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1: Structure 1994 Dec 15;2(12):1169-80

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Crystal structure of a bacterial chitinase at 2.3 A resolution.

Perrakis A, Tews I, Dauter Z, Oppenheim AB, Chet I, Wilson KS, Vorgias CE.

European Molecular Biology Laboratory, Hamburg, Germany.

BACKGROUND: Chitinases cleave the beta-1-4-glycosidic bond between the N-acetyl-D-glucosamine units of which chitin is comprised. Chitinases are present in plants, bacteria and fungi, but whereas structures are available for two prototypic plant enzymes, no structure is available for a bacterial or fungal chitinase. RESULTS: To redress this imbalance, the structure of native chitinase A from Serratia marcescens has been solved by multiple isomorphous replacement and refined at 2.3 A resolution, resulting in a crystallographic R-factor of 16.2%. The enzyme comprises three domains: an all beta-strand amino-terminal domain, a catalytic alpha/beta-barrel domain, and a small alpha+beta-fold domain. There are several residues with unusual geometries in the structure. Structure determination of chitinase A in complex with N,N',N",N"'-tetra-acetylo-chitotetraose, together with biochemical and sequence analysis data, enabled the positions of the active-site and catalytic residues to be proposed. CONCLUSIONS: The reaction mechanism seems to be similar to that of lysozyme and most other glycosylhydrolases, i.e. general acid-base catalysis. The role of the amino-terminal domain could not be identified, but it has similarities to the fibronectin III domain. This domain may possibly facilitate the interaction of chitinase A with chitin.

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