<table>
<tr><td> </td><td colspan="2">Experiment title: FRANKFURT BAG:</td><td>Experiment number:
MX-135</td></tr>
<tr><td>Beamline:
ID14 EH2</td><td colspan="2">Date of experiment:
from: 14-MAY-2003 to: 16-MAY-2003</td><td rowspan="2">Date of report:
13-Jan-2004
Received at ESRF:</td></tr>
<tr><td>Shifts:
3/5</td><td colspan="2">Local contact(s):
Dr. Cecile JAMIN</td></tr>
<tr><td colspan="4">Names and affiliations of applicants (* indicates experimentalists):
J.Koepke, R. Diem, G.Fritzsch</td></tr>
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Report:

Photosynthetic Reaction Center from *Rhodobacter spheroides*
(J. Koepke*, R. Diem*, and G. Fritzsch*)

Two datasets were collected from reaction center crystals soaked in glycerol soaking buffer with a pH value adjusted by the potassium phosphate buffer to pH9. The crystals were illuminated at our home rotating anode with laser light of 594nm to achieve charge separation between the special pair and the secondary quinone. After illumination they were shock frozen in the LN_2 gas stream and a test image was made. The smaller crystal measured first was of insufficient quality, why a second dataset to higher resolution was collected. The secondary quinone was found in two orientations with different occupancy. The proximal orientation was occupied by 40%, whereas the position distal to the non-heme iron was 60% occupied.

Strictosidine Synthase

(J. Koepke[1]*, G. Fritzsch[1]*, X. Ma[2]*, and J. Stoeckigt[2])
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To improve the resolution and data quality, a dataset with high redundancy and longer exposure times was collected. Unfortunately the quality could not be improved considerably compared to the data collected at ID29, although with 98.4% the dataset is now almost complete. The spacegroup R3 could be confirmed.

DFPase

(J.Koepke[1*], G.Fritzsch[1*], V.Katsemi[2], C.Luecke[2] and H.Rueterjans[2])

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The unit cell constants have shrunk in a and b considerably, why the structure could only be solved by molecular replacement with the native model. Density for the loop region of the residues 137 to 152 is missing. In addition the C-terminal end has changed, since the last residue Phe 314 has been mutated to alanine to avoid an observed sterical conflict with the active site of a neigbouring molecule in the crystal packing. Although the mutation generates free space in this region, no additional density for the inhibitor molecule could be identified, but instead the C-terminus of the neighbouring symmetry equivalent DFPase molecule points now directly into the active site and replaces there a water molecule.