Protein Structural Models
for CHEM 527

Proteins are made by linking amino acids

20 common amino acids
Tertiary folds are often the result of layering of secondary structures.
Alcohol dehydrogenase is a homotetramer
Peptide Plane Reduces the Number of Parameters

Tortion angles

\( \phi \)  PHI

\( \Psi \)  PSI

Tortion kinemage: C1basics.kin

Ramachandran Plot to Evaluate Outliers of “Good Protein Geometry”

Ramachandran plot from htADH

- Core (%) 91.3 %
- Allowed (%) 8.2 %
- Generously allowed 0.4 %
- Disallowed none

Plot statistics:

- Residues (unique/total residues) 120/265
- Residues (unique/totally allowed) 112/265
- Residues (unique/ambiguously allowed) 8/265
- Number of Ramachandran outliers 170
- Number of outliers (or equivalent helix angles) 170
- Total number of outliers 170
RMSD from Ideal Protein Geometry

RMSD from ideal geometry for htADH structure

- bonds (Å) 0.007
- angles (°) 1.30
- dihedrals (°) 23.60
- impropers (°) 0.85

Hydrogen Bonding Connection

- L²O ...... W₆ιH
- Y¹O ...... L'ιH
- T¹O ...... K²ιH
- G¹⁰ιH ...... G¹⁵ιH
- G¹¹ιH ...... G¹⁶ιH
- W₆ιHE3 ...... R¹⁸ιO
- L¹O ...... G¹³ιH
- W²O ...... G¹⁴ιH
Molecular Dynamic Simulation of a designed mini-protein (Trp-cage)

From the Duan lab
http://www.duanlab.ucdavis.edu/

The movie shown 2 slides ahead is 69.5 MB and can be downloaded here