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| | Experiment title: BAG-Frankfurt, Sodium-Proton-Antiporter NhaA from E.coli | Experiment number: MX-135 |
| Beamline: ID29 | Date of experiment: from: 17.03.03 to: 18.03.03 | Date of report: 19.01.04 <i>Received at ESRF:</i> |
| Shifts: 1.5/3 | Local contact(s): : Dr. Gordon LEONARD | |
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Report:

NhaA is the main Na^+/H^+ antiporter in *Escherichia coli*. The protein plays an important role in adaptation of the cells at high sodium concentrations and pH homeostasis. Its activity has a pronounced pH dependence. High resolution structural information for NhaA is not available. The crystals are generally smaller than $0.2 \times 0.1 \times 0.1 \text{ mm}^3$ and diffraction cannot be tested at home radiation sources. Crystal quality has been continuously improved and during the last beamtime, for the first time full data sets of native crystals have been collected ($\sim 4 \text{ \AA}$ resolution). Crystals of Selenomethionine (SeMet) containing NhaA were grown accordingly and measured during this beamtime. SeMet-Nha crystals showed similar properties as the native ones. They diffract to $\sim 4 \text{ \AA}$ resolution. The unit cell has been determined to be P21 with $a=109 \text{ \AA}$, $b=126$, $c=\text{\AA} 122 \text{ \AA}$ and $\beta=90.1^\circ$. However, variations of up to 5 \AA of unit cell axes have been found among crystals of the same conditions.

Furthermore, the angle beta varies considerably. Therefore, data collection was aimed to obtain phases via SAD. NhaA has a mass of 43 kDa and contains 22 methionine residues. Fluorescence scans confirmed the presence of selenomethionine. Selecting from several crystals five data sets were collected at a single wavelength: 1. 4.5 Å, R_{sym} 8.3 %, 98 % complete; 2. 4.5 Å, R_{sym} 8.9 %, 97 % complete; 3. 6.0 Å, R_{sym} 7.4 %, 99 % complete; 4. 4.5 Å, R_{sym} 9.2 %, 97 % complete. However, the combination of small crystals, relatively long exposure time per frame and the high number of frames limits the quality of the data. Radiation damage during collection of the data set results in gradual loss of diffraction level and quality. Structure determination has not been successful with the obtained data.