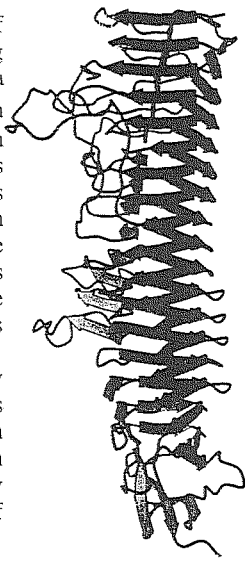
cules, yielding an R-factor of 18.7 % for 7363 reflections between 6.0-1.8 Å. ImmE7 protein contains four antiparallel α-helices and based on the genetic, kinetic and our structural data, a region rich in acidic residues is identified. Presumably this area is involved in the specific protein-protein interactions. We suggest that all the DNase-type immunity proteins, as well as colicins, must share a "homologous-structural framework" and the specific interaction is relied upon how well these two proteins' charged residues match on the interaction surface. These model can be described as a key and lock analogy, that not only the key must fit into a lock (homologous framework), but also the teeth of the key need to completely match the pitches of the lock, thus leading to the specific immunity of the colicin.

MS04.17.03 P69 PERTACTIN: LRR, PRR AND EFFICACIOUS VACCINE. Paul Emsley, Ian Charles, Neil F. Fairweather, & Neil W. Isaacs. Department of Chemistry, University of Glasgow, Glasgow G12 8QQ, UK.

Bordetella pertussis is the bacterial agent causing the respiratory disease known as whooping cough. In the course of the disease, *B. pertussis* binds to the pulmonary epithelial cells. One of these adhesins has been identified as pertactin. Pertactin is an Arg-Gly-Asp(RGD) sequence-containing protein. Such sequences has been known to mediate the interaction of a range of extracellular proteins to a family of cell surface adhesion receptors called integrins. The nature of the interaction of such proteins and integrins is of importance to cell attachment and mobility. Recent human trials of acellular vaccines containing pertactin show considerable efficacy (1).

The X-ray crystal structure of pertactin has been solved to 2.5 Å using the MIRAS method. The strucuture is a 18 stranded β-helix mostly L-shaped in cross section(2) with 2 proline-rich regions (PRRs). The number of residues per turn varies between 18 and 25, but is typically 23. Pertactin has Leucine Rich Repeat (LRR) features, as does pectate lyase (2). There are several loops protruding from the helix. Two of these are extended proline-rich regions ($(GGPXX)_6$) and -$(PPQ)_5$).



The former loop is located directly after the RGD in the sequence, and is thought to mediate the interaction with epithelial cells, the latter is an immunodominant region. Pertactin may be a potential model for the structure of bacterial hemagglutinin (FHA).

(1) Science **269**, 307 (1995).
(2) M. D. Yoder, S. E. Lietzke, and F. Jurnak, *Structure* **1**, 241 - 251 (1993).

MS04.17.04 THE 1.0Å RESOLUTION REFINED STRUCTURE OF MATING PHEROMONE E*r*-1 FROM EUPLOTES RAIKOVI. Daniel H. Anderson, Manfred S. Weiss, David Eisenberg, Molecular Biology Institute and Department of Chemistry and Biochemistry, University of California, Los Angeles. Los Angeles, California, 90095-1570, USA

E*r*-1 is one of a family of protein pheromones that modulate self-non-self recognition for cell aggregation and mating in the 1-cell ciliated protozoan *Euplotes raikovi*. We summarize the course and results of the refinement of the E*r*-1 model against atomic resolution X-ray data. The model was refined with anisotropic thermal parameters, to a R-factor of 12.92%, and includes 4 disordered sidechains, 22 water molecules, a disordered ethanol, and "riding" hydrogen atoms. There is almost no net libration of the molecule, but the sidechains vibrate relative to the backbone. Post-refinement analysis of the model revealed that this dense crystal is perfused by hydrogen bonding networks of solvent and protein atoms. The ends of helices are capped by hydrogen bonding to solvent and symmetry related molecules. Water molecules mediate almost all of the interhelical hydrogen bonding, and many of the lattice interactions. Indirect evidence is presented that motions at the sites of discrete disorder may be correlated, and that protonation of acidic sidechains may switch the conformations.

MS04.17.05 THE SOLVENT STRUCTURE OF CONCANAVALIN A ANALYSED AT 2Å AND THEN 0.94Å RESOLUTION. T. Gleichmann, A. Deacon, S.Trapani and J. R. Helliwell, Department of Chemistry, University of Manchester M13 9PL, UK

Our investigation deals with the reliability and verification of water molecules in proteins found by X-ray crystallography at both room temperature (to 2Å resolution) and low temperature (0.94 Å resolution). At room temperature several 2Å coordinate sets of concanavalin A were used as test cases to determine the number of conserved sites i.e. within the solvent structures of different crystal packing arrangements of the sugar free and two distinct sugar bound forms of the protein. Within the sugar free crystal form it was found that three waters in the sugar binding site are conserved in a number of derivatives (Ni, Co, Mn, Cd substituted concanavalin A) and match the positions of three sugar-oxygen atoms (from the sugar bound crystal structures). Overall in the three different crystal packings a large number of solvent sites are conserved; within a distance range of 0 to 1.2Å, 73 water sites (49%) in a mannoside subunit and 80 water sites (54%) in a glucoside subunit are conserved compared to the cobalt-substituted sugar free concanavalin A subunit (at 1.6Å, the best room temperature crystal structure coordinate set we have). In order to assess methods' aspects of the reliability and precision of the water structure we also compared two Co-concanavalin A structures at room temperature.

One was obtained with Laue data (at 2Å) and the other was with the 1.6Å monochromatic data set. A total of 150 waters were found from the Laue refinement of which 119 agreed with the monochromatic refinement (including the three receptor binding site waters). Finally by use of of flash freezing, a short wavelength intense SR beam (CHESS) and a CCD area detector a resolution of 0.94 A has been achieved for the sugar free crystal form (this is a record for a protein of 25kDa molecular weight, to our knowledge!). This X ray data set comprises 117000 unique reflections (75.4% complete). In this low-temperature refined structure (R-factor, SHELXL93, 13.1%) the number of detected solvent sites has increased from 147 to 290 and the quality of the electron density greatly enhanced.