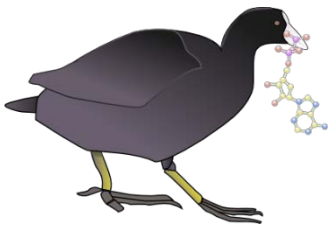
2015

Data Analysis of X-Ray Diffraction images using Phenix and CCP4 Suites

Phenix



CCP4

IMB 2015 XRF Boot Camp

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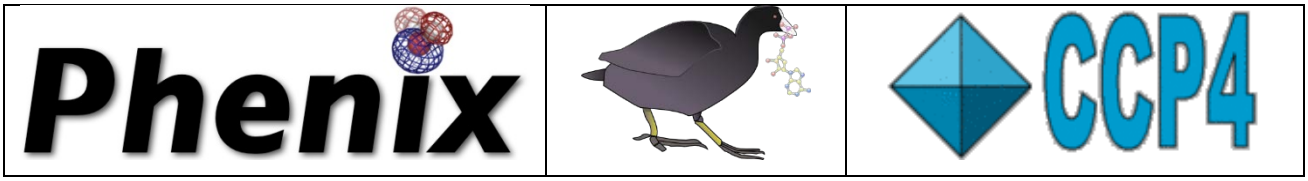
Data Analysis, Molecular Replacement, and Refinement

Xtriage, Phaser, Coot, and Refinement, using Phenix & CCP4 Suites

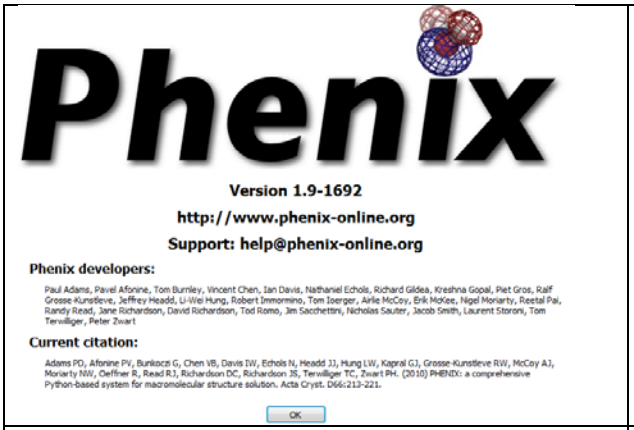


Introduction to data analysis

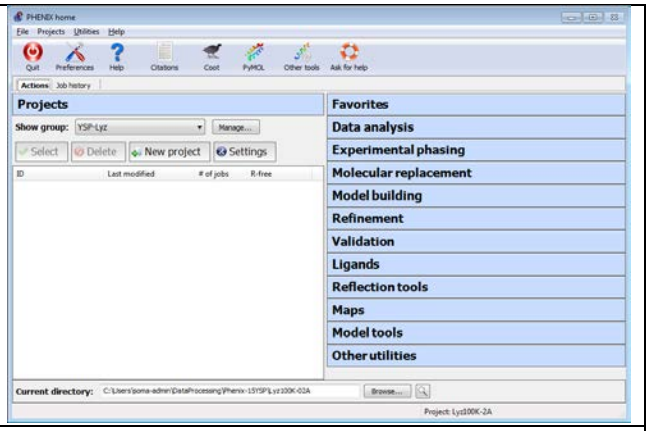
In this module we will learn to analyze the X-Ray diffraction data (images) we collected earlier for hen egg white tetragonal lysozyme crystal. We will use Phenix Suite of programs like Xtriage, Phaser, and Phenix Refine [**PHENIX: a comprehensive Python-based system for macromolecular structure solution**, P. D. Adams, P. V. Afonine, G. Bunkóczi, V. B. Chen, I. W. Davis, N. Echols, J. J. Headd, L.-W. Hung, G. J. Kapral, R. W. Grosse-Kunstleve, A. J. McCoy, N. W. Moriarty, R. Oeffner, R. J. Read, D. C. Richardson, J. S. Richardson, T. C. Terwilliger and P. H. Zwart. *Acta Cryst. D66, 213-221 (2010)*]. We will also use the program Coot [**Features and Development of Coot**, P Emsley, B Lohkamp, W Scott, and K Cowtan. *Acta Cryst. D66, 486-501 (2010)*] & CCP4 Suite [**Overview of the CCP4 suite and current developments**, M. D. Winn, C. C. Ballard, K. D. Cowtan, E. J. Dodson, P. Emsley, P. R. Evans, R. M. Keegan, E. B. Krissinel, A. G. W. Leslie, A. McCoy, S. J. McNicholas, G. N. Murshudov, N. S. Pannu, E. A. Potterton, H. R. Powell, R. J. Read, A. Vagin and K. S. Wilson. *Acta Cryst.* (2011). D67, 235-242 (2011)].

Phenix Suite, Coot, and CCP4 Suite can run on multiple operating systems like Windows, Macintosh, and Linux. So the tutorial will include programs and outputs run from multiple platforms. Many screen grabs were done under Windows platform but that shouldn't indicate any preference to that platform.

First, log into a computer using your username and password. Change to the directory where your data files from Scalepack (which is part of HKL Suite) are located. Start Phenix Suite by typing *phenix* (in Linux) or clicking on the Phenix-shortcut (in Windows or Mac platform). After an initial splash of Phenix logo you will see the PHENIX home screen shown below:

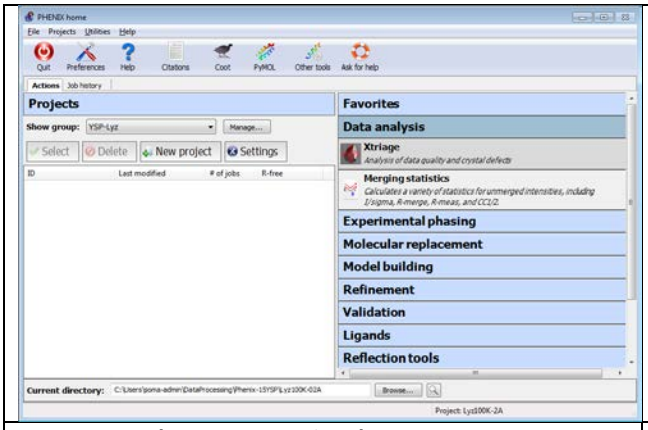


PHENIX logo

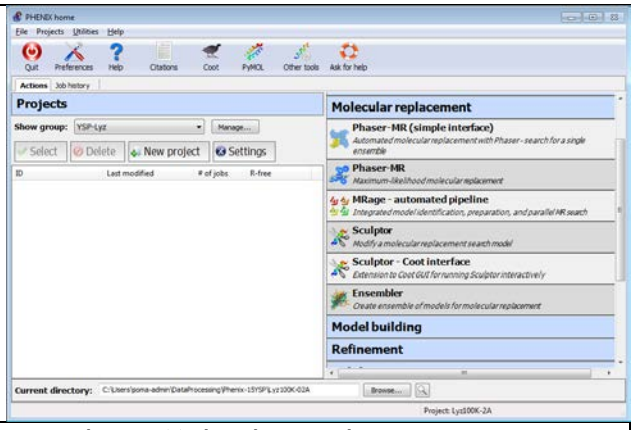


PHENIX home

Clicking on PHENIX HOME's right side sections like "Data Analysis" and "Molecular Replacement" reveal selection of programs available in that section (see below). The sections are grouped together with programs that carry out similar function or analysis.



Phenix Data Analysis section



Phenix Molecular Replacement section

In this tutorial will be analyzing the data following the sequence shown below:

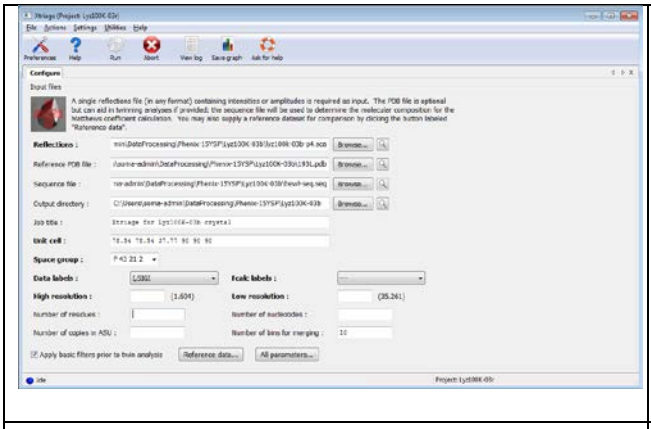
Xtriage > Phaser-MR (simple) > Coot > Phenix.Refinement >Coot

Toward the end of the tutorial we will analyze the data using programs from CCP4 Suite.

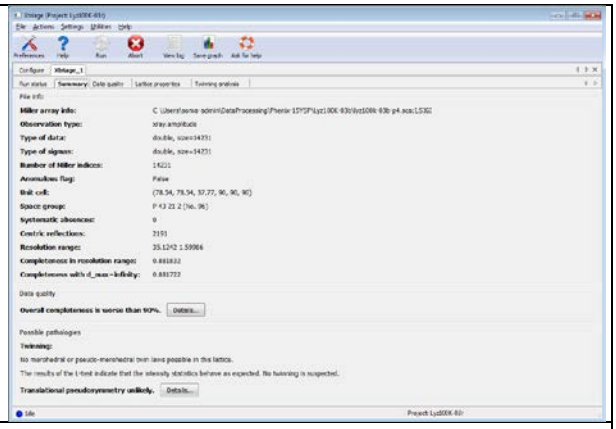
Phenix.Xtriage

Phenix.xtriage is program that checks the x-ray data quality and produces statistics on them. In our case, the program will read the *.sca (merged) output data file from our Scalepack program. Alternatively, we could run phenix.merging_statistics with unmerged (`no merge original index` in Scalepack) to produce other relevant statistics like (R-pim, CC*, etc).

First, click the "Data Analysis" section to reveal Xtriage program. Then click the Xtrigae program. This opens a new window which will require one input: *.sca file (merged data). Optionally, we can add sequence and PDB file. Here, we have `lyz100K-03b.sca` (only required file), `193L.pdb`, and `hewl-seq.seq` as inputs. Then click "Run". After few minutes of Xtriage running we get the "Output Summary" shown below:



Phenix.xtriage input



Phenix.xtriage output summary