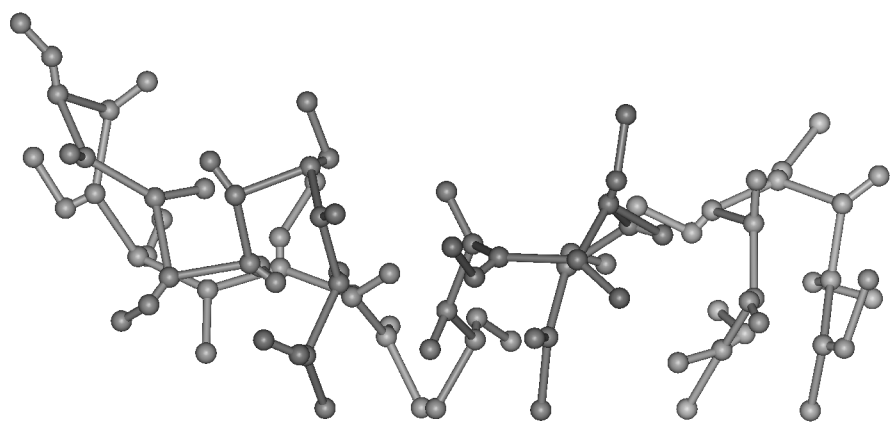


The Introduction of a New Hydrogen Bonding Energy Term into a Simplified Model of Three Hypervariable Loops

Allan Forster, Zhuan Qin, Heather L Gordon

Department of Chemistry, Brock University, St. Catharines, Ontario L2S 3A1 Canada

Antibodies contain six hypervariable loops that are responsible for antigen binding. Three hypervariable regions of the 8F5 antibody, which detects the pathogen human rhinovirus serotype 2 that causes the common cold, are being studied using Metropolis Monte Carlo simulations. The initial conformation of the antibody was taken from the protein data bank (1BBD). The overall objective is to generate all possible complementarity determining loop conformations, with and without a ligand, and to compare the two distributions to determine the mechanism with which the two bind. The specific goal of this project is to implement a new hydrogen bond correction potential into a smaller, simplified Wallqvist and Ullner description of a three loop system consisting of loops L1, L3, and H3. The new added potential allows for a greater number of β -sheet hydrogen bonds to be generated. This allows for more extended loops that better compare to the canonical structures that exist in nature. The figure below shows a sample conformation of the simplified three loop system.



L1 L3 H3