ESRF	**Experiment title:** X-ray crystallographic studies on MHC class I/peptide complexes.	**Experiment number:** LS-215
Beamline: ID13-BL1	**Date of Experiment:** from:10-Feb-95 to: 1l-Feb-95	**Date of Report:** 27-Feb-96 (update)
Shifts: 3	**Local contact(s):** Christian Riekel	*Received at ESRF :* [illegible]

Names and affiliations of applicants (*indicates experimentalists):

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Report:

Data from this experiment are included in:

S.W. Reid, K.J. Smith B. Jacobsen, C. O'Callaghan, H. Reyburn, K. Harlos, D.I. Stuart, A.J. McMichael, J.I. Bell and E.Y. Jones. (1996) 'Production and crystallization of MHC class I B allele single peptide complexes.' ***FEBS Lett. (In the*** press)

and are central to:

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)

Abstract (Reid *et al* 1996)

Major Histocompatability Complex Class I B alleles, HLA B8, B53 and B3501 have been cloned, expressed, refolded and crystallized in specific complexes with a number of different 8mer and 9mer peptides. For some of these crystallization was initiated by cross-seeding between different B allele complexes. All crystallize in the space group $P2_12_12_1$, with similar unit cell dimensions of approximately 52 Å x 81 Å x 112 Å, contain one complex per asymmetric unit and diffract to approximately 2.0 Å resolution.

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 $\alpha 2$ helix.