ESRF	Experiment title: **A number of Proteins from Bacteria to Eukarya and from Antarctic to Volcanic Areas**	**Experiment number**: LS-1954
Beamline: ID 14-1	**Date of experiment**: from: 13 Jul. 2001 to: 14 Jul. 2001	**Date of report**: 30/08/2001
Shifts: **3**	**Local contact(s)**: **: Dr. Stephanie MONACO**	*Received at ESRF:*

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Report:

Data collection report
Trematomus newnesi haemoglobin

Three complete data sets were collected at the beamline ID14-1 on intermediates of the unfolding pathway of the major haemoglobin component extracted from the Antarctic fish *Trematomus newnesi*.
The data set 1 was collected on a crystal obtained exposing the haemoglobin to air for 3 hours at pH 7.6. Two data collections were carried out to register both the low (up to 2.5 Å) and the high (up to 1.25 Å) resolution reflections with a high level of accuracy.
Data collection statistics are summarised in the following table (the values in parenthesis refer to the highest resolution shell 1.29-1.25 Å).

Space group	C2
Cell dimensions (Å,°)	a=88.46 b=87.66 c=55.50 β =99.2
Resolution (Å)	1.25
Total No. of reflections	470721
No.of independent reflections	114368
Completeness (%)	99.6 (98.-9)
Rsym(I) (%)	3.0 (33.2)

The data set 2 was collected on a crystal obtained exposing the haemoglobin to air for several days at pH 7.6. Two data collections were carried out to register both the low (up to 2.5 Å) and the high (up to 1.50 Å) resolution reflections with a high level of accuracy.
Data collection statistics are summarised in the following table (the values in parenthesis refer to the highest resolution shell 1.55-1.50 Å).

Space group	C2
Cell dimensions (Å,°)	a=87.25 b=87.31 c=55.49 β =98.3
Resolution (Å)	1.5
Total No. of reflections	264812
No.of independent reflections	65006
Completeness (%)	98.7 (95.9)
Rsym(I) (%)	3.2 (37.4)

The data set 3 was collected on a crystal obtained exposing the haemoglobin to air for several days at pH 6.0. Data collection statistics are summarised in the following table (the values in parenthesis refer to the highest resolution shell 1.74-1.70 Å).

Space group	C2
Cell dimensions (Å,°)	a=88.02 b=87.17 c=55.40 β =99.0
Resolution (Å)	1.7
Total No. of reflections	159820
No.of independent reflections	45449
Completeness (%)	99.8 (99.8)
Rsym(I) (%)	4.4 (27.5)

The structures of these three forms have been solved by molecular replacement.
The refinement is currently in progress.