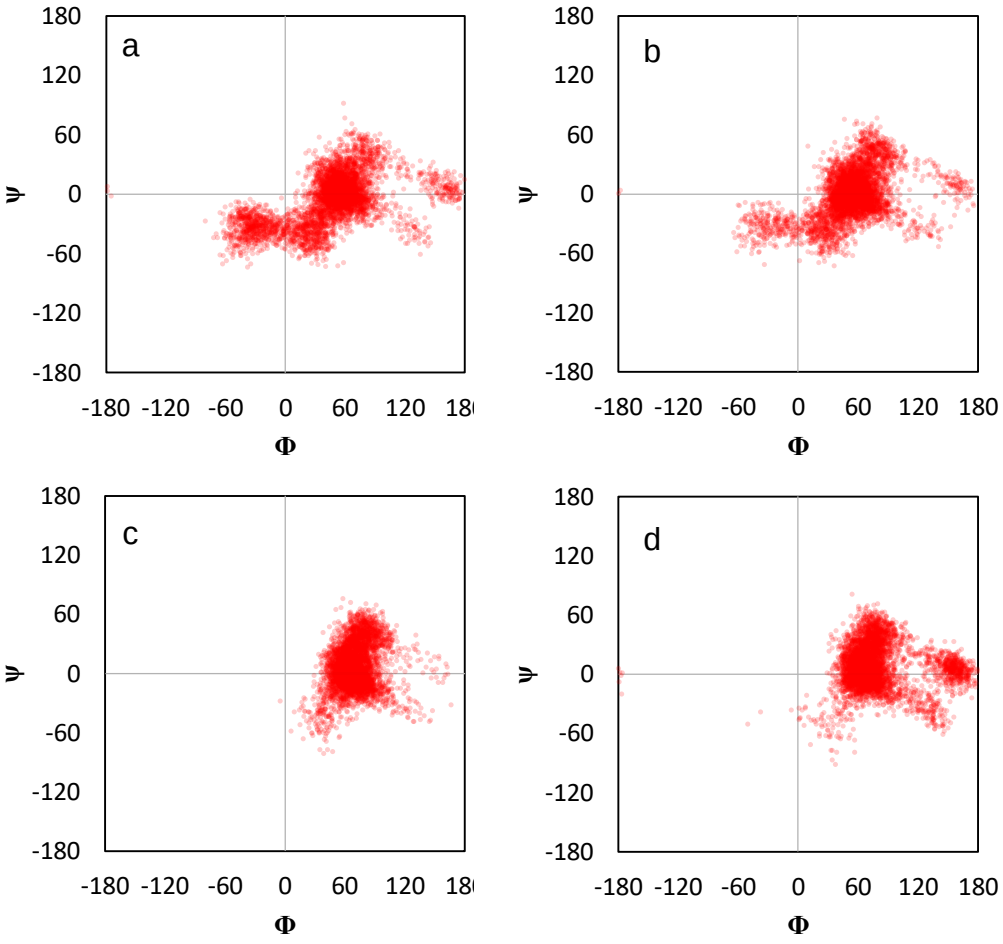

Figure S1. Torsional angle distribution patterns of Glc-Glc (a) in a cellulose chain, Glc-GlcN (b) in a GG chain, GlcN-GlcN (c) in a chitosan chain, and GlcN-Glc (d) in a GG chain during MD simulation (50-100 ns). Note that 1 dot per 10 ps.

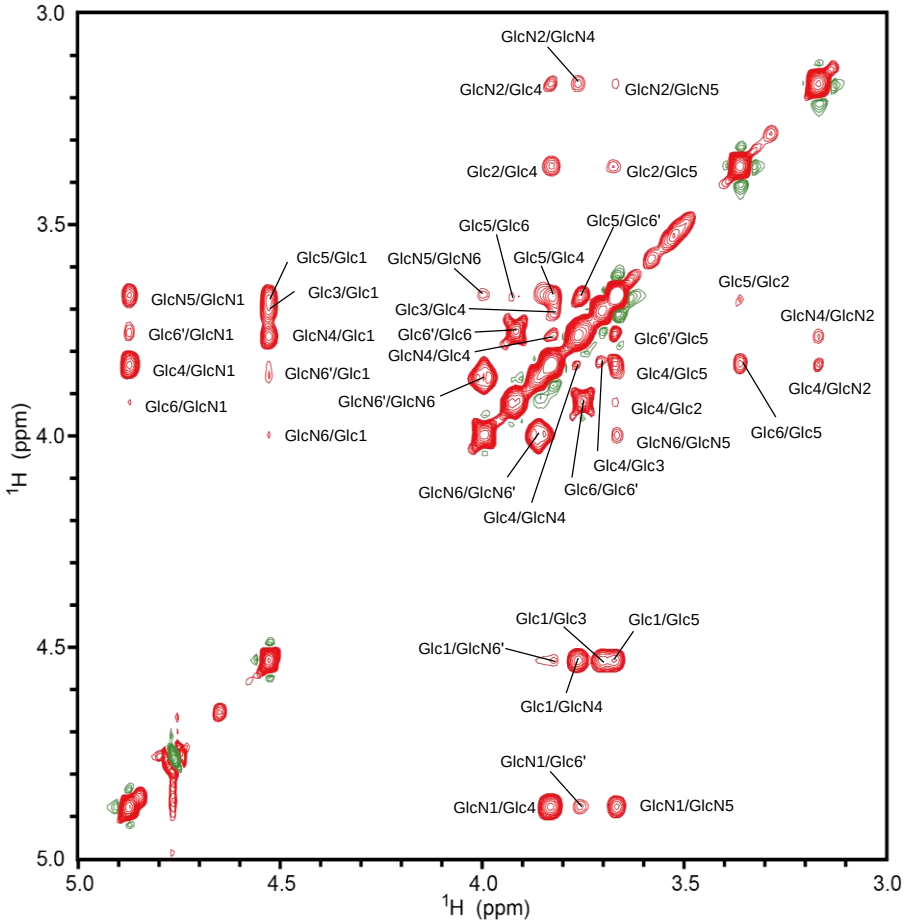

Figure S2. NOESY spectrum (80 ms) of GG. The crosspeaks (NOE signals) identified are designated as GlcN1/Glc4 (correlation between H1 of GalN and H4 of GlcN), etc. Positive and negative signals are indicated in red and green lines, respectively.

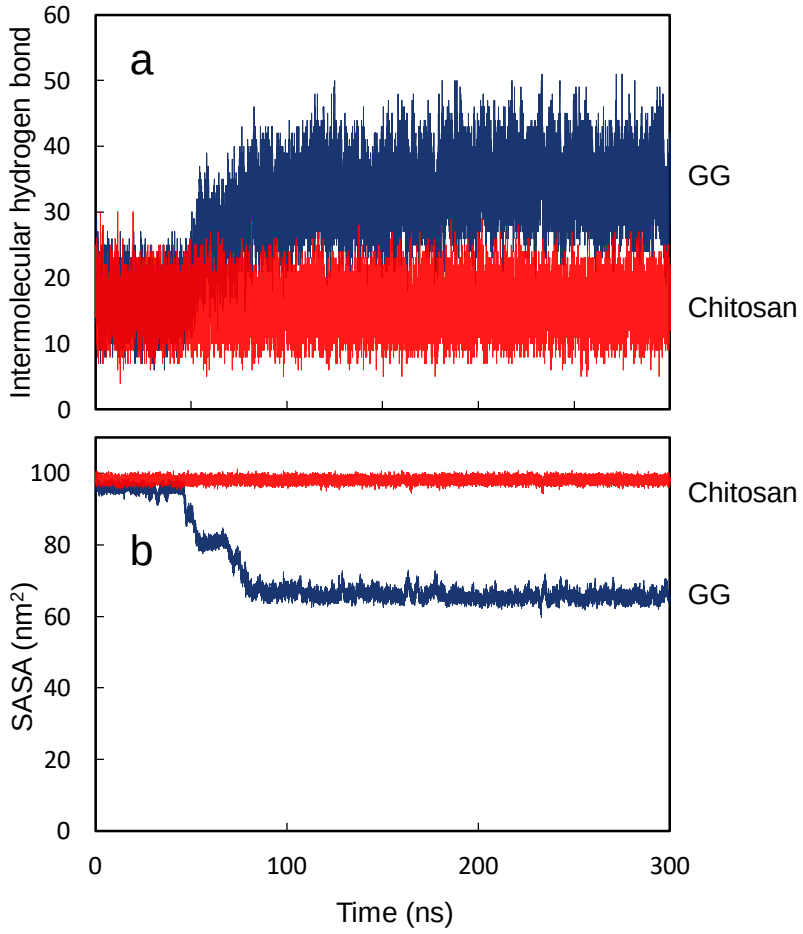

Figure S3. Time courses of interchain hydrogen bond number (a) and the total solvent-accessible surface area (b) during MD simulation of GG or chitosan chain (12 mer) in water. The data for GG correspond to the simulation whose structure is shown in Fig. 2. Abbreviation: SASA, total solvent-accessible surface area.

Supplementary material

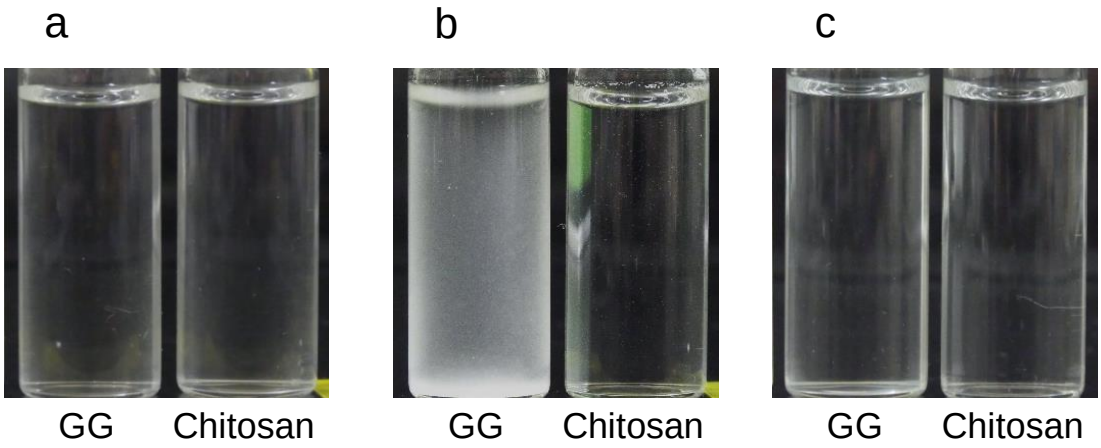

Fig. S4. Reversible insolubilization of GG in response to temperature. GG or chitosan (5 mg) was dissolved in 5 mL of 10 mM HCl containing 1 M NaCl. The solutions were kept at 25 °C for 24 h (a) and then at 4 °C for 24 h (b). After cooling, the solutions were heated at 50 °C for 2 min (c). Chitosan used for the experiment has deacetylation degree of 90% and molecular weight of $\geq 1 \times 10^5$ Da.

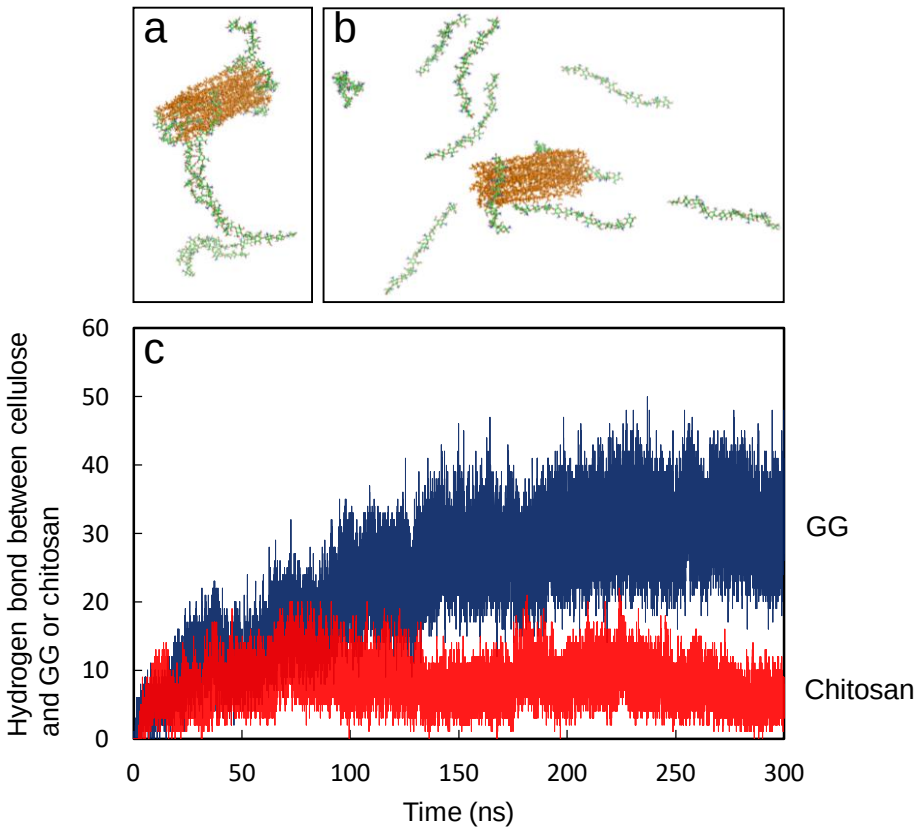

Figure S5. Adsorption of GG onto cellulose during MD simulation. The snapshots of the GG-cellulose (a) and chitosan-cellulose (b) systems at 300 ms show that cellulose adsorbs GG much more than chitosan. This observation was supported by the time courses of the number of hydrogen bond between cellulose and GG or chitosan during the simulations (c).

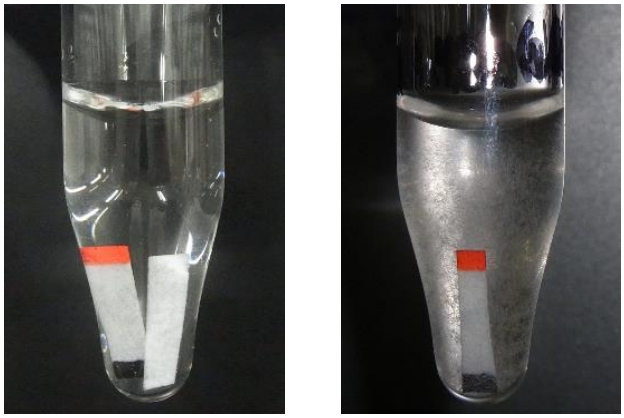

Figure S6. Cellulase tolerance of GG-treated cellulose. GG-treated (indicated by red and black edges) and non-treated paper strips were soaked in cellulase solution followed by incubation at 45 ^{o}C for 18 h.