Supporting information for:

Convergence and Sampling in Determining Free Energy Landscapes for Membrane Protein Association

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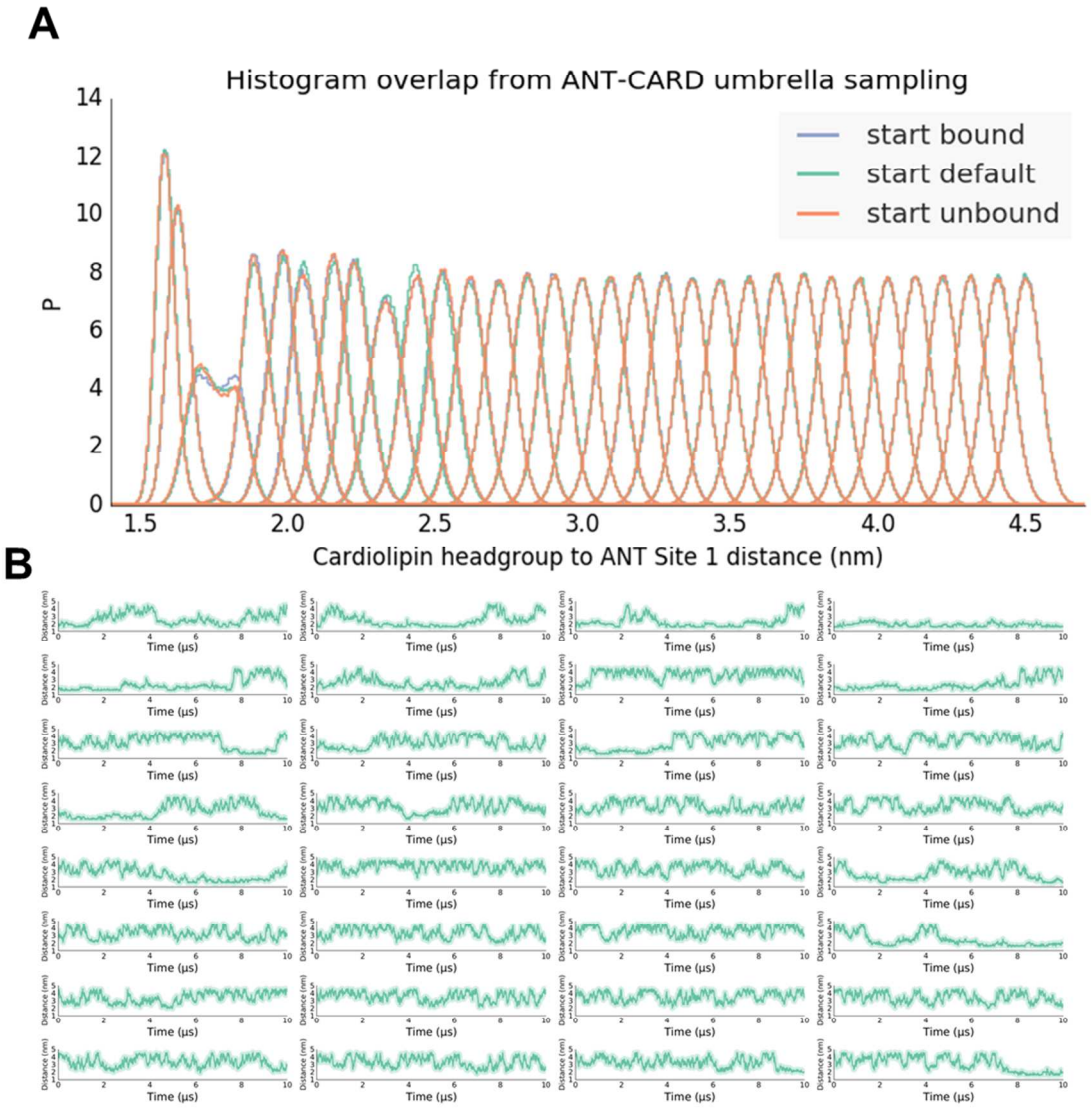
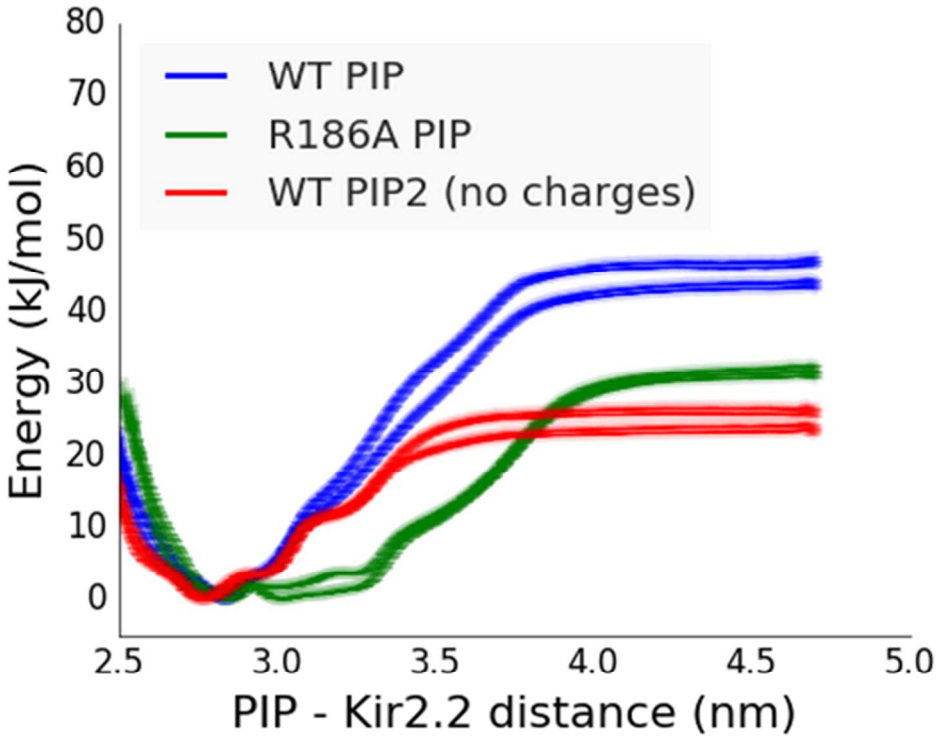


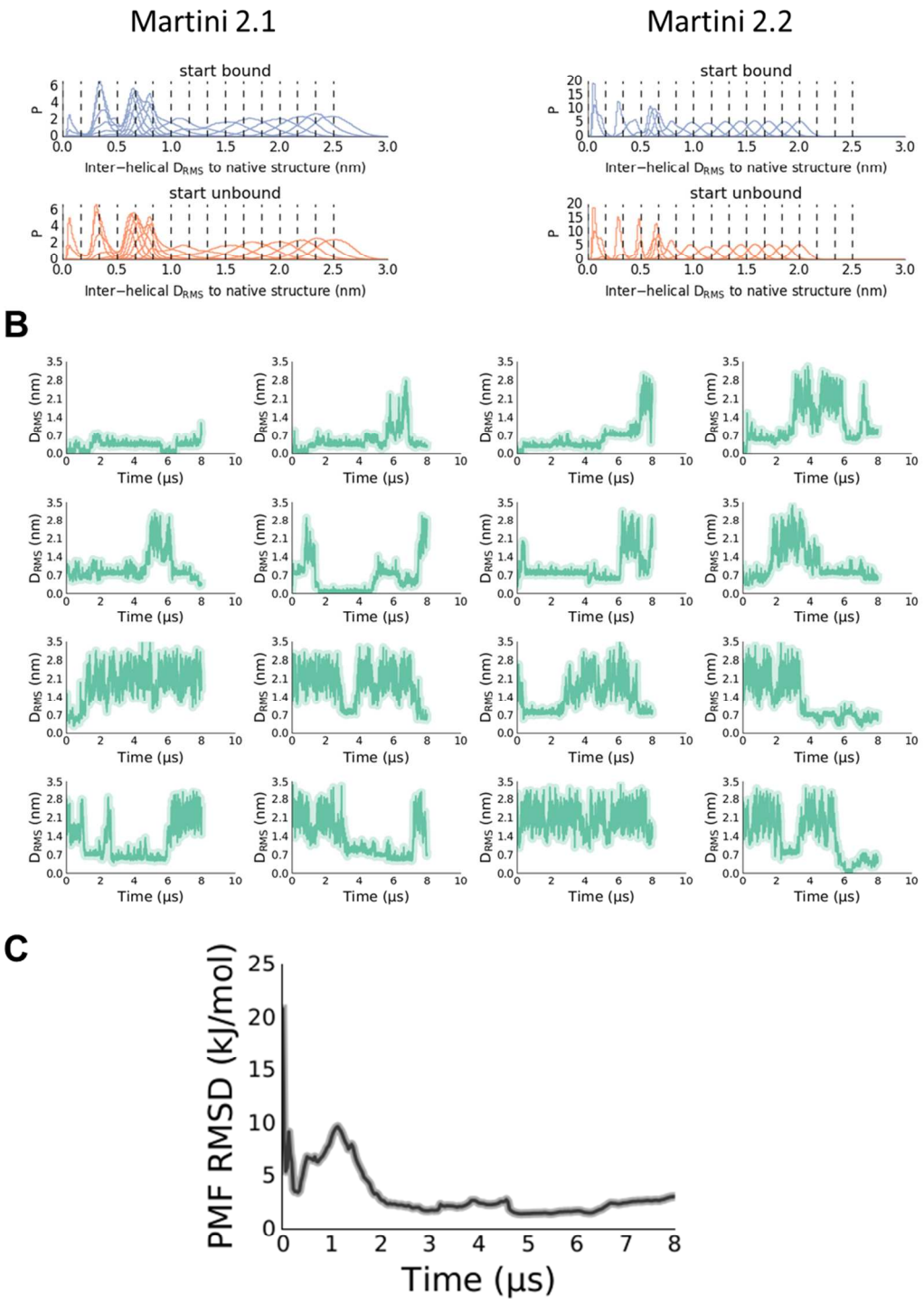
SI Figure S1:

(A) Histogram overlap for the ANT/CL distance-based collective variable, starting from three different initial configurations. (B) Continuous trajectories through the replica space, started from the default initial condition, showing multiple binding and unbinding events of the ANT/CL complex.



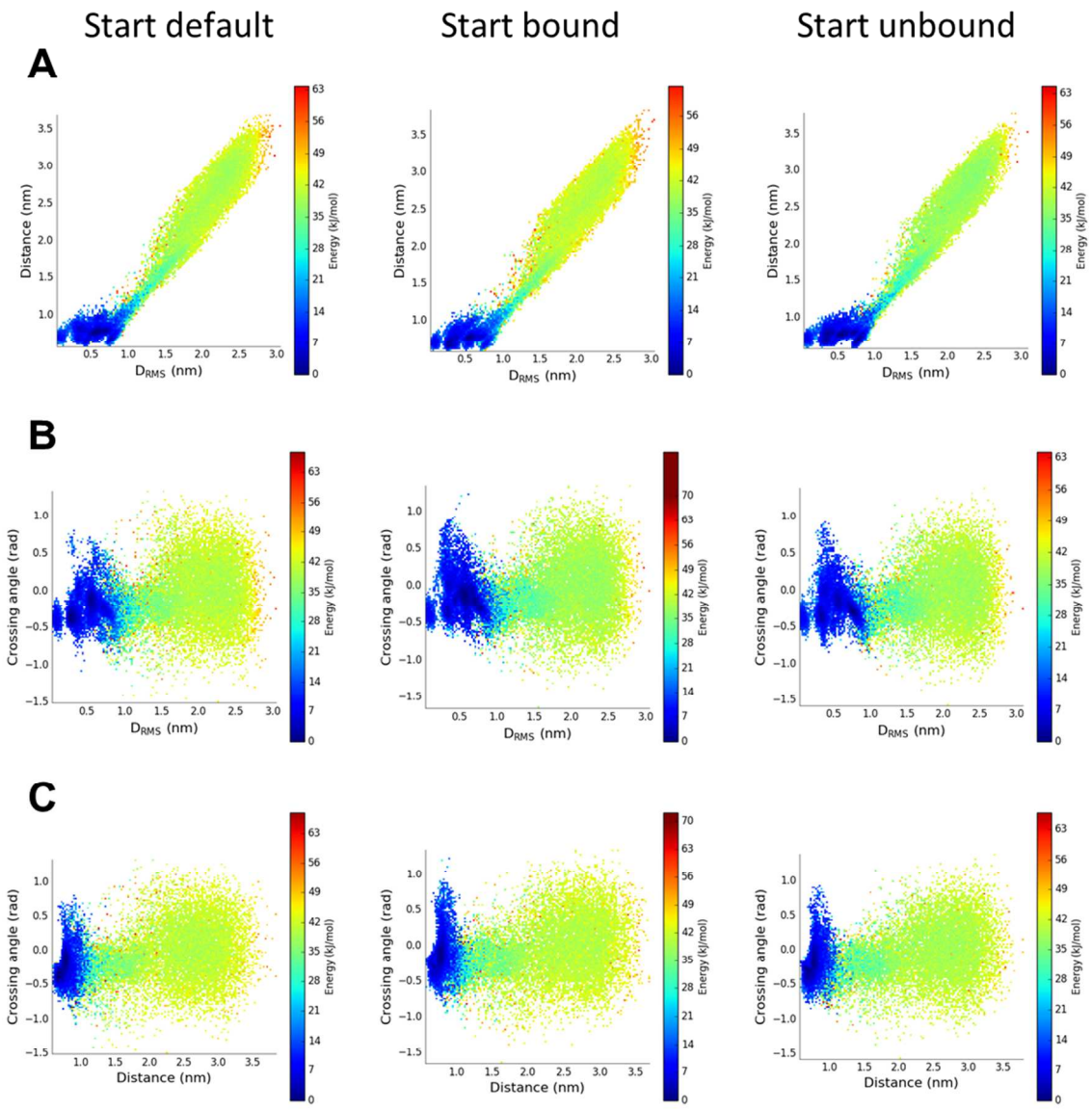
SI Figure 2:

Kir2.2/PIP_2 binding PMFs for the wild-type (blue) vs. R186A mutant (green) Kir2.2 and for the wild-type Kir2.2 with a neutral PIP_2 model (red).



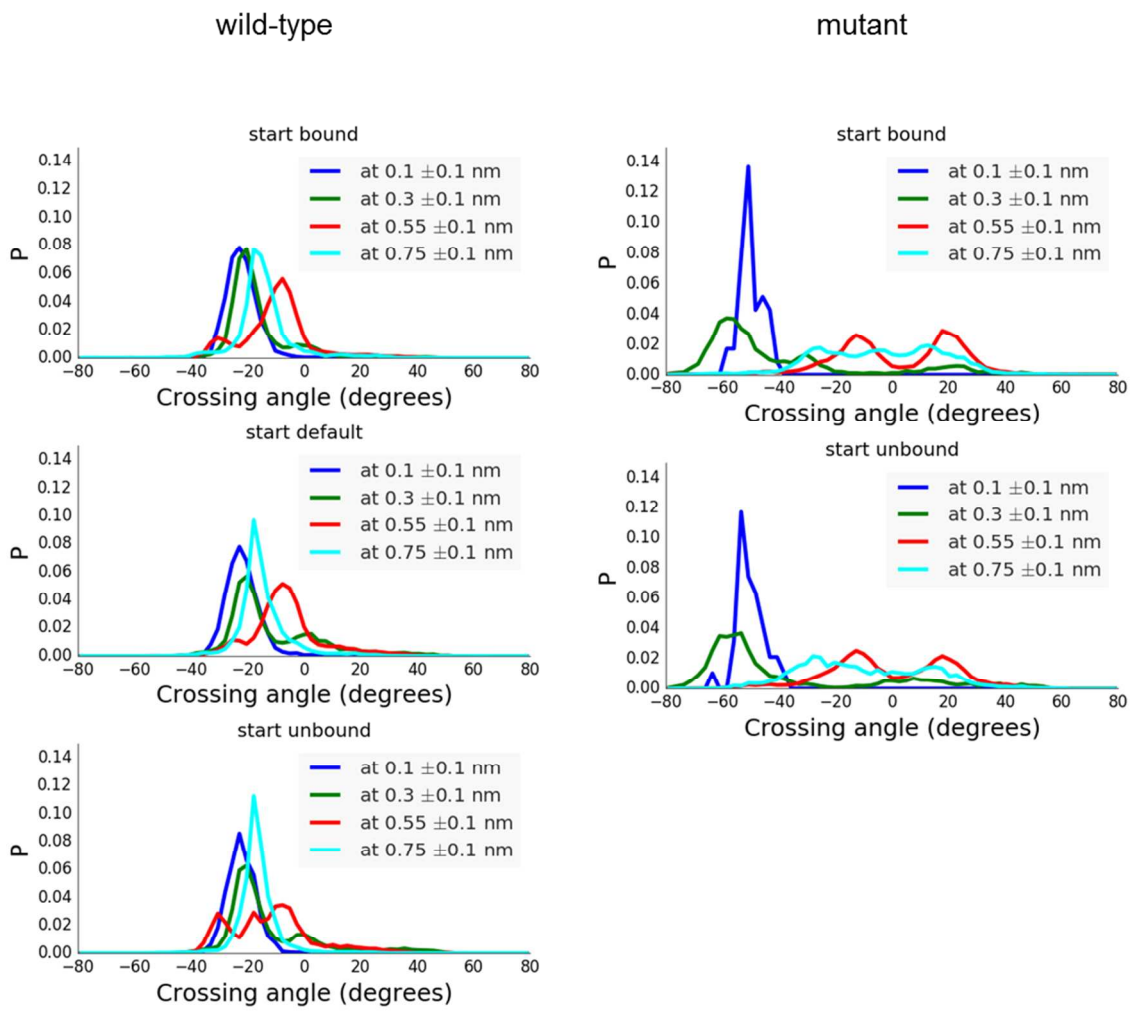
SI Figure 3:

Sampling and convergence of the glycophorin dimer. D_{RMS} histograms for starting from all bound and all unbound condition for Martini 2.1 (A, left panel) and Martini 2.2 (A, right panel. (B) Continuous trajectories through replica space for glycophorin dimerization PMFs, showing multiple binding and unbinding events, starting from the default initial condition. (C) RMSD of PMF starting from all bound and all unbound initial conditions.



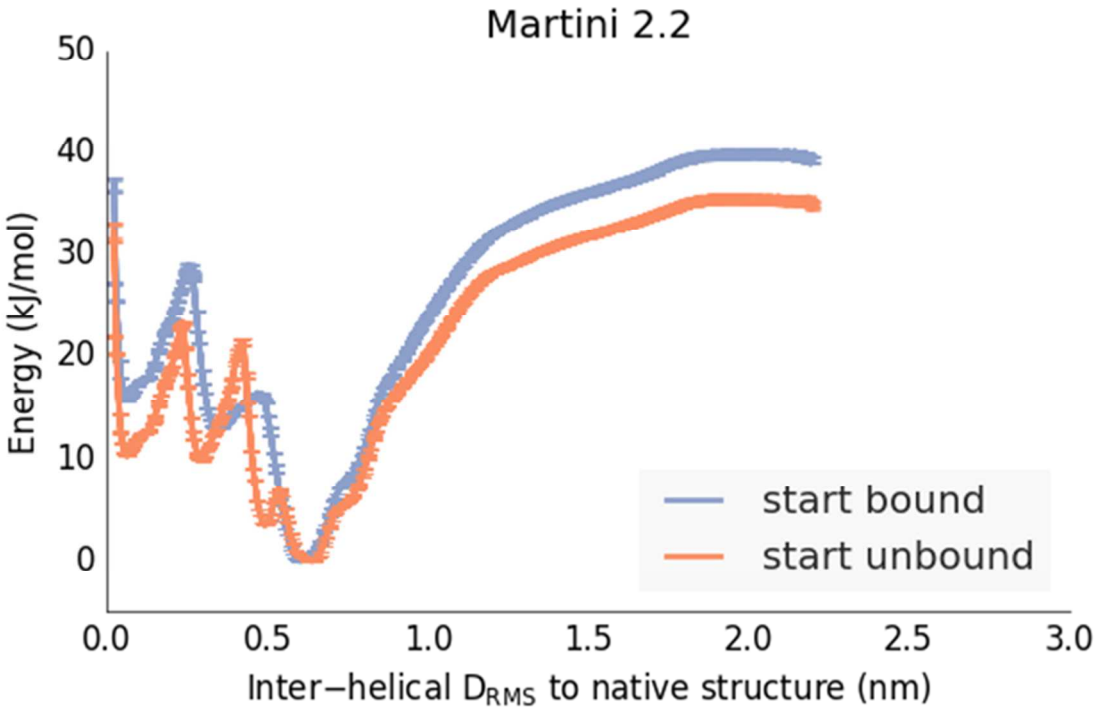
SI Figure 4:

2D PMFs of glycophorin dimerization projected on different collective variables, starting from 3 different initial conditions: (A) distance vs. D_{RMS}; (B) crossing angle vs. D_{RMS}; and (C) crossing angle vs. distance



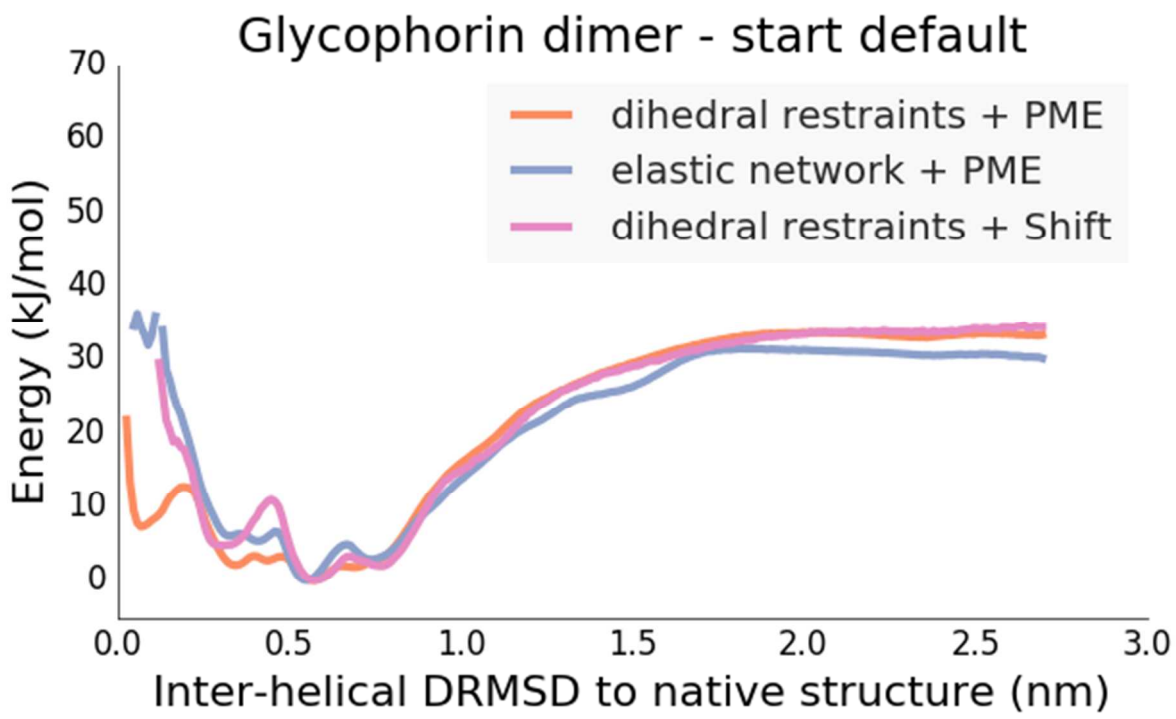
SI Figure 5:

Crossing angle distributions for different minima on the dimerization PMF of glycophorin, wild-type (left panel) and G83L mutant (right panel) with Martini 2.1.



SI Figure 6:

Dimerization PMF along inter-helical D_{RMS} for GpA G83L mutant with Martini 2.2, starting from all bound and all unbound initial conditions.



SI Figure 7:

Sensitivity of the GpA dimerization PMF to the choice of secondary structure restraint (dihedral vs. elastic network) and electrostatic treatment (PME vs. shifted) within Martini, starting with the replicas uniformly spaced along the reaction coordinate.

Input/setup files and code

Simulation setup files for ANT, Kir2.2 and GpA systems can be obtained from:
https://github.com/bestlab/SamplingPaper

The modified version of plumed (2.2-hrex) used to run the simulations is in available at:
https://github.com/bestlab/plumed2/tree/intermolecular-drmsd