

Methyl-donated Hydrogen Bonding in Hyaluronate Lyase Affects Enzyme Function

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Hyaluronate lyase (HL) is an enzyme utilized by the bacterium *Streptococcus pneumoniae* (spn) to degrade components of the victim extracellular matrix to initiate infection. We present computational studies using a fragment model of spnHL (A249Me-N254Me) from several x-ray diffraction conformations of the enzyme. We show that an interaction between a methyl group of V252 with the carbonyl oxygen of A249 meets the criteria for a hydrogen bond (HB), and this of a type frequently not understood even to exist. This bond modulates forces within an HB network, altering the configuration of traditional N—H--O and O—H--O HBs. Motion studies demonstrate a hinge-like movement of α -helix-5 with a fulcrum localized at the fragment model. Force vector calculations show the fragment model exerts a torque acting to rotate the helix in the direction of its observed movement, showing the interaction is significant for the tertiary structure and function of the protein.

