

K-Ras Q61L: An oncogenic mutation

Q61L

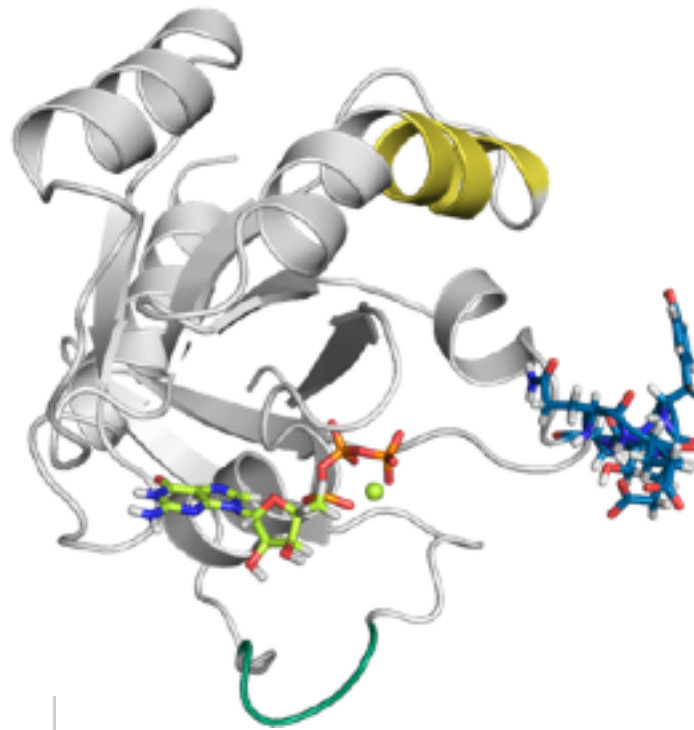
- residue 61 is part of switch 2
- change a charged residue to hydrophobic
- known to be oncogenic (more relevant in H-Ras than K-Ras)

TPS simulations

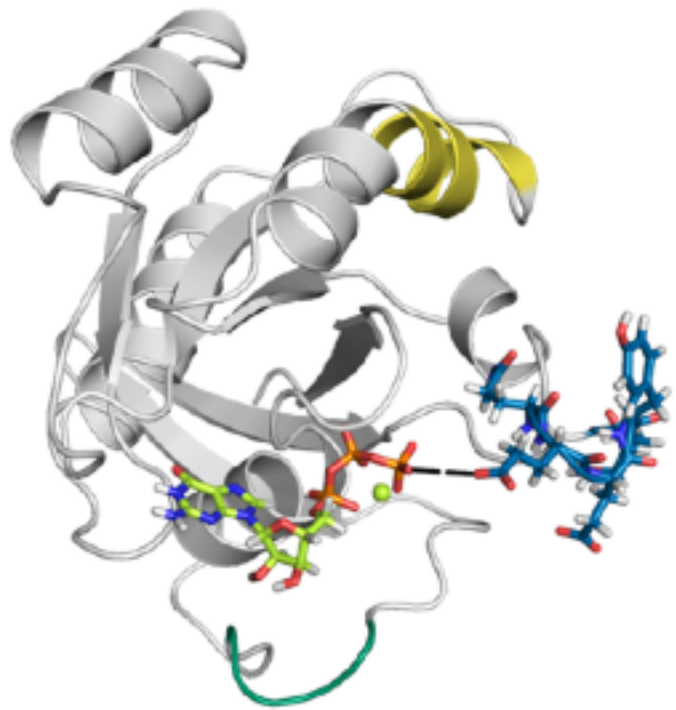
- multiple state transition path sampling
- separate runs for switch 1 and switch 2 (3 states in each)
- separate runs for wild type and mutant

4 different simulations; only going to look at switch 2 results

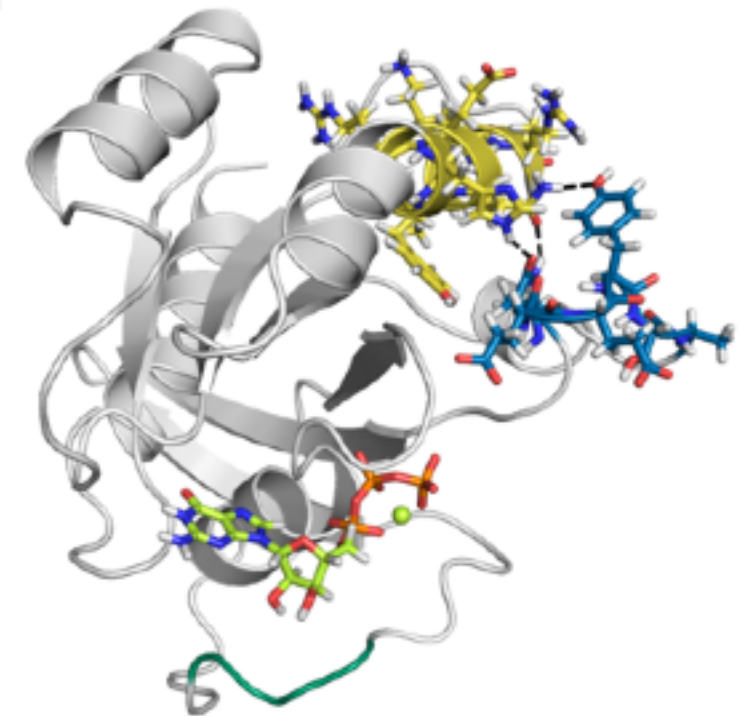
Switch 2 States



S2 open



S2 GTP-bound



S2 α3-bound