muscle and yeast enzymes. A model of one subunit was built using the computer graphics program Bilder designed and written by R. Diamond. The model comprises a short N-terminal peptide plus three domains A, B and C containing a total of 515 residues compared with the 529 contained in the sequence. There appears to be no electron density for either the N-terminal or the C-terminal residues. This model was used as the starting point for a restrained parameter, least squares refinement using the Konnert program implemented on the S.E.R.C. Cray-1 computer. The final crystallographic R-factor for the 2.6Å data was 0.283 and the final structure deviated from ideal bond lengths by an overall root-mean-square deviation of 0.019Å.

The active site has been located by studying the binding of bivalent cations, PEP and ATP. The overall homology between the muscle and yeast sequences is about 42% and side-chains close to the active site are highly conserved. Results of model-building experiments will be described.

02.1–25 MOLECULAR MODELLING APPROACHES TO THE CORRELATION OF STRUCTURE AND SOLUTION PROPERTIES OF THE SERINE PROTEASES. By T. F. Kumosinski[1], E. M. Brown[1], and M. N. Liebman[2]. [1]Eastern Regional Research Center, USDA, Philadelphia, PA 19118, and [2]Mt. Sinai School of Medicine, SUNY, N. Y., NY 10029, USA.

Serine proteases are responsible for a variety of biological control processes, such as fertilization and complement activation, via so-called limited proteolysis. These control processes involve exact macromolecular recognition. We have initiated studies of this recognition using calculations based on the three-dimensional X-ray crystallographic coordinates in conjunction with solution physical chemical methods. The modelling techniques used consisted in topological analysis (electrostatic potential surface mappings, partioned distance matrix analysis, van der Waals and accessible surface mappings) and a new internal energy profile analysis (dipole moment alignments, hydrophobicity indices, dipole-dipole, charge-dipole, and charge-charge interactions in a matrix representation). Sedimentation equilibrium and circular dichroism analyses on both enzyme and macromolecular inhibitor were performed to determine the free energy change on complex formation (ΔG_c) and the extent of autoproteolysis, as well as the influence of Ca binding and pH on ΔG_c and the regulation of autoproteolysis. The results for a number of serine proteases verified the existence of eight soft β-turns distributed on either side of the active site (MNL). They suggest point-site mutations which could modify the specificity of these natural protease inhibitors. (MNL is the recipient of a Revson Foundation Fellowship.)

02.1–26 CRYSTALLOGRAPHIC STUDIES OF BLUE PROTEIN FROM A. FAECALIS AT 2.8Å. E.T. Adman, Dept. of Biological Structure, Univ. of Washington, Seattle, Wash. 98115 and T. Beppu and H. Watanabe, Dept. of Agricultural Chemistry, Univ. of Tokyo, Bunkyo-ku, Tokyo 113

The blue protein from Alcaligenes faecalis strain S-6 is a Type I blue copper protein (cupredoxin) which is specifically required for transfer of electrons to a copper containing nitrite reductase, both in the normal electron transfer pathway whereby nitrates are converted to N_2, and in an abortive pathway whereby the reductase is inactivated in the presence of O_2.

Partial sequence information, the amino acid composition, and the molecular weight (intermediate to the two other blue copper proteins with known structure, plastocyanin and azurin) suggest that while A. faecalis blue protein probably has the same chromophore, it may have different folding, and may well represent a structural subclass of these cupredoxins.

This cupredoxin crystallizes in space group $P6_{5}$ with cell dimensions a = b = 49.9Å, c = 98.4Å, γ = 120°. The ratio of cell volume to molecular weight is 2.95, consistent with one 12,000 unit in the asymmetric unit with 60% solvent. Native diffraction data has been collected on a Picker FACS-1 diffractometer to 2.8Å resolution; data from a uranyl nitrate soaked crystal has also been collected to 2.8Å. The Patterson indicates one major heavy atom site.

Progress in determination of this structure will be reported. Support for ETA from NIH grant GM13666 is gratefully acknowledged.

02.1–27 X-RAY CRYSTALLOGRAPHY OF FAB FRAGMENTS OF ANTI-DIGOXIN AND ANTI-ARSONATE ANTIBODIES. D.R.Rose[1], G.A.Petsko[1], M.Margolies[2], J.Novotny[2], E.Haber[2] and M.Gefter[3], Depts. of [1]Chemistry and [3]Biology, M.I.T., and [2]Mass. General Hospital, Boston, Mass., U.S.A.

Crystals have been obtained of Fab fragments of monoclonal antibodies to the cardiac glycoside, digoxin. The Fab's are of clinical use in reversing the toxic effects of digoxin overdose[4]. Preliminary data on crystals of Fab 26-10 grown from mixtures of MPD and PEG(6000) will be presented.

Crystals of three anti-phenylarsonate hybridoma Fabs have been grown. Two(36-71 and 36-65) display the major idiotype of anti-arsonate antibodies in the A/J strain mouse and one (36-60) displays a minor idiotype. Data have been taken from Fab 36-71 crystals ($P2_1$, a=65.1, b=73.2, c=45.2Å, β=104.6°, grown from PEG(6000) at 20°C). Fab 36-60 crystallized at 4°C from PEG(6000) solutions in tetragonal space group $P4_32_12$ or enantiomorph with cell dimensions 68.6, 68.6, 247.0Å. A report on the progress of the structure solutions will be presented.

Abbreviations: MPD, 2-methyl-2,4-pentanediol, PEG, Polyethylene Glycol

[4]Margolies, M., Mudgett-Hunter, M., T. Smith, J. Novotny, and E. Haber (1981) in: Monoclonal Antibodies and T Cell Hybridomas (Hammerling, Hammerling, Kearney, eds.), Elsevier/North Holland, New York, 367-374.