Methods: Insertion of bacteriorhodopsin into the membrane

Authors: Christian Kappel and Helmut Grubmuller

First, a pre-equilibrated membrane patch was taken and lipid molecules which would overlap with the proteins were removed so that 9 lipid molecules per bacteriorhodopsin monomer were left. As next step, the volume occupied by the proteins was then defined using the program MSMS (41). Because bacteriorhodopsin in lipid membranes forms a 2D crystal lattice, periodic images in the x-y plane had also to be taken into account. Bacteriorhodopsin was inserted in the pre-equilibrated membrane patch according to the protocol described in ref. (40).

Results

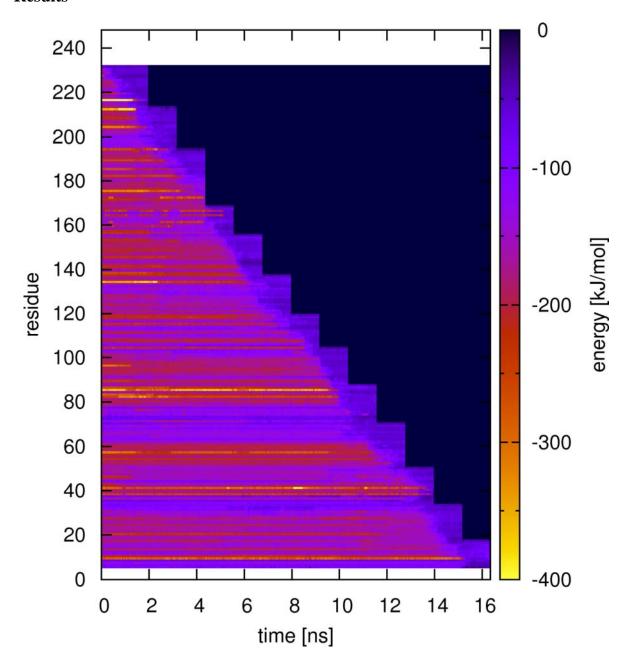


Figure S1: Time development of the sum of Coulombic and Lennard-Jones interactions between each individual residue and the rest of the protein during extraction and unfolding. Colors represent the strength of interaction.

Results: Anchor point stabilization

Anchor point (helix)	End of helix (hydrogen bond)	Center of helix (hydrogen bond)	Center of helix (hydrophobic contact)
Thr17 (A)		X	
Leu48 (B)			X
Tyr79 (C)	X		
Thr89 (C)		X	
Leu111 (D)			X
Ile119 (D)			X
Arg134 (E)	X		
Met145 (E)			X
Val179 (F)		X	
Pro200 (G)	X		

Table S1: Anchor points determined from extraction simulations towards the cytoplasmic side categorized by their location and stabilization.

Results: Fit results from the relaxation simulations

	partially unfolded helix G	partially unfolded helix F
\mathbf{F}_1	(4070±50) pN	(920±20) pN
F ₂	(460±40) pN	(302±2) pN
F _{final}	(10±40) pN	(107±1) pN
τ_1	(730±5) ps	(95±2) ps
τ_2	(55000±6000) ps	(4810±60) ps

Table S2: Values for all parameters from the bi-exponential fits employed to describe the forces in the relaxation simulations.