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.