Characterizing a Histidine Switch Controlling pH-Dependent Conformational Changes of the Influenza Virus Hemagglutinin

Mohamad R. Kalani,[†‡] Abdulvahab Moradi,[‡] Mahmoud Moradi,[†] and Emad Tajkhorshid[†]*

[†]Department of Biochemistry, College of Medicine, Beckman Institute for Advanced Science and Technology, and Center for Biophysics and Computational Biology, University of Illinois at Urbana-Champaign, Urbana, Illinois; and [‡]Faculty of Advanced Medical Technology, Golestan University of Medical Sciences, Gorgan, Iran

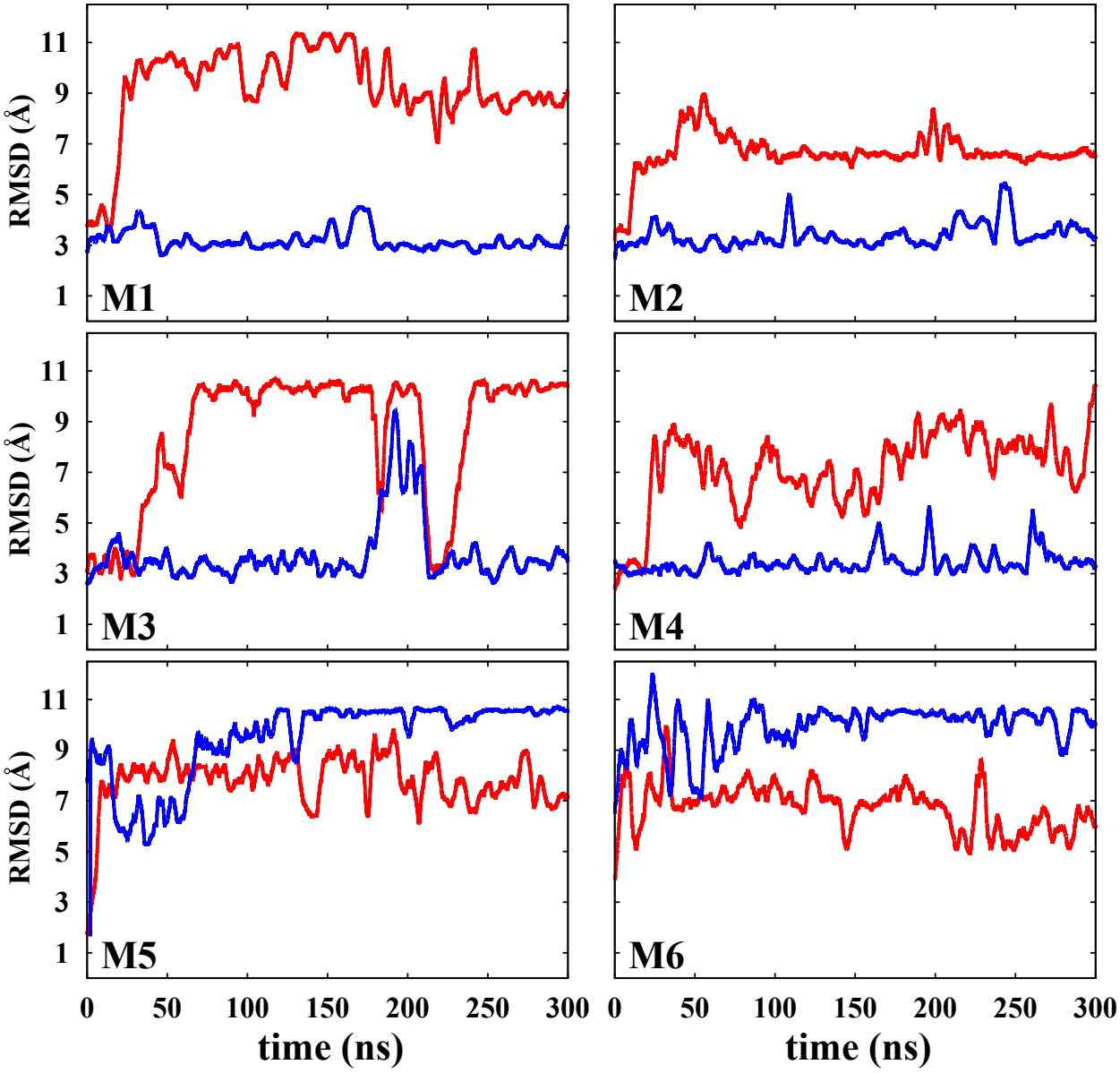

Fig. S1: RMSD time series during the implicit solvent simulations of systems with either protonated (red lines) or neutral (blue lines) hinge histidine over the first 300 ns of the trajectories of each model.

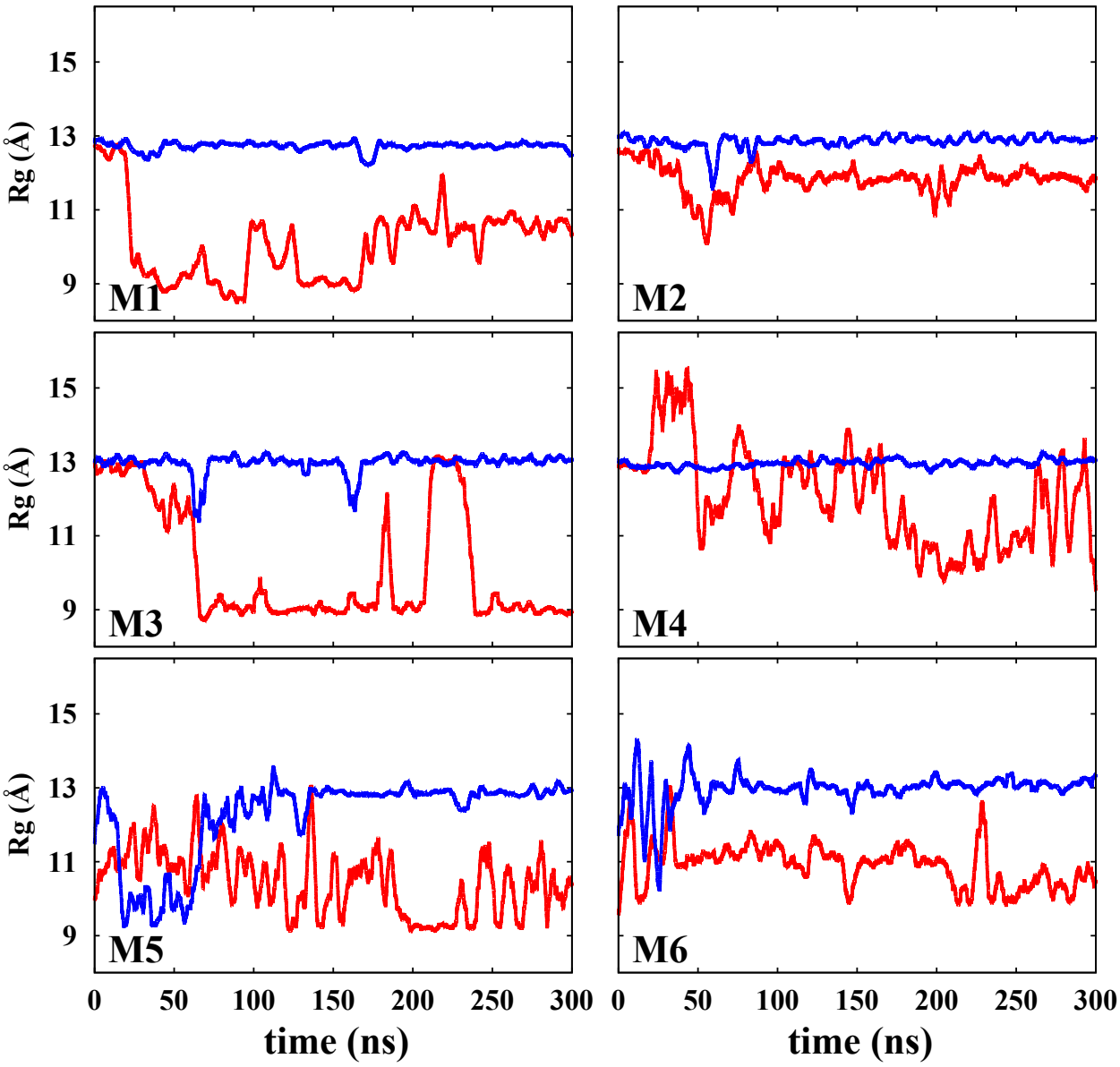

Fig. S2: Radius of gyration (Rg) time series during the implicit solvent simulations of systems with either protonated (red lines) or neutral (blue lines) hinge histidine over the first 300 ns of the trajectories of each model.