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**Conflicting thermal response of a monomer and a tandem dimer of a membrane protein segment (hHv1)** PANISAK BOONAMNAJ, Chulalongkorn University, SUNITA SUBEDI PAUDEL, University of Southern Mississippi, WARIN JETSADAWISUT, Chulalongkorn University, SUNAN KITJARUWANKUL, Kasetsart University Sriracha Campus, PORNTHEP SOMPORNPISUT, Chulalongkorn University, RAS PANDEY, University of Southern Mississippi — Using all-atom Molecular Dynamics and a coarse-grained Monte Carlo computer simulations, we study the thermal response of the structure of monomer and dimer of C-terminal domain of the protein hHv1 which is critical for dimer assembly and regulation of proton permeation through the membrane. A knowledge-based residue-residue (KBRR) interaction matrix is used as input for the Metropolis algorithm in coarse-grained (CG) model. We are able to examine a number of local and global physical quantities as a function of temperature (T) effectively due to efficiency of the CG model. We find that the radius of gyration (Rg) of the protein increases on increasing the temperature, as one would expect, over a well-defined range. All-atom simulation data, in contradiction, shows the opposite, i.e. Rg decreases with raising the temperature. The reverse-thermal response also appears in CGMC but only in low T range. Attempts are made to understand the dichotomy by performing large-scale simulations over the entire temperature regime.

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