Other fun PDB features for you to explore:

The PDB has many other molecular viewing programs that allow you to look at the whole protein. Ligand Explorer is fabulous if you just want to focus on the metal ion and what’s binding to it, however, if you want to explore more of the protein, programs like Simple Viewer and Protein Workshop are useful. These viewers are accessible from the structure summary page for the molecule, like Ligand Explorer. You can find links to them at the bottom of the “Biological Assembly” box on the right side of the structure summary page. They also use Java Web Start, but if you can get Ligand Explorer to work, these should work as well. Once you’ve launched the programs, you can load new files from there PDB ID numbers using the File:Open PDB ID menu item just as in Ligand Explorer.

Simple Viewer is just what its name implies. It allows you to rotate and zoom in and out on the molecule (same controls as Ligand Explorer), but that’s about the extent of what you can do. Protein Workshop also lets you view, rotate and zoon in on the structure, but also allows you to change the style and colors in the structure and visualize and label certain amino acids. The PDB has online help pages for both of these programs; links are given below:

Simple Viewer: <http://www.pdb.org/pdb/staticHelp.do?p=help/viewers/simpleViewer_viewer.html>

Protein Workshop: <http://www.pdb.org/pdb/staticHelp.do?p=help/viewers/proteinWorkshop_viewer.html>

Exploring protein structures beyond the PDB:

There are many other web resources aside from the PDB that one can use to explore the structures of proteins; a few are described below.

One website that I have used is MIT’s StarBiochem (<http://star.mit.edu/biochem/>). This program is user friendly and fairly powerful in terms of visualizing proteins. There are video tutorials available as well as a user manual on the website. My favorite thing about this website is that it has several excellent sample exercises that students can go through (both guided and unguided) that make great in class activities.

Another protein viewing program that has been around for a very long time is the Swiss PDB Viewer (<http://spdbv.vital-it.ch/>). This program is very powerful and has lots of great features (ability to measure distances, angles, make mutations, etc.). It does have a user guide and tutorials available, but be prepared to invest some time in learning how to use this program. However, if you need to be able to use some of these more advanced features, this program is well worth learning how to use.

PyMol (<http://www.pymol.org/>) is another powerful program that can be used to view and make images from PDB files. There is an educational version of this software that students and instructors can access free of charge.

MetalPDB (<http://metalweb.cerm.unifi.it/>) is a database specifically for accessing information on metal sites in biological molecules from the PDB. It has a great advanced search feature that allows you to search for particular metal/ligand combinations. A more complete description of this website, along with a comparison to other databases that focus on metals in biology, can be found in the following reference: Andreini C, Cavallaro G, Lorenzini S, Rosato A., MetalPDB: a database of metal sites in biological macromolecular structures., *Nucleic Acids Research,* 2013, *v. 41 (Database Issue)*, D312-D319 (doi: 10.1093/nar/gks1063).

Metal MACiE (<http://www.ebi.ac.uk/thornton-srv/databases/Metal_MACiE/home.html>) is a database that describes the properties and functions of metals involved in enzymatic reactions. It allows you to search by enzyme name, metal ions, and PDB code. It has a nice feature that allows you to see not only the overall reaction of the enzyme but also step-by-step diagrams of the reaction mechanism as well.

Further reading:

Most bioinorganic textbooks contain a chapter or section describing how amino acids (and nucleic acids) bind to metal ions. For example, Chapter III in Bertini, Gray, Steifel, and Valentine’s *Biological Inorganic Chemistry: Structure & Reactivity* is a very good resource on this topic as is Chapter 3 in Lippard and Berg’s *Principles of Bioinorganic Chemistry*.

A literature article that also may be helpful is: Yamashita, M.M., Wesson, L., Eisenman, G., and Eisenberg, D. Where Metal Ions Bind in Proteins, *Proc. Acad. Sci. USA*, 1990, *87*, 5648-5652.