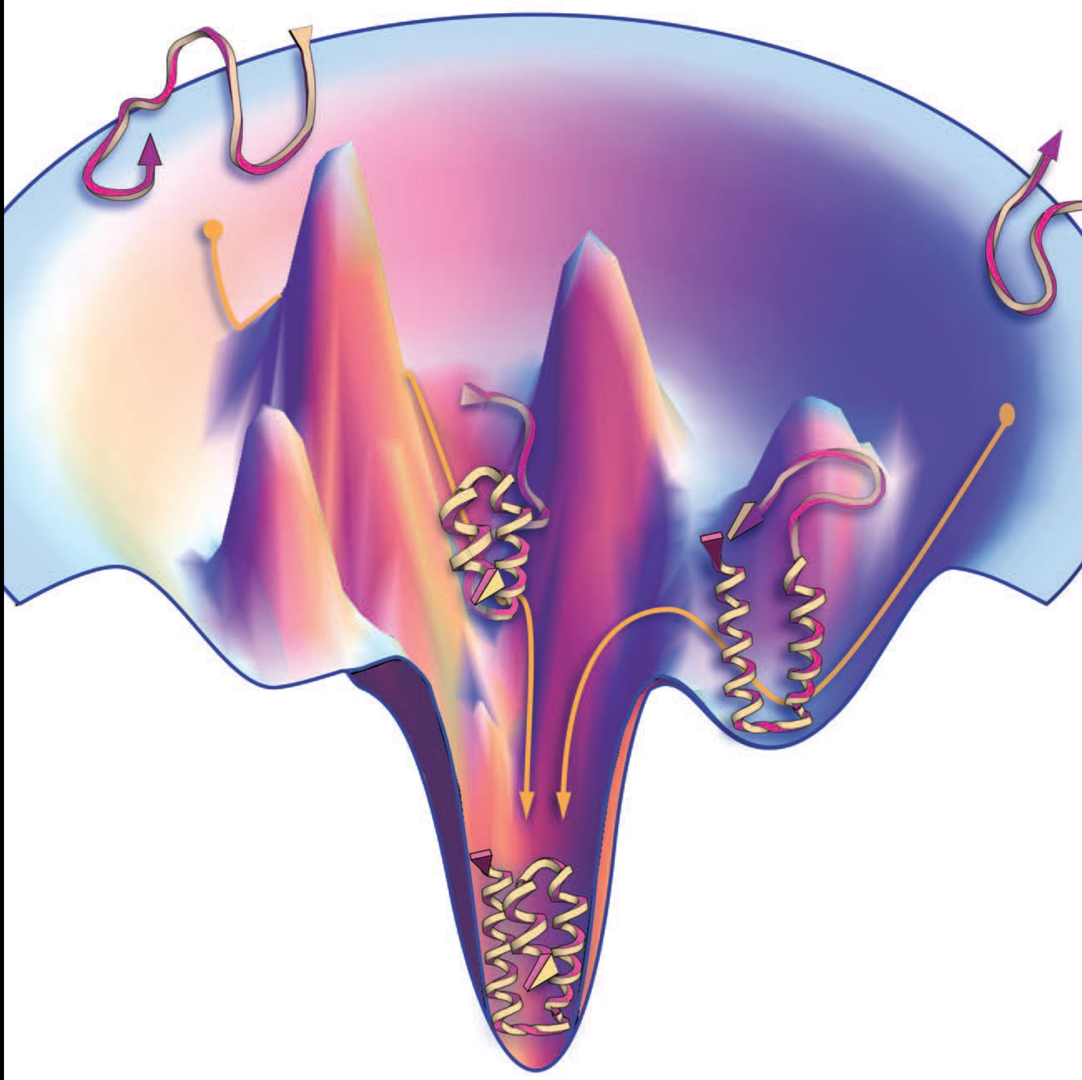
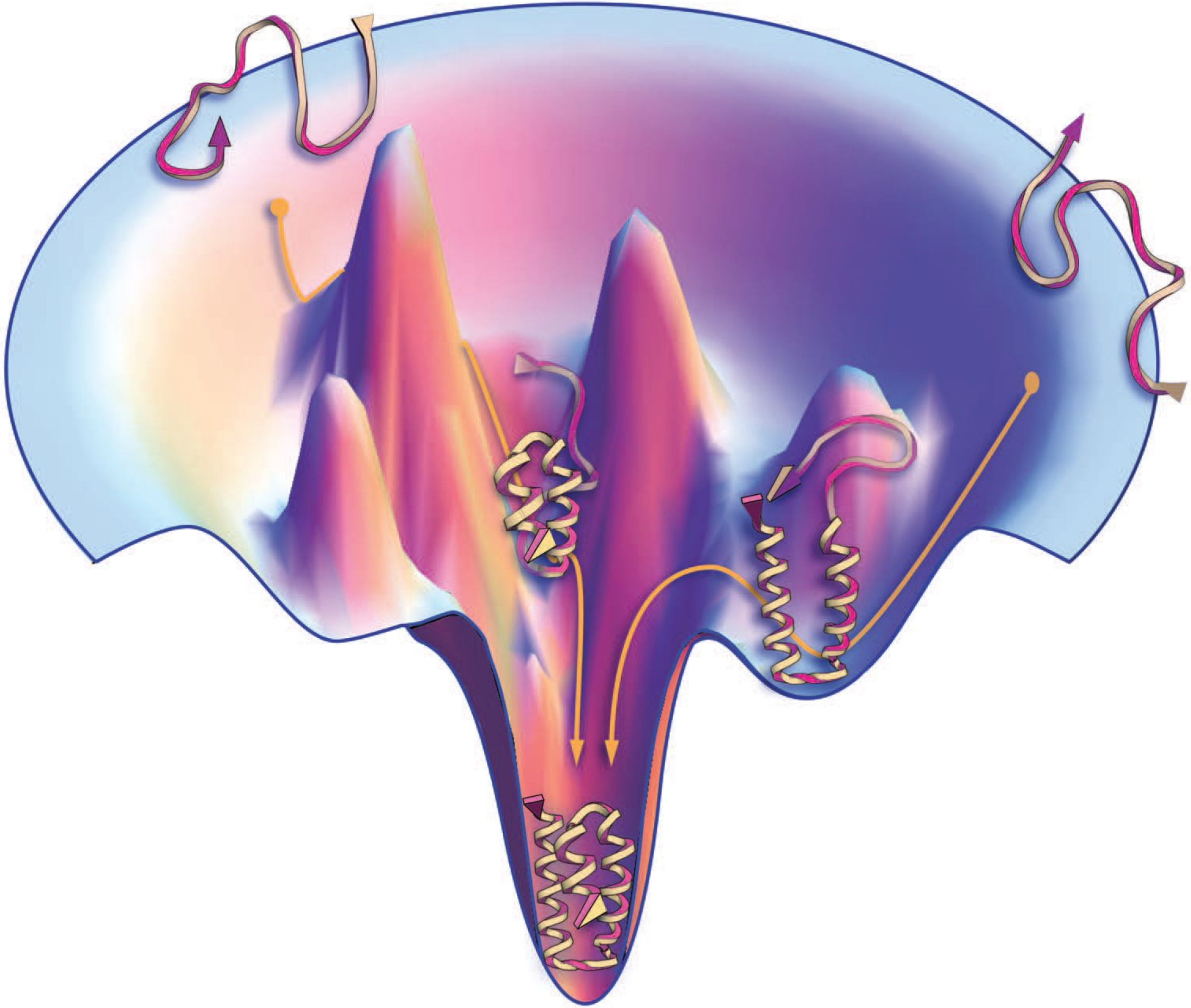
Minimizing in Foldit

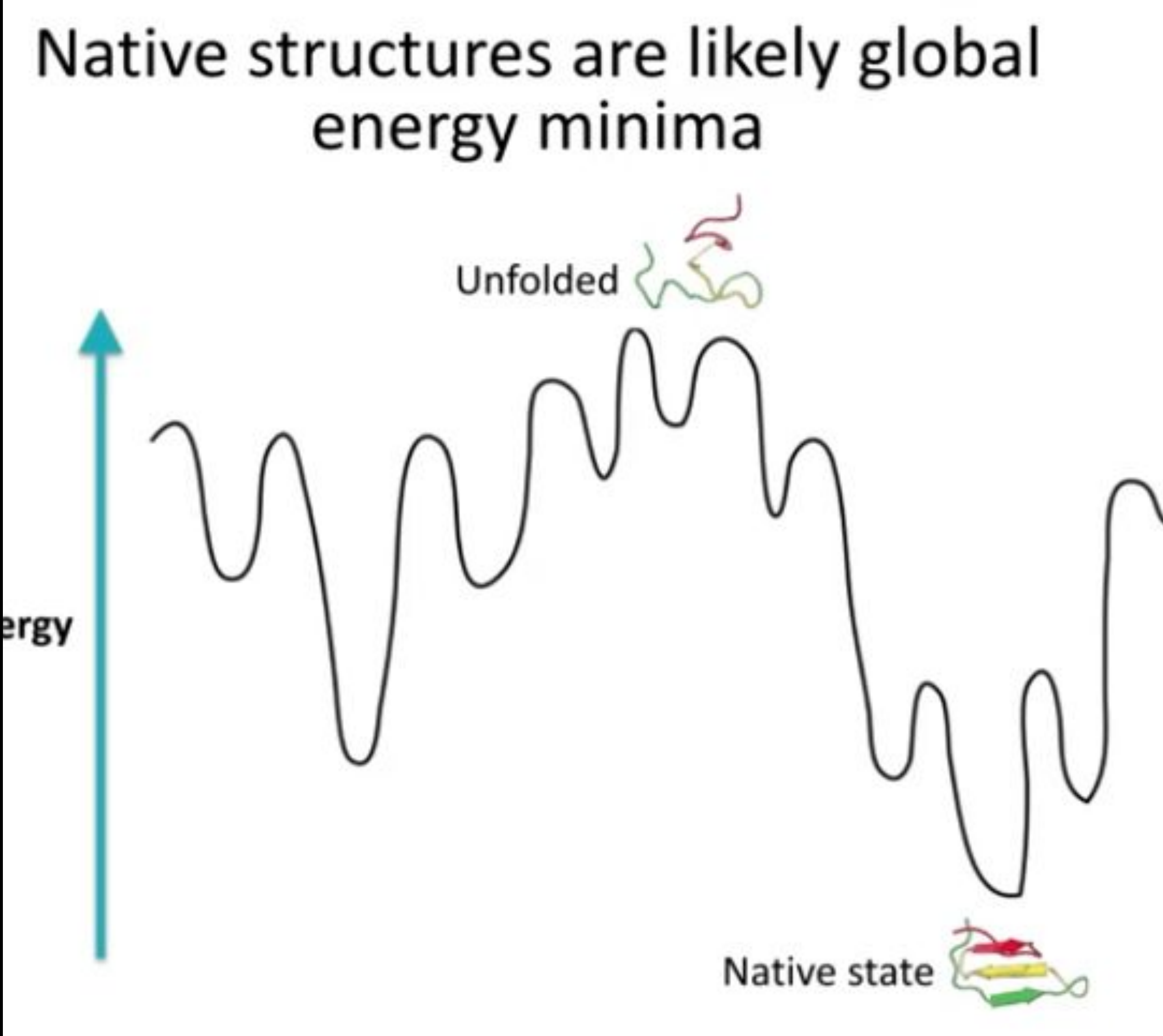
What is minimization and why do we need to minimize?



Explain this figure: what's going on here?

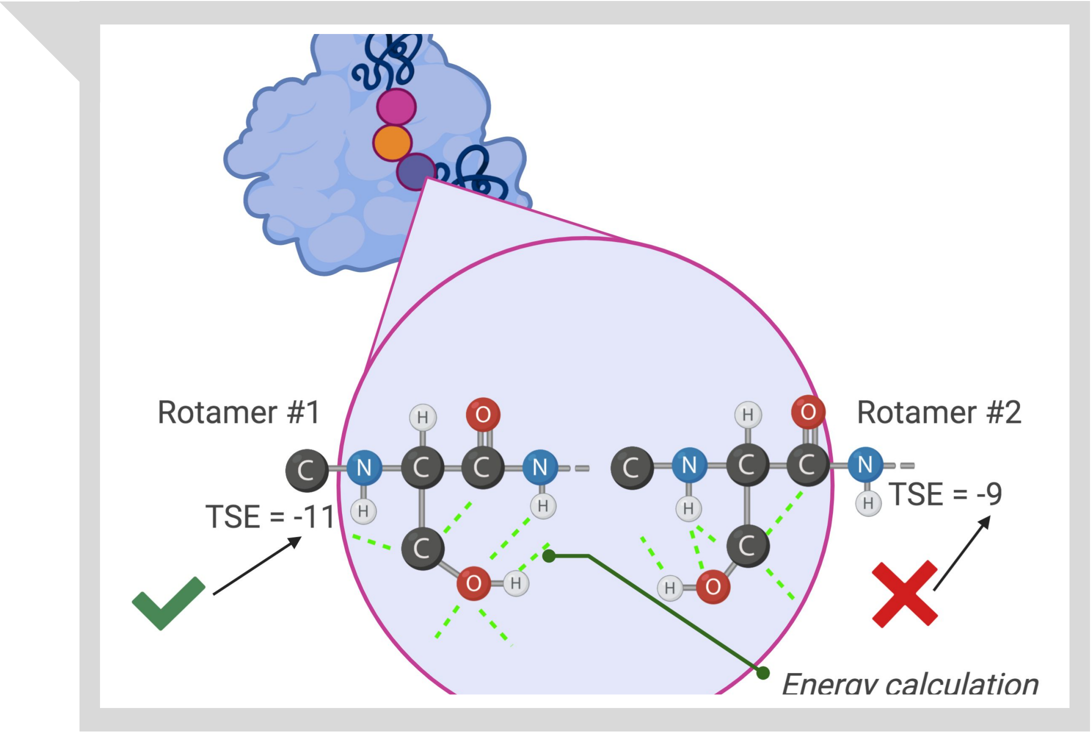


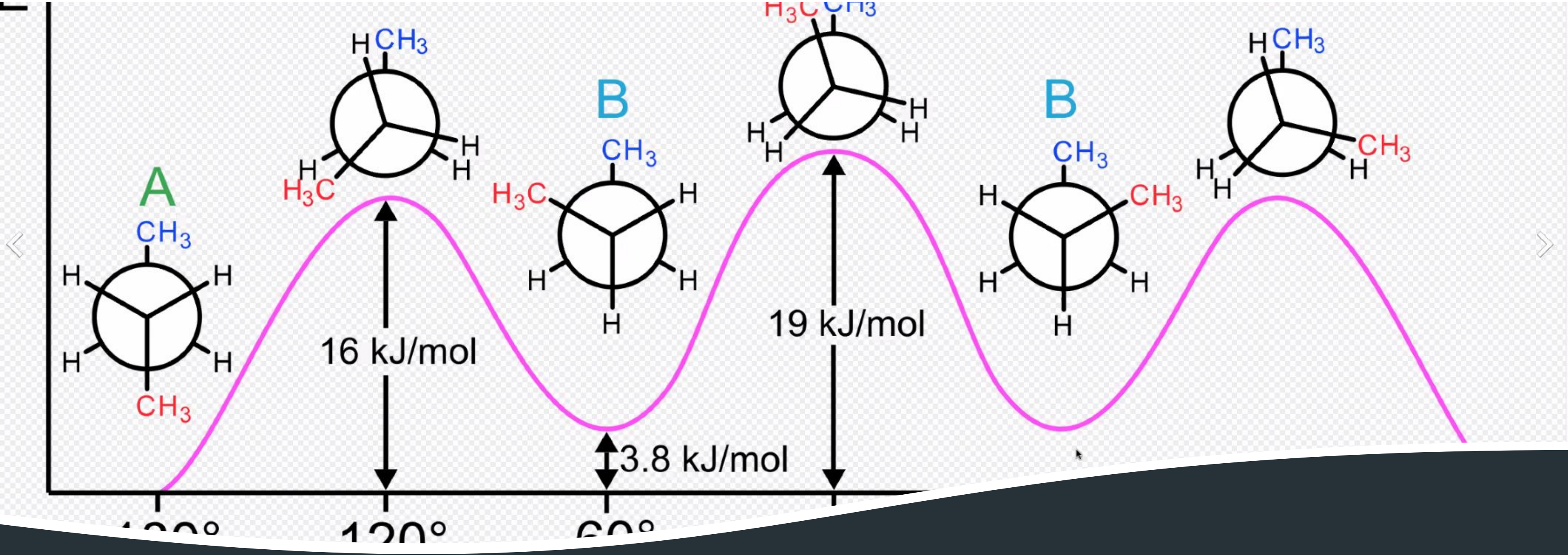
Another way to look at this (2D)



Native structures are likely global energy minima

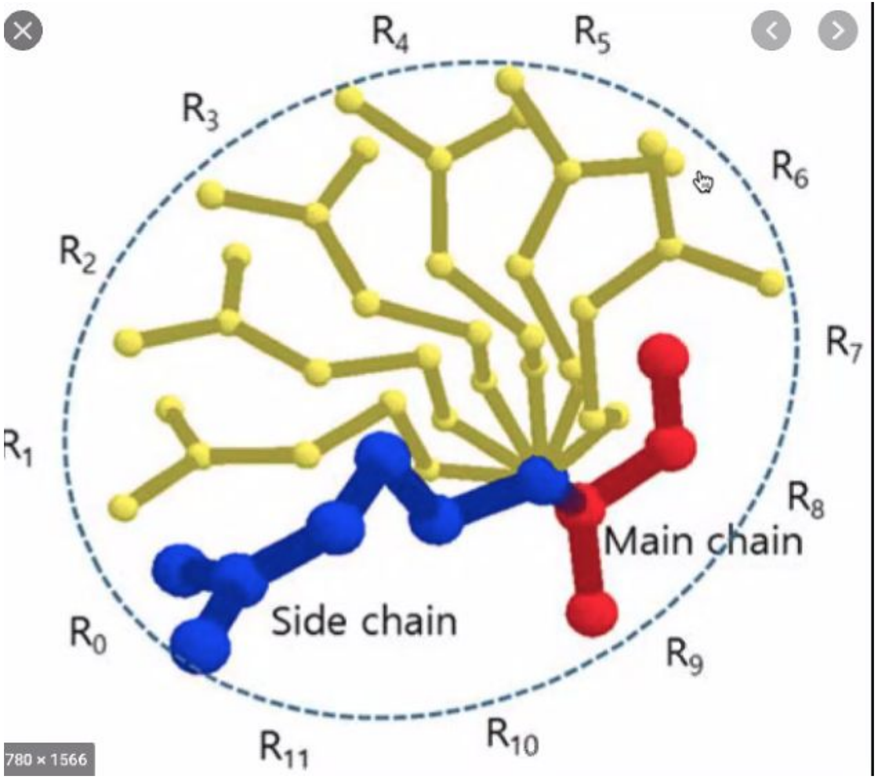
Thinking about not just backbone structure but actual rotamers





And the energy landscape of rotamers

And one other cool way to look at them. Here you can imagine the spaces between the rotamers… (this will be important soon)



Modeling in Foldit: translating concepts to game moves

Repack/Shake (S)	**Wiggle (W)**	**Minimize (E)**
The shake tool optimizes all of the protein side chains by rotating in different combinations to f**ind the best-scoring position for each one using the rotamer library**, based on gaussian angles.	Wiggle tries to optimize the backbone and the side chains in a more refined way than shake. You can imagine landing at a rotamer position, suggested by the library but that with a little tweaking you can **explore space between the rotamers defined in the library**, which might drop you to a lower “energy well”. Wiggle (W) will explore small movements in the backbone and sidechain to find those most favorable confirmations beyond what’s suggested by the library rotamers.	Minimize is a **version of wiggle that restricts the backbone** movement and only moves the sidechains between the library-defined rotamers