



ESRF

**Experiment title: Structural studies of an HIV-1 protease-inhibiting antibody**

**Experiment number: LS-1032**

**Beamline:**  
ID14

**Date of experiment:**  
from: 21 Sept 1998 to: 22 Sept. 1998

**Date of report:**  
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**Shifts: 3**

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**Report:**

The monoclonal antibody 1696 inhibits the HIV-1 and HIV-2 proteases by dissociating the active homodimeric enzyme into the inactive monomeric form. The single-chain Fv fragment of 1696 has been expressed as a recombinant protein in *E. coli* and crystallised. The crystals belong to the space group  $P2_12_12_1$  with cell dimensions  $a=126.93 \text{ \AA}$ ,  $b=61.21 \text{ \AA}$ ,  $c=57.30 \text{ \AA}$ . There are 2 independent molecules in the asymmetric unit, giving a  $V_m$  of  $2.2 \text{ \AA}^3/\text{Da}$ . Diffraction data were measured on the beam line ID14 between the resolution limits of 20 to  $1.7 \text{ \AA}$  using three crystals (size about  $0.2 \times 0.1 \times 0.1 \text{ mm}^3$ ). Details of the data processing are as follows:

No. of observations: 227,672

No. of unique observations: 45,422

Completeness: 91.3%

Rmerge: 9.1%

$\langle I/\sigma(I) \rangle$  : 34.3

The structure was solved by molecular replacement using the known structure of Fab 1696 (Lescar *et al.*, Protein Science, in press), and the refinement of the structure is in progress. The current refinement statistics are as follows:

No. of reflections $F > 3\sigma$ (all):	37539 (44305)
R-factor:	21.5% (23.4%)
R-free:	28.7% (30.4%)
No. of residues:	462
No. of solvent molecules:	233
r.m.s. deviations on bonds:	0.011 Å
r.m.s. deviations in angles:	1.70°