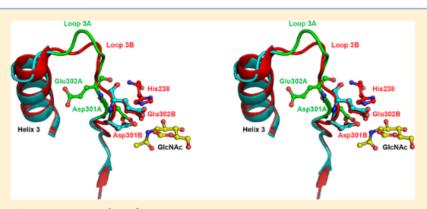


Structure and Activity of the *Streptomyces coelicolor* A3(2) β -N-Acetylhexosaminidase Provides Further Insight into GH20 Family Catalysis and Inhibition

Nhung Nguyen Thi,^{†,‡,§,⊥,||} Wendy A. Offen,[○] François Shareck,[†] Gideon J. Davies,[○] and Nicolas Doucet*,^{†,‡,§}

Supporting Information



ABSTRACT: β-N-acetylhexosaminidases (HEX) are glycosidases that catalyze the glycosidic linkage hydrolysis of gluco- and galacto-configured N-acetyl-β-D-hexosaminides. These enzymes are important in human physiology and are candidates for the biocatalytic production of carbohydrates and glycomimetics. In this study, the three-dimensional structure of the wild-type and catalytically impaired E302Q HEX variant from the soil bacterium Streptomyces coelicolor A3(2) (ScHEX) were solved in ligand-

[†]INRS-Institut Armand-Frappier, Université du Québec, 531 Boul. des Prairies, Laval, Québec H7V 1B7, Canada

[‡]PROTEO, the Québec Network for Research on Protein Function, Structure, and Engineering, 1045 Avenue de la Médecine, Université Laval, Québec, Québec GIV 0A6, Canada

[§]GRASP, the Groupe de Recherche Axé sur la Structure des Protéines, 3649 Promenade Sir William Osler, McGill University, Montréal, Québec H3G 0B1, Canada

¹Military Institute of Science and Technology, 17 Hoang Sam, Hanoi, Vietnam

Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Hanoi, Vietnam

OStructural Biology Laboratory, Department of Chemistry, University of York, York YO10 5DD, United Kingdom