

Abstract

Detailed conformational analysis of β -alanine in aqueous solution is presented. Previous calculations using the continuum solvation method failed to match the experimental finding of a purely statistical distribution; as a solution, explicit solvation methods using molecular dynamics simulations and *ab initio* quantum mechanics at varying levels are explored. Furthermore, van der Waal's and electrostatic contributions to the total explicit solvent energy are examined and compared with their continuum analogs. This work helps to provide a basis by which future researchers can decide on a solvation method to use based on available resources and the type of system to be modeled. This type of conformational analysis is relevant to some of the foremost scientific problems of our time: our ability to accurately predict material properties and protein folding characteristics relies on our understanding of simple systems such as this.