MD simulation of protein-DNA complex by GROMACS

One terminal of the protein drifted away after 10 ns

One end drifting away may be due to the shortness of the filament. An intuitive assumption would be extending the protein filament by adding more units would help stabilize the central body of the protein. From this angle, it is reasonable to perform a simulation in which positions of atoms of the protein are restrained.
Curves structural analysis on the 10 ns DNA in simulations with or without protein.
In pure DNA simulation, there was more base-pairing remaining after 10 ns. And the parameters were more likely to stay around 0 Å, though there were exceptional base pairs. The abnormal values arising in pure DNA simulation were probably due to preparation of the initial structure where the DNA was forced to go along a designed helical path.
Structural analysis of human nucleosomal sequences of different positioning strength

Figure 3 Averaged predicted minor groove width of human nucleosomal sequences grouped by strength of positioning.

Figure 3 seems to be saying, the higher G/C content it is, the stronger positioning would be expected.