

## Experimental report

### Beamtime the 05 Nov. 2017 on ID23-1 (originally ID30A-3)

Although our beamtime was initially scheduled on beamline ID30A-3, we were relocated to beamline ID23-1 as there was a technical problem on the former. We could however collect data for two projects.

(1) Sodium/proton antiporters, or exchangers, are present in all kingdoms of life and the dysfunction of human  $\text{Na}^+/\text{H}^+$  exchangers are linked to several diseases. We expressed the sodium proton antiporter (STNhaA) protein from *Salmonella typhimurium* in *E. coli*, purified it and crystallized it using a Fab antibody fragment as crystallization helper. This approach allowed obtaining crystals easily thus enabling a systematic structural analysis of the protein. Data at resolutions up to 2.5 Å had been obtained in the past and the structure was refined (unpublished data). In order to determine the  $\text{Na}^+$  pathway in ST-NhaA, crystals were soaked with  $\text{Ti}^+$ , an alkali ion mimic, using various protocols. We, collected data from several crystals at the  $\text{Ti}^+$  L-III edge, as well as at a slightly longer wavelength to confirm the nature of the anomalous scattering element in order to determine the best, reproducible conditions for  $\text{Ti}^+$  soaking. Overall, we collected diffraction data from about 40 STNhaA crystals. Among those, several diffracted x-rays in the range of 2.5-3.5 Å-resolution.

(2) We collected data from two crystal forms from a glycosyltransferase from *Yersinia enterocolitica* (YeGT). This protein was purified as is currently being biochemically characterized by our collaboration partners Dr. Thomas Jank and Prof. Klaus Aktories and their team. YeGT is homolog to the PaToxG protein we have characterized both biochemically and structurally a few years ago (Jank et al, NSMB, 2013). A first crystal form was obtained with the ligand free protein only. Several datasets were collected from each crystal. The best of those tetragonal crystals was diffracting X-rays to 2.3 Å-resolution. The second crystal form was only obtained when using YeGT in complex with its substrate. The rod shape of the crystals allowed collecting multiple datasets from each of them using a small beam. The best crystals diffracted to 1.3 Å-resolution with P21 as space group. Using the PaToxG model and molecular replacement, both structures could be solved and are currently being refined and analyzed.