Crystal Structure of Biphenyl Dioxygenase

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Biphenyl dioxygenase is the enzyme that catalyzes the stereospecific dioxygenation of the aromatic ring. This enzyme has attracted the attention of researchers due to its ability to oxidize polychlorinated biphenyls (PCBs), which is one of the serious environmental contaminants. Here we present the crystal structure of the terminal oxygenase component of the biphenyl dioxygenase (BphA1A2) derived from *Rhodococcus* strain sp. RHA1. This is the first crystal structure of the biphenyl dioxygenase. We also determined the crystal structure of the BphA1A2-biphenyl complex. Structural comparison between the substrate free and complex forms revealed that the substrate-binding pocket makes significant conformational changes upon substrate binding to accommodate the substrate into the pocket. The analysis with the two crystal structures suggested that the residues in the substrate-binding pocket can be classified into three groups, which respectively seem to be responsible for the catalytic reaction, the orientation/conformation of the substrate, and the conformational changes of the substrate-binding pocket.

Keywords: oxygenase, substrate binding, conformational change