peptides all bind to Fab 58.2 more tightly than their non-Aib containing counterparts, and unpublished NMR work has shown that the Aib residue confers additional structure on the peptides in solution. The addition of the Aib residue to the peptides does not significantly change their conformation while bound to Fab. The structures for the peptides as bound to the different Fabs will be compared and contrasted.

PS04.15.35 THE THREE DIMENSIONAL STRUCTURE OF STAPHYLOCOCCAL ENTEROTOXIN C2 FROM TWO CRYSTAL FORMS. S. Swaminathan, W. Furey, J. Pletcher and M. Sax, Biocrystallography Laboratory, VA Medical Center, University Drive C, PO Box 12055, Pittsburgh, PA 15240 & Department of Crystallography, University of Pittsburgh, Pittsburgh, PA 15260 USA.

Bacterial superantigens induce massive T cell proliferation when presented by major histocompatibility complex class II (MHCII) molecules. These superantigens induce all T cells bearing particular types of Vb elements irrespective of other variable elements present in the T cell receptor by forming a ternary complex with MHCII and T cell receptor (TCR). Staphylococcal enterotoxins produced by *Staphylococcus aureus* are both toxins and superantigens. As toxins they cause vomiting and diarrhea in humans. There are five distinct serotypes of staphylococcal enterotoxins which are labeled A through E. SEC is further subdivided into SEC1-3 due to minor epitope variations. Even though all staph enterotoxins possess a common SE-fold the mode of association of these with MHCII molecule appear to be different. Further, in spite of very high sequence homology the Vb specificity of these also differ, though there is some overlap. The crystal structure of SEC2 was determined to better understand the reasons for the differences in the mode of association and Vb specificities.

SEC2 crystallizes in two forms. The monoclinic form is in space group P21 with cell dimensions a = 43.43, b = 69.92, c = 42.22Å and β = 90.1° and has two molecules in the unit cell . The tetragonal form is in space group $P4_32_12$ and has cell dimensions a = b = 42.98 and c = 289.3Å . The crystal structure determination of these two forms by the molecular replacement method will be presented. The differences in the structures of SEB and SEC2 will also be discussed.

PS04.15.36 CRYSTAL STRUCTURE OF ANTI-P-GLYCOPROTEIN FAB MRK-16 IN COMPLEX WITH ITS PEPTIDE EPITOPE. S. Vasudevan, K. Johns and D.R. Rose, Ontario Cancer Institute and Department of Medical Biophysics, University of Toronto, Toronto, M5G 2M9 Canada

Cancer cells undergoing chemotherapy can develop multidrug resistance, one form of which is associated with the overexpression of a membrane protein, P-glycoprotein (pgp). Pgp is an ATP-binding cassette (ABC) transporter that consists of two putative membrane-spanning domains and two cytoplasmic ATPase domains. Pgp has been shown to participate in energy-dependent efflux of a wide range of common anti-cancer drugs as well as other substrates. Inhibition of pgp function can improve the effectiveness of chemotherapy.

Monoclonal antibody MRK-16 binds to a discontinuous epitope consisting of two extracellular loops distant in the amino-acid sequence of pgp. It has been used as an adjuvant in anti-cancer treatments. We are studying MRK-16 firstly to understand its mode of interaction with pgp with the possible goal of improved pgp inhibitors, and secondly as part of a broad strategy to use antibodies as tools towards the structure of pgp itself. We report here the crystal structure of the MRK-16 Fab. Crystals were grown in the presence of a synthetic peptide representing one of the epitope loops. The space group is P2(1) with unit cell dimensions(a,b,c) of 54.5, 67.8, 117.2Å, β=97.6deg., and there are two Fab's per asymmetric unit. The structure was determined by standard molecular replacement techniques and refined to 2.8Å resolution with x-plor. Due to crystal packing, only one of the Fab's is complexed with peptide, permitting a comparison of liganded and unliganded structures in the same crystal. The elbow angles of the two copies of the Fab differ by about 7 degrees and there are some intriguing differences in the conformations of some of the complementarity-determining loops that make up the binding site. Conclusions based on the structure reported here, in the light of information on other pgp inhibitors, will be discussed.

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PS04.15.37 STRUCTURE OF AN IMMUNODOMINANT 38-kDa PROTEIN ANTIGEN b (Pab) FROM *MYCOBACTERIUM TUBERCULOSIS*. Nand K. Vyas, Meenakshi N. Vyas, Abha Choudhary, Zengyi Chang and Florante A. Quiocho, Department of Biochemistry and Howard Hughes Medical Institute. Baylor College of Medicine. Houston, TX-77030.

Mycobacterium tuberculosis, an etiological agent of tuberculosis, infects about one-third of the world's human population. Tuberculosis remains the largest cause of deaths (3 million each year) from a single infectious agent. Among well characterized secreted protein antigens, the 38-kDa protein antigen b (Pab) from *M. tuberculosis* is of great current interest in the immunology of tuberculosis because its B and T cell epitopes are species-specific and immunodominant. Amino acids sequence of the 38kDa protein has 30 % similarity with the periplasmic phosphahe-binding protein (PBP) from *Escherichia coli* (*E. coli*). The 38-kDa gene from *M. tuberculosis* has been subcloned and overexpressed in the nonpathogenic *E. coli* for structure-function studies. We have determined an X-ray structure of the recombinant 38-kDa at 3.0 Å resolution by the MIR method. Results of the 38-kDa structure determination and further refinement will be presented. The structure of the 38-kDa will be used for topographic mapping of known B and T cell epitopes to understand cooperation between B and T cells in immune responses. In addition, the 38-kDa structure will be used for comparison with the known structure of the PBP (*E. coli*). Crystallization of the 38- kDa by vapor diffusion and repeated seeding methods produced crystals in two distinct forms. The orthorhombic form, space group $P2_12_12$, has cell dimensions: a= 125.45 Å b= 72.27 Å and c= 73.43 Å, whereas monoclinic form, space group $P2_1$, has cell dimensions: a= 67.42 Å b= 113.38 Å, c= 42.68 Å and ß= 108.53°. Asymmetric unit of each crystal form contains two molecules of the 38-kDa. Both crystal forms diffract X-rays to 2.0 Å resolution.