Visualization

Problem Solving in GBCB
Types of Representations

- Physical (e.g., wire, plastic, etc.)
- Computer
Computer Representations

- 1980’s - Expensive graphics workstations
- Personal computers
  - Kinemage (KiNG - Java-based visualizer)
  - RasMol
  - Chime
  - Swiss-PDB Viewer
  - VMD
  - UCSF Chimera
  - Cn3D
  - Jmol
Kinemage

- Kinetic image
- “Kinemages are set up to illustrate a particular idea about a three-dimensional object, rather than neutrally displaying that object; they incorporate the author’s selection, emphasis, and viewpoint …” ¹
- Self-directed exploration not possible

¹Richardson, J.S. and Richardson, D.
Rasmol

- Raster¹ Molecules
- Rastop (Windows only)
- Functions as a stand-alone program

Chime

- Derived from RasMol
- A browser plug-in
Swiss-PDB Viewer (DeepView)

- Structure analysis and display tools
- In conjunction with SWISS-MODEL, used for homology modeling
- Energy computation
- Computation of electrostatic properties
- Ramachandran plots
VMD
http://www.ks.uiuc.edu/Research/vmd/

- **Visual Molecular Dynamics**
- Provides a wide variety of methods for rendering and coloring molecules
- Animate and analyze the trajectory of a molecular dynamics (MD) simulation
- No limits on the number of molecules, atoms, residues or number of animation frames
- Reads many molecular data file formats
UCSF Chimera

- Successor to UCSF MidasPlus
- Available for Windows, Linux, MacOSX, SGI IRIX, HP Unix
Pymol

- Python-enhanced molecular graphics tool
- 3D visualization of proteins, small molecules, density, surfaces, and trajectories
- Includes molecular editing, ray tracing, and movies
Cn3D

- “See in 3D”
- Developed at NCBI (National Center for Biotechnology Information)
- Interface to Entrez’s molecular biology search engine (e.g., relate sequence to structure)
- MMDB (Molecular Modeling Database) derived from PDB
- ASN.1 format
Jmol

• Open source molecular viewer written in Java
• Run as Web browser applet or stand-alone application
• Rasmol/Chime script compatibility
• Testimonial

“Jmol v10: I can't believe it's Java! But it's also open-source, so there's simply no question about it. Get your copy now, before they run out of those virtual Java machine thingies. It's just in time (JIT) for Christmas, from what I hear!”

Warren L. DeLano - author of Pymol
**VRML**

- Virtual reality modeling language
- Can generate nice representations of molecules, but not as easy to use as others
- Designed for any object, not just molecules
- Less stable than other viewers
PDB Format
(http://www.rcsb.org/)

| REMARK   | Header information |
| REMARK   | More header information |
| CRYS1    | 74.600  74.600  42.900  90.00  90.00  120.00  P6522 |
| ATOM     | 1  N   ILE A   1       4.215  43.479  11.411  1.00  0.00 |
| ATOM     | 2  CA  ILE A   1       5.632  43.867  11.583  1.00  0.00 |
| ATOM     | 3  C   ILE A   1       6.080  44.642  10.339  1.00  0.00 |
| ATOM     | 4  O   ILE A   1       5.670  44.319   9.181  1.00  0.00 |
| ATOM     | 5  CB  ILE A   1       6.378  42.575  11.755  1.00  0.00 |
| ATOM     | 6  CG1 ILE A   1       7.684  42.510  11.025  1.00  0.00 |
| ATOM     | 7  CG2 ILE A   1       5.595  41.348  11.326  1.00  0.00 |
| ATOM     | 8  CD1 ILE A   1       8.504  41.218  11.283  1.00  0.00 |
| ATOM     | 9  N   ARG A   2       6.900  45.676  10.596  1.00  0.00 |
| ATOM     | 10  CA  ARG A   2       7.423  46.581  9.567   1.00  0.00 |
| ATOM     | 11  C   ARG A   2       8.915  46.451  9.224   1.00  0.00 |
| ATOM     | 12  O   ARG A   2       9.698  47.420  9.352   1.00  0.00 |
| ATOM     | 13  CB  ARG A   2       7.199  48.002 10.039   1.00  0.00 |
| ATOM     | 14  CG  ARG A   2       5.819  48.583  9.695   1.00  0.00 |
| ATOM     | 15  CD  ARG A   2       5.893  49.746  8.795   1.00  0.00 |
| ATOM     | 16  NE  ARG A   2       4.924  49.746  7.722   1.00  0.00 |
| ATOM     | 17  CZ  ARG A   2       5.036  50.457  6.564   1.00  0.00 |
ASN.1 Format

- Abstract Syntax Notation number one
- International standard that aims in specifying data used in common protocols
- Can be used for more than protein or nucleic acid data
- Can contain more information than PDB file (i.e., annotations)