

calculations on the different states of the mechanism show differences in the degree of protonation of this residue, showing that it may provide protons necessary for the initial steps of oxygen reduction to water. To corroborate these findings we have studied the role of glutamate 498 (E498), through crystal structure determination of three different mutant enzymes in which this residue was replaced by site-directed mutagenesis, in an attempt to further understand several structural and functional aspects of the enzyme mechanism. Being located within hydrogen bonding distance of a water molecule in the dioxygen entrance channel and directly interacting with the dioxygen moiety that binds between the two type 3 copper atoms, not only we confirm that E498 acts as an important proton donor during the catalytic mechanism, but we also take a step further demonstrating the role of this residue in the stabilization of the dioxygen reduction site as a whole.

Keywords: diamond light source; macromolecular crystallography; beamlines

[1] Bento I., Carrondo M.A., Lindley P.F., *J. Biol. Inorg. Chem.*, **2006**, 11, 539. [2] Kataoka K., Sugiyama R., Hirota S., Inoue M., Urata K., Minagawa Y., Seo D., Sakurai T., *J. Biol. Chem.*, **2009**, ahead of printing. [3] Solomon E.I., Augustine A.J., Yoon J., *Dalton Trans.*, **2008**, 30, 3921.

Keywords: CotA laccase; site-directed mutagenesis; biomolecular modelling

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The Phase 1 MX Beamlines at Diamond Light Source: Experience from Operation and Commissioning. Ralf Flaig^a, Macromolecular Crystallography Group^a. ^a*Diamond Light Source, Harwell Science and Innovation Campus, Chilton, Didcot, Oxfordshire, OX11 0DE, UK.*
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Diamond Light Source [1] is the new UK third generation synchrotron located south of Oxford. In January 2007 Diamond welcomed first users.

In Phase 1 seven beamlines are funded which includes three beamlines for macromolecular crystallography (MX) [2]. These are currently running a user programme for both academic and industrial users. Commissioning time is also scheduled with the aim for optimisation of operation. The beamlines are similar in design and take radiation from an in-vacuum undulator. A double crystal monochromator and a Kirkpatrick-Baez mirror arrangement are the main optical components. All beamlines are fully tuneable and are equipped with automatic sample changers.

Experience and results from operation and commissioning of the MX beamlines will be presented. This will include discussion of the beam properties, status and performance of the optical components and diagnostics in the optics hutch as well as results from commissioning of the equipment in the experimental end station. The software environment and results from data collections will also be discussed. Latest developments and a future outlook will be presented.

[1] <http://www.diamond.ac.uk>. [2] <http://www.diamond.ac.uk/MX>