# Protein Folding Simulations Proteins, Aminos, Folding, and Trajectories

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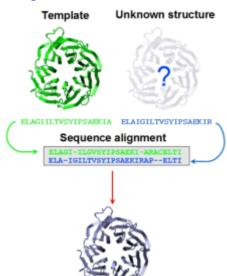
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#### Protein Structure Prediction Methods

- Homology modeling
- Fold recognition
- Fragment Assembly
- Molecular dynamics

# Homology Modeling



### Protein Folding Simulations

v(t)

#### **Molecular Dynamics**

t x(t)1. Assign
2. Calcu

I. Assign velocities to all atoms

2. Calculate forces on all atoms

3. Use Newton's second law to calculate acceleration on each atom F=ma

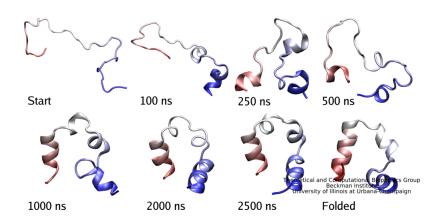


4. Calculate velocities for the next timestep

5. Use change of velocities to get coordinates for next timestep

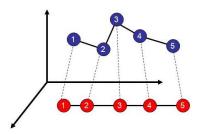
6. Go to step 2.

# Protein Folding Simulations

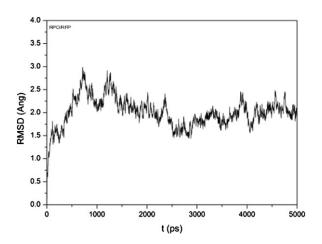


#### Comparison between structures

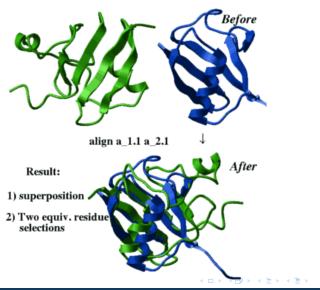
Using RMSD to find the optimal superposition



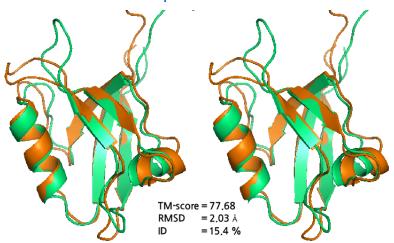
# Protein Folding Trajectories



# Protein Comparison



#### Metrics for Protein Comparison



RMLPRLCCLEKGPNGYGFHLHGEKG---KLGQYIRLVEPGSPAE-KAGLLAGDRLVEVNGENVEKETHQQVVSRIRAALNAVRLLVVDPETDEQL---GAITYTVELKRYGGPLGITISG1--EPFPDFIIISSLIKGGLAERTGAINIGDRILAINSSSLKGKPLSEAIHLLDWAGETVILKIKKGTDAO--PASS