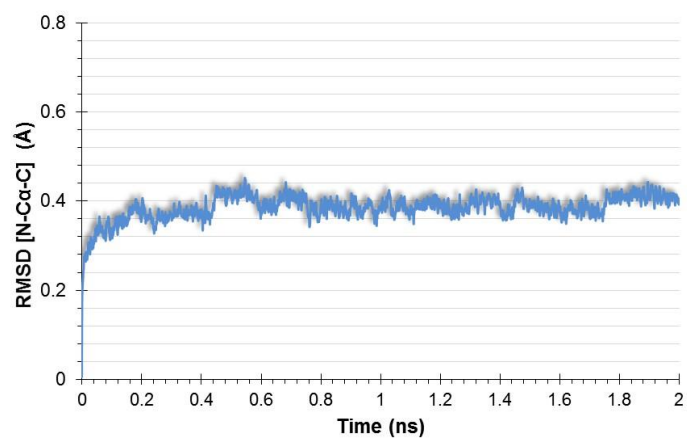


## **SupportingInformation**



**Figure S1.** Time-dependent evolution of the RMSD of the protein backbone atoms along the 2 ns QM/MM MD simulation of HG-3.