Project Name: Auto-Rickshaw

Name of pipeline: Auto-Rickshaw

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Current Status: Running on 16 processors cluster and used by EMBL-Hamburg beamline users

Purpose

e.g. What is the scope and purpose of the pipeline?

To validate the X-ray diffraction experiment at the beamline and build as complete model as possible.

High Level Description

e.g. A brief description of the pipeline components and architecture

The pipeline contains CCP4, SHELXC/D/E, MLPHARE, NANTMRF, BP3, SHARP, DM, RESOLVE, MAPMAN, ESSENS, and ARP/wARP.

Jiffies

e.g. Describe any custom utilities which had to be written for the pipeline, for example a function to convert between different file formats

Yes, many

Decision Making

e.g. A description of the types of decision which are made within the pipeline

Decisions are made based on the specific crystallographic problem which program to choose and what parameters would be necessary.

Data Standards and Management

e.g. How is data stored and transferred within the pipeline?

The data is stored internally as variable and in various formats which are then used by required program within the pipeline.

Languages

e.g. What languages is the pipeline implemented in?

The pipeline is written in *Cshell* and user-interface prepared using *java, perl, and html*

External dependencies

e.g. Does the pipeline use any external libraries or toolboxes? No

Context/Audience/Environment

e.g. Is the pipeline intended to be run only at the beamline by experts, or on a laptop by a novice user? No, it runs at cluster and accessible from EMBL-Hamburg beamline computers.

Links to Supporting Documents

e.g. Links to project homepages http://www.embl-hamburg.de/Auto-Rickshaw/

References

e.g. Publications which contain further information
Panjikar, S., Parthasarathy, V., Lamzin, V. S., Weiss, M. S. & Tucker, P. A. (2005). *Auto-Rickshaw* - An automated crystal structure determination platform as an efficient tool for the validation of an X-ray diffraction experiment. *Acta Cryst.* D (in press).