Lactoferrin, a member of the transferrin family of proteins is an iron binding glycoprotein (M₀ - 80 000 daltons), present in mamalian milks, mucous secretions and white blood cells. Because of its ability to bind iron tightly, (K (f) 10⁻¹⁰) lactoferrin exerts a bacterio­static effect in vitro by depriving micro-organisms of essential iron (Bullem, J.J., Rogers, H.J. & Leigh, L. Brit. Med. J., 1972, 3, 69-75). As well as a role in non-immunological host defence, there are reports which suggest it may modulate immune and inflammatory pro­cesses (Birgens, E.R. & Aisen, E.N. Baker, & Dodson, Department of Chemistry, University of United Kingdom, 1984, 32, 225-230) and prevent the catalytic formation of potent­ially harmful oxygen radicals (Baldwin, D.A., Jenny, E.B. & Aisen, P. J. Biol. Chem., 1984, 259, 13901-13914).

The three dimensional structure of lactoferrin determined at 3.2Å resolution is presented. The 703 amino acid residues are organized into two homologous lobes that are connected by a short g helix. Each of these lobes carries on of the binding sites, one carbohydrate chain, and is divided into two domains of supersecondary structure. The iron is found at the domain interface where it is bonded to four protein ligands, 2 tyrosine, 1 histidine and 1 aspartate. The fifteenth and sixth coordination sites correspond with a region of positive electron density adjoining the iron and provide a possible location for the associated anion (CO₃²⁻ or HCO₃⁻). This region is adjacent to an arginine sidechain and a helix N-terminals. Some remarkable structural simi­larities between lactoferrin and certain other binding proteins are also apparent.

Human des-B30 insulin in which there is a peptide bond formed between Lys B29 and Gly A1 by the synthetic action of trypsin is a byproduct of the industrial conversion of pig to human insulin. This modification leaves the hormone without detectable activity. Rhombohedral crystals of this insulin have been grown in conditions that produce 4 Zn insulin with native hormone. The crystals' cell dimensions are 261Å x 261Å x 261Å. The electron density for the chymotrypsinogen a molecule isolated from bovine insulin, was determined. The crystals are orthorhombic, with space group P2₁₂₁₂₁, and cell dimensions a = 60.2Å, b = 228Å, c = 222Å.

Matthews (J. Mol. Biol., 1968) has found that for protein crystals the value of the crystal volume per unit mass, Vm, lies within the range 1.8 to 3.6 with a median value of 2.4. For a Vm of 1.8 the asymmetric unit of these crystals would contain 36 insulin molecules and for a Vm of 3.6 there would be 18 molecules. Assuming the insulin exists as a hexamer, for a Vm of 2.7, which is close to the median of observed values, there would be 24 molecules or 4 hexamers in the asymmetric unit.

A model for the structure, based on the packing of nearly spherical hexamers subject to the constraints of the space group symmetry, has been obtained. The crystals diffract to a resolution of about 3.0Å on precession photographs. The same crystals can be obtained from bovine insulin.

Bowman-Birk inhibitors found in the seeds (beans) of the leguminous plants are small proteins which inhibit the serine proteases by making stable enzyme-inhibitor complexes. The inhibitors usually consist of 60-80 amino acid residues including 7 disulfide linkages, all are evolutionarily conserved. They are double-headed inhibitors consisting of two tandem homologous domains each with a binding site. Each domain consists of three peptide loops made by disulfide linkages, and each loop is made of 8-11 residues. Crystals have been obtained of AB-I and IIa from azuki beans, A-I, II and IIa from peanuts, and their complexes with trypsin or chymo­trypsin.

A-II, 3 A study: The molecule has an elongated shape with an approximate dimension of 45x10x15 Å, consisting of two distinct domains which are connected by two rather flexible chains (Fig. 1.1). The structures of the domains are very similar to each other and are related by an intramolecular pseudo two-fold symmetry. The binding sites are in the outermost loops, which protrude from the core of the molecule to the opposite direction. The electron densities for both binding sites are very low, indicating a considerable flexibility or a disorder in the conformation.

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AB-I(trypsin complex, 2.3 A study: The SIR method with the MR method solved the structure. Of the inhibitor only the structure of the trypsin-binding domain could be determined. The electron density for the chymotryp­sin-binding domain, however, is so low that any model could not be built. The structure was refined to R=0.21 including trypsin, the trypsin-binding domain of 29 amino acid residues has been constructed.