muscle and yeast enzymes. A model of one subunit was built using the computer graphics program Bildner 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 Konkert program implemented on the S.D.R.C. Cray-1 computer. The final crystallographic R-factor for the 2.6A data was 0.263 and the final structure deviated from ideal bond lengths by an overall root-mean-square deviation of 0.019A.

The active site has been located by studying the binding of bivalent cations, mean-square deviation of 0.283 and the final structure deviated from ideal bond lengths by an overall root-mean-square deviation of 0.019A.

Results of model-building experiments will be presented. The active site has been located by studying the binding of bivalent cations, using the Konkert program implemented on the S.D.R.C. Cray-1 computer. The final crystallographic R-factor for the 2.6A data was 0.263 and the final structure deviated from ideal bond lengths by an overall root-mean-square deviation of 0.019A.

The active site has been located by studying the binding of bivalent cations, mean-square deviation of 0.283 and the final structure deviated from ideal bond lengths by an overall root-mean-square deviation of 0.019A.

The modelling techniques used consisted in topological analysis (electrostatic potential surface mappings, charge-charge, and charge-dipole interactions in a matrix representation). Sedimentation equilibrium and circular dichroism analyses on both enzyme and macromolecular inhibitor were presented. 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 Sevion Foundation Fellowship.)