

Molecular Graphics

7.51 September 2001

RasMol and PDB files.

The simplest graphics program on Athena is called *RasMol*. To use this program, you will need to copy files that contain the coordinates of a molecule (called PDB files) into your directory. Some of these files are located in the 7.51 locker. At present, they include:

| | |
|------------------|--|
| BPTI.pdb | (bovine pancreatic trypsin inhibitor) |
| bDNA.pdb | (a model of B-form DNA) |
| 1PAR.pdb | (Arc repressor bound to operator DNA) |
| 5rsa.pdb | (ribonuclease A) |
| 256b.pdb | (cytochrome b562) |
| 1mbn.pdb | (sperm whale myoglobin) |
| 4gcr.pdb | (gamma crystallin) |
| 1rbp.pdb | (retinol-binding protein) |
| 1tim.pdb | (triosephosphate isomerase) |
| 4fxn.pdb | (flavodoxin) |
| 2cro.pdb | (phage 434 Cro repressor) |
| lake.pdb | (adenylate kinase with inhibitor) |
| lhgj.pdb | (influenza virus hemagglutinin) |
| lhtm.pdb | (influenza virus hemagglutinin ectodomain) |
| loel.pdb | (groEL) |
| lrno.pdb | (ribonuclease A) |
| lrpg.pdb | (ribonuclease A with inhibitor) |
| 2zta.pdb | (leucine zipper) |
| 4ake.pdb | (adenylate kinase) |
| 6cha.pdb | (alpha-chymotrypsin with inhibitor) |
| trp_apo.pdb | (trp repressor) |
| trp_rep.pdb | (trp repressor) |
| trypsin_bpti.pdb | (trypsin-BPTI complex) |

To copy one or more files, log on to Athena (for example in the basement of Bldg. 66) and after the Athena prompt (Athena %), type:

```
add 7.51
```

To list the files, type:

```
ls /mit/7.51
```

To copy the bDNA.pdb file into your directory, type:

```
cp /mit/7.51/bDNA.pdb .
```

Note that the period at the end of the line is important. It means copy to the current directory. To copy all of the pdb files type:

```
cp /mit/7.51/*.pdb .
```

To launch the RasMol graphics program, type:

add rasmol

and then type:

rasmol

You should now see the RasMol window. To load a structure, use **Open** under the **File** menu and then type the name of the pdb file in the command window after the prompt:

RasMol >
PDB file name:

The structure should now appear in the graphics window. You can rotate and move the structure using the mouse. To identify an atom, click on it and look in the command window. Experiment with different views, colors, etc. using the Display, Color, and Option menus. There's a good tutorial by Andrew Coulson (Univ. Edinburgh, UK). It's located in a text file in the 7.51 locker named *rasmol.tutorial*. For on-line help while running RasMol, type:

help commands

to list the various commands (Backbone, Load, Select, etc.), To get information about a specific command such as Select, type:

help select

For more information about RasMol and related topics, visit the RasMol homepage on the WWW (<http://www.umass.edu/microbiol/rasmol/>). If you want to install your own version of RasMol on a Mac, PC, or Unix machine, this Web site has all of the information that you need.

GETTING YOUR OWN PDB FILES.

The coordinates for most known X-ray and NMR structures (and some theoretical structures) are deposited in the Protein Data Bank (<http://www.rcsb.org/pdb/>). You can get PDB files from the PDB using Netscape. To launch Netscape from Athena, type:

add infoagents

and then type:

netscape &

Click all of the necessary buttons and enter the address (<http://www.pdb.bnl.gov>). When the PDB Homepage comes up, enter keywords into the search engine provided to find structures of interest. Use the {EXPLORE} and then the Download/Display File to get the coordinates. For some oligomers, the PDB file will only have a subset of the subunits (the rest are related by crystallographic symmetry). To get a files with all of the subunits, use the Other Sources option in Structural Explorer and then click on the PDB code under the EBI MSD Macromolecule File Server heading. This will take you to a database where files with the ending .mmol should have the coordinates for the native oligomer. WARNING—sometimes it's not clear whether a crystallographic oligomer exists or functions in solution.