

Molecular Dynamics Analysis of the Rx-RxRE Complex of HTLV-1

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Adult T-cell leukemia, caused by a virus called human T-cell leukemia virus type-1 (HTLV-1), infects 10 to 20 million people throughout the world. Rex, a critical viral protein, prevents the host cell from breaking down viral RNA. Rex binds to a specific sequence in viral RNA called the Rex Response Element (RxRE). The purpose of this study is to better understand the roles that arginine-rich motifs and the presence of water play in Rex recognition of RxRE. Systems have been built under 200 mM KCl in the presence of explicit water molecules, and simulations have run for 30-60ns. The thermodynamics of the systems have been analyzed for the convergence of equilibration parameters, the presence of hydrogen bonds between arginines and the backbones has been compared across multiple models, and sites of high water density have been examined.