



Experiment title: Truncated Hemoglobin N from Mycobacterium tuberculosis: analysis of mutants and soaking with various ligands.

Experiment number:
MX394

Beamline: ID14-2	Date of experiment: from: 21/7/05 to: 22/7/05	Date of report: 1/8/05 <i>Received at ESRF:</i>
Shifts: 3	Local contact(s): Rana ROY	

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Report:

M. tuberculosis truncated Hemoglobin N (hbn) is characterized by a system of molecular cavities linking the protein active site to the solvent. In order to study the features of the active site and its accessibility to various hydrophobic compound we are performing mutants and ligands analysis. The crystals belong to orthorhombic space group P212121 accommodating 2 molecules in the asymmetric unit. Here you have the result of actual experiments:

Mutant: hbn qellv
mosaicity 2°
resolution 2.1 Å
Rsym 14.3 % (64.7%)*; *(2.2-2.1)
compl 73.2 (69.9)
molt. 2.5 (2.4)
I/sig 4.5 (1.2)
refinement: R/Rfree=20.8/28.5%

hbn cocrist. with linoleic acid 5 mM
stab. with linoleic 20 mM
mosaicity 1.5°
res. 2.1 Å
Rsym 11.7 % (78.8%)*; *(2.2-2.1)
compl 92.2% (84.3)
molt 3.1 (3.0)
I/sig 4.3 (1.0)

ref. R/Rfree=24.5/29.2%
no ligand bound.

hbn soaking with oleic acid 20 mM
mosaicity 1.4°
res. 2.1
Rsym 11.0 % (60.4%)*; *= 2.1-2.2
compl. 96% (79.9)
molt. 3.2 (2.5)
I/sig 6.2 (1.3)
ref. R/Rfree=19.5/26.1%
no ligand bound

hbn cocrist. with pentanol 5 mM
stab.. pentanol 20 mM
mosaicity parto da 1.5
res. 2.0
Rsym 8.4 % (64.2%)*; *=2.0-2.1
compl 91.5% (89.3)
molt 3.1 (2.9)
I/sig 7.8 (1.2)
ref. R/Rfree=19.3/25.0%
one pentanol molecule in sub A

hbn aquo met
mosaicity 1.5°
res. 1.8 Å
Rsym 5.8 % (53.6%)*; *=1.80-1.89
compl. 80.1 (69.2)
molt. 3.3 (3.2)
I/sig 11.4 (1.4)
ref. R/Rfree=18.8/24.3%

