



Experiment title: BAG-LEBS-2003-2	Experiment number: MX-204	
Beamline: BM14	Date of experiment: from: 18/09/2003 at 8h00 to: 19/09/2003 at 8h00	Date of report: 23/02/2003
Shifts: 3	Local contact(s): Dr. Pierre LEGRAND (e-mail: legrand@embl-grenoble.fr)	<i>Received at ESRF:</i>
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Report:

M. Graille + N. Leulliot (3 shifts): yeast *Saccharomyces cerevisiae* Structural Genomics project

The systematic names of the genes are used. More details on every orf can be found on <http://genomics.eu.org/targets.html>

1)YHR049w (target 91).

Spacegroup $P2_12_12_1$ a=48A; b=128A; c=255A.

Resolution 2.4A

Completion 99.2%

This protein is of unknown structure and function. During this beamtime, we have collected a SAD dataset that allowed us to solve the structure. We have also collected a 1.7A resolution dataset (space group P1), which was used for structure refinement. The protein adopts an hydrolase fold.

2)YML079w (target 136).

Spacegroup C2 a=149A; b=66A; c=122A; beta=104°.

Resolution 2.6A.

Completion 95%

Rsym=3.9%

This orf codes for a protein of unknown function. We have solved the structure by SAD method in space group I432. The protein adopts a jelly roll structure already observed in seed storage proteins and in epimerase. The crystal form used for phasing was grown in the presence of ATP and analysis of the electron density map revealed the presence of the nucleotide bound to the molecule. To get more information, we

have co-crystallized this protein with a nucleotide derivative. During that session, we have collected a 2.6Å resolution dataset in a new space group. Analysis of the electron density map did not revealed the presence of the ligand bound to the molecule.

3) YHR029c (target 188)

Spacegroup P6122 a=b=60Å; c=110Å.

Resolution 2.3Å.

Completion 100%

Rsym=6%

This protein is the target number 188 of the Yeast Structural Genomics initiative. It is a 200 residues protein of unknown function with no structurally related homologue known to date. Small crystals of this protein have diffracted to 2.3 Å. Phases are needed to solve the structure.

4) NCS mutant complexed to testosterone.

Spacegroup P4₁ a=b=44Å; c=55Å.

Resolution 1.7Å.

Completion 100%

Rsym=7.7%

Neocarzinostatin (NCS) is an antitumour antibiotic protein isolated from the actinomycetes *Streptomyces carzinostaticus* whose structure has been solved to 1.5Å resolution. A directed evolution strategy was used to confer to this protein the ability to bind a human hormone. This mutant has been crystallized in different conditions according to the absence or the presence of the hormone. We have collected high resolution data from a crystal obtained with a NCS mutant co-purified with a testosterone derivative. The ligand is well defined in electron density. Unexpectedly, two steroid molecules are bound to one NCS mutant.