Selection of input parameters:

Download the protein 1MSE.pdb, and use it for training purposes.
For example:

**Position:** 139
**Chain:** C
**Original Amino Acid (One letter abbreviation):** N
**Mutated Amino Acid (One letter abbreviation):** E

The change of binding free energy due to mutation from SAMPDI and experimental results are 0.67 kcal/mol and 1.3 kcal/mol respectively. Note that this change is mutant minus wild-type binding free energies. Thus, positive change implies mutation destabilizes the protein-DNA interaction.

Be aware that NAMD energy minimization does not result in identical structures, if repeated several times on the same file. Because of that, if you run the same mutation via SAMPDI, the results may be slightly different.