SUPPORTING MATERIAL

A Practical Implicit Membrane Potential for NMR Structure Calculations of Membrane Proteins.

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Supplementary Table

Table S1. *eefxPot* Membrane insertion energy (kcal/mol) obtained for Ala_{25} and Leu_{25} with different values of the dielectric screening parameter *a*.

	$a = 0.85$		$a = 0$	
	Ala_{25}	Leu_{25}	Ala_{25}	Leu_{25}
$\Delta E_{EEF\text{-}IMM}$	1.6	-45.7	-364.7	-317.4
ΔE_{ELEC}	-42.6	-26.5	-408.9	-298.2
ΔE_{SLV}	44.2	-19.2	44.2	-19.2

For each peptide helix, the membrane-inserted state was generated by positioning the center of mass at the membrane center ($z = 0$) and the helix axis parallel to the membrane normal, while the surface-adsorbed state had the center of mass at the membrane surface ($z = T/2$) and helix axis perpendicular to the membrane normal. After subjecting each state to a 300-step minimization, the free energy of insertion was evaluated as the difference between the energies in the two states.

Supplementary Figures

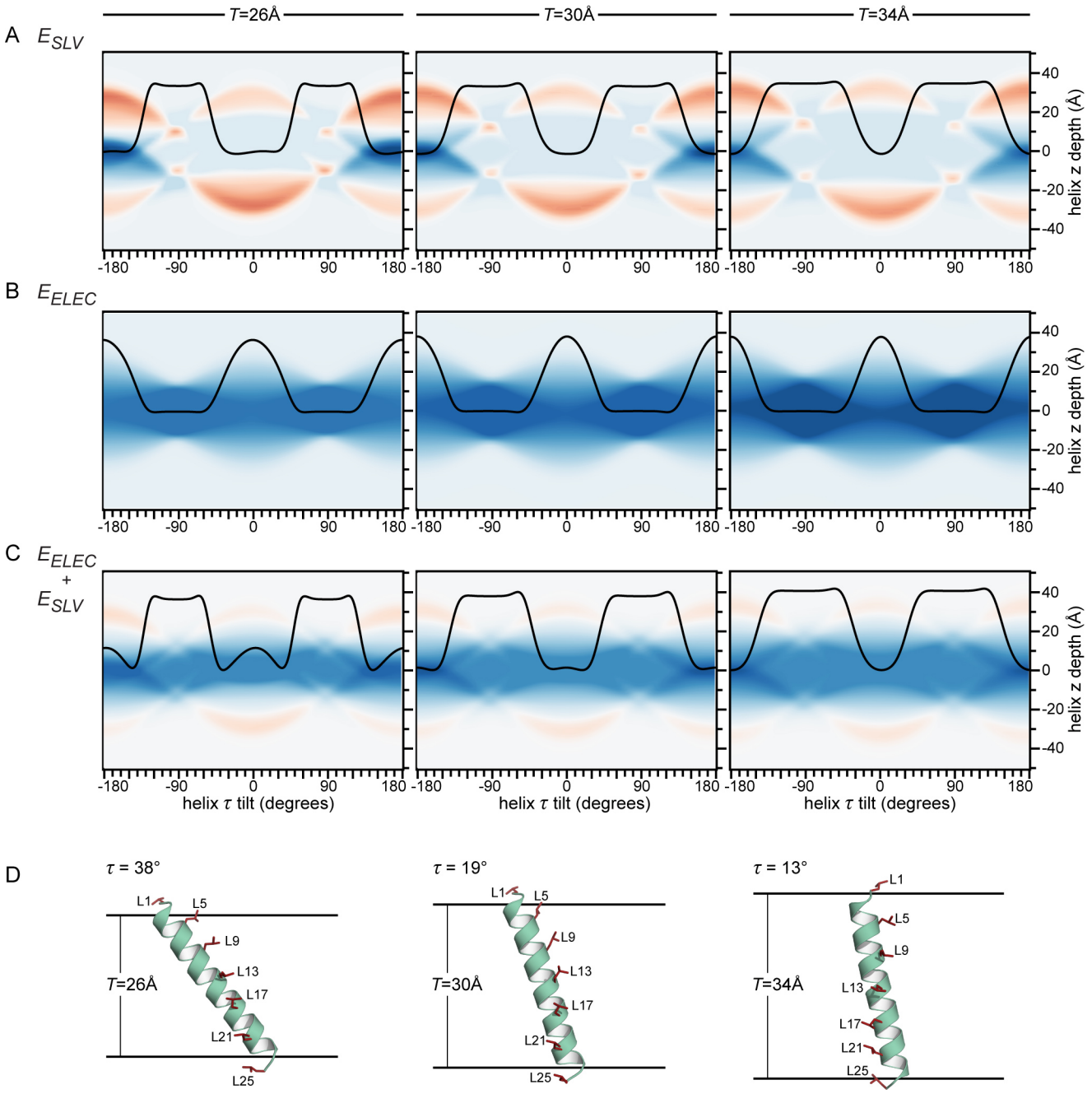

Fig. S1. Energy landscape and position of Leu_{25} in *eefxPot* membranes of thickness T = 26 Å, 30 Å and 34 Å. (A-C) The landscape was mapped by holding the peptide helix as a rigid body, placing it at various membrane depths along the membrane z axis and rotating through 360° around the membrane y axis. Solid lines trace the energy profiles for peptide helix tilt at a membrane depth of z = 0Å. Since the peptide backbone and side chains were treated as one rigid body in this calculation, the value of E_{VDW} remains constant and was not included in the analysis. **(D)** The transmembrane helix tilt of Leu_{25} depends on the model membrane thickness. Structures were generated with 200 ps of unrestrained *eefxPot* MD simulation in the three different membrane thicknesses. The membrane is represented by horizontal lines separated by thickness T. Simulations were performed at 300 K.

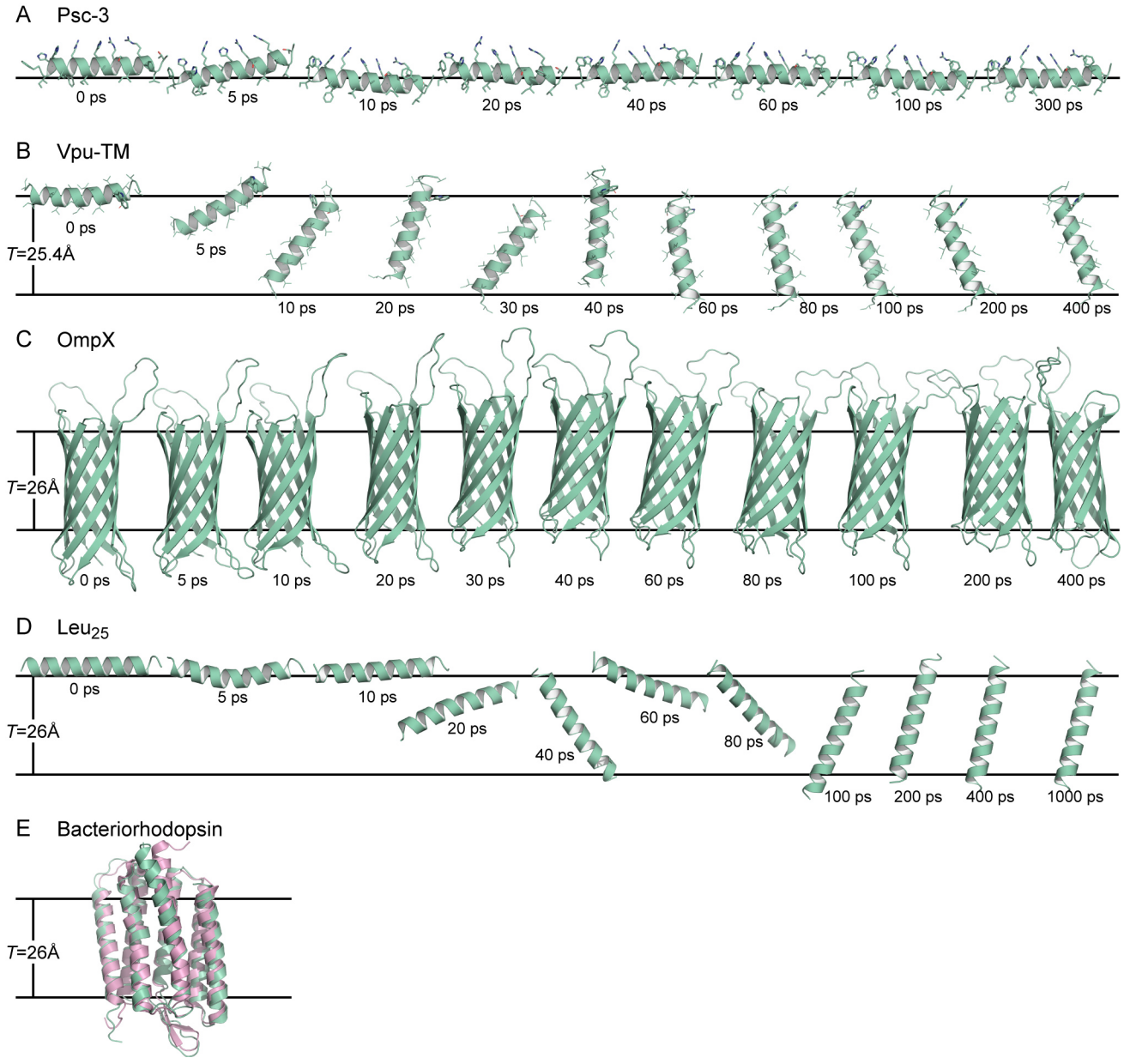

Fig. S2. Structure snapshots taken from unrestrained *eefxPot* MD simulations of Psc-3 (PDB 2MCW), Vpu-TM (PDB 1PI7), OmpX (PDB 2M06) and bacteriorhodopsin (PDB 1M0L). The membrane is represented by horizontal lines separated by thickness *T*. Simulations were performed at 300 K.