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

www.umass.edu/microbio/chime/explorer

by Eric Martz, May 2000

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Your Name _____ PDB ID Code _____

Name of Molecule

A. How many chains are there?

Chain Name*	Protein, DNA, or RNA?	Number of Residues? **	Disulfides?	Alpha helices? ***	Beta strands? Parallel or antiparallel? ***

Hint: click on the chain and look for the one-letter "name" in the message window. **Hint: use the Sequence display (click the red/yellow icon, then Sequences). ***Hint: in QuickViews, DISPLAY Cartoon, COLOR Structure.

B. Is water present?

C. 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.)

D. 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.)

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

F. Comments/special features?