	Experiment title: Crystallographic studies on the interactions between collagen type II peptides and molecules from the immune system	**Experiment number**: MX-568
Beamline: ID23-2	**Date of experiment**: from:13-9-2006 to:14-9-2006	**Date of report**: 13-6-2007
Shifts: 2	**Local contact(s)**: Sean McSweeney	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Huseyin Usyal*, Marjolein Thunnissen* Dep. Molecular Biophysics, kemicentrum, Lund University. Getingevägen 60 S22100 Lund Sweden

Report:

Our goal was to collect data on class II A^q molecule with a bound collagen peptide. The structure of this complex would give us information on the interactions the peptide makes with the MHC molecule and give clues on the recognition of the glycosylated peptide. The crystals had been tested before at Max-lab and were aftrwards stored in a storage dewar for 4 months prior to travelling to the ESRF. Unfortunately when we started datacollection of these crystals at the ESRF it became apparent that they had not survived the storage. This was a major set-back for us.

We used the remaining time to test several crsyals we had obtained for other projects. Many of these small crsyatls turned out to be various salt crystals however for one project, the IgD binding domain of MID (Morexella catarhallis IgD binding protein) several of the tested crystal were protein crystals that diffracted to 4-5Å, 3.5Å and 2.1Å for the various forms. We collected a full native dataset for the crystal form that diffracted to 2.1Å. The crystal was very radiation sensitive and we had to expose several different pars of the crystal to obtain a full dataset. the crystal belonged to space group C2 with cell dimensions a = 254.70Å, b = 54.10Å, c = 39.40Å, $\alpha = 90°$, $\beta = 95.1°$ and $\gamma = 90°$. Further statistics on datacollection can be found in table 1.

Since the protein does not share any sequence homolgy with proteins in the PDB database we have to solve the structure by *de novo* methods. The crystal does not contain any Cys orMmet residues therefore we can not try to use seleno-Met variants in a MAD experiment. We are therefore trying to solve the structure by MIR methods and a search for appropriate heavy metal substitutes is ongoing.

Table 1: Statistics on datacollection

Diffraction limits (Å	2.1- 25Å
Wavelength collected at	0.8726
R_{merge}[a] (%)	11.3 (23.4)
Completeness (%)	99.7 (100)
Mean I/s	9.87 (5.45)
Unique reflections in data set	31383
Multiplicity of observation	4.7 (4.8)
Spacegroup	C2
No of different segments used	9