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Conformational changes of Gag HIV-1 on a lipid bilayer measured by neutron reflectivity provides insights into viral particle assembly H. NANDA, NIST Center for Neutron Research, Gaithersburg, MD, S.A.K. DATTA, National Cancer Institute, Frederick, MD, F. HEINRICH, M. LOESCHE, Carnegie Mellon University, Pittsburgh, PA, and NIST Center for Neutron Research, Gaithersburg, MD, A. REIN, National Cancer Institute, Frederick, MD, S. KRUEGER, NIST Center for Neutron Research, Gaithersburg, MD — Formation of the HIV-1 is mediated by the Gag polyprotein at the cytoplasmic membrane surface of the infected host cell. Studies suggest large conformational changes in the Gag protein may occur during self-assembly on the membrane [Current Biology, 1997 (7) p.729, J. Mol. Biol. 2007 (365) p. 812]. The one-dimensional profile of Gag bound to a lipid bilayer interface was determined at angstrom resolution by neutron reflectometry. This was done using a novel method for modeling reflectivity data by a Monte Carlo simulation technique. The results show conditions under which the Gag protein can be made to extend or stay compact on the membrane surface. Further atomic detail was obtained using atomistic models to fit the one-dimensional Gag structural data. This involved combining X-ray resolution structures of the ordered protein domains with conformational sampling of the flexible linker region.

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