Zheng and Qin, http://www.jgp.org/cgi/content/full/jgp.201411335/DC1

DataS1.txt: Atomic coordinates of the ICD obtained from five MD trajectories in the C state (10 frames/trajectory).

DataS2.txt: Atomic coordinates of the ICD obtained from five MD trajectories in the O state (10 frames/trajectory).

DataS3.txt: Results of residue conservation analysis from the ConSurf server.

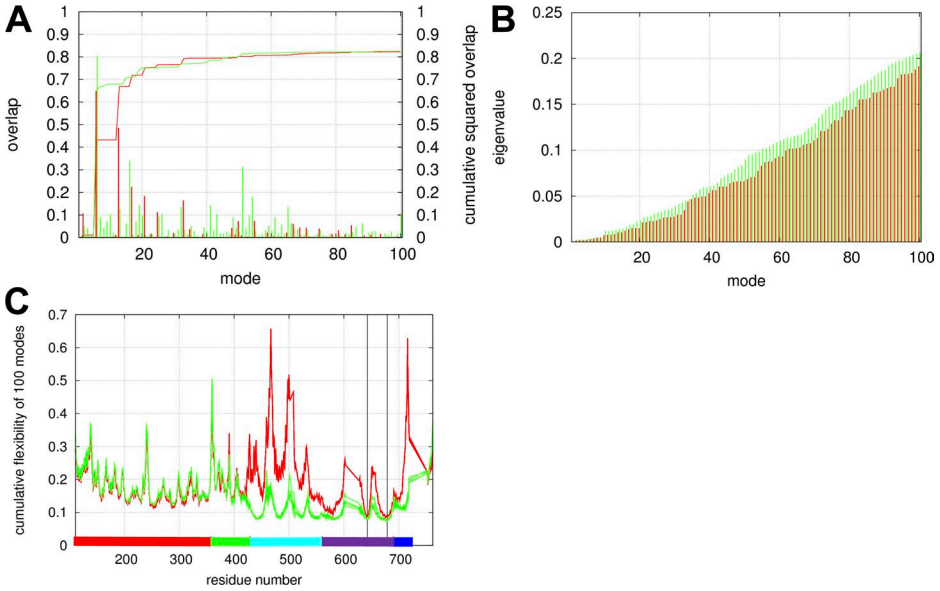


Figure S1. Results of NMA for the lowest 100 modes calculated in the absence (red) or presence (green) of lipids. (A) The overlap and cumulative squared overlap as a function of mode number (shown as impulses and lines, respectively). (B) The eigenvalue as a function of mode number. (C) The cumulative flexibility as a function of residue number. In C, the ranges of residue numbers are colored as follows: red, ARD; green, MPD; cyan, S1–S4 helices; purple, S5–S6 helices; blue, CTD. The positions of residues G643 and I679 are marked by vertical lines.

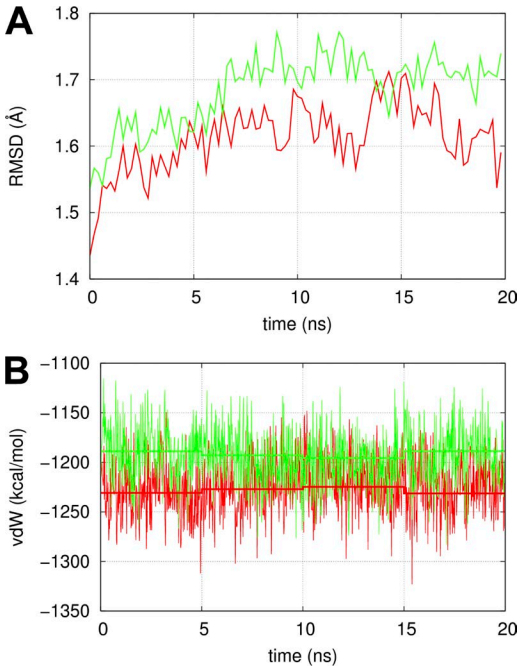


Figure S2. Convergence analysis of MD simulation. (A) Root mean squared deviation of nonhydrogen atoms (relative to the experimental structure) as a function of time for a representative MD trajectory of ICD in C state (red) and O state (green). (B) vdW energy as a function of time for a representative MD trajectory of ICD in C state (red) and O state (green). In panel B, the average vdW energy for the first, second, third, and fourth 5-ns window (shown as plateaus) exhibits no significant time-dependent drift.

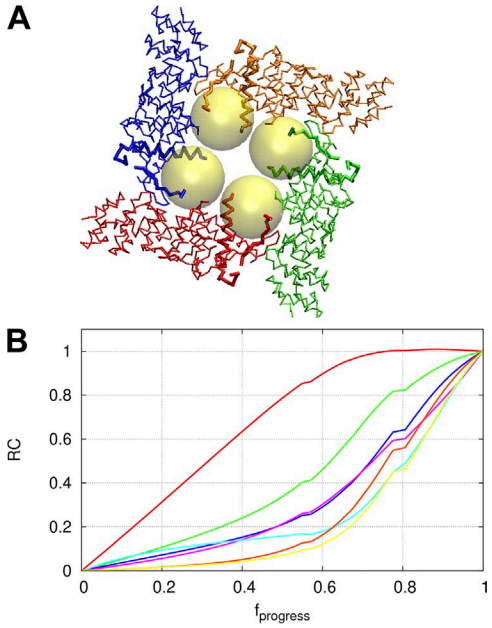
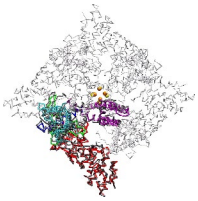
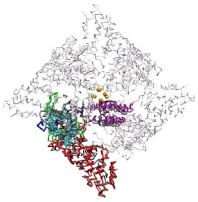


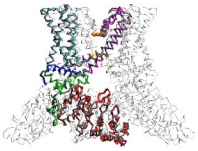
Figure S3. Results of transition pathway modeling in the presence of more complete CTDs. In panel A, the four subunits are colored in blue, red, green, and orange. The TMDs are removed for clarity. The cryo-EM–resolved parts of CTDs are shown as thick traces. The missing residues of CTDs are modeled as four large beads with a radius of 13 Å (colored in yellow). In B, reaction coordinates along the closed-to-open transition pathway are shown for the following functional parts of TRPV1: ARD (red), MPD (green), CTD (blue), helices S1–S4 (cyan), helices S5–S6 (purple), and residues G643 (orange) and I679 (yellow).



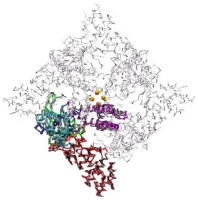
Video 1. Collective motion described by mode 6 using the same top view and color scheme as in Fig. 1 B. For comparison, the O-state conformation of a representative subunit is also shown (colored in gray).



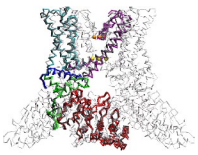
Video 2. Collective motion described by mode 13 using the same top view and color scheme as in Fig. 1 B. For comparison, the O-state conformation of a representative subunit is also shown (colored in gray).



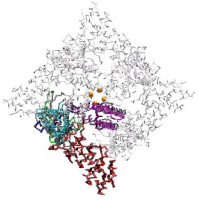
Video 3. Predicted transition pathway from C state to O state of TRPV1 in the side view. The same color scheme as in Fig. 1 (A and B). For comparison, the O-state conformation of a representative subunit is also shown (colored in gray).



Video 4. Predicted transition pathway from C state to O state of TRPV1 in the top view. The same color scheme as in Fig. 1 (A and B). For comparison, the O-state conformation of a representative subunit is also shown (colored in gray).



Video 5. Predicted conformational changes induced by activation of the ICDs of TRPV1 in the side view. The same color scheme as in Fig. 1 (A and B). For comparison, the O-state conformation of a representative subunit is also shown (colored in gray).



Video 6. Predicted conformational changes induced by activation of the ICDs of TRPV1 in the top view. The same color scheme as in Fig. 1 (A and B). For comparison, the O-state conformation of a representative subunit is also shown (colored in gray).