ESRF	**Experiment title:** BAG Barcelona – Clade I Catalases	**Experiment number**: LS1936
Beamline: ID14-2	**Date of experiment**: from: 13-7-01 to: 15-7-01	**Date of report**: 10-Aug-01
Shifts: 3	**Local contact(s)**: Stephanie Monaco	*Received at ESRF:*

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Report:

Catalase (hydrogen peroxide:hydrogen peroxide oxidoreductase, EC:1.11.1.6) which is present in most eukaryotic and aerobic prokaryotic organisms can utilise hydrogen peroxide as both electron donor and electron acceptor in a dismutation reaction that yields water and molecular oxygen: $2H_2O_2 \rightarrow 2H_2O + O_2$
To date, the structures of six heme-containing catalases, all of them belonging to the Clade II and III groups, have been determined at almost atomic resolution. However, no structural work has yet been reported with catalases from the Clade I group, which includes all plant and also some bacterial enzymes. This group of catalases present a number of major singularities such as the absence of NADP(H) binding (observed in clade II catalases) and of the C-terminal domain found in clade III catalases.

Diffraction data corresponding to crystals of Clade I catalases from *Pseudomonas,* has been collected at the ESRF. Crystals were monoclinic (space group $P2_1$ with unit cell parameters a=61., b=154. and c=109.Å and β=102.8°). These crystals diffracted beyond 1.5 Å resolution at the ESRF but presented a strong decay even when cooled at liquid nitrogen temperatures (Figure 1).

Refinement, with a data set at 1.8 Å resolution (overall completeness 98%), is now been completed (present values Rfactor=26%, Rfree=31%). The asymmetric unit contains a whole molecule with more than two thousand residues.

Structure Factor Check
catF

Title: Pseudomonas catF
Date: Jun'00
PDB code: ps_catF

Crystal

Cell parameters:

a: 60.63 Å b: 153.88 Å c: 109.19 Å
α: 90.00° β: 102.85° γ: 90.00°

Space group: P 1 21 1

Structure Factors

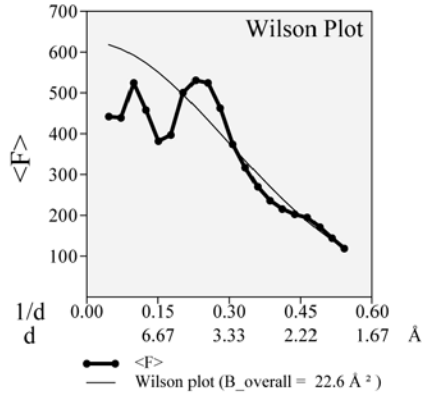
Input

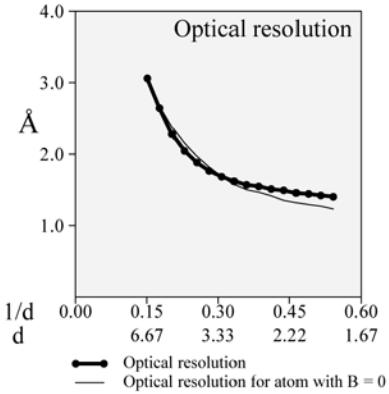
Nominal resolution range:		29.87 □ 1.80 Å
Reflections in file:		175342
Unique reflections	above 0:	175342
	above 1σ:	174494
	above 3σ:	120550

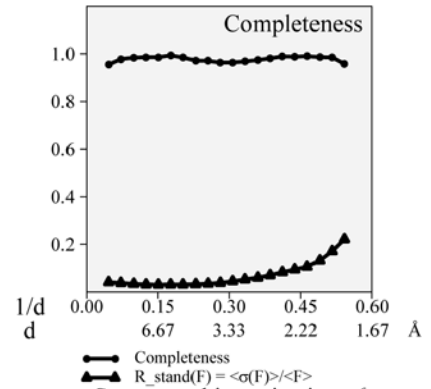
SFCHECK

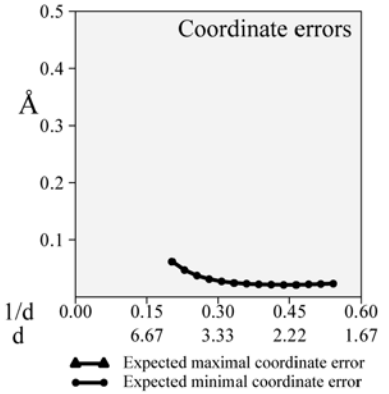
Nominal resolution range: (max. from input data, min. from author)	29.87 □ 1.80 Å
Used reflections:	175342
Completeness:	97.9 %
R_stand(F) = <σ(F)>/<F> :	0.084
Anisotropic distribution of Structure Factors ratio of eigen values:	1.0000 0.6560 0.7401
B_overall (by Patterson):	22.6 Å ²
Optical resolution:	1.41 Å
Expected opt. resol. for complete data set:	1.41 Å
Estimated minimal error:	0.024 Å

Structure Factor Check
catF

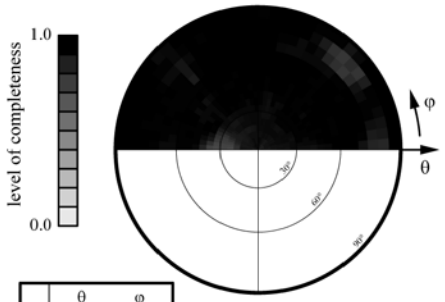


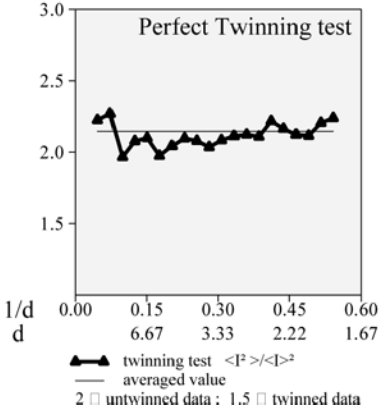






Stereographic projection of the averaged radial completeness



	θ	φ
h	77.15	0.00
k	90.00	90.00
l	0.00	0.00

polar coordinates of the crystallographical axes