A study of extremely pure dipalmitoyl-phosphatidylcholine (DPPC) by X-ray analysis and X-ray scattering has revealed several features not reported previously. The experimental observations were very sensitive to sample purity and experimental procedure. Nevertheless, reproducible results have been obtained. From both single crystal and powder X-ray patterns we have shown that the crystallographic parameters used have already been refined by FPT least-squares method; Sakabe et al., proceeding of the symposium on proinsulin, insulin and C-peptide, p75, 1979, Excerpta Medica was refined by using block-diagonal least-squares method with X-ray diffraction data to 1.1Å resolution collected at 4°C, and the structure of insulin and gramicidin were reobtained with SUPCOMFIT program. The ordered atoms whose isotropic temperature factors were less than 30Å² were refined with anisotropic temperature factors in this procedure. A value reduced to 0.155 with 33030 data which correspond to 96.3% of the theoretical number of reflection to 1.1Å. 90% of hydrogen atoms bonded to insulin appeared at expected positions on Fourier maps. Thus the refinement with anisotropic temperature factors is effective to refine hydrogen atoms. Hydrogen atom is bonded to N atom of BIGHis but is not bonded to the N atom in this crystal, and those of terminal methyl groups of side chains keep a staggered conformation though they may move as a flipping mode. The geometrical analysis of hydrogen bonds was carried out about helical parts, β-sheet and β-bends and the geometrical analysis between two molecules in an asymmetric unit. α-helix from 810 to 815 is a bit curved against inside of the molecule and the cooperation of hydrogen bonds exists in β-sheet. The dynamic behavior was analyzed with anisotropic temperature factors of individual atoms. We calculated translational vibration and libration of hexamer, two monomers and α-helix in B-chain by using Tl or TlS method.

The activation domain of the trypsinogen molecule is disordered. Upon complex formation with basic pancreatic trypsin inhibitor (PTI), trypsinogen under electron microscope gives a trypsin-like state, in which the activation domain is ordered (Huber & Bode, Acc. Chem. Res. 1978), 41, 114).

In the flexible activation domain of trypsinogen, the disulfide Cys121-Cys220 can be selectively reduced and mercerated. The crystal structures of such modified trypsinogen have been analyzed in its native form and in its complex with PTI and the dipeptide Ile-Val. The mercury atom, covalently bound between the two sulfur atoms, is crystallographically undetectable in the free form of trypsinogen, whereas well defined in the complexed form. After crystallographic refinement of the complex at 2.0Å resolution, the R value was 0.20.

A trypsinogen crystal was crystallographically analyzed and refined at 173K. The coordinates as well as the thermal parameters were compared with the room temperature data. The overall B-factor is reduced by 4.4Å². A number of additional ordered water molecules are observed. The order of the activation domain is not increased detectably at 173K. Residues at the boundaries of the flexible segments, except at the N-terminus, indicate a considerable contribution of temperature independent static disorder. Within the significance level of our measurements it seems that most of the other residues behave like harmonic oscillators.