Figure 3: Free energy as a function of the distance between the biased Mg$^{2+}$ and the center of mass of RNA (CoM$_{RNA}$). The curves shown on the figure were obtained from the control simulations performed on a flexible $\text{GGGGCC}$ duplex contained in a large simulation box ($\approx$11000 explicit water molecules) with a buffer of KCl at 0.1 M concentration (red curve), then the same box and a buffer with KCl and MgCl$_2$ at 0.1 M and 0.05 M concentration respectively (black curve) and lastly on a smaller box ($\approx$2100 explicit water molecules) and a buffer of KCl at 0.1 M concentration (blue curve). $\Delta G$ is computed as $\Delta G(d) = -k_B T \log P(d) + k_B T \log d^2$, where $P(d)$ is the probability to find Mg$^{2+}$ at distance $d$ from CoM$_{RNA}$. The error is shown by the red, gray and blue shades of the respective curves and it was calculated using block analysis over 4 blocks. The free-energy curves are aligned on the minimum and the bulk region is defined by the flat free energy part (shown by the light-gray and light-blue boxes) corresponding to the Mg$^{2+}$ unbound states. Since Mg$^{2+}$-RNA distance is evaluated with minimal image convention, it is not possible for this distance to be larger than half the box size. The profile consistently increases at that distance.