

Protein structural visualization

The main feature of computer visualization programs is interactivity, which allows users to visually manipulate the structural images through a graphical user interface. At the touch of a mouse button, a user can move, rotate, and zoom an atomic model on a computer screen in real time, or examine any portion of the structure in great detail, as well as draw it in various forms in different colors. Further manipulations can include changing the conformation of a structure by protein modeling or matching a ligand to an enzyme active site through docking exercises. Because a Protein Data Bank (PDB) data file for a protein structure contains only x, y, and z coordinates of atoms, the most basic requirement for a visualization program is to build connectivity between atoms to make a view of a molecule.

The visualization program should also be able to produce molecular structures in different styles, which include wire frames, balls and sticks, space-filling spheres, and ribbons.

- A wire-frame diagram is a line drawing representing bonds between atoms. The wire frame is the simplest form of model representation and is useful for localizing positions of specific residues in a protein structure, or for displaying a skeletal form of a structure when C α atoms of each residue are connected.
- Balls and sticks are solid spheres and rods, representing atoms and bonds, respectively. These diagrams can also be used to represent the backbone of a structure.
- In a space-filling representation (or Corey, Pauling, and Koltan [CPK]), each atom is described using large solid spheres with radii corresponding to the Van der Waals radii of the atoms.
- Ribbon diagrams use cylinders or spiral ribbons to represent α -helices and broad, flat arrows to represent β -strands. This type of representation is very attractive in that it allows easy identification of secondary structure elements and gives a clear view of the overall topology of the structure. The resulting images are also visually appealing.

Different representation styles can be used in combination to highlight a certain feature of a structure while deemphasizing the structures surrounding it. For example, a cofactor of an enzyme can be shown as space-filling spheres while the rest of the protein structure is shown as wire frames or ribbons.

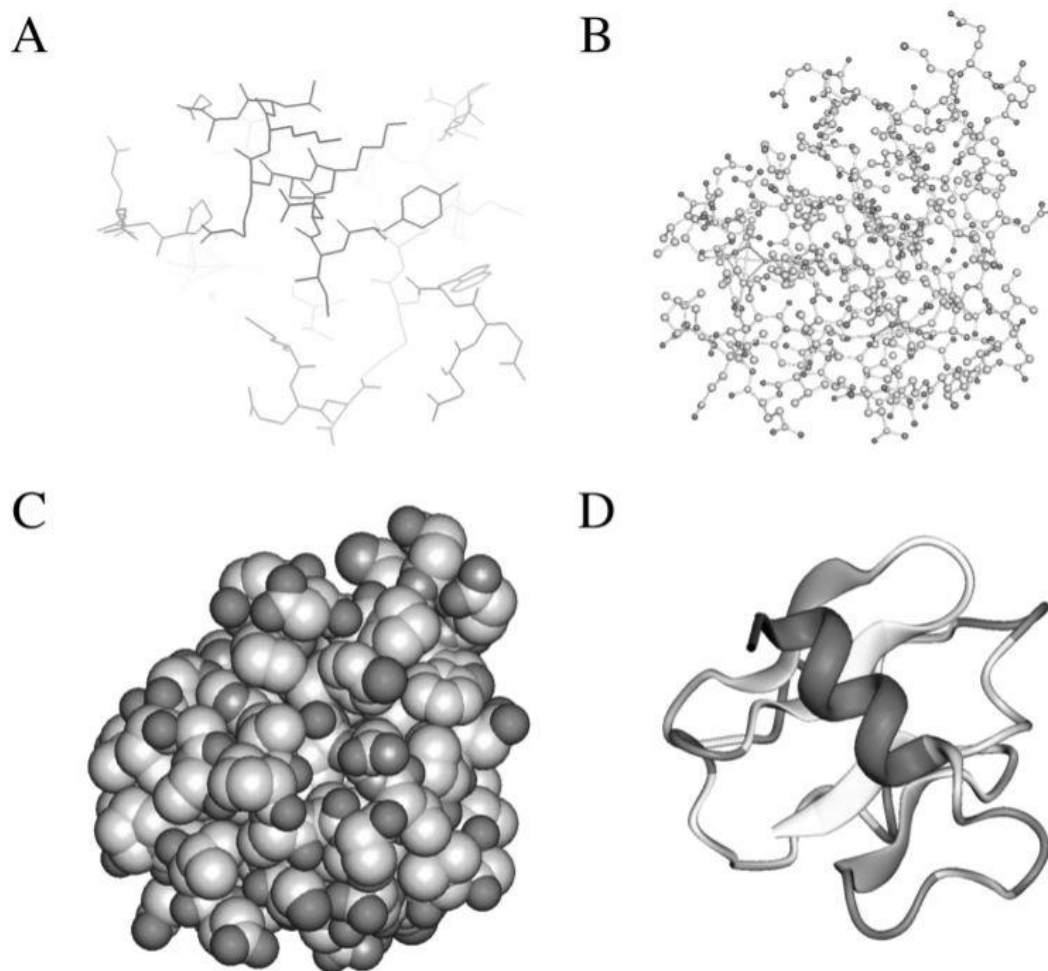


Figure 13.1: Examples of molecular structure visualization forms. **(A)** Wireframes. **(B)** Balls and sticks. **(C)** Space-filling spheres. **(D)** Ribbons (see color plate section).

RasMol (<http://rutgers.rcsb.org/pdb/help-graphics.html#rasmol> download) is a command-line-based viewing program that calculates connectivity of a coordinate file and displays wireframe, cylinder, stick bonds, α -carbon trace, space-filling (CPK) spheres, and ribbons. It reads both PDB and mmCIF formats and can display a whole molecule or specific parts of it. It is available in multiple platforms: UNIX, Windows, and Mac. RasTop (www.geneinfinity.org/rastop/) is a new version of RasMol for Windows with a more enhanced user interface.

Swiss-PDB Viewer (www.expasy.ch/spdbv/) is a structure viewer for multiple platforms. It is essentially a Swiss-Army knife for structure visualization and modeling because it incorporates so many functions in a small shareware program. It is capable of structure visualization, analysis, and homology modeling. It allows display of multiple structures at the same time in different styles, by charge distribution, or by surface accessibility. It can measure distances, angles, and even mutate residues. In addition, it can calculate molecular

surface, electrostatic potential, Ramachandran plot, and so on. The homology modeling part includes energy minimization and loop modeling.

Molscript (www.avatar.se/molscript/) is a UNIX program capable of generating wire-frame, space-filling, or ball-and-stick styles. In particular, secondary structure elements can be drawn with solid spirals and arrows representing α -helices and β -strands, respectively. Visually appealing images can be generated that are of publication quality. The drawback is that the program is command-line-based and not very user friendly.

A modified UNIX program called Bobscrip (www.strubi.ox.ac.uk/bobscrip/) is available with enhanced features.

Ribbons (<http://sgce.cbse.uab.edu/ribbons/>) another UNIX program similar to Molscript, generates ribbon diagrams depicting protein secondary structures. Aesthetically appealing images can be produced that are of publication quality. However, the program, which is also command-line-based, is extremely difficult to use.

Grasp (<http://trantor.bioc.columbia.edu/grasp/>) is a UNIX program that generates solid molecular surface images and uses a graded coloring scheme to display electrostatic charges on the surface. There are also a number of web-based visualization tools that use Java applets. These programs tend to have limited molecular display features and low-quality images. However, the advantage is that the user does not have to download, compile, and install the programs locally, but simply view the structures on a web browser using any kind of computer operating system. In fact, the PDB also attempts to simplify the database structure display for end users. It has incorporated a number of light-weight Java-based structure viewers in the PDB web site.

WebMol (www.cmpharm.ucsf.edu/cgi-bin/webmol.pl) is a web-based program built based on a modified RasMol code and thus shares many similarities with RasMol. It runs directly on a browser of any type as an applet and is able to display simple line drawing models of protein structures. It also has a feature of interactively displaying Ramachandran plots for structure model evaluation. Chime (www.mdlchime.com/chime/) is a plug-in for web browsers; it is not a standalone program and has to be invoked in a web browser. The program is also derived from RasMol and allows interactive display of graphics of protein structures inside a web browser.

Cn3D (www.ncbi.nlm.nih.gov/Structure/CN3D/cn3d.shtml) is a helper application for web browsers to display structures in the MMDB format from the NCBI's structural database. It can be used on- or offline as a stand-alone program. It is able to render three-dimensional molecular models and display secondary structure cartoons. The drawback is that it does not recognize the PDB format.

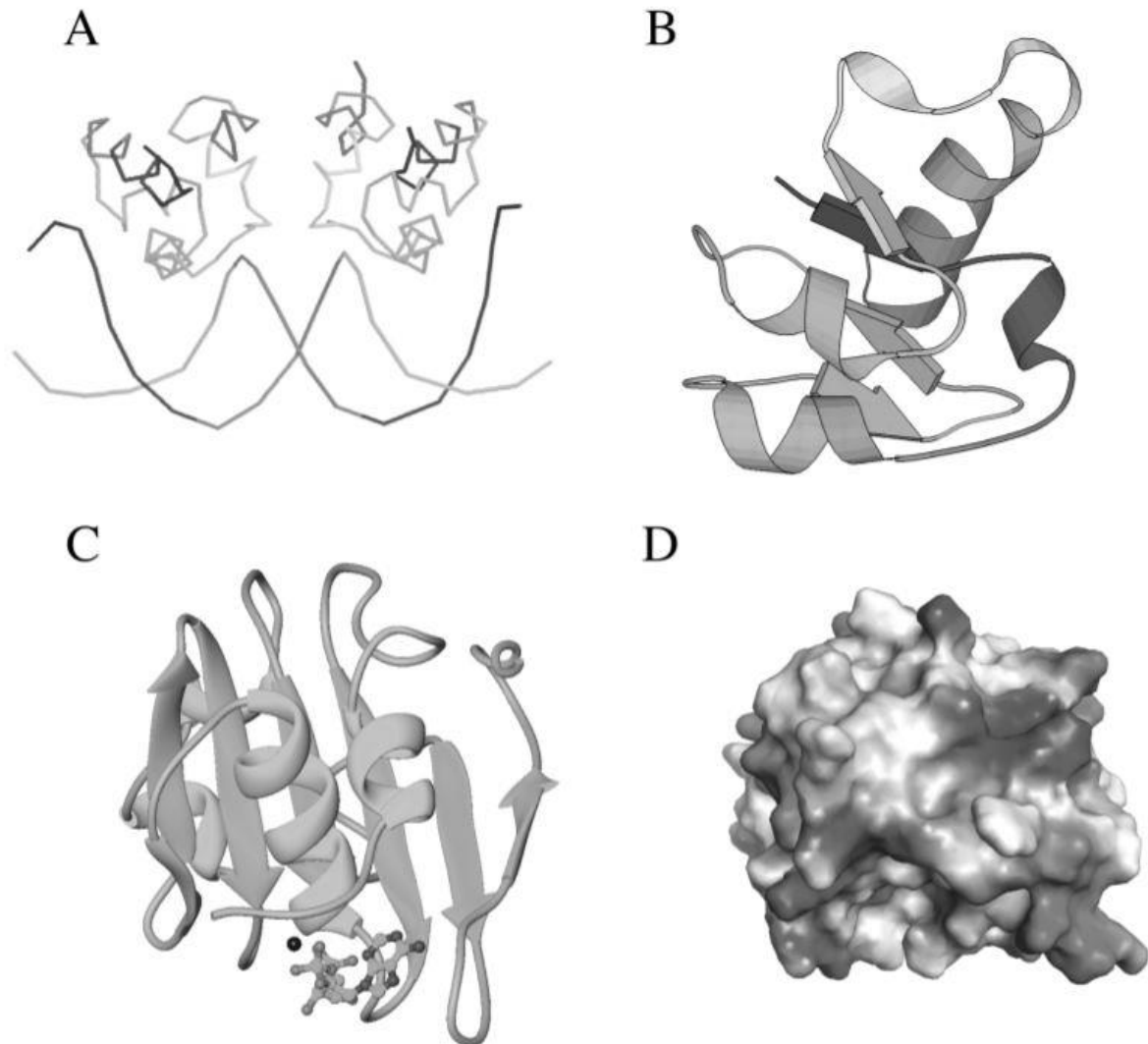


Figure 13.2: Examples of molecular graphic generated by (A) Rasmol, (B) Molscript, (C) Ribbons, and (D) Grasp (see color plate section).