ESRF	**Experiment title:** Crystal Structures of Two H-2D^b/Glycopeptide Complexes Suggests a Molecular Basis for CTL Cross-Reactivity	**Experiment number:** LS-1128
Beamline: BM14	**Date of experiment:** Various from: 1998 to: 1999	**Date of report:** 22/03/00
Shifts: 1	**Local contact(s):** Vivian Stojanoff	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Dr J. Tormo
Professor EY Jones

Report:

Two synthetic O-GlcNAc bearing peptides that elicit H-2D^b-restricted glycopeptide-specific cytotoxic T cells (CTL) have been shown to display nonreciprocal patterns of cross-reactivity. Here, we present the crystal structures of the H-2D^b glycopeptide complexes to 2.85 Å resolution or better. In both cases, the glycan is solvent exposed and available for direct re cognition by the T cell receptor (TCR). We have modeled the complex formed between the MHC-glycopeptide complexes and their respective TCRs, showing that a single saccharide residue can be accommodated in the standard TCR-MHC geometry. The mdoels also reveal a possible molecular basis for the observed cross-reactivity patterns of the CTL clones, which appear to be influenced by the length of the CDR3 loop and the nature of the immunizing ligand.