

Supplementary Information

Probing the Conformational and Energy Landscapes of KRAS membrane orientation

Priyanka Prakash¹ and Alemayehu A. Gorfe^{1,2*}

¹ McGovern Medical School, University of Texas Health Science Center at Houston, Department of Integrative Biology and Pharmacology, 6431 Fannin St., Houston, Texas 77030

^{1,2} MD Anderson Cancer Center UTHealth Graduate School of Biomedical Sciences, Houston, Texas, 77030, USA.

*Correspondence to: Alemayehu.g.abebe@uth.tmc.edu

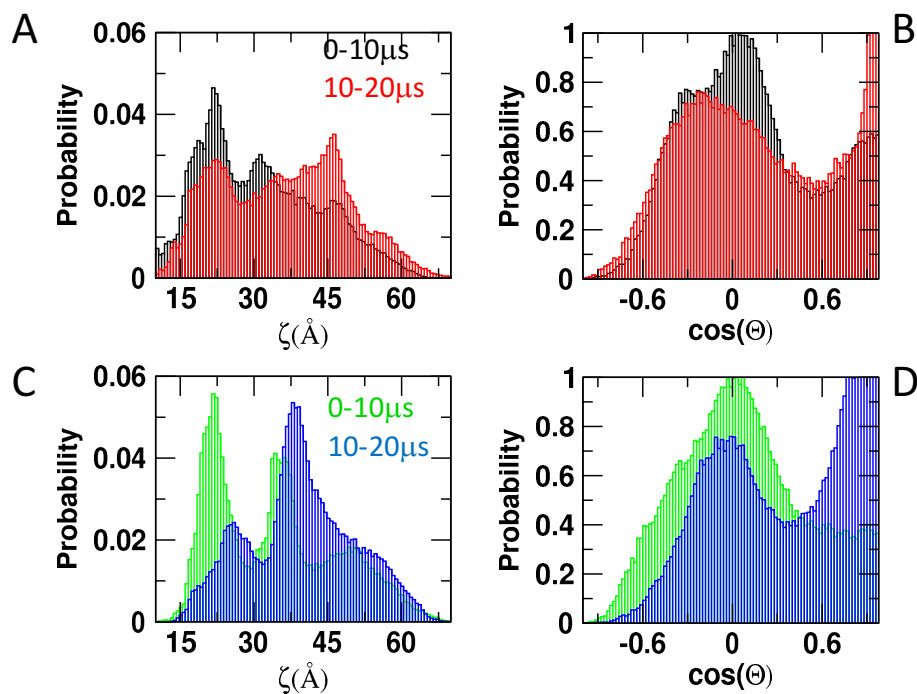


Figure S1: Conformational fluctuations of membrane-bound G12D (A & C) and Q61H (B & D) KRAS mutants during the first- and second-halves of a 20 μs MD simulation. (A, B) Normalized histograms of ζ (distance between the C α atoms of D132 and T183). (C, D) Normalized histograms of $\cos(\Theta)$ (cosine of the angle between a vector along beta-strand 1 (residues 5-9) and the membrane normal).