

MOLECULAR GRAPHICS OVERVIEW

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Why learn to use molecular graphics programs?

Humans are highly visually oriented beings. In Biochemistry, our ability to communicate information about the structure and function of biological molecules, and even to ask the right questions about them, is critically linked to our ability to effectively visualize them from any desired point of view and to see them both in part and in whole. The effective use of molecular graphics is part art and part science.

The "Art" of Molecular Graphics

Molecular graphics is used to *portray* structures.

Lines from a PDB file containing coordinates:

```
ATOM 1 N VAL 1 -2.900 17.600 15.500 1.0 0.0  
ATOM 2 CA VAL 1 -3.600 16.400 15.300 1.0 0.0
```

```
HETATM 1262 OH HEM 1 16.700 27.100 4.800 1.0 0.0
```

are turned by molecular graphics programs such as RASMOL into pictures. Commands in such programs can tailor the picture to highlight key features or views of a structure without necessarily showing all the atoms explicitly:



This picture shows myoglobin (blue) with its alpha-helices drawn in a "ribbon" format that emphasizes their helical shape. The picture also shows the heme ligand in a "stick" format (yellow) that highlights its characteristic ring-containing atomic structure. The iron atom (green) in the center is shown in a "space-filling" format to emphasize its central importance in oxygen binding. When a biochemist uses molecular graphics in a presentation or a publication, there is an art to getting the view, the colors, the drawing styles just right to make the point clearly.

The "Science" of Molecular Graphics

Molecular graphics is also used to interactively *ask questions* about structures.

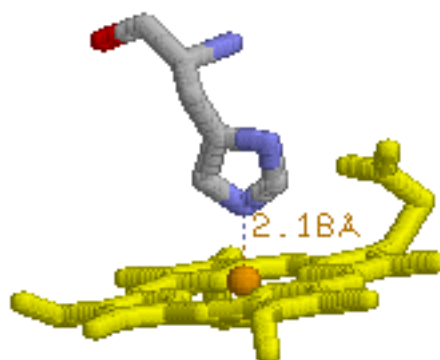
"Is there a hydrogen bond between those two atoms?"

"Is residue 43 in an alpha helix?"

"Is Tyrosine 47 of myoglobin buried in the interior of the protein or is it exposed to the solvent?"

"How similar are the structures of myoglobin and hemoglobin?"

"What amino acid side chains are responsible for contacting the substrate in serine protease enzymes?"



The above picture shows a measurement of the distance between a nitrogen on histidine 93 of myoglobin and an iron atom from the heme. The geometry of this interaction might be important for understanding how the histidine affects the ability of the heme to bind oxygen on its other face.

Fine then. What molecular graphics programs will we learn?

RASMOL (version 2.6)

This shareware free program is the easiest visualization tool used today. The software excels in displaying macromolecular structures in multiple formats (cpk, cartoon ribbons, ball-and-stick, etc.) and is available for many different computing platforms. Its scripting language is relatively easy to learn and use, but the command-line interface is a little cumbersome at times.

Download RASMOL version 2.6 (even though there is a 2.7 version, please download 2.6)
<http://www.umass.edu/microbio/rasmol/getras.htm>

RASMOL Manual* (for version 2.6) <http://www.umass.edu/microbio/rasmol/distrib/rasman.htm> (Roger Sayle, Glaxo)

* Two copies of the RASMOL Manual are available in the computer lab. They are not to be removed. They will NOT be replaced. Highly highly suggest obtaining your own copy for reference throughout your project.

RASMOL Tutorials

- Gale Rhodes (U. Southern Maine) <http://www.usm.maine.edu/~rhodes/RasTut/index.html>
- Montfort/Wells/Little (U. Arizona) <http://www.biochem.arizona.edu/classes/bioc568/rasstart.htm>
- Amoia/Cordes (U. Arizona) (1) [Introduction to Basic Commands](#) (2) [Creating and Running Scripts](#) (Required - In Class!)

DEEP VIEW (version 3.7)

(Formerly called SWISS-PDB VIEWER)

This shareware free software is a more robust visualization program and is commonly used by many structural biologists. Although the rendering is not as nice as in RASMOL, it provides a number of powerful tools for displaying and manipulating macromolecular structure that RASMOL cannot. The user can display multiple structures, display electron density or electrostatic maps, display crystal symmetry (useful for displaying an entire molecule), create 'mutants', perform sequence alignments, superimpose related molecules, perform energy minimizations, and so on. If you are interested in structural biology research, you should learn how to use this program thoroughly.

DEEP VIEW Umbrella Page (Expasy) <http://us.expasy.org/spdbv/>

Download DEEP VIEW version 3.7 <http://us.expasy.org/spdbv/text/disclaim.htm> (help directions if needed: <http://www.usm.maine.edu/%7Erhodes/0Help/GetSPdbV.html>)

DEEP VIEW User Guide <http://us.expasy.org/spdbv/text/main.htm>

DEEP VIEW Tutorials

- Gale Rhodes (U. Southern Main) <http://www.usm.maine.edu/~rhodes/SPVTut/index.html> (Required - Out of Class!)
 - Two copies of the Gale Rhodes Tutorial (Sections 1-8, 10,11) are available in the computer lab. They are not to be removed. They will NOT be replaced.
- From DEEP VIEW Homepage (Expasy) <http://us.expasy.org/spdbv/text/tutorial.htm>