Abstract

Tinkering a distorted α/β barrel

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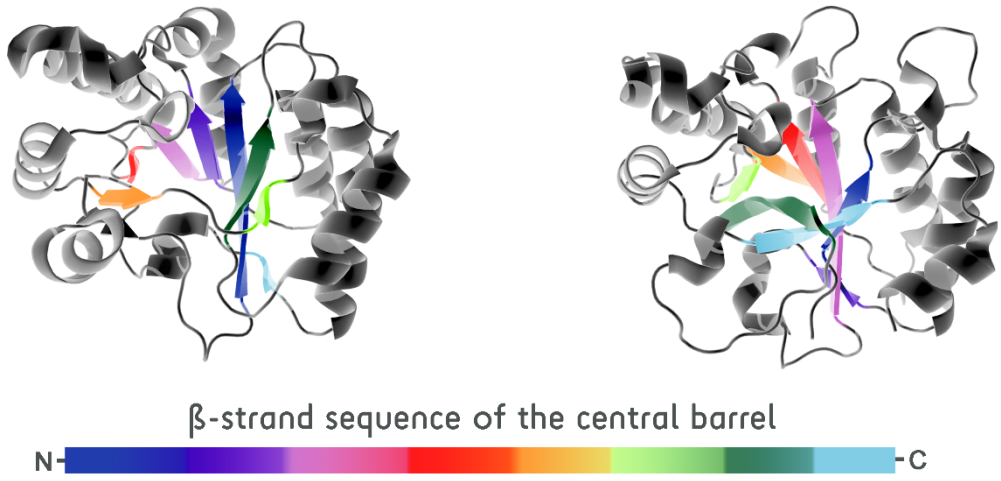
Peptidoglycan deacetylases from *B. cereus*, *B. anthracis* and other closely related bacteria have been described as required for evasion to lysozyme and innate immune responses. There are 11 coding sequences found in *B. anthracis* that all share the same core domain, along with several other carbohydrate esterases, hydrolases and other unidentified enzymes from a variety of organisms. This domain has been described as the NodB, a distorted (beta/alpha) barrel fold comprising eight parallel beta-strands, with the C-terminal ends of five of these strands forming the solvent exposed active site region. Reverse-engineering an inert deacetylase back to an active state has revealed the importance of hydrogen bonding capacity in the oxyanion hole of the active site and has shed light into yet unknown architectural characteristics of the NodB. A comparative analysis of structurally characterized NodB domains revealed two distinct topological domains and several new important motifs and properties. Further investigation of the NodB domain reveals a highly modular scaffold that has evolved to adopt a variety of enzymatic states and biological functions.



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