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 HOMOLOGUES. U. Stallings, K.A. Pattridge, 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 HN3, has been determined at 4.4-Å resolution by local averaging of electron density maps calculated by isomorphous replacement. The enzyme crystallizes from ammonium sulfate at pH 5.7 and pH 7.0 in space group $P4_12_12$ with $a = 146.6$ and $c = 55.6$. 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-45 occur 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.

02.1-46 AN X-RAY DIFFRACTION STUDY OF A PEPTIDE HORMONE DEMAMINE-OXYTOCIN. By T. L. Blundell, S. Cooper, J-T. Li, J. E. Pitz, I. J. Tickle, A. C. Preham and S. P. Wood, Laboratory of Molecular Biology, Department of Crystallography, Birkbeck College, University of London, London WC1E 7HX, UK; V. J. Hruby, Department of Chemistry, University of Arizona, Tucson, Arizona 85721, USA; and H. R. Wamsbord, Department of Physiology and Biophysics, Mount Sinai Medical Centre, New York 10029, USA.

Oxytocin, a nanopeptide hormone composed of a twenty-membered ring and acyclic tail, has hormonal activities eliciting smooth muscle contraction in mammary glands and uterus. The highly potent 6-sulphur demamine oxytocin has been crystallised in the dry form with space group $P3_1$ and cell dimensions $a = 27.01$, $b = 9.06$, $c = 22.98$, $\beta = 102.1^\circ$ and data collected to 1.92 Å resolution. The 6-seleno demamine oxytocin analogue crystallised isomorphously with cell dimensions $a = 27.01$, $b = 9.14$, $c = 22.98$, $\beta = 102.2^\circ$ and data have been collected to 1.92 Å resolution. The phases were calculated using anomalous differences and the models refined with restraints using SHELX and RESTRAIN (Moss, Moffew, Haneef, Stanford and Borkakoti). There are type II $\beta$-turns between residues 2 to 5 of the rings and type I $\beta$-turns involving residues 6 to 9. There is conformational disorder at the disulphide bridge. The crystal structure will be compared to conformations from NMR and other spectroscopic studies in water and DMSO and in terms of binding to neurophysin and receptors.