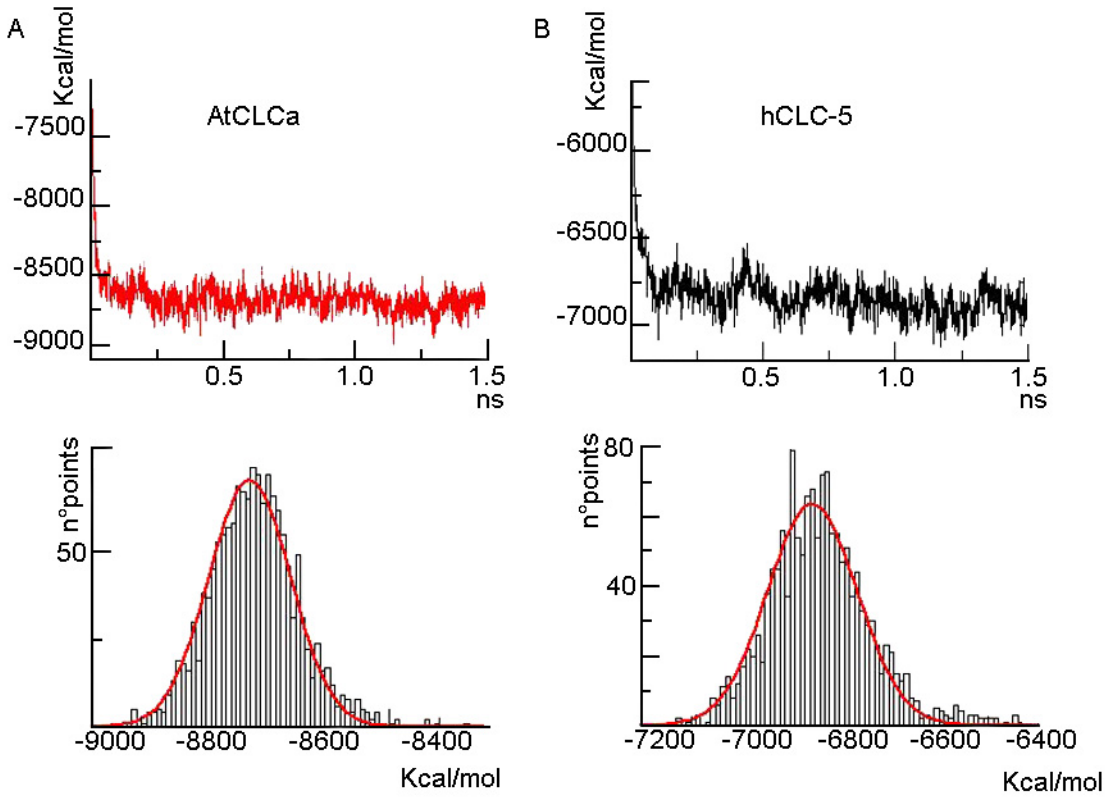
Supplementary Figure 4.



Time course potential energy of the C-terminus of AtCLCa wild-type model in complex with ATP (**A**, upper panel) and of hCLC-5 (**B,** upper panel). MD simulation of 1.5 ns was recorded for each model. After 50 ps in both proteins the internal energy did not vary significantly, therefore these first 50 ps were discarded for the calculation of the ΔG_{bind}. The histograms for the potential energy presented in the lower panels whow that the distributions are well described by a single Gaussian curve, indicating that during the simulation the C-terminus domains were in a single conformation.