cheaper than PB

MM-GBSA

↳ only good for relative energy differences (not absolute)

☆ Start with a single structure
- also the minimized 19F Xtals

* Collect conformations every 100ps from equilibrated portion of simulations

* Calculate

E_{bond}
$E_{dihedral}$
E_{vdw}
E_{elec}
ΔG_{solv}

* Explore using molecular surface area vs. van der Waal radii for ΔG_{SA}

ΔG_{SA} ← surface area dependent term $= \gamma(SA)$ ↑

ΔG_{GB} - Generalized Born

$-T\Delta S_{config}$

normal mode approx

molecular surface

van der Waals radii

better method but a good coeff needed (γ)

• see literature: How to calc error in MM/GBSA