Protein Structure Review and Refinement Introduction

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Proteins are made by linking amino acids

Several Ways to Visualize Amino Acids
20 common amino acids

Primary Sequence → Secondary Structure
Alcohol dehydrogenase is a homotetramer
The Peptide Plane

Peptide Plane Reduces the Number of Parameters

Tortion angles

$\phi$ PHI

$\Psi$ PSI
Ramachandran Plot to Evaluate Outliers of “Good Protein Geometry”

Ramachandran plot from hADH
- core (%) 91.3%
- allowed (%) 8.2%
- generously allowed 0.4%
- disallowed none

Macromolecular Protein Crystallography
Experimental Data Points vs. Refined Parameters

X-ray Diffraction Reflections
Experimental Data Points

Electron Density Map and Refined Model of Enzyme

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
Least Squares Refinement Summed Over all Atoms and Data Points

From Crystallography Made Crystal Clear

Chapter 7. Obtaining and Judging the Molecular Model

\[ \Phi = \sum_{hkl} w_{hkl} \left( |F_{o,hkl}| - |F_{c,hkl}| \right)^2 + \sum_j w_j \left( d_j^{\text{ideal}} - d_j^{\text{model}} \right)^2 + \sum_j w_j \left( \phi_j^{\text{ideal}} - \phi_j^{\text{model}} \right)^2 \]

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
Trp Cage Peptide Sequence

1  5  10  15  20
N L Y I Q W L K D G P S S G R P P S

Hydrogen Bonding Connection

L2:O-------W6:H
Y3:O-------L1:H
I4:O-------K8:H
G10:O-------S13:H
G11:O-------S14:H
W6:H---E1---R16:O
L1:O-------G12:H
W6:O-------G13:H