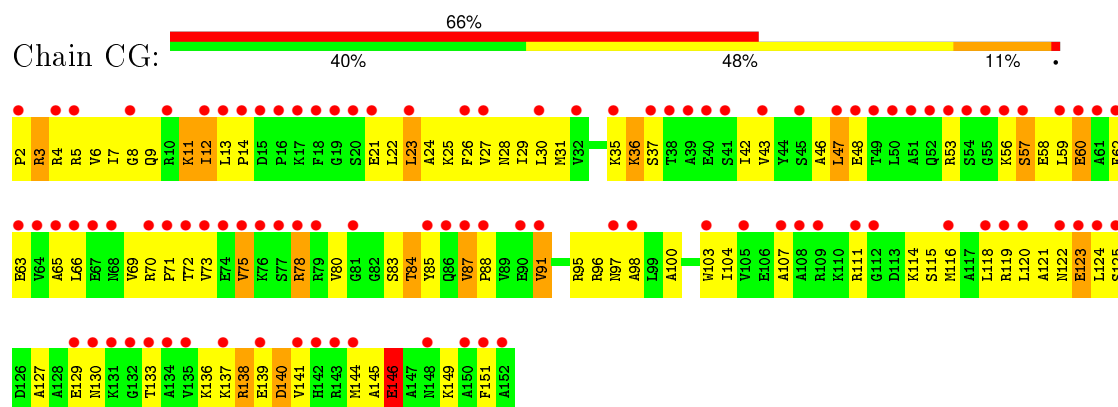


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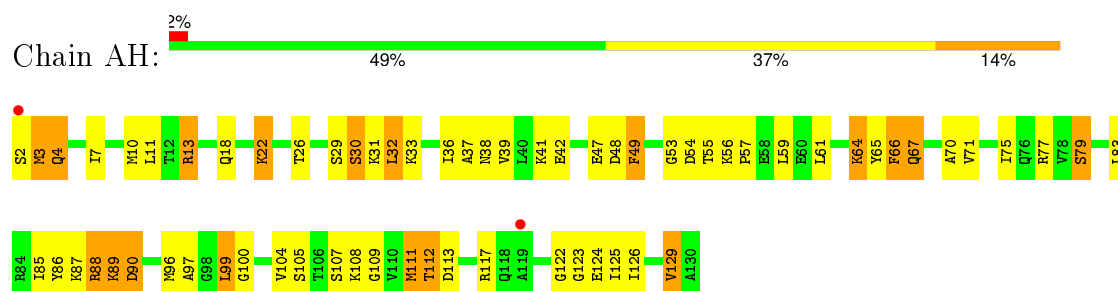




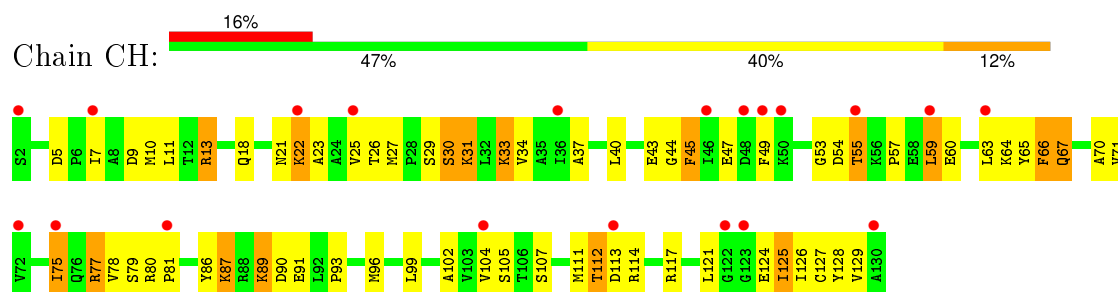
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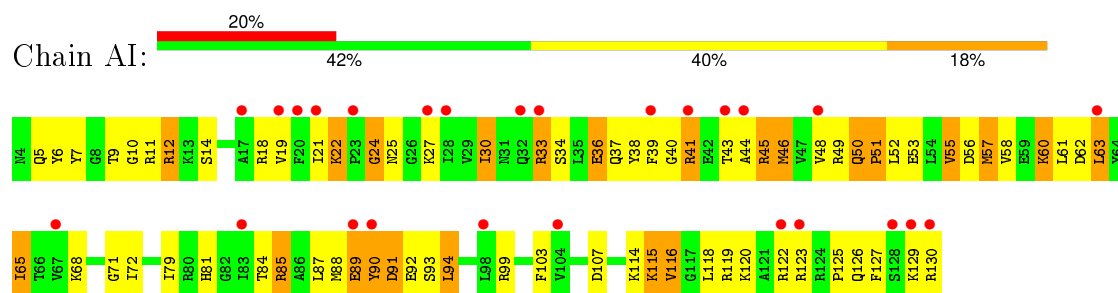
• Molecule 8: 30S ribosomal protein S8



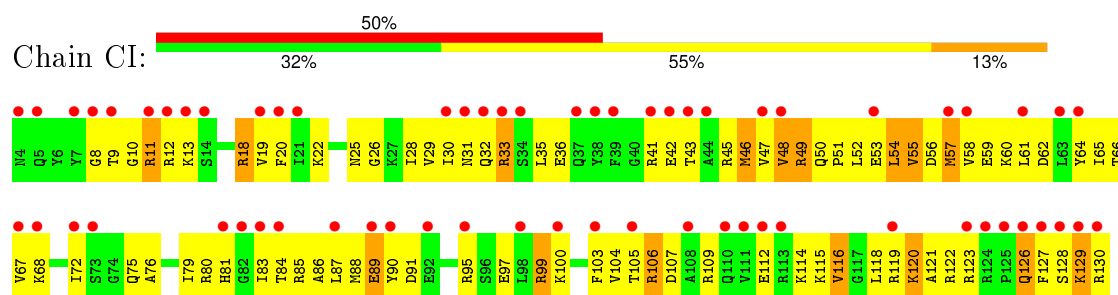
• Molecule 8: 30S ribosomal protein S8



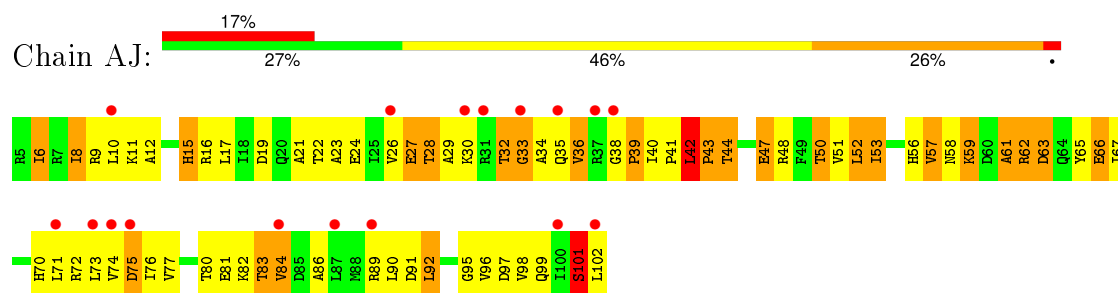
• Molecule 9: 30S ribosomal protein S9



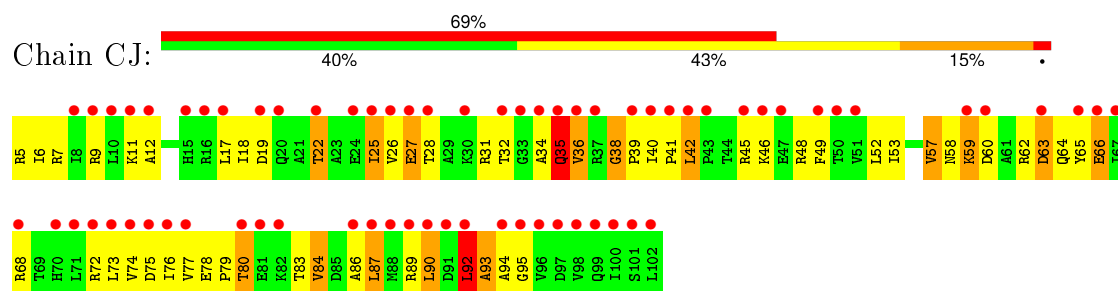
• Molecule 9: 30S ribosomal protein S9



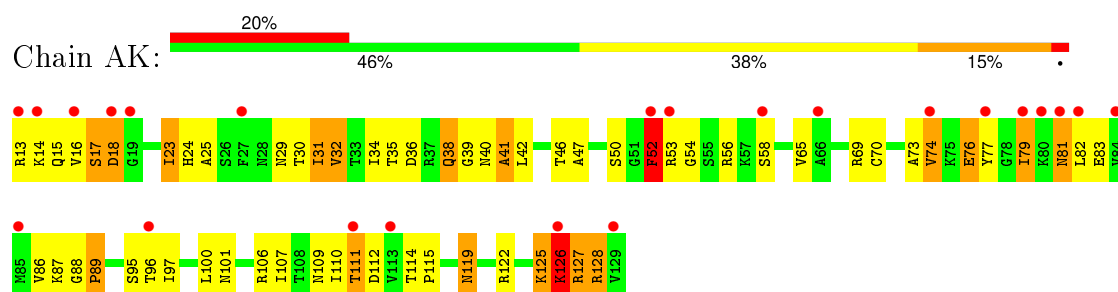
- Molecule 10: 30S ribosomal protein S10



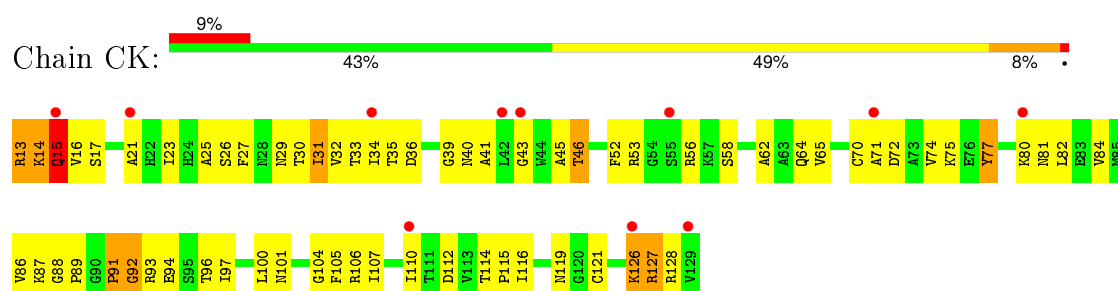
- Molecule 10: 30S ribosomal protein S10



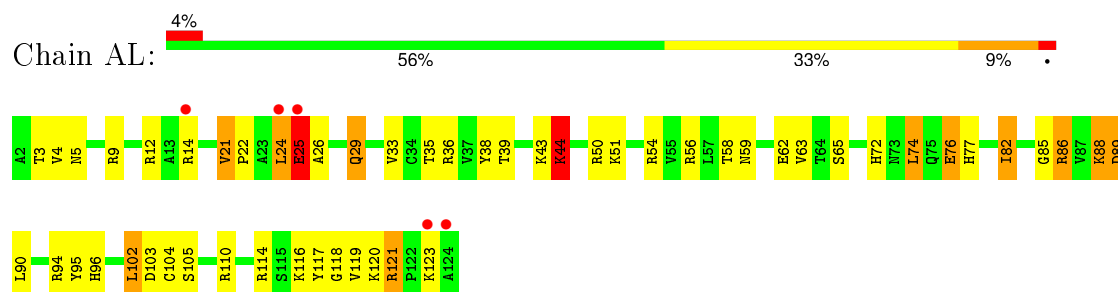
- Molecule 11: 30S ribosomal protein S11



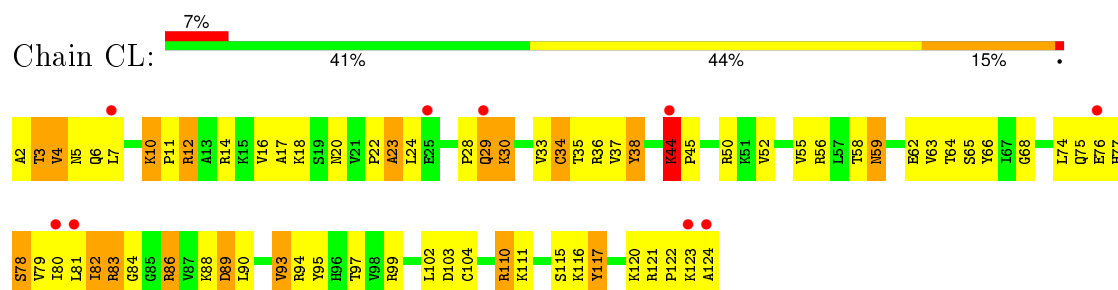
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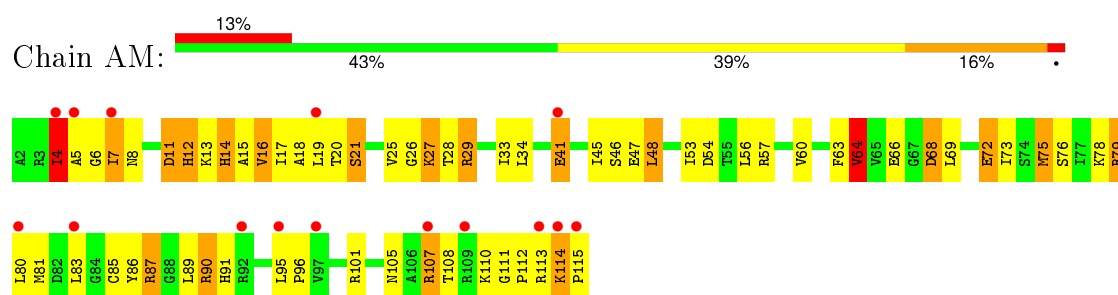
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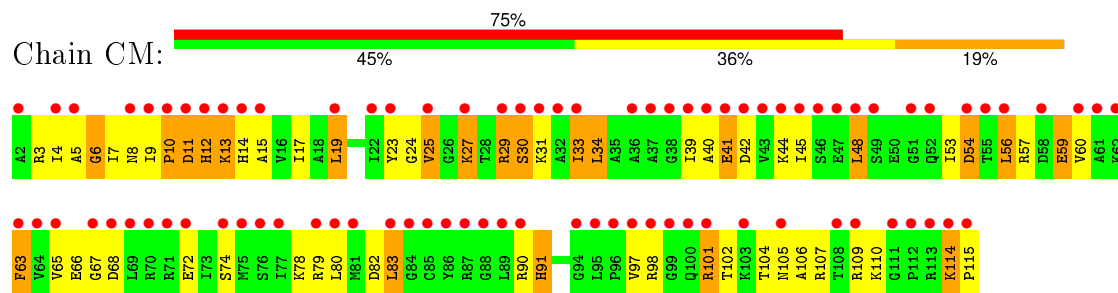
- Molecule 12: 30S ribosomal protein S12



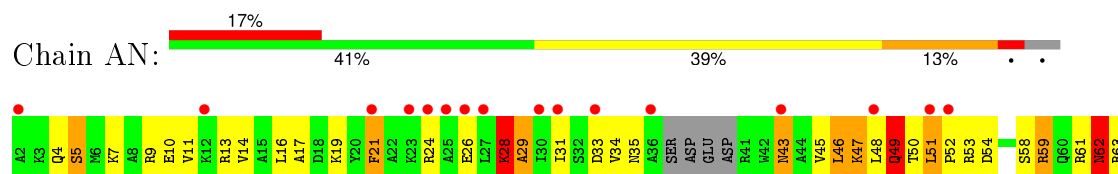
- Molecule 13: 30S ribosomal protein S13

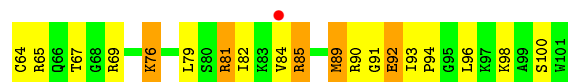


- Molecule 13: 30S ribosomal protein S13

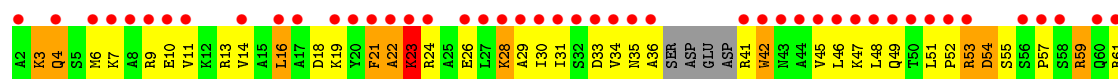


- Molecule 14: 30S ribosomal protein S14

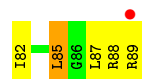




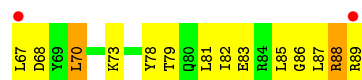
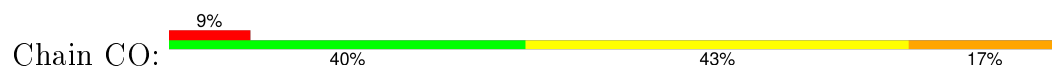
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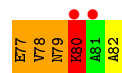
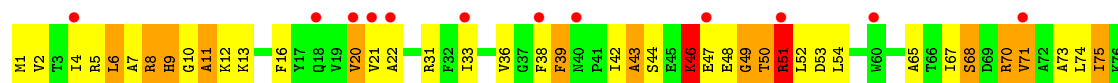
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

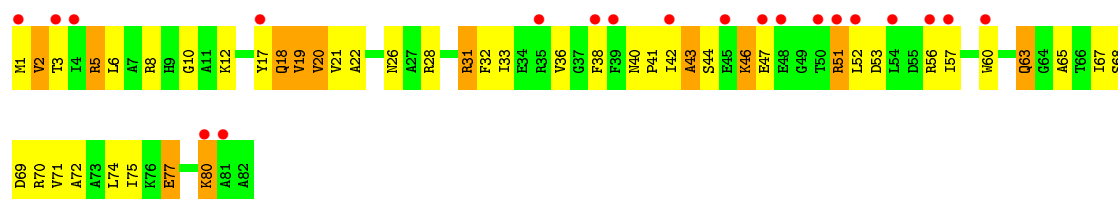


- Molecule 16: 30S ribosomal protein S16

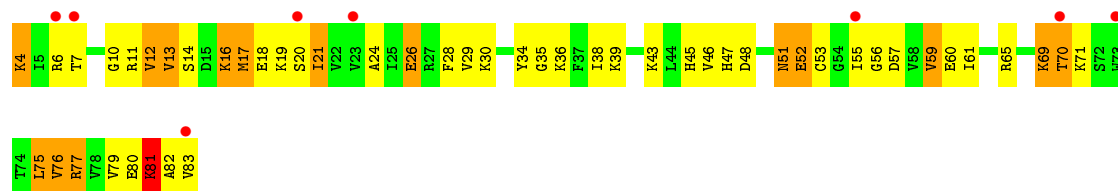


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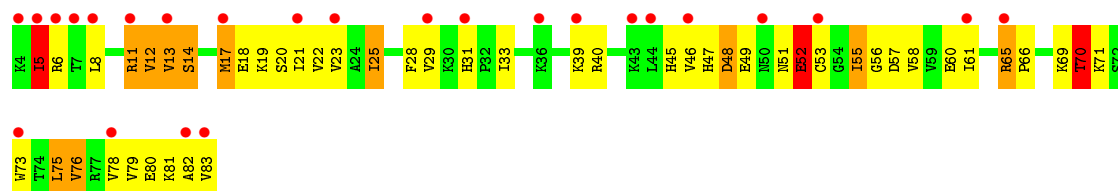




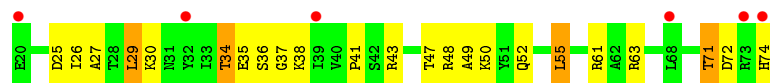
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



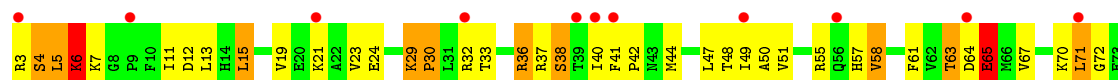
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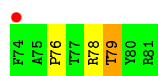


- Molecule 18: 30S ribosomal protein S18

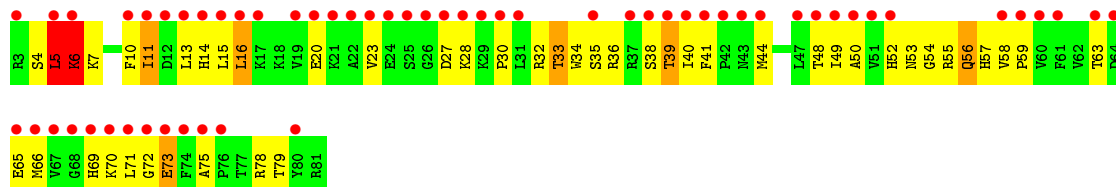
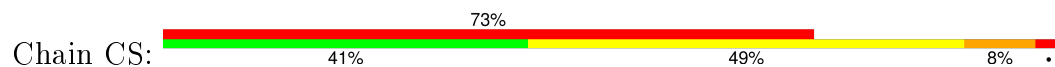


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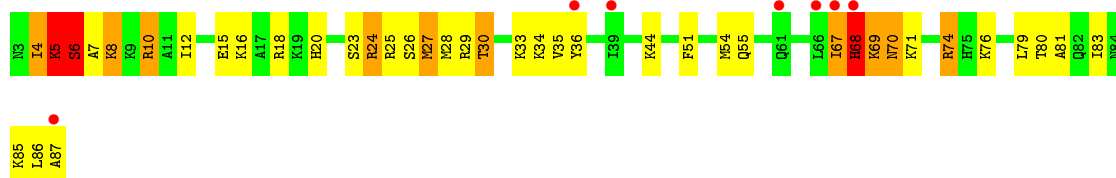




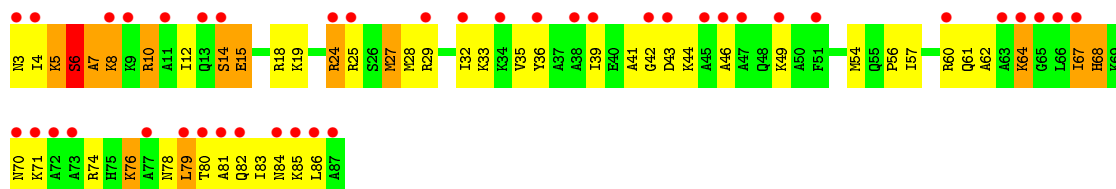
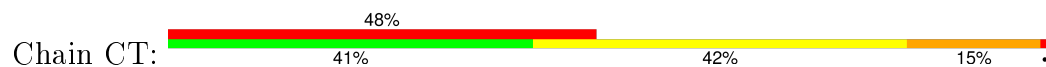
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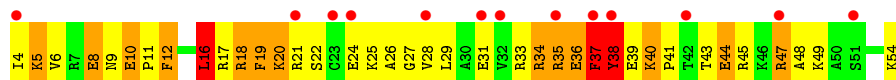
- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



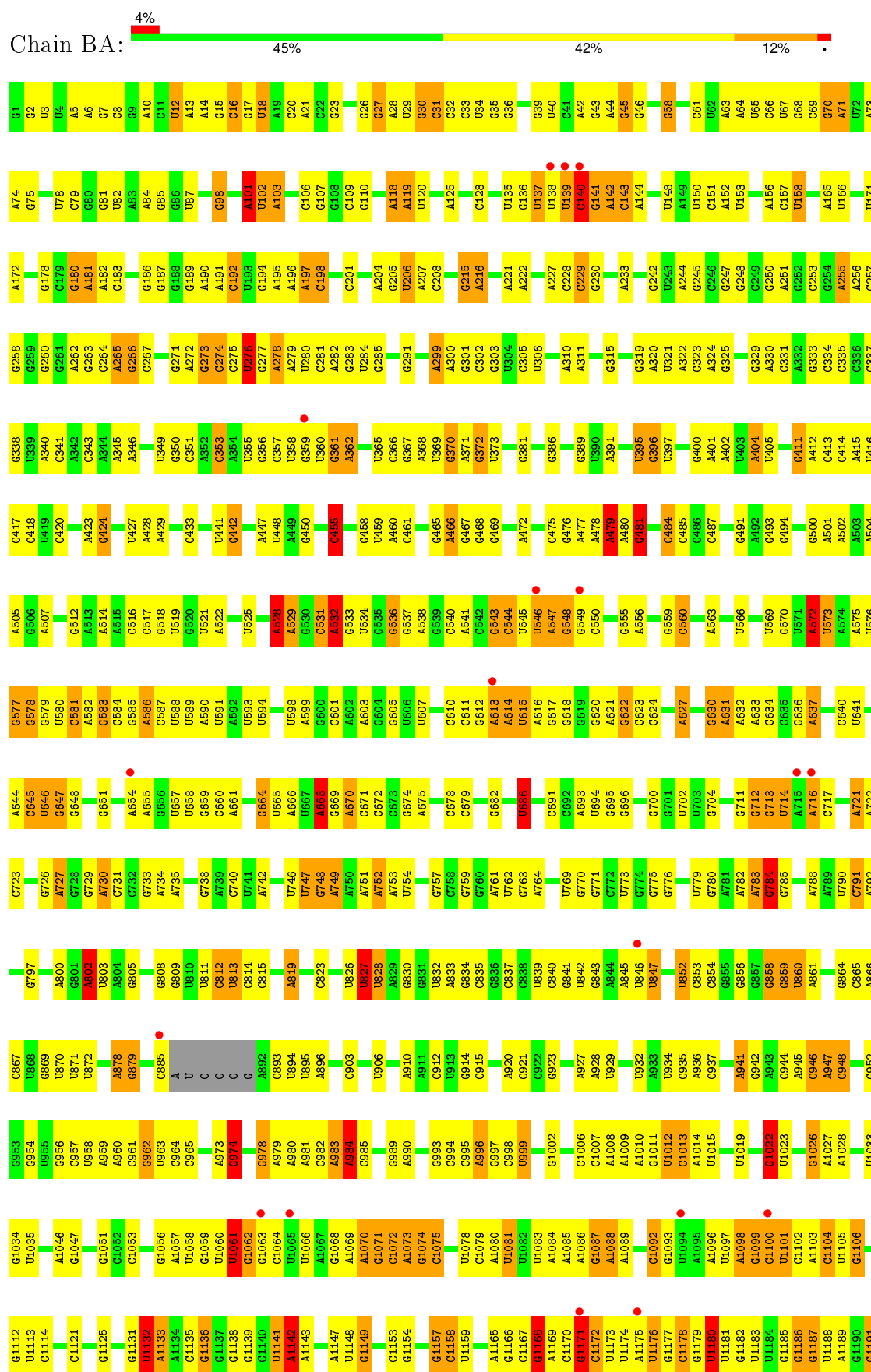
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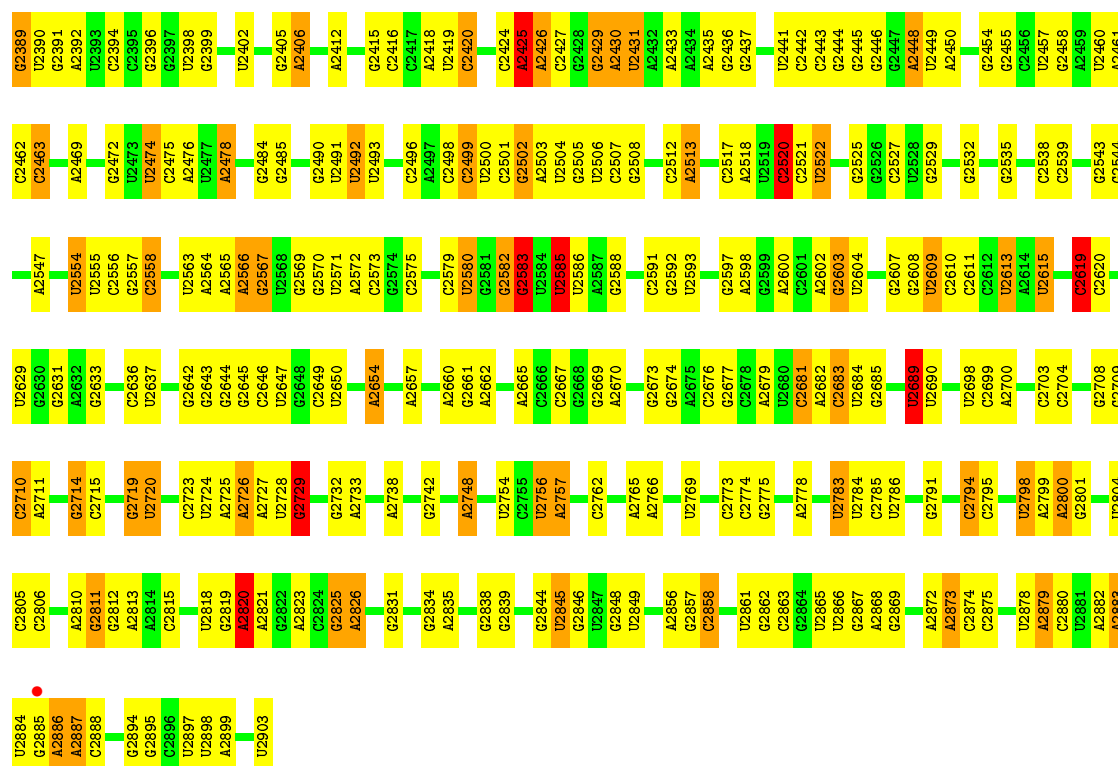
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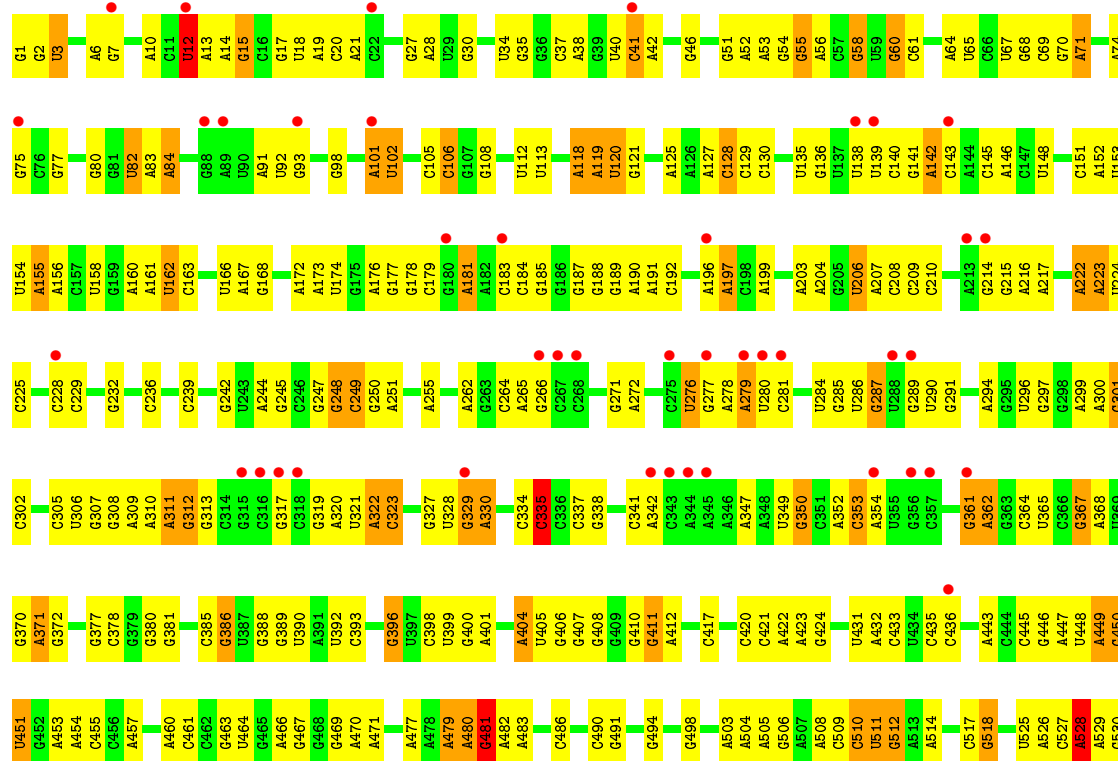
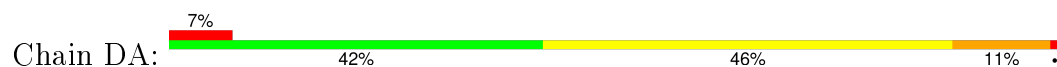
- Molecule 22: 23S rRNA

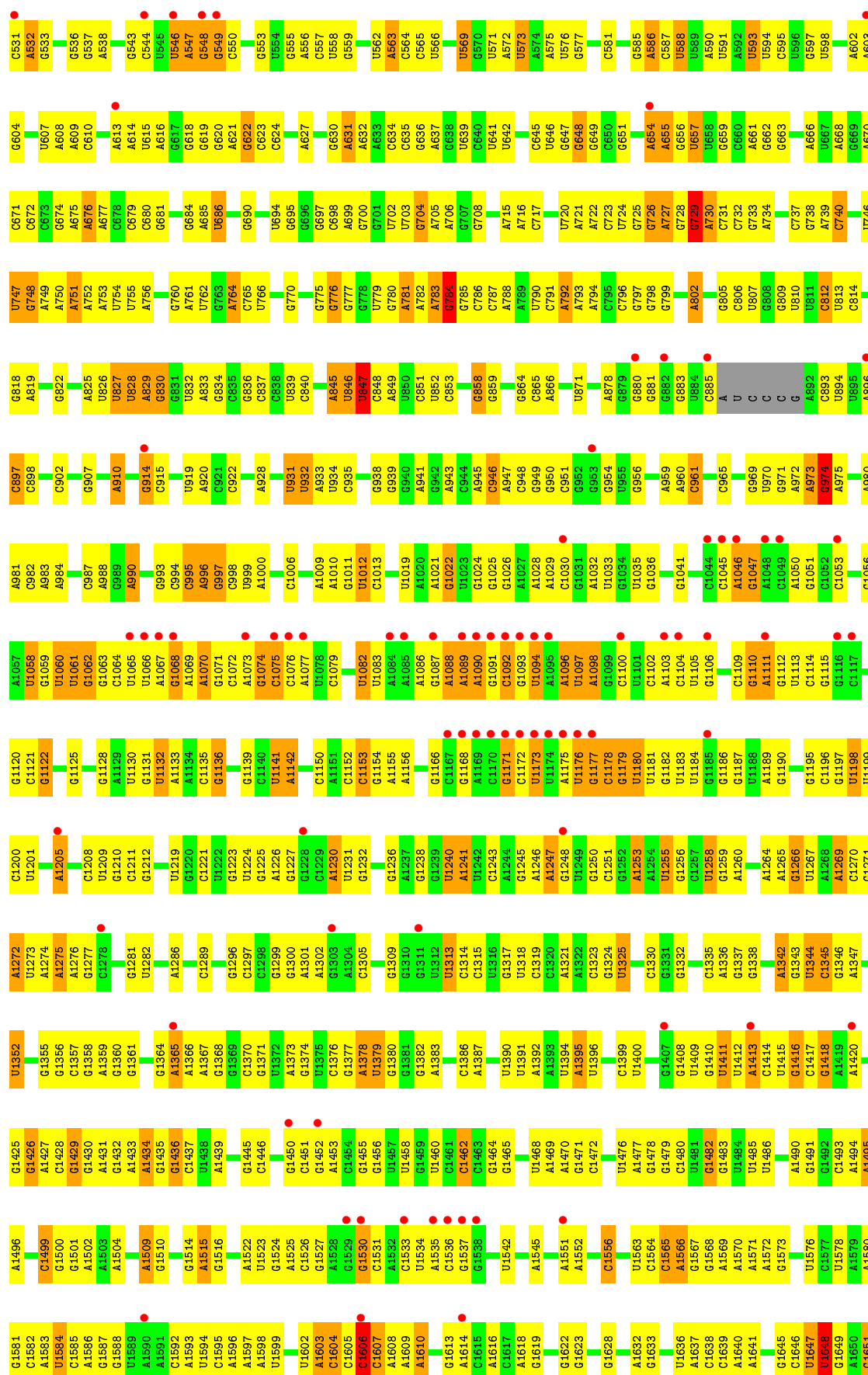


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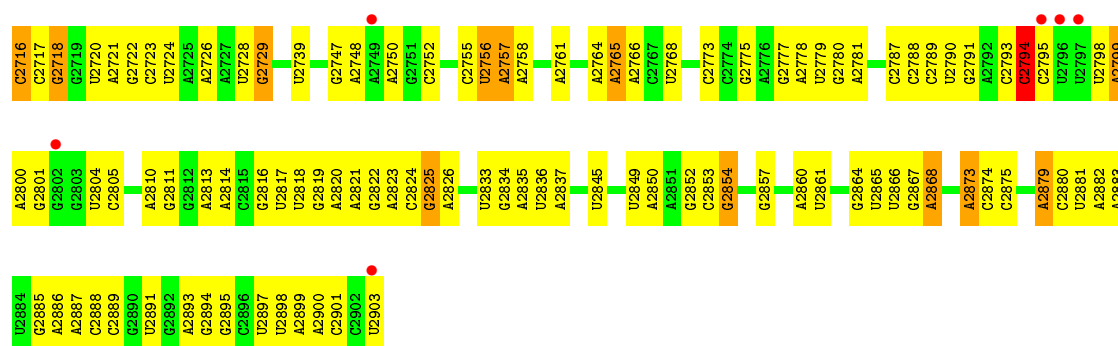


Molecule 22: 23S rRNA

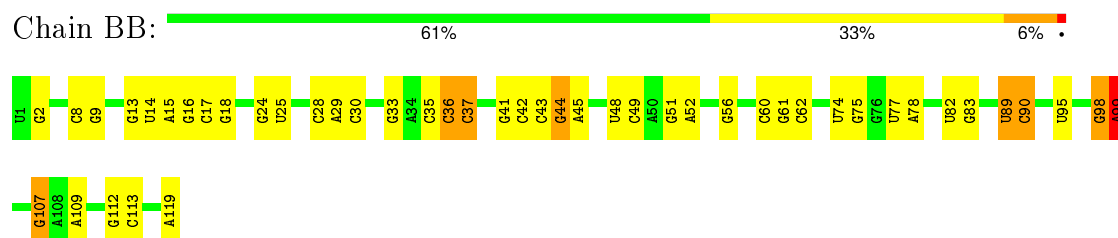




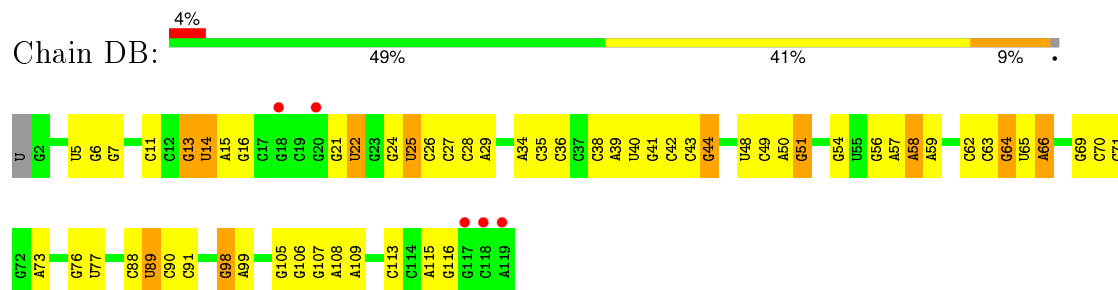
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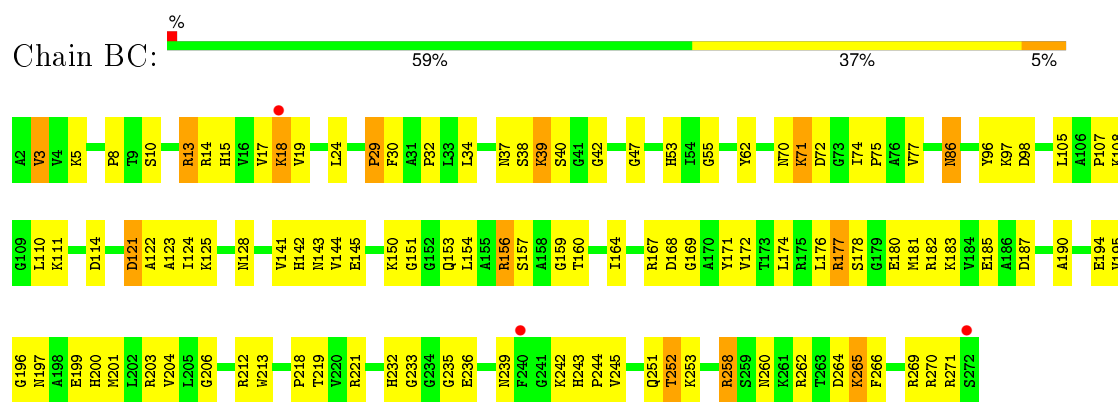
• Molecule 23: 5S rRNA



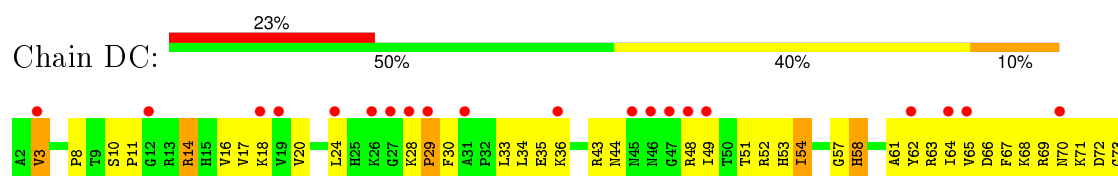
• Molecule 23: 5S rRNA

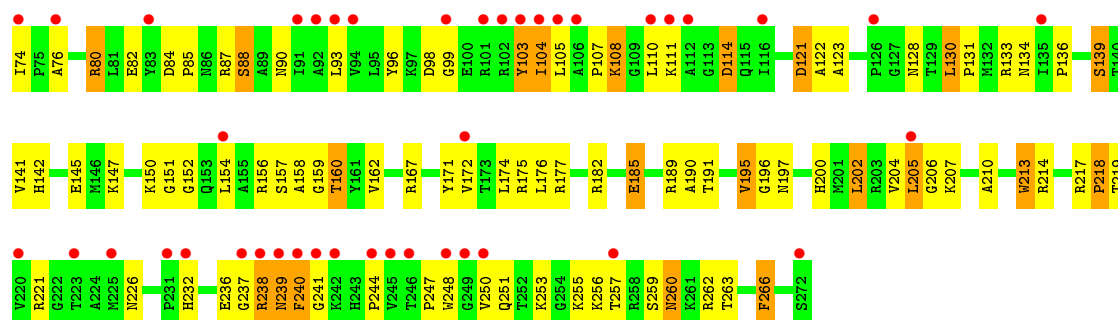


• Molecule 24: 50S ribosomal protein L2



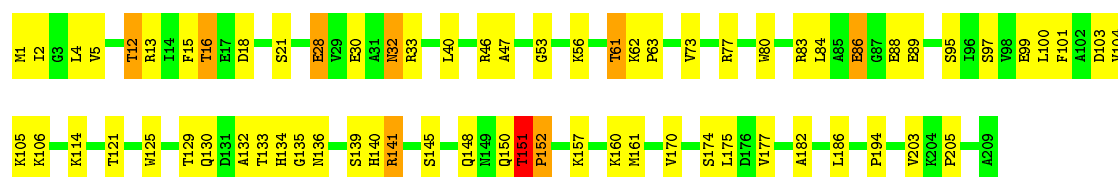
• Molecule 24: 50S ribosomal protein L2





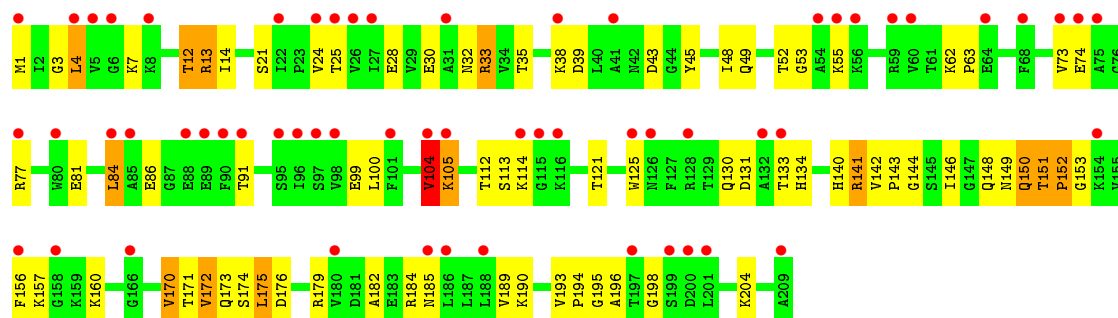
- Molecule 25: 50S ribosomal protein L3

Chain BD: 67% 29% 4%



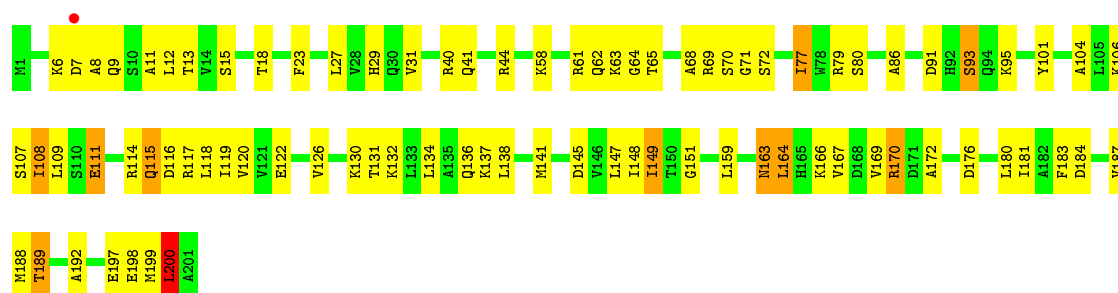
- Molecule 25: 50S ribosomal protein L3

Chain DD: 28% 62% 32% 6%



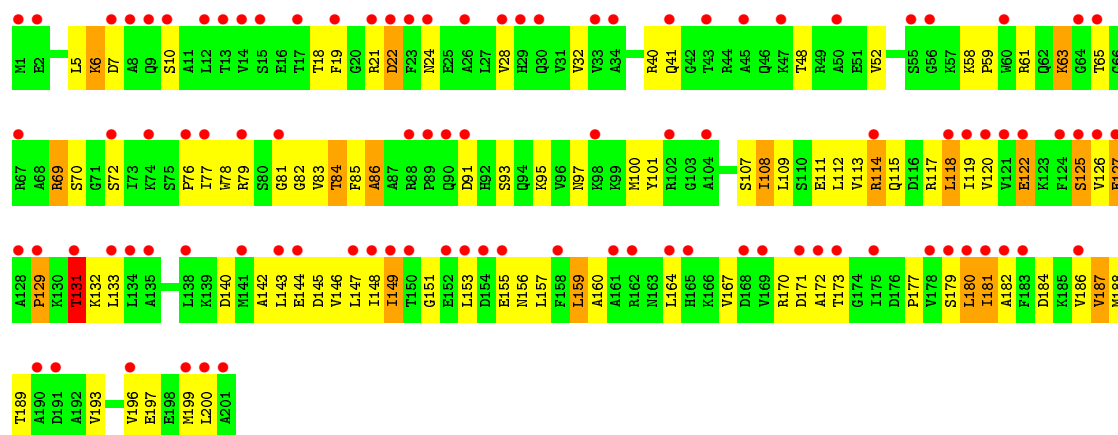
- Molecule 26: 50S ribosomal protein L4

Chain BE: 58% 36% 6%

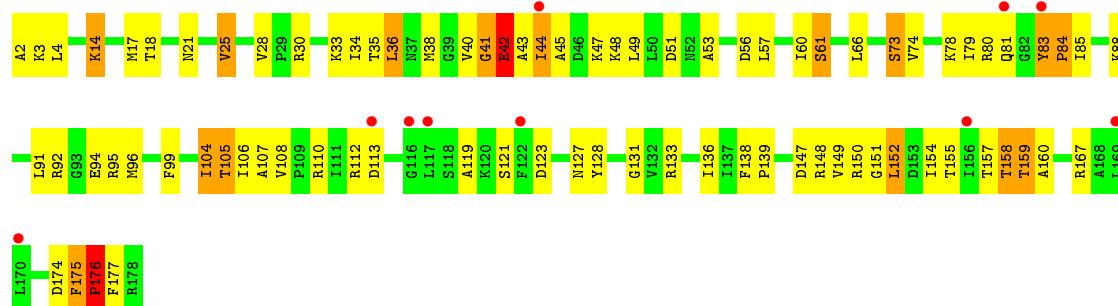


- Molecule 26: 50S ribosomal protein L4

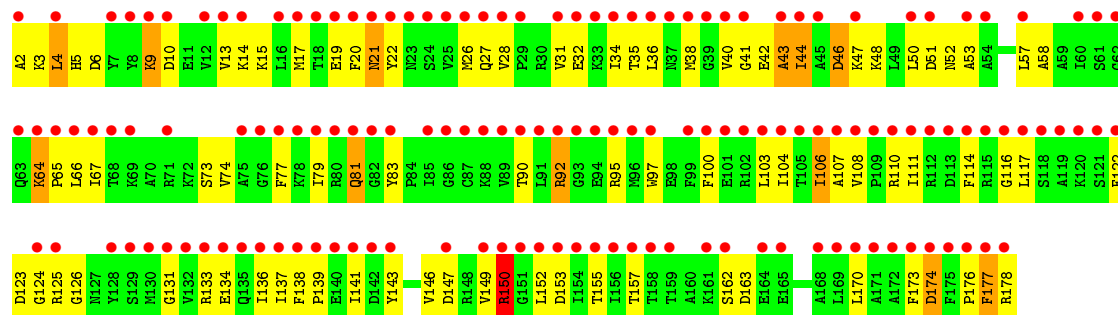
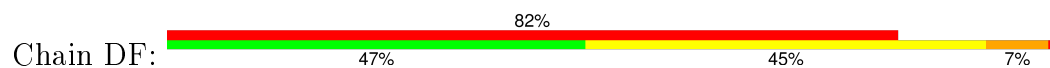
Chain DE: 49% 52% 38% 9%



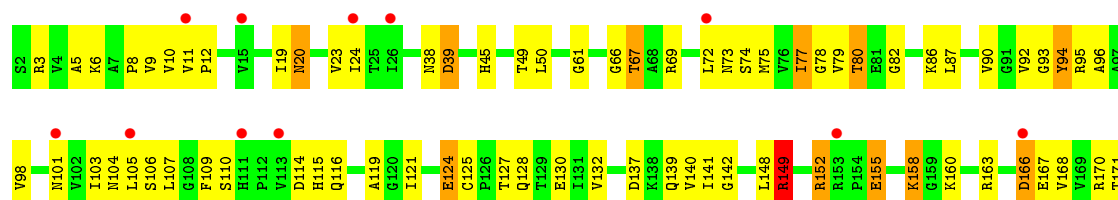
• Molecule 27: 50S ribosomal protein L5

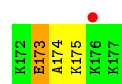


• Molecule 27: 50S ribosomal protein L5

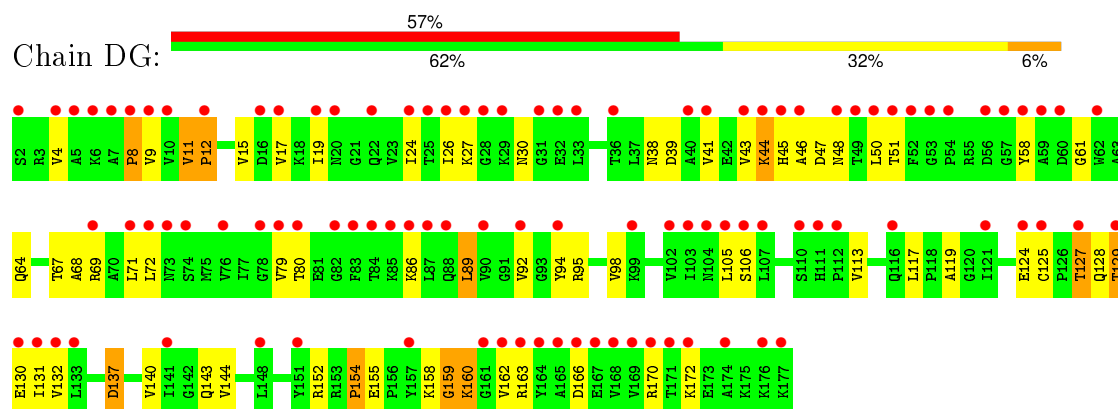


• Molecule 28: 50S ribosomal protein L6

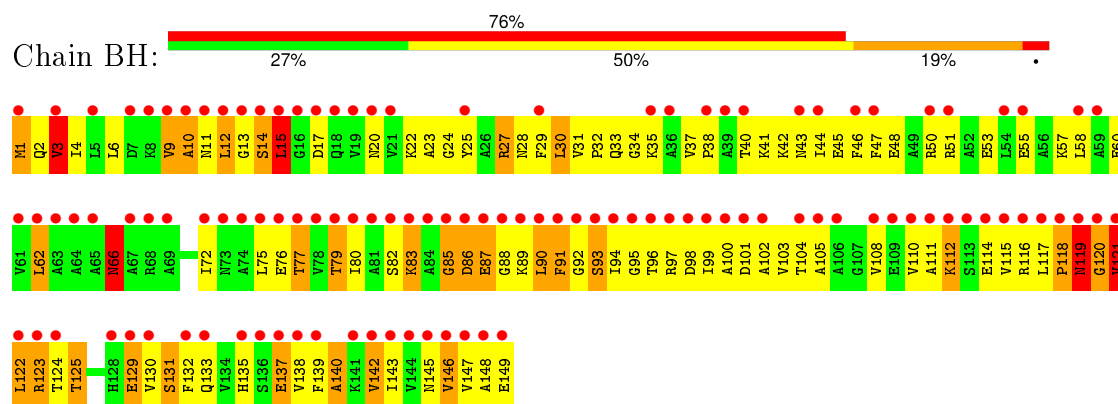


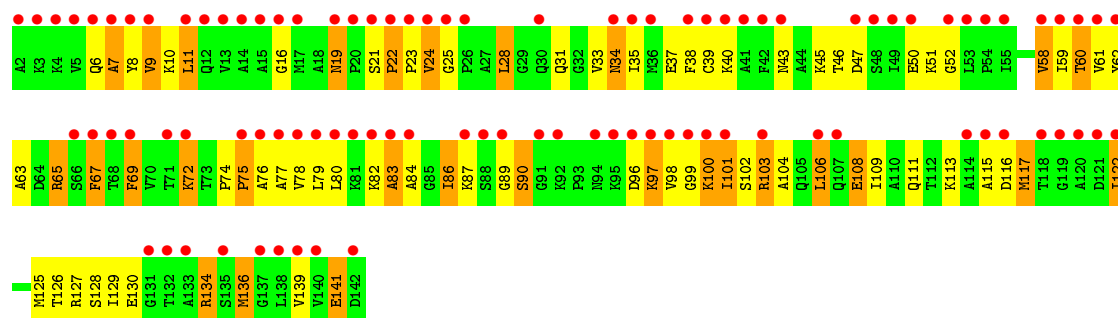


• Molecule 28: 50S ribosomal protein L6

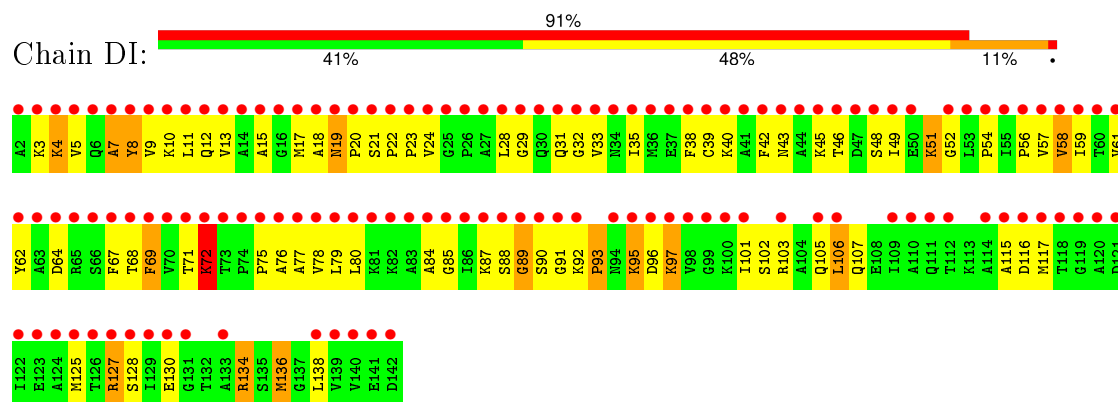


• Molecule 29: 50S ribosomal protein L9

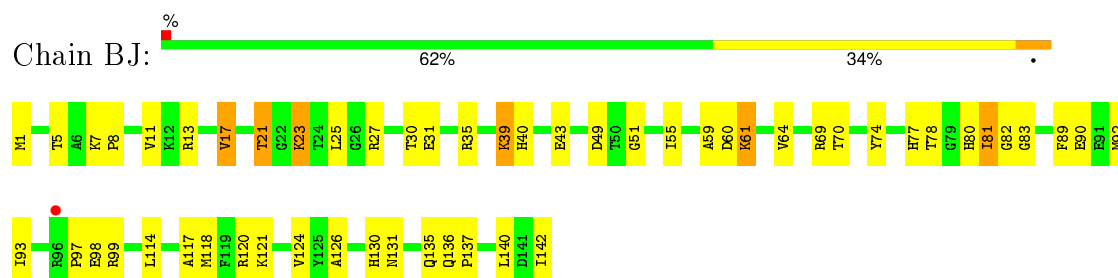




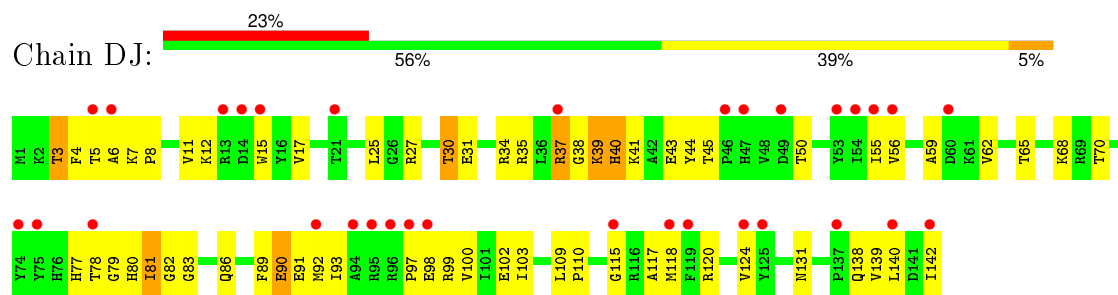
- Molecule 30: 50S ribosomal protein L11



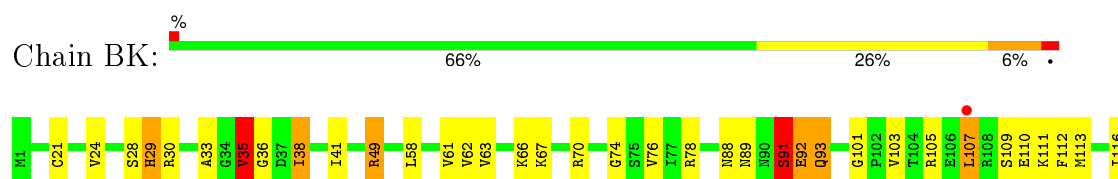
- Molecule 31: 50S ribosomal protein L13



- Molecule 31: 50S ribosomal protein L13



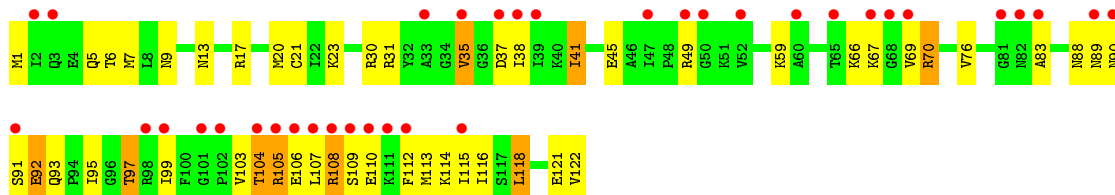
- Molecule 32: 50S ribosomal protein L14



S117
L118
A119
P120
E121
V122

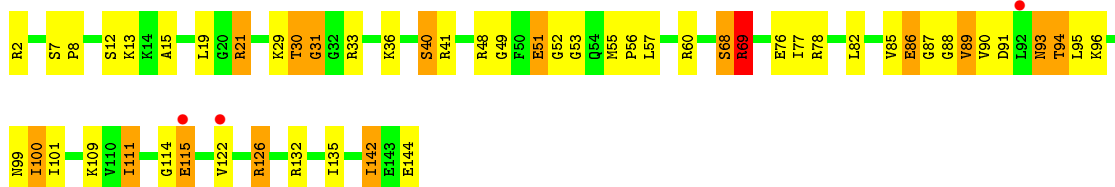
• Molecule 32: 50S ribosomal protein L14

Chain DK: 



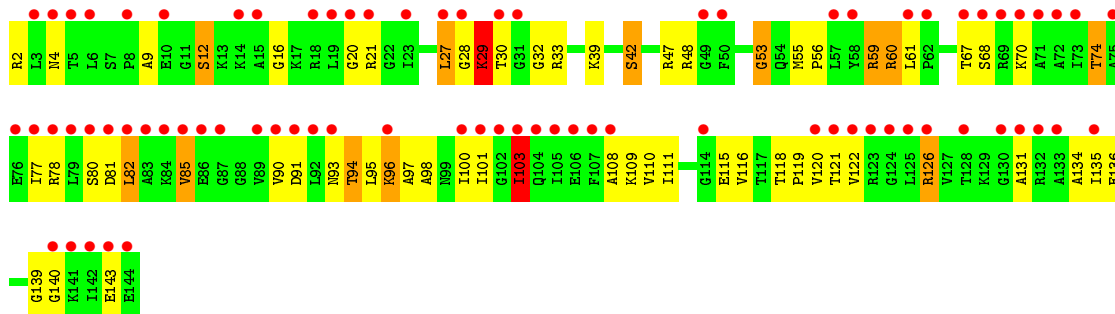
• Molecule 33: 50S ribosomal protein L15

Chain BL: 



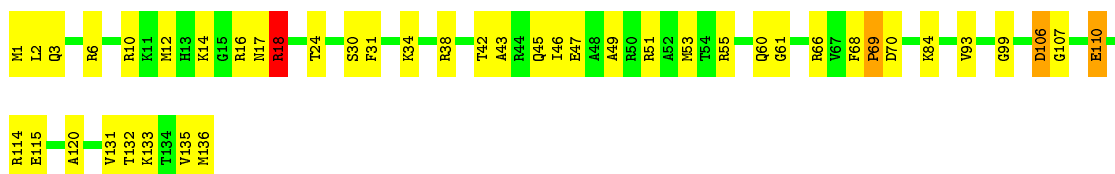
• Molecule 33: 50S ribosomal protein L15

Chain DL: 



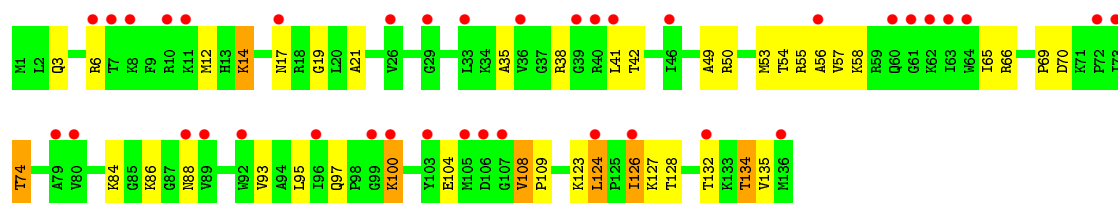
• Molecule 34: 50S ribosomal protein L16

Chain BM: 



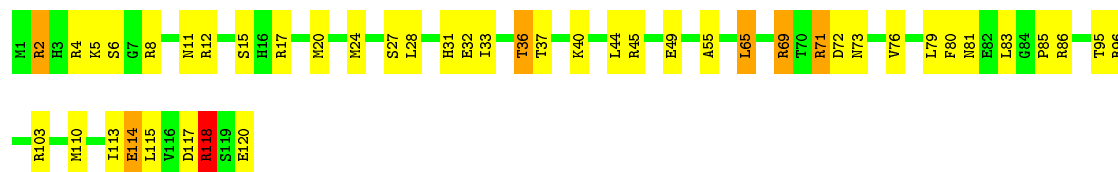
• Molecule 34: 50S ribosomal protein L16

Chain DM: 



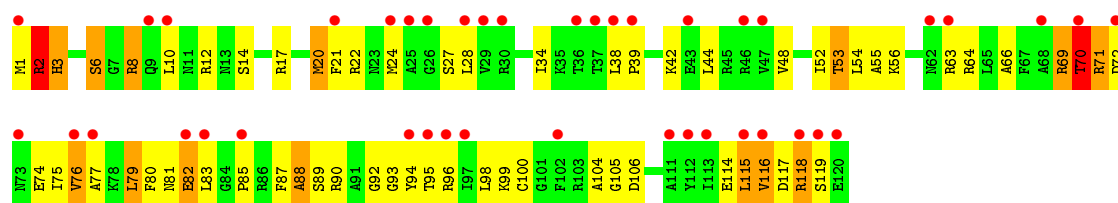
• Molecule 35: 50S ribosomal protein L17

Chain BN: 63% 32% 5% •



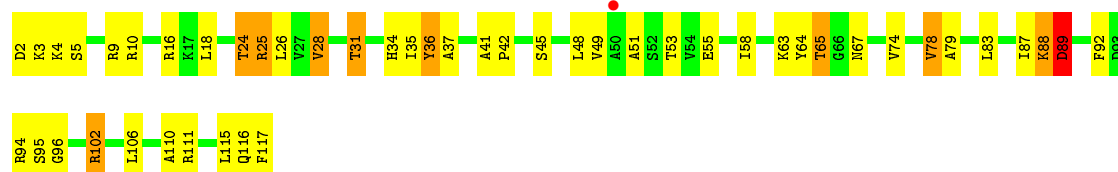
• Molecule 35: 50S ribosomal protein L17

Chain DN: 47% 40% 12% •



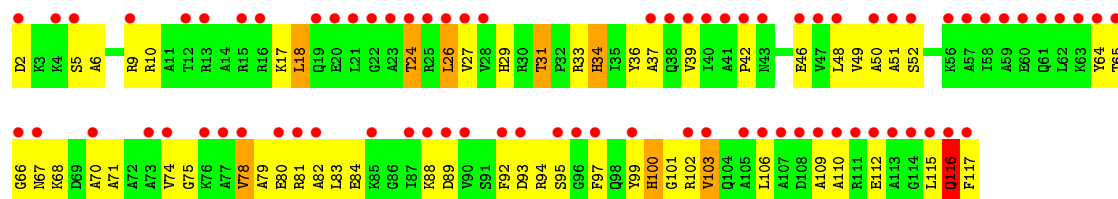
• Molecule 36: 50S ribosomal protein L18

Chain BO: 59% 33% 8% •



• Molecule 36: 50S ribosomal protein L18

Chain DO: 49% 43% 7% •

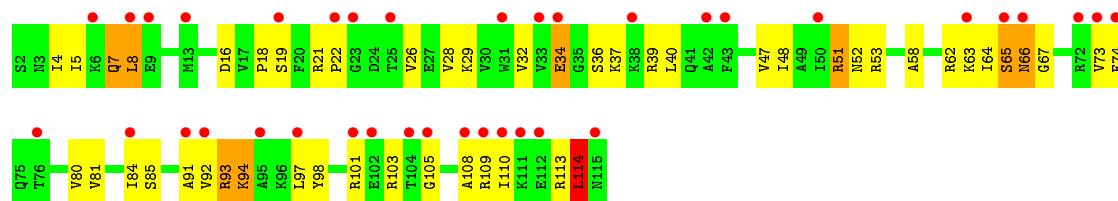


• Molecule 37: 50S ribosomal protein L19

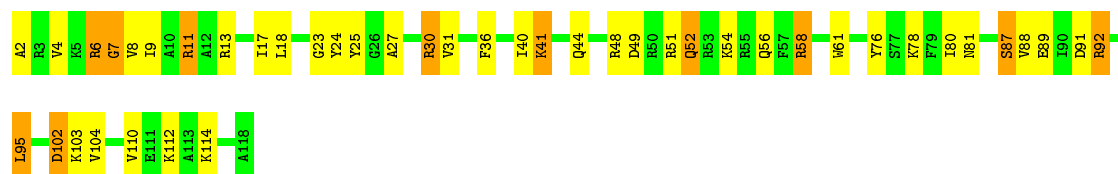
Chain BP: 58% 36% 5% •



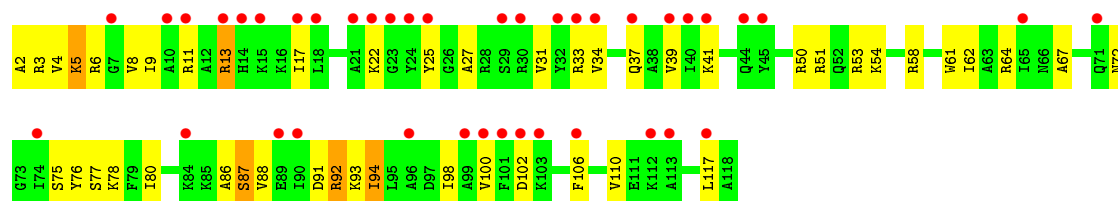
• Molecule 37: 50S ribosomal protein L19



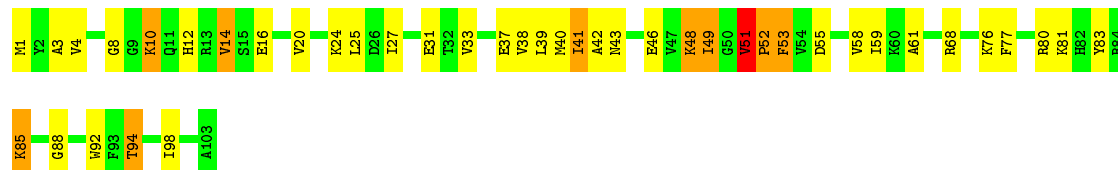
• Molecule 38: 50S ribosomal protein L20



• Molecule 38: 50S ribosomal protein L20

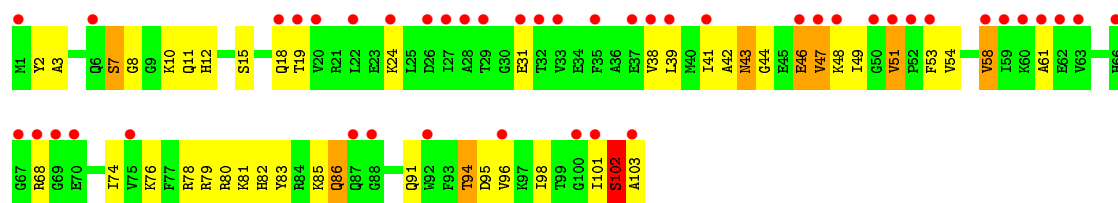


• Molecule 39: 50S ribosomal protein L21

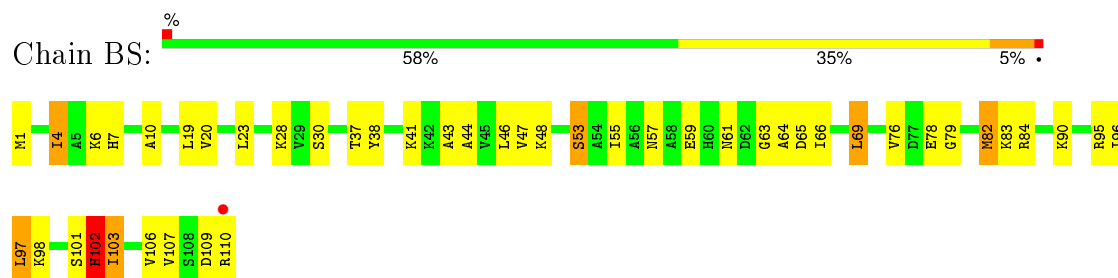


• Molecule 39: 50S ribosomal protein L21

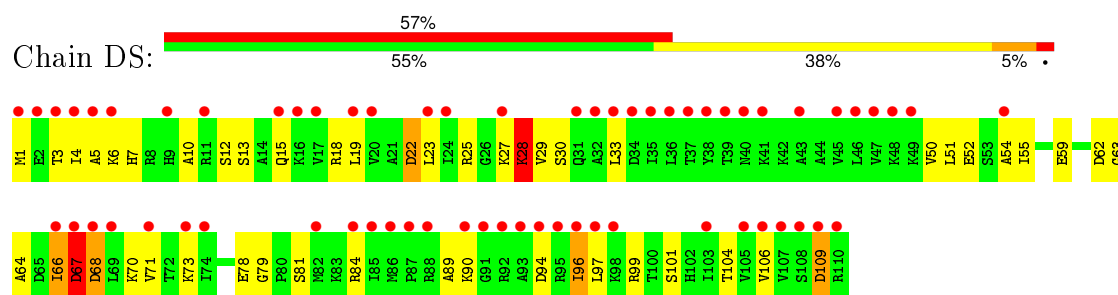




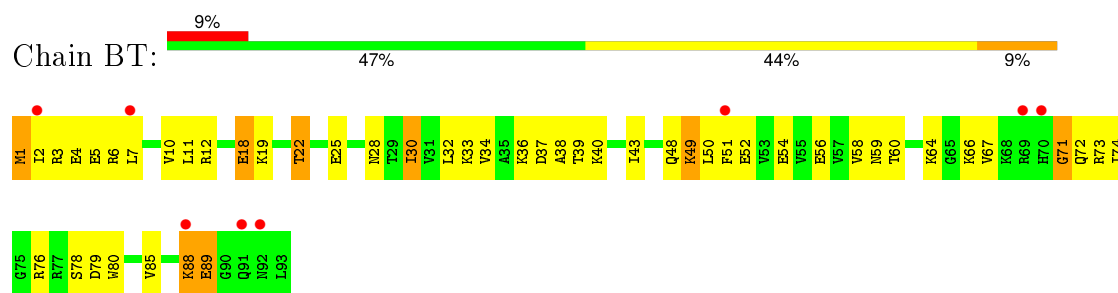
• Molecule 40: 50S ribosomal protein L22



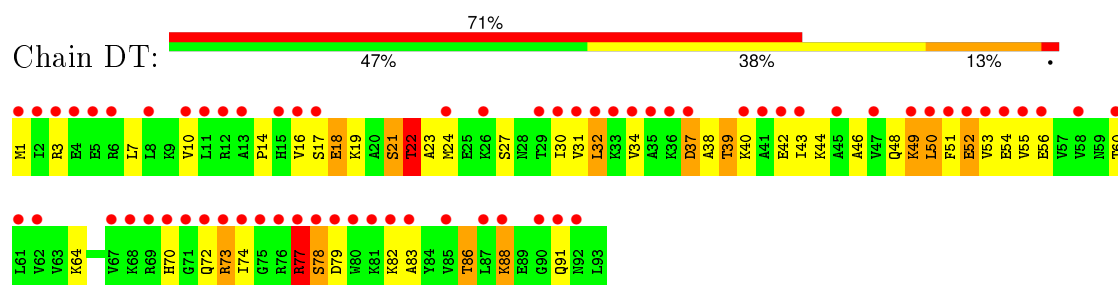
• Molecule 40: 50S ribosomal protein L22



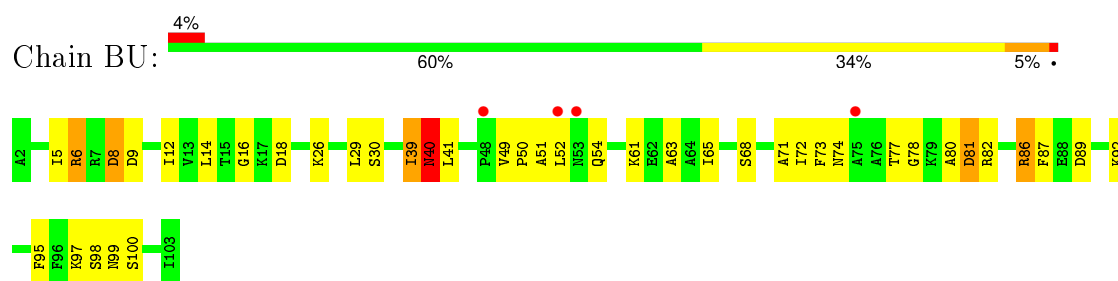
• Molecule 41: 50S ribosomal protein L23



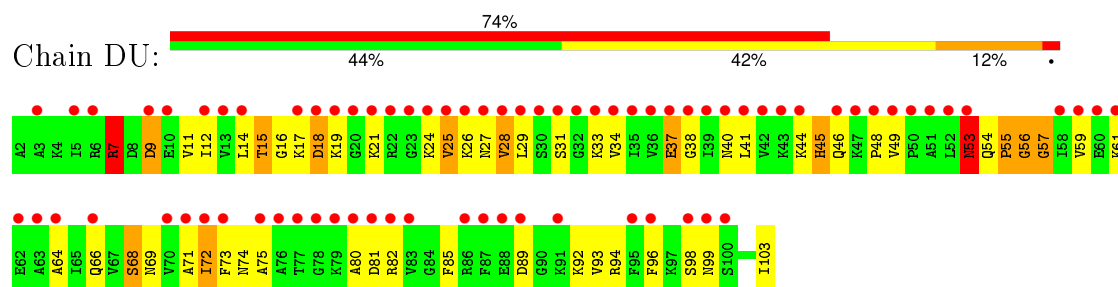
• Molecule 41: 50S ribosomal protein L23



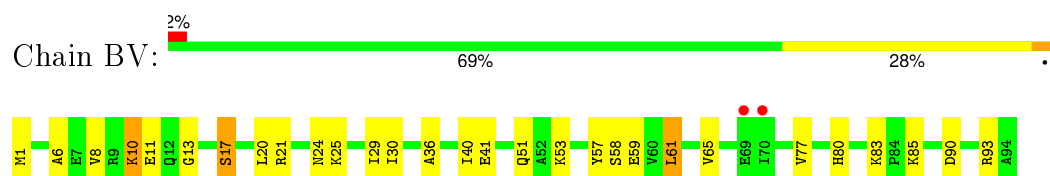
• Molecule 42: 50S ribosomal protein L24



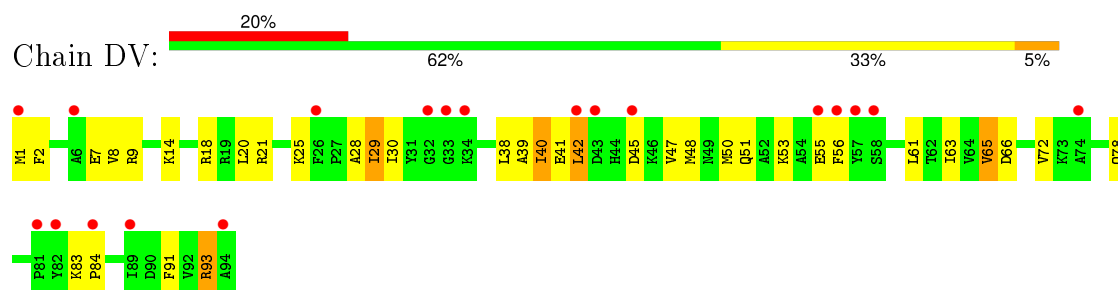
- Molecule 42: 50S ribosomal protein L24



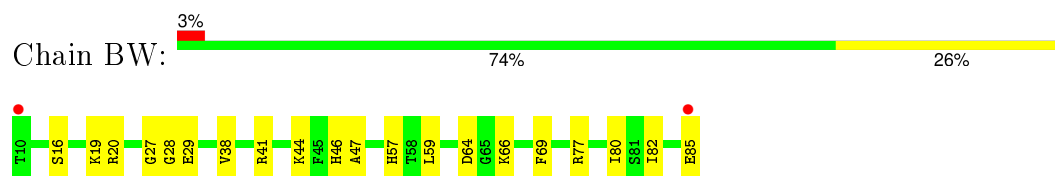
- Molecule 43: 50S ribosomal protein L25



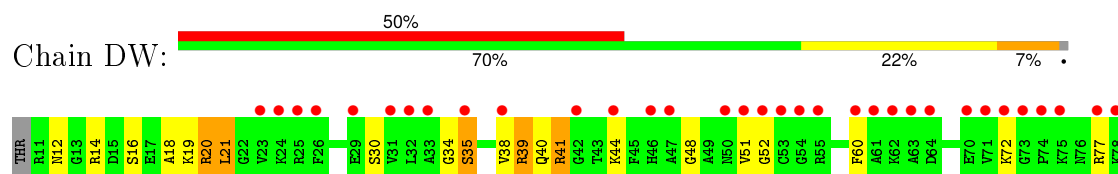
- Molecule 43: 50S ribosomal protein L25

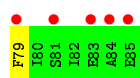


- Molecule 44: 50S ribosomal protein L27

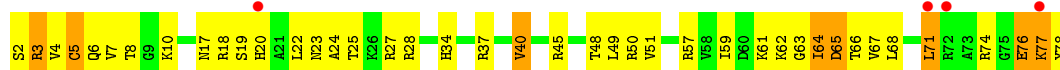


- Molecule 44: 50S ribosomal protein L27

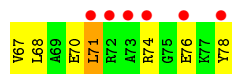
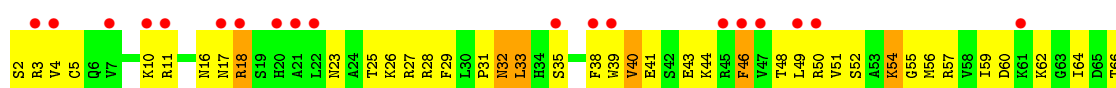
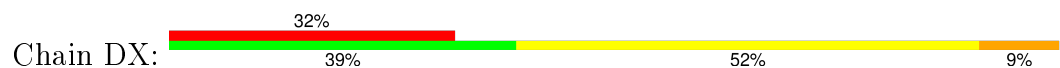




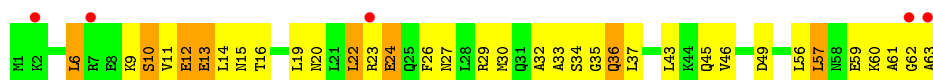
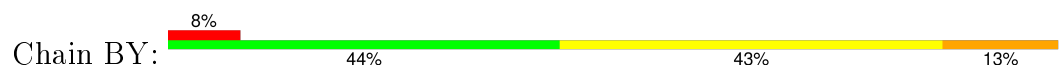
- Molecule 45: 50S ribosomal protein L28



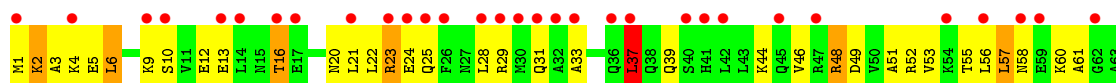
- Molecule 45: 50S ribosomal protein L28



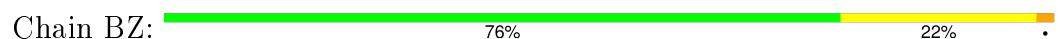
- Molecule 46: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L29



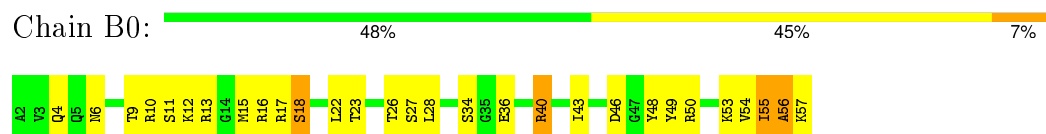
- Molecule 47: 50S ribosomal protein L30



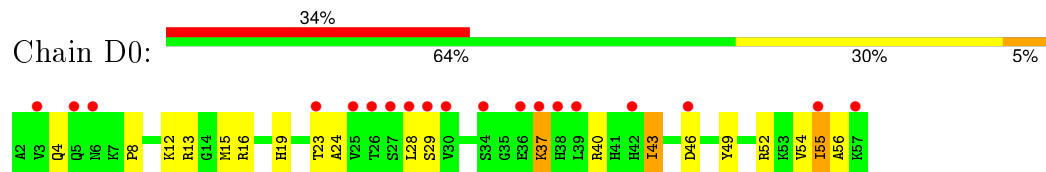
- Molecule 47: 50S ribosomal protein L30



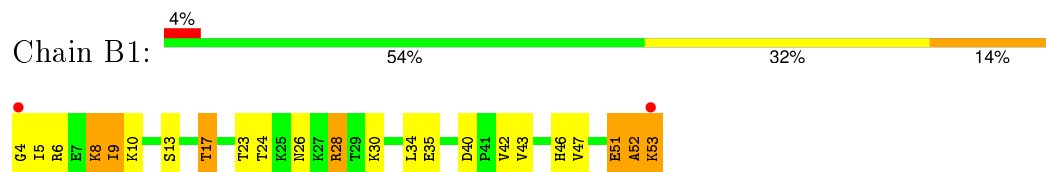
- Molecule 48: 50S ribosomal protein L32



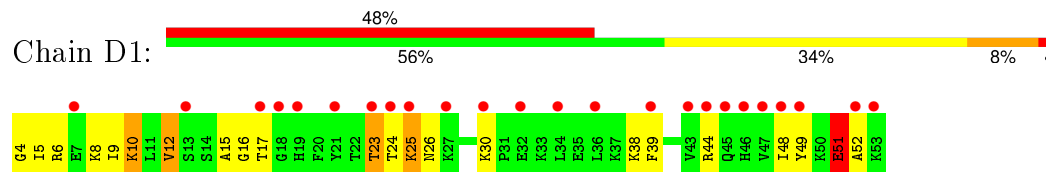
- Molecule 48: 50S ribosomal protein L32



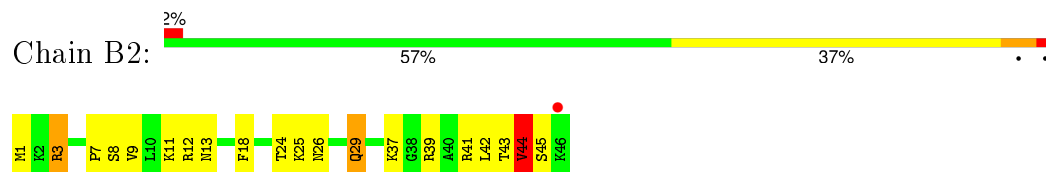
- Molecule 49: 50S ribosomal protein L33



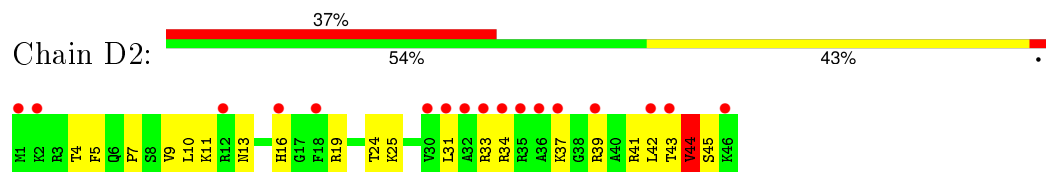
- Molecule 49: 50S ribosomal protein L33



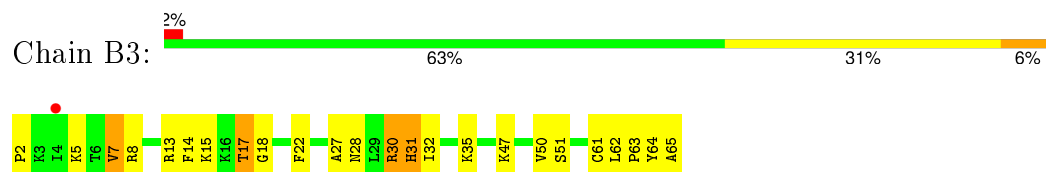
- Molecule 50: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L35

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.08Å 432.73Å 631.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.68 – 2.95 68.68 – 2.95	Depositor EDS
% Data completeness (in resolution range)	93.2 (68.68-2.95) 93.2 (68.68-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.248 , 0.282 0.255 , 0.289	Depositor DCC
R_{free} test set	4515 reflections (0.41%)	DCC
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1118451 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	288328	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DBB, MG, 004, MHV, MHW, MHT, 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	0.44	0/36944	1.04	74/57632 (0.1%)
1	CA	0.39	0/36966	0.99	74/57666 (0.1%)
2	AB	0.36	0/1736	0.72	1/2338 (0.0%)
2	CB	0.33	0/1736	0.70	0/2338
3	AC	0.35	0/1652	0.65	2/2225 (0.1%)
3	CC	0.32	0/1652	0.58	1/2225 (0.0%)
4	AD	0.35	0/1665	0.68	0/2227
4	CD	0.38	0/1665	0.71	1/2227 (0.0%)
5	AE	0.38	0/1119	0.74	0/1504
5	CE	0.37	0/1119	0.73	0/1504
6	AF	0.39	0/836	0.71	2/1128 (0.2%)
6	CF	0.34	0/836	0.68	0/1128
7	AG	0.32	0/1196	0.59	0/1602
7	CG	0.31	0/1196	0.56	0/1602
8	AH	0.36	0/989	0.67	0/1326
8	CH	0.30	0/989	0.59	0/1326
9	AI	0.32	0/1034	0.65	1/1375 (0.1%)
9	CI	0.32	0/1034	0.64	0/1375
10	AJ	0.35	0/797	0.65	0/1077
10	CJ	0.30	0/797	0.66	2/1077 (0.2%)
11	AK	0.35	0/893	0.63	0/1205
11	CK	0.32	0/893	0.63	0/1205
12	AL	0.39	0/969	0.69	0/1300
12	CL	0.35	0/969	0.72	0/1300
13	AM	0.33	0/893	0.69	0/1193
13	CM	0.33	0/893	0.65	0/1193
14	AN	0.31	0/785	0.66	0/1043
14	CN	0.29	0/785	0.57	0/1043
15	AO	0.31	0/718	0.61	0/959
15	CO	0.30	0/718	0.61	0/959
16	AP	0.39	0/659	0.72	1/884 (0.1%)
16	CP	0.33	0/659	0.59	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.37	0/658	0.72	1/881 (0.1%)
17	CQ	0.38	0/658	0.63	0/881
18	AR	0.31	0/463	0.60	0/621
18	CR	0.30	0/463	0.57	0/621
19	AS	0.32	0/653	0.63	0/877
19	CS	0.33	0/653	0.59	0/877
20	AT	0.36	0/671	0.64	0/888
20	CT	0.32	0/671	0.62	0/888
21	AU	0.43	0/431	0.75	0/570
21	CU	0.45	0/431	0.78	0/570
22	BA	0.68	6/69659 (0.0%)	1.32	534/108672 (0.5%)
22	DA	0.38	0/69659	0.99	76/108672 (0.1%)
23	BB	0.62	1/2850 (0.0%)	1.22	7/4444 (0.2%)
23	DB	0.32	0/2828	0.92	2/4410 (0.0%)
24	BC	0.45	0/2122	0.71	0/2852
24	DC	0.34	0/2122	0.62	0/2852
25	BD	0.50	0/1586	0.74	1/2134 (0.0%)
25	DD	0.32	0/1586	0.59	0/2134
26	BE	0.42	0/1571	0.70	0/2113
26	DE	0.34	0/1571	0.62	1/2113 (0.0%)
27	BF	0.37	0/1435	0.63	0/1926
27	DF	0.30	0/1435	0.56	0/1926
28	BG	0.39	0/1343	0.69	1/1816 (0.1%)
28	DG	0.31	0/1343	0.55	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	0.38	0/1046	0.69	0/1410
30	DI	0.35	0/1046	0.67	0/1410
31	BJ	0.49	0/1152	0.70	0/1551
31	DJ	0.31	0/1152	0.59	0/1551
32	BK	0.51	0/948	0.73	0/1268
32	DK	0.34	0/948	0.58	0/1268
33	BL	0.45	0/1054	0.80	2/1403 (0.1%)
33	DL	0.32	0/1054	0.62	0/1403
34	BM	0.48	0/1093	0.73	1/1460 (0.1%)
34	DM	0.30	0/1093	0.57	0/1460
35	BN	0.47	0/974	0.77	0/1301
35	DN	0.33	0/974	0.59	0/1301
36	BO	0.43	0/902	0.66	0/1209
36	DO	0.29	0/902	0.53	0/1209
37	BP	0.47	0/929	0.72	1/1242 (0.1%)
37	DP	0.32	0/929	0.59	1/1242 (0.1%)
38	BQ	0.56	0/960	0.73	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.32	0/960	0.53	0/1278
39	BR	0.53	0/829	0.82	1/1107 (0.1%)
39	DR	0.34	0/829	0.66	0/1107
40	BS	0.71	2/864 (0.2%)	0.89	2/1156 (0.2%)
40	DS	0.33	0/864	0.63	0/1156
41	BT	0.45	0/745	0.70	0/994
41	DT	0.33	0/745	0.61	0/994
42	BU	0.43	0/788	0.72	0/1051
42	DU	0.37	0/788	0.61	0/1051
43	BV	0.40	0/766	0.67	1/1025 (0.1%)
43	DV	0.28	0/766	0.54	0/1025
44	BW	0.52	0/587	0.69	0/776
44	DW	0.29	0/576	0.54	0/762
45	BX	0.39	0/635	0.67	0/848
45	DX	0.32	0/635	0.61	0/848
46	BY	0.39	0/510	0.76	0/677
46	DY	0.32	0/510	0.64	0/677
47	BZ	0.52	0/453	0.74	0/605
47	DZ	0.30	0/453	0.56	0/605
48	B0	0.52	0/450	0.75	0/599
48	D0	0.31	0/450	0.61	0/599
49	B1	0.44	0/417	0.69	0/554
49	D1	0.32	0/417	0.56	0/554
50	B2	0.48	0/380	0.80	0/498
50	D2	0.30	0/380	0.58	0/498
51	B3	0.43	0/513	0.71	0/676
51	D3	0.29	0/513	0.49	0/676
52	B4	0.52	0/303	0.66	0/397
52	D4	0.37	0/303	0.58	0/397
53	B5	0.32	0/1145	0.69	1/1556 (0.1%)
54	B6	1.71	0/13	2.43	1/15 (6.7%)
54	D6	1.45	0/13	2.67	2/15 (13.3%)
All	All	0.47	9/310652 (0.0%)	1.01	796/464396 (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
2	CB	0	1
5	AE	0	1

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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	984	A	N9-C4	-9.06	1.32	1.37
22	BA	1142	A	N9-C4	-8.98	1.32	1.37
40	BS	102	HIS	CB-CG	-6.45	1.38	1.50
22	BA	1936	A	N9-C4	-5.92	1.34	1.37
23	BB	99	A	N9-C4	-5.46	1.34	1.37

The worst 5 of 796 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	984	A	C2-N3-C4	-12.57	104.31	110.60
1	AA	1054	C	O5'-P-OP2	-12.23	94.69	105.70
22	BA	1936	A	C2-N3-C4	-10.65	105.28	110.60
25	BD	151	THR	C-N-CD	-10.63	97.20	120.60
22	BA	1142	A	C2-N3-C4	-10.48	105.36	110.60

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	123	VAL	Peptide
11	AK	126	LYS	Peptide
21	AU	39	GLU	Peptide
21	AU	8	GLU	Peptide
25	BD	151	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	608	14
1	CA	33015	0	16616	645	0
2	AB	1705	0	1732	135	0
2	CB	1705	0	1732	109	0
3	AC	1625	0	1696	75	0
3	CC	1625	0	1696	67	0
4	AD	1643	0	1707	93	0
4	CD	1643	0	1707	74	0
5	AE	1106	0	1148	60	0
5	CE	1106	0	1148	72	0
6	AF	818	0	808	37	0
6	CF	818	0	808	35	0
7	AG	1182	0	1238	47	0
7	CG	1182	0	1238	49	0
8	AH	979	0	1031	38	0
8	CH	979	0	1031	43	0
9	AI	1022	0	1070	51	0
9	CI	1022	0	1070	64	0
10	AJ	787	0	828	60	0
10	CJ	787	0	828	44	0
11	AK	877	0	887	54	0
11	CK	877	0	887	39	0
12	AL	955	0	1016	38	0
12	CL	955	0	1016	48	0
13	AM	884	0	941	49	0
13	CM	884	0	941	40	0
14	AN	774	0	824	44	0
14	CN	774	0	824	44	0
15	AO	710	0	728	20	0
15	CO	710	0	728	38	0
16	AP	649	0	666	34	0
16	CP	649	0	666	30	0
17	AQ	649	0	691	30	0
17	CQ	649	0	691	33	0
18	AR	456	0	478	12	0
18	CR	456	0	478	25	0
19	AS	638	0	665	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	638	0	665	31	0
20	AT	665	0	714	31	0
20	CT	665	0	714	34	0
21	AU	426	0	449	39	0
21	CU	426	0	449	29	0
22	BA	62195	0	31280	1058	0
22	DA	62195	0	31280	1193	1
23	BB	2549	0	1291	19	0
23	DB	2529	0	1281	44	0
24	BC	2083	0	2154	76	0
24	DC	2083	0	2154	94	0
25	BD	1565	0	1616	48	0
25	DD	1565	0	1616	55	0
26	BE	1552	0	1619	47	0
26	DE	1552	0	1619	63	0
27	BF	1411	0	1444	51	0
27	DF	1411	0	1444	50	0
28	BG	1323	0	1371	44	0
28	DG	1323	0	1371	39	0
29	BH	1110	0	1145	196	0
29	DH	1110	0	1148	91	13
30	BI	1032	0	1085	52	0
30	DI	1032	0	1085	54	0
31	BJ	1129	0	1162	28	0
31	DJ	1129	0	1162	48	0
32	BK	939	0	1012	30	0
32	DK	939	0	1012	29	0
33	BL	1045	0	1117	38	0
33	DL	1045	0	1117	46	0
34	BM	1074	0	1157	30	0
34	DM	1074	0	1157	20	0
35	BN	961	0	1000	35	0
35	DN	961	0	1000	47	0
36	BO	892	0	923	25	0
36	DO	892	0	923	42	0
37	BP	917	0	962	39	0
37	DP	917	0	962	34	0
38	BQ	947	0	1019	35	0
38	DQ	947	0	1019	44	0
39	BR	816	0	839	37	0
39	DR	816	0	839	34	0
40	BS	857	0	922	34	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AT	2	0	0	0	0
57	AU	1	0	0	1	0
57	B2	1	0	0	0	0
57	B3	3	0	0	0	0
57	B4	2	0	0	0	0
57	BA	619	0	0	59	0
57	BB	13	0	0	1	0
57	BC	8	0	0	1	0
57	BD	3	0	0	2	0
57	BE	3	0	0	0	0
57	BF	1	0	0	1	0
57	BG	1	0	0	0	0
57	BL	5	0	0	1	0
57	BN	5	0	0	1	0
57	BS	1	0	0	0	0
57	BV	1	0	0	0	0
57	CA	189	0	0	10	0
57	CL	1	0	0	0	0
57	CN	3	0	0	0	0
57	CT	4	0	0	0	0
57	CU	1	0	0	1	0
57	D0	1	0	0	0	0
57	D2	2	0	0	1	0
57	D3	1	0	0	0	0
57	D4	1	0	0	0	0
57	DA	612	0	0	63	0
57	DB	13	0	0	0	0
57	DC	7	0	0	1	0
57	DD	4	0	0	1	0
57	DE	4	0	0	0	0
57	DL	4	0	0	0	0
57	DN	1	0	0	0	0
57	DQ	2	0	0	0	0
57	DT	3	0	0	0	0
57	DV	1	0	0	0	0
All	All	288328	0	192913	6784	14

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 6784 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:83:LYS:HD2	1:CA:55:A:O2'	1.21	1.29
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
29:BH:117:LEU:O	29:BH:121:VAL:CG2	1.95	1.14
29:BH:123:ARG:O	29:BH:124:THR:CG2	2.01	1.09
29:BH:97:ARG:HD2	1:CA:369:G:O2'	1.51	1.09

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

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	DC	269/271 (99%)	209 (78%)	42 (16%)	18 (7%)	1	6
25	BD	207/209 (99%)	183 (88%)	19 (9%)	5 (2%)	7	33
25	DD	207/209 (99%)	173 (84%)	29 (14%)	5 (2%)	7	33
26	BE	199/201 (99%)	171 (86%)	22 (11%)	6 (3%)	5	26
26	DE	199/201 (99%)	157 (79%)	29 (15%)	13 (6%)	1	7
27	BF	175/177 (99%)	144 (82%)	23 (13%)	8 (5%)	3	15
27	DF	175/177 (99%)	146 (83%)	17 (10%)	12 (7%)	1	6
28	BG	174/176 (99%)	147 (84%)	15 (9%)	12 (7%)	1	6
28	DG	174/176 (99%)	138 (79%)	25 (14%)	11 (6%)	2	8
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	1
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	1	2
30	BI	139/141 (99%)	78 (56%)	37 (27%)	24 (17%)	0	0
30	DI	139/141 (99%)	80 (58%)	44 (32%)	15 (11%)	0	2
31	BJ	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	4	21
31	DJ	140/142 (99%)	123 (88%)	15 (11%)	2 (1%)	14	49
32	BK	120/122 (98%)	98 (82%)	13 (11%)	9 (8%)	1	5
32	DK	120/122 (98%)	100 (83%)	14 (12%)	6 (5%)	3	13
33	BL	141/143 (99%)	109 (77%)	20 (14%)	12 (8%)	1	4
33	DL	141/143 (99%)	105 (74%)	29 (21%)	7 (5%)	3	13
34	BM	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	13	47
34	DM	134/136 (98%)	112 (84%)	19 (14%)	3 (2%)	8	35
35	BN	118/120 (98%)	96 (81%)	21 (18%)	1 (1%)	24	64
35	DN	118/120 (98%)	97 (82%)	11 (9%)	10 (8%)	1	4
36	BO	114/116 (98%)	95 (83%)	15 (13%)	4 (4%)	4	22
36	DO	114/116 (98%)	96 (84%)	14 (12%)	4 (4%)	4	22
37	BP	112/114 (98%)	98 (88%)	9 (8%)	5 (4%)	3	15
37	DP	112/114 (98%)	91 (81%)	16 (14%)	5 (4%)	3	15
38	BQ	115/117 (98%)	107 (93%)	3 (3%)	5 (4%)	3	16
38	DQ	115/117 (98%)	108 (94%)	6 (5%)	1 (1%)	21	61
39	BR	101/103 (98%)	86 (85%)	8 (8%)	7 (7%)	1	6
39	DR	101/103 (98%)	77 (76%)	20 (20%)	4 (4%)	4	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BS	108/110 (98%)	100 (93%)	5 (5%)	3 (3%)	6	28
40	DS	108/110 (98%)	89 (82%)	14 (13%)	5 (5%)	3	15
41	BT	91/93 (98%)	70 (77%)	13 (14%)	8 (9%)	1	4
41	DT	91/93 (98%)	70 (77%)	9 (10%)	12 (13%)	0	1
42	BU	100/102 (98%)	80 (80%)	12 (12%)	8 (8%)	1	4
42	DU	100/102 (98%)	73 (73%)	17 (17%)	10 (10%)	1	2
43	BV	92/94 (98%)	85 (92%)	6 (6%)	1 (1%)	17	56
43	DV	92/94 (98%)	82 (89%)	8 (9%)	2 (2%)	8	35
44	BW	74/76 (97%)	67 (90%)	7 (10%)	0	100	100
44	DW	73/76 (96%)	65 (89%)	6 (8%)	2 (3%)	6	29
45	BX	75/77 (97%)	72 (96%)	1 (1%)	2 (3%)	6	29
45	DX	75/77 (97%)	64 (85%)	9 (12%)	2 (3%)	6	29
46	BY	61/63 (97%)	40 (66%)	12 (20%)	9 (15%)	0	1
46	DY	61/63 (97%)	49 (80%)	8 (13%)	4 (7%)	1	7
47	BZ	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
47	DZ	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	4	21
48	B0	54/56 (96%)	46 (85%)	5 (9%)	3 (6%)	2	11
48	D0	54/56 (96%)	41 (76%)	11 (20%)	2 (4%)	4	20
49	B1	48/50 (96%)	38 (79%)	6 (12%)	4 (8%)	1	4
49	D1	48/50 (96%)	37 (77%)	8 (17%)	3 (6%)	2	8
50	B2	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	3	15
50	D2	44/46 (96%)	38 (86%)	4 (9%)	2 (4%)	3	15
51	B3	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	12	45
51	D3	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	12	45
52	B4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
52	D4	36/38 (95%)	33 (92%)	1 (3%)	2 (6%)	2	11
53	B5	183/228 (80%)	94 (51%)	54 (30%)	35 (19%)	0	0
54	B6	2/8 (25%)	2 (100%)	0	0	100	100
54	D6	2/8 (25%)	2 (100%)	0	0	100	100
All	All	11422/11688 (98%)	8887 (78%)	1654 (14%)	881 (8%)	1	5

5 of 881 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	PHE
2	AB	22	TYR
2	AB	34	ALA
2	AB	64	LYS
2	AB	73	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	113 (63%)	67 (37%)	0	1
2	CB	180/180 (100%)	129 (72%)	51 (28%)	0	2
3	AC	170/170 (100%)	132 (78%)	38 (22%)	1	4
3	CC	170/170 (100%)	131 (77%)	39 (23%)	1	4
4	AD	172/172 (100%)	129 (75%)	43 (25%)	1	3
4	CD	172/172 (100%)	138 (80%)	34 (20%)	1	7
5	AE	113/113 (100%)	85 (75%)	28 (25%)	1	3
5	CE	113/113 (100%)	85 (75%)	28 (25%)	1	3
6	AF	87/87 (100%)	64 (74%)	23 (26%)	0	2
6	CF	87/87 (100%)	63 (72%)	24 (28%)	0	2
7	AG	124/124 (100%)	94 (76%)	30 (24%)	1	3
7	CG	124/124 (100%)	91 (73%)	33 (27%)	0	2
8	AH	104/104 (100%)	79 (76%)	25 (24%)	1	3
8	CH	104/104 (100%)	83 (80%)	21 (20%)	1	6
9	AI	105/105 (100%)	74 (70%)	31 (30%)	0	1
9	CI	105/105 (100%)	77 (73%)	28 (27%)	0	2
10	AJ	86/86 (100%)	64 (74%)	22 (26%)	0	2
10	CJ	86/86 (100%)	67 (78%)	19 (22%)	1	4
11	AK	90/90 (100%)	66 (73%)	24 (27%)	0	2
11	CK	90/90 (100%)	69 (77%)	21 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	103/103 (100%)	84 (82%)	19 (18%)	2	9
12	CL	103/103 (100%)	78 (76%)	25 (24%)	1	3
13	AM	92/92 (100%)	74 (80%)	18 (20%)	1	7
13	CM	92/92 (100%)	70 (76%)	22 (24%)	1	3
14	AN	79/83 (95%)	61 (77%)	18 (23%)	1	4
14	CN	79/83 (95%)	68 (86%)	11 (14%)	4	17
15	AO	75/76 (99%)	59 (79%)	16 (21%)	1	5
15	CO	75/76 (99%)	57 (76%)	18 (24%)	1	3
16	AP	65/65 (100%)	52 (80%)	13 (20%)	1	7
16	CP	65/65 (100%)	49 (75%)	16 (25%)	1	3
17	AQ	74/74 (100%)	52 (70%)	22 (30%)	0	1
17	CQ	74/74 (100%)	53 (72%)	21 (28%)	0	2
18	AR	48/48 (100%)	41 (85%)	7 (15%)	4	16
18	CR	48/48 (100%)	39 (81%)	9 (19%)	2	8
19	AS	70/70 (100%)	57 (81%)	13 (19%)	2	9
19	CS	70/70 (100%)	55 (79%)	15 (21%)	1	5
20	AT	65/65 (100%)	46 (71%)	19 (29%)	0	2
20	CT	65/65 (100%)	48 (74%)	17 (26%)	0	2
21	AU	44/44 (100%)	27 (61%)	17 (39%)	0	0
21	CU	44/44 (100%)	32 (73%)	12 (27%)	0	2
24	BC	216/216 (100%)	190 (88%)	26 (12%)	6	24
24	DC	216/216 (100%)	180 (83%)	36 (17%)	3	11
25	BD	164/164 (100%)	147 (90%)	17 (10%)	9	30
25	DD	164/164 (100%)	144 (88%)	20 (12%)	6	23
26	BE	165/165 (100%)	138 (84%)	27 (16%)	3	12
26	DE	165/165 (100%)	133 (81%)	32 (19%)	2	7
27	BF	148/148 (100%)	121 (82%)	27 (18%)	2	9
27	DF	148/148 (100%)	118 (80%)	30 (20%)	1	6
28	BG	137/137 (100%)	117 (85%)	20 (15%)	4	16
28	DG	137/137 (100%)	123 (90%)	14 (10%)	9	31
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%)	86 (79%)	23 (21%)	1	5
30	DI	109/109 (100%)	84 (77%)	25 (23%)	1	4
31	BJ	116/116 (100%)	103 (89%)	13 (11%)	7	27
31	DJ	116/116 (100%)	102 (88%)	14 (12%)	6	23
32	BK	103/103 (100%)	93 (90%)	10 (10%)	10	35
32	DK	103/103 (100%)	90 (87%)	13 (13%)	5	22
33	BL	102/102 (100%)	85 (83%)	17 (17%)	3	11
33	DL	102/102 (100%)	81 (79%)	21 (21%)	1	6
34	BM	109/109 (100%)	97 (89%)	12 (11%)	8	27
34	DM	109/109 (100%)	97 (89%)	12 (11%)	8	27
35	BN	100/100 (100%)	87 (87%)	13 (13%)	5	20
35	DN	100/100 (100%)	83 (83%)	17 (17%)	2	11
36	BO	86/86 (100%)	64 (74%)	22 (26%)	0	2
36	DO	86/86 (100%)	72 (84%)	14 (16%)	3	12
37	BP	99/99 (100%)	88 (89%)	11 (11%)	8	27
37	DP	99/99 (100%)	80 (81%)	19 (19%)	2	8
38	BQ	89/89 (100%)	74 (83%)	15 (17%)	2	11
38	DQ	89/89 (100%)	76 (85%)	13 (15%)	4	16
39	BR	84/84 (100%)	73 (87%)	11 (13%)	5	20
39	DR	84/84 (100%)	70 (83%)	14 (17%)	3	11
40	BS	93/93 (100%)	78 (84%)	15 (16%)	3	12
40	DS	93/93 (100%)	77 (83%)	16 (17%)	2	10
41	BT	80/80 (100%)	68 (85%)	12 (15%)	3	15
41	DT	80/80 (100%)	66 (82%)	14 (18%)	2	10
42	BU	83/83 (100%)	68 (82%)	15 (18%)	2	9
42	DU	83/83 (100%)	64 (77%)	19 (23%)	1	4
43	BV	78/78 (100%)	66 (85%)	12 (15%)	3	14
43	DV	78/78 (100%)	67 (86%)	11 (14%)	4	17
44	BW	57/58 (98%)	53 (93%)	4 (7%)	19	53
44	DW	56/58 (97%)	49 (88%)	7 (12%)	6	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BX	67/67 (100%)	55 (82%)	12 (18%)	2	9
45	DX	67/67 (100%)	55 (82%)	12 (18%)	2	9
46	BY	55/55 (100%)	48 (87%)	7 (13%)	5	21
46	DY	55/55 (100%)	43 (78%)	12 (22%)	1	5
47	BZ	48/48 (100%)	43 (90%)	5 (10%)	9	30
47	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	6
48	B0	47/47 (100%)	40 (85%)	7 (15%)	4	15
48	D0	47/47 (100%)	42 (89%)	5 (11%)	8	29
49	B1	45/45 (100%)	38 (84%)	7 (16%)	3	13
49	D1	45/45 (100%)	39 (87%)	6 (13%)	5	19
50	B2	38/38 (100%)	32 (84%)	6 (16%)	3	13
50	D2	38/38 (100%)	32 (84%)	6 (16%)	3	13
51	B3	51/51 (100%)	46 (90%)	5 (10%)	10	34
51	D3	51/51 (100%)	46 (90%)	5 (10%)	10	34
52	B4	34/34 (100%)	30 (88%)	4 (12%)	6	24
52	D4	34/34 (100%)	28 (82%)	6 (18%)	2	10
53	B5	61/180 (34%)	48 (79%)	13 (21%)	1	5
54	B6	2/2 (100%)	2 (100%)	0	100	100
54	D6	2/2 (100%)	2 (100%)	0	100	100
All	All	9390/9522 (99%)	7570 (81%)	1820 (19%)	2	7

5 of 1820 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BU	81	ASP
4	CD	138	SER
39	DR	43	ASN
45	BX	48	THR
2	CB	68	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
45	BX	34	HIS

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Mol	Chain	Res	Type
3	CC	176	HIS
41	DT	59	ASN
2	CB	18	HIS
2	CB	51	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	357 (23%)	16 (1%)
1	CA	1538/1539 (99%)	337 (21%)	9 (0%)
22	BA	2895/2903 (99%)	563 (19%)	28 (0%)
22	DA	2895/2903 (99%)	643 (22%)	34 (1%)
23	BB	118/119 (99%)	23 (19%)	0
23	DB	117/119 (98%)	25 (21%)	0
All	All	9100/9122 (99%)	1948 (21%)	87 (0%)

5 of 1948 RNA backbone outliers are listed below:

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

5 of 87 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2286	G
1	CA	559	A
22	DA	2296	U
22	BA	2326	C
1	CA	96	U

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	MHW	B6	1	54	9,9,10	1.44	1 (11%)	8,11,13	2.39	2 (25%)
54	DBB	B6	3	54	4,5,6	1.42	1 (25%)	3,5,7	2.22	2 (66%)
54	MHU	B6	5	54	13,15,16	1.71	2 (15%)	15,19,21	1.25	1 (6%)
54	MHV	B6	6	54	7,9,10	1.34	1 (14%)	8,11,13	4.22	4 (50%)
54	004	B6	7	54	9,10,11	1.57	1 (11%)	10,12,14	2.63	5 (50%)
54	MHW	D6	1	54	9,9,10	1.52	1 (11%)	8,11,13	3.10	3 (37%)
54	DBB	D6	3	54	4,5,6	1.09	0	3,5,7	1.83	1 (33%)
54	MHU	D6	5	54	13,15,16	1.95	3 (23%)	15,19,21	1.83	2 (13%)
54	MHV	D6	6	54	7,9,10	0.89	0	8,11,13	3.73	3 (37%)
54	004	D6	7	54	9,10,11	0.52	0	10,12,14	1.61	1 (10%)

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

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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	7	004	CB-CA	-4.46	1.48	1.52
54	B6	6	MHV	CB-CG	-2.75	1.45	1.50
54	B6	3	DBB	CB-CA	-2.40	1.46	1.53
54	B6	5	MHU	CD2-CE2	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D6	5	MHU	CD2-CE2	2.41	1.43	1.38

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	MHV	CD2-CE-N	-9.82	90.50	109.82
54	B6	6	MHV	CD2-CE-N	-8.95	92.22	109.82
54	B6	6	MHV	CA-CB-CG	-6.31	104.80	111.87
54	B6	7	004	CB-CA-N	-4.83	101.15	112.54
54	D6	1	MHW	CG2-CD-CE	-4.75	111.55	118.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	0.08	42 (2%) 58 37	15, 50, 134, 177	0
1	CA	1539/1539 (100%)	0.41	109 (7%) 19 10	29, 71, 143, 177	0
2	AB	218/218 (100%)	1.01	42 (19%) 2 1	39, 71, 98, 131	0
2	CB	218/218 (100%)	1.56	79 (36%) 0 0	55, 80, 108, 126	0
3	AC	206/206 (100%)	0.37	13 (6%) 23 12	36, 56, 81, 95	0
3	CC	206/206 (100%)	1.58	66 (32%) 1 0	52, 73, 93, 114	0
4	AD	205/205 (100%)	0.81	25 (12%) 5 3	33, 55, 80, 109	0
4	CD	205/205 (100%)	0.40	14 (6%) 20 11	23, 40, 75, 93	0
5	AE	150/150 (100%)	0.44	5 (3%) 50 31	32, 49, 82, 111	0
5	CE	150/150 (100%)	0.66	11 (7%) 18 9	35, 56, 83, 105	0
6	AF	100/100 (100%)	0.36	7 (7%) 19 10	34, 55, 75, 85	0
6	CF	100/100 (100%)	0.89	16 (16%) 3 1	44, 72, 97, 105	0
7	AG	151/151 (100%)	1.15	34 (22%) 1 1	48, 73, 96, 107	0
7	CG	151/151 (100%)	3.18	100 (66%) 0 0	75, 92, 105, 113	0
8	AH	129/129 (100%)	0.33	2 (1%) 74 55	28, 47, 71, 80	0
8	CH	129/129 (100%)	0.93	20 (15%) 3 1	46, 63, 83, 90	0
9	AI	127/127 (100%)	1.09	26 (20%) 1 1	42, 68, 96, 115	0
9	CI	127/127 (100%)	2.17	63 (49%) 0 0	64, 87, 106, 131	0
10	AJ	98/98 (100%)	1.09	17 (17%) 2 1	42, 62, 93, 120	0
10	CJ	98/98 (100%)	3.41	68 (69%) 0 0	66, 89, 108, 122	0
11	AK	117/117 (100%)	0.92	23 (19%) 1 1	29, 61, 88, 106	0
11	CK	117/117 (100%)	0.63	11 (9%) 11 5	35, 63, 82, 91	0
12	AL	123/123 (100%)	0.42	5 (4%) 41 24	23, 36, 72, 102	0
12	CL	123/123 (100%)	0.81	9 (7%) 18 9	38, 50, 80, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.67	15 (13%) 4 2	43, 66, 91, 105	0
13	CM	114/114 (100%)	3.49	85 (74%) 0 0	80, 98, 113, 118	0
14	AN	96/100 (96%)	0.83	17 (17%) 2 1	39, 56, 93, 108	0
14	CN	96/100 (96%)	2.81	57 (59%) 0 0	60, 88, 106, 119	0
15	AO	88/88 (100%)	0.48	6 (6%) 20 11	31, 49, 66, 99	0
15	CO	88/88 (100%)	0.76	8 (9%) 11 6	42, 62, 84, 108	0
16	AP	82/82 (100%)	0.97	14 (17%) 2 1	35, 46, 80, 103	0
16	CP	82/82 (100%)	1.59	20 (24%) 1 1	43, 61, 87, 105	0
17	AQ	80/80 (100%)	0.69	8 (10%) 9 5	30, 55, 85, 123	0
17	CQ	80/80 (100%)	1.63	25 (31%) 1 0	42, 69, 97, 108	0
18	AR	55/55 (100%)	0.70	6 (10%) 7 4	38, 51, 76, 113	0
18	CR	55/55 (100%)	0.94	9 (16%) 2 1	40, 54, 83, 113	0
19	AS	79/79 (100%)	0.90	12 (15%) 3 1	45, 66, 92, 97	0
19	CS	79/79 (100%)	4.05	58 (73%) 0 0	79, 98, 113, 126	0
20	AT	85/85 (100%)	0.73	7 (8%) 14 7	35, 48, 74, 115	0
20	CT	85/85 (100%)	2.33	41 (48%) 0 0	52, 69, 91, 98	0
21	AU	51/51 (100%)	1.52	13 (25%) 1 1	49, 70, 92, 105	0
21	CU	51/51 (100%)	1.07	9 (17%) 2 1	43, 67, 92, 107	0
22	BA	2897/2903 (99%)	0.31	121 (4%) 40 23	3, 18, 128, 196	0
22	DA	2897/2903 (99%)	0.58	194 (6%) 21 11	42, 82, 142, 182	0
23	BB	119/119 (100%)	-0.19	0 100 100	6, 26, 52, 94	0
23	DB	118/119 (99%)	0.40	5 (4%) 40 23	68, 109, 131, 143	0
24	BC	271/271 (100%)	0.07	3 (1%) 82 65	8, 24, 44, 65	0
24	DC	271/271 (100%)	1.29	62 (22%) 1 1	40, 60, 76, 84	0
25	BD	209/209 (100%)	0.09	0 100 100	4, 15, 42, 69	0
25	DD	209/209 (100%)	1.43	59 (28%) 1 0	47, 64, 83, 99	0
26	BE	201/201 (100%)	0.06	1 (0%) 91 81	4, 27, 54, 95	0
26	DE	201/201 (100%)	2.19	98 (48%) 0 0	38, 76, 96, 108	0
27	BF	177/177 (100%)	0.41	10 (5%) 28 15	23, 44, 86, 104	0
27	DF	177/177 (100%)	3.96	145 (81%) 0 0	79, 97, 113, 125	0
28	BG	176/176 (100%)	0.49	12 (6%) 20 11	21, 39, 66, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	2.49	101 (57%) 0 0	66, 85, 103, 117	0
29	BH	149/149 (100%)	4.67	113 (75%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	2.46	74 (49%) 0 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	3.88	95 (67%) 0 0	80, 104, 120, 136	0
30	DI	141/141 (100%)	5.77	129 (91%) 0 0	91, 110, 121, 124	0
31	BJ	142/142 (100%)	-0.05	1 (0%) 89 76	5, 12, 32, 54	0
31	DJ	142/142 (100%)	1.32	32 (22%) 1 1	49, 64, 80, 96	0
32	BK	122/122 (100%)	-0.06	1 (0%) 87 73	7, 16, 40, 68	0
32	DK	122/122 (100%)	1.42	36 (29%) 1 0	47, 60, 81, 95	0
33	BL	143/143 (100%)	0.14	3 (2%) 67 46	4, 26, 49, 80	0
33	DL	143/143 (100%)	2.50	77 (53%) 0 0	45, 72, 90, 111	0
34	BM	136/136 (100%)	-0.06	0 100 100	6, 16, 34, 93	0
34	DM	136/136 (100%)	1.31	38 (27%) 1 0	40, 64, 82, 110	0
35	BN	120/120 (100%)	-0.04	0 100 100	7, 13, 25, 70	0
35	DN	120/120 (100%)	1.89	41 (34%) 0 0	50, 71, 88, 109	0
36	BO	116/116 (100%)	0.13	1 (0%) 85 70	18, 29, 52, 59	0
36	DO	116/116 (100%)	3.15	78 (67%) 0 0	64, 86, 100, 113	0
37	BP	114/114 (100%)	0.09	2 (1%) 71 51	10, 22, 49, 73	0
37	DP	114/114 (100%)	1.44	37 (32%) 1 0	51, 66, 84, 91	0
38	BQ	117/117 (100%)	-0.03	0 100 100	3, 8, 21, 57	0
38	DQ	117/117 (100%)	1.51	40 (34%) 0 0	46, 65, 79, 83	0
39	BR	103/103 (100%)	-0.08	0 100 100	4, 15, 37, 64	0
39	DR	103/103 (100%)	2.04	45 (43%) 0 0	49, 72, 86, 96	0
40	BS	110/110 (100%)	0.03	1 (0%) 85 70	4, 9, 27, 89	0
40	DS	110/110 (100%)	2.52	63 (57%) 0 0	53, 69, 89, 97	0
41	BT	93/93 (100%)	0.59	8 (8%) 13 6	15, 28, 83, 100	0
41	DT	93/93 (100%)	3.21	66 (70%) 0 0	60, 79, 102, 111	0
42	BU	102/102 (100%)	0.17	4 (3%) 43 25	15, 32, 62, 95	0
42	DU	102/102 (100%)	4.19	75 (73%) 0 0	61, 82, 103, 109	0
43	BV	94/94 (100%)	0.03	2 (2%) 67 46	11, 24, 48, 59	0
43	DV	94/94 (100%)	1.14	19 (20%) 1 1	60, 78, 93, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	0.14	2 (2%) 59 38	10, 17, 37, 56	0
44	DW	75/76 (98%)	2.27	38 (50%) 0 0	49, 75, 86, 107	0
45	BX	77/77 (100%)	0.17	4 (5%) 31 17	11, 28, 53, 81	0
45	DX	77/77 (100%)	1.56	25 (32%) 1 0	49, 66, 84, 89	0
46	BY	63/63 (100%)	0.60	5 (7%) 15 8	21, 42, 71, 93	0
46	DY	63/63 (100%)	2.35	31 (49%) 0 0	63, 86, 95, 104	0
47	BZ	58/58 (100%)	-0.01	0 100 100	7, 11, 34, 40	0
47	DZ	58/58 (100%)	1.34	18 (31%) 1 0	50, 69, 82, 89	0
48	B0	56/56 (100%)	-0.09	0 100 100	4, 14, 38, 77	0
48	D0	56/56 (100%)	2.05	19 (33%) 0 0	49, 69, 90, 106	0
49	B1	50/50 (100%)	0.25	2 (4%) 42 25	19, 33, 61, 95	0
49	D1	50/50 (100%)	2.17	24 (48%) 0 0	63, 79, 91, 103	0
50	B2	46/46 (100%)	0.11	1 (2%) 65 44	8, 14, 22, 97	0
50	D2	46/46 (100%)	1.96	17 (36%) 0 0	47, 64, 78, 100	0
51	B3	64/64 (100%)	0.18	1 (1%) 74 55	10, 16, 26, 37	0
51	D3	64/64 (100%)	1.80	25 (39%) 0 0	53, 67, 79, 83	0
52	B4	38/38 (100%)	0.42	1 (2%) 59 38	13, 23, 38, 60	0
52	D4	38/38 (100%)	2.98	24 (63%) 0 0	56, 71, 84, 96	0
53	B5	191/228 (83%)	7.17	185 (96%) 0 0	71, 107, 119, 133	0
54	B6	2/8 (25%)	0.34	0 100 100	6, 6, 6, 8	0
54	D6	2/8 (25%)	1.07	1 (50%) 0 0	41, 41, 41, 44	0
All	All	20738/20810 (99%)	0.95	3532 (17%) 2 1	3, 61, 117, 196	0

The worst 5 of 3532 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	BH	96	THR	24.6
53	B5	111	PHE	23.5
30	DI	2	ALA	21.9
29	BH	113	SER	20.6
30	DI	3	LYS	20.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
54	004	D6	7	10/11	0.90	0.20	-	38,42,48,48	0
54	MHU	B6	5	15/16	0.97	0.23	-	0,5,18,21	0
54	MHV	B6	6	9/10	0.98	0.16	-	2,6,13,14	0
54	MHW	D6	1	9/10	0.77	0.33	-	49,54,56,59	0
54	MHW	B6	1	9/10	0.95	0.21	-	12,14,18,21	0
54	004	B6	7	10/11	0.97	0.29	-	3,6,7,10	0
54	DBB	D6	3	6/7	0.91	0.28	-	37,40,41,43	0
54	MHU	D6	5	15/16	0.89	0.36	-	37,42,54,56	0
54	MHV	D6	6	9/10	0.92	0.16	-	39,40,42,43	0
54	DBB	B6	3	6/7	0.97	0.22	-	6,8,10,15	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
55	MG	BA	3040	1/1	0.88	0.45	27.33	7,7,7,7	0
55	MG	BA	3178	1/1	0.91	0.46	27.24	20,20,20,20	0
55	MG	AA	1669	1/1	0.84	0.55	20.06	43,43,43,43	0
55	MG	DA	3057	1/1	0.78	0.62	17.12	54,54,54,54	0
55	MG	DA	3162	1/1	0.84	0.45	13.43	46,46,46,46	0
55	MG	BA	3186	1/1	0.98	0.35	12.55	18,18,18,18	0
55	MG	DA	3157	1/1	0.95	0.40	11.36	47,47,47,47	0
55	MG	DA	3153	1/1	0.93	0.48	10.59	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3170	1/1	0.91	0.29	10.49	35,35,35,35	0
55	MG	DA	3002	1/1	0.89	0.41	10.01	52,52,52,52	0
55	MG	BA	3168	1/1	0.71	0.32	9.32	18,18,18,18	0
55	MG	BA	3116	1/1	0.86	0.31	8.59	11,11,11,11	0
55	MG	BA	3113	1/1	0.92	0.32	8.46	10,10,10,10	0
55	MG	AA	1622	1/1	0.91	0.27	7.80	21,21,21,21	0
55	MG	BA	3070	1/1	0.94	0.25	7.67	9,9,9,9	0
55	MG	DA	3027	1/1	0.84	0.45	7.63	51,51,51,51	0
55	MG	BA	3108	1/1	0.78	0.28	6.43	1,1,1,1	0
55	MG	DA	3165	1/1	0.93	0.38	5.72	34,34,34,34	0
55	MG	BA	3130	1/1	0.95	0.24	4.49	4,4,4,4	0
55	MG	DA	3013	1/1	0.78	0.37	3.92	45,45,45,45	0
55	MG	DA	3124	1/1	0.76	0.38	3.78	59,59,59,59	0
55	MG	DA	3109	1/1	0.93	0.24	3.70	37,37,37,37	0
55	MG	DA	3070	1/1	0.38	0.35	3.33	58,58,58,58	0
55	MG	BA	3152	1/1	0.97	0.22	3.17	11,11,11,11	0
55	MG	BA	3163	1/1	0.93	0.23	3.16	27,27,27,27	0
55	MG	BA	3153	1/1	0.95	0.30	3.00	2,2,2,2	0
55	MG	DA	3005	1/1	0.35	0.23	2.92	66,66,66,66	0
55	MG	DA	3008	1/1	0.86	0.42	2.61	51,51,51,51	0
55	MG	DA	3071	1/1	0.90	0.28	2.56	59,59,59,59	0
55	MG	BA	3188	1/1	0.75	0.18	2.13	27,27,27,27	0
55	MG	BA	3161	1/1	0.84	0.22	2.02	24,24,24,24	0
55	MG	DA	3116	1/1	0.83	0.20	1.97	51,51,51,51	0
55	MG	BA	3155	1/1	0.92	0.27	1.92	15,15,15,15	0
55	MG	CA	1640	1/1	0.95	0.21	1.82	23,23,23,23	0
55	MG	DA	3047	1/1	0.70	0.31	1.65	66,66,66,66	0
55	MG	BA	3175	1/1	0.83	0.18	1.47	27,27,27,27	0
55	MG	BA	3053	1/1	0.96	0.20	1.41	4,4,4,4	0
55	MG	DA	3040	1/1	0.64	0.26	1.41	57,57,57,57	0
55	MG	DA	3031	1/1	0.80	0.23	1.41	50,50,50,50	0
55	MG	BA	3159	1/1	0.92	0.19	1.40	19,19,19,19	0
55	MG	BA	3107	1/1	0.97	0.20	1.30	6,6,6,6	0
55	MG	BA	3184	1/1	0.96	0.17	1.08	23,23,23,23	0
55	MG	DA	3046	1/1	0.47	0.25	1.05	53,53,53,53	0
55	MG	AA	1662	1/1	0.93	0.19	0.94	41,41,41,41	0
55	MG	AA	1630	1/1	0.65	0.20	0.73	49,49,49,49	0
55	MG	BA	3109	1/1	0.89	0.20	0.64	9,9,9,9	0
55	MG	BA	3034	1/1	0.89	0.20	0.64	18,18,18,18	0
55	MG	CA	1615	1/1	0.88	0.16	0.62	35,35,35,35	0
55	MG	BA	3062	1/1	0.96	0.21	0.57	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3068	1/1	0.86	0.19	0.45	52,52,52,52	0
55	MG	DA	3114	1/1	0.94	0.33	0.40	64,64,64,64	0
55	MG	BA	3104	1/1	0.97	0.20	0.27	1,1,1,1	0
55	MG	AA	1641	1/1	0.95	0.18	0.26	20,20,20,20	0
55	MG	BA	3012	1/1	0.91	0.21	0.23	4,4,4,4	0
55	MG	DA	3063	1/1	0.93	0.19	0.18	41,41,41,41	0
55	MG	BA	3063	1/1	0.98	0.20	0.15	0,0,0,0	0
55	MG	BA	3047	1/1	0.78	0.14	0.02	34,34,34,34	0
56	ZN	B4	101	1/1	0.96	0.21	-0.22	131,131,131,131	0
55	MG	BA	3105	1/1	0.88	0.19	-0.30	4,4,4,4	0
55	MG	AA	1634	1/1	0.72	0.17	-0.34	36,36,36,36	0
55	MG	BA	3132	1/1	0.91	0.19	-0.40	27,27,27,27	0
55	MG	CA	1603	1/1	0.83	0.14	-0.41	44,44,44,44	0
55	MG	DA	3105	1/1	0.92	0.17	-0.44	37,37,37,37	0
55	MG	AA	1636	1/1	0.97	0.20	-0.47	26,26,26,26	0
55	MG	DA	3018	1/1	0.71	0.18	-0.48	57,57,57,57	0
55	MG	BA	3097	1/1	0.97	0.19	-0.53	6,6,6,6	0
55	MG	AA	1617	1/1	0.77	0.18	-0.55	44,44,44,44	0
55	MG	BA	3165	1/1	0.97	0.16	-0.56	2,2,2,2	0
55	MG	DA	3108	1/1	0.95	0.18	-0.60	35,35,35,35	0
55	MG	BA	3036	1/1	0.90	0.19	-0.61	19,19,19,19	0
55	MG	CA	1630	1/1	0.88	0.26	-0.69	66,66,66,66	0
55	MG	BA	3013	1/1	0.93	0.19	-0.77	0,0,0,0	0
55	MG	DA	3023	1/1	0.64	0.18	-0.79	35,35,35,35	0
55	MG	AA	1607	1/1	0.91	0.15	-0.84	33,33,33,33	0
55	MG	DA	3022	1/1	0.93	0.15	-0.87	54,54,54,54	0
55	MG	DA	3081	1/1	0.93	0.15	-0.94	43,43,43,43	0
55	MG	DA	3107	1/1	0.90	0.14	-1.20	49,49,49,49	0
55	MG	DA	3012	1/1	0.80	0.16	-1.21	40,40,40,40	0
55	MG	DA	3132	1/1	0.88	0.11	-1.25	45,45,45,45	0
55	MG	CA	1614	1/1	0.87	0.09	-1.25	44,44,44,44	0
55	MG	DA	3062	1/1	0.77	0.14	-1.29	44,44,44,44	0
55	MG	DA	3096	1/1	0.93	0.17	-1.40	52,52,52,52	0
55	MG	BA	3112	1/1	0.94	0.16	-1.48	11,11,11,11	0
55	MG	DA	3104	1/1	0.77	0.14	-1.56	54,54,54,54	0
55	MG	BA	3134	1/1	0.87	0.17	-1.58	8,8,8,8	0
56	ZN	D4	101	1/1	0.97	0.05	-1.61	79,79,79,79	0
55	MG	BA	3049	1/1	0.91	0.14	-1.65	9,9,9,9	0
55	MG	DA	3077	1/1	0.61	0.08	-1.79	59,59,59,59	0
55	MG	BA	3071	1/1	0.89	0.16	-1.85	11,11,11,11	0
55	MG	AA	1604	1/1	0.87	0.10	-1.88	45,45,45,45	0
55	MG	CA	1635	1/1	0.60	0.18	-1.91	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1629	1/1	0.95	0.12	-1.94	43,43,43,43	0
55	MG	BA	3120	1/1	0.83	0.16	-1.94	7,7,7,7	0
55	MG	DA	3079	1/1	0.82	0.11	-1.98	62,62,62,62	0
55	MG	AA	1642	1/1	0.96	0.13	-2.01	24,24,24,24	0
55	MG	BB	201	1/1	0.76	0.10	-2.17	28,28,28,28	0
55	MG	DA	3136	1/1	0.59	0.10	-2.21	57,57,57,57	0
55	MG	BA	3021	1/1	0.92	0.16	-2.21	1,1,1,1	0
55	MG	BA	3022	1/1	0.96	0.16	-2.22	3,3,3,3	0
55	MG	CA	1617	1/1	0.72	0.15	-2.24	35,35,35,35	0
55	MG	DA	3049	1/1	0.63	0.10	-2.26	49,49,49,49	0
55	MG	CA	1632	1/1	0.92	0.13	-2.28	54,54,54,54	0
55	MG	DA	3128	1/1	0.91	0.10	-2.31	57,57,57,57	0
55	MG	BA	3064	1/1	0.90	0.17	-2.44	2,2,2,2	0
55	MG	CA	1624	1/1	0.85	0.13	-2.51	33,33,33,33	0
55	MG	BA	3023	1/1	0.76	0.15	-2.53	15,15,15,15	0
55	MG	BA	3077	1/1	0.83	0.08	-2.54	26,26,26,26	0
55	MG	DA	3095	1/1	0.80	0.10	-2.60	49,49,49,49	0
55	MG	DA	3134	1/1	0.86	0.10	-2.60	34,34,34,34	0
55	MG	AA	1618	1/1	0.81	0.11	-2.62	35,35,35,35	0
55	MG	DA	3053	1/1	0.92	0.12	-2.75	43,43,43,43	0
55	MG	AA	1616	1/1	0.87	0.10	-2.78	42,42,42,42	0
55	MG	BA	3136	1/1	0.96	0.14	-2.79	24,24,24,24	0
55	MG	DA	3078	1/1	0.71	0.10	-2.98	64,64,64,64	0
55	MG	DA	3021	1/1	0.79	0.12	-3.03	38,38,38,38	0
55	MG	DA	3145	1/1	0.95	0.10	-3.05	37,37,37,37	0
55	MG	DA	3026	1/1	0.69	0.10	-3.10	53,53,53,53	0
55	MG	CA	1621	1/1	0.70	0.11	-3.14	53,53,53,53	0
55	MG	BA	3008	1/1	0.82	0.12	-3.18	9,9,9,9	0
55	MG	DA	3097	1/1	0.88	0.08	-3.30	44,44,44,44	0
55	MG	BA	3129	1/1	0.95	0.16	-3.34	5,5,5,5	0
55	MG	BA	3024	1/1	0.94	0.14	-3.34	7,7,7,7	0
55	MG	BA	3177	1/1	0.94	0.09	-3.37	24,24,24,24	0
55	MG	BA	3066	1/1	0.89	0.13	-3.57	6,6,6,6	0
55	MG	BA	3050	1/1	0.92	0.11	-3.70	11,11,11,11	0
55	MG	CA	1616	1/1	0.93	0.11	-3.72	29,29,29,29	0
55	MG	BA	3068	1/1	0.90	0.17	-3.79	6,6,6,6	0
55	MG	CA	1601	1/1	0.72	0.11	-3.83	33,33,33,33	0
55	MG	CA	1610	1/1	0.96	0.09	-3.88	47,47,47,47	0
55	MG	DA	3120	1/1	0.90	0.09	-3.96	49,49,49,49	0
55	MG	BA	3059	1/1	0.94	0.14	-3.97	16,16,16,16	0
55	MG	BA	3079	1/1	0.77	0.11	-4.05	28,28,28,28	0
55	MG	DB	201	1/1	0.92	0.06	-4.12	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1619	1/1	0.93	0.11	-4.23	26,26,26,26	0
55	MG	AA	1606	1/1	0.95	0.09	-4.24	31,31,31,31	0
55	MG	BA	3017	1/1	0.97	0.13	-4.25	6,6,6,6	0
55	MG	BA	3065	1/1	0.97	0.11	-4.30	7,7,7,7	0
55	MG	AA	1613	1/1	0.90	0.11	-4.55	20,20,20,20	0
55	MG	BA	3027	1/1	0.89	0.09	-4.72	22,22,22,22	0
55	MG	DA	3038	1/1	0.81	0.09	-4.76	42,42,42,42	0
55	MG	DA	3050	1/1	0.94	0.07	-4.82	29,29,29,29	0
55	MG	AA	1640	1/1	0.91	0.06	-4.83	39,39,39,39	0
55	MG	DA	3017	1/1	0.80	0.13	-4.97	40,40,40,40	0
55	MG	CA	1626	1/1	0.81	0.08	-5.07	42,42,42,42	0
55	MG	BA	3009	1/1	0.78	0.13	-5.22	6,6,6,6	0
55	MG	BA	3101	1/1	0.92	0.14	-5.57	2,2,2,2	0
55	MG	BA	3110	1/1	0.89	0.08	-5.71	23,23,23,23	0
55	MG	DA	3073	1/1	0.84	0.10	-5.77	37,37,37,37	0
55	MG	BA	3058	1/1	0.94	0.08	-5.80	13,13,13,13	0
55	MG	CA	1607	1/1	0.89	0.10	-6.05	42,42,42,42	0
55	MG	AA	1633	1/1	0.94	0.09	-6.32	31,31,31,31	0
55	MG	BA	3118	1/1	0.96	0.07	-6.54	11,11,11,11	0
55	MG	AA	1625	1/1	0.97	0.07	-6.69	31,31,31,31	0
55	MG	CA	1622	1/1	0.95	0.05	-6.74	40,40,40,40	0
55	MG	AA	1609	1/1	0.96	0.08	-6.98	20,20,20,20	0
55	MG	DA	3129	1/1	0.94	0.11	-7.08	38,38,38,38	0
55	MG	BA	3073	1/1	0.86	0.12	-7.12	13,13,13,13	0
55	MG	BA	3096	1/1	0.97	0.11	-7.45	5,5,5,5	0
55	MG	DA	3065	1/1	0.94	0.06	-7.54	33,33,33,33	0
55	MG	DA	3058	1/1	0.96	0.05	-7.98	37,37,37,37	0
55	MG	BA	3002	1/1	0.89	0.08	-9.89	15,15,15,15	0
55	MG	BA	3131	1/1	0.93	0.11	-10.21	35,35,35,35	0
55	MG	BA	3005	1/1	0.97	0.05	-12.66	31,31,31,31	0
55	MG	BA	3028	1/1	0.92	0.11	-24.90	4,4,4,4	0
55	MG	AA	1665	1/1	0.90	0.16	-	34,34,34,34	0
55	MG	DA	3025	1/1	0.72	0.45	-	49,49,49,49	0
55	MG	DA	3092	1/1	0.77	0.45	-	62,62,62,62	0
55	MG	AA	1626	1/1	0.92	0.19	-	26,26,26,26	0
55	MG	BA	3067	1/1	0.93	0.20	-	5,5,5,5	0
55	MG	BA	3102	1/1	0.91	0.33	-	23,23,23,23	0
55	MG	BA	3115	1/1	0.89	0.19	-	35,35,35,35	0
55	MG	AA	1647	1/1	0.98	0.18	-	39,39,39,39	0
55	MG	BA	3151	1/1	0.89	0.20	-	31,31,31,31	0
55	MG	BA	3037	1/1	0.98	0.23	-	2,2,2,2	0
55	MG	DA	3043	1/1	0.66	0.21	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3187	1/1	0.90	0.17	-	28,28,28,28	0
55	MG	BA	3045	1/1	0.68	0.20	-	13,13,13,13	0
55	MG	AA	1623	1/1	0.78	0.13	-	42,42,42,42	0
55	MG	DA	3084	1/1	0.78	0.30	-	56,56,56,56	0
55	MG	BA	3146	1/1	0.95	0.25	-	23,23,23,23	0
55	MG	BA	3080	1/1	0.91	0.10	-	18,18,18,18	0
55	MG	CA	1631	1/1	0.82	0.25	-	62,62,62,62	0
55	MG	BA	3085	1/1	0.77	0.15	-	7,7,7,7	0
55	MG	DA	3086	1/1	0.65	0.13	-	53,53,53,53	0
55	MG	CA	1612	1/1	0.98	0.05	-	30,30,30,30	0
55	MG	BA	3141	1/1	0.98	0.42	-	4,4,4,4	0
55	MG	AA	1610	1/1	0.72	0.17	-	49,49,49,49	0
55	MG	BA	3169	1/1	0.95	0.12	-	24,24,24,24	0
55	MG	BB	202	1/1	0.94	0.08	-	11,11,11,11	0
55	MG	DA	3054	1/1	0.78	0.28	-	44,44,44,44	0
55	MG	BA	3086	1/1	0.91	0.21	-	9,9,9,9	0
55	MG	BA	3093	1/1	0.87	0.16	-	16,16,16,16	0
55	MG	CA	1649	1/1	0.92	0.16	-	35,35,35,35	0
55	MG	BA	3154	1/1	0.79	0.20	-	29,29,29,29	0
55	MG	DA	3066	1/1	0.86	0.11	-	39,39,39,39	0
55	MG	CA	1609	1/1	0.31	0.21	-	58,58,58,58	0
55	MG	AM	201	1/1	0.93	0.29	-	29,29,29,29	0
55	MG	BA	3142	1/1	0.94	0.41	-	15,15,15,15	0
55	MG	DA	3141	1/1	0.93	0.20	-	28,28,28,28	0
55	MG	CA	1636	1/1	0.30	0.26	-	79,79,79,79	0
55	MG	BA	3011	1/1	0.95	0.07	-	13,13,13,13	0
55	MG	DA	3080	1/1	0.81	0.11	-	39,39,39,39	0
55	MG	DA	3072	1/1	0.95	0.12	-	42,42,42,42	0
55	MG	BA	3126	1/1	0.88	0.28	-	7,7,7,7	0
55	MG	BA	3174	1/1	0.95	0.12	-	20,20,20,20	0
55	MG	BA	3038	1/1	0.88	0.14	-	8,8,8,8	0
55	MG	AA	1643	1/1	0.91	0.16	-	19,19,19,19	0
55	MG	AA	1650	1/1	0.94	0.17	-	35,35,35,35	0
55	MG	AA	1644	1/1	0.82	0.26	-	32,32,32,32	0
55	MG	BA	3143	1/1	0.96	0.28	-	7,7,7,7	0
55	MG	DA	3056	1/1	0.64	0.24	-	51,51,51,51	0
55	MG	DA	3032	1/1	0.85	0.06	-	49,49,49,49	0
55	MG	AA	1603	1/1	0.95	0.15	-	34,34,34,34	0
55	MG	DA	3123	1/1	0.86	0.17	-	47,47,47,47	0
55	MG	AA	1632	1/1	0.78	0.14	-	40,40,40,40	0
55	MG	DB	202	1/1	0.90	0.05	-	42,42,42,42	0
55	MG	CA	1653	1/1	0.96	0.31	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3014	1/1	0.85	0.09	-	43,43,43,43	0
55	MG	DA	3009	1/1	0.65	0.12	-	57,57,57,57	0
55	MG	BA	3082	1/1	0.89	0.19	-	15,15,15,15	0
55	MG	BA	3158	1/1	0.94	0.18	-	20,20,20,20	0
55	MG	BA	3171	1/1	0.96	0.14	-	29,29,29,29	0
55	MG	DA	3117	1/1	0.78	0.06	-	49,49,49,49	0
55	MG	BA	3167	1/1	0.94	0.15	-	28,28,28,28	0
55	MG	BA	3121	1/1	0.93	0.08	-	22,22,22,22	0
55	MG	DA	3060	1/1	0.47	1.18	-	61,61,61,61	0
55	MG	DA	3036	1/1	0.84	0.16	-	61,61,61,61	0
55	MG	DA	3024	1/1	0.80	0.17	-	45,45,45,45	0
55	MG	CA	1644	1/1	0.96	0.25	-	32,32,32,32	0
55	MG	DA	3074	1/1	0.84	0.10	-	41,41,41,41	0
55	MG	BA	3010	1/1	0.84	0.15	-	3,3,3,3	0
55	MG	BA	3076	1/1	0.84	0.19	-	17,17,17,17	0
55	MG	BA	3166	1/1	0.92	0.21	-	25,25,25,25	0
55	MG	DA	3034	1/1	0.76	0.29	-	56,56,56,56	0
55	MG	CA	1646	1/1	0.91	0.14	-	40,40,40,40	0
55	MG	DA	3152	1/1	0.92	0.16	-	41,41,41,41	0
55	MG	DA	3061	1/1	0.79	0.99	-	53,53,53,53	0
55	MG	BA	3015	1/1	0.58	0.41	-	52,52,52,52	0
55	MG	AA	1671	1/1	0.93	0.20	-	35,35,35,35	0
55	MG	BA	3083	1/1	0.92	0.21	-	32,32,32,32	0
55	MG	BA	3078	1/1	0.92	0.10	-	33,33,33,33	0
55	MG	BA	3125	1/1	0.88	0.20	-	8,8,8,8	0
55	MG	AA	1638	1/1	0.62	0.12	-	51,51,51,51	0
55	MG	DA	3133	1/1	0.81	0.58	-	57,57,57,57	0
55	MG	DA	3158	1/1	0.83	0.16	-	55,55,55,55	0
55	MG	DB	203	1/1	0.85	0.06	-	56,56,56,56	0
55	MG	CA	1606	1/1	0.78	0.29	-	52,52,52,52	0
55	MG	BA	3176	1/1	0.93	0.14	-	24,24,24,24	0
55	MG	BA	3018	1/1	0.96	0.09	-	27,27,27,27	0
55	MG	DA	3111	1/1	0.66	0.12	-	42,42,42,42	0
55	MG	DA	3125	1/1	0.85	0.17	-	51,51,51,51	0
55	MG	CA	1627	1/1	0.83	0.12	-	59,59,59,59	0
55	MG	BA	3191	1/1	0.93	0.24	-	35,35,35,35	0
55	MG	CA	1654	1/1	0.85	0.14	-	26,26,26,26	0
55	MG	AA	1645	1/1	0.98	0.13	-	39,39,39,39	0
55	MG	BA	3150	1/1	0.80	0.24	-	42,42,42,42	0
55	MG	AA	1605	1/1	0.80	0.16	-	32,32,32,32	0
55	MG	DA	3137	1/1	0.82	0.47	-	42,42,42,42	0
55	MG	DA	3166	1/1	0.87	0.15	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1648	1/1	0.93	0.19	-	42,42,42,42	0
55	MG	BA	3052	1/1	0.70	0.15	-	8,8,8,8	0
55	MG	AA	1664	1/1	0.91	0.19	-	36,36,36,36	0
55	MG	AA	1663	1/1	0.93	0.17	-	35,35,35,35	0
55	MG	BA	3084	1/1	0.94	0.12	-	12,12,12,12	0
55	MG	AA	1621	1/1	0.93	0.06	-	33,33,33,33	0
55	MG	AA	1648	1/1	0.78	0.29	-	38,38,38,38	0
55	MG	DA	3167	1/1	0.83	0.12	-	59,59,59,59	0
55	MG	BA	3031	1/1	0.84	0.14	-	8,8,8,8	0
55	MG	DA	3159	1/1	0.80	0.17	-	39,39,39,39	0
55	MG	DA	3041	1/1	0.66	0.36	-	53,53,53,53	0
55	MG	DA	3067	1/1	0.95	0.10	-	49,49,49,49	0
55	MG	DA	3144	1/1	0.97	0.04	-	52,52,52,52	0
55	MG	CA	1645	1/1	0.97	0.19	-	41,41,41,41	0
55	MG	BA	3147	1/1	0.98	0.46	-	13,13,13,13	0
55	MG	AA	1659	1/1	0.77	0.52	-	34,34,34,34	0
55	MG	BA	3069	1/1	0.97	0.07	-	39,39,39,39	0
55	MG	DA	3139	1/1	0.98	0.36	-	31,31,31,31	0
55	MG	AA	1608	1/1	0.67	0.21	-	24,24,24,24	0
55	MG	BA	3185	1/1	0.90	0.17	-	11,11,11,11	0
55	MG	AA	1653	1/1	0.95	0.30	-	24,24,24,24	0
55	MG	DA	3100	1/1	0.88	0.07	-	43,43,43,43	0
55	MG	DA	3138	1/1	0.86	0.72	-	41,41,41,41	0
55	MG	BA	3060	1/1	0.82	0.38	-	33,33,33,33	0
55	MG	BA	3123	1/1	0.86	0.13	-	18,18,18,18	0
55	MG	BA	3192	1/1	0.94	0.16	-	15,15,15,15	0
55	MG	BA	3048	1/1	0.72	0.09	-	16,16,16,16	0
55	MG	BA	3072	1/1	0.98	0.20	-	4,4,4,4	0
55	MG	BA	3189	1/1	0.97	0.20	-	3,3,3,3	0
55	MG	DA	3010	1/1	0.69	0.11	-	48,48,48,48	0
55	MG	DA	3083	1/1	0.88	0.27	-	61,61,61,61	0
55	MG	BA	3194	1/1	0.99	0.17	-	28,28,28,28	0
55	MG	BA	3103	1/1	0.84	0.12	-	9,9,9,9	0
55	MG	DA	3029	1/1	0.81	0.28	-	41,41,41,41	0
55	MG	AA	1646	1/1	0.89	0.20	-	44,44,44,44	0
55	MG	DA	3127	1/1	0.58	0.13	-	47,47,47,47	0
55	MG	BA	3014	1/1	0.91	0.11	-	6,6,6,6	0
55	MG	DA	3112	1/1	0.83	0.28	-	52,52,52,52	0
55	MG	DA	3131	1/1	0.54	0.89	-	71,71,71,71	0
55	MG	AA	1661	1/1	0.94	0.20	-	22,22,22,22	0
55	MG	DA	3090	1/1	0.71	0.21	-	58,58,58,58	0
55	MG	AA	1658	1/1	0.96	0.08	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3128	1/1	0.88	0.22	-	9,9,9,9	0
55	MG	DA	3076	1/1	0.80	0.33	-	48,48,48,48	0
55	MG	DA	3135	1/1	0.67	0.24	-	47,47,47,47	0
55	MG	DA	3037	1/1	0.77	0.10	-	45,45,45,45	0
55	MG	CA	1638	1/1	0.62	0.21	-	55,55,55,55	0
55	MG	BA	3160	1/1	0.90	0.26	-	7,7,7,7	0
55	MG	BA	3039	1/1	0.95	0.18	-	1,1,1,1	0
55	MG	CA	1643	1/1	0.95	0.28	-	44,44,44,44	0
55	MG	BA	3030	1/1	0.79	0.28	-	10,10,10,10	0
55	MG	BB	204	1/1	0.98	0.29	-	4,4,4,4	0
55	MG	AA	1652	1/1	0.88	0.20	-	43,43,43,43	0
55	MG	DA	3089	1/1	0.94	0.22	-	58,58,58,58	0
55	MG	DA	3082	1/1	0.97	0.06	-	50,50,50,50	0
55	MG	DA	3085	1/1	0.93	0.10	-	42,42,42,42	0
55	MG	DA	3048	1/1	0.35	0.20	-	51,51,51,51	0
55	MG	CA	1641	1/1	0.93	0.83	-	46,46,46,46	0
55	MG	DA	3006	1/1	0.81	0.37	-	64,64,64,64	0
55	MG	DA	3122	1/1	0.85	0.18	-	42,42,42,42	0
55	MG	BA	3094	1/1	0.91	0.05	-	17,17,17,17	0
55	MG	DA	3088	1/1	0.92	0.29	-	51,51,51,51	0
55	MG	BA	3190	1/1	0.90	0.25	-	33,33,33,33	0
55	MG	BA	3054	1/1	0.90	0.11	-	5,5,5,5	0
55	MG	AA	1668	1/1	0.88	0.18	-	18,18,18,18	0
55	MG	AA	1620	1/1	0.80	0.11	-	44,44,44,44	0
55	MG	AA	1667	1/1	0.86	0.20	-	37,37,37,37	0
55	MG	DA	3160	1/1	0.79	0.30	-	35,35,35,35	0
55	MG	DA	3044	1/1	0.83	0.10	-	61,61,61,61	0
55	MG	DA	3154	1/1	0.87	0.13	-	45,45,45,45	0
55	MG	CA	1651	1/1	0.90	0.15	-	48,48,48,48	0
55	MG	AA	1654	1/1	0.96	0.33	-	40,40,40,40	0
55	MG	DA	3118	1/1	0.81	0.12	-	45,45,45,45	0
55	MG	DA	3069	1/1	0.85	0.08	-	63,63,63,63	0
55	MG	CA	1613	1/1	0.90	0.15	-	19,19,19,19	0
55	MG	AA	1612	1/1	0.84	0.14	-	24,24,24,24	0
55	MG	BA	3057	1/1	0.75	0.20	-	20,20,20,20	0
55	MG	BA	3193	1/1	0.96	0.13	-	12,12,12,12	0
55	MG	DA	3020	1/1	0.95	0.36	-	42,42,42,42	0
55	MG	AA	1601	1/1	0.92	0.14	-	49,49,49,49	0
55	MG	BA	3032	1/1	0.95	0.17	-	8,8,8,8	0
55	MG	BA	3098	1/1	0.77	0.34	-	58,58,58,58	0
55	MG	DA	3143	1/1	0.71	0.29	-	46,46,46,46	0
55	MG	BA	3099	1/1	0.89	0.14	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1656	1/1	0.94	0.12	-	37,37,37,37	0
55	MG	DA	3015	1/1	0.66	0.63	-	56,56,56,56	0
55	MG	BA	3003	1/1	0.83	0.11	-	20,20,20,20	0
55	MG	BA	3007	1/1	0.87	0.08	-	25,25,25,25	0
55	MG	CA	1628	1/1	0.78	0.40	-	64,64,64,64	0
55	MG	BA	3162	1/1	0.93	0.19	-	21,21,21,21	0
55	MG	DA	3148	1/1	0.90	0.26	-	45,45,45,45	0
55	MG	BA	3091	1/1	0.88	0.07	-	28,28,28,28	0
55	MG	DA	3151	1/1	0.85	0.40	-	45,45,45,45	0
55	MG	DA	3087	1/1	0.69	0.14	-	51,51,51,51	0
55	MG	DA	3115	1/1	0.70	0.18	-	58,58,58,58	0
55	MG	DA	3051	1/1	0.90	0.07	-	35,35,35,35	0
55	MG	BA	3144	1/1	0.97	0.19	-	25,25,25,25	0
55	MG	DA	3156	1/1	0.96	0.13	-	30,30,30,30	0
55	MG	BA	3181	1/1	0.91	0.22	-	14,14,14,14	0
55	MG	BA	3055	1/1	0.89	0.22	-	23,23,23,23	0
55	MG	CA	1623	1/1	0.93	0.29	-	40,40,40,40	0
55	MG	BA	3149	1/1	0.97	0.15	-	1,1,1,1	0
55	MG	AA	1639	1/1	0.82	0.06	-	51,51,51,51	0
55	MG	CA	1634	1/1	0.89	0.07	-	49,49,49,49	0
55	MG	BA	3164	1/1	0.96	0.45	-	21,21,21,21	0
55	MG	AA	1627	1/1	0.83	0.34	-	43,43,43,43	0
55	MG	BB	203	1/1	0.82	0.09	-	10,10,10,10	0
55	MG	DA	3033	1/1	0.76	0.23	-	45,45,45,45	0
55	MG	DA	3093	1/1	0.68	0.14	-	65,65,65,65	0
55	MG	CA	1642	1/1	0.94	0.27	-	27,27,27,27	0
55	MG	DA	3101	1/1	0.95	0.10	-	40,40,40,40	0
55	MG	BA	3006	1/1	0.94	0.10	-	20,20,20,20	0
55	MG	AA	1602	1/1	0.90	0.07	-	33,33,33,33	0
55	MG	DA	3155	1/1	0.57	0.74	-	44,44,44,44	0
55	MG	AA	1619	1/1	0.88	0.26	-	43,43,43,43	0
55	MG	BA	3145	1/1	0.90	0.21	-	15,15,15,15	0
55	MG	DA	3019	1/1	0.95	0.16	-	47,47,47,47	0
55	MG	BA	3061	1/1	0.79	0.47	-	55,55,55,55	0
55	MG	BA	3122	1/1	0.94	0.24	-	2,2,2,2	0
55	MG	DA	3119	1/1	0.68	0.63	-	68,68,68,68	0
55	MG	DA	3146	1/1	0.89	0.21	-	35,35,35,35	0
55	MG	DA	3106	1/1	0.62	0.13	-	56,56,56,56	0
55	MG	BA	3172	1/1	0.96	0.19	-	23,23,23,23	0
55	MG	BA	3133	1/1	0.86	0.39	-	40,40,40,40	0
55	MG	AA	1637	1/1	0.78	0.18	-	18,18,18,18	0
55	MG	BA	3019	1/1	0.82	0.24	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3113	1/1	0.66	0.16	-	42,42,42,42	0
55	MG	BA	3041	1/1	0.96	0.12	-	11,11,11,11	0
55	MG	DA	3130	1/1	0.87	0.09	-	51,51,51,51	0
55	MG	CA	1605	1/1	0.76	0.37	-	57,57,57,57	0
55	MG	CA	1637	1/1	0.73	0.37	-	51,51,51,51	0
55	MG	BA	3148	1/1	0.95	0.24	-	16,16,16,16	0
55	MG	CA	1655	1/1	0.82	0.61	-	44,44,44,44	0
55	MG	DA	3028	1/1	0.80	0.08	-	50,50,50,50	0
55	MG	DA	3035	1/1	0.96	0.15	-	38,38,38,38	0
55	MG	AA	1615	1/1	0.70	0.12	-	46,46,46,46	0
55	MG	DA	3099	1/1	0.49	0.18	-	53,53,53,53	0
55	MG	BA	3033	1/1	0.91	0.24	-	4,4,4,4	0
55	MG	DA	3094	1/1	0.85	0.30	-	59,59,59,59	0
55	MG	BA	3182	1/1	0.93	0.21	-	22,22,22,22	0
55	MG	CA	1650	1/1	0.86	0.49	-	40,40,40,40	0
55	MG	CA	1652	1/1	0.71	0.16	-	39,39,39,39	0
55	MG	AA	1660	1/1	0.94	0.22	-	40,40,40,40	0
55	MG	AA	1666	1/1	0.91	0.22	-	30,30,30,30	0
55	MG	BA	3114	1/1	0.90	0.20	-	19,19,19,19	0
55	MG	CA	1625	1/1	0.91	0.21	-	25,25,25,25	0
55	MG	BA	3025	1/1	0.78	0.25	-	40,40,40,40	0
55	MG	CA	1633	1/1	0.67	0.45	-	54,54,54,54	0
55	MG	DA	3059	1/1	0.89	0.35	-	53,53,53,53	0
55	MG	BA	3042	1/1	0.91	0.17	-	6,6,6,6	0
55	MG	DA	3103	1/1	0.74	0.14	-	48,48,48,48	0
55	MG	BA	3117	1/1	0.98	0.15	-	4,4,4,4	0
55	MG	BA	3056	1/1	0.97	0.11	-	10,10,10,10	0
55	MG	BA	3020	1/1	0.93	0.11	-	7,7,7,7	0
55	MG	DA	3126	1/1	0.89	0.14	-	57,57,57,57	0
55	MG	BA	3075	1/1	0.86	0.15	-	15,15,15,15	0
55	MG	BA	3157	1/1	0.96	0.26	-	26,26,26,26	0
55	MG	BA	3092	1/1	0.93	0.09	-	20,20,20,20	0
55	MG	DA	3140	1/1	0.96	0.44	-	37,37,37,37	0
55	MG	AA	1651	1/1	0.96	0.27	-	32,32,32,32	0
55	MG	DA	3004	1/1	0.46	0.33	-	64,64,64,64	0
55	MG	CA	1618	1/1	0.92	0.16	-	28,28,28,28	0
55	MG	CA	1629	1/1	0.85	0.08	-	63,63,63,63	0
55	MG	CA	1639	1/1	0.94	0.12	-	34,34,34,34	0
55	MG	BA	3195	1/1	0.86	0.12	-	20,20,20,20	0
55	MG	BA	3026	1/1	0.97	0.07	-	7,7,7,7	0
55	MG	DA	3098	1/1	0.87	0.56	-	63,63,63,63	0
55	MG	BA	3087	1/1	0.81	0.10	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1631	1/1	0.77	0.13	-	42,42,42,42	0
55	MG	CA	1608	1/1	0.89	0.30	-	50,50,50,50	0
55	MG	DA	3091	1/1	0.67	0.66	-	71,71,71,71	0
55	MG	BA	3001	1/1	0.95	0.08	-	10,10,10,10	0
55	MG	DA	3163	1/1	0.56	0.31	-	51,51,51,51	0
55	MG	DA	3039	1/1	0.93	0.17	-	53,53,53,53	0
55	MG	BA	3043	1/1	0.99	0.08	-	15,15,15,15	0
55	MG	DA	3142	1/1	0.87	0.34	-	38,38,38,38	0
55	MG	DA	3007	1/1	0.80	0.27	-	54,54,54,54	0
55	MG	AA	1624	1/1	0.66	0.17	-	39,39,39,39	0
55	MG	DA	3149	1/1	0.90	0.32	-	36,36,36,36	0
55	MG	AA	1614	1/1	0.64	0.44	-	53,53,53,53	0
55	MG	DA	3055	1/1	0.76	0.50	-	53,53,53,53	0
55	MG	BA	3137	1/1	0.99	0.45	-	4,4,4,4	0
55	MG	BA	3119	1/1	0.86	0.34	-	21,21,21,21	0
55	MG	AA	1635	1/1	0.81	0.18	-	37,37,37,37	0
55	MG	DA	3011	1/1	0.78	0.17	-	46,46,46,46	0
55	MG	BA	3074	1/1	0.95	0.07	-	20,20,20,20	0
55	MG	CM	201	1/1	0.79	0.32	-	46,46,46,46	0
55	MG	AA	1611	1/1	0.98	0.07	-	18,18,18,18	0
55	MG	BA	3106	1/1	0.96	0.33	-	0,0,0,0	0
55	MG	AA	1655	1/1	0.92	0.12	-	34,34,34,34	0
55	MG	BA	3140	1/1	0.89	0.20	-	14,14,14,14	0
55	MG	AA	1649	1/1	0.96	0.22	-	27,27,27,27	0
55	MG	BA	3046	1/1	0.94	0.22	-	8,8,8,8	0
55	MG	BA	3089	1/1	0.94	0.10	-	12,12,12,12	0
55	MG	AA	1657	1/1	0.64	0.62	-	40,40,40,40	0
55	MG	DA	3110	1/1	0.82	0.37	-	57,57,57,57	0
55	MG	CA	1604	1/1	0.51	0.17	-	70,70,70,70	0
55	MG	BA	3127	1/1	0.96	0.09	-	1,1,1,1	0
55	MG	CA	1647	1/1	0.94	0.19	-	24,24,24,24	0
55	MG	CA	1602	1/1	0.53	0.10	-	61,61,61,61	0
55	MG	BA	3051	1/1	0.86	0.12	-	6,6,6,6	0
55	MG	BA	3035	1/1	0.93	0.15	-	2,2,2,2	0
55	MG	DA	3102	1/1	0.53	0.21	-	45,45,45,45	0
55	MG	AA	1670	1/1	0.97	0.37	-	26,26,26,26	0
55	MG	BA	3124	1/1	0.96	0.25	-	21,21,21,21	0
55	MG	BA	3088	1/1	0.94	0.16	-	32,32,32,32	0
55	MG	DA	3150	1/1	0.93	0.22	-	42,42,42,42	0
55	MG	BA	3081	1/1	0.98	0.17	-	1,1,1,1	0
55	MG	BA	3138	1/1	0.91	0.40	-	4,4,4,4	0
55	MG	DA	3161	1/1	0.92	0.10	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1620	1/1	0.92	0.10	-	46,46,46,46	0
55	MG	BA	3016	1/1	0.92	0.07	-	17,17,17,17	0
55	MG	BA	3095	1/1	0.97	0.09	-	8,8,8,8	0
55	MG	BA	3173	1/1	0.94	0.19	-	20,20,20,20	0
55	MG	DA	3052	1/1	0.91	0.08	-	35,35,35,35	0
55	MG	BA	3100	1/1	0.93	0.14	-	6,6,6,6	0
55	MG	DA	3045	1/1	0.75	0.21	-	53,53,53,53	0
55	MG	AA	1628	1/1	0.93	0.05	-	37,37,37,37	0
55	MG	DA	3147	1/1	0.94	0.19	-	49,49,49,49	0
55	MG	BA	3111	1/1	0.90	0.12	-	23,23,23,23	0
55	MG	BA	3029	1/1	0.71	0.11	-	15,15,15,15	0
55	MG	BA	3004	1/1	0.61	0.15	-	33,33,33,33	0
55	MG	BA	3044	1/1	0.57	0.15	-	20,20,20,20	0
55	MG	DA	3064	1/1	0.96	0.08	-	38,38,38,38	0
55	MG	DA	3003	1/1	0.92	0.09	-	52,52,52,52	0
55	MG	BA	3180	1/1	0.92	0.26	-	25,25,25,25	0
55	MG	BA	3156	1/1	0.98	0.24	-	12,12,12,12	0
55	MG	BA	3135	1/1	0.96	0.09	-	17,17,17,17	0
55	MG	BA	3090	1/1	0.80	0.08	-	17,17,17,17	0
55	MG	DA	3016	1/1	0.68	0.41	-	53,53,53,53	0
55	MG	DA	3042	1/1	0.91	0.11	-	49,49,49,49	0
55	MG	BA	3179	1/1	0.77	0.47	-	39,39,39,39	0
55	MG	DA	3121	1/1	0.70	0.16	-	41,41,41,41	0
55	MG	CA	1611	1/1	0.59	0.19	-	55,55,55,55	0
55	MG	BA	3139	1/1	0.91	0.40	-	1,1,1,1	0
55	MG	DA	3001	1/1	0.53	0.19	-	43,43,43,43	0
55	MG	DA	3075	1/1	0.96	0.11	-	48,48,48,48	0
55	MG	DQ	201	1/1	0.86	0.25	-	32,32,32,32	0
55	MG	DA	3164	1/1	0.96	0.13	-	47,47,47,47	0
55	MG	BA	3183	1/1	0.96	0.17	-	24,24,24,24	0
55	MG	DA	3030	1/1	0.95	0.15	-	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.