

E0037

Distribution of Water Around Amino Acid Side Chains: Statistical and Computational Analysis.

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The structure of water around proteins is of interest to explain protein folding and stability, as well as function. In crystallography, knowledge of water structure is important for refining protein structures determined by X-ray. The calculated model for a protein, based on electron density derived from x-ray diffraction data, usually refines with a significantly higher residual factor (R value) than that for small molecules. Knowledge of structural propensities for water in protein crystals can provide additional parameters in refinement, which ultimately improve the accuracy of the calculated model (reflected in a lower R value). A better understanding of the role(s) and function(s) of water molecules requires a general 'map' of localized hydrogen bonding interactions between the side chains and water. Here, we present the results from theoretical calculations and statistical analyses, which show strong agreement for the distances, locations, as well as orientations of water molecules around the 20 amino acid side chains. These distribution data indicate that water structures around amino acid side chains exhibit propensities that can be used to parameterize and improve X-ray crystallographic refinement.

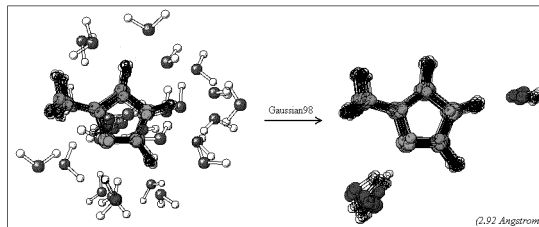


Figure B. Superimposed 25 histidine-water complexes using Gaussian98 and GaussView.