Supporting Information

Parameter	Value
Gaussian Height	0.5 kj/mol
Gaussian width	0.1
Bias Factor	6
Gaussian Drop rate	6ps
Swap rate	20ps
Number of tics	2
Feature Space	Dihedrals
Normalized Features	False

Table 1: Set of parameters used for the Bias-exchange tICA-Metadynamics simulations of Alanine dipeptide across 3 different FFs

Parameter	Value
Gaussian Height	0.5 kj/mol
Gaussian width	0.05
Bias Factor	6
Gaussian Drop rate	5ps
Swap rate	5ps
Number of tics	2
Simulation Temp	395 K
Number of walkers	15/tIC
Interval	#Based upon the WW-FIP Anton dataset tic_1: -1.07,1.95 tic_2: -12.11,1.83
Feature Space	Dihedrals + Closest Heavy atom contacts (Beta =10)
Normalized Features	True

Table 2: Set of parameters used for the Bias-exchange tICA-Metadynamics simulations of FIP and GTT mutants of WW domain. Each pair of tIC walkers is connected via MPI but the walkers themselves are only sharing the biases via a shared folder. For the closest heavy atom contacts, we used Plumed's definition of closest heavy atoms to make the contacts differentiable.

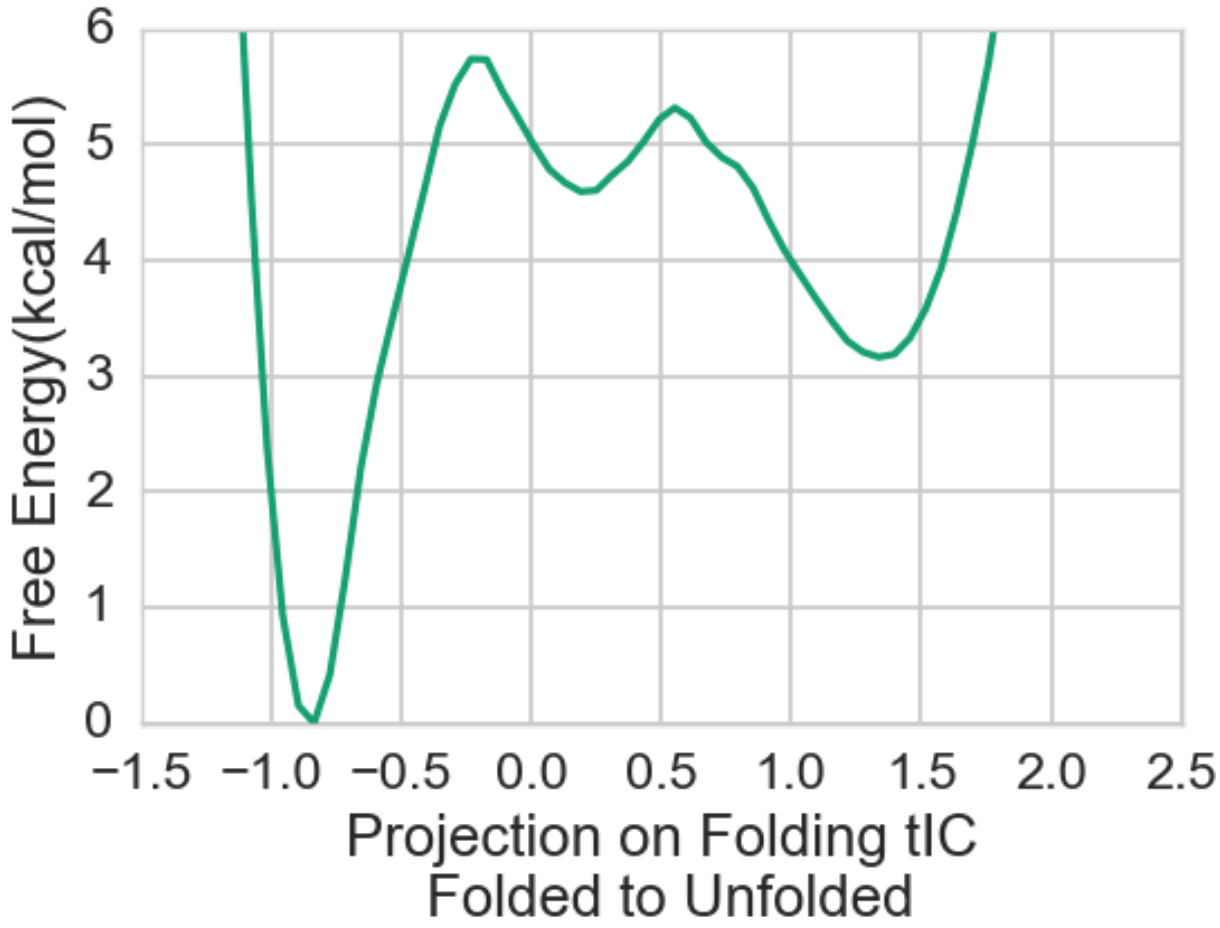

Figure 1: Anton - MSM solution to the FIP's free energy projection along the dominant tIC coordinate.