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The $gp41_{659-671}$ HIV-1 antibody epitope: a structurally challenging small peptide YUAN ZHANG, CELESTE SAGUI, Department of Physics, North Carolina State University — We present the results of extensive Molecular Dynamics (MD) simulations of the tridecapeptide corresponding to residues 659-671 of the envelope glycoprotein gp41 of HIV-1, which spans the 2F5 monoclonal antibody epitope ELDKWA. The most recent AMBER force fields ff99SB and ff12SB in both implicit and explicit solvents have been used for a cumulative time longer than 7.2 μs. We have analyzed the conformational ensembles of the peptide both with and without applied tensile restraints, and found that: (1) The amount of helical populations is important in aqueous solution, but this structure forms part of a flexible conformational ensemble with a rugged free energy landscape with shallow minima, which agrees well with the bulk of the experimental observations; (2) our results are more consistent with the experimental results than those from previous simulations; (3) under uniaxial tension, the disordered peptide first becomes fully helical before melting into turns, loops and 3_{10}-helices.

Yuan Zhang
Department of Physics, North Carolina State University

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