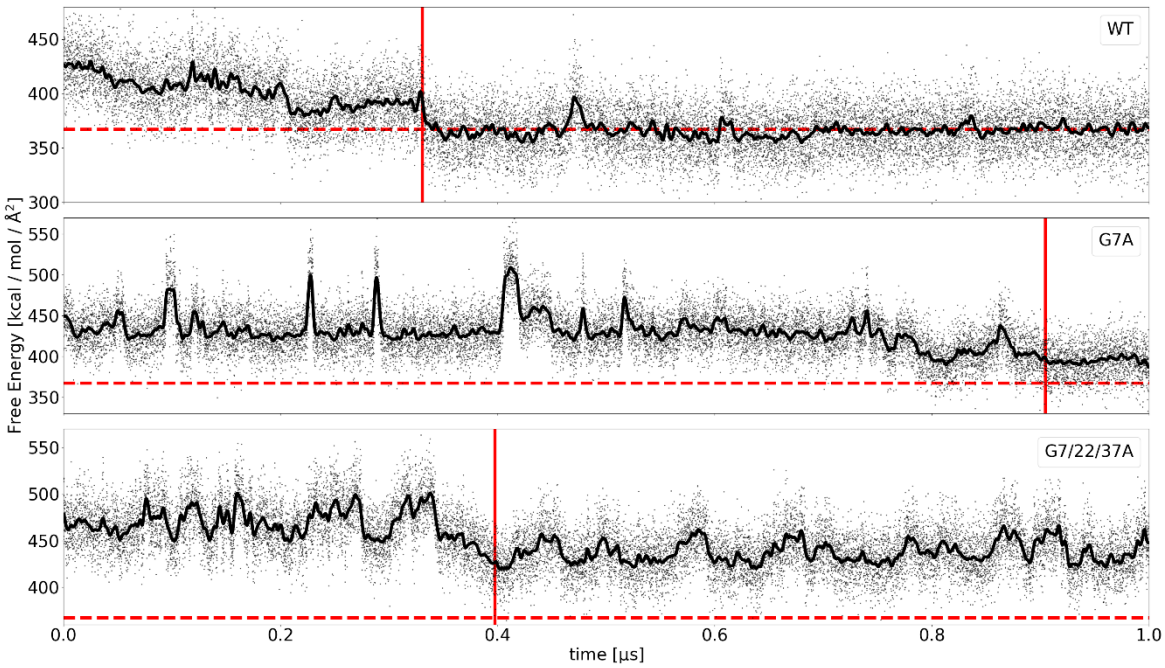

S13_Fig. Time course of the MMGBSA energy during three exemplary simulations. Red vertical lines indicate the time point when the RMSD of the N-Terminus reached values of a folded helix for the first time. The red dashed line displays the mean energy of a folded helix. In the first example a successful folding process of a wild-type peptide is shown (Figure 1 and S4_Fig (example 7)). The second example presents a peptide with one G7aA mutation in one strand (the letter a indicates chain A of the triple helix), which folded around 900ns, but the final energy was increased compared to a folded wild-type. The third example shows a peptide with three mutations (at position 7 of each chain) which temporarily got close to the folded state, but unfolded subsequently.