Introduction to RasMol

The Beta Globin Exercise:

1. Download 1A3N (pdb file of hemoglobin) from the Protein Data Bank
2. Start RasMol and open 1A3N
3. Change Background color
4. Isolate the beta subunit of hemoglobin
5. On the navigation bar, select "display" and then "backbone" from the pull-down menu.
6. Moving the molecule
7. Increase the size of the backbone
8. Center the betaglobin
9. Boolean Operators
   Group exercise to demonstrate Boolean operators (and/or/not)
10. Add the heme group
11. Select alpha helices and color red
12. If there were beta sheets in this molecule, you would select them using the select command the pre-defined term "sheets"
13. Return the helices to CPK coloring
14. Display histidine residues associated with heme group
15. Identify the histidine residue numbers closest to the heme group.
    Use the mouse to click on the residue.
    A message will appear in the command line box identifying the residue.
    Q: Which two histidine residues are closest to the heme group?
16. Display only the histidines associated with the heme group
17. Selectively display the 2 histidines associated with the heme group
18. Select chain B and the heme group associated with this chain and then change the display to spacefill from the pull-down menu from the display menu.
19. Select non-polar amino acids and color yellow
20. Select charged (polar) amino acids
    Q: Where are these amino acids located?
21. select the heme group and color it cyan
22. Slab the protein to see the internal residues
    Q: Which type of amino acid is predominantly located in the interior of the protein?
23. Save a file with this current design.
24. Close RasMol and load your script file