

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
RasMol>background white
4. Isolate the beta subunit of hemoglobin
RasMol> restrict *b
5. On the navigation bar, select “display” and then “backbone” from the pull-down menu.
6. Moving the molecule
Mouse/keyboard controls
7. Increase the size of the backbone
RasMol> backbone 250
8. Center the betaglobin
RasMol>center *b
9. Boolean Operators
Group exercise to demonstrate Boolean operators (and/or/not)
10. Add the heme group
RasMol> select hem and *b
RasMol> spacefill 200
RasMol> wireframe 150
11. Select alpha helices and color red
RasMol> select helices and *b
RasMol> color cyan
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
RasMol> select helices
RasMol> color cpk
14. Display histidine residues associated with heme group
RasMol> select *b and his
RasMol> spacefill 200
RasMol> wireframe 150
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?
A: *Histidine 63 and Histidine 92*
16. Display only the histidines associated with the heme group
RasMol>spacefill off
RasMol>wireframe off (since we still have the histidines selected, these commands will turn off the display of all of the histidine)
17. Selectively display the 2 histidines associated with the heme group
RasMol> select *b and (his63 or his92)
RasMol>spacefill 200

- RasMol>wireframe 150
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.
RasMol> select (*b and hem) or *b
19. Select non-polar amino acids and color yellow
RasMol> select hydrophobic
RasMol> color yellow
Q: Where are these amino acids located?
A: mostly in the middle (interior), but since this subunit interacts with 3 others, there are some "surface" non-polar amino acids that would interact with the other subunits.
20. Select charged (polar) amino acids
RasMol> select charged
RasMol> color red
Q: Where are these amino acids located?
A: on the surface; charged (polar) amino acids are hydrophilic, meaning that they "like" interacting with water. In a cell, the proteins are surrounded by an aqueous solution (the cytoplasm) and therefore, polar amino acids will be predominantly located on the surface of the protein and non-polar amino acids will be located predominantly in the interior of the protein (away from the aqueous environment).
21. select the heme group and color it cyan
RasMol> select *b and hem
RasMol> color cyan
22. Slab the protein to see the internal residues
RasMol>slab 50
Q: Which type of amino acid is predominantly located in the interior of the protein?
A: the non-polar (yellow) amino acids
23. Save a file with this current design.
RasMol>save script 1a3n.spt
24. Close RasMol and load your script file
RasMol>script 1a3n.spt