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Collapse of an HIV-1 protease (1DIFA-dimer) in an effective solvent medium by a Monte Carlo simulation[1] RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — HIV-1 protease (1DIFA) consists of two polypeptide chains, each monomer with 99 residues where two aspartic acid residues (Asp^{25}) form the active catalytic site. The conformation and dynamics of the protein chain (with 198 residues) are investigated on a cubic lattice where empty sites represent effective solvent. Specificities of residues are captured via an interaction matrix (residue-residue, residue-solvent) of the Lennard-Jones potential. We examine global properties such as the variation of the root mean square displacement and radius of gyration with the time steps for a range of solvent interaction strength. Local quantities include energy and mobility profiles of residues to understand the active segments (useful in proteolysis). The hydrophobic residues possess higher energy and lower mobility while the electrostatic and polar residues are more mobile despite their lower interaction energy. We find that the radius of gyration of the protein collapses (globular structure) in a narrow range of solvent interaction strength.

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