Figure S1. A snap shot of cellulose chains in cellulose I$_\beta$ at 300 K. All the hydroxymethyl groups are in $tg$ conformation.
Figure S2: Distribution of the glycosidic angles ($\tau$, $\phi$, $\psi$) and exocyclic hydroxymethyl group ($\omega$) in the heating phase as a function of temperature simulated with the standard torsional parameter $K_1 = 9.35$ kJ/mol (a, c) and with modified torsional parameter $K_1 = 4.5$ kJ/mol (b, d).
Figure S3: Distribution of the glycosidic angles ($\tau$, $\phi$, $\psi$) and exocyclic hydroxymethyl group ($\omega$) in the cooling phase as a function of temperature simulated with the standard torsional parameter $K_1 = 9.35$ kJ/mol (a, c) and with modified torsional parameter $K_1 = 4.5$ kJ/mol (b, d).
Figure S4: Distribution of the puckering parameters (Q, Θ, Φ) of the pyranose rings in the heating phase as a function of temperature simulated with the standard torsional parameter $K_1 = 9.35 \text{ kJ/mol}$ (a) and with modified torsional parameter $K_1 = 4.5 \text{ kJ/mol}$ (b). Since the puckering parameters are polar coordinates, Φ has little impact on the overall shape of the sugar as far as the value of Θ is close to zero.
Figure S5: Distribution of the puckering parameters (Q, Θ, Φ) of the pyranose rings in the cooling phase as a function of temperature with the standard torsional parameter $K_1 = 9.35$ kJ/mol (a) and with modified torsional parameter $K_1 = 4.5$ kJ/mol (b).
Figure S6: The unit cell parameters ($a$, $b$, $c$, $\gamma$) as a function of temperature in the heating (red) and cooling (green) phases simulated with the standard torsional parameter $K_1 = 9.35$ kJ/mol (A) and with modified torsional parameter $K_1 = 4.5$ kJ/mol (B).