

## SUPPLEMENTARY MATERIAL

**Table S1.** All atom pairwise root-mean-square derivatives among the nine lowest energy structures

Pairwise RMSD	2	3	4	5	6	7	8	9
Structure 1	0.28	0.28	0.32	0.39	0.39	0.24	0.36	0.36
Structure 2		0.29	0.26	0.31	0.33	0.40	0.49	0.31
Structure 3			0.15	0.41	0.41	0.40	0.37	0.35
Structure 4				0.39	0.38	0.42	0.39	0.32
Structure 5					0.26	0.51	0.49	0.44
Structure 6						0.39	0.39	0.29
Structure 7							0.33	0.31
Structure 8								0.41

**Table S2.** Average values with standard deviation of all the backbone torsion angles and glycosidic dihedral angles for all the nine structures

	$\alpha$	$\beta$	$\epsilon$	$\zeta$	$\chi$	$\delta$	$\gamma$
<b>A5</b>	-	-	-171.5 ( $\pm 1.5$ )	97.0 ( $\pm 3.0$ )	-120.5 ( $\pm 2.5$ )	136.5 ( $\pm 4.5$ )	58.0 ( $\pm 2.0$ )
<b>G6</b>	-77.5 ( $\pm 1.5$ )	-180.0 ( $\pm 1.0$ )	-178.5 ( $\pm 0.5$ )	-108.0 ( $\pm 0.0$ )	-118.0 ( $\pm 0.0$ )	132.5 ( $\pm 0.5$ )	51.5 ( $\pm 0.5$ )
<b>G7</b>	-69.0 ( $\pm 1.0$ )	-177.5 ( $\pm 0.5$ )	-177.5 ( $\pm 0.5$ )	-105.0 ( $\pm 1.0$ )	-123.5 ( $\pm 0.5$ )	135.0 ( $\pm 1.0$ )	56.0 ( $\pm 0.0$ )
<b>A8</b>	-71.0 ( $\pm 1.0$ )	-173.5 ( $\pm 1.5$ )	-177.5 ( $\pm 0.5$ )	-104.0 ( $\pm 1.0$ )	-120.5 ( $\pm 1.5$ )	134.0 ( $\pm 1.0$ )	54.0 ( $\pm 1.0$ )
<b>T9</b>	-68.0 ( $\pm 1.0$ )	-178.0 ( $\pm 1.0$ )	-174.5 ( $\pm 1.5$ )	-97.5 ( $\pm 1.5$ )	-127.0 ( $\pm 2.0$ )	129.0 ( $\pm 1.0$ )	56.0 ( $\pm 1.0$ )
<b>C10</b>	-70.5 ( $\pm 1.5$ )	-176.0 ( $\pm 2.0$ )	-173.0 ( $\pm 1.0$ )	-104.5 ( $\pm 1.5$ )	-123.5 ( $\pm 2.5$ )	135.0 ( $\pm 1.0$ )	51.5 ( $\pm 1.5$ )
<b>C11</b>	-79.0 ( $\pm 3.0$ )	-173.0 ( $\pm 4.0$ )	180.5 ( $\pm 4.5$ )	80.5 ( $\pm 4.5$ )	-100.0 ( $\pm 15.0$ )	145.0 ( $\pm 2.0$ )	51.5 ( $\pm 2.5$ )
<b>T12</b>	-78.5 ( $\pm 1.5$ )	-176.0 ( $\pm 2.5$ )	175.5 ( $\pm 0.5$ )	-85.8 ( $\pm 0.5$ )	-163.0 ( $\pm 1.0$ )	124.5 ( $\pm 2.5$ )	50.0 ( $\pm 3.0$ )
<b>U13</b>	175.7 ( $\pm 1.5$ )	-176.5 ( $\pm 0.5$ )	-176.0 ( $\pm 1.0$ )	-170.0 ( $\pm 3.0$ )	15.5 ( $\pm 0.5$ )	91.0 ( $\pm 0.0$ )	-163.5 ( $\pm 0.5$ )
<b>T14</b>	72.0 ( $\pm 0.0$ )	-73.0 ( $\pm 5.0$ )	-173.0 ( $\pm 5.0$ )	-124.0 ( $\pm 14.0$ )	24.0 ( $\pm 3.0$ )	88.5 ( $\pm 1.5$ )	-162.5 ( $\pm 2.5$ )
<b>T15</b>	-78.5 ( $\pm 3.5$ )	-182.0 ( $\pm 5.0$ )	-178.5 ( $\pm 8.5$ )	-83.0 ( $\pm 3.0$ )	-122.0 ( $\pm 5.0$ )	132.5 ( $\pm 7.5$ )	50.0 ( $\pm 2.0$ )
<b>G16</b>	-64.5 ( $\pm 1.5$ ) <sup>a</sup> 150.0 ( $\pm 3.0$ ) <sup>b</sup>	-183.0 ( $\pm 13.0$ )	-177.0 ( $\pm 2.0$ )	-104.5 ( $\pm 2.5$ )	-109.0 ( $\pm 16.0$ )	134.0 ( $\pm 12.0$ )	65.5 ( $\pm 1.5$ ) <sup>a</sup> -174.0 ( $\pm 1.0$ ) <sup>b</sup>
<b>G17</b>	-68.0 ( $\pm 2.0$ )	-180.0 ( $\pm 3.5$ )	-175.5 ( $\pm 1.5$ )	-108.5 ( $\pm 3.5$ )	-121.0 ( $\pm 2.0$ )	134.5 ( $\pm 1.5$ )	54.0 ( $\pm 2.0$ )
<b>A18</b>	-73.5 ( $\pm 1.5$ )	-173.5 ( $\pm 1.5$ )	-175.5 ( $\pm 0.5$ )	-109.05 ( $\pm 1.5$ )	-120.5 ( $\pm 1.5$ )	137.5 ( $\pm 1.5$ )	51.5 ( $\pm 0.5$ )
<b>T19</b>	-70.0 ( $\pm 1.0$ )	-177.5 ( $\pm 1.5$ )	-174.0 ( $\pm 1.0$ )	-115.5 ( $\pm 1.5$ )	-121.0 ( $\pm 1.0$ )	135.5 ( $\pm 2.5$ )	55.0 ( $\pm 1.0$ )
<b>C20</b>	-69.5 ( $\pm 0.5$ )	-178.5 ( $\pm 0.5$ )	-175.5 ( $\pm 0.5$ )	-115.5 ( $\pm 1.5$ )	-127.5 ( $\pm 0.5$ )	140.5 ( $\pm 0.5$ )	57 ( $\pm 1.0$ )
<b>C21</b>	-68.5 ( $\pm 0.5$ )	-175.5 ( $\pm 0.5$ )	-178.0 ( $\pm 0.0$ )	-103.0 ( $\pm 0.0$ )	-127.0 ( $\pm 0.0$ )	139.5 ( $\pm 1.0$ )	56.0 ( $\pm 0.0$ )
<b>T22</b>	-67.0 ( $\pm 0.0$ )	-175.0 ( $\pm 0.0$ )			-122.5 ( $\pm 0.5$ )	138.0 ( $\pm 0.0$ )	54.0 ( $\pm 0.0$ )

The value in parenthesis is the deviation from average.

<sup>a</sup>Average of five structures.

<sup>b</sup>Average of four structures.