Figure S1. Dynamic changes of the secondary structure profile for (A) WT, (B) A52V mutant, (C) E203K mutant and (D) P124S mutant MEK-1 throughout the simulation. The colored bar represented different secondary structures as follows: coil (C), π-helix (I), helix (G), α-helix (H), β-Bridge (B), β-bugle (E), turn (T).

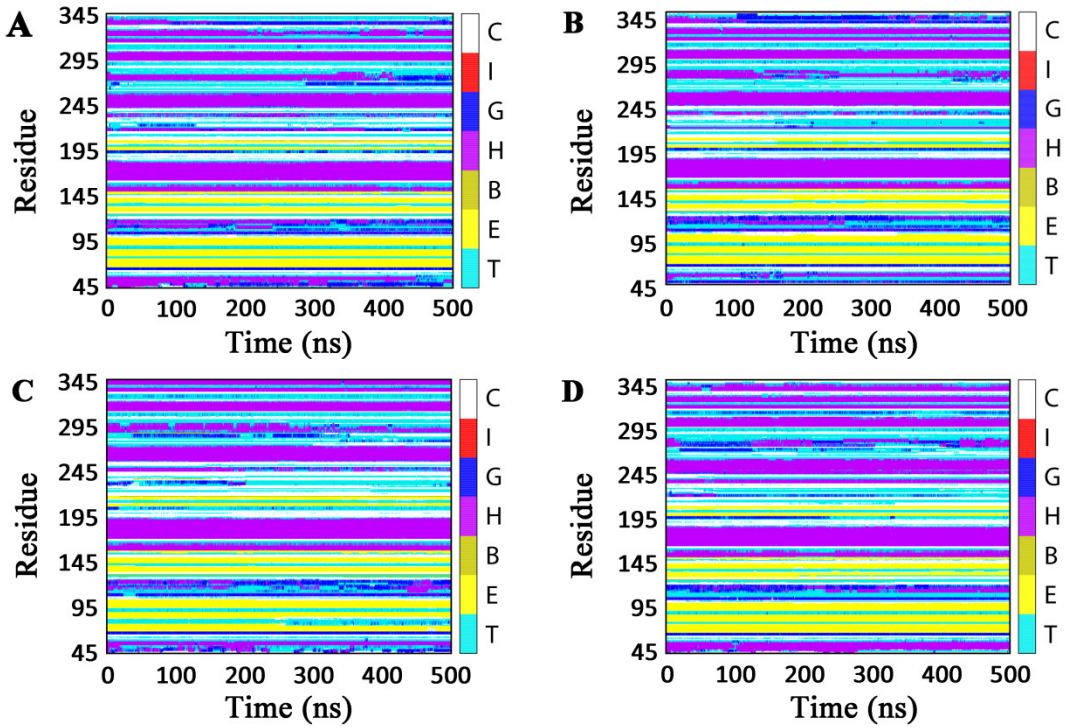

Figure S2 Typical force profiles of ligands pulled out of the MEK1 pocket along the unbinding pathway.

