01. DETERMINATION OF MACROMOLECULAR STRUCTURES

01.61 SRLSQ REFINEMENT OF TRICLINIC LYSOZYME. by M. Ramachandran, Neutron Physics Division, Raja Ramanna Centre, Bombay 400085, India, and, L.C. Siekert and L.G. Jensen, Department of Biological Structure, University of Washington, Seattle, WA 98195, USA.

The x-ray structure refinement of triclinic hen egg-white lysozyme by the method of stereochemically restrained least-squares (SRLSQ) at 2Å resolution has recently been completed. The 1270-atom structure (1001 protein non-hydrogen atoms, 5 NO₃ groups and 249 water oxygen atoms) was refined to an R-value of 0.124 using 7075 independent x-ray structure amplitudes with 1090 Dₚ·1.97Å. The refinement had also resulted in an excellent agreement between the model and the ideal geometries. The R-value came down to 0.169.

General interactive graphics system, the PROTEIN model in the residue range 1.5-2Å resolution has recently been completed. This allowed the use of all observed SF in a least squares refinement. Coupled with the measurement of the crystal density by a density gradient technique, the evaluation of the solvent scattering makes it possible to determine the amount of salt present in the solvent space.

01.62 NEUTRON STRUCTURE ANALYSIS OF PLASTOCYANIN. By W.B. Church, T.P.J. Garrett, H.C. Freeman, Department of Inorganic Chemistry, University of Sydney, Sydney 2006, Australia, and B.P. Schoenborn, Biology Department, Brookhaven National Laboratory, Upton, New York 11973, USA.

Plastocyanin is a 10,500 dalton protein containing one Cu(II)-plastocyanin from poplar leaves has previously been solved and refined using X-ray data at a resolution of 1.6Å. The intramolecular hydrogen bonds which can be inferred from the distances between pairs of non-hydrogen atoms include several that stabilize the protein configuration near the Cu site. Of particular interest is a N-H ... O bond to a Cu-binding cysteine side-chain, which appears to be analogous to such bonds at the active sites of a number of other metalloproteins. The possible importance of hydrogen bonding in relation to the electron transfer function of plastocyanin has generated an interest in the experimental determination of the hydrogen bond positions. Neutron diffraction data for deuterated poplar plastocyanin have been measured at the Brookhaven National Laboratory High-Flux Beam Reactor. The intensities of 64% of the reflections to 1.7Å are significant [1 ± 2σ(1)]. Even the initial nuclear scattering density difference maps provided evidence for well-ordered hydrogen atoms. In this paper, we report progress in the neutron structure analysis of the deuterated protein and in a parallel refinement of the structure using new X-ray counter data to 1.6Å resolution.