ESRF	**Experiment title**: Crystal Structures of HLA-B*5101 Complexed with HIV Immunodominant Epitopes	**Experiment number**: LS-1128
Beamline: ID14	**Date of experiment**: from: 1998 to: 1999	**Date of report**: 01/09/00
Shifts: **2**	**Local contact(s)**: Edward Mitchell	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Dr K. Maenaka*

Mrs T. Maenaka*

Professor E.Y. Jones*

Report:

The crystal structures of the human MHC class I allele HLA-5*5101 in complex with 8-m34, TAFTIPSI, and 9-mer, LPPVAKEI, immunodominant pepetide epitopes from HIV-1 have been determined by x-ray crystallography. In both complexes, the hydrogen-bonding network in the N-terminal anchor (P1) is rearranged as a result of the replacement of the standard tyrosine with histidine at position 171. This results in a nonstandard positioning of the peptide N terminus, which is recognised by B*5101-restructed T cell clones. Unexpectedly, the P5 peptide residues appear to act as anchors, drawing the peptides unusually deeply into the peptide-binding groove of B51. The unique characteristics of P1 and P5 are likely to be responsible for the zig-zag conformation of the 9-mer peptide and the slow assembly of B*5101. A comparison of the surface characteristics in the α1-helix C-terminal region for B51 and other MHC class I alleles highlights mainly electrostatic differences that my be important in determining the specificity of human killer cell Ig-like receptor binding. *The Journal of Immunology, 2000, 165: 0000-0000.*