isomorphous replacement and anamolous scattering from a single mercuric iodide derivative (Freymann, Metcalf, Turner and Wiley, unpublished). The electron density map indicates a rod-shaped dimer, with a core of four 80 Å long alpha-helices.

The human histocompatability antigen HLA-A2 is active in tissue graft rejection and immunological recognition during surveillance by "T-killer" cells. The papain-solubilized HLA is a 2 chain structure (46,000 daltons), which is purified from human tissue culture cells. This is a technically challenging problem as the crystals are very thin plates. X-ray data to 2.8 Å resolution for the native and a platinum tetrachloride derivative were collected at the EMBL synchrotron outstation in Hamburg from crystals 10-30 microns thick. Three platinum sites have been determined from the three-dimensional difference Patterson (Bjorkman, Bennett and Wiley, unpublished). An antigenically distinct HLA, A28, forms an isomorphous crystal. Further progress in this analysis will be discussed.

02. X–8 THE STRUCTURE OF NEURAMINIDASE. By P.M. Colman, J.N. Varghese and W.G. Laver, CSIRO Division of Protein Chemistry, Parkville 3052, Australia and Australian National University, Canberra, Australia.

The three dimensional structure of the N2 subtype of influenza neuraminidase has been determined by a combination of the multiple isomorphous replacement method in one crystal form with noncrystallographic symmetry averaging in a second crystal form where two copies of the polypeptide are found in the asymmetric unit. The two crystal types used are of neuraminidases from naturally occurring field isolates from 1957 and 1967 with sequence homology of ∿90%. Neuraminidase was liberated from the viral membrane by pronase digestion.

The chain folding has revealed a new class of tertiary structure in which six twisted β sheets, all with 'W' topology, are arranged like the blades of a propeller to form one of the four subunits of the enzyme. Four of the five potential glycosylation sequences carry carbohydrate. One of these oligosaccharides is involved in stabilisation of the circularly symmetric tetramer.

The enzyme active centre has been identified by difference Fourier analysis of sialic acid soaked crystals. The binding site is in a cavity on that surface of the tetramer distal to the viral membrane, and near the corners of the box shaped tetramer. The cavity is lined with nine acidic groups, six basic groups and three hydrophobic groups which are strictly conserved in amino acid sequences of neuraminidases both within and between subtypes of influenza.

Sites of field strain sequence variation have been mapped on to the structure and reveal a nearly continuous surface of variation encircling the catalytic cavity.

02. X–9 STRUCTURES OF SEVERAL BINDING PROTEINS INVOLVED IN ACTIVE TRANSPORT AND CHEMOTAXIS. by F.A. Quiocho, N.K. Vyas, J.W. Pflugrath, M.A. Saper, and M.N. Vyas, Department of Biochemistry, Rice University, Houston, Texas 77251, U.S.A.

Binding proteins located in the periplasm of Gram-negative bacteria are essential components of osmotic-shock sensitive active transport and chemotaxis. The following binding proteins have been solved in our laboratory at the resolution indicated: L-arabinose-binding protein (1.7 Å), sulfate-binding protein (2.0 Å), leucine, isoleucine, valine-binding protein (2.8 Å), and the D-galactose-binding protein (2.5 Å). With the exception of the amino acid binder, each structure has been solved with bound ligand. The arabinose- and sulfate-binding proteins have been refined by restrained least squares method to R-factors of 13.7% and 14.0%, respectively. Despite lack of significant sequence homology, these proteins have a high degree of overall structural similarity; all four proteins are elongated and composed of two globular domains with a central β-pleated sheet sandwiched between helices. As a group these proteins are unusual since each domain is folded from two separate polypeptide chain segments. These proteins have a common ligand binding site located in the cleft between the two domains. The interaction of L-arabinose and sulfate with respective receptor protein revealed novel features. Either α- or β-L-arabinose is bound in the same site of the binding protein, and all sugar hydroxyls and ring oxygen in both anomers form identical extensive networks of hydrogen-bonds with side chain residues. The sulfate bound to the sulfate-binding protein forms hydrogen-bonds with seven residues none of which are charged; three of these residues are peptide NH from the N-termini of three helices. The bound arabinose or sulfate is inaccessible to the bulk solvent. (Research supported by NIH, NSF and the Robert A. Welch Foundation.)

02. X–10 THE STRUCTURE OF GLYCOLATE OXIDASE FROM SPINACH. By Y. Lindqvist and C.-I. Brändén, Department of Chemistry and Molecular Biology, Swedish University of Agricultural Sciences, S-750 07 Uppsala, Sweden.

Glycolate oxidase is one of the key enzymes in the photorespiration of plants, where it oxidizes glycolate to glyoxylate. It is a flavin enzyme using FMN as cofactor. Structure determination of glycolate oxidase from spinach to 5.5 Å resolution showed (Y. Lindqvist & C.I. Brändén, J. Mol. Biol. (1980) 143, 201-211) that two thirds of the electron density could be interpreted as eight αβ-units wound up as a barrel as in triose-phosphate-isomerase (D.C. Phillips, M.J.E. Sternberg, J.M. Thornton & I.A. Wilson J. Mol. Biol. (1978) 119, 329-351). The data have been extended to 2.5 Å resolution and an electron density map based on two heavy atom derivatives $Hg(CN)_4^{2-}$ and $Pt(NH_3)_2Cl_2$ was calculated. From this map it was possible to build in the β-strands and some of the helices of the αβ-barrel but several helices were poorly defined. For density not belonging to the αβ-barrel it was not possible to trace the main chain. Since our platinum derivative did not contribute much to the phasing we had in actual fact SIR phases. We therefore tried the ISIR-ISAS program package written by Bi-Cheng Wang (Acta Cryst A, in press). This program defines a protein-solvent boundary from the map, flattens the solvent and after backtransformation of the filtered map combines the phases using Sim weighting. This is done in several iterative cycles. The result on our data was striking and gave a map where the helices of the αβ-barrel can now be clearly defined and additional helices in the extra density regions have been identified. We are presently building a model on a graphics display and the result of this work will be presented.