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The Macromolecular Crystallography Beamlines for Phase 1 at Diamond

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Diamond [1] is the new third generation synchrotron source which is currently being built in the United Kingdom south of Oxford. In Phase 1 seven beamlines are funded which includes three beamlines for macromolecular crystallography (MX). Radiation from three in-vacuum undulators will be used for these beamlines. The undulators will be canted to allow for a second one to be placed in the straight to provide radiation for a side station. All three MX beamlines will be tunable over a wavelength range of 0.5-2.5 Å to allow for multiple anomalous dispersion experiments. Significant emphasis is being placed on the automation of each beamline, both in terms of hardware and software. The implemented diagnostics tools will also allow for a remote monitoring and control of the beam. The experimental stations will be equipped with large area detectors, with robotic sample changers to enable automatic mounting of cryocooled and room temperature samples as well as a high quality crystal viewing system. Next to the beamlines the users will find support laboratories to prepare for their experiments. The MX beamlines are scheduled for commissioning in 2006 and will come on-line for users in 2007.

[1] http://www.diamond.ac.uk.

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Complete automation of molecular replacement

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Analysis of the PDB shows that this year around 67% of all the deposited structures are solved by molecular replacement. With better algorithms and organisation of data bank it can be expected that this number will be substantially higher. This talk will describe a complete automation of molecular replacement. There are three main components of this work: (1) Reorganisation of database of proteins. All entries in the PDB have been analysed and only non-redundant sets of protein structure, domains and tertiary information were stored. Hierarchical database according to sequence identities was organised. It means that search for similar structure is very fast (less than 10 seconds). (2)Automatic molecular replacement system was designed using python. The system requires only experimental data - sequence the reflection data. The system begins searching the database and extracting candidate structures. It also analyses the experimental data and makes such decisions as resolution limit, existence of pseudo-translation. Then the system starts molecular replacement and refinement on the candidate structures using several protocols (3) Programs such as MOLREP, REFMAC. We have already tested more than 1000 cases and success rate is more than 75%. It is expected that more than 80% of structures will be solved completely automatically.