Oligomerization State of Photosynthetic Core Complexes is Correlated with the Dimerization Affinity of a Transmembrane Helix

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Supporting Information

Movies

MovieS1a Trajectory of the 15-ns equilibrium molecular dynamics simulation with a *Rba. blasticus* PufX monomer in a POPE bilayer (simulation *blasticus-Monomer-POPE* in Table 1 in the text). Coloring scheme in this movie, as well as in subsequent movies, is the same as in Figure 2 in the text.

MovieS1b Trajectory of the 15-ns equilibrium molecular dynamics simulation with a *Rba. capsulatus* PufX monomer in a POPE bilayer (simulation *capsulatus-Monomer-POPE* in Table 1 in the text).

MovieS1c Trajectory of the 15-ns equilibrium molecular dynamics simulation with a *Rba. veldkampii* PufX monomer in a POPE bilayer (simulation *veldkampii-Monomer-POPE* in Table 1 in the text).

MovieS2a Trajectory of the 50-ns equilibrium molecular dynamics simulation with a *Rba. blasticus* PufX dimer in a POPE bilayer (simulation *blasticus-Dimer-POPE* in Table 1 in the text).

MovieS2b Trajectory of the 50-ns equilibrium molecular dynamics simulation with a *Rba. capsulatus* PufX dimer in a POPE bilayer (simulation *capsulatus-Dimer-POPE* in Table 1 in the text).

MovieS2c Trajectory of the 100-ns equilibrium molecular dynamics simulation with a *Rba. veldkampii* PufX dimer in a POPE bilayer (simulation *veldkampii-Dimer-POPE* in Table 1 in the text).

Additional figures and results

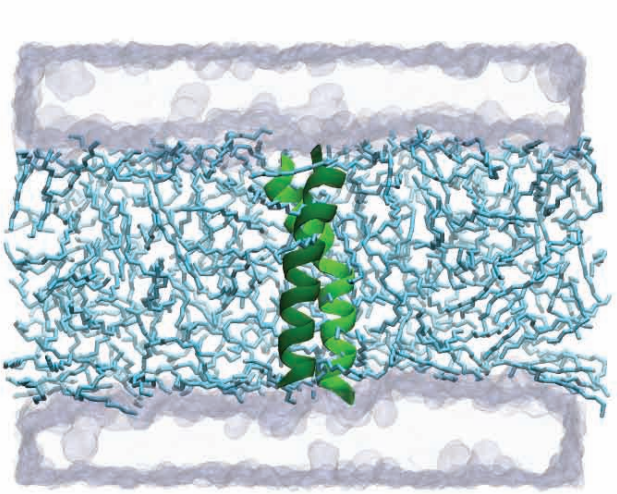

Figure S1: An example setup of a molecular dynamics simulation using a dodecane patch as a lipid mimetic. Shown here is the configuration for simulation *capsulatus-Dimer-DODE-1* in Table 1 in the text. Water is shown in transparent blue, dodecane molecules are shown in cyan, and the two transmembrane segments of *Rba. capsulatus* PufX are shown in green and dark green.

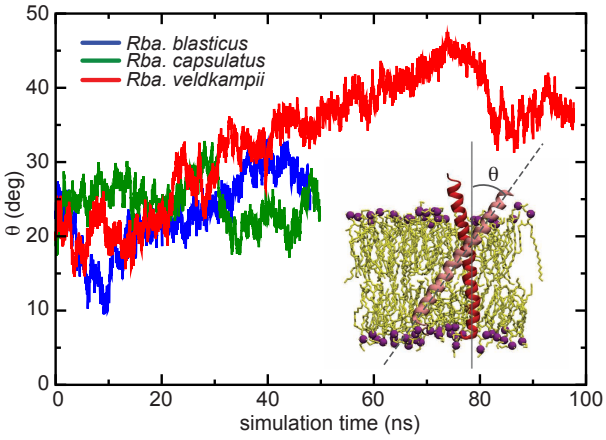

Figure S2: Measurement of helix tilt with respect to the membrane normal during the equilibrium simulations *blasticus-Dimer-POPE* (blue trace), *capsulatus-Dimer-POPE* (green trace), and *veldkampii-Dimer-POPE* (red trace).

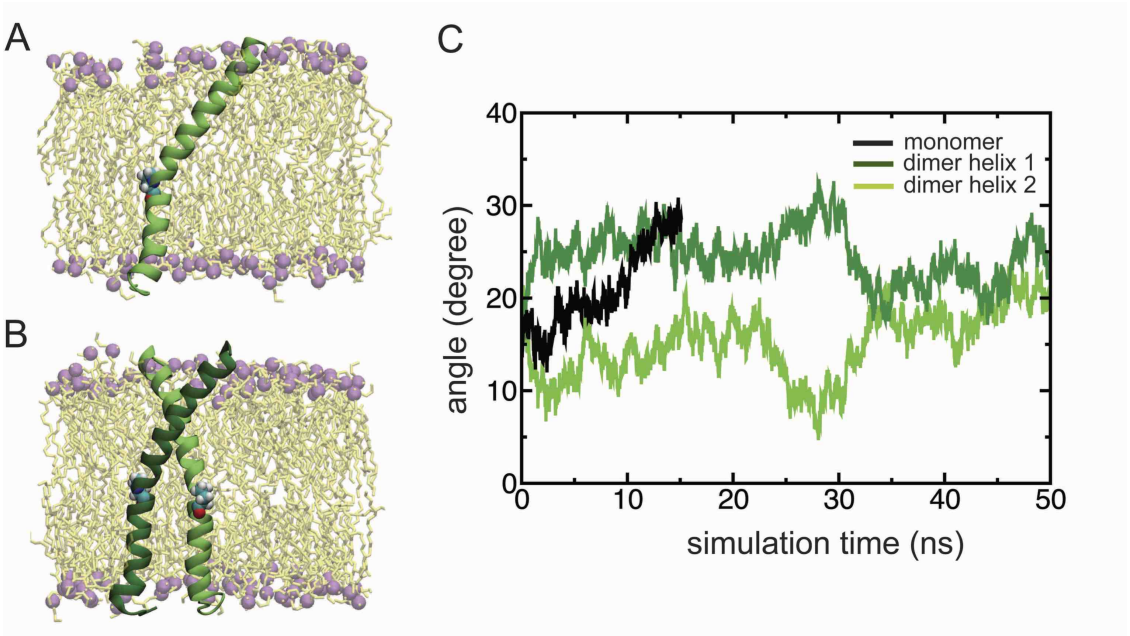

Figure S3: Location of the transmembrane proline residue in *Rba. capsulatus* PufX. (A) Protein-membrane system from simulation *capsulatus-Monomer-POPE* at 15 ns. PufX is shown in green, with the proline residue at location 36 (P36) shown in sphere representation. Membrane is shown in transparent with the same color scheme as in Figure 2 of the main text. (B) Protein-membrane system from simulation *capsulatus-Dimer-POPE* at 35 ns. The two PufX helices are colored in green and dark green for distinction. The P36 residues can be seen to point away from the helix-helix association interface. (C) Measurement of the helix kink near the P36 residue during simulation *capsulatus-Monomer-POPE* (black trace) and *capsulatus-Dimer-POPE* (dark green and light green traces).

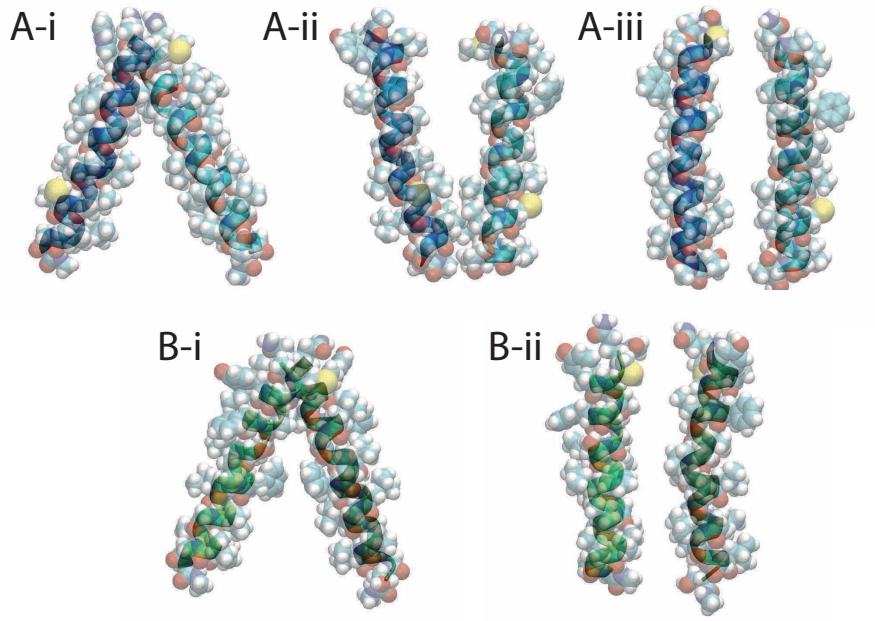

Figure S4: Common conformations of PufX helices seen in ABF simulations with a helix-helix separation of 14.9-15.1 Å. A) The three most common conformations for the transmembrane segments of *Rba. blasticus* PufX seen in *blasticus-Dimer-DODE-ABF-1*. A-i) Conformation with helices associated at the N-terminal ends via close contacts near Gly29. A-ii) Conformation with helices interacting transiently at the C-terminal ends via van der Waals contacts between large side chains (most notably Leu43, Leu44, and Thr47). A-iii) Conformation with the helices separated. The conformation in A-ii is only observed for the case of *Rba. capsulatus*. For example, for the case of the transmembrane segments of *Rba. capsulatus* PufX seen in *capsulatus-Dimer-DODE-ABF-1*, only two common conformations are observed with a helix-helix separation of 14.9-15.1 Å, one with associated N-terminal ends also mediated by the Gly29 contact (B-i), and another with completely separated helices (B-ii).

Complete citation for ref 31

(31) MacKerell, Jr., A. D.; Bashford, D.; Bellott, M.; Dunbrack Jr., R.L.; Evanseck, J.D.; Field, M.J.; Fischer, S.; Gao, J.; Guo, H.; Ha, S.; Joseph-McCarthy, D.; Kuchnir, L.; Kuczera, K.; Lau, F.T.K.; Mattos, C.; Michnick, S.; Ngo, T.; Nguyen, D.T.; Prodhom, B.; Reiher, III, W.E.; Roux, B.; Schlenkrich, M.; Smith, J.C.; Stote, R.; Straub, J.; Watanabe, M.; Wiorkiewicz-Kuczera, J.; Yin, D.; Karplus, M. "All-atom empirical potential for molecular modeling and dynamics studies of proteins." *The Journal of Physical Chemistry B*. **1998**, *102*:3586-3616.