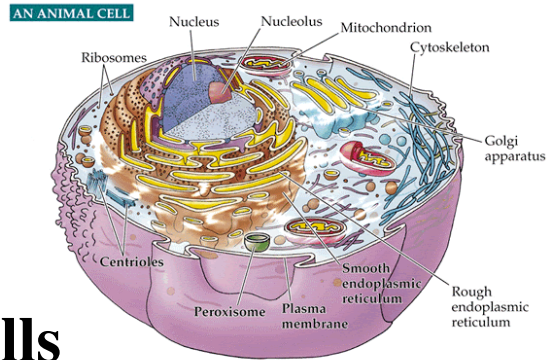


Introduction to:

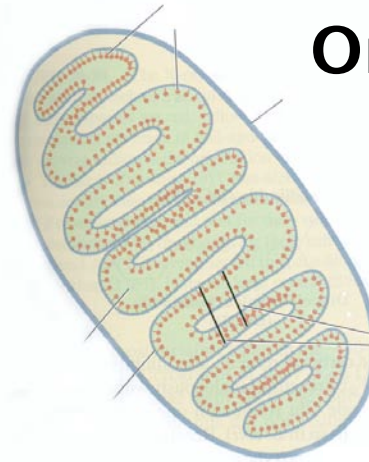
Visual **M**olecular **D**ynamics

Cells

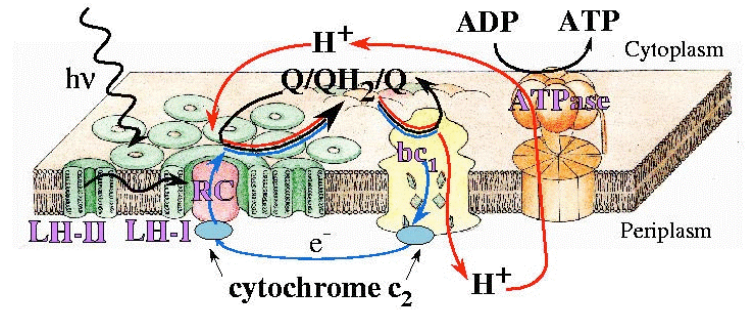


© 2001 Sinauer Associates, Inc.

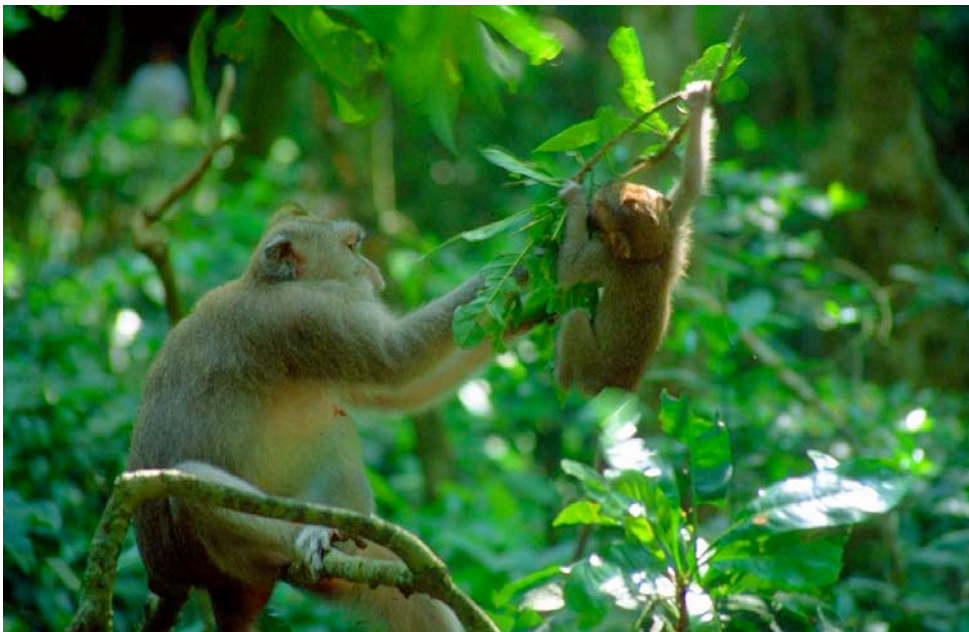
Organelles



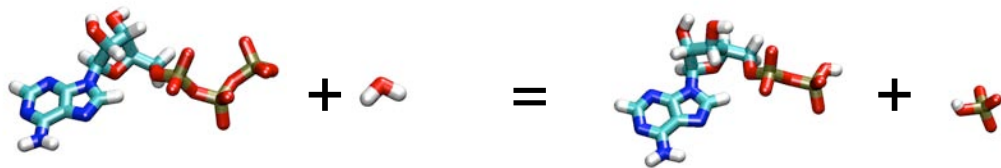
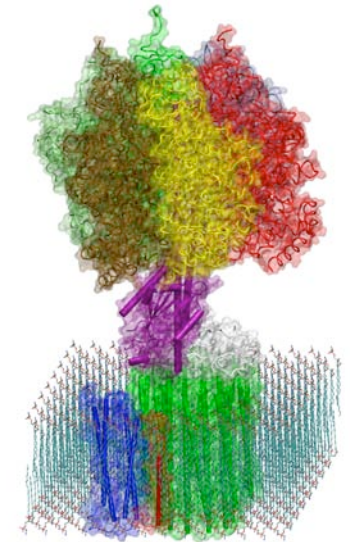
Integral units



Theoretical Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign

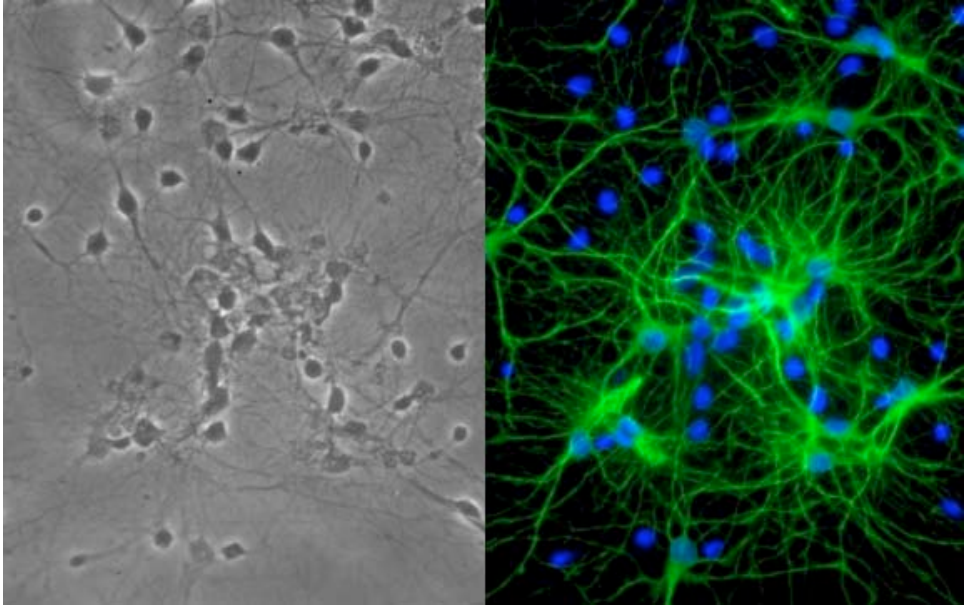


Protein machines

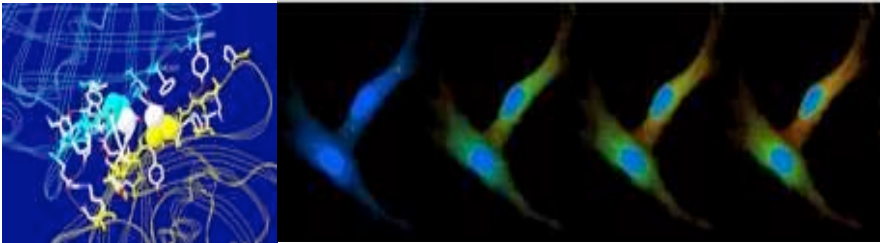


Chemical reactions

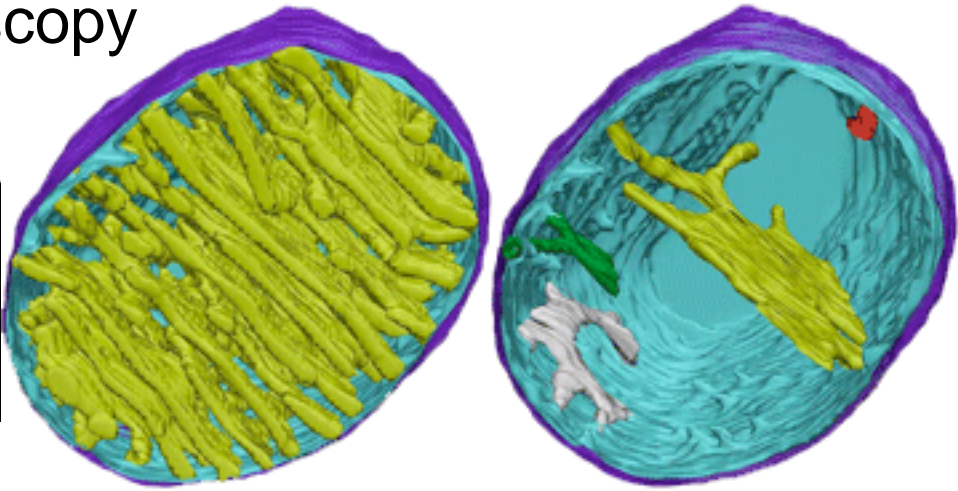
Visualization biomolecular organization



Optical and fluorescence microscopy

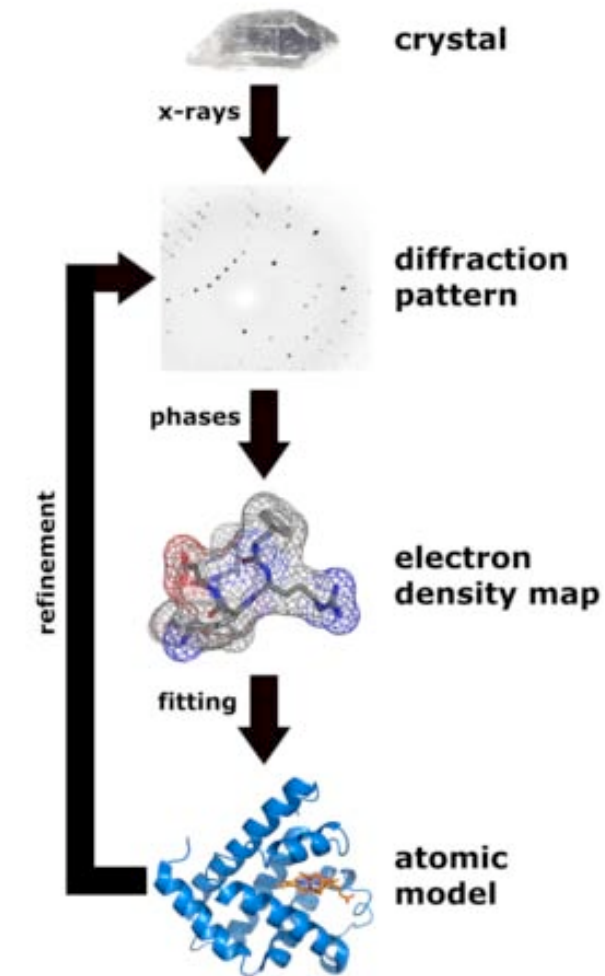


FRET

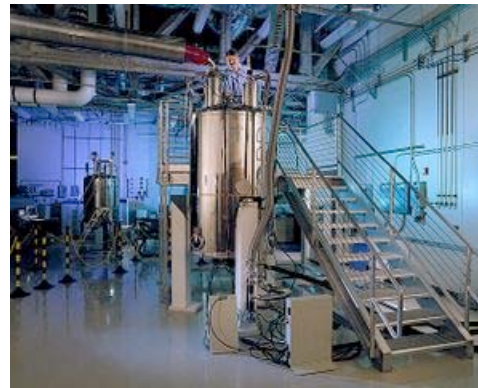


Electron tomography

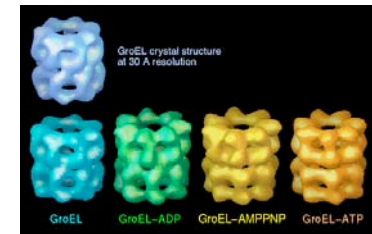
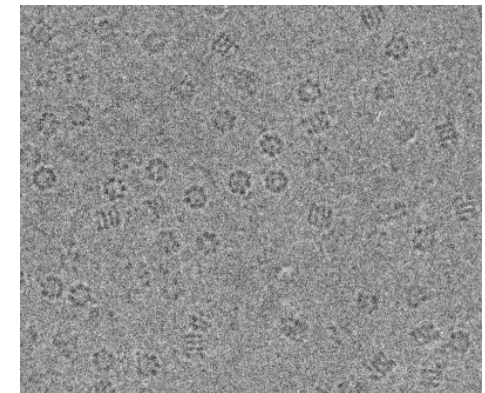
Sources of atomic-scale structural information



X-ray crystallography

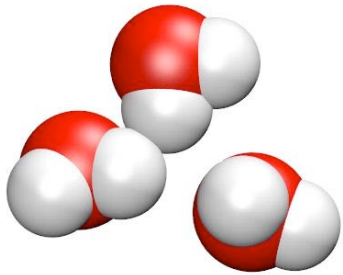


NMR

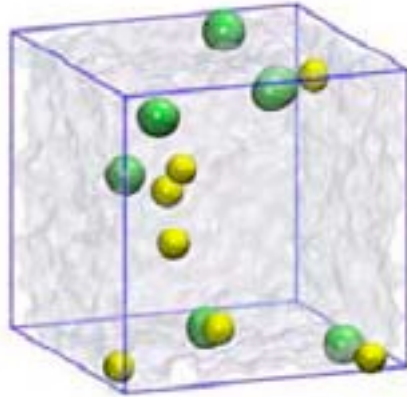


Electron Microscopy

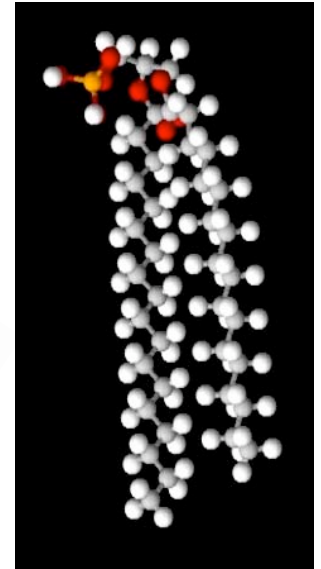
Cell components



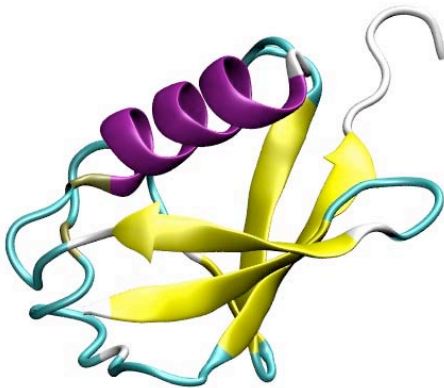
Water



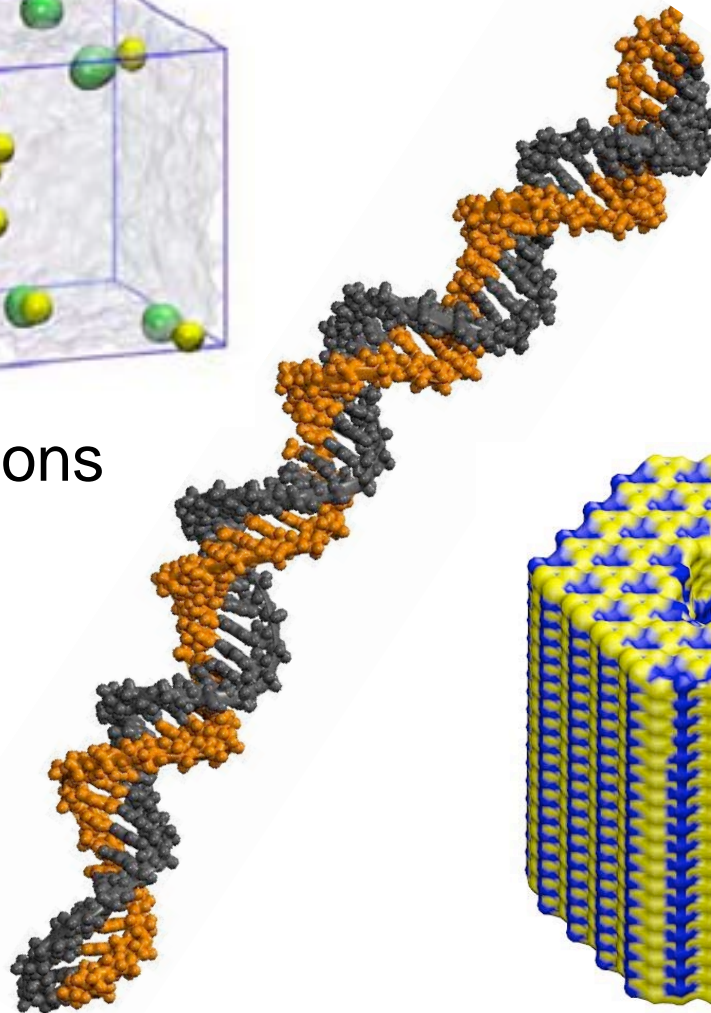
Ions



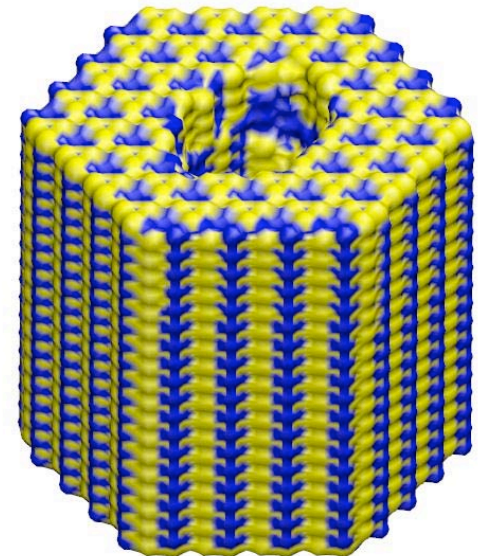
lipids



proteins

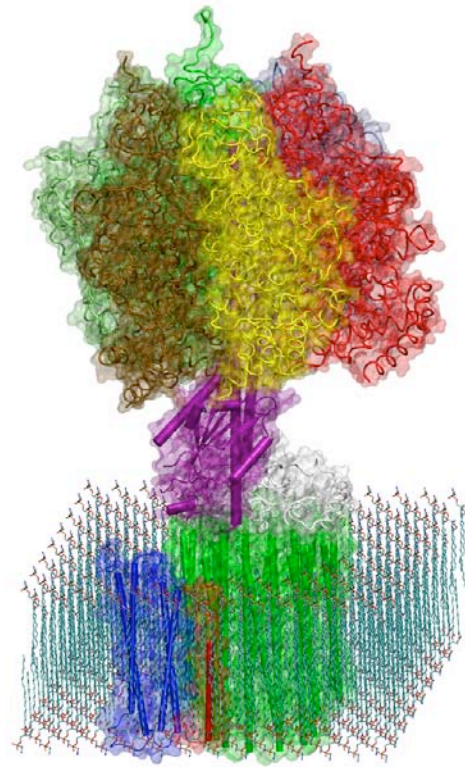


DNA

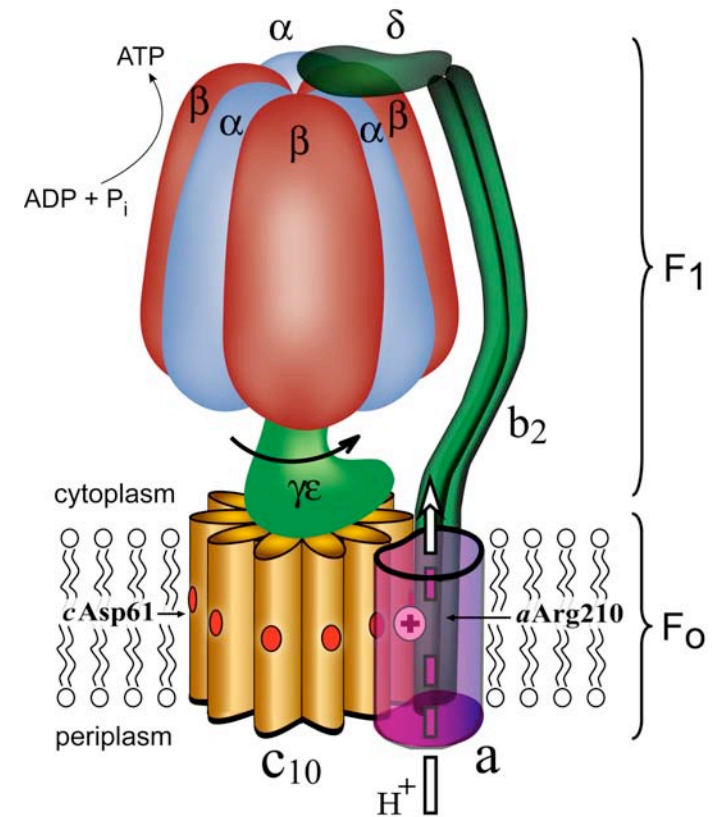


Synthetic components

Humans perceive information through vision

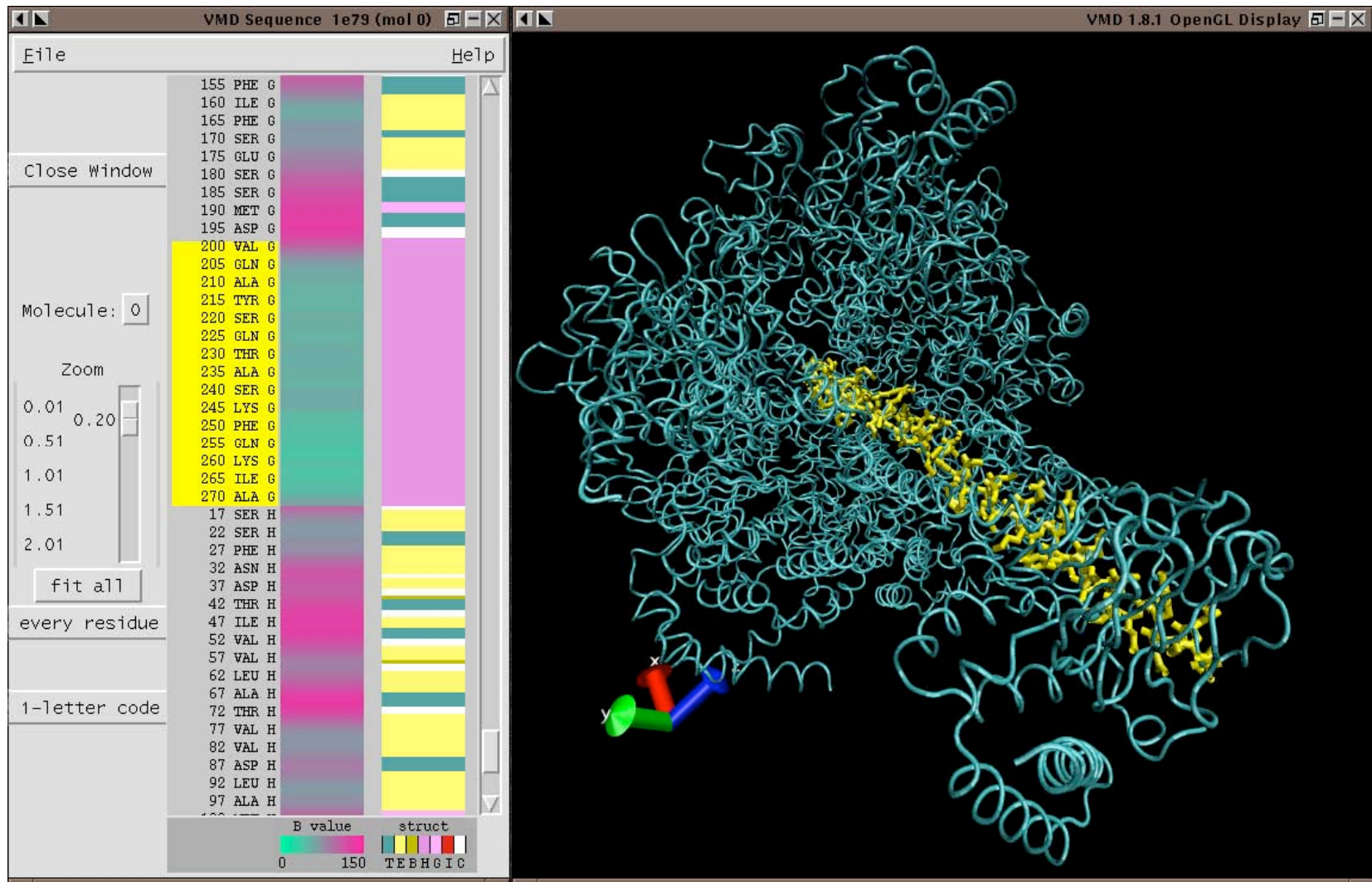


Molecular structure of FoF1-ATP synthase

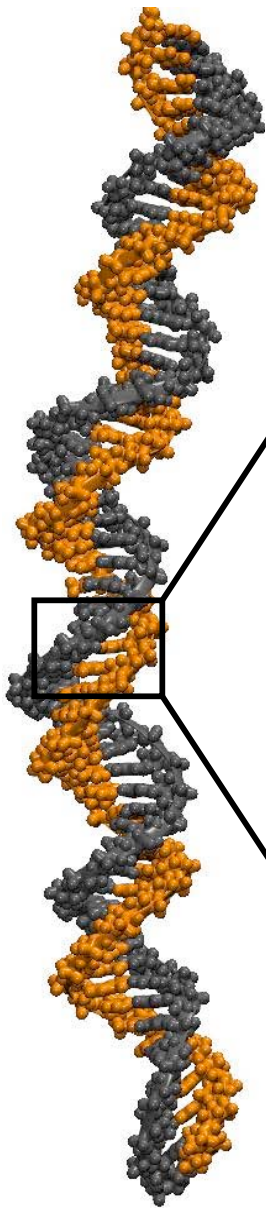


No real image - use schematics

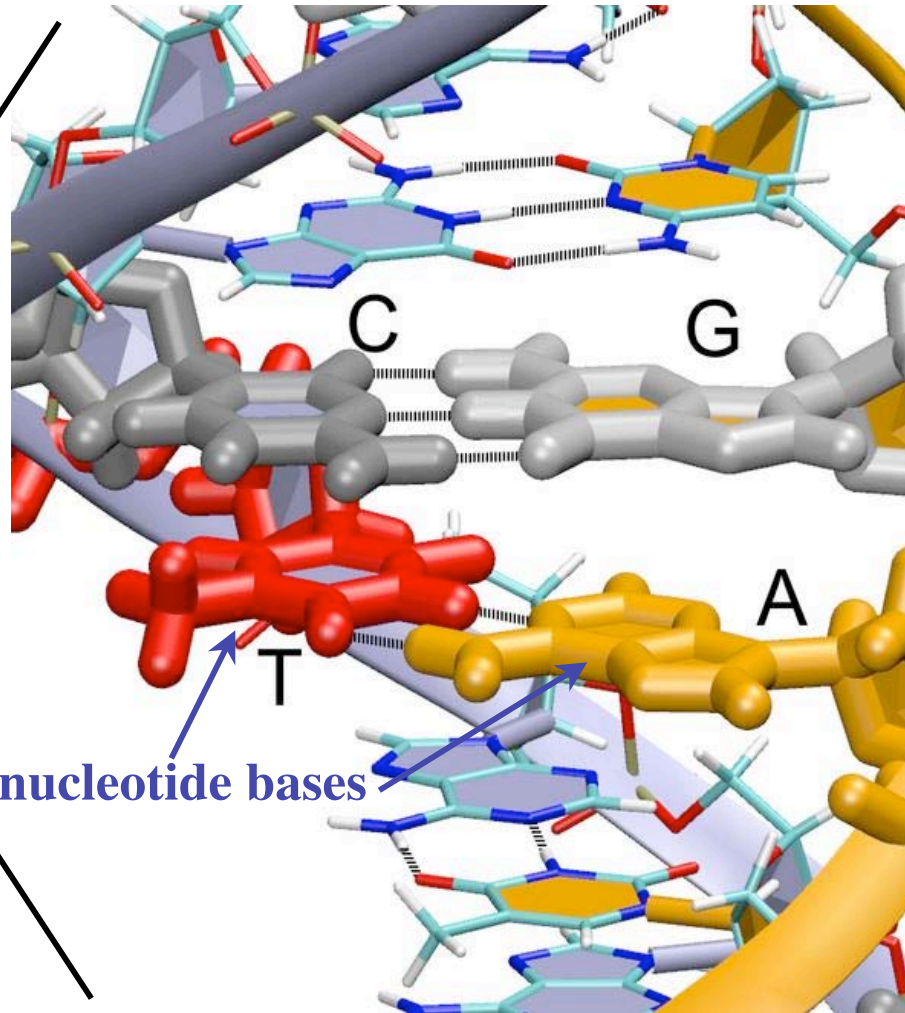
VMD - a program for looking at biomolecules



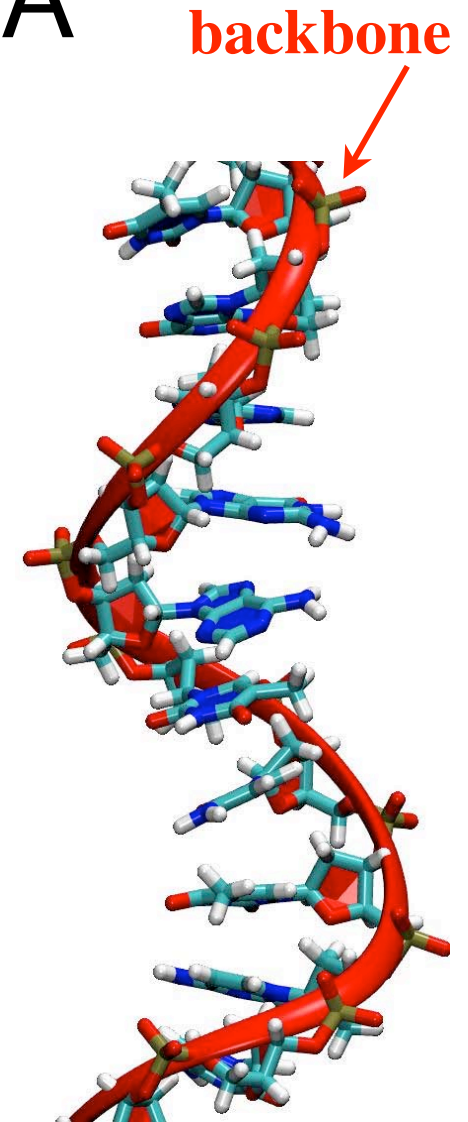
Learn by looking: DNA



Double stranded DNA

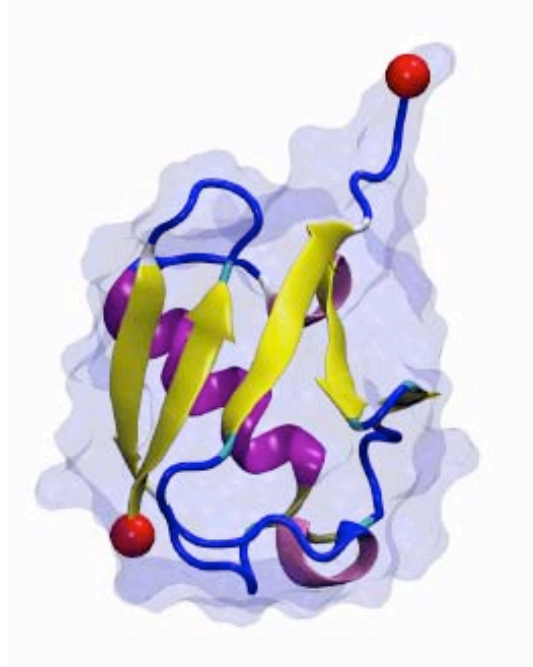


5'-AAGCTGGTTCAG-3'



Single stranded DNA

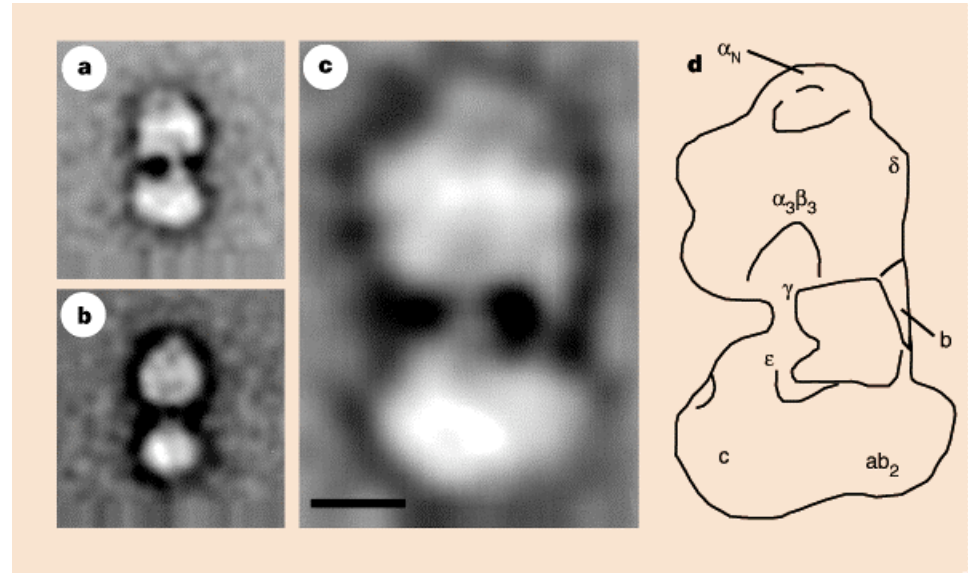
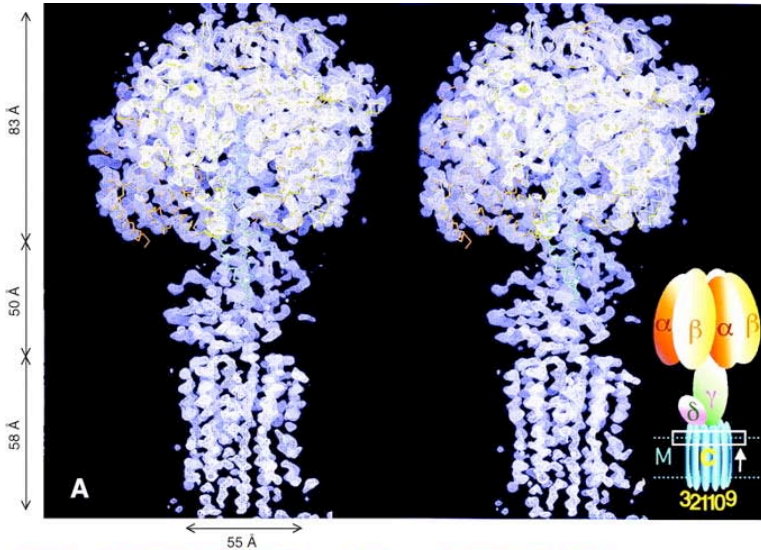
VMD Molecular Graphics



VMD Developer: John Stone

Jordi Cohen
Marcos Sotomayor
Elizabeth Villa
October 2006

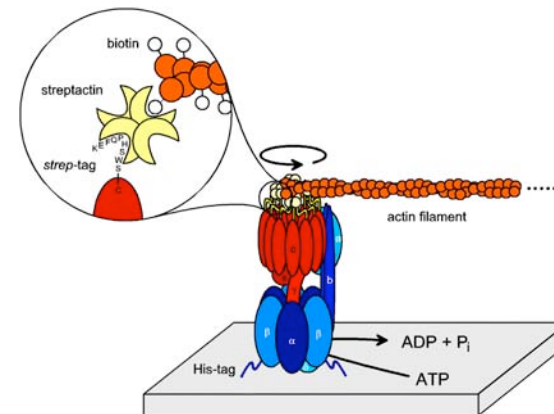
ATPase Structure Data



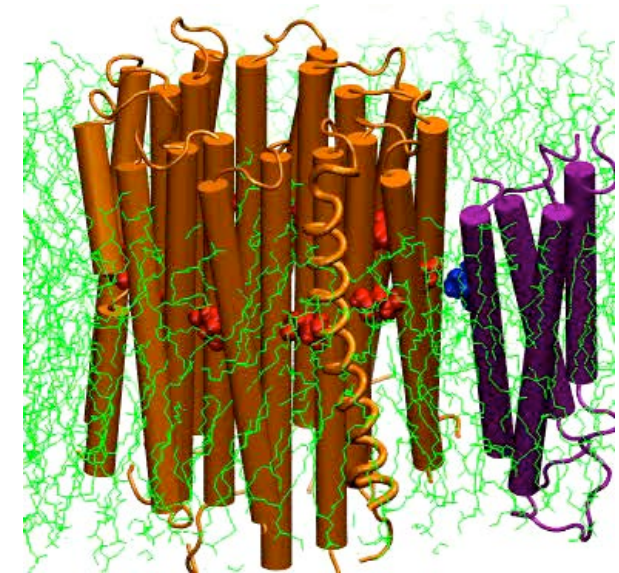
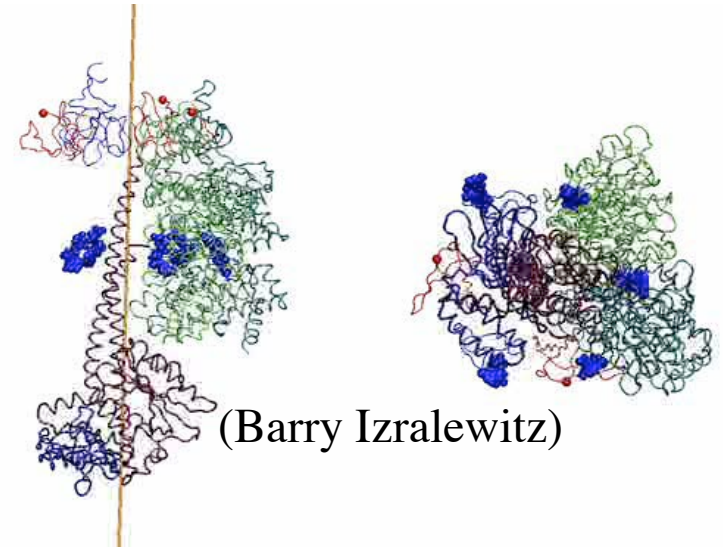
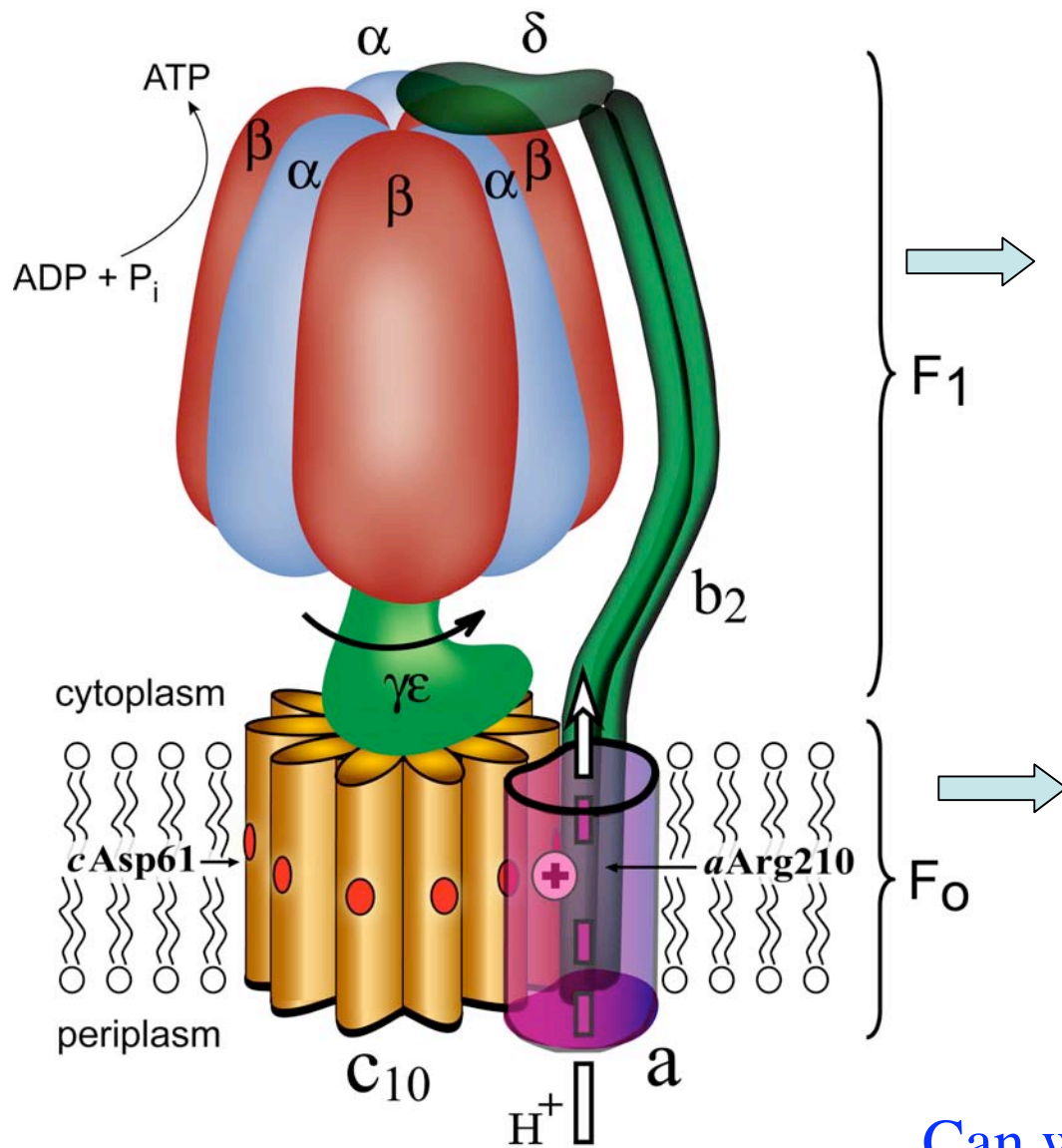
X-ray structure, 3.9Å
Stock et al., Science (1999)



(Wolfgang Junge)

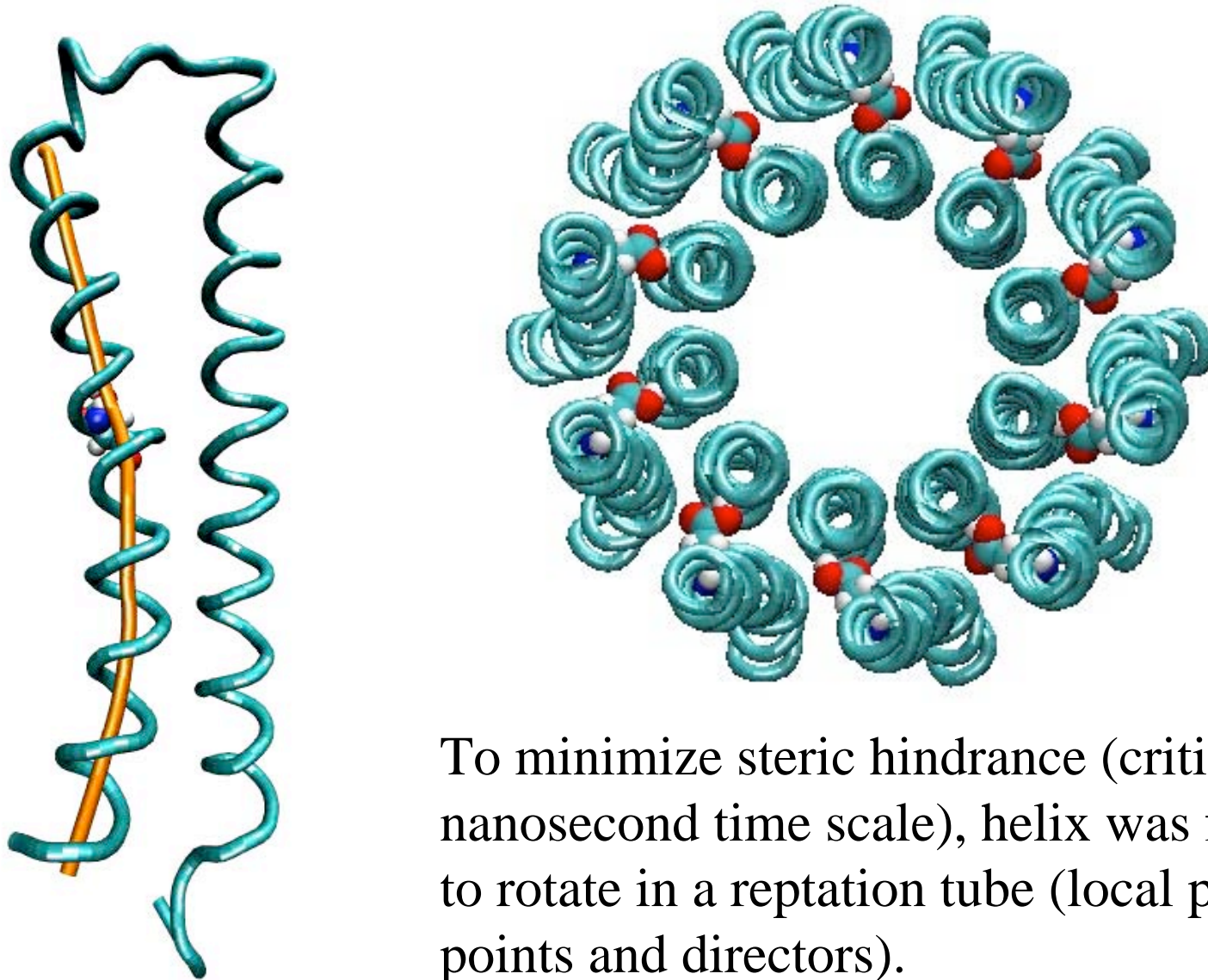


Learn by looking: F-ATP synthase



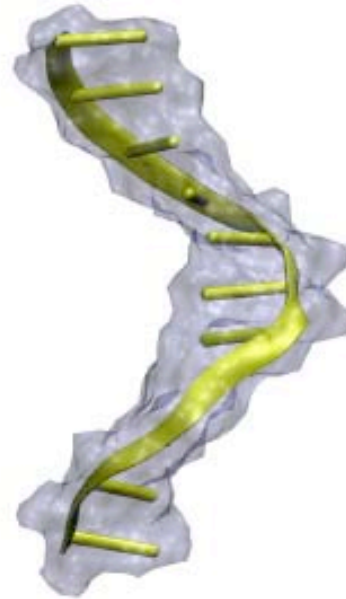
Can work in reverse!

Structure of the Fo ring



To minimize steric hindrance (critical on nanosecond time scale), helix was forced to rotate in a reptation tube (local pivot points and directors).

Images and Movies Tutorial



Alek Aksimentiev

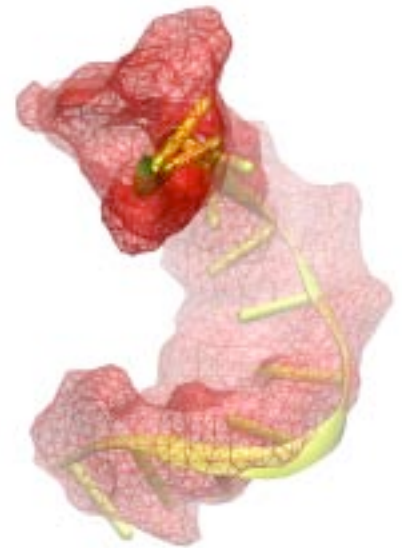
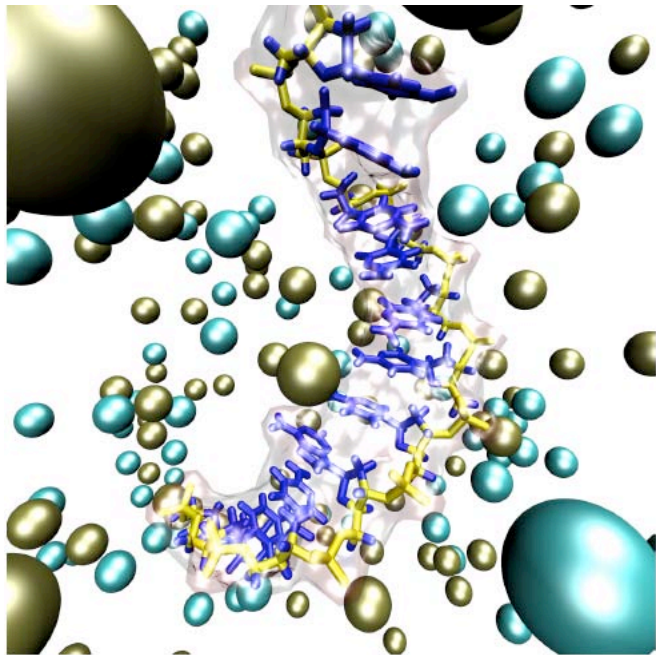
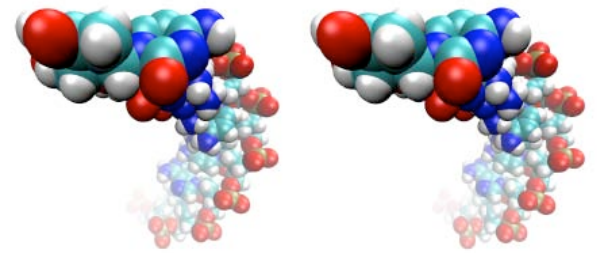
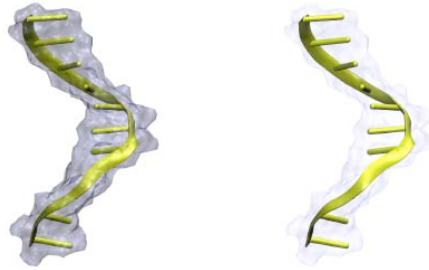
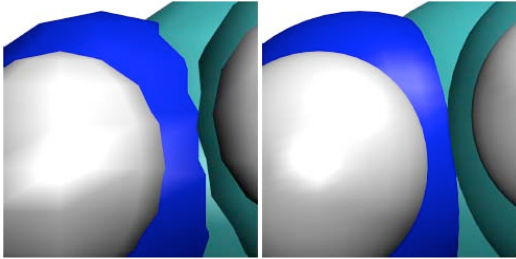
John Stone

David Wells

Marcos Sotomayor

November 2006

Highlights



Highlights

