02. X–1 STRUCTURE OF BACTERIORHODOPSIN.
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Two structures for bacteriorhodopsin have been determined to resolutions of 6-7 Å. One is from native (p3) purple membrane as isolated from Halobacterium halobium (Blaurock and Stoeckenius, 1971). The other is an in vitro form produced using Triton X-100 and DTAC. It is orthorhombic ($p22_12_1$) with a totally different packing of the molecules (Michel et al., 1980).

In both structures, seven rod-shaped densities stretch from one side of the membrane to the other having roughly the same length as the thickness of lipid bilayer. The rods are at angles of from 3° to 23° to the perpendicular to the membrane. Most of the polypeptide in these rods is probably α-helical.

Many other experiments on the structure have been tried to determine which part of the structure is the cytoplasmic surface, to find where the retinal is, and to try to label different parts of the structure with heavy atoms. However, the main work being pursued at the moment is to try to solve the structure at 3 Å resolution. For this model building (using standard α-helices) and molecular averaging have given some success using the 3 Å intensity data from the two crystal forms. However, the maps have not been good enough to interpret. Further progress depends on two further methods currently being tried. One is heavy atom derivatives followed by isomorphous replacement. The other is high resolution imaging. Both of these methods and where we have reached will be discussed.

References
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02. X–2 STRUCTURAL STUDIES ON A TRANSMEMBRANE CHANNEL, MATRIX PORIN FROM E.coli. By
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Matrix porin, an integral membrane protein from the outer membrane of E.coli, is being studied by high resolution X-ray crystallography. Large, single crystals of matrix porin (space group $P4_2$, a=b=154.9 Å, c =172.4 Å) have been grown from detergent-solubilized protein in the presence of polyethylene glycol and NaCl. At room temperature, a 4.0 Å native data set has been collected on film at the synchrotron facility of the EMBL Outstation in Hamburg. After processing, merging of film data yielded 9.5% on F for 33,742 reflections. A high resolution data set (~2.8 Å) has been collected at -15°C. These data are being evaluated.

From earlier X-ray results it was determined that there are two trimers in the $P4_2$ asymmetric unit. The direct diffraction data display evidence for 2-fold non-crystallographic symmetry in the hkO plane. This is supported by rotation function analyses. We have tentatively located the molecular 3-fold axes of the two trimers. The diffraction data also display interesting characteristics suggesting the existence of protein-bound, quasi-ordered detergent in the crystal. These results as well as the current status of the X-ray project will be discussed.

02. X–3 CRYSTALLIZATION OF MEMBRANE PROTEINS AND STRUCTURE OF PHOTOSYNTHETIC REACTION CENTRES. By
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Several integral membrane proteins like bacteriorhodopsin, photosynthetic reaction centres and light harvesting complexes could be crystallized from detergent containing solutions by salt precipitation. Most likely the membrane proteins are crystallized with detergents bound to their hydrophobic surface domains. The detergents used must be small, and in several cases small amphiphilic molecules like heptane-1,2,3-triol have to be added to obtain crystals . The best of the crystals are suited for high-resolution X-ray crystallography.

Crystals of the photosynthetic reaction centre from Rhodopseudomonas viridis diffract X-rays to beyond 2.5 A resolution. The reaction centres, which are a complex of four different proteins, 6 bacteriochlorophyll- and bacteriopheophytin-, and 2 quinone molecules, are still functionally active in the crystals: They perform light-driven electron transport. Three different heavy atom derivatives were obtained by conventional soaking of the crystals. The M.I.R. phases were improved by solvent flattening and phase combination. An electron density map at 3 A resolution could be calculated. This electron density map is interpreted at present. The secondary structure of the proteins is mainly helical. Atomic models for the bacteriochlorophyll- and bacteriopheophytin molecules have already been built.

02. X–4 DYNAMICS OF PROTEIN FOLDING. By
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Recent progress in the analysis of the architecture of proteins has shown that with certain exceptions the large number of different structures now known can be classified into a relatively small number of categories (alpha-helical proteins, beta-sheet proteins and mixed alpha-helical, beta-sheet proteins). This suggests that the dynamics of protein folding may not be as complicated and many faceted as implied by elementary statistical considerations based on the number of possible configurations of a polypeptide chain. A proposed mechanism for protein folding, the diffusion-collision model, takes account of the secondary structural elements and makes use of their properties to provide estimates of the kinetic parameters involved in the folding process. The diffusion-collision model is a mechanism into which it has been possible to introduce specific physical magnitudes to estimate the kinetic parameters. The diffusion-collision model is discussed and elaborated with regard to a) the nature of the elementary step of folding, and b) the combination of such steps to yield the overall folding kinetics. The model calculations for the elementary step are compared to simplified molecular dynamics simulations of a twenty-four residue polypeptide chain consisting of two eight-residue alpha-helical segments connected