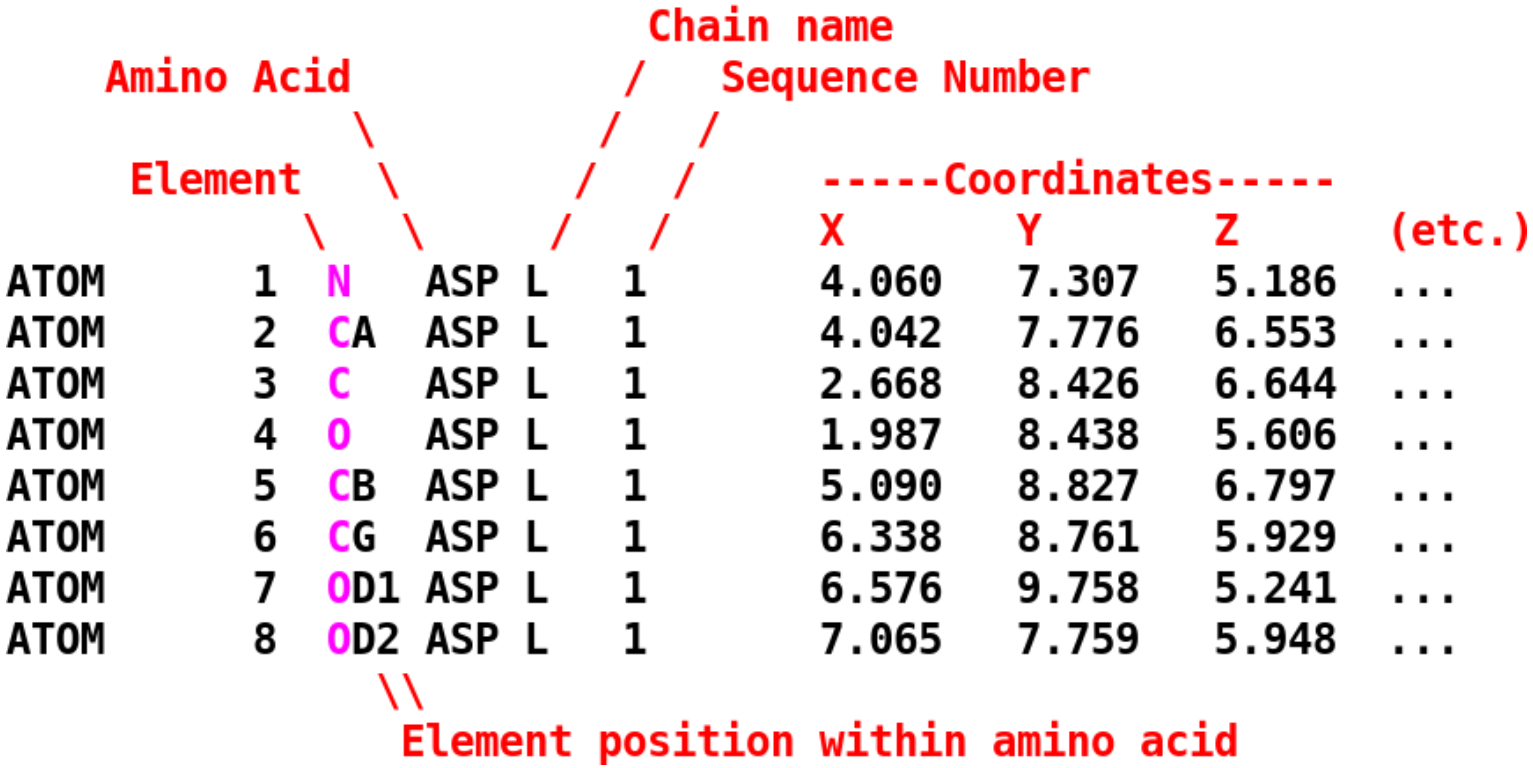
CS612 - Algorithms in Bioinformatics

Visualization and Representation

March 5, 2025

The PDB File Format

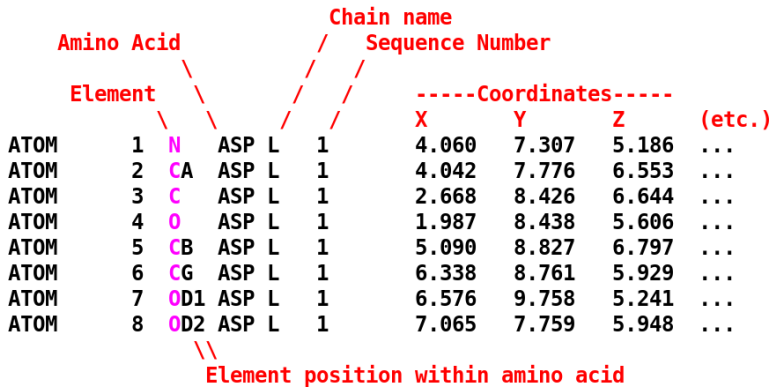


Modeling and Visualization of Protein Structures

- Computer graphics, scientific visualization and geometry to create a 3-D visual model of molecular structures.
- Facilitates structure, dynamic and function analysis.
- The PDB represents molecular structures as a set of Cartesian coordinates in 3-D.
- Internal coordinates – bond lengths, angles and dihedrals (more about them later...).
- Possible to switch back and forth.

Cartesian Coordinates

- Representing each atom as a set of (x, y, z) coordinates
- Easy and convenient to render on screen.
- Every line in a PDB file represents the 3-D location of the atom center with respect to some (arbitrary) axis system.
- Using a graphics package, simply draw a dot for each atom.



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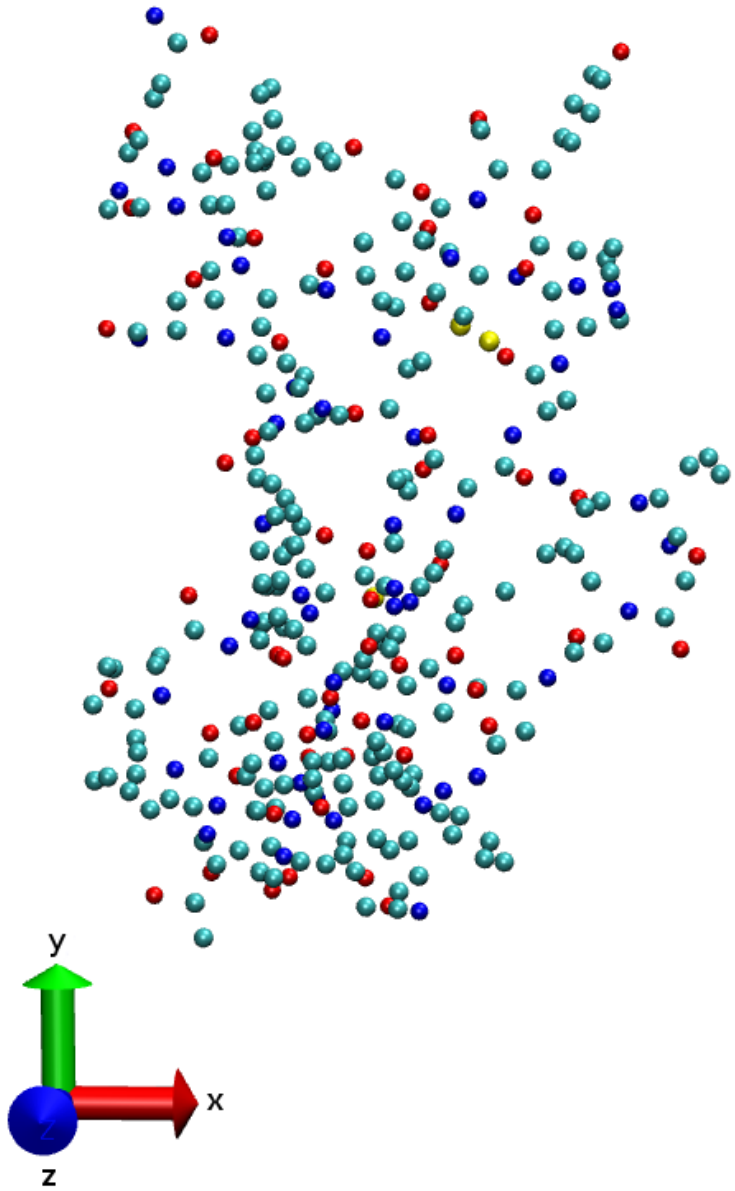


Visualization of Protein Structures

- Numerous tools are available for visualizing the structures stored in the PDB and other repositories.
- Most such tools allow a detailed examination of the molecule in a variety of rendering modes.
- For example, sometimes it may be useful to have a detailed image of the surface of the molecule as experienced by a molecule of water.
- For other purposes, a simple, cartoonish representation of the major structural features may be sufficient.

Visualization Tools

- "Full featured" academic packages
  - UCSF Chimera (`http://chimera.ucsf.edu/`)
  - PyMOL (`http://pymol.sourceforge.net/`)
  - VMD (`http://www.ks.uiuc.edu/Research/vmd/`)
- Viewers
  - RasMol/Chime (`http://www.openrasmol.org/`)
  - Jmol (`http://jmol.sourceforge.net/`)
  - SwissProt PDB-Viewer (DeepView) (`https://spdbv.unil.ch`)
  - RCSB Protein 3D viewer (`https://www.rcsb.org/3d-view`)

Modeling Tools

- Amber (`http://amber.scripps.edu/`)
- Charmm (`http://www.charmm.org/`)
- NAMD (`http://www.ks.uiuc.edu/Research/namd/`)
- Gaussian (`http://www.gaussian.com/`)
- ModBase (`http://modbase.compbio.ucsf.edu/`)
- Modeller (`http://www.salilab.org/modeller/`)
- DOCK (`http://dock.compbio.ucsf.edu/`)
- Many, many more.

Comparison of Visualization Packages

- JMol
  - Best-in-class viewer
  - Web enabled
  - Scriptable
  - Input only
  - Compatible with RasMol scripts
  - Limited analytical capabilities
  - Mostly through Javascript wrappers

Comparison of Visualization Packages

- PyMol
  - Best-in-class for peptidometics, speed
  - Single-screen interface (+command line)
  - Extensible
  - Some modeling capabilities
  - Good publication tools (built-in ray tracer)
  - Scriptable

Comparison of Visualization Packages

- VMD
  - Best-in-class for MD (integrated with NAMD) and other analysis tools
  - Scriptable
  - Excellent stereo capabilities
  - Embedded ray tracer (Tachyon)
  - Extensible
  - Now supports Python, previously was only TCL/TK

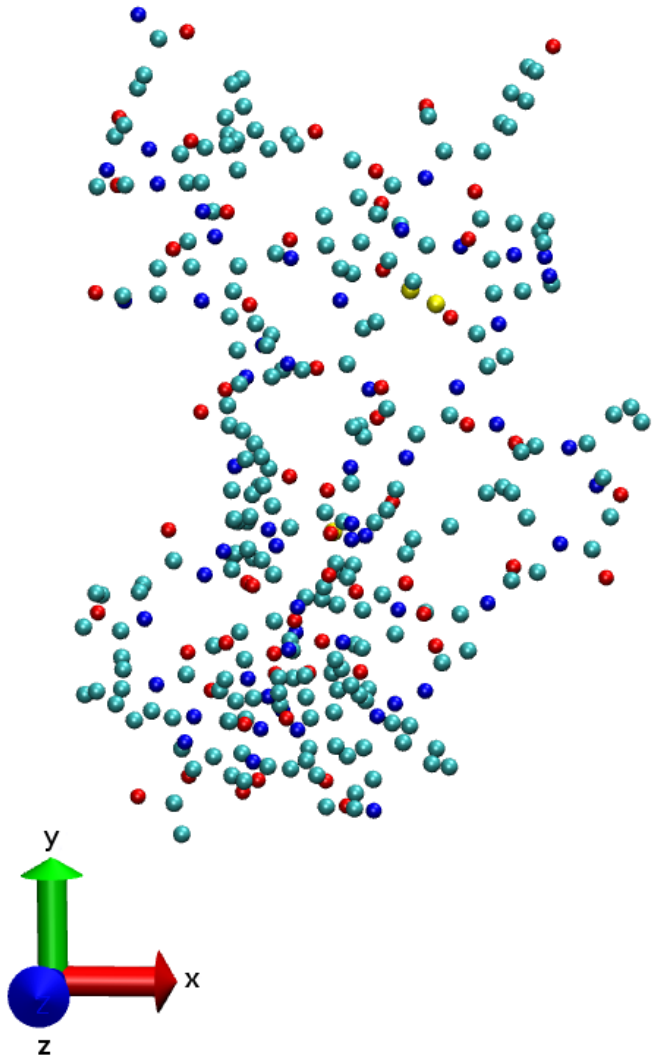
Comparison of Visualization Packages

- Chimera
  - Best-in-class for visualizing very large structures
  - Multiscale extension, volume viewer
  - Focus on extensibility, broad functionality
  - Primarily analytical interface
  - Familiar GUI interface (+command line)
  - Scriptable
  - Reasonable tools for publication & presentation
  - Embedded ray tracer (POV-Ray)
  - Excellent sequence/structure capabilities
  - Eeasonable interface to modeling programs

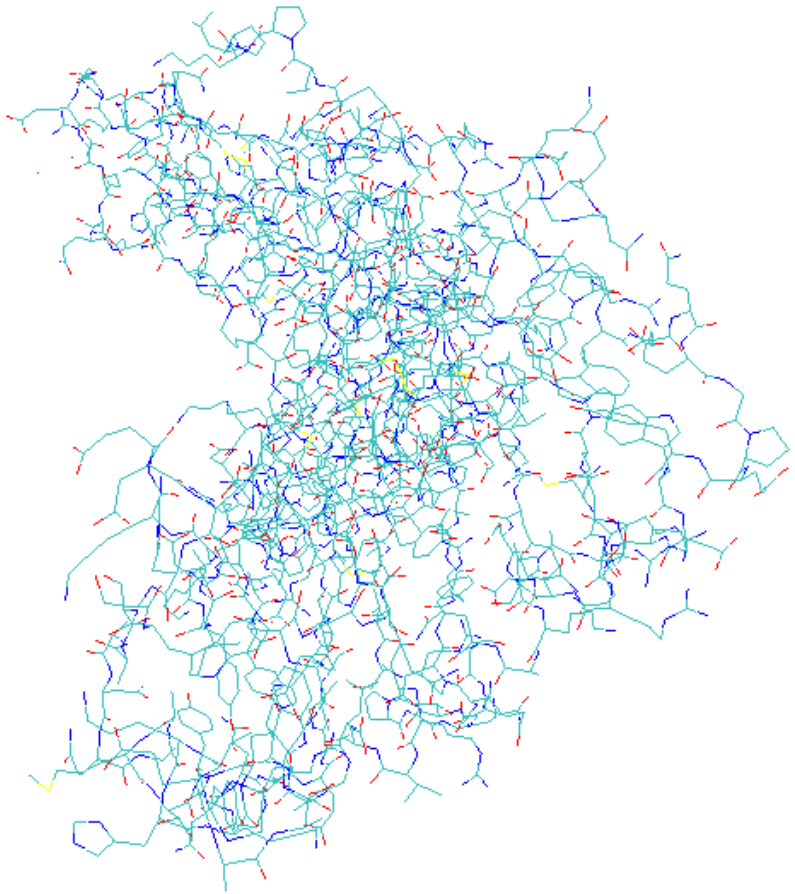
Comparison of Visualization Packages

- There is no "best" package for everything (IMHO)
- YMMV (Your Mileage May Vary)
  - What we think is easy, you may think is hard
  - What we think is hard, you may think is easy
- Choosing the best package for you
  - Does what you need
  - Good documentation
  - Good support (either local or from the authors)

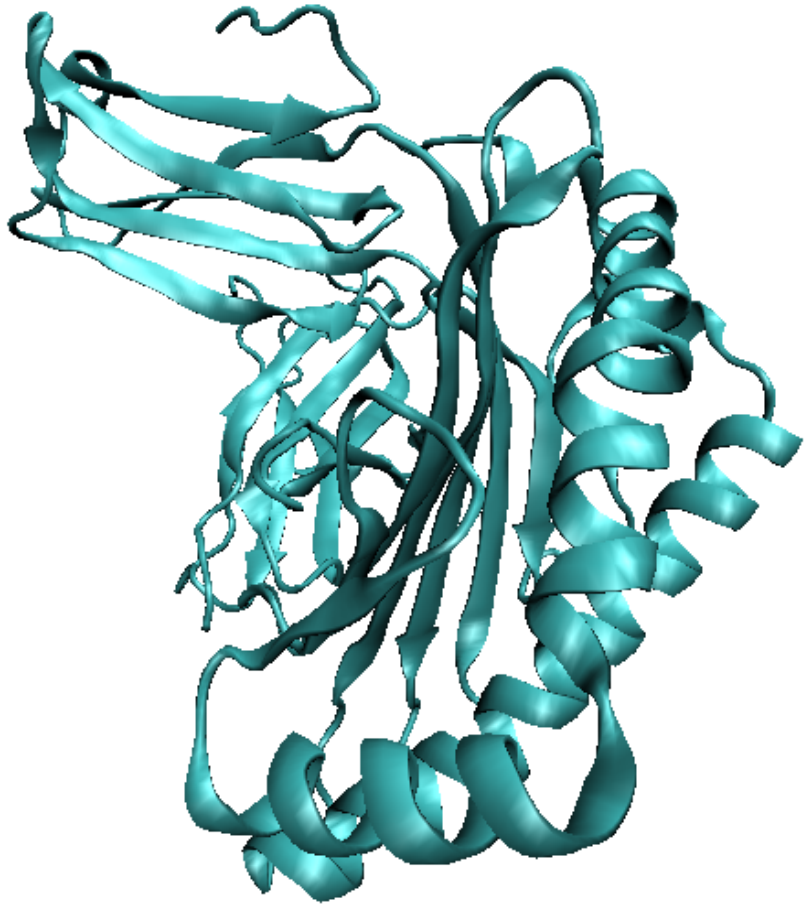
Representation of Protein Structures – Set of Dots



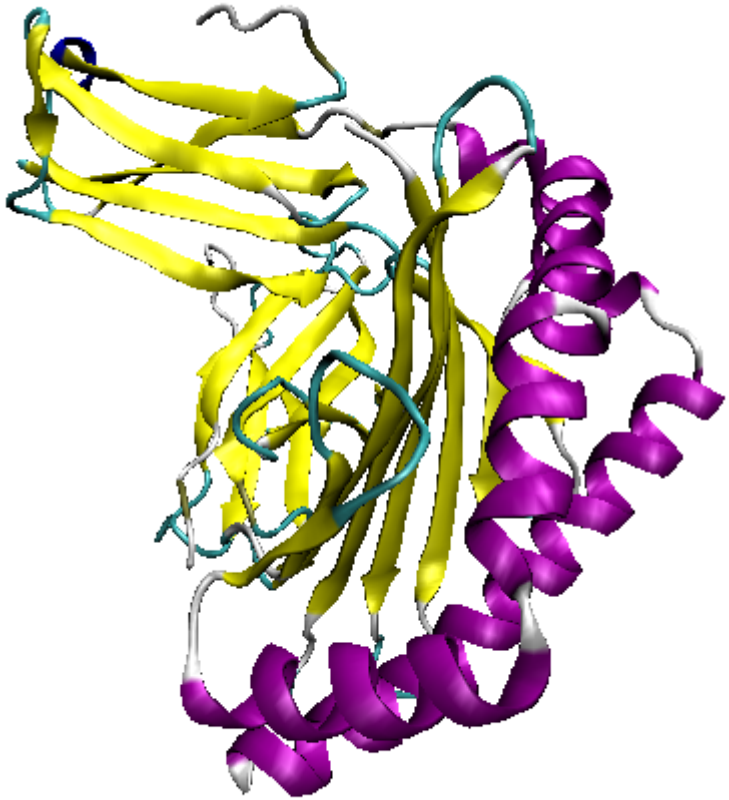
Representation of Protein Structures – Wireframe



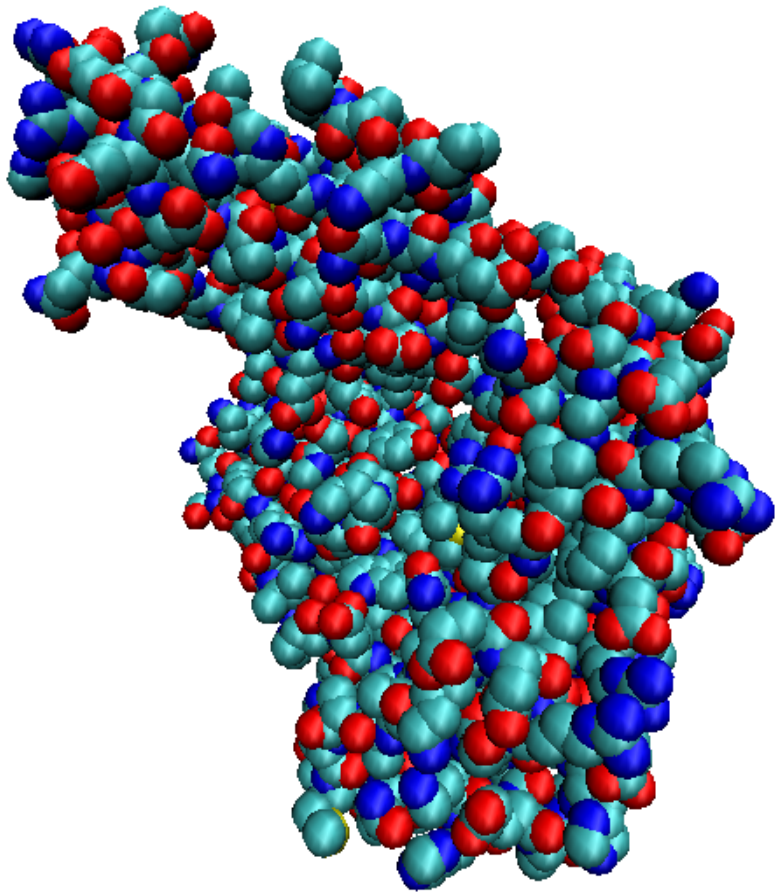
Representation of Protein Structures – Cartoon



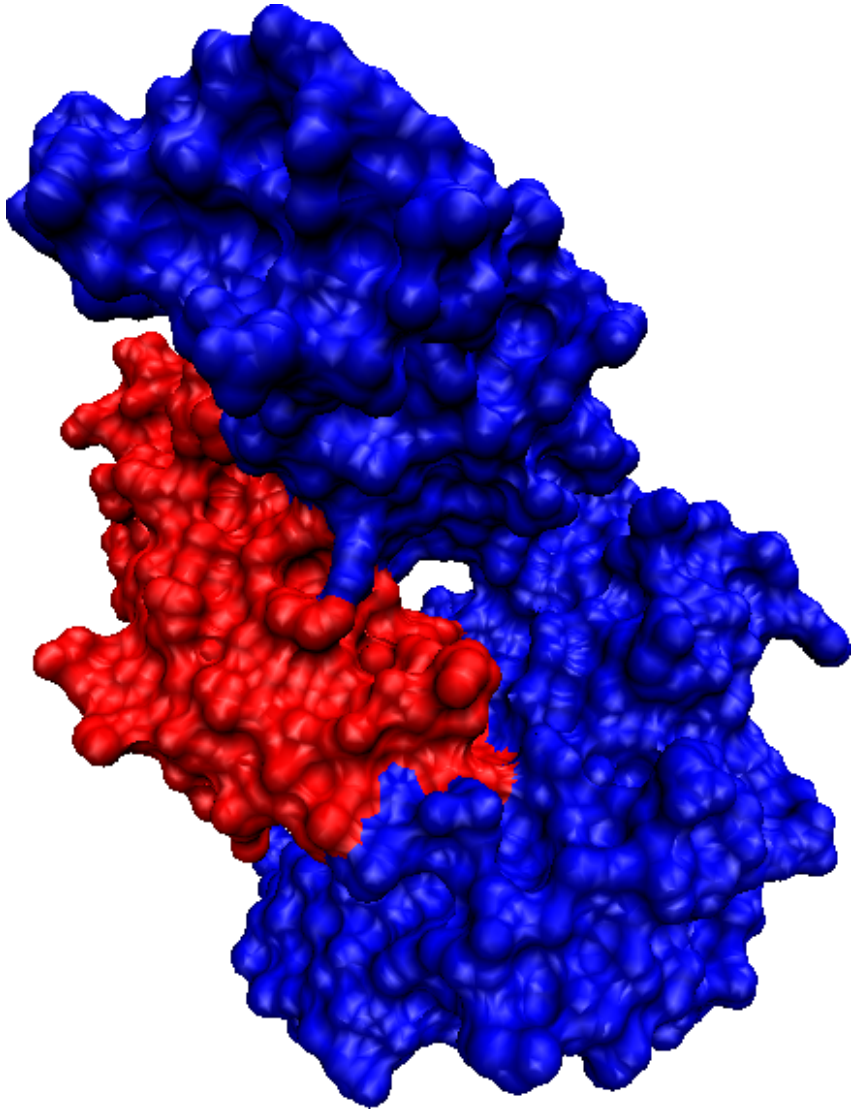
Representation of Protein Structures – Color by Secondary Structure



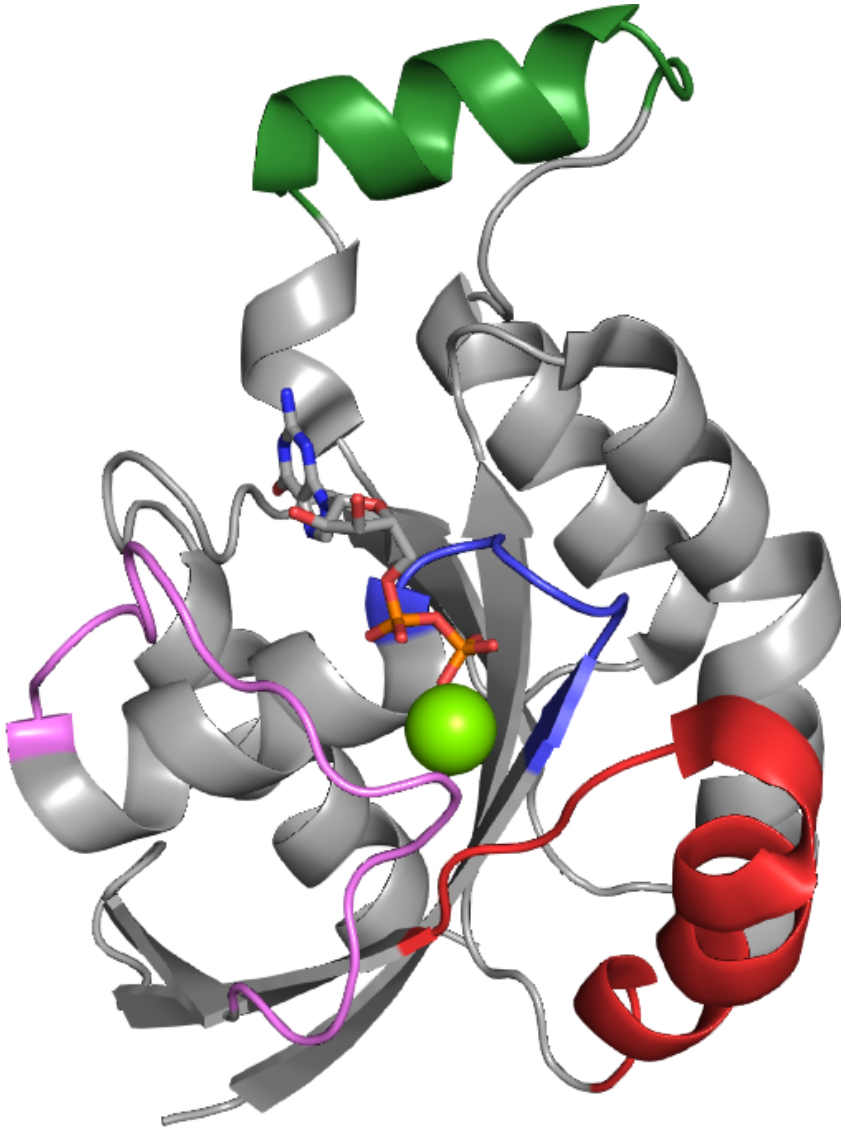
Representation of Protein Structures – Spheres



Representation of Protein Structures – Solvent Accessible Surface, Colored by Chain



Representation of Protein Structures – Mixed View



Representation of Protein Structures – Transparency