

Supporting Information

Molecular Dynamics Investigations of Cello-oligosaccharide Recognition by Cel9G-CBM3c from *Clostridium cellulovorans*

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Supporting Information

1. **Figure S1.** Initial enzyme-substrate for G18 and BG6 models.
2. **Figure S2.** The root mean square deviation (RMSD) of protein backbone atoms compared to the X-ray structure.
3. **Figure S3.** Dihedral angles along the dynamic time between planes of H125/Y416 and G+2 sugar unit for G18 model in wild type and D58A.

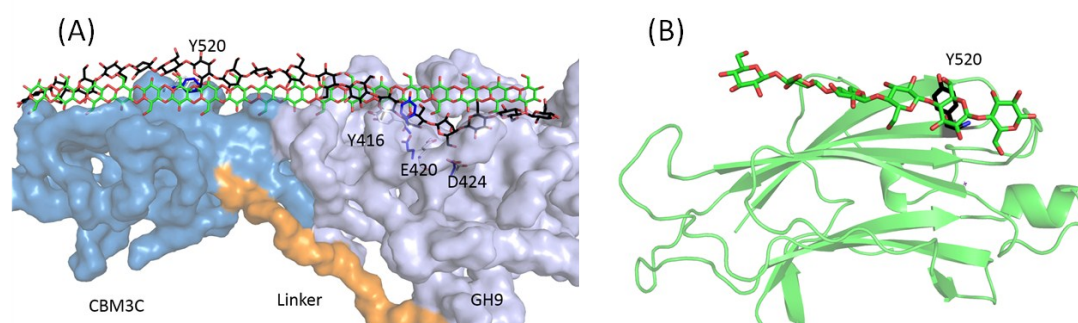


Figure S1. (A) Initial enzyme-substrate complex model (carbon in green color). For comparison, we include one snapshot at 100 ns extracted from MD trajectory (carbon in black color). (B) The initial CBM3c complexed with cellobiose molecule. Carbon atoms of Y520 is labeled in black color.

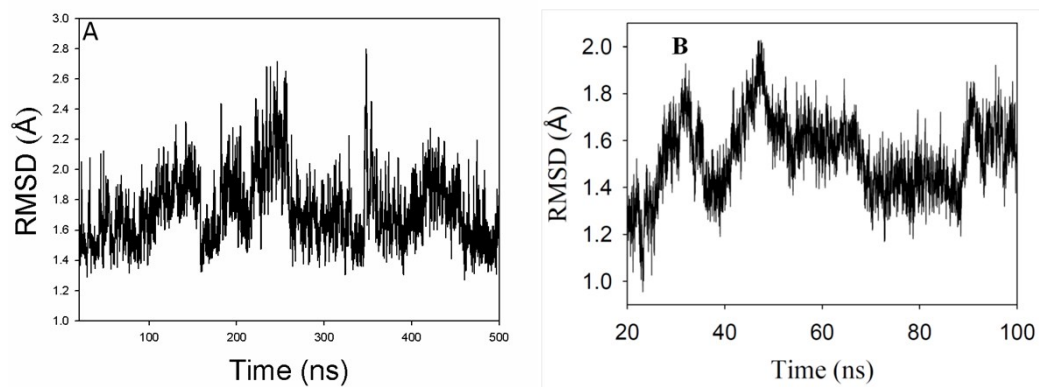


Figure S2. Root mean square deviations (RMSDs) of protein backbone atoms for models of (A) G18 and (B) BG6 as a function of simulation time.

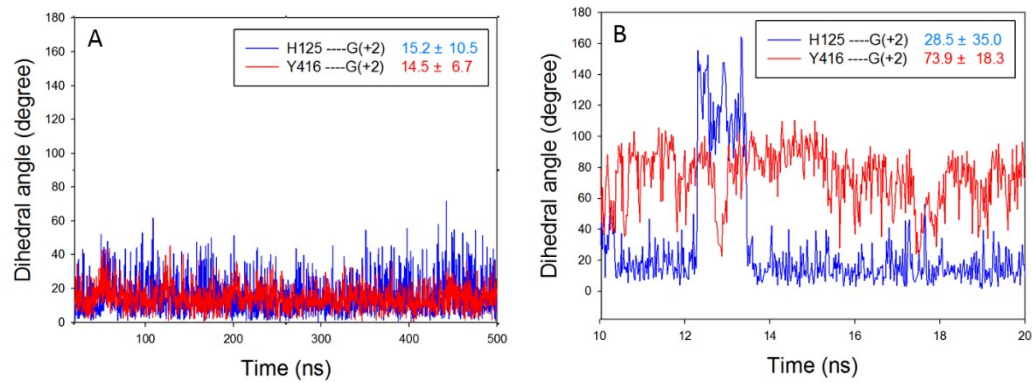


Figure S3. Dihedral angles along the dynamic time between planes of H125/Y416 and G+2 sugar unit for G18 model in wild type and D58A.