



	<b>Experiment title:</b> PROTEIN CRYSTALLOGRAPHY AT AFMB-CNRS, MARSEILLE	<b>Experiment number:</b> LS1657
<b>Beamline:</b> ID14-1/2	<b>Date of experiment:</b> from: 03.03.00 to: 04.03.00	<b>Date of report:</b> Aug00
<b>Shifts:</b> 3	<b>Local contact(s):</b> Stephanie Monaco, Ed MITCHELL	<i>Received at ESRF:</i>
<b>Names and affiliations of applicants (* indicates experimentalists):</b>  Silvia SPINELLI*, Christian CABBILLAU		

### Report:

Protein name: CAB10 anti amylase VHH

Size: 14353 Daltons, 131 aa

.Data collection of complex amylase and VHH CAB10

Crystals were frozen to 100K, without cryoprotectant.

The space group and unit cell dimensions were confirmed from a preliminary exposure to be P1, a=57.34 Å, b=60.74 Å c=107.21 Å, alpha=98.705, beta=100.879 and gamma=101.259 degree

Two data set were collected to 100K, one to high resolution with an exposure time of 30 s per degree, and the other to low resolution with an 5 s exposure by degree.

.The structure of the complex amylase-VHHCAB10 was determined using the molecular replacement method with the AMoRe program.

The search models were amylase structure personal communication (F.Payan) and the VHH anti Lysozyme (PDB code:1mel)

The model is refined with CNS, slow cooling and energy minimisation, using all data between 30 and 1.6 Å.

Details of data collection and refinement are shown in the table below.

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Total number of observation	716803
number of unique reflections	175069
overall % data > 1sigma (last shell)	95.9(95.9)
overall R-merge (%) (last shell)	7.4(19.4)
overall I/sigma(I) (last shell)	4.6(1.8)
resolution	30.0-1.6 A
refinement resolution:	30 - 1.6 A
final Rfactor/Rfree	0.24/0.21
total number of refl. in resol. range:	181958 ( 100.0 % )
total number of reflections used:	172727 ( 99.9 % )
number of reflections in working set:	169390 ( 89.6 % )
number of reflections in test set:	3337 ( 10.3 % )
number of protein atoms:	10185

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