02.1-43 STRUCTURAL STUDIES OF RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE. By W.W. Smith, S.W. Suh, D. Eisenberg, Molecular Biology Institute, University of California, Los Angeles, and R. Hamlin, A. Howard, C. Nielsen, N.h. Xuong, Department of Physics, University of California, San Diego, California.

Ribulose bisphosphate Carboxylase/Oxygenase (RuBisCO) catalyzes the initial step common to both the pathways of photosynthesis and photorespiration, and is said to be the most abundant protein on earth. RuBisCO from tobacco contains eight large subunits (M_r = 55,000) and eight small subunits (M_r = 14,000), arranged with symmetry 422. The enzyme crystallizes in space group I422 with a = 148.7 Angstroms and c = 137.5 Angstroms. We have determined the structure of this enzyme to a resolution of 5.0 Angstroms and have interpretted the electron density in terms of the subunit locations. All of the data used in the structure determination were collected on the Mark I multiwire area detector currently in operation at UCSD. Native data to 2.9 Angstroms resolution have been obtained using the Mark II version of the area detector. This enzyme is the first structure of this size to be solved with the use of the multiwire area detector. We have also determined (Johal, et. al., J. Biol. Chem., 255, 8873-8880 (1980)) that crystals of RuBisCO from other plant species are isomorphous with those from tobacco. This may be related to the tendency of RuBisCO to be crystalline in the chloroplast.

02.1-44 TYROSYL-tRNA SYNTHETASE FORMS A NUCLEOTIDE BINDING FOLD. By P. Brick, T.N. Bhat and D.M. Blow, Blackett Laboratory, Imperial College, London SW7 2BZ.

Tyrosyl-tRNA synthetase from B.stearothermophilus is a dimeric molecule of approximately 90,000 daltons. The crystal structure originally reported by Irwin et al. (J.Mol.Biol. (1976) 105, 577) has been reinterpreted using a new density modification technique (Bhat and Blow, this volume). The structure consists of an amino-terminal α/β domain, a domain containing five α-helices, and a region of at least 95 amino-acids at the carboxyl-terminus which appears to be disordered. The re-interpretation reveals two new α-helices in the α/β domain, and some changes in chain connections. The strands of the β-sheet are in the order A F E B C D, with A antiparallel to the others. The arrangement of strands B to F is topologically identical to arrangements found in many other proteins, including the first five strands of the sheet in the NAD-binding domain of the dehydrogenases.

In the complex with tyrosyl adenylate (Rubin and Blow, J.Mol.Biol. (1980) 145, 489), an intermediate in the reaction catalysed by the enzyme, the adenine lies near the carboxyl-terminal end of strands E and F of the β-sheet, with the ribose between the ends of strands B and E. This is similar to the nicotinamide position in dehydrogenases. The tyrosine moiety occupies a pocket at one side of the sheet, close to strands B and C. This tyrosine orientation is quite different from any part of the coenzyme in dehydrogenases.

02.1-45 REFINEMENT OF CARBONIC ANHYDRASE ISOZYMES B AND C AT 2Å RESOLUTION. By M. Ramanadham and K.K. Kannan, Neutron Physics Division, Bhabha Atomic Research Centre, Trombay, Bombay 400 085, India.

The structures of human erythrocyte carbonic anhydrase isozymes B and C are refined by the method of stereochemically restrained least-squares. Initial model for the B enzyme has been improved by model fitting using an interactive graphics display and real-space refinement. Restraints on 5,515 inter-atomic distances, 345 planar groups and 298 chiral centers have been imposed, while refining 5,931 positional parameters from 1,977 atoms (including one Zn^{2+} ion), against 3,723 structure amplitudes in the d-spacing range of 5 to 3Å chosen from 15,524 observations with $d \geqslant 1.98$ Å. The molecular model has significantly improved in 4 cycles of refinement during which the R-factor has changed from 0.415 to 0.365. Work is currently underway to locate the remaining 7 residues of the protein and solvent molecules and to refine the structure further. Similar procedure is persued in the refinement of C enzyme also. The initial model has 2,039 atoms from 256 residues (out of a total of 259) and one Zn^{2+} ion. Thus a total of 6,120 positional parameters are refined using structure-amplitude data in the d-spacing range of 5 to 3Å chosen from more than 17,000 observations with $d \geqslant 1.97$Å. Restraints on 5,717 distances, 353 planar groups and 298 chiral centers are imposed during the refinement. A comparison of the two carbonic anhydrase structures and function in the light of the refinement will be discussed.

02.1-46 THE STRUCTURE OF LIPASE AT 2.5 Å RESOLUTION. By Y. Hata, N. Tanaka, M. Kakudo, A. Sugihara*, M. Iwai* and Y. Tsujisaka*, Institute for Protein Research, Osaka University, Suita, Osaka 565, Japan; * The Osaka Municipal Technical Research Institute, Kitaogimachi, Kita-ku, Osaka 530, Japan.

Lipase from *Geotrichum candidum* (ATCC34614) is a hydrolase of three ester bonds in fats and fatty oils, especially triolein. The molecule (Mr=55,000) consists of a protein (430 amino acid residues) and 7% of carbohydrate. The primary sequence is not known. The crystals were grown from 3% enzyme solution, pH 5.6, kept at 10°C; space group $P2_1$, Z=2, a=59.5, b=83.6, c=56.1 Å, β=99.9°. These crystals were crosslinked with 0.37% glutaraldehyde in order to reduce their solubility in solutions of heavy-atom reagents. A 2.5 Å resolution electron density map was calculated with double isomorphous replacement technique (K_2PtCl_4, $UO_2(AcO)_2$). The density was tentatively interpreted and the polypeptide backbone model (2 cm/Å) was built with an optical comparater.

The molecule is ellipsoidal with approximate dimensions 70 x 50 x 50 Å. About 20% of amino acid residues are in α-helix conformation and about 4% in β-structure. The molecule is composed of two parts from a viewpoint of the arrangement of the secondary structure. One part (part A) is rich in α-helices and contains seven of the nine α-helices. The other (part B) consists of three β-strands and two α-helices which form a β-sheet sandwiched between the α-helices. The active site of the enzyme was estimated as around one of the Pt atoms which inactivates the enzyme by binding to the histidyl residue in the active site (J. Biochem., 86, 1821 (1979)). The possible active site is in the vicinity of the longest α-helix. A long channel leads to the surface from the site and its end is surrounded with α-helices.