

RasMol - A short introduction

RasMol is a free, open-source molecular graphics program which can be obtained from <http://www.openrasmol.org/> This guide provides a very short introduction to using the RasMol CD which you have been given to view a structure.

A full manual may be obtained at http://www.rasmol.org/software/RasMol_Latest_Manual.html and interactive help is available within RasMol.

Tutorials are available at a number of sites online. For example:

<http://www.umass.edu/microbio/rasmol/rasquick.htm>

<http://spdbv.vital-it.ch/TheMolecularLevel/RasTut/>

http://www.mrc-lmb.cam.ac.uk/rlw/text/rasmol_tutorial

https://ww2.chemistry.gatech.edu/~lw26/bCourse_Information/4581/labs/tbp/rasmol/rasmol_tbp_fset.html

A list of tutorials is available at:

<http://www.umass.edu/microbio/rasmol/rastut.htm>

Starting RasMol

To start RasMol, simply double click on its icon. Where the icon (three balls joined with sticks) lives, depends on where it is installed! If you are running it from CD, then:

RasMol will start with a window with a black background and menus at the top.

When RasMol starts, a second window is also opened where you can type commands to control the program. However, when this opens, it is immediately shrunk down onto the task bar at the bottom of the screen - **you need to click the box on the task bar to open it.**

Loading a Structure

In the RasMol window, click the **File** menu and select **Open**.

Use the file browser to select a protein structure file (a PDB file) to be loaded. PDB files may be downloaded from <http://www.pdb.org/>

Manipulating the Structure

To rotate the structure, click in the window with the **left mouse button** and drag the mouse.

To rotate the structure about the axis coming out of the screen, hold down the **shift** key, click in the window with the **right mouse button** and drag the mouse up and down.

To move (translate) the structure, click in the window with the **right mouse button** and drag the mouse.

To zoom the structure, hold down the **shift** key, click in the window with the **left mouse button** and drag the mouse up and down.

Modifying the View

Most modifications to the view can be made from the menus:

rendering style (**Display** menu): wireframe (bonds represented by lines), space-filled (atoms represented by spheres), cartoons (cartoon backbone trace of helices, strands and coil), etc.

colouring scheme (**Colours** menu): CPK (colour by atom type), chain (colour by chain), temperature (colour by temperature factor), structure (colour by secondary structure), etc.

More Control

To obtain more control over the picture you obtain, you need to use the command language rather than the menus. To access the command prompt, **click the RasMol command window icon in the task bar**. A window will open where you can type commands.

The usual reason for requiring more control is when you wish to apply different colouring or rendering styles to different parts of the structure. For example, you might want to show the structure in cartoon style, but show the active site residues space-filled. To gain this type of control you only need to learn a few commands.

Colour

The Colour command gives much more flexibility than the colours menu. You can access all the functions of the menu, but you can also do simpler things such as specifying that the atoms in the current atom selection (see below) should be red.

The colour command always applies the colouring to the atoms selected by the last SELECT command (described below). For example:

COLOUR red	Colours all atoms in the current select red. Most other common colour names will also work.
COLOUR cpk	Colour according to atom type (carbon: white, oxygen: red, nitrogen: blue)

Rendering

As above, most rendering can be specified from the **Display** menu. However, you can obtain more control from the command line – you can modify the thickness of lines or the size of spheres used in space-fill. The commands are WIREFRAME, BACKBONE, SPACEFILL, CARTOONS. Each can take 'on' or 'off' as a parameter or a number to define the size.

e.g.

WIREFRAME off	Switch off the wireframe
WIREFRAME 100	Draw a thick wireframe
BACKBONE 50	Draw a medium thickness backbone
SPACEFILL 20	Draw very small speheres for each atom
CARTOONS on	Switch on the cartoons representation

Select

Select is the most important command - it specifies amino acids ranges to which other commands should apply. Here are some examples:

SELECT *	Select everything - all atoms of all chains
SELECT *:A	Select all atoms of the chain labelled A
SELECT 24-34	Select residues 24-34 in all chains
SELECT 24-34:A	Select residues 24-34 in chain A
SELECT water	Select all water residues
SELECT not protein	Select all non-protein atoms
SELECT ser	Select all serine residues
SELECT ser:A	Select all serine residues in chain A
SELECT 24-34 OR 50-56:A	Select residues 24-34 in all chains plus residues 50-56 in chain A.

Note, in the last example, the use of 'OR' to combine two selections. Intuitively you might expect 'AND' to be used. However, each selection restricts what is to be included, so you are selecting atoms which match the first restriction (24-34) OR the second restriction (50-56:A)

The examples are fairly self explanatory. When you specify numbers you are specifying a residue range. This applies to all chains and all atoms within those residues unless you specify otherwise. To restrict a selection to a particular chain, use a colon (:) followed by the chain name.

To restrict the selection to a particular atom, use a full-stop (.) followed by the atom name. Unfortunately, this is rather buggy in the standard versions of RasMol. You can only do this when the part immediately after the SELECT command starts with a character and not a number. So you can do:

SELECT *.CA	Select the CA atoms in all chains
SELECT *:A.CA	Select CA atoms of the chain labelled A
SELECT tyr23.ca	Select the CA atoms of Tyrosine 23

However, owing to limitations in RasMol (which really should be fixed!) you CANNOT do:

SELECT 24-34.CA	Select the CA atoms of residues 24-34 in all chains
SELECT 24-34:A.CA	Select the CA atoms of residues 24-34 in chain A

The way around this, is to combine the atom selection with the residue selection using an 'AND':

SELECT 24-34 AND *.CA	Select the CA atoms of residues 24-34 in all chains
SELECT 24-34:A AND *.CA	Select the CA atoms of residues 24-34 in chain A

Remember the 'AND' is used in a true Boolean sense – the atoms that are selected, must match the first criterion AND the second one.

Certain keywords (such as 'water' and 'protein') are also allowed and 'not' inverts the selection.