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Auto-Rickshaw: An Automated Crystal Structure Determination as an Efficient Tool to Validate an X-Ray Diffraction Experiment. M.S. Weiss, V. Parthasarathy, V. Lamzin, P.A. Tucker, S. Panjikar. EMBL Hamburg Outstation, c/o DESY, Notkestr. 85, D-22603 Hamburg, Germany.

The EMBL-Hamburg automated crystal structure determination platform (aka Auto-Rickshaw) combines various macromolecular crystallographic software packages with several decision-making steps. Auto-Rickshaw is able to automatically determine macromolecular crystal structures as soon X-ray data are collected and processed. A large number of structure solution paths are encoded in the system and the optimal path through the system is selected by the computer-coded decision-makers as the structure solution evolves. The primary aim of the pipeline is to validate the crystallographic experiment at the synchrotron site while the crystal is still at or near the beam line. Thus, the system has been optimized for speed, so that typically within a few minutes the answer is provided as to whether the collected data are of sufficient quality to allow successful structure determination.

The platform is installed on a 16-processor Linux cluster and the web-server is accessible for Hamburg beamline users and EMBL staff. An overview of the pipeline with its design, functionality, some examples and the way this platform is used as a feedback system for X-ray data collection or validation of X-ray experiment, will be discussed.