World Academy of Science, Engineering and Technology
International Journal of Bioengineering and Life Sciences
Vol:11, No:03, 2017

Binding Studies and Structure Determination of the Recombinantly Produced Type-II 3-Dehydroquinate Dehydratase from Acinetobacter Baumannii

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Abstract : Dehydroquinase (3-dehydroquinate dehydratase, DHQD, EC 4.2.1.10) is involved in shikimate pathway and catalyzes the conversion of dehydroquinate to dehydroshikimate. Shikimate pathway is important drug target as this pathway is absent in mammals. DHQD from Acinetobacter baumannii (AbDHQD) was cloned, expressed and purified to homogeneity. The binding studies showed that compounds quinic acid and citrazinic acid bound to AbDHQD at micromolar concentrations. AbDHQD was crystallized using 30% PEG-3350, 50mM tris-HCl, and 1.0M MgSO4 at PH 8.0. Crystals of AbDHQD were stabilized by transferring them into reservoir solution to which 25% glycerol was added for data collection at 100K. The X-ray intensity data were collected to 2.0Å resolution. The crystals belong to monoclinic space group P21 with cell dimensions, a = 82.3, b = 95.3, c = 132.3Å and β = 95.7°. The structure was solved with molecular replacement method and refined to Rcryst/Rfree factors of 0.200/0.232. The structures of 12 crystallographically independent molecules in the asymmetry unit were identical with r.m.s shifts for the C□ atoms ranging from 0.3 Å to 0.8 Å. They formed a dodecamer with four trimers arranged in a tetrahedral manner. The classical lid adopted an open conformation although a sulfate ion was observed in the substrate binding site. As a result of which, the compounds quinic acid and citrazinic acid did not bind to AbDHQD.

Keywords : acinetobacter Bauman Nii, dehydroquinate dehydratase, dodecamer, open conformation
Conference Title : ICCMB 2017 : International Conference on Cellular and Molecular Biology
Conference Location : Prague, Czechia
Conference Dates : March 23-24, 2017