

BCH 258 – Fall 2009

Instructions for Individual Report

Due Mon. Oct 12, by email or on a CD.

The report uses one or more PDB files and is organized around a paper from the primary literature (you can of course add information from a related paper that complements or differs with your central one), on a topic of interest to you and that uses the 3D macromolecular structure to make a point important to the argument of the paper.

In many cases, the paper would be the one that reports the structure in the related PDB file(s), so that paper is the “JNRL” reference in the PDB header. Otherwise the paper might refer to an earlier structure and would cite the PDB code for it.

The report is in written form (.doc or .pdf), plus a kinemage graphics file of the structure that shows how you documented the structural evidence for the point(s) made in the paper, or perhaps how you disagree with some part of it. A pdf of the paper should also be included. The kinemage should have saved views for the relevant parts, and whatever lines, labels, etc. needed to let someone else see the critical things; the text should explain what to do or look for in the graphics. If you are an expert in some other suitable graphics (e.g., PyMol, Coot) you may use that (with an accompanying text file) – but then you will need to come in and show it to one of us in person.

1) PDB codes must be given!

2) This is probably quite unlike any report that you have ever written before. The text should NOT be just a summary and discussion of the paper with 2D pictures.

3) There must be a tight coupling between text and graphics. i.e. text should refer explicitly to views, labels, drawn, and colored parts. The graphics must clearly show what the text discusses. Any 2D figures within the text must clearly have added value to a specific view or feature shown in the kinemage. The exception would be something like blob diagrams to show context of components not included in the 3D structure coordinates.

4) DO NOT just write a text report with just a vaguely related set of kinemage illustrations as an extra file. Ideally, the kinemage graphics (with labels, etc.) could tell the story in itself – the text is just the glue that leads the reader through the graphics report.

Possible ways to find your topic:

Search, or ask people, for a suitable paper & structure on a molecule central to your research interests.

Look thru a recent issue of a relevant major journal.

Search at the PDB site for structures related to a topic of interest, and look up their JNRL papers.

If you have doubts about whether you've selected an appropriate paper, PDB, and point – come ask Dave, Jane, or Lorena or send email.