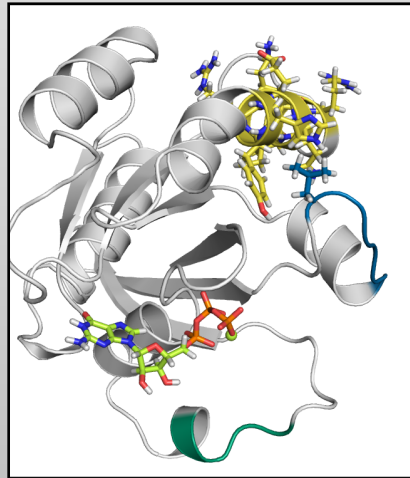
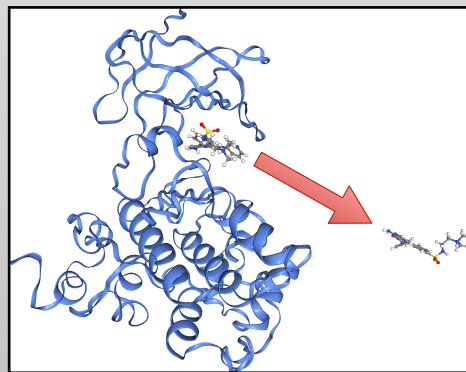


# Questions



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?

# Simulation philosophy

- ***Unbiased dynamics:*** Make as few assumptions as possible about what degrees of freedom are important
- ***Full atomistic:*** High resolution in space and time
- ***Calculate rates, observe mechanisms:***  
Compare with experiment and provide new insight