#asca2015
@alwaysonthejazz

CCP4 i2

A new graphical interface for the CCP4 suite

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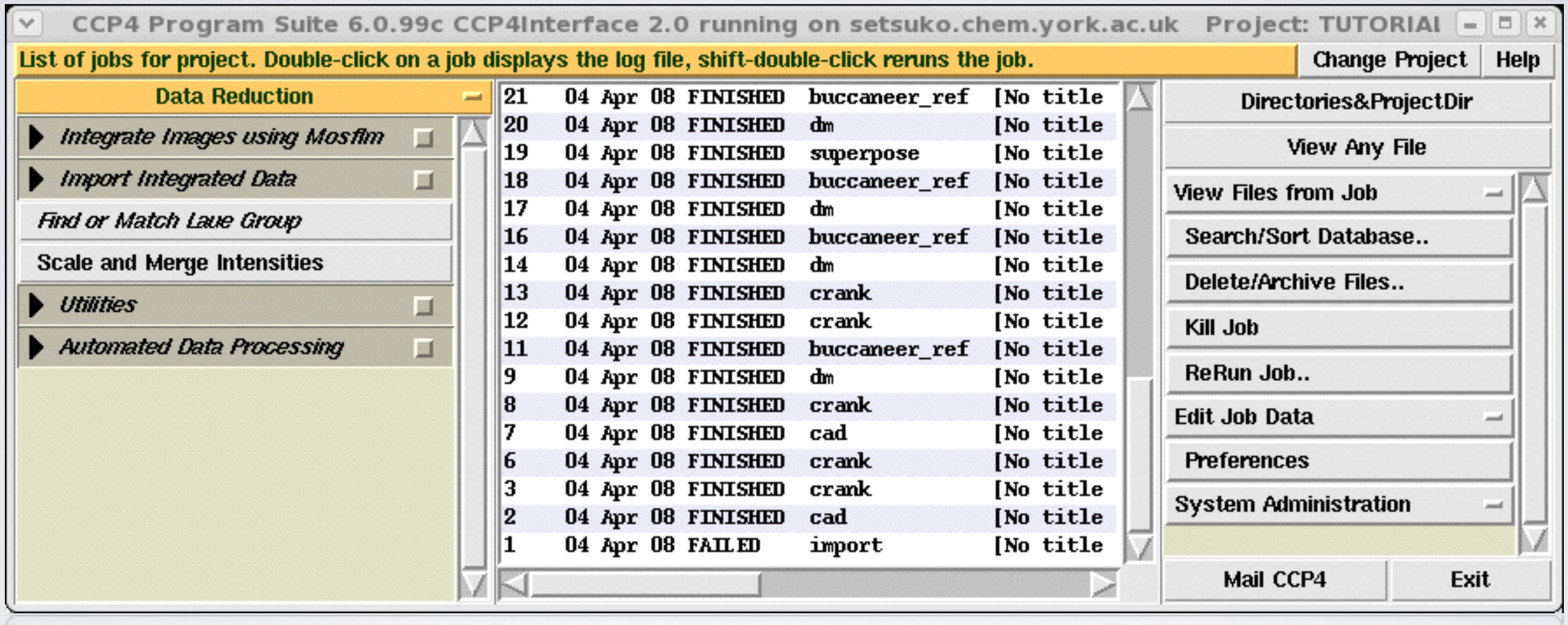
BRIEF OVERVIEW

- Why have we developed a new interface?
- Functionality and programs included
- Release plans

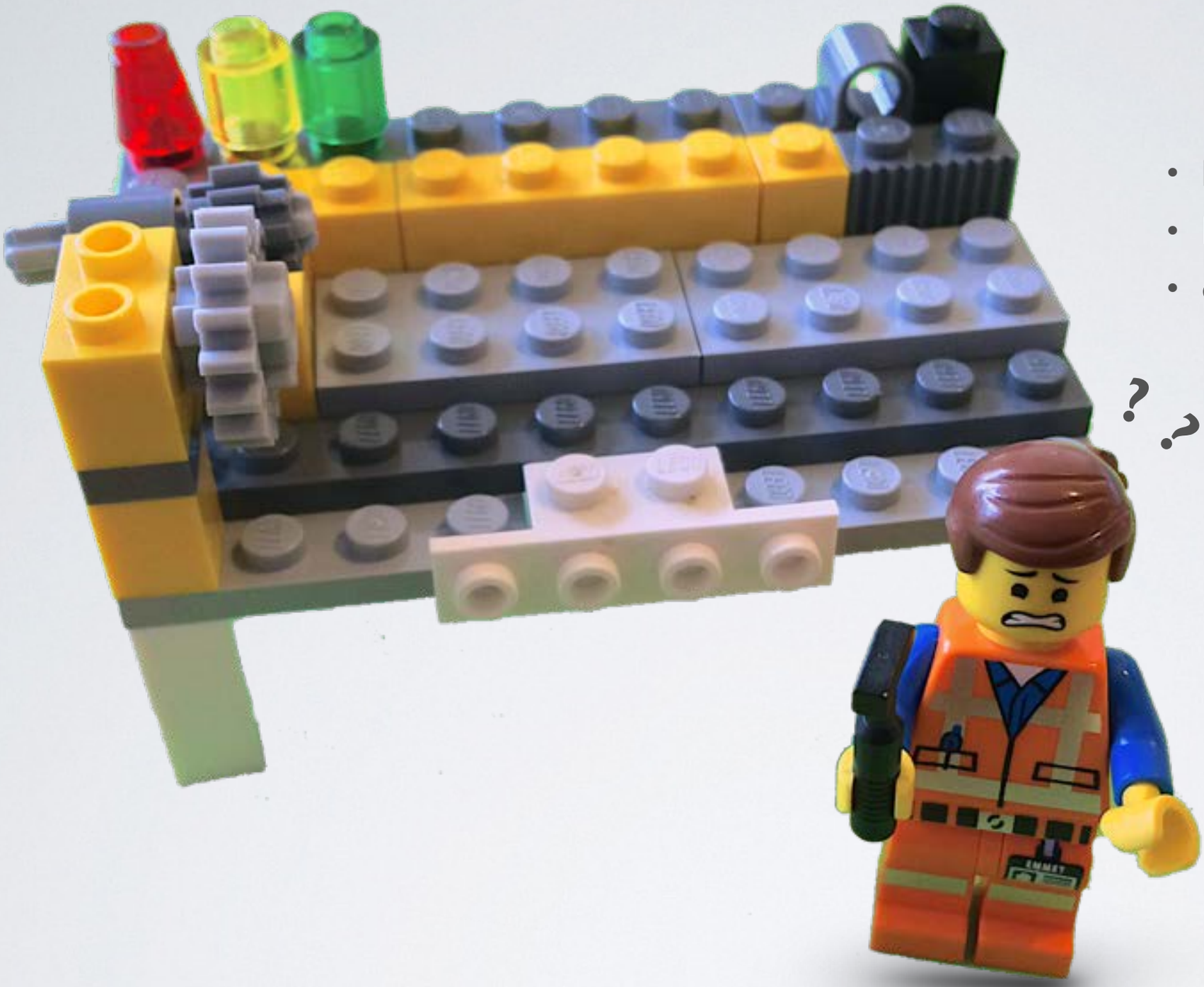
CCP4i

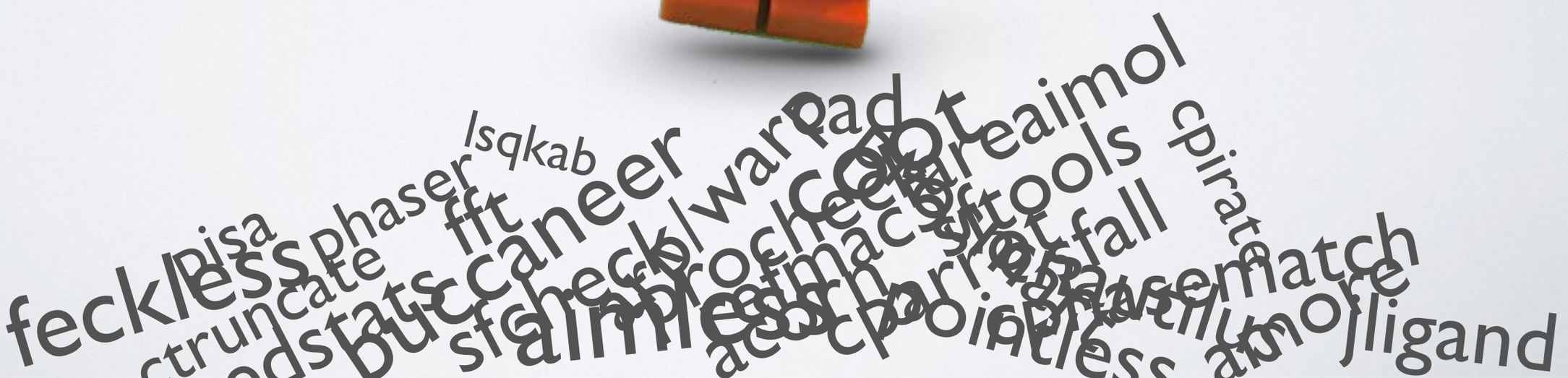


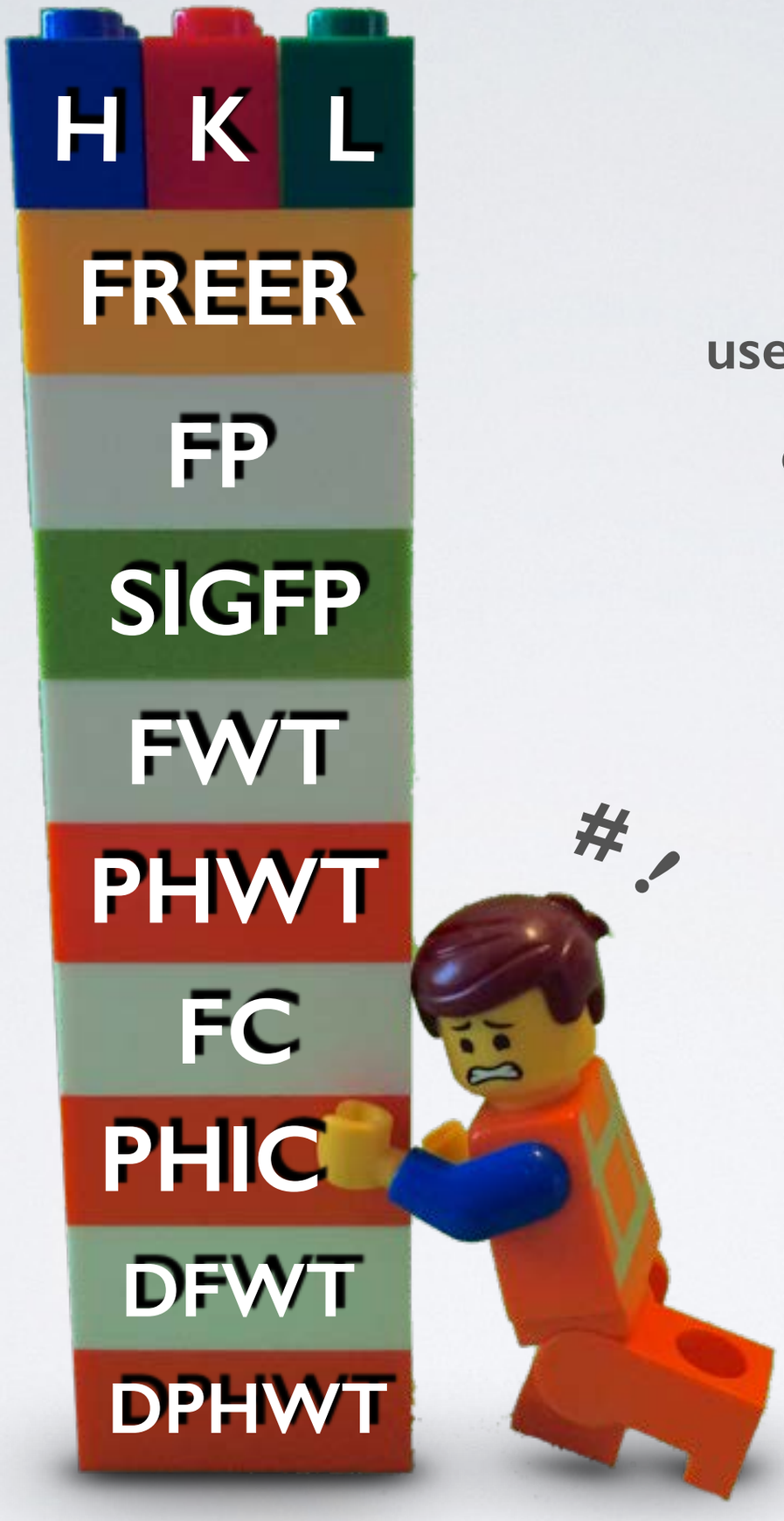
Designed in 1997, when GNU/Linux was taking off
Done in TCL/TK (not very popular nowadays)

CCP4i

- **barebones interface**
- **little automation**
- **difficult for amateurs**







CCP4i

uses bulky MTZ files

columns have cryptic labels

Which columns do I use?

Has Refmac5 modified my FP, SIGFP columns?

ON TOP OF THAT

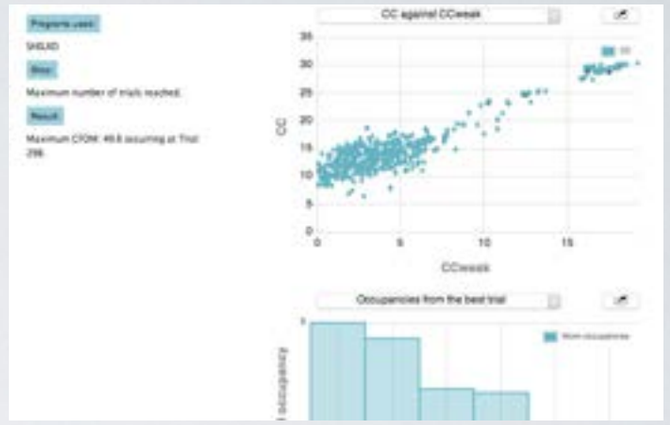
- Barebones database, little tracking, almost no facilities for Research Data Management
- Limited pipelining capabilities
- No access to crystallographic libraries from TCL/TK

Time for a new interface!

CONCEPTS BEHIND CCP4i2

Interface

Reports



python

Engine

CCP4

→ clipper-python

→ biopython

→ cctbx **Libraries**

SQLite **Database**

New concept: data objects miniMTZ

Reflection data

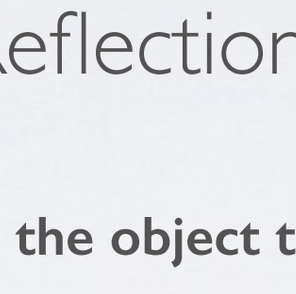
Column names and types are tied to the object type

H, K, L

F

SIGF

=



New concept: miniMTZ

Map coefficients

Column names and types are tied to the object type

H, K, L

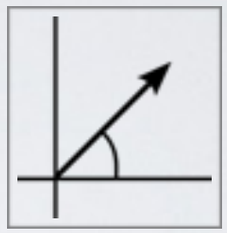
F

PHI

=

input and output

Pipelines

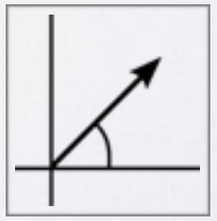


buccaneer → refmac5

python

coot

prosmart



FUNCTIONALITY AND PROGRAMS INCLUDED

dit History Utilities Projects Help

CCP4i2 alpha-0 CCP4i2 Welcome

Run file:///Users/jon/ccp4i2/docs/general/welcome.html

CCP4i2 Welcome

Close tab

CCP4i2

Welcome

New to CCP4i2?

Try the ten minute Quickstart introduction.

View any file

Use this window as a web browser - select Open file from the File pull-down menu.

Open an existing project

Use the Project pull-down menu

Start a new crystallography project

Create a project. More about CCP4i2 projects.

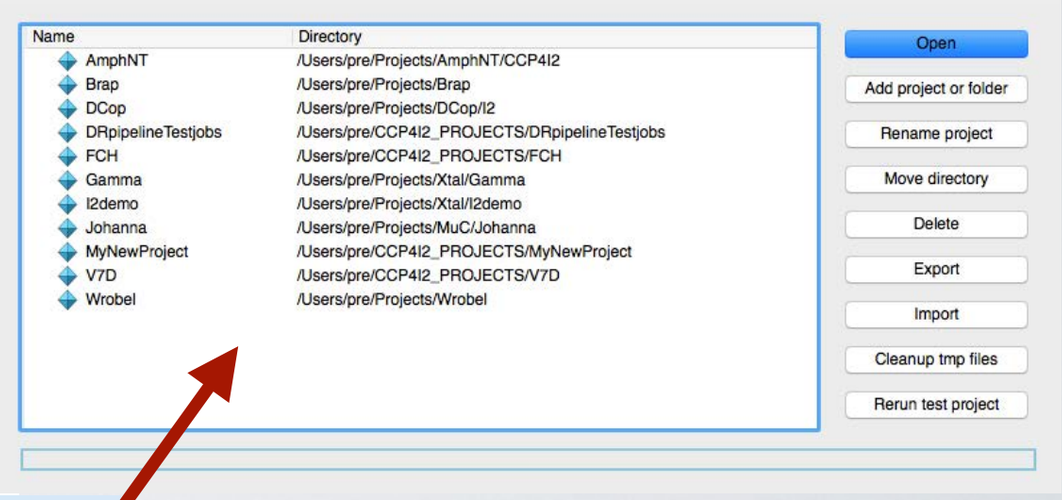
Work in a 'General' project

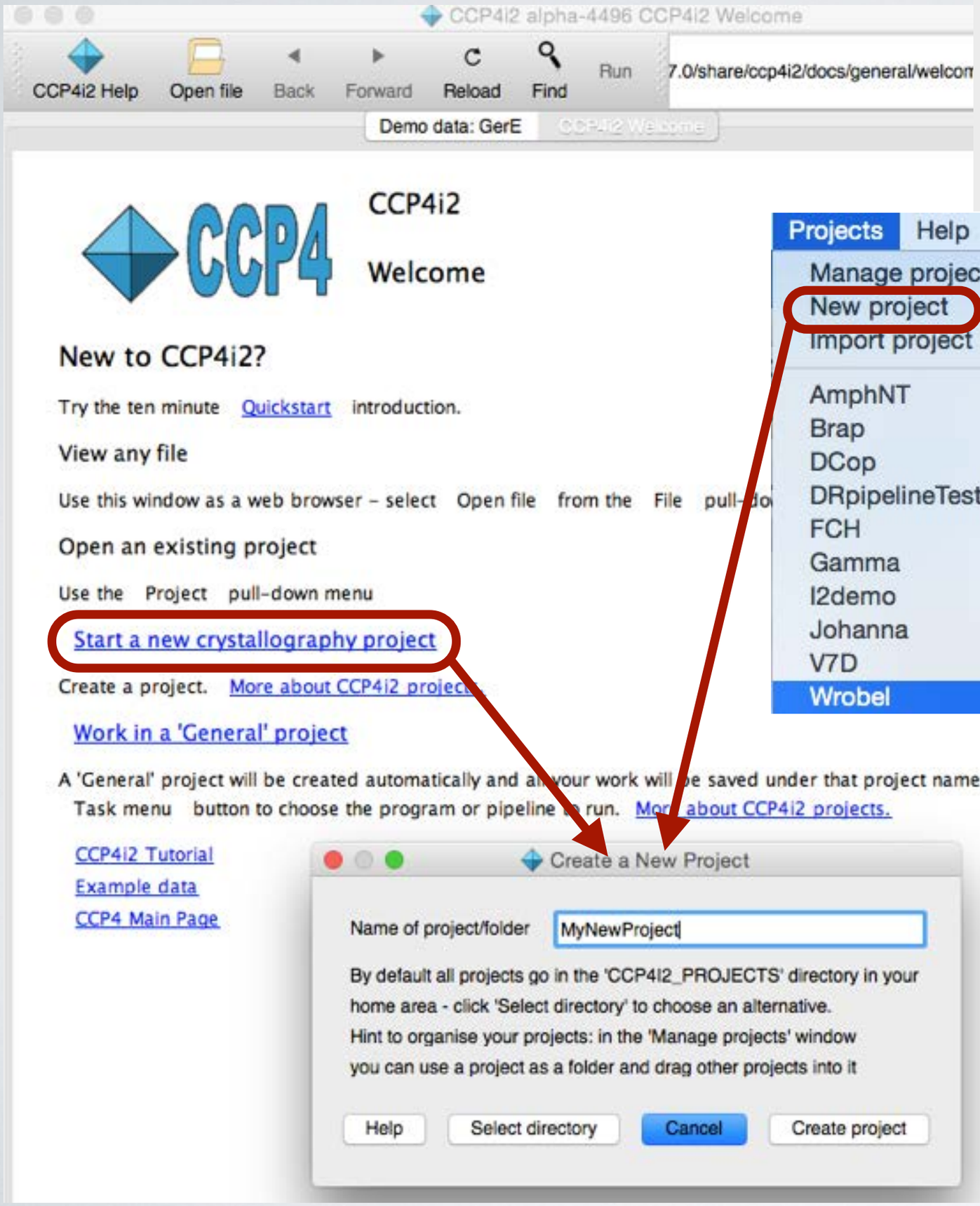
A 'General' project will be created automatically and all your work will be saved under that project name. Then click the Task menu button to choose the program or pipeline to run. More about CCP4i2 projects.

CCP4i2 Tutorial
Example data
CCP4i2 Programmers Documentation
CCP4 Main Page

Known issues with current release Test page

Creating a new project



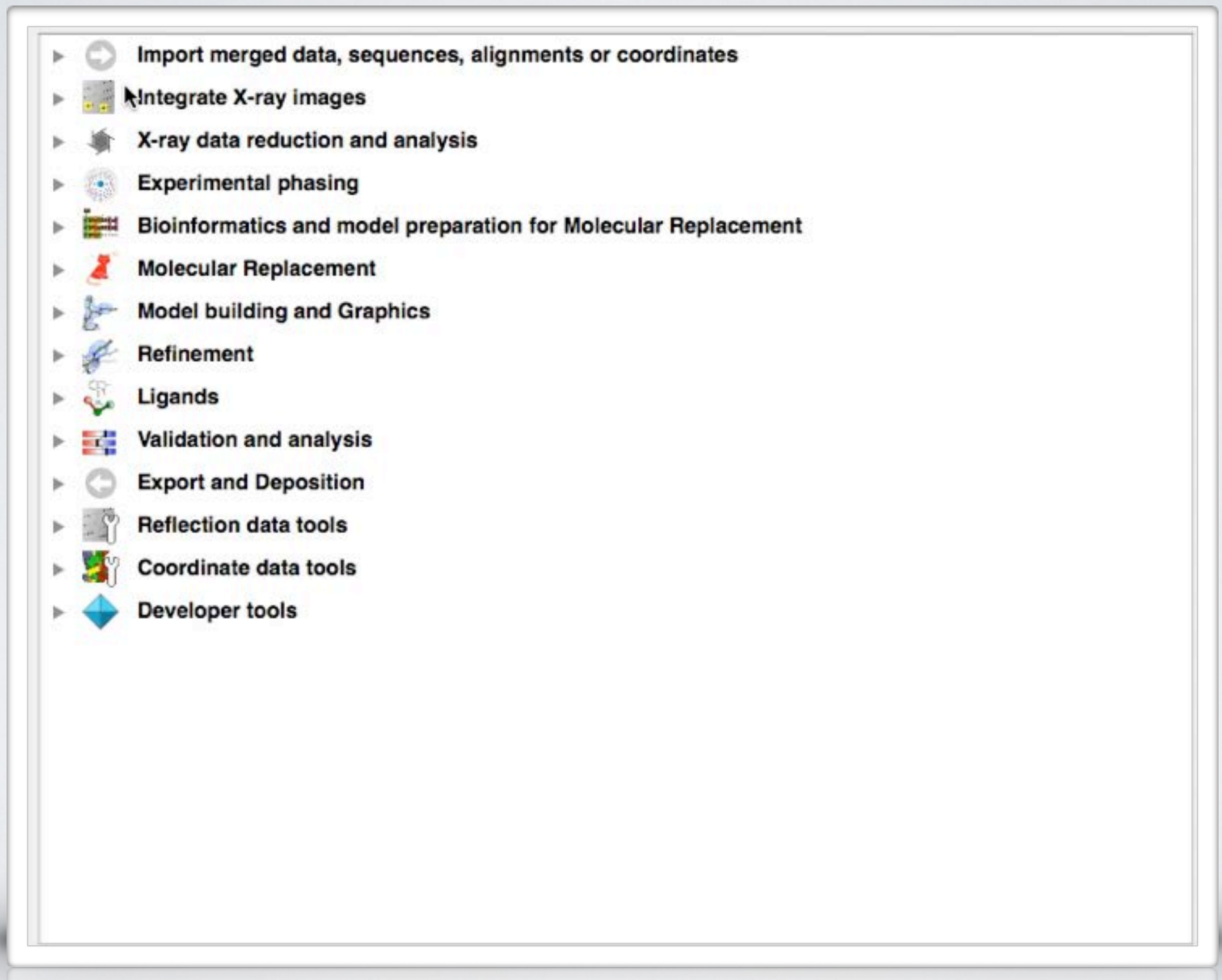


Manage all projects

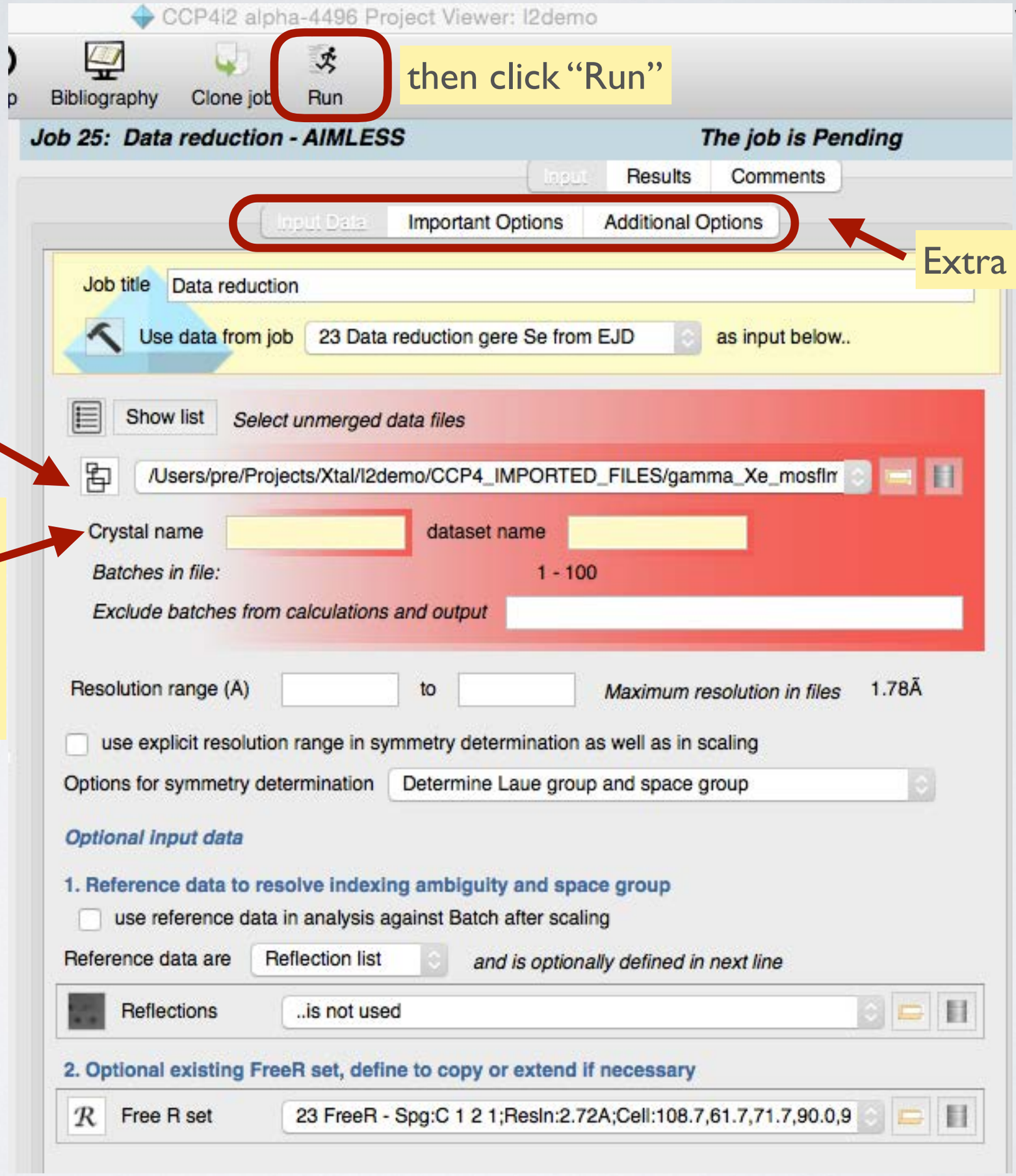
By default projects are created in $HOME/CCP4I2_PROJECTS but you can put them anywhere

Avoid spaces in project names (and other names)

THE TASK MENU



Set input

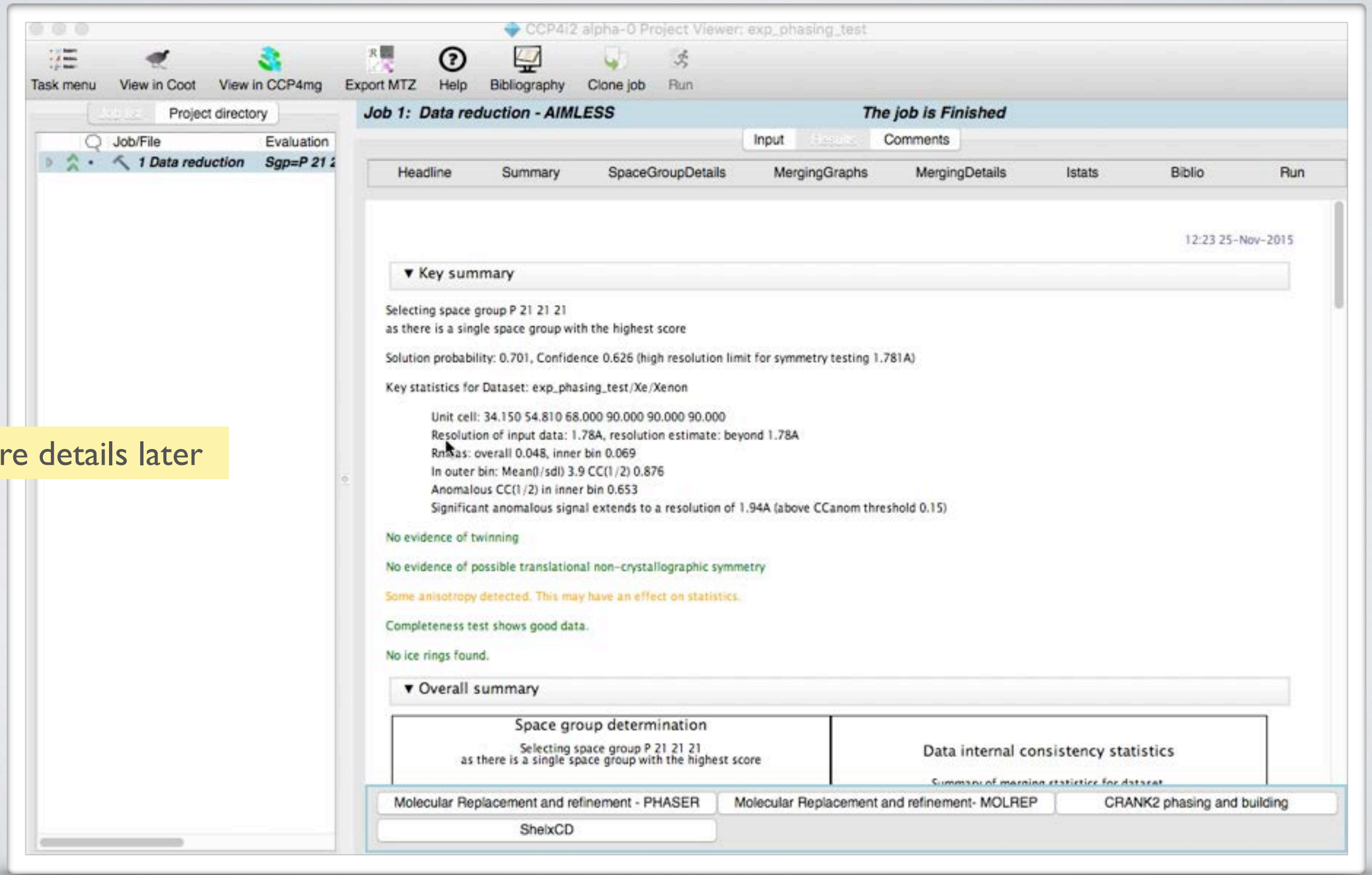


Choose input data

Compulsory (red) crystal and dataset names, used to identify data object
Short, no spaces!

Reports

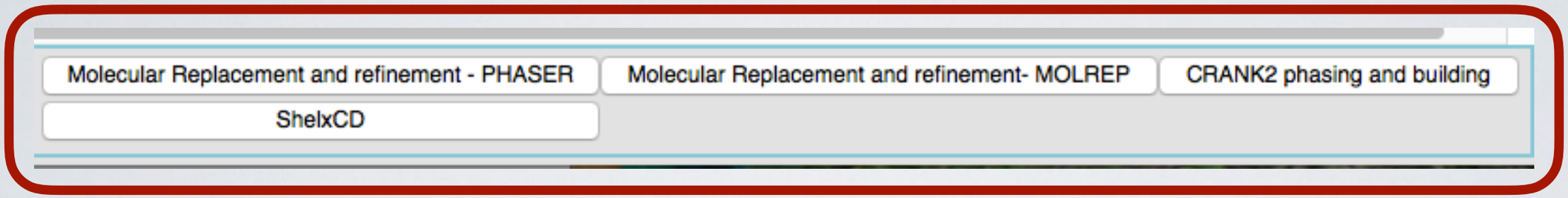
Some tasks give live updates (though not this one yet)
More will in future



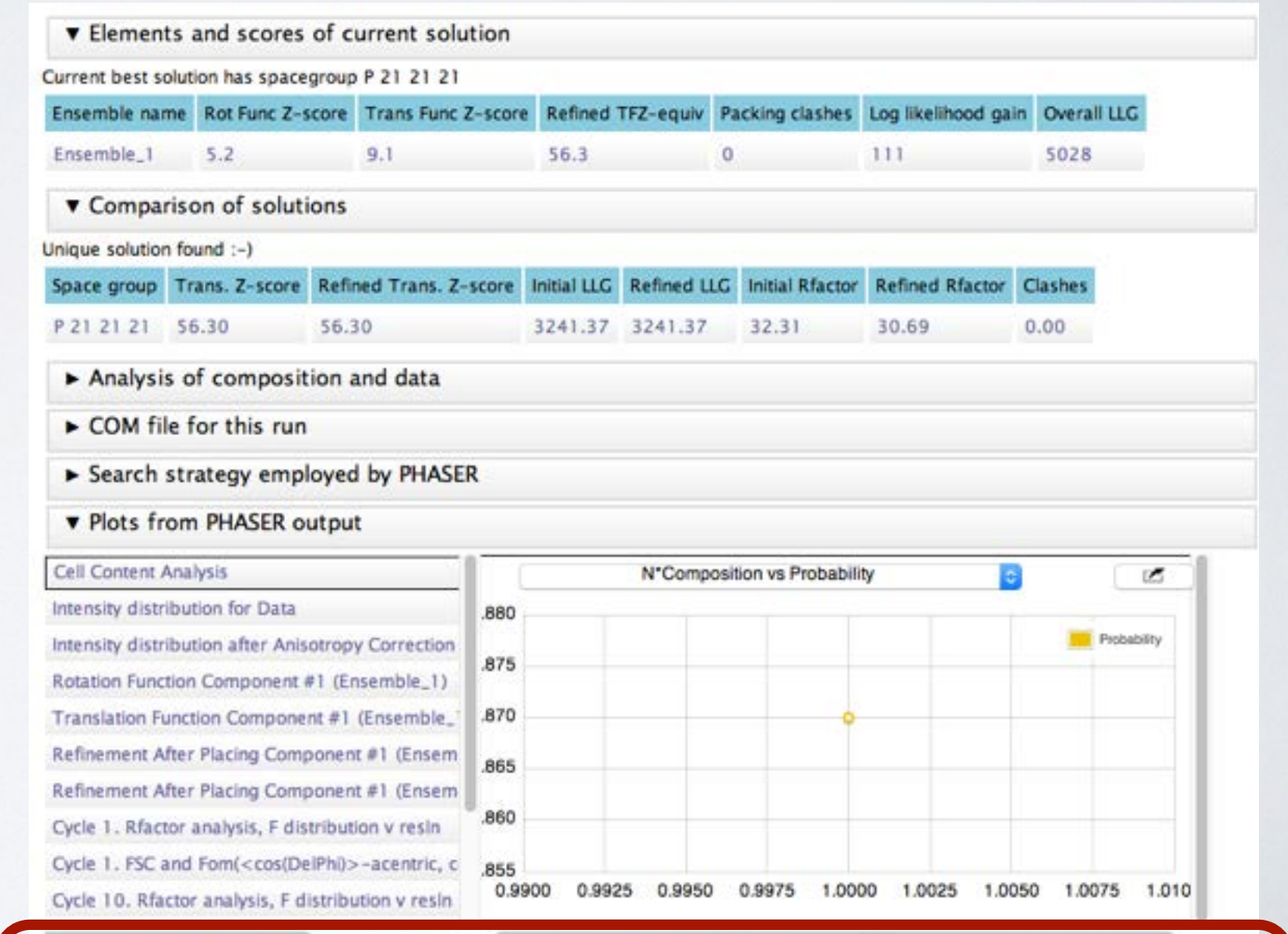
More details later

Follow-on

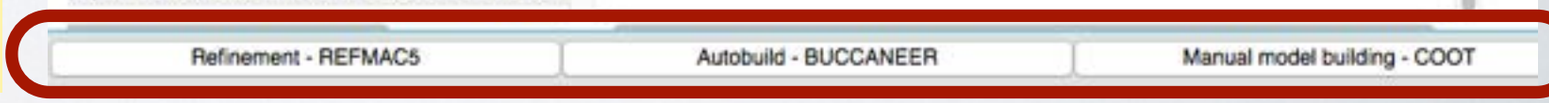
Next job suggestions, with main inputs filled in automatically



From Data Reduction
Solve structure by Molecular replacement or
Experimental phasing



From Molecular Replacement
Refine, Model build or
Manual building



RELEASE PLANS

- First version to roll out with CCP4 7.0 in late December

- Updates will incorporate new programs. Next: Arcimboldo, ACORN

- Alpha-test version available now. Contact me if you want to test it: jon.agirre@york.ac.uk

To start ccp4i2

Usually type “ccp4i2”

BUT here type “locali2”

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Eugene Krissinel
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Ronan Keegan
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Marcin Wojdyr
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