

Project Name: Chart
Name of pipeline: Chart
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Current Status: Not Yet Released for 5.0.2

Purpose
From scaled and truncated data use programs of the CCP4 Suite and SHELXD to provide an interpretable map and then use ARP/wARP to build into it if requested.
High Level Description
Create command files and run them. Analyse the log files and prepare further command files. Chart was started several years ago now and was based around MLPHARE and SHELXS. mlphare is still seems to do a reasonably good job but SHELXS has been superseded by SHELXD. When available, PHASER will be integrated into the system.
Jiffies
awk-based mlphare-log analyser
Decision Making
Resolution ranges for shelx/rantan, sensible shelx solutions, repeated potential heavy atom solution sets, best solution set from mlphare, bad atoms in mlphare (are extra sites real?), hand checking by DM output analysis.
Data Standards and Management
Derivative info is held internally. Com and log files are written to disk. Deposition harvesting remains a dream.
Languages
scsh (scheme (lisp)). It is Free.
External dependencies
CCP4 and SHELXD
Context/Audience/Environment
The pipeline primarily intended to be run at the beamline by novice users.
Links to Supporting Documents
http://www.chem.gla.ac.uk/~paule/chart