Record of 3D Macromolecular Structure Observations for Protein Explorer (Advanced Level Form)

by Eric Martz, May 2000 (revised August 2000)   **Advanced PDF**   **Basic Level Form**
To type into this form, use Netscape's File menu, Edit Page.
Protein Explorer development is supported by the National Science Foundation.

Your Name _____   PDB ID Code _____

Name of Molecule _____

Resolution _____   R_free _____   Date Deposited at PDB _____

Authors _____

EXPDTA _____   Organism _____

A. How many chains are there?

Chain Name*	Protein, DNA, or RNA?	Disulfides? Nonbridge Cysteines?	Alpha helices? ***	Beta strands? Parallel/antiparallel ? ***

Chain Name*	Number of Residues? **	Nature of Gaps or Insertions (if any)?	Number of cation-pi's? (any between chains?)	Number of salt bridges? (any between chains?)

*Hint: click on the chain and look for the one-letter "name" in the message window.
**Hint: use the Sequence display (click 🔴, then Sequences). Compare with SEQRES in the PDB file header.
***Hint: in QuickViews, DISPLAY Cartoon, COLOR Structure.

B. Does the 3D structure represent the entire length of the naturally occuring protein? (Hint: Click 🔴and use the links to PDB File Header; and RCSB Structure Explorer, where you can click Other Sources. You may need to click All to open the *Sequence Data* block of links).

C. Is water present? Approximately what percentage of the water truly in the crystal is visible?

D. Are bound ligands present (non-solvent "hetero" atoms)? If so, are they held by covalent or noncovalent bonds? To what types of residues? (Hint: SELECT Ligand, DISPLAY Contacts. Click on bonded atoms to identify their residues.)

E. In soluble proteins, hydrophobic residues are buried in the cores of domains. Large hydrophobic patches on the surface may be sites of protein-protein interaction. Where do you see concentrations of hydrophobic residues? (Hint: DISPLAY Spacefill, COLOR Polarity3.)

F. If there is protein bound to nucleic acid, which nucleotides are recognized in a sequence-specific manner? Which are bound nonspecifically to the backbone? (Hint: SELECT Protein, DISPLAY Contacts, click on bound atoms to identify residues.)

G. Are hydrogen atoms present? If so, are all hydrogens present, or only a subset? (Hint: in FirstView, click on Water, and then on the link to "more about hydrogen".)

H. How many models are present, and why?

I. What other protein has greatest *structural* similarity to yours, without regard to sequence similarity? Try **http://cl.sdsc.edu/ce/all-to-all/all-to-all.html**. If you find one of interest, check it, click the [Get Alignment] button. Click Download Alignment as a PDB File. Use Netscape's File, Save As and name the file **aligned.pdb**. Enter "bare" Protein Explorer or use the "Different Molecule" link and Browse to find and load aligned.pdb. To see both molecules, you will need to go to Advanced Explorer, NMR Model Selection, and accept the offer to color by N-C Rainbow.

J. Validation? (PDBREPORT http://www.cmbi.kun.nl/gv/pdbreport)

K. Comments/special features? (Noncovalent bonding between moieties? MSA3D?)