Supporting Information

Silva et al. 10.1073/pnas.0904505106

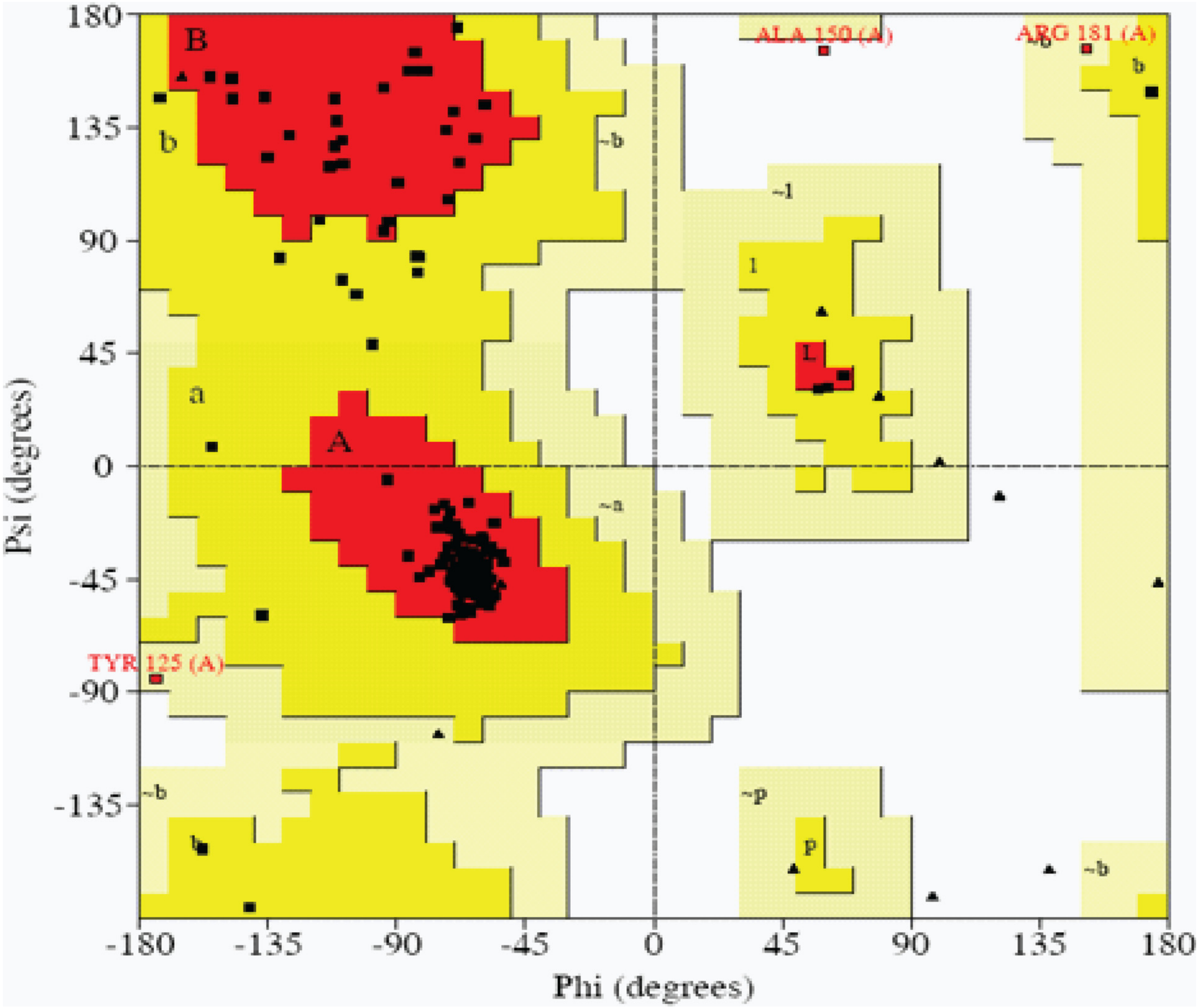


Fig. S1. Ramachandran plot. Red regions are highly favored in terms of steric interactions, yellow regions are allowed, white regions are unfavored. Triangles are glycine residues (unrestricted by φ and ψ because of lack of a side chain), all other residues are indicated by squares. Residues in disallowed regions, by the steric criteria, are in red.

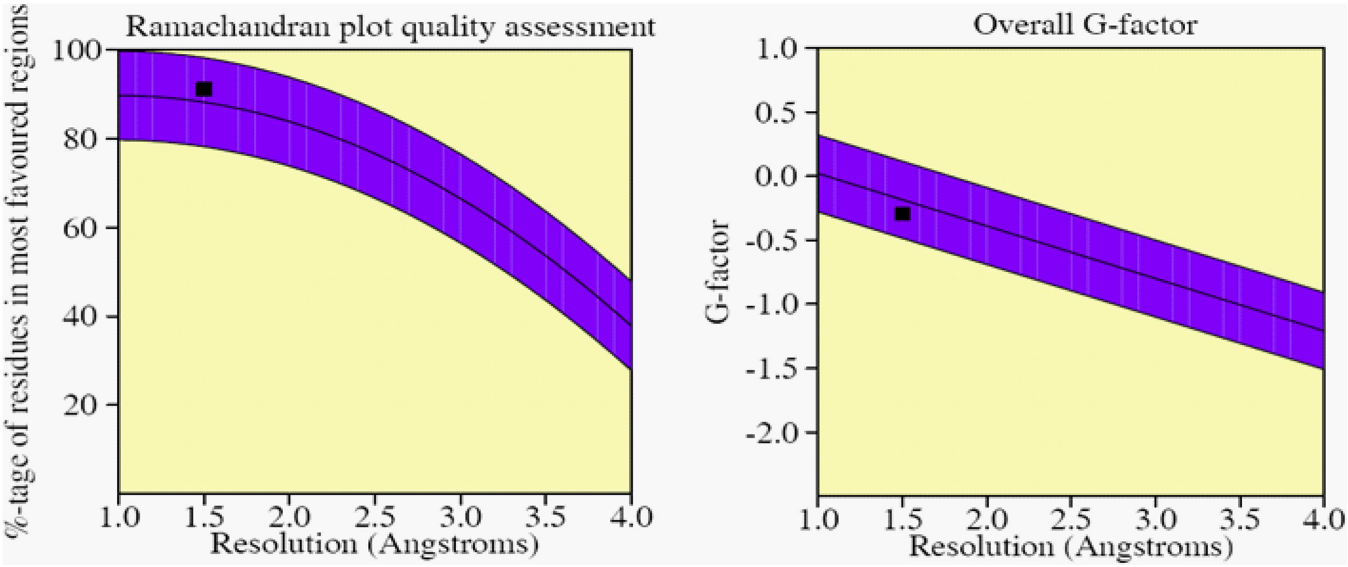


Fig. S2. Procheck assessment. Comparison of Ramachandran plot and G-factor to known structures. For the Ramachandran plot, as the crystal becomes better resolved more residues tend to be found in the favored regions (90% in the highest resolution structures), which is what we observe. The G-factor is a similar comparison, but includes many more criteria such as the angles of the side chains for each residue, bond lengths and planarity (2).

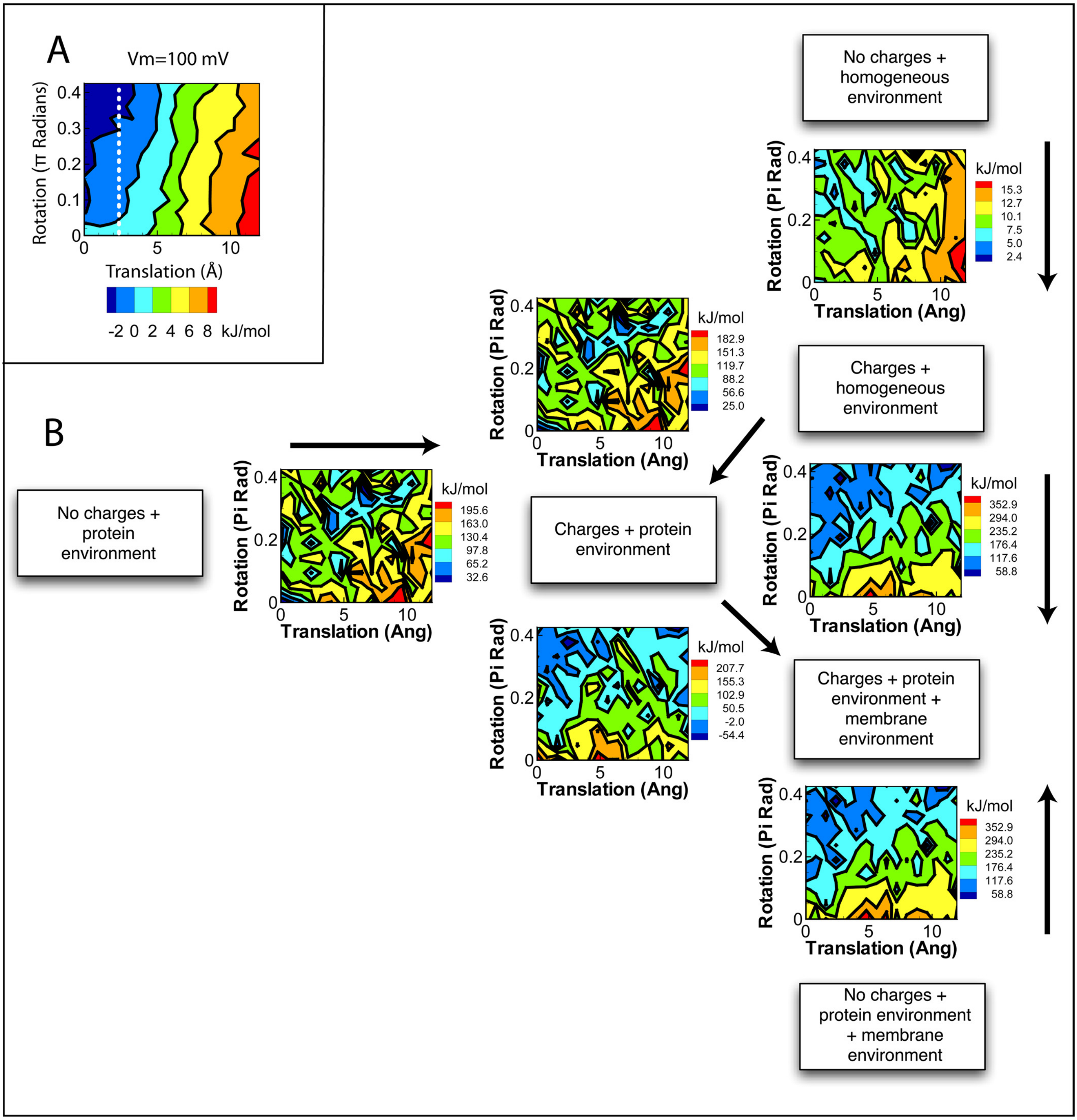
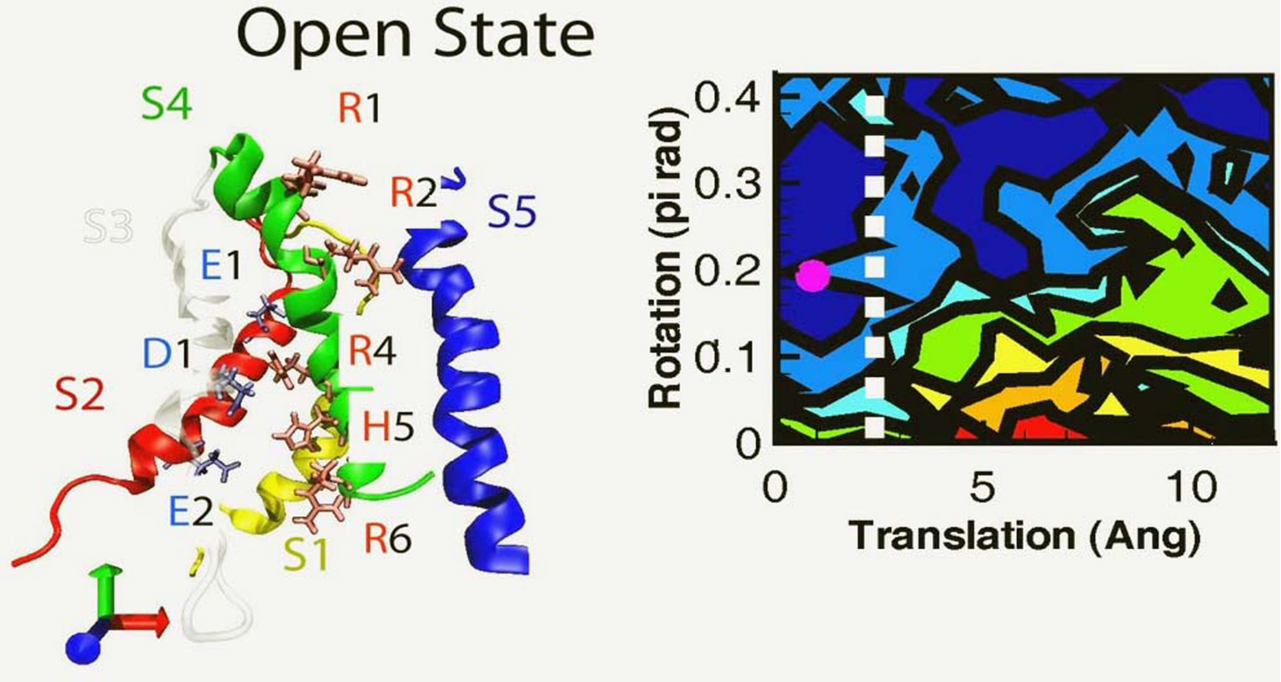


Fig. S3. Estimation of error in energy calculations. (*A*) Membrane potential $V_m = 100$ mV causes stabilization of the open state and introduces a net difference of ≈10 kJ/mol between closed and open configurations. (*B*) Energy cycle. Each energy landscape represents the energy difference between two different environments as indicated. Difference is from conditions (indicated in boxes) at arrow head to those at arrow tail. For example, the topmost energy landscape on the right represents ''Charges+Homogeneous Environment'' minus ''No Charges+Homogeneous Environment''. The dielectric constant for the homogeneous environment is $\varepsilon = 78$. Large increases within the energy landscape are associated with the introduction of the protein environment and further by the presence of the membrane environment. Scaling of the energy landscape was performed to account for the effect of individual water molecules and other environmental contribution not explicitly computed in the simulations. With this correction, the energy barriers are in the range of V_m as required.



Movie S1. Movie shows S4 movement through the energy landscape from open to closed. At stable conformation (open, intermediate, closed, deep closed) the protein is rotated showing 3D structure.

Movie S1 (AVI)

Other Supporting Information Files

SI Appendix (PDF)