

Crystal structure of Arabidopsis CELLULOSE SYNTHASE3 (CESA3) catalytic domain with its substrate UDP-Glucose provides insight into the molecular mechanism behind cellulose synthesis

Zhu Qiao, Edwin R. Lampugnani, Xin-Fu Yan, Ghazanfar Abbas Khan, Saw Wuan Geok, Patrick Hannah, Feng Qian, Jacob Calabria, Yansong Miao, Gerhard Grüber, Staffan Persson, Yong-Gui Gao

School of Biological Sciences, Nanyang Technological University, Singapore 637551, Singapore)

Email of communicating: zhu.qiao@ntu.edu.sg

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Cellulose is synthesized by cellulose synthases (CESAs) from the Glycosyltransferase GT-2 family. In plants, the CESAs form a six-lobed rosette-shaped CESA complex (CSC). Here we report crystal structures of the catalytic domain of *Arabidopsis thaliana* CESA3 (AtCESA3^{CatD}); both in apo and UDP-Glucose bound forms (1) (Figure. 1). The AtCESA3^{CatD} has an overall GT-A fold core domain sandwiched between a plant-conserved region (P-CR) and a class-specific region (C-SR). By superimposing the structure of AtCESA3^{CatD} onto the bacterial cellulose synthase BcsA, we found that the coordination of the UDP-Glc differs, indicating different substrate coordination during cellulose synthesis in plants and bacteria. Moreover, structural analyses revealed that the AtCESA3^{CatD} can form a homodimer mainly via interactions between specific beta strands. We confirmed the importance of specific amino acids on these strands for homo-dimerization through yeast and *in planta* assays using point-mutated full-length AtCESA3. Our work provides molecular insights into how the substrate UDP-Glc is coordinated in the CESAs and how the CESAs might dimerize to eventually assemble into CSCs in plants.

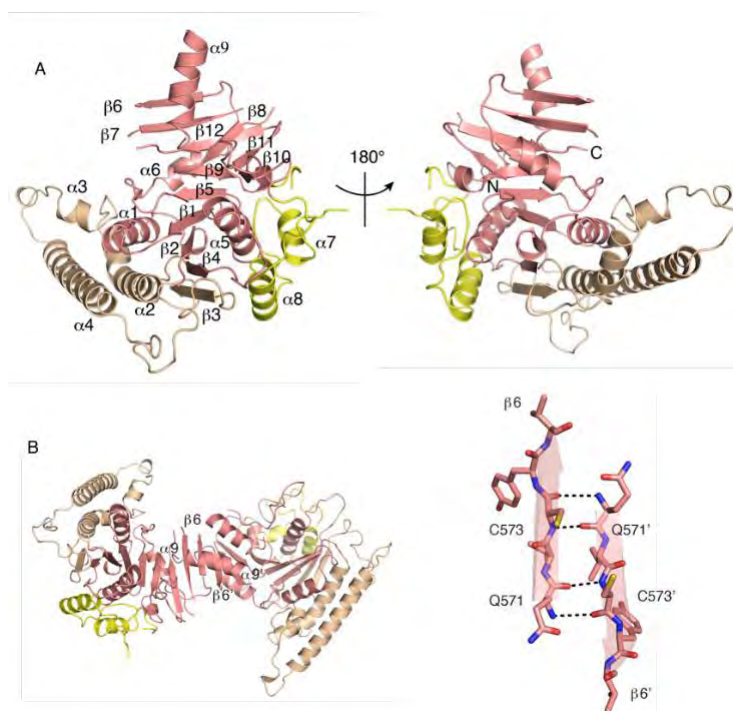


Figure 1. Crystal structural of Arabidopsis CESA3 catalytic domain (AtCESA3^{CatD}).

[6] The crystal structure of AtCESA3^{CatD} is shown as a cartoon. The P-CR domain, C-SR domain, and the core GT domain of AtCESA3^{CatD} are colored wheat, yellow and salmon, respectively. Secondary structure elements are labeled numerically. The unmodeled region is connected by dashed lines. B: Crystal structure of two paired AtCESA3^{CatD} molecules resolved in an asymmetric unit. Details of homo-dimerization mechanism of AtCESA3^{CatD} dimer formation. The $\beta 6$ of AtCESA3^{CatD} is shown as sticks and cartoon with amino acids labeled, with atoms N, O, and C colored blue, red, and salmon, respectively. Hydrogen bonds are indicated as dashed lines. Note that the prime (ϕ) indicates the second protomer in the homodimer.