



Experiment title:
HCV non-structural protein 3 protease domain (NS3)
bound to a X inhibitor

**Experiment
number:**
LS-1517

Beamline:
ID14 EH1

Date of experiment:
from: 20/11/99 to: 21/11/99

Date of report:
29.02.00

Shifts: 1

Local contact(s): H.Belrhali

Received at ESRF:

Names and affiliations of applicants (* indicates experimentalists):

Martin Walsh, Cara Vaughan
IRBM, Rome

Report:

Background: Hepatitis C virus (HCV) currently infects approximately 3% of the world's population. The HCV protease domain of NS3 is a serine protease with a chymotrypsin-like fold and is a potential antiviral target. Reversible covalent inhibitors have been designed. The crystal structures of these inhibitors will shed light on the mode of binding of these compounds allowing a structure-directed approach to the design of more potent inhibitors.

Results: A 2.2 Å resolution data set of the NS3 protease with a covalent peptide inhibitor was collected on beamline ID14-EH1. Data were 96.5% complete in the 20-2.2 Å range with an overall R_{merge} of 6.2%.