12 Leucines from 4 helices around the 4-fold axis make a hydrophobic channel. The 3-fold channel is very hydrophilic. Each subunit donates a SER, ASP and GLU.

Ribbon diagram of the apoferritin dimer and parts of two other subunits. The hydrophobic face of the short helix facing the 4-fold channel is shaded.

02.1-44 MANGANESE AND IRON SUPEROXIDE DISMUTASES ARE STRUCTURAL HOMOLOGS. U. Stallings, S.A. Partridge, and N.L. Ludwig, Biophysics Research Division and Department of Biological Chemistry, University of Michigan, Ann Arbor, MI 48109.

The crystal structure of a tetrameric manganese superoxide dismutase from a thermophilic bacterium, Thermus thermophilus HB8, has been determined at 4.4 Å resolution by local averaging of electron density maps calculated from isomorphous replacement. The enzyme crystallizes from ammonium sulfate at pH 5.7 and pH 7.0 in space group P2_12_12 with a = 144.6 Å and c = 55.6 Å. The spatial arrangement of the principal secondary structural features of iron superoxide dismutase is repeated in manganese dismutase, as demonstrated by superposition of the polypeptide chains of Fe and Mn dismutases. Density peaks corresponding to bound Mn are observed at locations equivalent to the Fe positions in iron dismutase, indicating one metal binding site per chain, or four sites per tetramer. The Mn dismutase tetramers have molecular 222 symmetry with one of the twofold axes coincident with a crystallographic diad. The tetramer is approximately rectangular in shape and appears to be constructed with only two unique interfaces. One set of interchain contacts closely resembles the dimer interface of Fe dismutase, but the other interface utilizes a polypeptide segment, inserted between the first and second helices, that has no equivalent in Fe dismutase.

02.1-45 THE STRUCTURE ANALYSIS OF DIPHTHERIA TOXIN by B. McKeever and R. Sarma, Biochemistry Department, State Univ. of New York, Stony Brook, N.Y. 11794, U.S.A.

The diphteria toxin, produced by Corynebacterium diphtheriae is responsible for the observed lesions associated with that disease. The Protein is a single polypeptide chain of molecular weight 60,000. It is made of two domains, the C terminal domain recognizes and binds to receptors on susceptible cell surface and internalizes the N terminal domain, which upon entering the cytoplasm catalyzes the hydrolysis of NAD and the ADP ribosylation of a unique diphthamide residue on the eukaryotic elongation Factor-2, resulting in the termination of Protein synthesis.

The purified Protein can be isolated into sixteen fractions with different identifiable properties; monomer-dimer, polypeptide bound or free and so on. The bound dimer fraction yields diffraction quality crystals belong to the space group P3_1_2 or its enantiomorph with unit cell dimensions a=b=97.9 Å; c=100.3 Å. The diffraction data is being collected using oscillation photographs and the structure is being determined using multiple isomorphous replacement method. The results of the electron density map will be presented.