

## Side chain flexibility

In physics, **degrees of freedom** refers to the number of variables required to describe the system. It is an analog to the same idea in statistics, but used for different things.

- A single particle in space has 3 degrees of freedom (x,y,z)
- A 3D object in space has 6 degrees of freedom (x,y,z,yaw,pitch,roll)

In summary...

- for each residue we have two torsional degrees of freedom (DOF) in the main chain ( $\phi$  and  $\psi$ )
- each residue also has 0-4 DOF in its side chain, which affects the local form of this side chain
- therefore, a residue can have up to 6 DOF

## Why do proteins fold?

- reduce energy levels
- polar side chains want to interact with the water and with each other
- reducing hydrophobic surface area: non-polar side chains want to stay away from the water and polar side chains and interact with each other
- condensed non-polar residues cause protein to compact and assume a globular shape

## Secondary structure

Folded proteins form regular structure patterns (secondary structures) to increase hydrogen bonding and reduce steric clashing.

- $\alpha$  helices
  - most common
  - they have *handedness* (or chirality); most are right-handed (left-handed helices have steric constraints)
  - can be amphipathic
  - has periodicity: residues 3-4 spaces apart may have the same face
- $\beta$  strands/sheets
  - can be formed from both parallel and antiparallel peptide strands
  - parallel sheets are always buried, but antiparallel sheets are more stable
- $\beta$  turns: smallest secondary structure, stabilized by hydrogen bonding

## Calculations

- If we have Cartesian coordinates of each amino acid, can we calculate bond lengths, bond angles, and torsional angles?
- Inversely, if we have bond lengths, bond angles, and torsional angles, can we calculate Cartesian coordinates?