ESRF	**Experiment title:** X-ray crystallographic studies on MHC class I/peptide complexes.	**Experiment number:** LS-417
Beamline: D14-BL19	**Date of Experiment:** from: 2-Feb-96 to: 4-Feb-96	**Date of Report:** 27-Feb-96 (prelim)
Shifts: 6	**Local contact(s):** Andy Thompson	*Received at ESRF:* 04 MAR 1996

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Report:

Data from this experiment will answer key structure/functions questions raised in:

K.J. Smith, S.W. Reid, D.I. Stuart, A.J. McMichael, E.Y. Jones and J.I. Bell. (1996) 'An altered position of the alpha 2 helix of MHC class I is revealed by the crystal structure of HLA B*3501.' *Immunity* (In the press)

The data are currently being analysed.

Abstract (Smith *et al* 1996)

The crystal structure of the human Major Histocompatibility Complex class I B allele HLA B*3501 complexed with the 8mer peptide epitope HIV- 1 nef 75-82 (VPLRPMTY) has been determined at 2.0Å resolution. Comparison with the crystal structure of the closely related allele HLA B*5301 reveals the structural basis for the tyrosine specificity of the B *3501 F pocket. The structure also reveals a novel conformation of the 8mer peptide within the binding groove. The positions of the peptide N and C termini are nonstandard, but the classic pattern of hydrogen bonding to nonpolymorphic MHC class I residues is maintained, at the N terminus by addition of a water molecule, and at the C terminus by a substantial shift in the α2 helix.

The data collected on BL19 are for HLA B35 complexed with a 9mer peptide. The previous work (as detailed in the above abstract for Smith *et al* 1996) raised functionally important questions which centre on which of the nonstandard features of the HLA B35/nef peptide complex structure arise because of the short (8mer) nef peptide and which are inherent to the HLA B35 allele. The current analysis will address these questions.