	Experiment title: Structural studies of Fv1696 as a complex with the 8 N-terminal residues of HIV protease	**Experiment number:** LS-1685
Beamline: ID14-1	Date of experiment 12.5.2000	**Date of report:** 29.8.2000
Shifts: 2	**Local contact(s):** J. Lescar	*Received at ESRF:*

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Report:

The monoclonal antibody 1696, obtained from immunisation of mice with the HIV-1 protease, inhibits the viral enzyme by binding to the N-terminal residues, thus causing dissociation of the active homodimer into inactive monomeric subunits. We have previously solved the Fab fragment of 1696 in the uncomplexed state with data measured at the ESRF (experiment LS-1032, publication: J. Lescar, J. Brynda, P. Rezacova, R. Stouracova, M.-M. Riottot, V. Chitarra, M. Fabry, M. Horejsi, J. Sedlacek & G. A. Bentley. (1999). « Inhibition of the HIV-1 and HIV-2 proteases by a monoclonal antibody ». *Protein Science*. **8**, 2686-2696).

More recently, we have crystallised the recombinant Fv fragment of 1696 as a complex with an 8-residue peptide corresponding to the first 7 N-terminal residues of the HIV-1 protease with an additional C-terminal Arg residue included to increase the solubility of the peptide. The crystals were small (~ 0.15x0.05x0.05 mm^3) and invariably multiple. Several crystals were cryo-cooled and tested in the beam at ID14-1 before a usable data set was obtained.

The crystals belong to the space group $P2_1$ with cell dimensions a=45.56 Å, b=57.17 Å, c=91.17 Å, β=97.07°, Z=4. A total of 14,309 unique reflections were obtained between the resolution lilits of 30.9-2.6 Å (R_{merge}=0.106, completeness=97%, 42,409 total reflections measured). Refinement of the structure is in progress: current R and R_{free} values are 0.295 and 0.325, respectively, with tight non-crystallographic symmetry restraints being applied to the two molecules in the asymmetric unit.