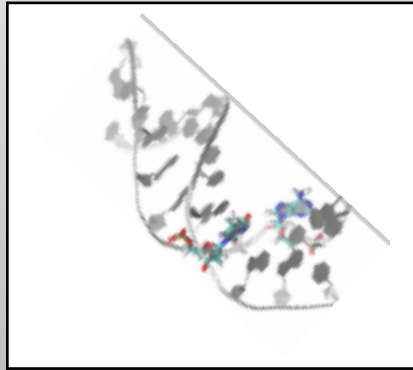
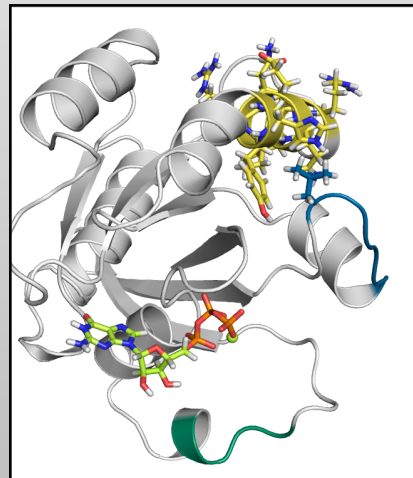


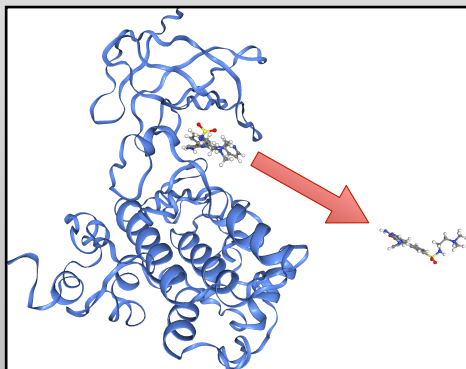
Questions



What is the mechanism of the Watson-Crick to Hoogsteen conformational transition in DNA?

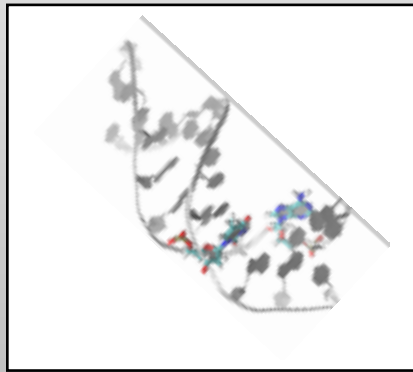


Are there fundamental differences in the dynamics of wild type and oncogenic mutant proteins?

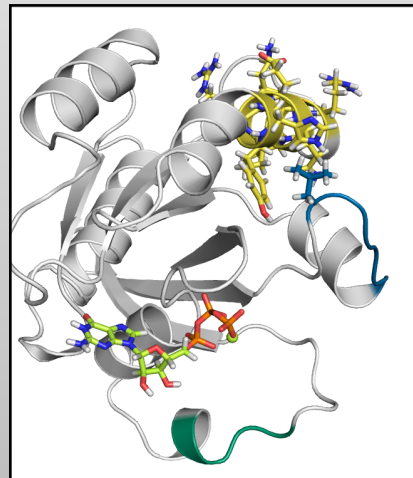


How does a drug bind/unbind from its target site? What role do non-target short-lived binding poses play?

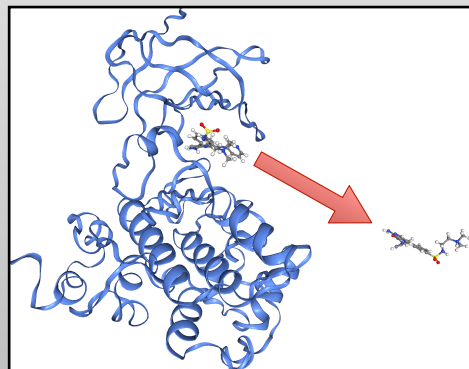
Answers



Path sampling simulations show that the outside channel is preferred in the WC-HG transition in DNA.



Path sampling simulations identify the differences in dynamics that lead to the K-Ras Q61L mutant causing cancer.



New on-the-fly state definitions in path sampling will help us characterize the role of intermediates in drug unbinding.