local environment and hydrogen bonding networks of each water molecule. A correlation between the environment of each unique water molecule and its energetic properties such as dipole moment and binding energy was seen. Moreover, non-pair additive effects were found to be non-negligible. However, agreement between predicted and experimental results was not as good as the agreement between the different predicted asymmetric units (which were all simulated independently of the crystal symmetry constraints). This implies that there is room for improvement in the potential energy functions in order to obtain closer agreement with experimental data. Therefore, we have been studying modifications to these potentials which include either all hydrogen atoms or polar hydrogen atoms explicitly rather than the united atom approach used initially. Further studies involve a more specific solute potential combined with our PE water model.

In the second part of this study of hydration of nucleotides, both accessible and contact areas have been calculated for di-, tetra- and dodeca- nucleotides in the classical A, B and Z helical forms. Changes in the solvent exposure of some residues have been found e.g. the free phosphate oxygens have increased contact and accessible areas as one goes from the A to the B to the Z form, and the 5' sugars have less solvent exposed areas than the 3' sugars but this is due to a different balance of atomic accessibilities in the A and B forms. Sequence specific changes to these solvent exposures have also been investigated as a function of the number and type of neighbouring bases. Similar calculations are being undertaken for (a) dinucleotide drug crystal structures in order to compare the changes in solvent exposure on binding intercalating drugs and (b) oligonucleotide structures to look at the effects of local changes in structure compared with the classical forms.

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02.12–7 STRUCTURAL ANALYSIS OF THE PROTEIN CRAMBIN FROM X-RAY DIFFRACTION STUDIES AT 0.945 A. Martha M. Teeter, Department of Chemistry, Boston, University, Boston, MA 02215 USA.

Crambin is a small, hydrophobic plant protein (MW = 4700) with no known function. However, crystals of it diffract to 0.88 A (Teeter and Hendrickson, J. Mol. Biol. (1979) 127, 219-224). The model obtained from the structure solution and refinement at 1.5 A (Hendrickson and Teeter (1981) Nature 290, 107-113) has now been refined against the 0.945 A data by restrained least squares techniques (Hendrickson and Teeter, unpublished).

Crambin crystals contain 32% solvent. More than 80% of the solvent is ordered. Despite the fact that crystals were grown from 60% ethanol, very little ethanol (about 7%) has been located in the crystals. Most of the water found at the surface of crambin is bound to polar groups at the surface. These molecules connect donors and acceptors on the protein in lines. However, a cluster of waters at a hydrophobic intermolecular interface, sandwiched between charged protein side chains, form pentagon arrays around a methyl group on the surface. This is the first time such a cluster has been described at a protein surface and is reminiscent of the water clathrate structures of quaternary amines, aliphatic amines and alcohols. The significance of crambin's pentagonal water array for solvent ordering in general at hydrophobic protein surfaces is unclear and will be discussed.

The detailed geometry of crambin (bond lengths and angles, dihedral and planarity) will be described and compared with peptide geometry information available from analysis of the Cambridge Data File. Features of the secondary structure (hydrogen bonding patterns and distortions from ideal geometry) will be discussed.