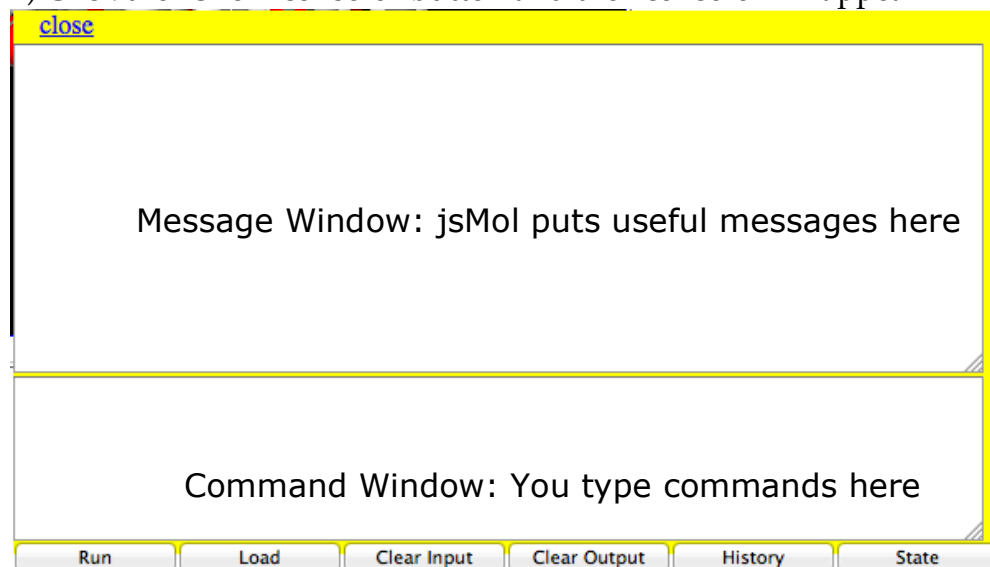


2) Click the “Show console” button and the “console will appear”:



3) Click in the bottom window of the console – the “Command window” – and type your commands there.

A few notes here:

- We’ll show commands in `this font`
- Commands must be entered exactly. Be careful about:
 - Leaving spaces between words
 - Capitalizing or not capitalizing
 - spelling
- Don’t forget to hit “return” or “enter” after each command.
- jsMol typically replies to each command with an informative message in the Message Window. For example, if you select something, it will tell you how many atoms you’ve selected. If this number is zero, you didn’t select anything, and probably made a mistake.

As a test, try the following:

- type: `select all`
- You should see “8087 atoms selected” in the Message Window
- type: `spacefill off`
- The display should go blank (you turned off all the atoms!)
- type: `select 100`
- You should see “14 atoms selected” in the Message Window; you’ve selected amino acid number 100.
- type: `spacefill on`
- You should see one little amino acid in spacefill mode.
- If you leave the cursor over it, a message will pop up telling you that it’s an ASN (Asparagine).
- You can also click on it and that same information will appear in the Message Window.
- Click “reset view” to get back to the starting view.

Some useful commands

- Selecting things (for example):
 - `select 27` – selects amino acid number 27
 - `select ala` – selects all alanines
 - `select ligand` – selects the ligand (aka “the substrate”)
 - `select ca` – selects the Calcium ion (Ca^{2+}) that is an important part of the structure
 - `select within (2.0, phe)` – selects all the atoms that are within 2.0 Angstroms of any of the phenylalanines. An atom is about 1-3 angstroms in diameter.
- Selecting more than one thing. This is a little counter-intuitive unless you are a computer scientist.
 - If you want to select BOTH amino acid 27 AND amino acid 100, you type: `select 27 or 100`. Note that, to jsMol, “or” means “select all the atoms that are either in 27 or in 100”.
 - `select 27 and 100` – selects no atoms since there are no atoms that are in both 27 and 100 at the same time.
 - `select within(2.0, phe) and not phe` – selects all the atoms that are both within 2.0 angstroms of a phenylalanine and not in a phenylalanine. That is, the nearby neighbors of phenylalanines.
- Showing things:
 - `spacefill on` – shows the selected atom(s) as big spheres
 - `spacefill off` – turns off the spacefill view of the selected atom(s)
 - if you want to show the selected atom(s) as “ball and stick”, it takes two commands:
 - `spacefill 0.5`
 - `wireframe 0.2`
 - remember that this shows single, double, and triple bonds as identical rods
 - to turn off “ball and stick” for the selected atom(s), it also takes two commands:
 - `spacefill off`
 - `wireframe off`
 - `dots on` – shows the selected atom(s) as dots
 - `dots off` – turns off the dots on the selected atom(s)
- Coloring things:
 - `color cpk` – colors the selected atom(s) by which atom they are using the scheme shown on the web page.
 - `color blue` – colors the selected atom(s) with the specified color. Some colors that work are red, blue, green, yellow, purple, white; you can try others.

You might want to play with this a little before you go further.

Reminder: The program shows the **covalent** bonds; your job is to infer the presence of various **non-covalent** interactions using your knowledge of structure and bonding. The chart on the next page outlines this process:

How to decide about non-covalent bonds:

1) Does one part have a **full**
(+) charge and the other have
a **full** (-) charge?

YES

NO

■ These parts of the two molecules *can* make an ionic bond.

■ These parts of the two molecules *cannot* make an ionic bond.

2) Does one part have a hydrogen donor
(OH or NH) and the other part have a
hydrogen acceptor (O: or N:)?

YES

NO

■ These parts of the two molecules *can* make a hydrogen bond.

■ These parts of the two molecules *cannot* make a hydrogen bond.

3) Can either part make either an ionic bond or a hydrogen bond?

YES

NO

■ These parts of the two molecules *cannot* make a hydrophobic interaction.

■ These parts of the two molecules *can* make a hydrophobic interaction.