of arthritis, cancer and asthma and there are correlations between expression levels and disease prognosis. However, the function of these secreted proteins is completely unknown. This project is aimed at uncovering the physiological roles of the chilectins, using a combination of structural biology and cell biological studies.

Keywords: chilectin, chitinase, arthritis

### P04.01.06

Acta Cryst. (2008). A64, C232

## A structural investigation in to the basis of Celiac disease

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Celiac disease (CD) is a common T cell mediated disease in which the body develops an inappropriate immune response to dietary gluten. Gluten ingestion by CD affected individuals' result in symptoms such as bloating, diarrhoea, and malabsorption. The only available treatment against these symptoms is strict adherence to a lifelong gluten free diet. Major Histocompatibility Complex (MHC) class II proteins HLA-DQ2 and/or HLA-DQ8, are critical for the development of a CD4+ T cell response towards gluten. The structures of both HLA-DO2 and HLA-DO8 were previously solved in complex with an antigenic gluten peptide. HLA-DQ2 was solved in complex with an a-gliadin-I gluten peptide, one of two strongly antigenic registers that overlap within an optimal peptide. The 2nd register, a-gliadin II, has been shown by functional studies to be a stronger antigen. Crystallization studies are underway to assess the functional and structural properties of this immunodominant epitope. The structure of HLA-DQ2/a-gliadin II gluten peptide complex will aid in our understanding of CD4+ T cell recognition of gluten epitopes in CD. No structures of a TcR specific for any HLA-DQ2/DQ8-gliadin peptide have been reported. Crystals have been optimised for solution of an apo gluten specific TcR, and I am attempting to crystallize a HLA-DQ2/DQ8-peptide-TcR complex. This project aims to structurally characterise the interactions between HLA-DQ8-gluten peptide complex, and an HLA-DQ8/peptide specific TCR. The ternary complex will identify important contact residues in the peptide that allow TcR recognition and hence may aid in the development of new treatments (e.g. peptide vaccine), and provide significant insight into the structural mechanism that results in the activation of CD4+ T cells in CD.

Keywords: MHC proteins, T cell receptor, X-ray crystallography of proteins

### P04.01.07

Acta Cryst. (2008). A64, C232

Purification, crystallization and preliminary X-ray analysis of photosystem II dimer from a red alga

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Photosystem II (PSII) is a membrane protein complex performing light-induced electron transfer and water-splitting reactions, leading to the evolution of molecular oxygen which is required for all oxygenic life on the earth. The central part of photosystem II is highly conserved from prokaryotic cyanobacteria to eukaryotes; however, there are some apparent differences in the extrinsic proteins involved in oxygen evolution among different organisms. So far, the crystal structure of PSII from cyanobacteria has been reported, whereas no reports have been published on the structure of any eukaryotic PSII. Red alga is one of the eukaryotic algae, and its PSII differs from that of cyanobacteria in that the former contains a 20 kDa protein, a unique, fourth extrinsic protein. In order to elucidate the structure of red algal PSII and its differences with cyanobacterial PSII, we purified and crystallized PSII from an acidophilic, thermophilic red alga Cyanidium caldarium. In order to obtain pure PSII dimer suitable for crystallization from the red alga, we improved the purification procedure published previously, which yielded a highly purified PSII dimer preparation with high oxygen-evolving activities comparable with that of thermophilic cyanobacterial PSII. We succeeded in the crystallization of red algal PSII dimer and obtained two types of crystals with different space group crystals. One type of the crystal had a space group of P2221 with unit cell dimensions of a = 146.8Å, b = 176.9Å, c = 353.7Å. Another type of the crystal had a space group  $P2_12_12_1$  with unit cell dimensions of a =209.2Å, b = 237.5Å, c = 299.8Å. Multiple data sets of native crystals have been collected and processed to 3.7 Å, which may enable us to resolve the structure of red algal PSII.

Keywords: photosynthesis, membrane proteins, crystallization

#### P04.01.08

Acta Cryst. (2008). A64, C232-233

# Structural analysis of ATP:Cob(I)alamin adenosyltransferase

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B12 is an important nutrient for maintaining life in all animals, lower eukaryotes, and prokaryotes, but is only synthesized by a prokaryotes. In mammalian, B12 should be converted to two biologically active cofactors, methylcobalamin (MeCbl) and adenosylcobalamin (AdoCbl), and these cofactors are used by enzymes, the functions of which are needed for the Acetyl-CoA synthesis, methyl transfer, ribonucleotide reduction, fermentation process, and methionine synthesis. Because B12 synthesis is limited within the micro-organisms, the adenosyltransferases that are able to transfer the 5'-deoxyadenosyl moiety from ATP to the cobalt atom of cob(I)alamin is needed to construct the complete biosynthetic pathway of AdoCbl in higher order organisms. Until now, two crystal structures of PduO enzyme with Mg-ATP are available in the RCSB protein data bank (2nt8, 2idx), and these structures indicates that the enzyme is a trimer and each subunit consists of five helixbundle. Further, co-crystal structure with Mg-ATP reveals that unseen ATP binding motif at the N-terminal of the protein in native crystal structure is visible in substrate-protein complex crystal