

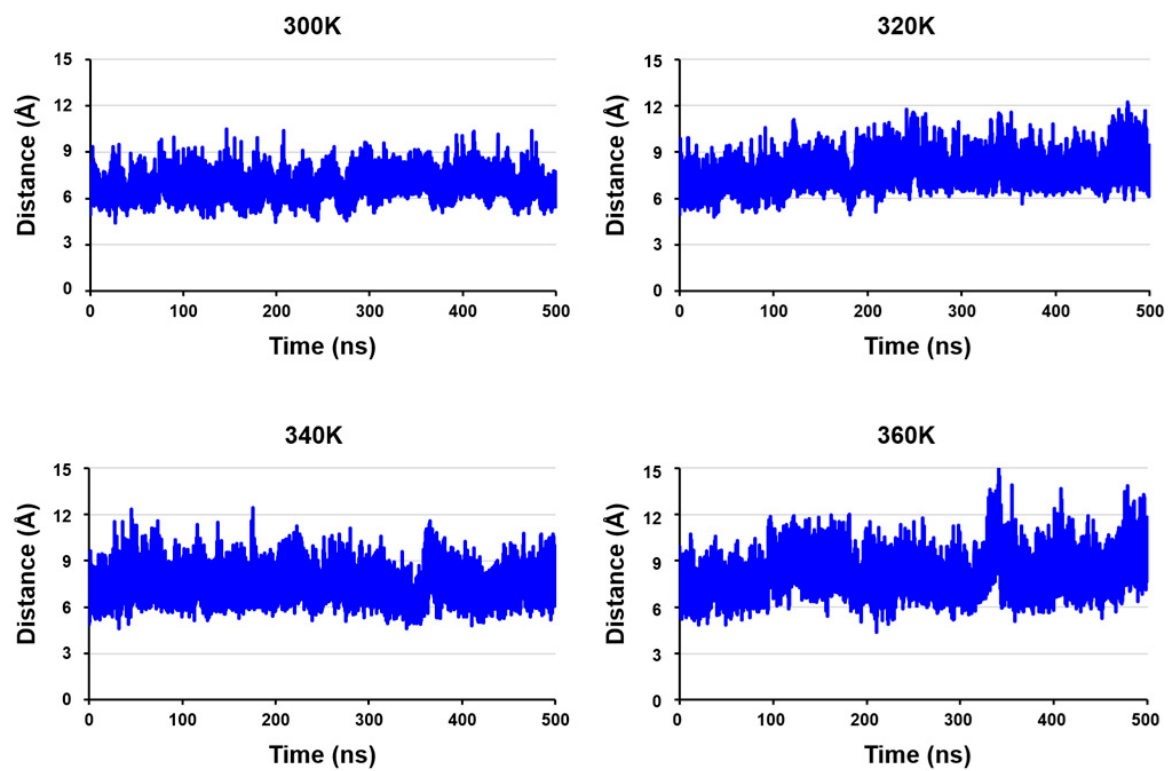
Supplementary Data

Temperature-dependent thumb domain dynamics of xylanase TsaGH11 revealed by molecular dynamics simulations

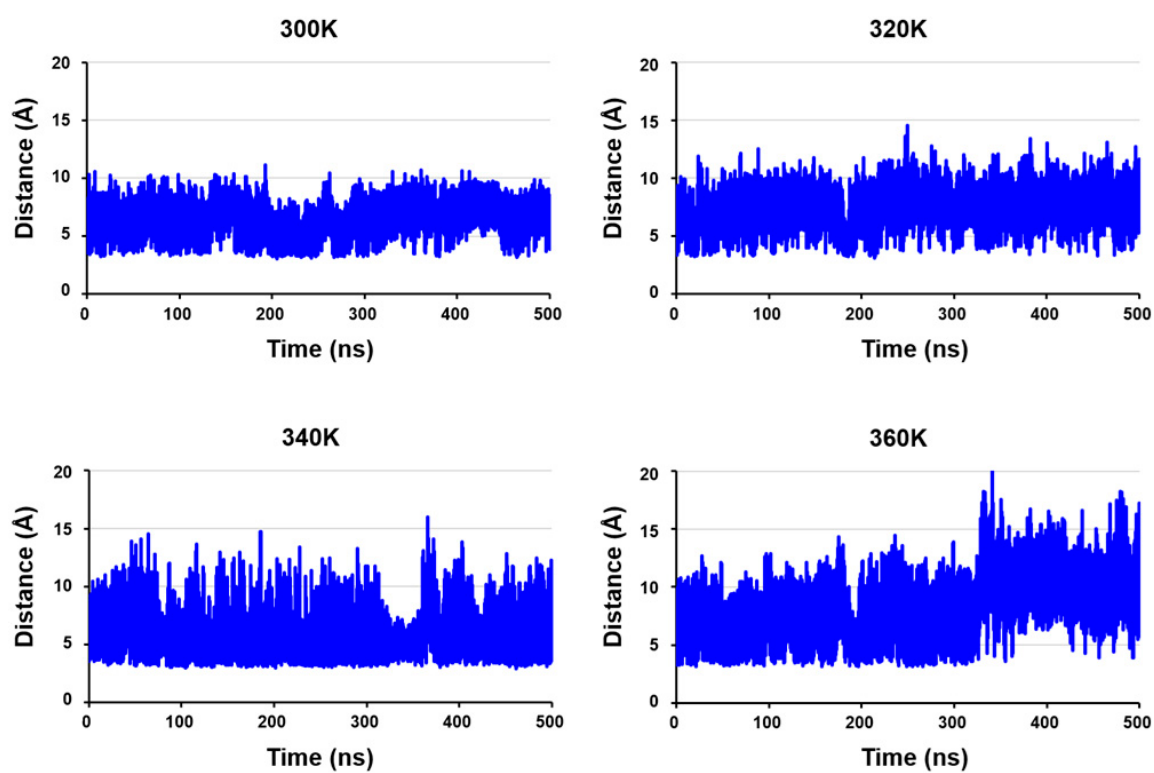
Ki Hyun Nam*

College of General Education, Kookmin University, Seoul 02707, Republic of Korea

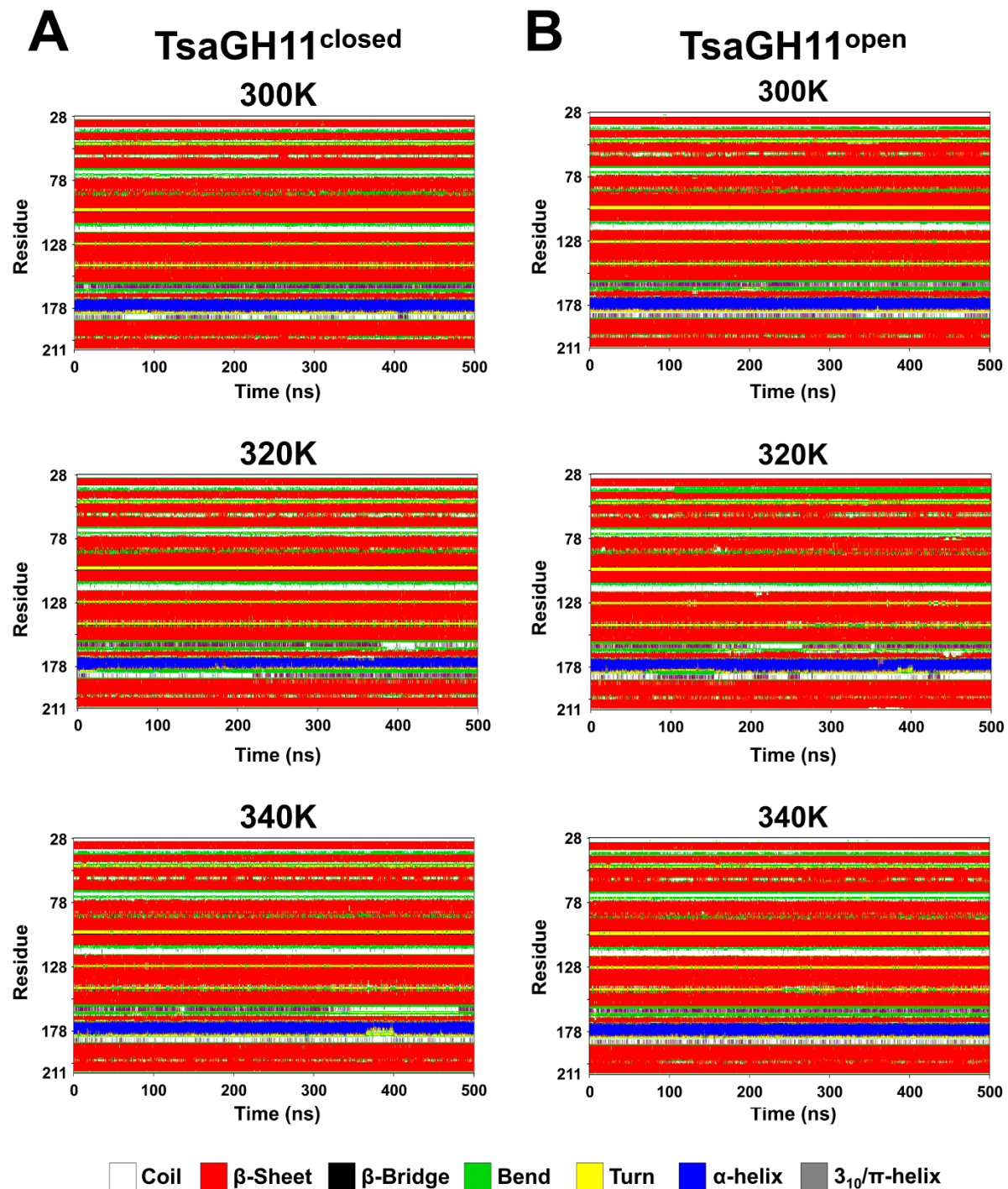
*Corresponding: structure@kookmin.ac.kr



Supplementary Figure S1. Time-series analysis of the Glu105–Glu198 distance during MD simulations of TsaGH11 at 300, 320, 340, and 360 K.



Supplementary Figure S2. Time-series analysis of the Trp36–Pro143 distance during MD simulations of TsaGH11 at 300, 320, 340, and 360 K.



Supplementary Figure S3. Time evolution of the secondary structures of (A) *TsaGH11*^{close} and (B) *TsaGH11*^{open} at 300, 320, and 360 K over the 500 ns molecular dynamics production trajectories.