A continuous feed-back mechanism between the process of data collection and that of data reduction has been developed. It enables modification of these procedures and their adjustment to account for the specific problems of ribosomal crystals.

Consequently, the quality of the data has significantly improved: Currently the evaluated data sets are of completeness and quality comparable to those obtained from crystalline proteins of average size (Rmerge 5-9%).

Special emphasis is put upon the accurate measurement and evaluation of the very low resolution reflections (below 150Å). These reflections are believed to be very important for low resolution phasing by methods other than MIR.

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PS-03.10.04 CRYSTALLOGRAPHY OF A MULTIENZYME COMPLEX CONTAINING RUBISCO. **By M.V.Hosur and K.K.Kannan**, Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Bombay-400085, INDIA.

The existence of multienzyme complexes functional inside living cells has been postulated lately, and crystal structures of two such complexes have been reported so far. We report here our results on one multienzyme complex isolated and purified from spinach leaves . The purified sample is assumed to contain the following enzymes: (1) RUBISCO (2) phosphoribulose isomerase and (3) phosphoribokinase. Single crystals grown by the hanging drop method, have the orthorhombic space group P21212 with a=173, b=134 and c=112Å, and contain two copies of the multienzyme complex in the unit cell. Diffraction data to 2.5Å resolution has been collected at the photon factory in Japan on Prof. Sakabe's oscillation-Weissenberg camera and the Image Plate system. The L4S4 part of the high resolution structure of spinach RUBISCO was the search model in the Molecular Replacement calculations carried out using the software package, MERLOT. The cross rotation function was calculated by including data between 10 and 5Å resolution limits, and for an integration radius of 29Å. The highest peak in this rotation function map was 7.8 times the standard deviation, and for this solution, the translation function calculations gave a consistent set of strong peaks (about 18 sigma) for all symmetry related pairs of molecules. These solutions to the rotation and translation problems led to an initial R-factor of 35.9% for all data between 10 and 3.5Å resolution. Preliminary electron density maps were then calculated using X-PLOR. There is a good deal of continuous electron density on the outside of the input RUBISCO molecule. This extra density represents the other components of the multienzyme complex. Refinement of the model and atomic interpretation of the extra density is currently under progress.

PS-03.10.05 A STUDY OF THE INTERACTION MODES FOR BILE SALTS. By A.R. Campanelli, S. Candeloro De Sanctis*, M. D'Alagni, A. D'Archivio, L. Galantini, E. Giglio, L. Scaramuzza, Dipartimento di Chimica, Università di Roma "La Sapienza", Roma, Italy.

Bile salts, the most important natural detergents, form molecular aggregates in aqueous solutions, which interact in bile and in the small intestines with several important biological compounds as, for example, bilirubin-IXα, cholesterol, phospholipids, glycerides and fatty acids.
There are many indications that the structures of the aggregates in solution are sometimes similar to those found in the crystals and, for this reason, the crystal structure of these compounds is of great interest.
The crystals, difficult to grow, are very seldom single and very often grow like a bunch of thin needles, sometimes unstable in the air. However, we have succeeded in solving a number of crystal structures and we have found that in the crystals the molecules are held together into very stable structural units, sometimes loosely bound to one another, this being a further indication that the aggregation scheme can be similar in the aqueous solutions. For two bile salts, sodium and rubidium deoxycholate, such similarity has been proved unambiguously.
We have found that different bile salts can have very similar aggregation patterns in the crystals and the structures examined so far can be grouped into three basic aggregation schemes.
Generally, the structures are helical (hexagonal, trigonal, twofold) stabilized by hydrogen bonds and ion-ion and ion-dipole interactions. Similarities and differences will be discussed, in particular concerning the hydrogen bond network, compaired with the other interactions through which the structures are stabilized.

PS-03.10.06 X-RAY ANALYSIS OF YEAST LIPOAMIDE DEHYDROGENASE AT 3.5Å RESOLUTION.
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The pyruvate dehydrogenase complex is one of the highly organized multienzyme complexes which catalyze serial reactions accurately and efficiently. To elucidate the reaction mechanism, we are analyzing the crystal structure of lipoamide dehydrogenase which is a component of the complex from yeast.
Crystals, newly obtained by a desalting method, have the same space group as, but are slightly different in the cell parameters from previous ones, the structure of which has already been X-ray analyzed at 4.5Å resolution[1]. Diffraction data were collected up to 2.98Å resolution (max. 2.49Å, 65%) using synchrotron radiation. The crystal structure was solved by molecular replacement with glutathione reductase. Three programs (X-PLOR, MERLOT, MOLREP) gave a significant unique solution with reasonable crystal packing. After several refinements of the poly peptides, validity of the structure was verified using omit maps. The R-factor was further improved by 2% with molecular dynamics. The present R-factor is 30.5% at 3.5Å resolution.
In the electron density map, the main chain could be easily traced, detecting the insertions and deletions of amino acids. Some residual densities are assignable to FAD and side chains. The whole molecular model is in construction.

1) Takenaka, A., Kizawa, K., Hata, T., Sato, S., Misaka, E., Tamura, C., Sasada, Y., J. Biochem. (1988). **103**, 463-469

