

Dynamics of O₂ in DpgC, a cofactor-independent oxygenase

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The reaction of molecular oxygen with organic substrates is a spin-forbidden transformation. The majority of known oxygenases rely on bound metals or flavin cofactors to activate triplet molecular oxygen. DpgC, an enzyme involved in the biosynthesis of vancomycin, belongs to a small class of enzymes that are able to perform this reaction without the use of cofactors or metals. The structure of this enzyme, bound to a substrate analogue, displays density consistent with molecular oxygen in a hydrophobic pocket next to the substrate. In this work, we use Molecular Dynamics simulations to study the dynamics of dioxygen in the enzyme. The results of this study will later be applied to the study of the reaction mechanism, which has not yet been elucidated.