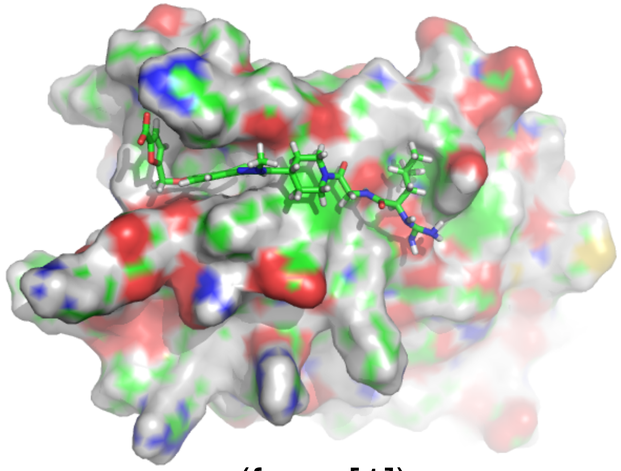
Docking approximates binding ΔG

- $\Delta G = \Delta H + T\Delta S$

- Docking score ~ ΔH
- It sometimes involves
  - ad hoc ΔS based on the number of rotatable bonds
  - ΔG_{solv}
- Docking is based on “optimal” orientations



(from [1])

How is ΔG/ΔA calculated from molecular simulations?