<table>
<tr><td>ESRF</td><td>Experiment title: X-ray structure determination of Azotobacter vinelandii molybdate binding proteins at atomic resolution.</td><td>Experiment number:
LS-936</td></tr>
<tr><td>Beamline:
ID14-4</td><td>Date of experiment:
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<tr><td>Shifts:
3</td><td>Local contact(s):
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Report:

Molybdenum is required for the cofactors of redox enzymes such as the iron-molybdenum cofactor of nitrogenase and the molybdenum cofactor of nitrate reductase. In the environment, molybdenum is available in trace quantities as the soluble oxydianion molybdate, which closely resembles sulfate and phosphate. Gram negative bacteria use a high affinity ABC transporter to bring molybdate into the cell. The 24 kDa binding protein, ModA, is responsible for the initial recognition and binding of molybdate within the periplasmic space. Once inside the cell the anion may interact with a number of cytoplasmic molybdate-binding proteins or molbindins, which are all similar to, or have domains that resemble, the tetrameric 28 kDa (4 x 7 kDa) Mop protein from *H. influenzae*. The equivalent protein in *A. vinelandii* is ModG, which is made up of 14 kDa subunits - each containing a tandem repeat of a Mop-like sequence. Gel filtration chromatography suggests that it is a dimer. Curiously ModA and the molbindins will bind both molybdate and tungstate, but not sulfate. Through our structural studies we intend to derive the molecular basis for this specificity. Furthermore, by solving the crystal structures of apo- and ligand-bound forms we hope to characterize the conformational changes associated with ligand binding.

A. vinelandii actually produces two ModAs sharing only 50% sequence identity, which we denote ModA1 and ModA2. We have determined the structure of ModA2 at 1.2 Å resolution and have a partially refined model for ModA1 at 2.25 Å resolution, both with ligand bound. They are typical periplasmic binding proteins, having ligand binding sites in a deep cleft formed at the interface of two αβ domains. We have recently solved the crystal structure of ligand-bound ModG and it is being refined to a resolution of 1.8 Å. In agreement with secondary structure predictions, it is comprised almost entirely of β-sheet, and two distinct types of molybdate-binding site have been identified.

During our recent beamtime allocation on ID14-4 we managed to collect data on both apo- and ligand-bound forms of ModA1 to a resolution of about 1.8 Å. Furthermore we collected data to a similar resolution on apo ModG. These data are still being analysed, and we are therefore unable to report any further details at present.