

## Crystal Structure of A Biopolyester-hydrolyzing Enzyme PHA Depolymerase.

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Polyhydroxyalkanoate (PHA) is a biodegradable polyester produced by a number of bacterial strains as an energy-storage material. Extracellular PHA depolymerases efficiently hydrolyze PHA, and are typically composed of three domains: catalytic, linker, and PHA-binding domains. Some fungal depolymerases are only composed of a single domain with an efficient affinity to PHA granules. We have determined the crystal structure of the type II PHA depolymerase composed of a single domain by a single isomorphous replacement/anomalous dispersion method. Refinement of coordinates of the model at 1.7 Å was converged to an *R*-factor of 19.6% (free-*R* 23.0%). The structure represents an  $\alpha/\beta$  hydrolase fold with a circular permuted connectivity. A crevice is formed on the surface of the protein, at the bottom of which catalytic triad residues Ser-19, Asp-101, and His-135 are located. Several hydrophobic residues which may interact with polymer chains are contributed to form the crevice. The catalytic site has no obvious lid structure and is open to bulk solvent. Several surface-exposed hydrophobic residues are arranged along the mouth of the crevice, suggesting a deformation mechanism of polyester chains during degradation of PHA.

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