

Crystal Structure of Chitin Binding Domain of Chitinase A1

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The crystal structure of the chitin-binding domain (ChBD) of chitinase A1 (ChiA1), from *B. circulans* WL-12 has been determined. ChiA1 is a glycosidase that hydrolyzes chitin, and ChBD, ranging from Ala⁶⁵⁵ to Gln⁶⁹⁹ located at the C-terminal, binds specifically to insoluble chitin.

The diffraction data of the ChBD_{ChiA1} crystal were collected at BL44XU at SPring-8, Japan, with the resolution of 0.95 Å. The phase was determined by the molecular replacement method using the structure previously determined by NMR as the model.

ChBD_{ChiA1} has a compact and globular structure with the topology of a twisted β -sandwich. The overall topology is similar to that of the cellulose-binding domain (CBD) of *Erwinia chrysanthemi* endoglucanase Z (CBD_{EGZ}). However, ChBD_{ChiA1} lacks the three aromatic residues (Trp¹⁸, Trp⁴³, and Tyr⁴⁴ in CBD_{EGZ}), aligned linearly and exposed to the solvent, which interact with cellulose. Mutation studies suggested that the loop region containing Trp⁶⁸⁷ interact with chitin. Moreover, ChBD_{ChiA1} is detached from chitin by decreasing the pH value in solution from 4 to 3, probably because the charge in the side-chain of Glu⁶⁸⁸ is involved in the chitin-binding. Therefore, the binding mechanism of ChBD_{ChiA1} is expected to be different from that proposed for CBDs.

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