Supporting Information
For
Transferring the PRIMO Coarse-Grained Force Field to the Membrane Environment: Simulations of Membrane Proteins and Helix-Helix Association

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Figure S1: Insertion energy of the designed peptides: CHARMM/HDGB versus experimental transfer free energies of side-chain analogs from water into cyclohexane versus PRIMO-M (A); and biological hydrophobicity scale versus CHARMM/HDGB (B). The corresponding correlation coefficients (r) are also provided. Charged residues were excluded from the scale since their insertion free energies are considerably overestimated by CHARMM/HDGB methodology

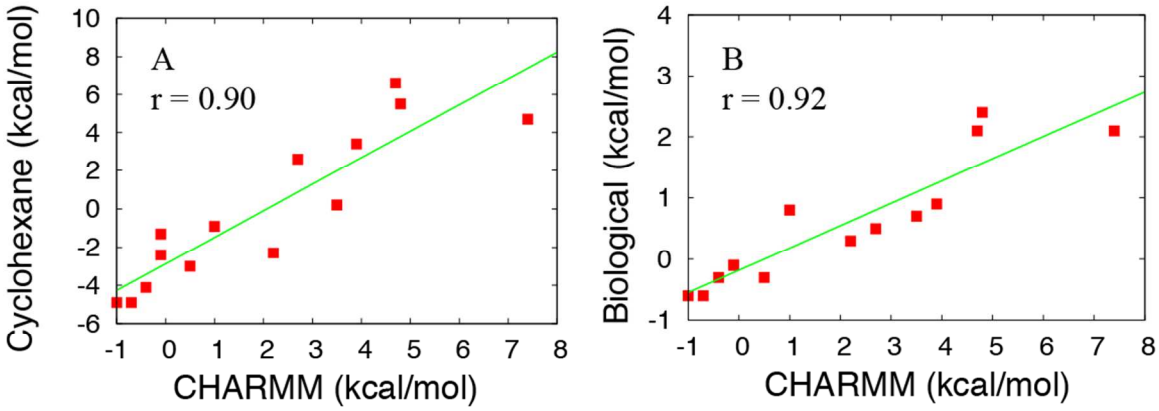

Figure S2: Time evolution of C_α RMSD during PRIMO-M MD simulations with nonbonded cutoff distances of 38 Å for selected proteins from their respective crystal structure

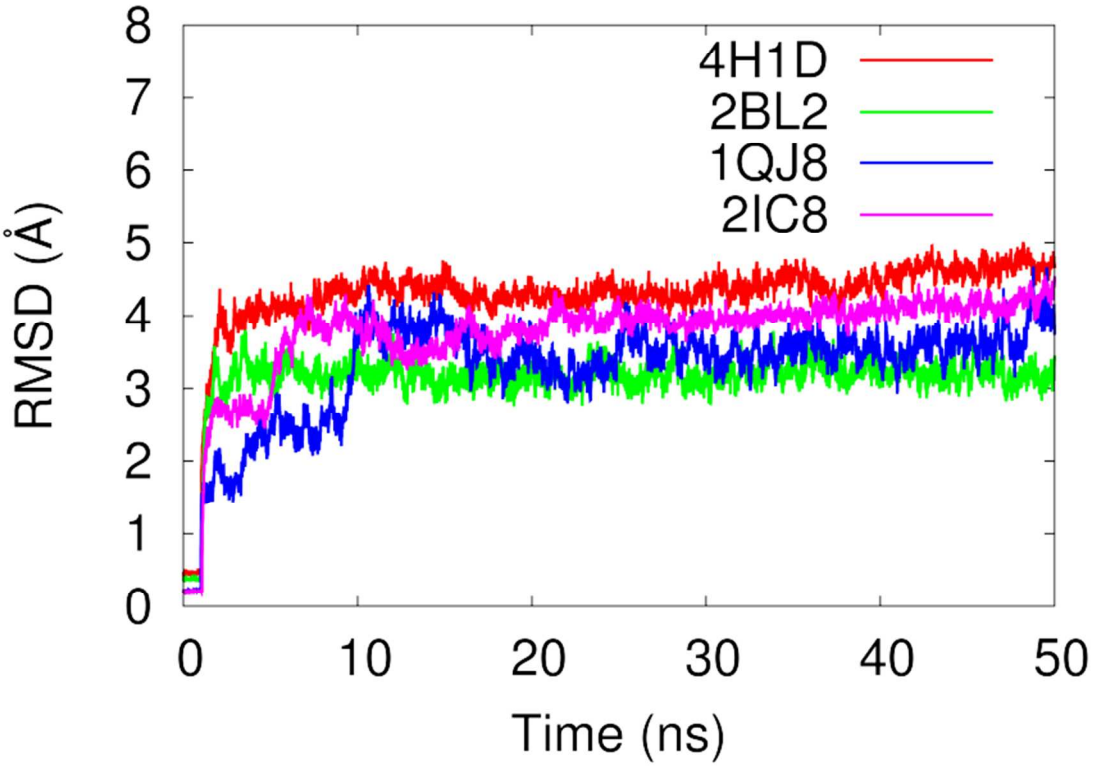

Figure S3: The B-factors of the C_α atoms were calculated from their root-mean-square fluctuations. The red line is from the PRIMO-M simulation while the blue line is from the PRIMO simulation in aqueous environment. The green line is from the experiment.

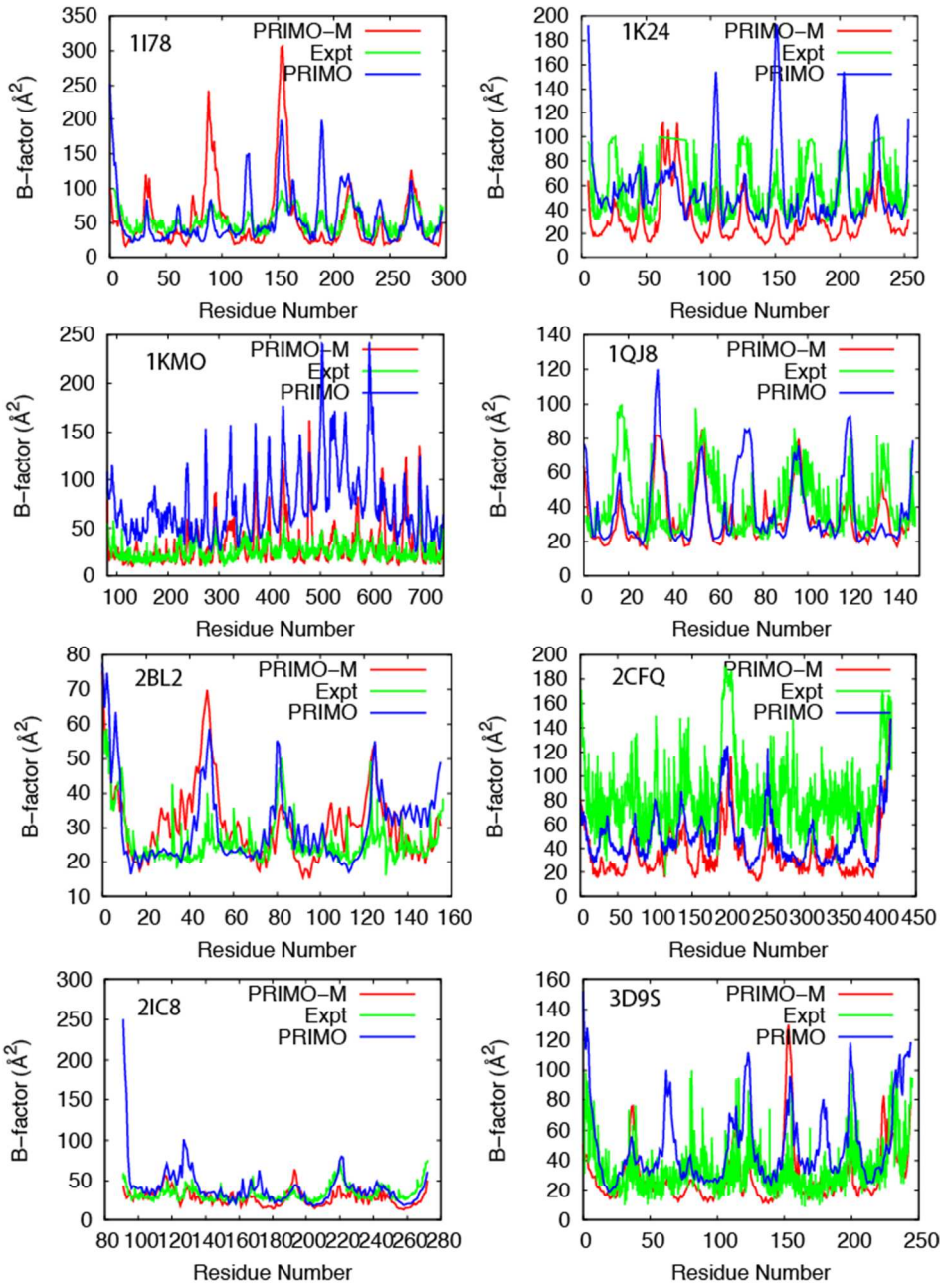

Figure S4: Time evolution of C_α RMSD during PRIMO MD simulations in the aqueous environment for selected proteins from their respective crystal structure.

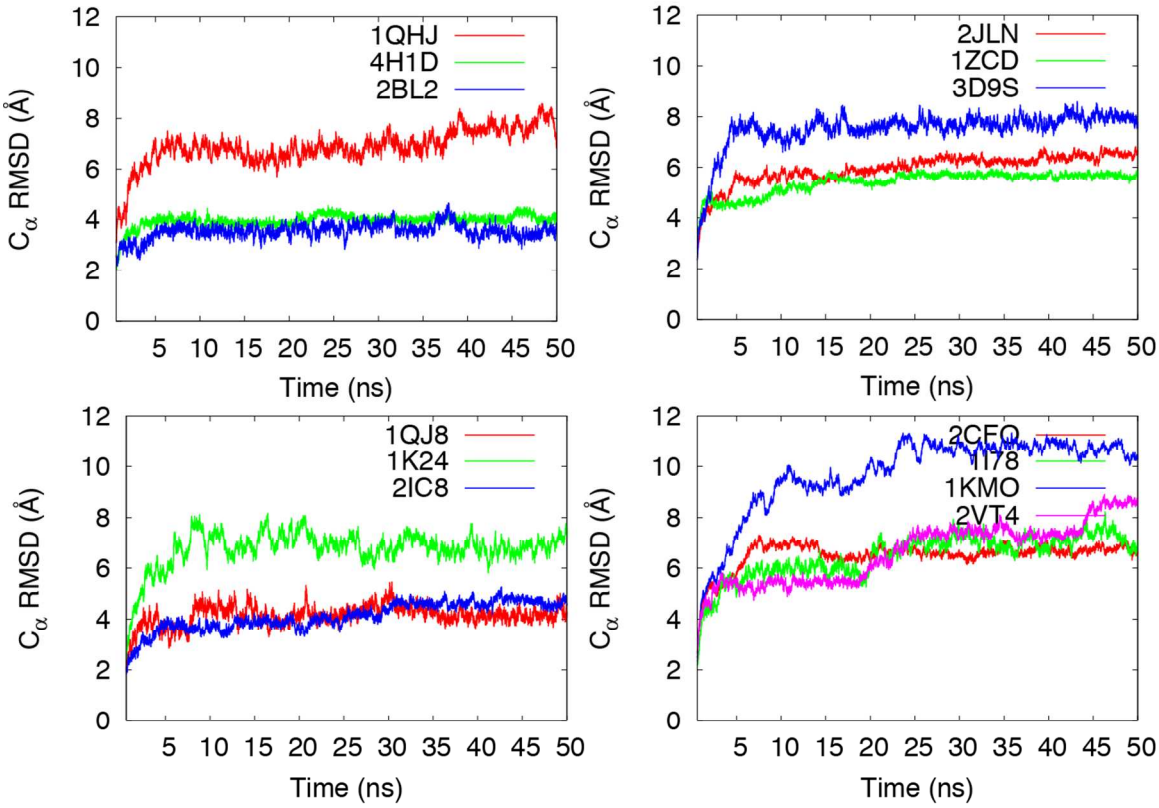

Figure S5: Helix-helix contact map obtained from the simulation. The native contacts are marked with 'X'. The color bar represents the probability of forming a contact.