ESRF	**Experiment title:** PROTEIN CRYSTALLOGRAPHY AT AFMB-CNRS, MARSEILLE	**Experiment number:** LS1657
Beamline: BM14	**Date of experiment:** from: 03.03.00 to: 04.03.00	**Date of report:** Aug00
Shifts: 3	**Local contact(s):** Andy THOMPSON	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

Protein name: MSA6OE7 anti bacterial VHH
Size: 12.000 Daltons, 116 aa

.Data collection of unliganded VHH MSA6OE7
Crystals were frozen to 100K, with 7% of MPD as cryoprotectant.
The crystals belong to the space group P3221, with dimensions
a=71.4 A, b=71.4 A c=74.84 A alpha=beta=90 gamma=120.000.
A data set was collected to 100K, with an exposure time of
30 s per degree

.The 3-dimensional structure was determined with MR using as search model a dromedary single domain VHH antibody fragment against the Ribonuclease A (PDB code:1bzq). The refinement using CNS is underway.

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

Total number of observation	192442
number of unique reflections	11594
overall % data > 1sigma (last shell)	99.8(99.8)
overall R-merge (%) (last shell)	4.0(19.5)
overall I/sigma(I) (last shell)	15.0(3.5)
resolution	24.0-2.19 A

refinement resolution: 20 - 2.2 A	
final Rfactor/Rfree	0.2377/0.2781
total number of refl. in resol. range:	11559 (100.0 %)
total number of reflections used:	11548 (99.9 %)
number of reflections in working set:	10358 (89.6 %)
number of reflections in test set:	1190 (10.3 %)
number of protein atoms:	1005
rms deviations from ideal values:	
Bonds (A):	0.012
Angles (degree)	1.5
Dihedral (degree)	26.4
Imporper (degree)	0.81
B-factors (A2):	
main chains	30.2
side chains	33.2
Solvent	39.5