Supplementary Data

Recognition of a Single β-D-Xylopyranose Molecule by Xylanase GH11 from *Thermoanaerobacterium saccharolyticum*

Ki Hyun Nam

College of General Education, Kookmin University, Seoul 02707, Republic of Korea; structure@kookmin.ac.kr

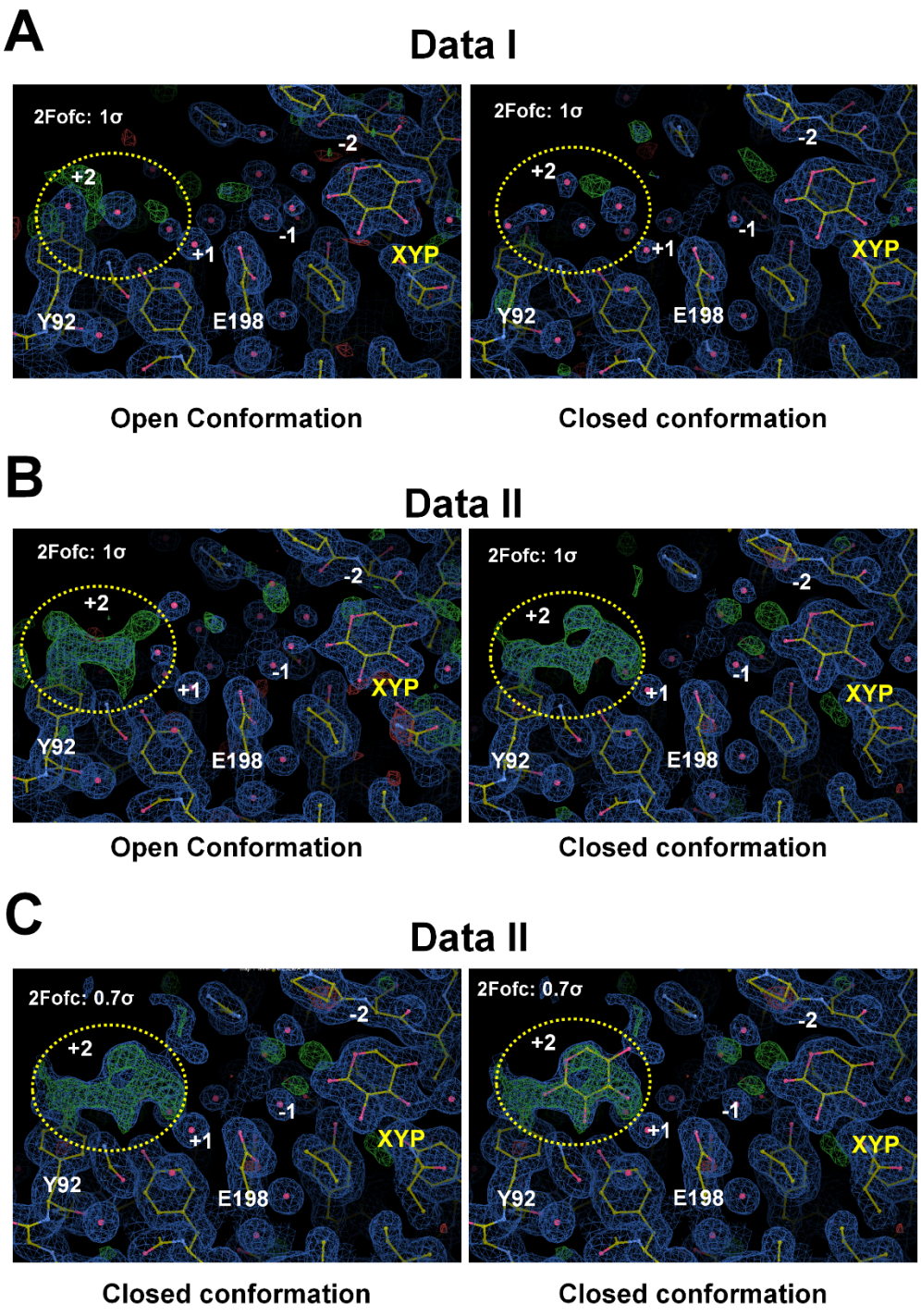

Figure S1. 2Fo-Fc electron-density maps (blue mesh) and Fo-Fc electron-density maps (+3 σ: green mesh; −3 σ: red mesh) of the TsaGH11-XYP molecule from (A) Data I and (B) Data II. (C) Modeling of the XYP molecule in a 2Fo-Fc electron-density map (0.7 σ, blue mesh) at the +2 subsite of the TsaGH11 closed conformation.

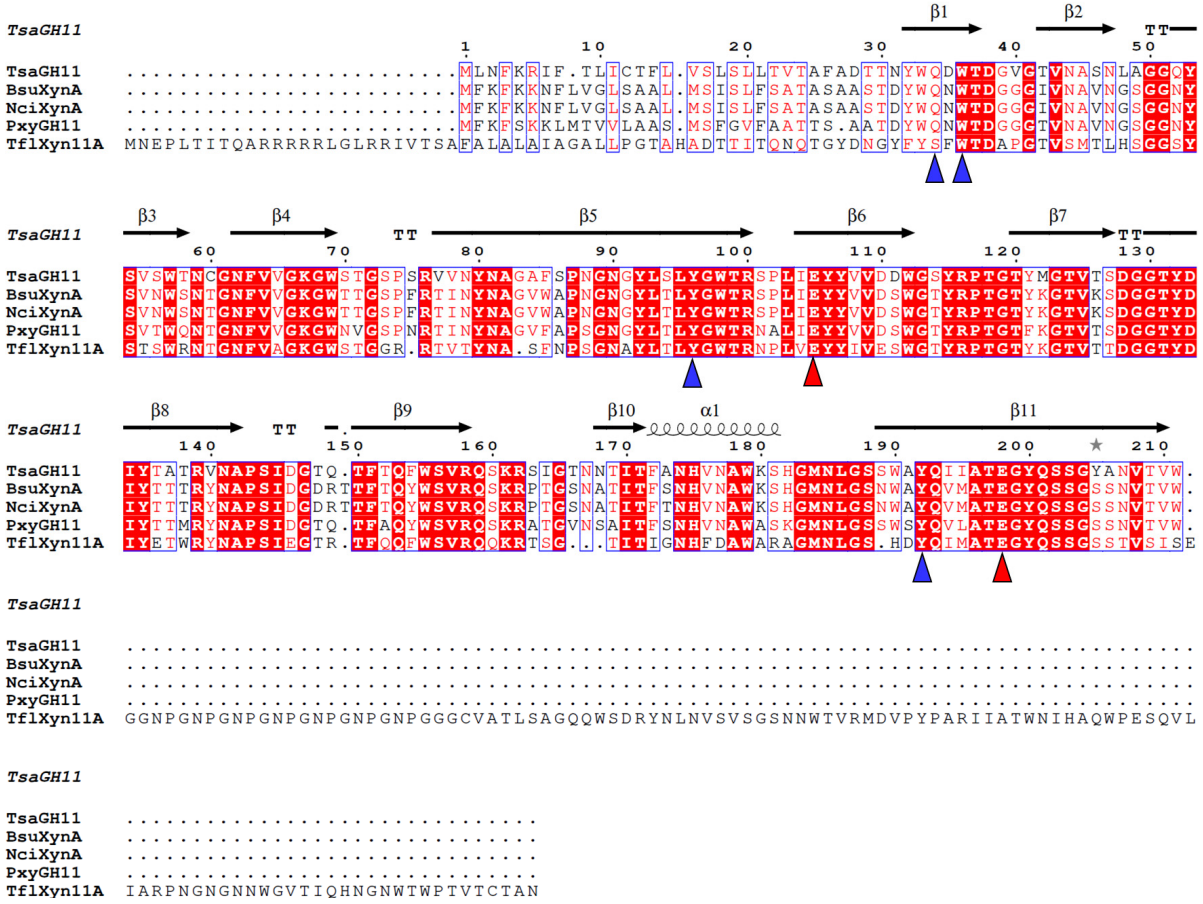

Figure S2. Structure-based multiple sequence alignment of .TsaGH11 (UniProt: I3VTR8) compared with BsXynA (P18429), NciXynA (P09850), PxyGH11 (A0A0M9BNX9), and TflXyn11A (Q8GMV7).

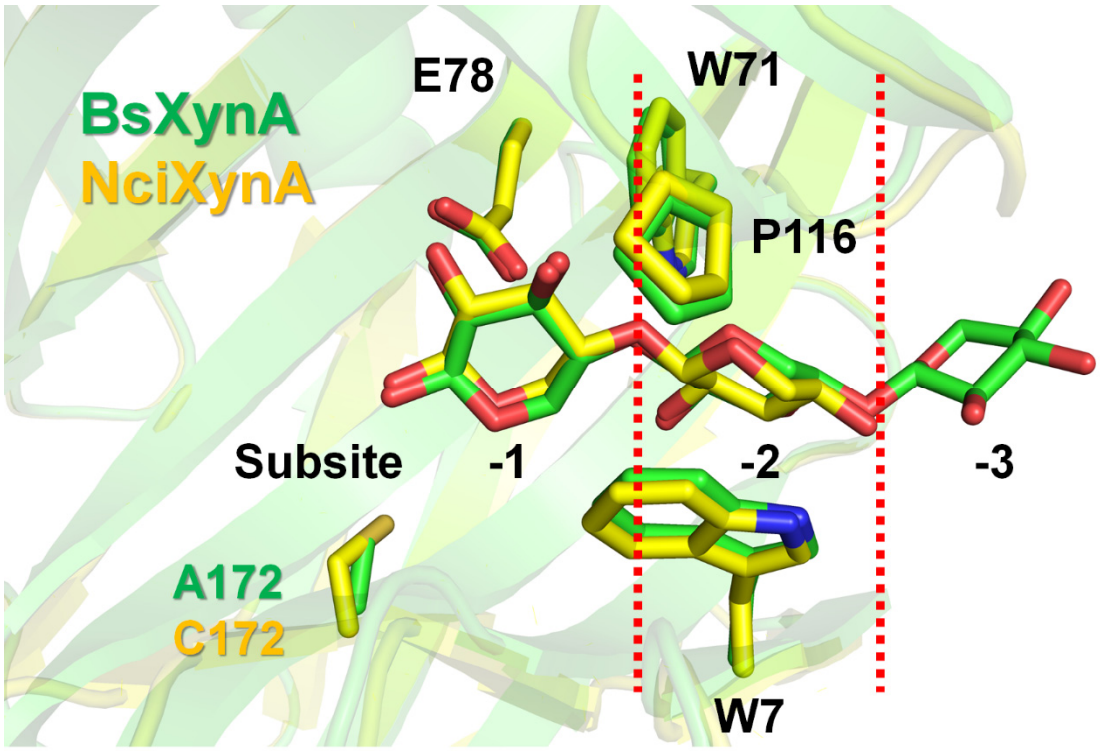

Figure S3. Superimposition of BsXynA-XYP3 (PDB code: 2QZ3, green) and NciXyn-XYP2 (1BCX, yellow). The position of the β-D-xylopyranose (XYP) molecule at the −2 subsite in BsXynA-XYP3 and NciXyn-XYP2 is almost similar.

Table S1. Interaction between TsaGH11 and the XYP molecule.

XYP	Residue (atom)	Data I		Data II	
		Open (Å)	Open (Å)	Open (Å)	Closed (Å)
O1	Tyr96 (OH)	3.70	3.21	3.46	3.31
	Glu105 (OH)	4.20	3.66	3.99	3.70
O_2	Tyr96 (OH)	3.33	3.05	3.17	3.02
	Qln34 (NE2)	3.90	3.53	3.59	3.68
	Tyr192 (OH)	3.00	2.84	2.87	2.92
O_3	Qln34 (NE2)	3.25	2.74	3.73	2.82
	Tyr192 (OH)	2.57	2.50	2.68	2.57
O4	Trp34 (NE1)	4.03	4.36	4.02	4.09
	Ser144 (O)	4.10	3.85	4.04	3.86
O5	Pro143 (O)	4.40	3.63	4.37	3.80
C5	Pro143 (CB)	5.01	4.07	4.92	4.04