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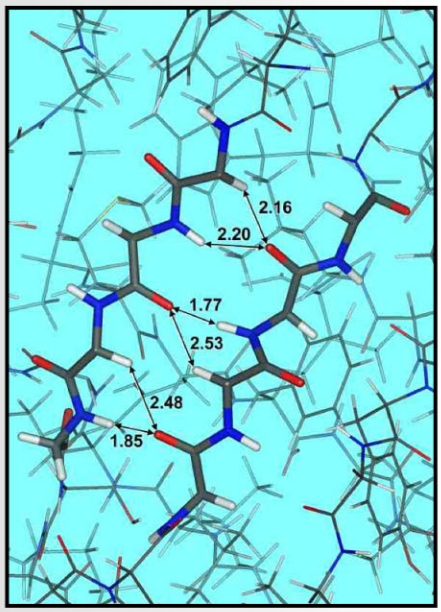
Environmental Molecular Sciences Laboratory



Annual Report 2000

Theory, Modeling, and Simulation

September 2001

Pacific Northwest
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Cover Photo: C^{α}–H···O=C hydrogen bonds in the β-sheet formed by the protein called *Achromobacter protease I*. Numbers indicate estimated distances (in angstroms) between the hydrogen atoms (white) and oxygen atoms (red). Carbon atoms are shown in gray and nitrogen atoms in blue. High-level *ab initio* calculations provide a lower limit of –2.1 kcal/mol for the C^{α}–H···O=C hydrogen bond. The magnitude of this interaction, roughly one-half the strength of the N–H···O=C hydrogen bond, suggests that C^{α}–H···O=C hydrogen bonding may represent a hitherto unrecognized contribution to protein conformation.

This collaborative research effort among scientists in the Theory, Modeling, and Simulation (TM&S) directorate and the Universidad Autónoma Metropolitana - Iztapalapa exemplifies the effective use of high performance computers in developing accurate force field parameters to provide a more quantitative understanding of complex biological systems. The TM&S directorate also operates the Molecular Science Computing Facility (MSCF), a national user resource, in support of environmental molecular research projects.

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D. A. Dixon, Associate Director
and the Staff of the Theory, Modeling,
and Simulation Program

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