

Protein structure homework: FAQ

Q: Did you tell us not to go to molecule and then information in RasTop to find info on the proteins but for us to open the protein files in notepad.

A: I did not tell you not to use the information button -- I warned you that it might be misreading and asked you to verify this information by comparing with what you see on the screen and what is in the actual pdb-file. That's why I suggested that you open this file with notepad or any other text editor.

Q: When I open a protein in notepad I don't understand what all the acronyms mean.

A: There are many acronyms there. Some of them are intuitive, but some aren't. The most important that you need to know are
"ATOM" -- means that the line contains atom coordinates (also atom number, name, residue name and residue number)
"HETATM" -- stands for "heteroatom" i.e. any atom that is not a part of amino acid (could be water, heme, etc)
"SEQRES" -- these lines list the amino acid sequence of a protein.
Some files also contain lines starting with "HELIX" or "SHEET" -- these list elements of secondary structure

Q: The number of amino acid residues in the protein sequence equals the atom number seen on the protein text file?

A: NO. there are more than one atom per residue, right? Residue number is listed in column 5 (in those lines starting with "ATOM"). Of course, there are other ways to get the number of residues:

You can count how many residues are in the protein sequence which is usually listed in the header part of a pdb-file (lines starting with SEQRES).

Another way of doing this is on the screen is to find the N- and C-termini and determine residue numbers corresponding to these residues by clicking on them. Then do the subtraction.

Q: To determine if there are any other molecules beside polypeptide chains, we should download the text file for that particular protein, correct?

A: Yes, this is probably the most straightforward way. You can also try to see them in the RasTop window, e.g. switching to "ball-and-stick" representation of bonds.

Q: You would want us to identify heme groups or water molecules this way?

A: You can try identifying them from what you see on the screen, but this might not be very easy or accurate. Probably the best way would be to look what is in the text file and then compare it with what you see on the screen and/or what the "information" button gives you.

Q: Is there a way to zoom in on the proteins.

A: Yes. As I used it many times in class: on the bottom of RasTop (left side) you will find three sliders. If you select (check out) "Translate-Zoom" instead of "Rotate", you should be able to use the z-slider to move the protein along the z-axis closer to you (i.e. zoom on it)

Q: For the supersecondary elements, do we reference our books to name them? I can highlight the helices and sheets and compare them to structures seen in the book.

A: There are some definitions/examples in the book. Some of them I also mentioned in my lecture (back in March). I just noticed, for example, that the book does not mention beta-hairpins (or maybe I missed it?). Just let your fantasy go.