Project Name: PHENIX

Name of pipeline: PHENIX

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Current Status: Close to first general alpha release

Purpose

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

Automated structure solution, starting from integrated intensities to final refined model.

High Level Description

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

Many fundamental algorithms from the Computational Crystallography Toolbox (cctbx), molecular replacement algorithms from PHASER, anomalous and isomorphous phasing from PHASER and SOLVE, density modification from RESOLVE, automated model building from RESOLVE and TEXTAL, structure refinement components from the cctbx. Components are brought together using the Python scripting language.

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

The cctbx contains many tools for data interpretation and conversion.

Decision Making

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

Decision making is made locally within components, within the strategy framework, and also within Python scripts that implement wizards.

Data Standards and Management

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

Data is stored in the Project Data Storage, which uses the Python pickle facility. Data is also transferred using the CCP4 MTZ and PDB coordinate formats.

Languages

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

Python, C/C++, Fortran

External dependencies

e.g. Does the pipeline use any external libraries or toolboxes?

The open source cctbx, the LGPL'd CCP4 MTZ library and monomer library, numerous open source libraries for the graphical environment.

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?

Both

Links to Supporting Documents

e.g. Links to project homepages

http://www.phenix-online.org/
http://cci.lbl.gov/cctbx_build/
http://www-structmed.cimr.cam.ac.uk/phaser/
http://solve.lanl.gov/
http://textal.tamu.edu:12321/

References

e.g. Publications which contain further information

See http://www.phenix-online.org/papers/index.html