



	Experiment title: Ligand binding experiments on human neuroglobin	Experiment number: LS-2183
Beamline: ID14-EH1	Date of experiment: from: 12-06-02 to: 14-06-02	Date of report: 01-09-2002
Shifts: 3	Local contact(s): Vincent Favre-Nicolin	<i>Received at ESRF:</i>

Names and affiliations of applicants (* indicates experimentalists):

Alessandra Pesce

X-ray Structural Biology Lab

Advanced Biotechnology Center

Largo Rosanna Benzi, 10

16132 Genova

Italy

Report:

Human neuroglobin is the first example of vertebrate globin with a hexacoordinated heme, as showed by the three-dimensional structure just solved.

The aim of this experiments was to bind a series of ligands to the protein, in order to break the hexacoordination and analyse if some structural changes occur from hexacoordination to pentacoordination.

Two data sets have been collected with the following data processing statistics

Soaking with sodium azide:

Space group: P2₁

Unit cell: $a = 39.6 \text{ \AA}$, $b = 94.9 \text{ \AA}$, $c = 68.5 \text{ \AA}$, $\beta = 95.5^\circ$

Resolution: 30 - 2.15 \AA

R_{sym}: 5.7 %

Soaking with imidazole

Space group: P2₁

Unit cell: $a = 39.6 \text{ \AA}$, $b = 95.3 \text{ \AA}$, $c = 70.5 \text{ \AA}$, $\beta = 92.6^\circ$

Resolution: 30 - 2.15 \AA

Rsym: 7.8 %

The ligand binding experiments were not successful. Analysis of the electron density map showed that the ligands were not bound.