**02.2-02** COMPARISON OF THE STRUCTURES OF KDPG ALDOLASE AND TRIOSE PHOSPHATE ISOMERASE. By L. Lebioda, M.H. Hatada, I. Mavridis and A. Tulinsky, Department of Chemistry, Michigan State University, East Lansing, Michigan 48824, U.S.A.

The structure of 2-keto-3-deoxy-6-phosphogluconate (KDPG) aldolase has been extended to 2.8 Å resolution using MIR methods. The final MIR phases were improved further with 3 cycles of refinement via electron density modification procedures coupled with inverse fast Fourier transform phase angle calculations. With the complete sequence of the enzyme now available (Suzuki, N. and Wood, W.A., J. Biol. Chem., 255, 3427 (1980)), a Kendrew model was constructed corresponding to the electron density of the final cycle. All 225 residues have been accounted for in the model. The main chain density is generally good except in the region 189-197 where it is weak and discontinuous; of the side chains, 139 residues have good density, 36 residues have only partial, and 29 residues have no side chain density, while 21 residues are Gly.

Of the approximately 50 residues not located in the 3.5 Å resolution map, about 40 have been found in the interior of the molecule as part of 8 strands of a β-barrel. The overall folding of KDPG aldolase is similar to that of triose phosphate isomerase (TIM) with adjacent strands of β-structure linked by α-helical segments. However, the content of regular secondary structure is lower: α helix 29 and 55%, β sheet 16 and 23% for KDPG aldolase and TIM, respectively. The similarity between the structure of KDPG aldolase and TIM was originally recognized by Richardson (Biochem. Biophys. Res. Comm., 90, 285 (1979)) at the 3.5 Å resolution level. This led her to propose 4 chain reconnections to create 4 additional β-strands and thus an 8 strand β-barrel. Richardson's proposed reconnections are necessarily approximately correct topologically, however, since most of the additional residues of the 2.8 Å resolution map were found in the interior as part of the β-barrel, the details of the barrel are different. The very prominent electron density of the helical periphery of the molecule probably affected the generally weaker interior density adversely at lower resolution.

The C-$C_\alpha$ coordinates of KDPG aldolase have been measured with the aid of a surveyor's transit and a cathetometer. The $C_\alpha$ structure is being compared to that of TIM. The primary structures and the active site regions of KDPG aldolase and TIM are also being compared. Depending upon the degree of significance of correlations, a comparison of the side chain structure might also be carried out.

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**02.2-03** TWO ANALYSES OF PROTEIN STRUCTURES : 1. THE ROLE OF THE AMINO AND CARBOXY TERMINI. 2. SALT BRIDGES AND THE DISTRIBUTION OF CHARGED GROUPS. By J. Thornton and L. Chakauya, Department of Crystallography, Birkbeck College, Malet Street, London, WC1E 7HX, UK.

1. A survey of the N and C terminal regions in proteins of known structure has been performed. We have considered conformation, accessibility, proximity and specific interactions between termini, relationship to the active site and functional regions, domain linking and dimerisation and the asymmetry of the termini. The results suggest that the termini fulfil certain specific roles in maintaining the stable native conformation.

2. The distribution of salt bridges and charged groups in proteins of known structure has been analysed. The survey includes residue type, conformation, acessibility and function. The role of salt bridges and charged groups in proteins is considered.

**02.2-04** CALCULATING MOLAR VOLUMES OF PROTEINS FROM ATOMIC COORDINATES : PROBLEMS OF VOLUME PARTITIONING AND WATER-PROTEIN INTERACTIONS. By B. J. Gellatly and J. L. Finney, Crystallography Dept, Birkbeck College, Malet Street, London, WC1E 7HX, England.

An ability to calculate accurate molar volumes of proteins is a strong test of a model of solvent-protein interactions, and is desireable if we are to understand pressure effects. Moreover, increasing use of low-angle neutron scattering measurements of radius of gyration require a knowledge of excluded volume for full interpretation. However, attempts to perform such calculations have been so far unsuccessful (Richards, J. Mol. Biol. 82, 1(1974); Finney, ibid, 96, 721(1975)), because of (a) technical problems of physically reasonable space partitioning, and (b) an inadequate knowledge of where to position bounding solvent. Richards' use of a surrounding ordered water lattice resulted in calculated volumes greater than experiment. Finney used a variety of surface treatments and managed to obtain a range of results which encompassed the experimental value. However the use of van der Waals surfaces was unjustified with respect to hydrogen bonding interactions. The present availability of high resolution structures including much of the first shell water suggests further progress can now be made in solving this problem. We report here the initial results of studies on several small but well-defined proteins.

(1) Volume partitioning between protein and the surroundings was performed using the Voronoi construction, which places dividing planes midway between atom pairs, and the Radical Plane generalisation (Fisher et al, Neues Jahrb. Min. Monat. 227(1971)), in which the dividing plane is drawn at a distance which is a function of the sizes of the two atoms concerned (cf. Richards' "method B"). Its application to protein packing will be