CCP4 from a user perspective

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Overview

- File formats
- CCP4 Website
- CCP4 Help
- CCP4BB
- CCP4 Program Suite
- CCP4 Interface
- Interaction with other programs
- Example(s) of Use

File formats

- Reflection files (mtz format)
- Coordinate files (pdb format)

Provide ways in and out of CCP4 Suite

MTZ files

- Columns, columns, columns
- Labels
- Types
- Non-ascii
- Viewers

PDB files

- ‘standard’
- Ascii
- Widely used

CCP4 Website

- http://www.ccp4.ac.uk
- Downloads
- Problem pages
- Documentation
- Meetings
- Jobs

CCP4 Help

- Documentation
- General crystallography
- Help in interface

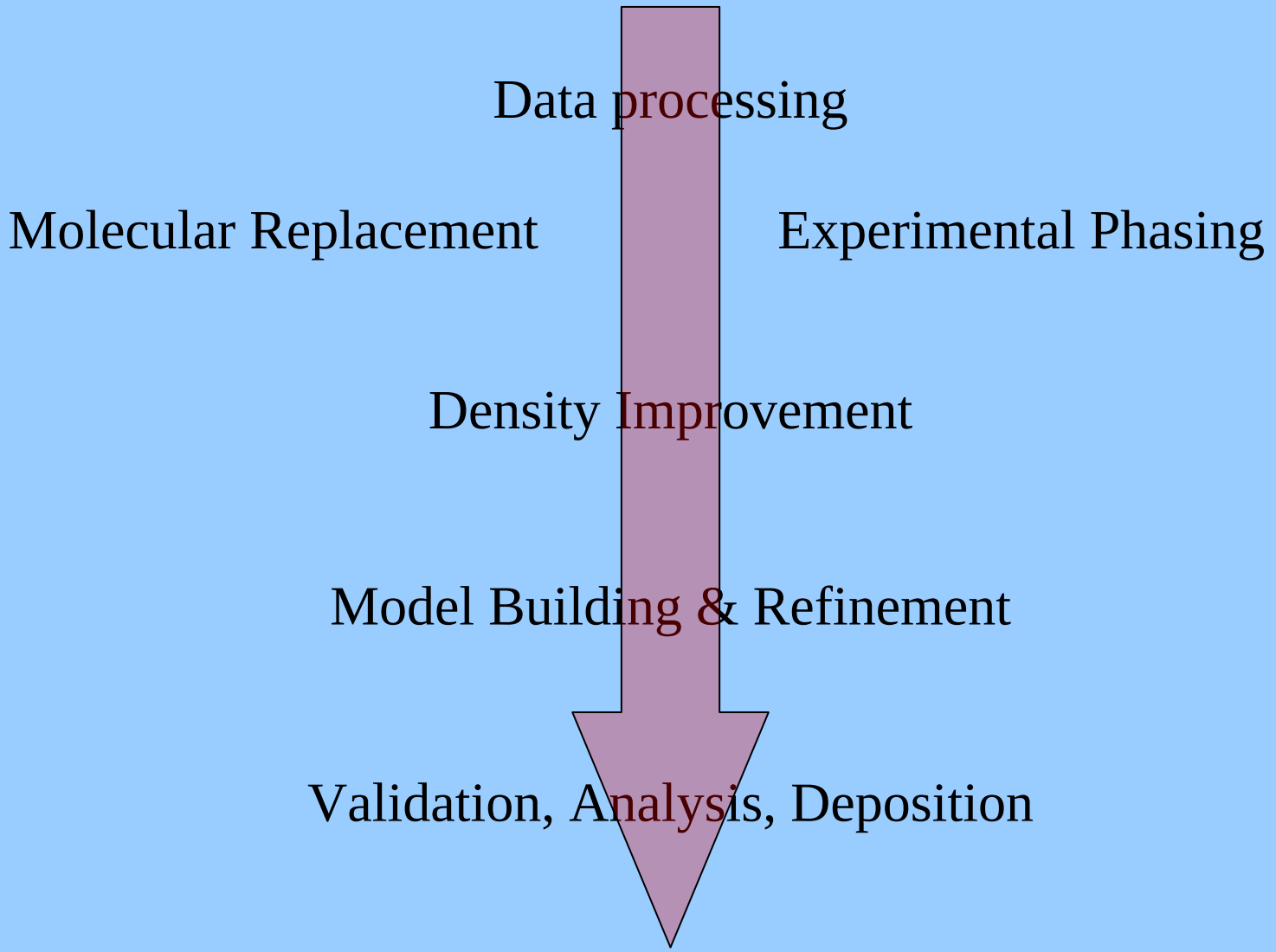
CCP4BB

- Members from all over the world
- Fast, expert help from colleagues
- Useful tips
- Non-CCP4 topics
- Heated (entertaining) discussions

CCP4 Program Suite

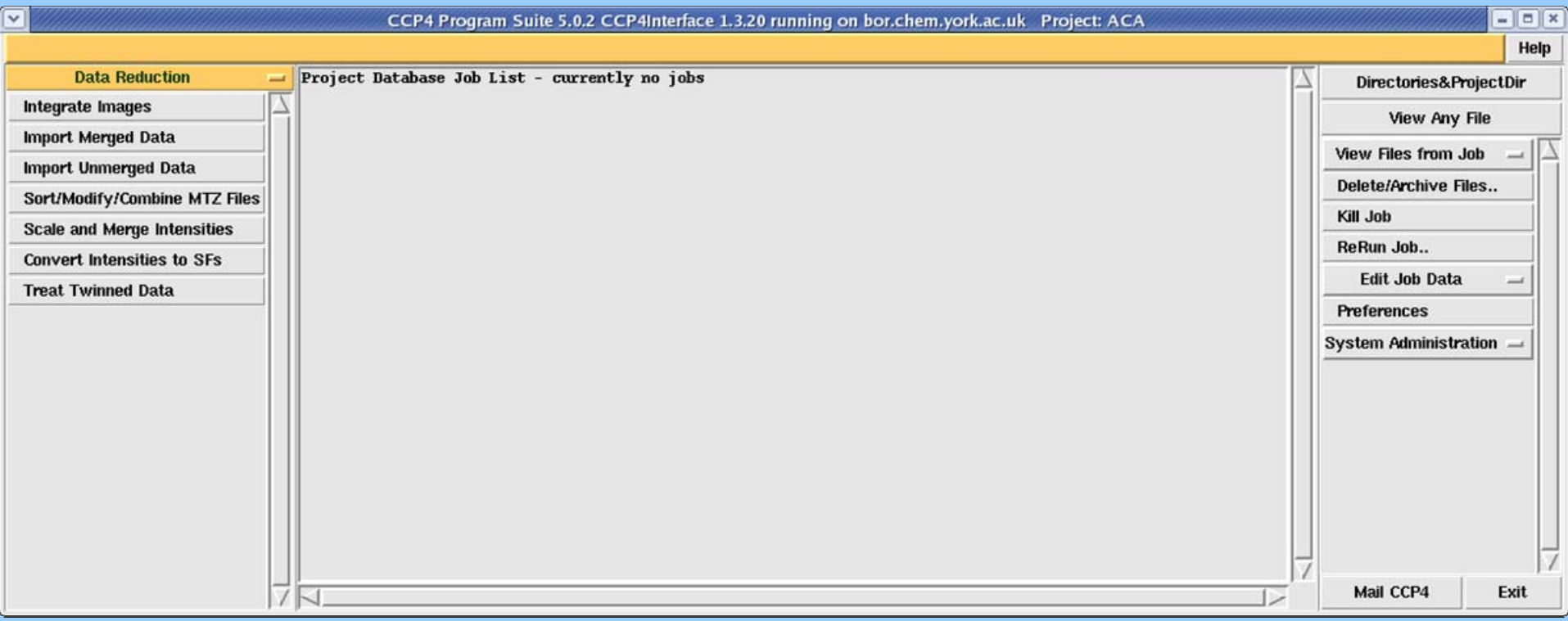
- ***Many*** programs from many authors
- All aspects of crystallography

Overview

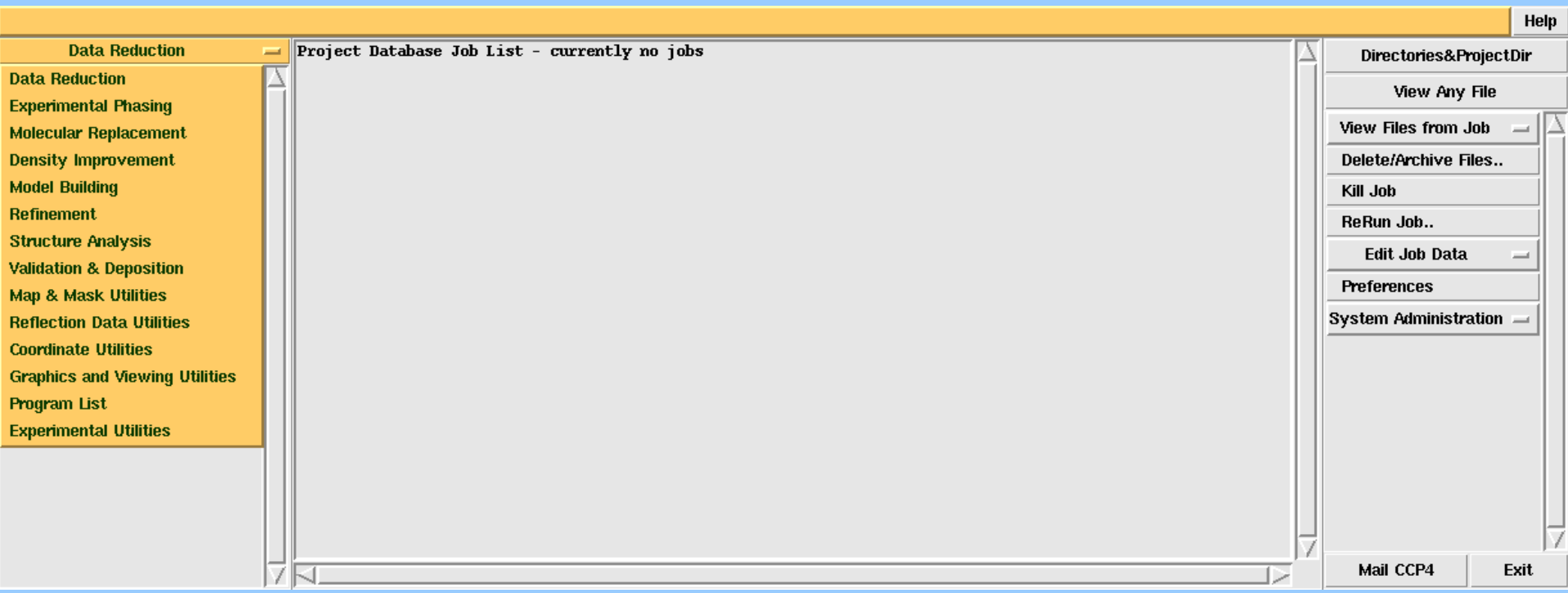

Data processing
Molecular Replacement
Experimental Phasing
Density Improvement
Model Building & Refinement
Validation, Analysis, Deposition

Interface

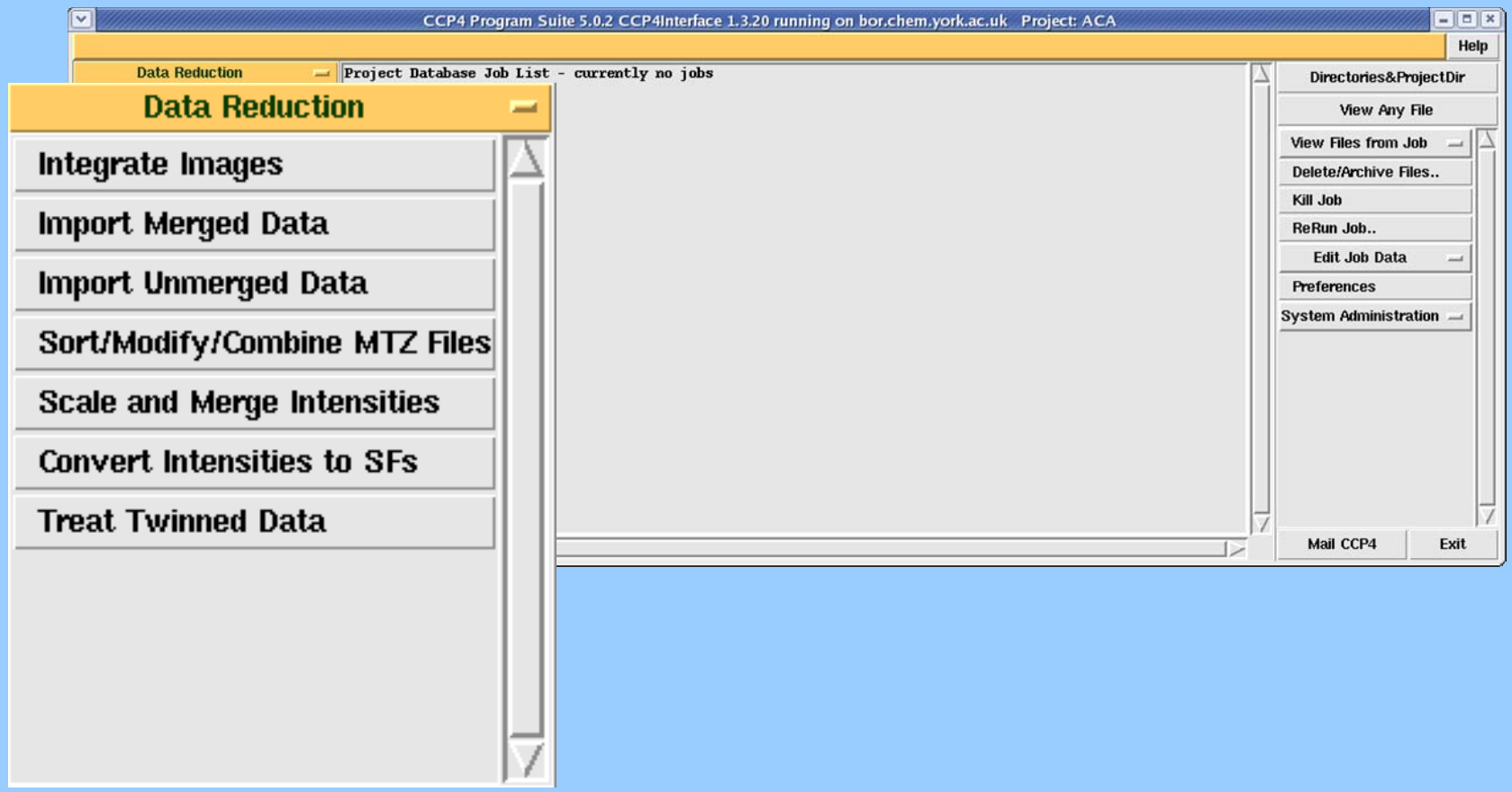
- No more typos
- Import/Export
- Help
- Defaults
- Project Management !!
- Tasks (logical sequence)
- Graphs from log files

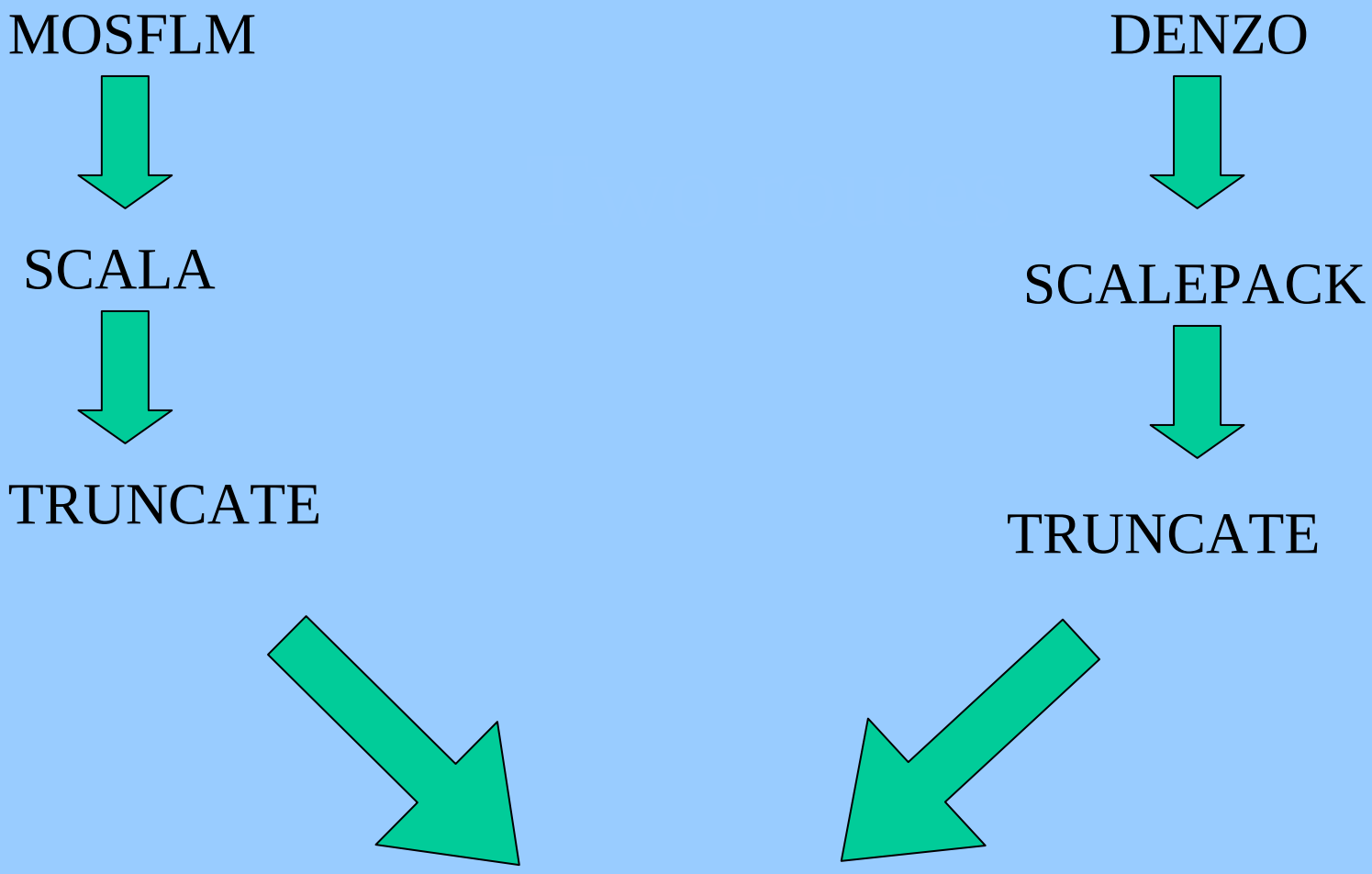

CCP4 Program Suite 5.0.2 CCP4Interface 1.3.20 running on bor.chem.york.ac.uk Project: ACA
Help
Data Reduction
Integrate Images
Import Merged Data
Import Unmerged Data
Sort/Modify/Combine MTZ Files
Scale and Merge Intensities
Convert Intensities to SFs
Treat Twinned Data
Project Database Job List - currently no jobs
Directories&ProjectDir
View Any File
View Files from Job
Delete/Archive Files..
Kill Job
ReRun Job..
Edit Job Data
Preferences
System Administration
Mail CCP4
Exit

Modules


Help
Data Reduction
Data Reduction
Experimental Phasing
Molecular Replacement
Density Improvement
Model Building
Refinement
Structure Analysis
Validation & Deposition
Map & Mask Utilities
Reflection Data Utilities
Coordinate Utilities
Graphics and Viewing Utilities
Program List
Experimental Utilities
Project Database Job List - currently no jobs
Directories&ProjectDir
View Any File
View Files from Job
Delete/Archive Files..
Kill Job
ReRun Job..
Edit Job Data
Preferences
System Administration
Mail CCP4
Exit

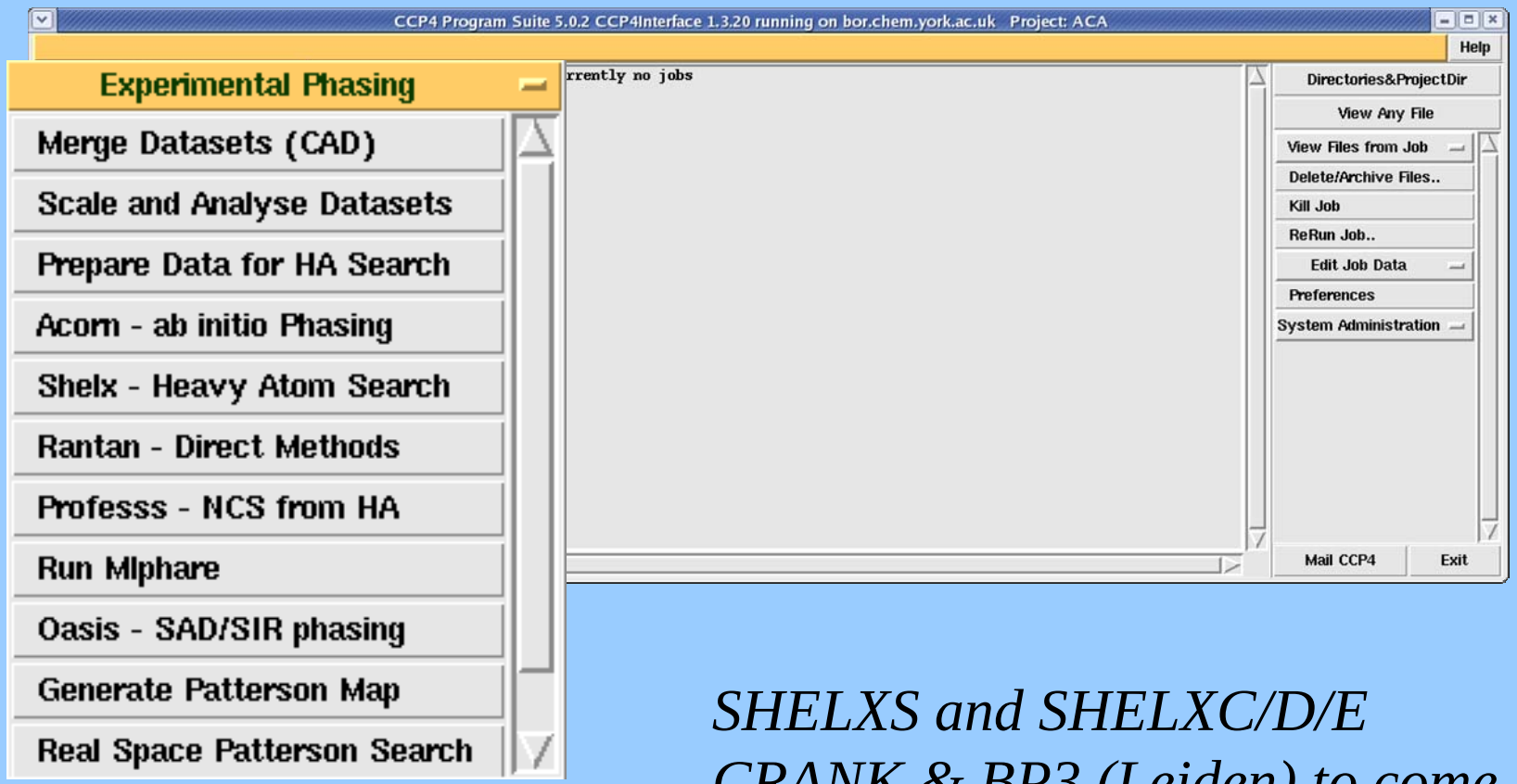
Data Reduction





MTZ file with structure factors etc.

Experimental Phasing



SHELXS and SHELXC/D/E
CRANK & BP3 (Leiden) to come

ACORN

- Heavy atom substructures
- Locating secondary structure elements
- Density modification

- At high resolution, complete ‘density’ determination

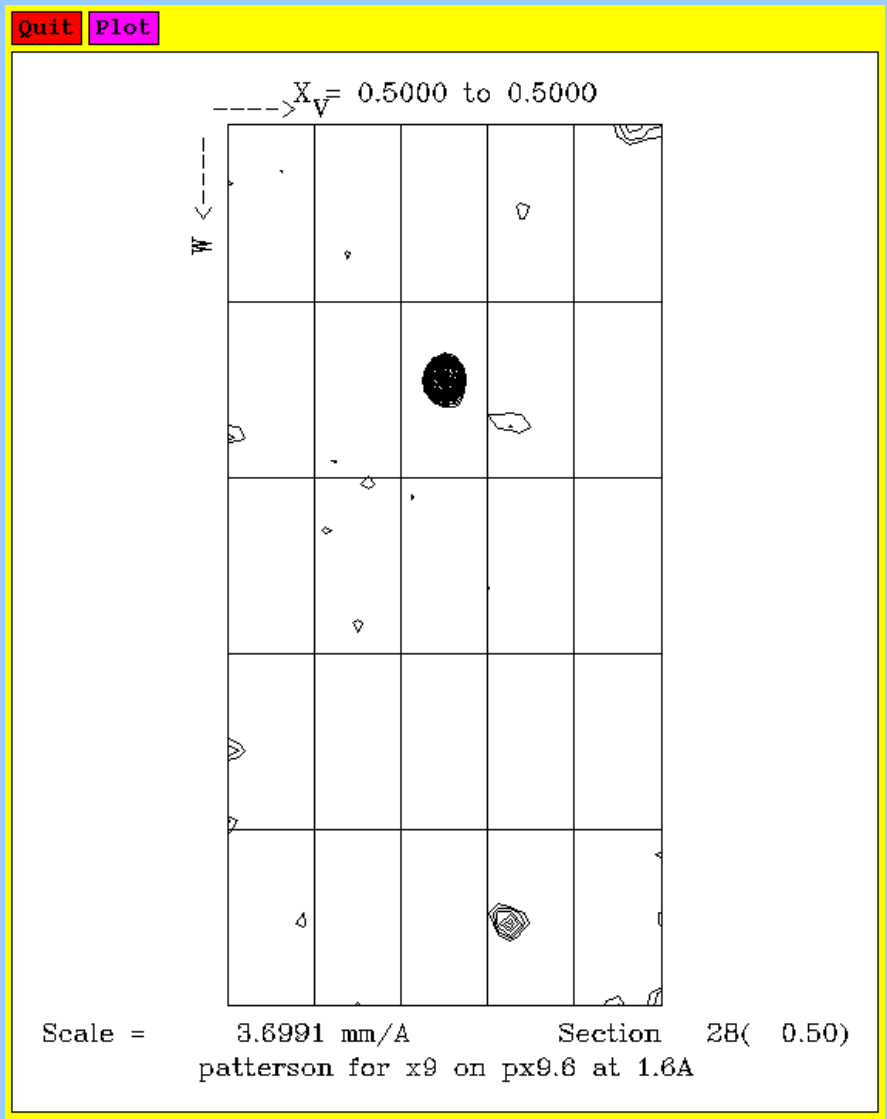
Foadi,J., Woolfson,M.M., Dodson,E.J., Wilson,K.S., Yao Jia-xing and Zheng Chao-de (2000) *Acta. Cryst.* **D56**, 1137-1147.

ACORN on a CBM

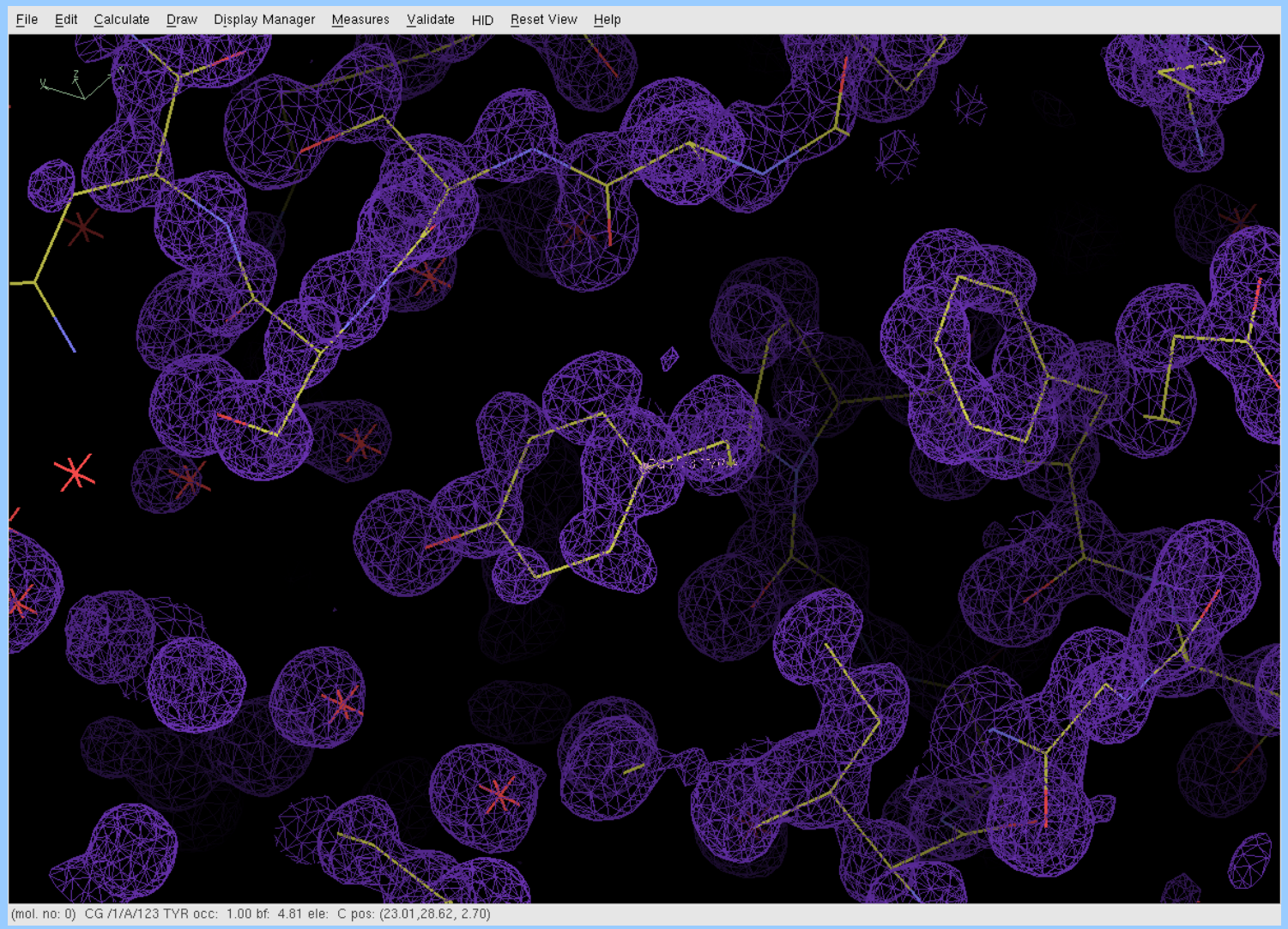
- Data to 1.0A on Se form at l = 0.87Å (SRS)
- Patterson shows Se very clearly
- ACORN gave excellent map in 18 min on SGI

Ab initio structure determination and functional characterization of CBM36: A new family of calcium-dependent carbohydrate binding modules
Jamal-Talabani S, Boraston AB, Turkenburg JP, Tarbouriech N, **Ducros VMA**, Davies GJ
STRUCTURE
12 (7): 1177-1187 JUL 2004

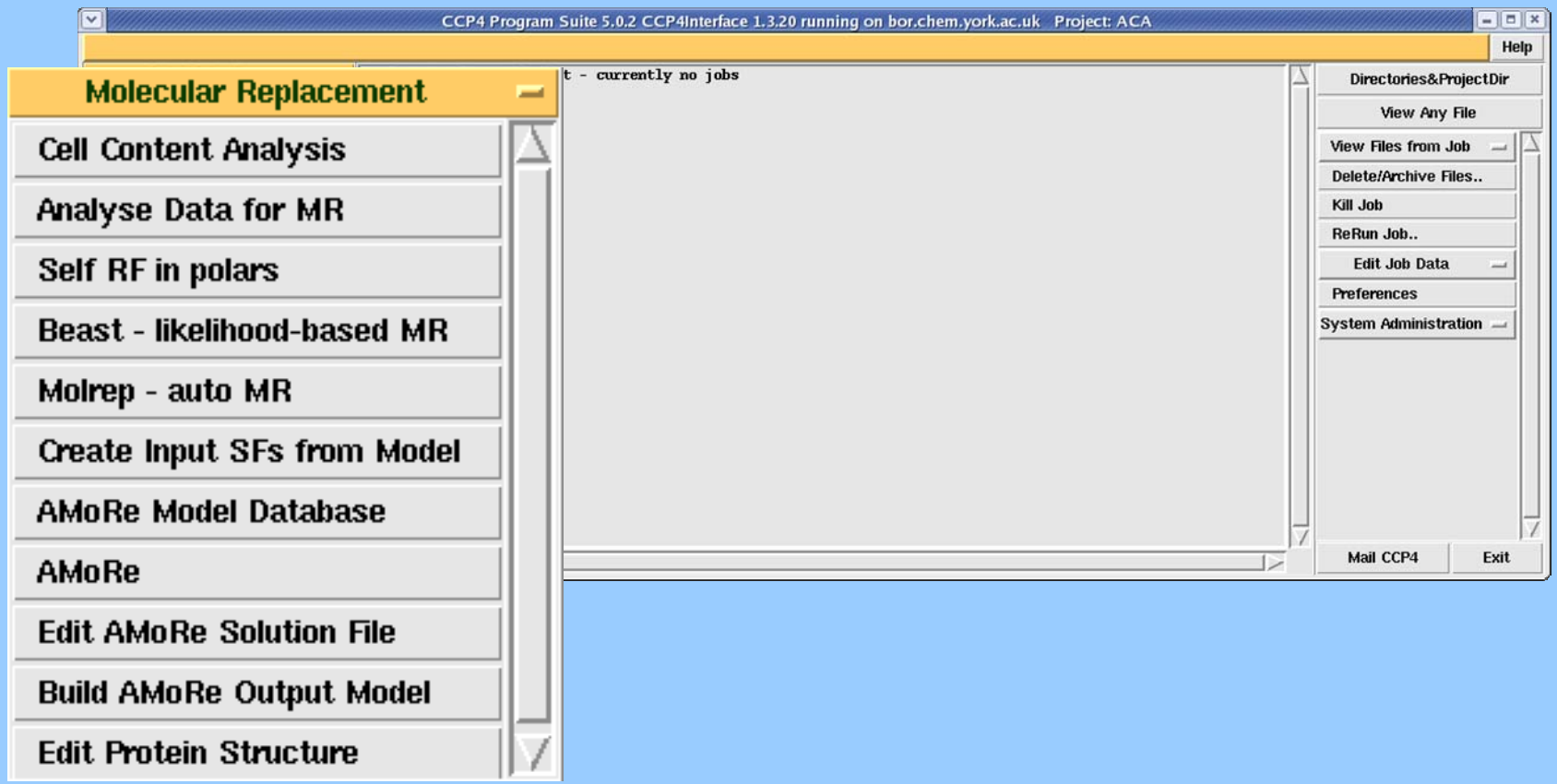
Patterson


Quit
Plot
X_V = 0.5000 to 0.5000
W
Scale = 3.6991 mm/A
Section 28(0.50)
patterson for x9 on px9.6 at 1.6A

CBM ACORN map & final model



Molecular Replacement



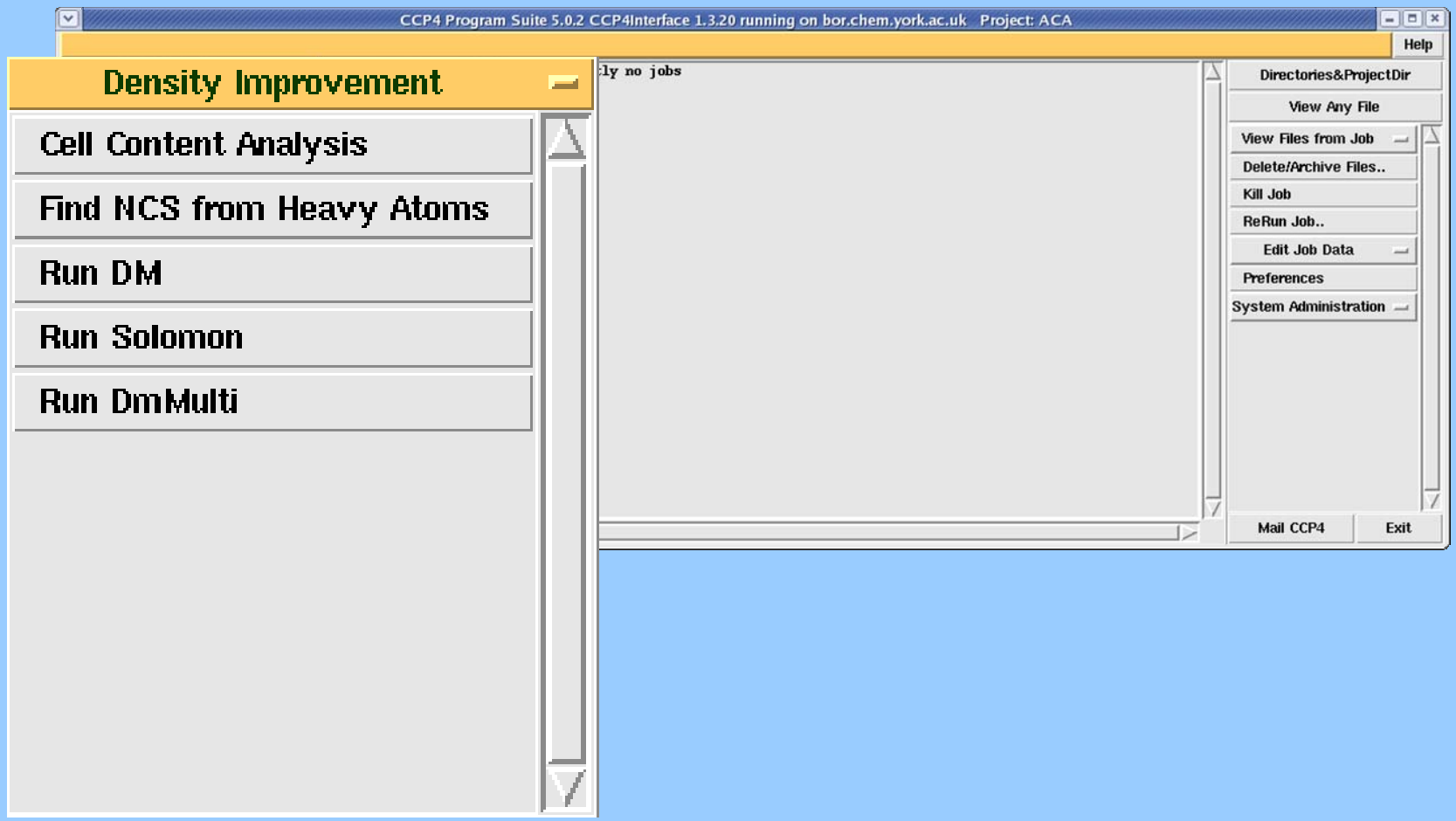
MR programs

- Molrep
- AMoRe
- Phaser (Randy Read, Tuesday morning)

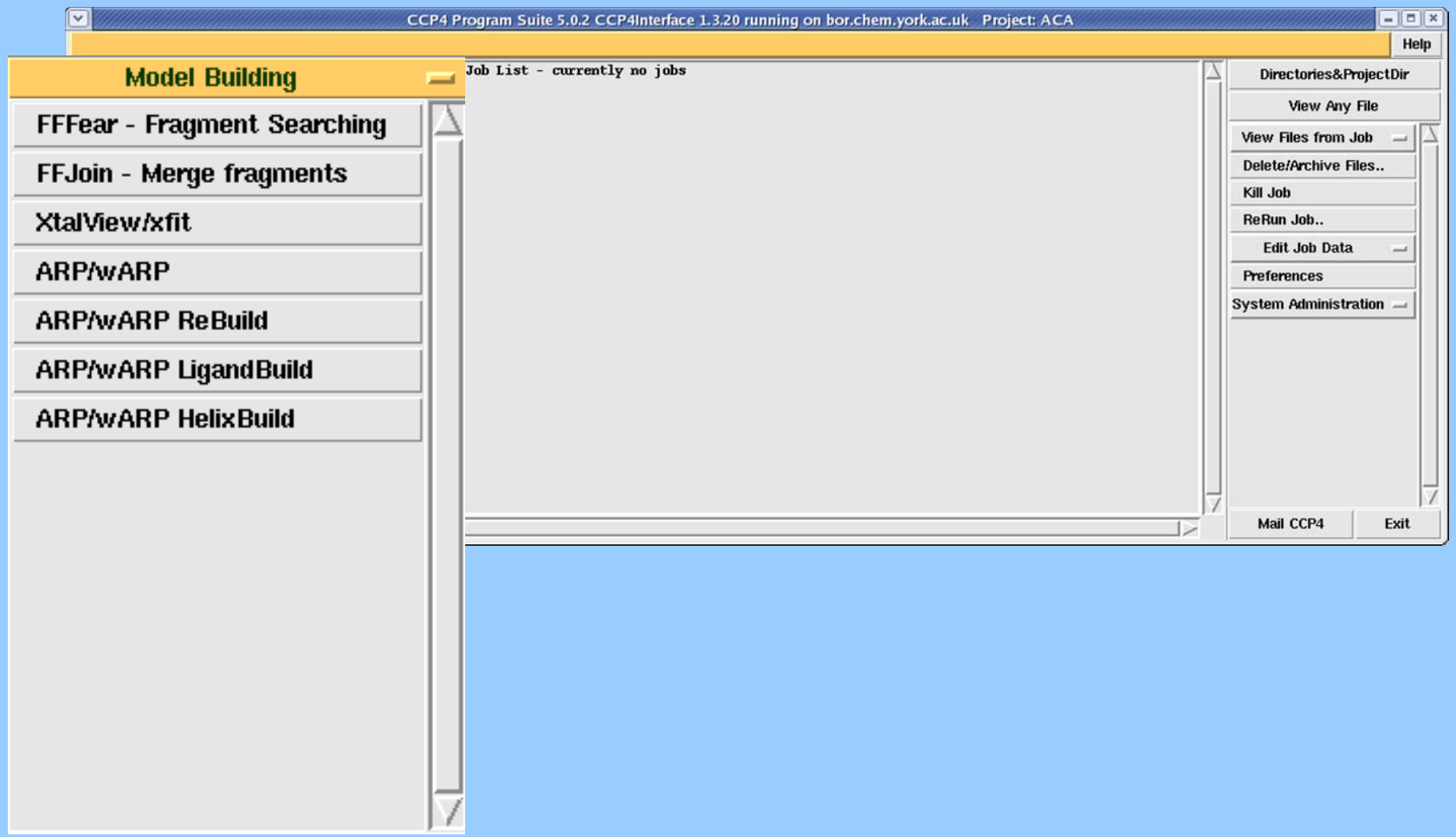
- Many utilities

MR Utilities

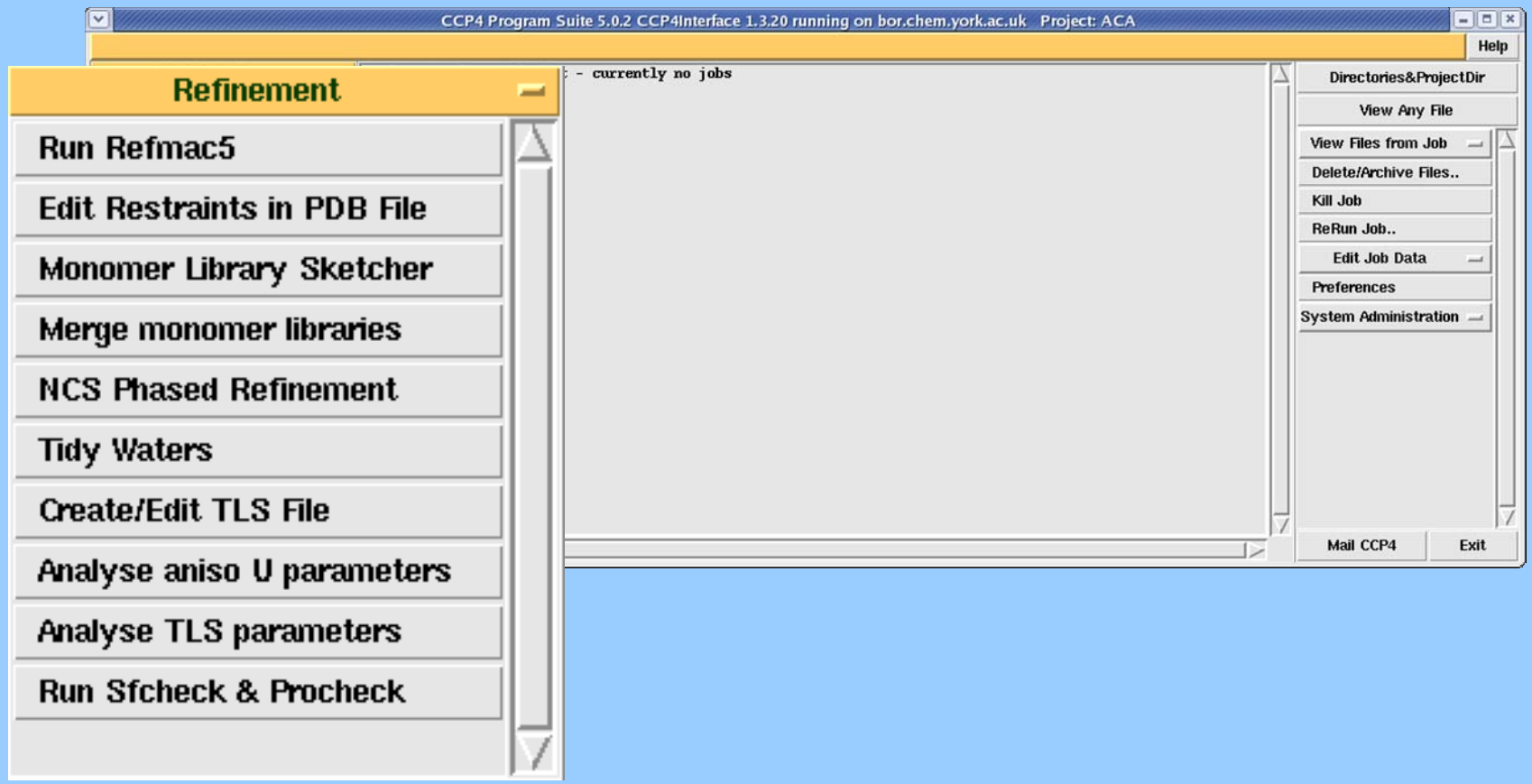
Density Improvement



Model Building



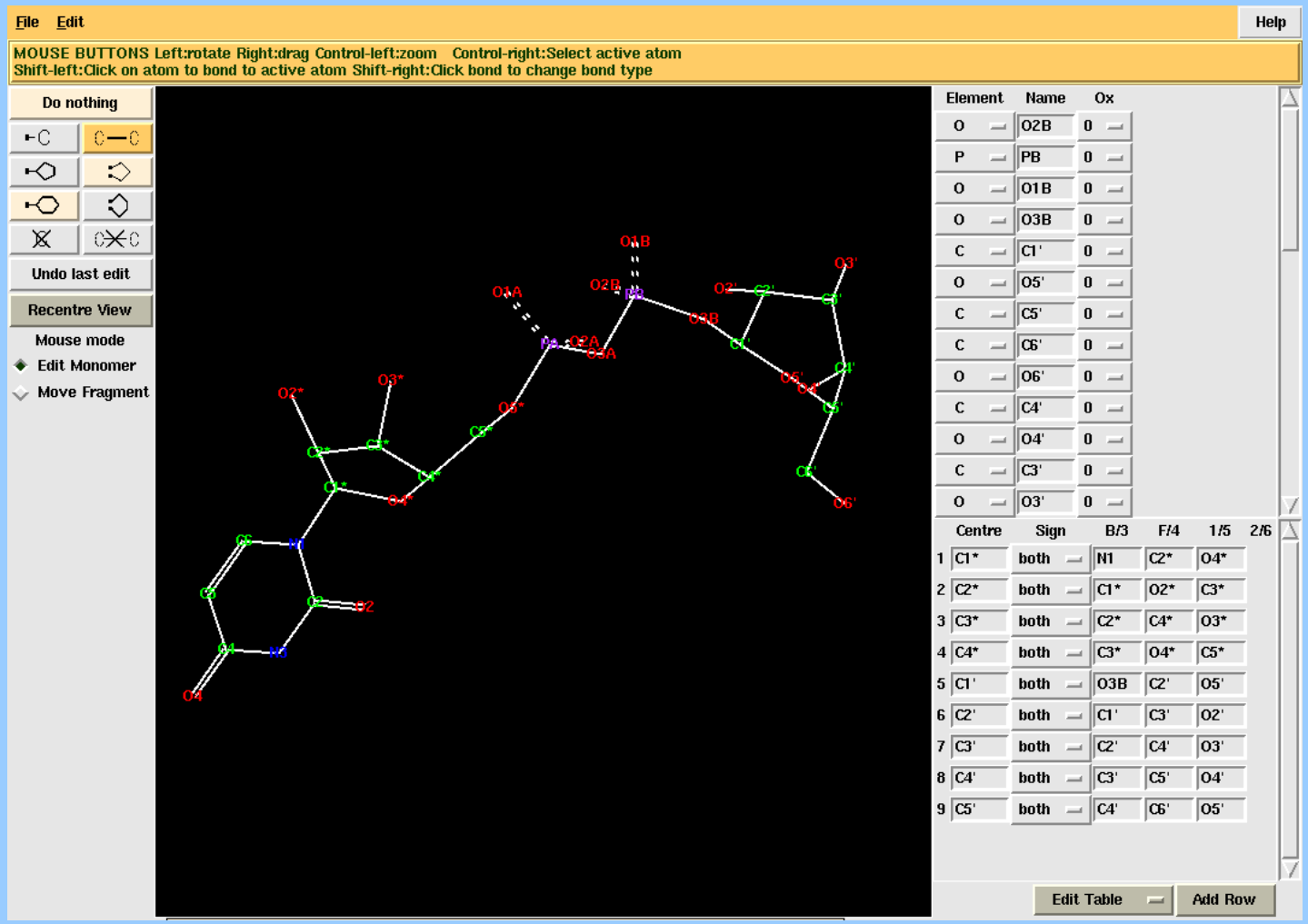
Refinement


CCP4 Program Suite 5.0.2 CCP4Interface 1.3.20 running on bor.chem.york.ac.uk Project: ACA
Help
Refinement
Run Refmac5
Edit Restraints in PDB File
Monomer Library Sketcher
Merge monomer libraries
NCS Phased Refinement
Tidy Waters
Create/Edit TLS File
Analyse aniso U parameters
Analyse TLS parameters
Run Sfcheck & Procheck
- currently no jobs
Directories&ProjectDir
View Any File
View Files from Job
Delete/Archive Files..
Kill Job
ReRun Job..
Edit Job Data
Preferences
System Administration
Mail CCP4
Exit

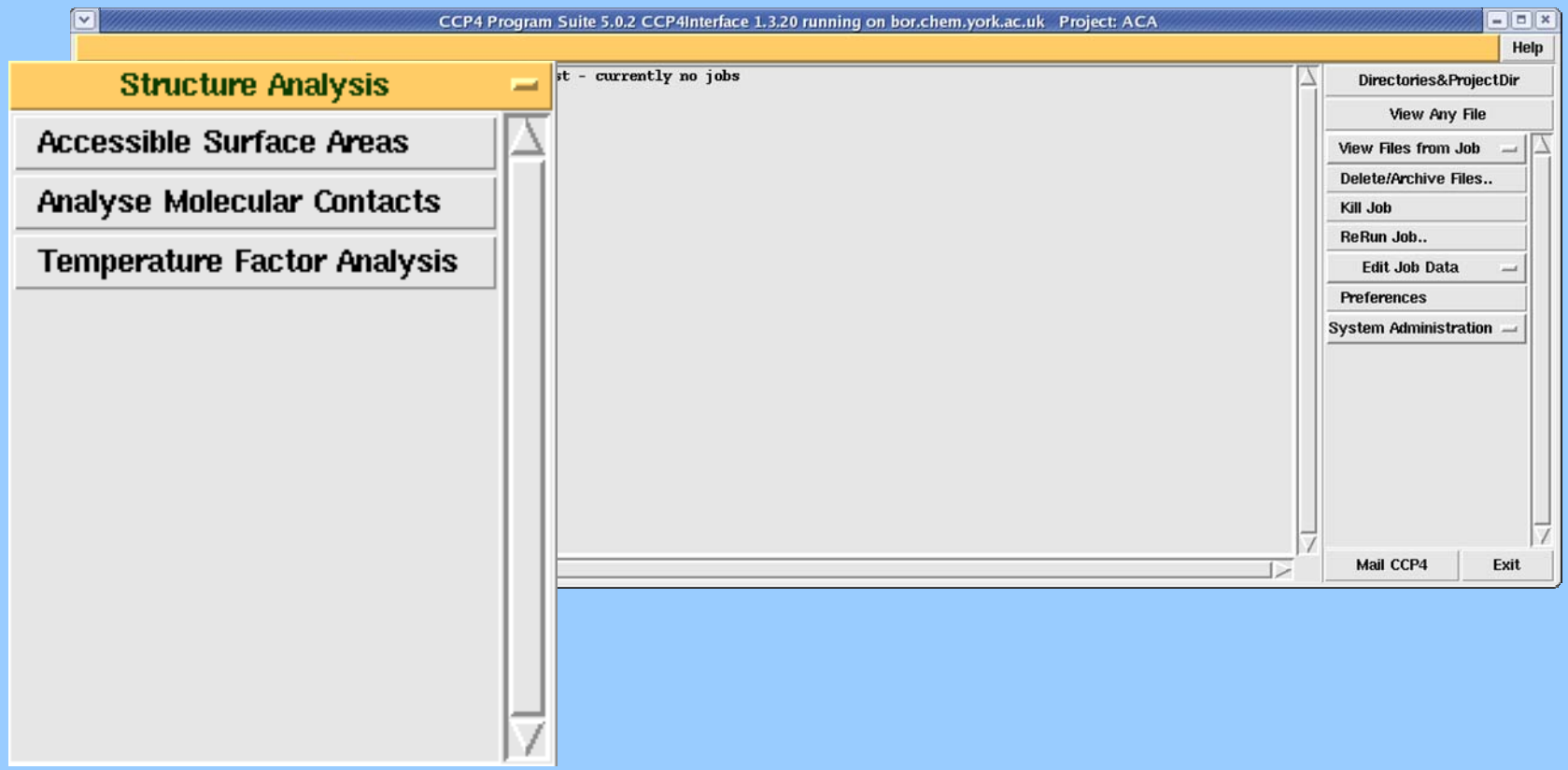
REFMAC

- Algorithms
- Scaling
- Restraints (geometric & NCS)
- TLS
- Combines with ARP/wARP
- Easy to use in interface

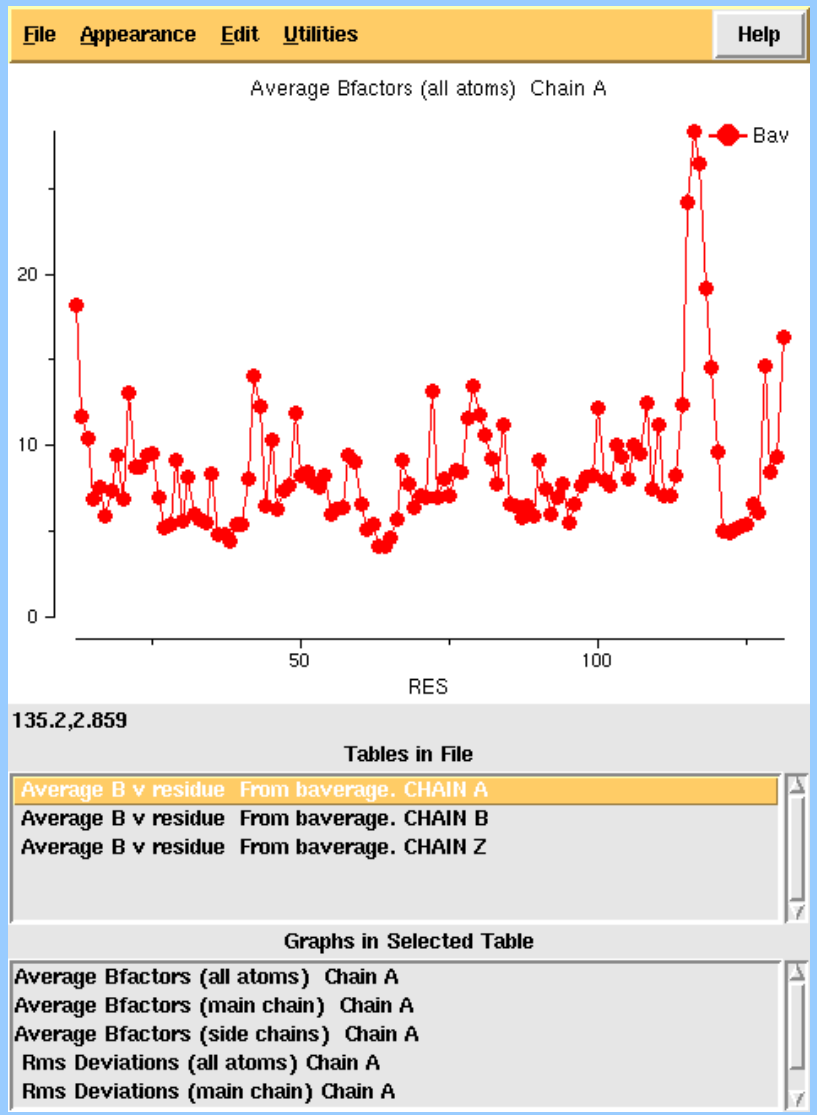
Monomer library sketcher



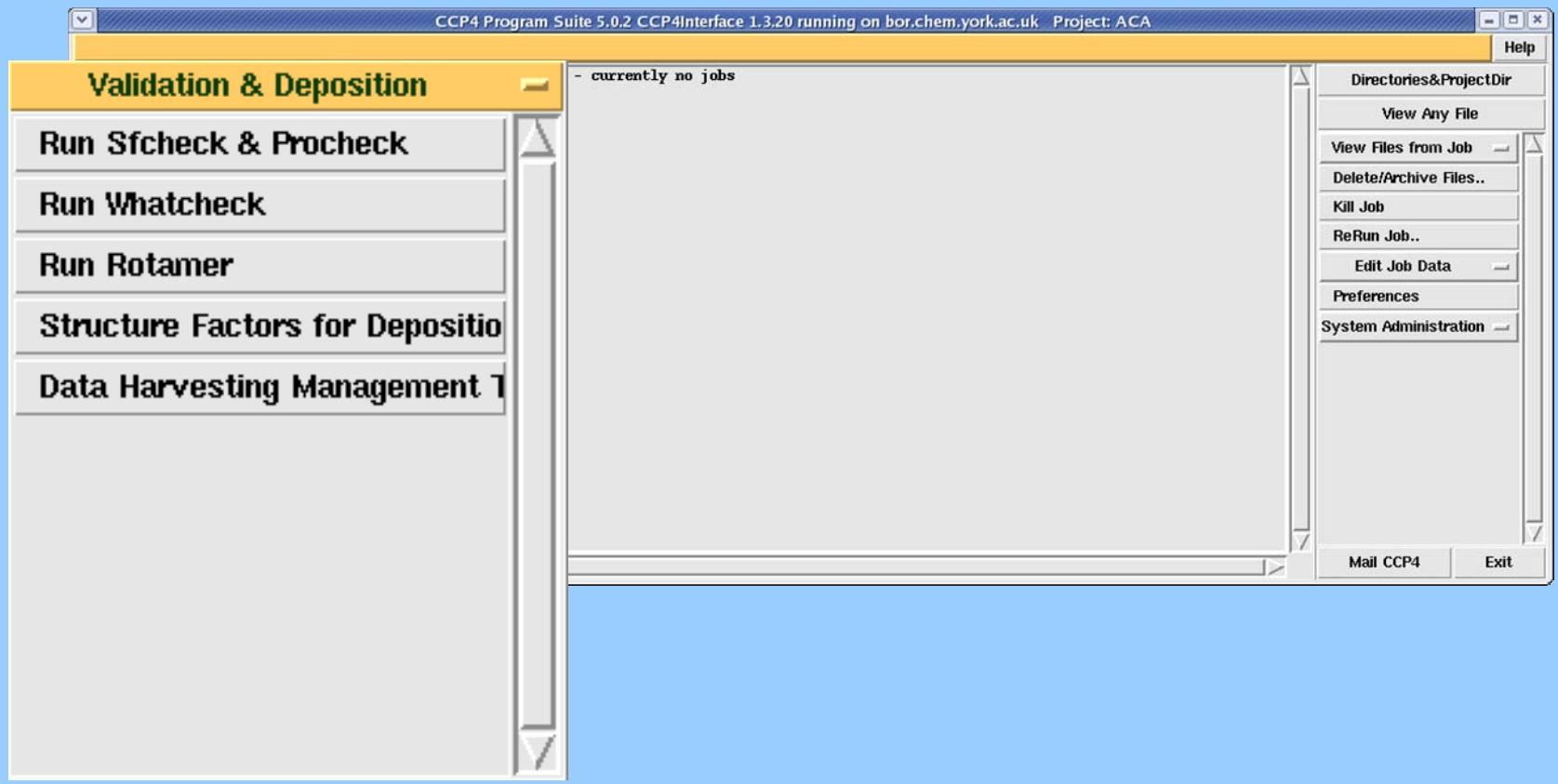
Structure Analysis



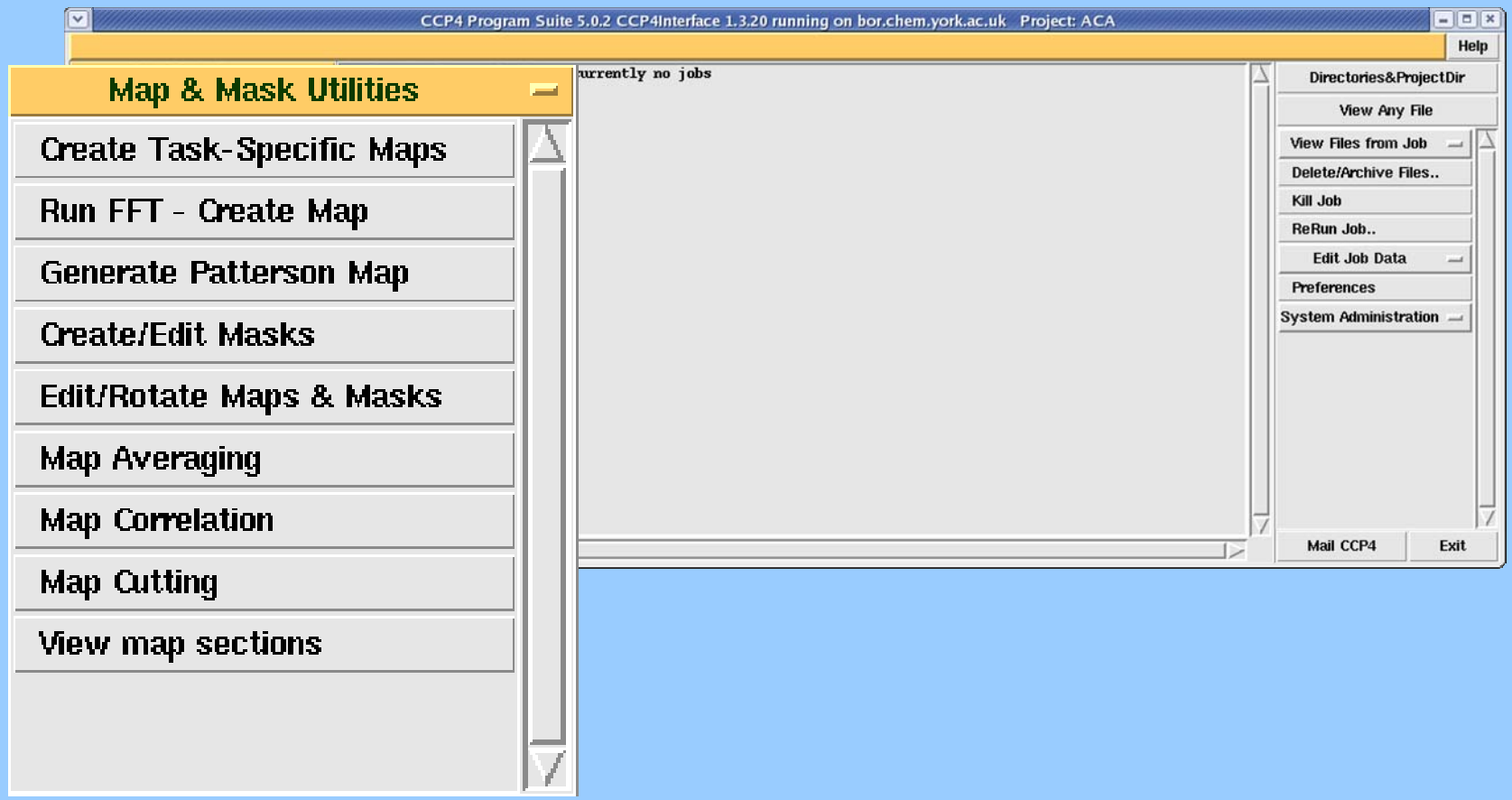
Temperature factor analysis



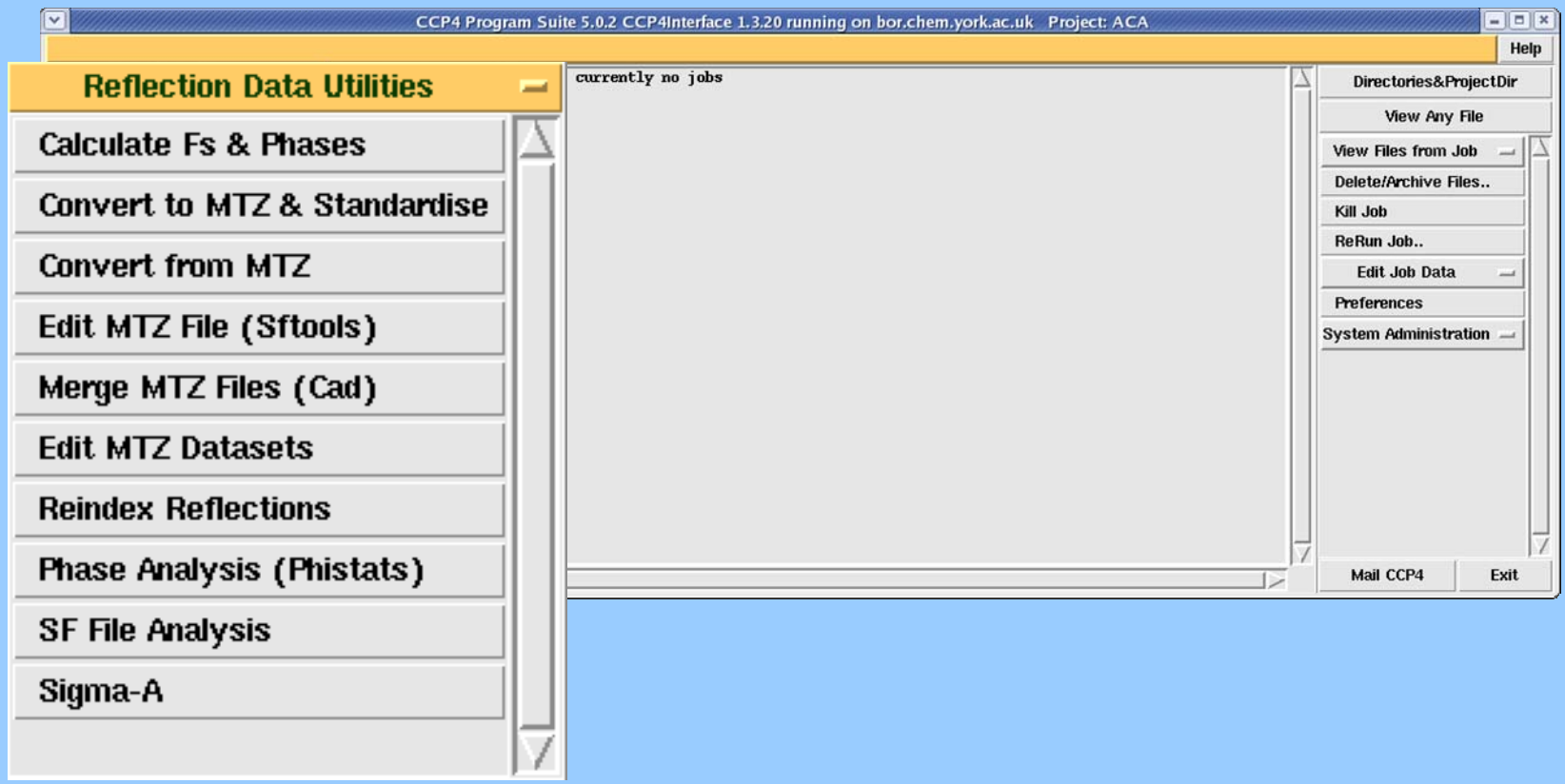
Validation & Deposition



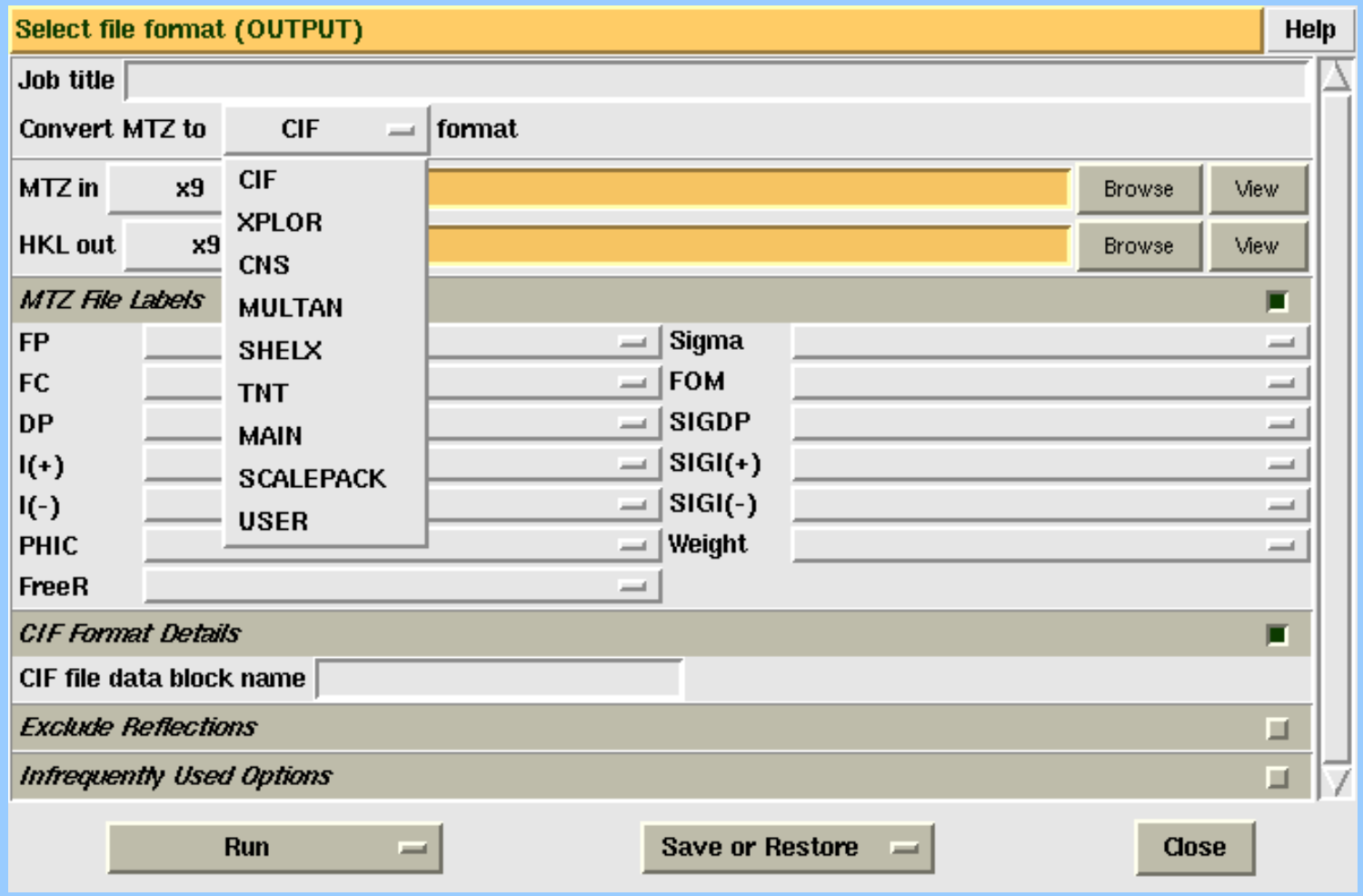
Map & Mask Utilities



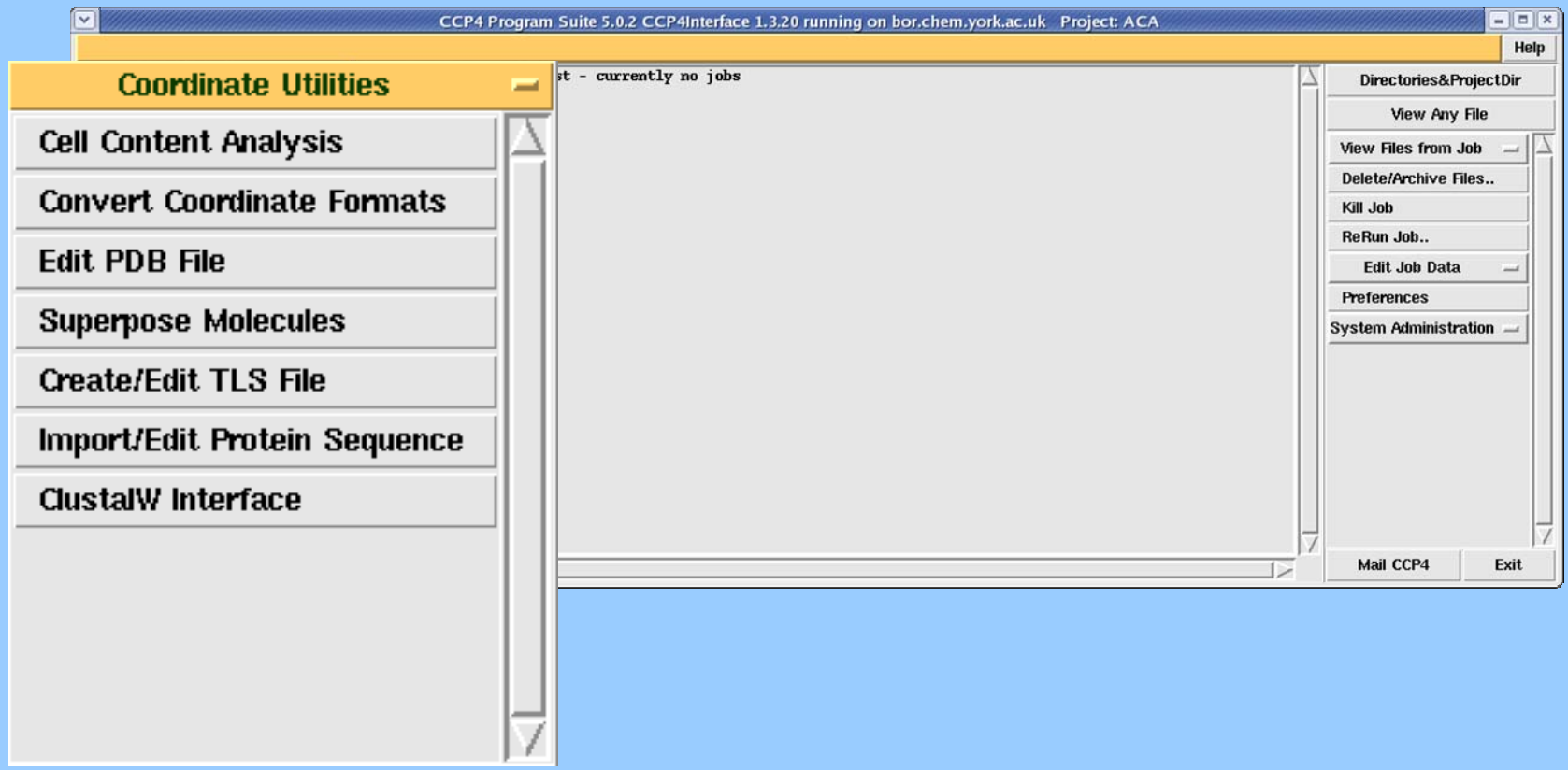
Reflection Data Utilities



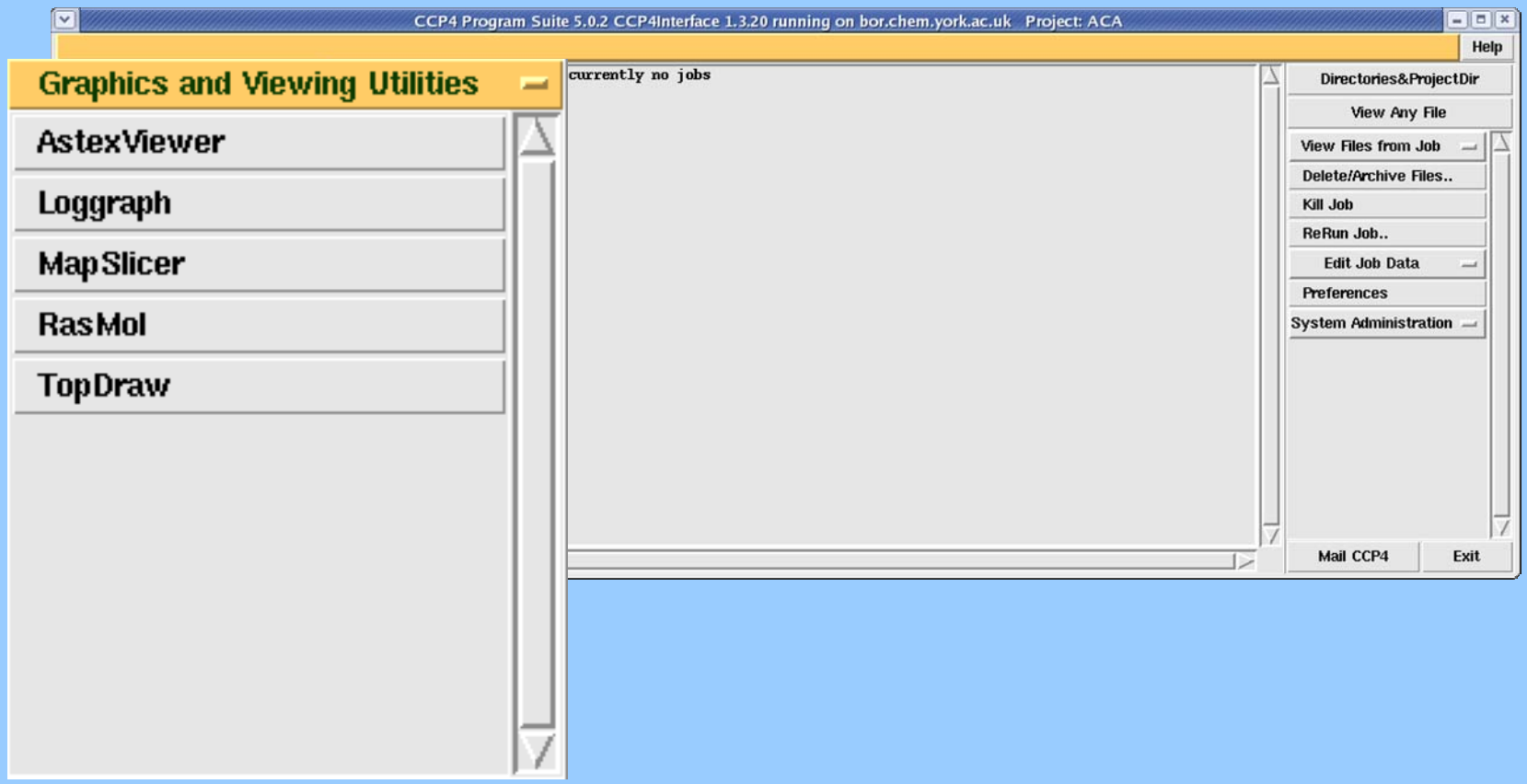
Convert from MTZ



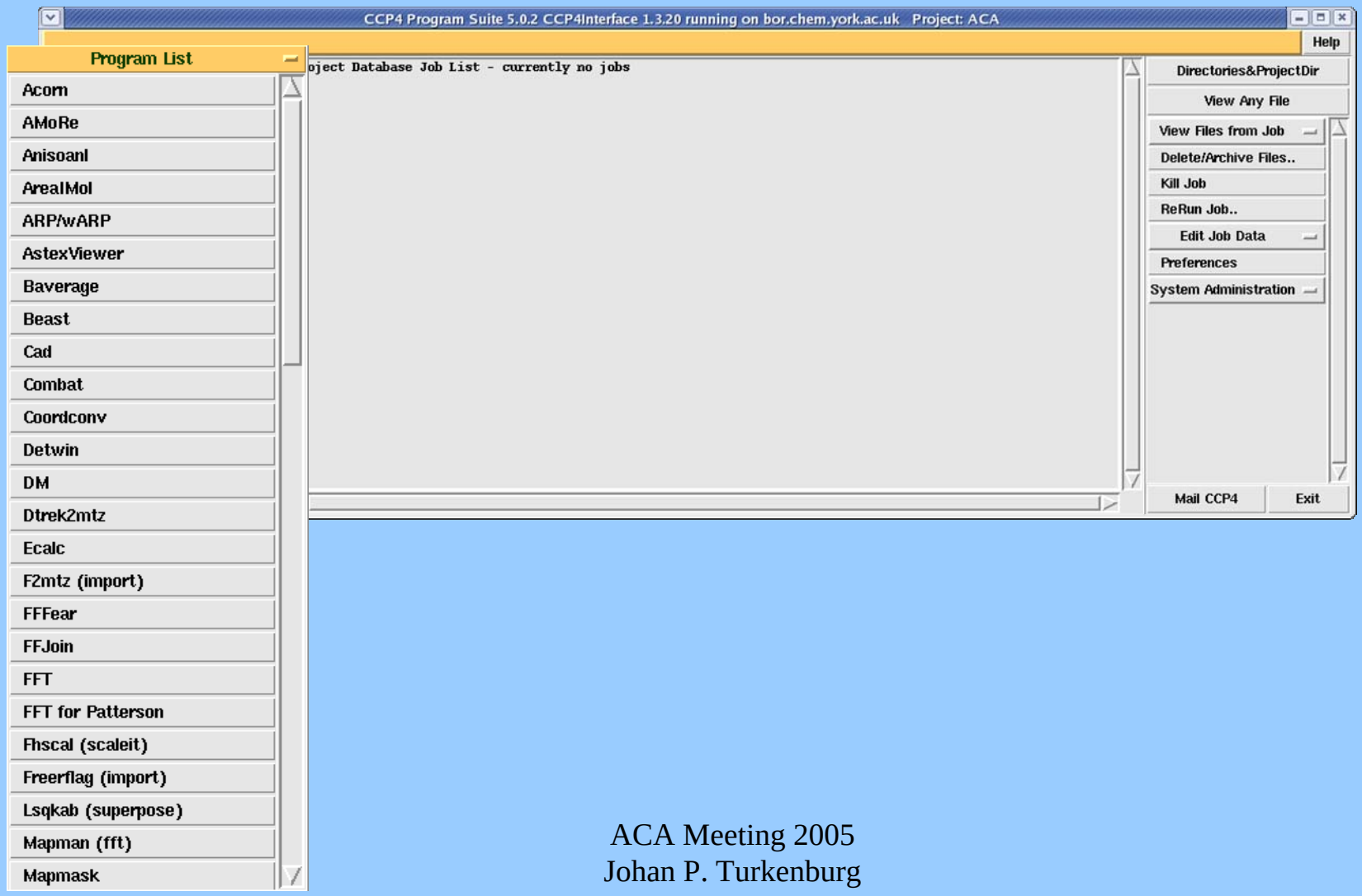
Coordinate Utilities



Graphics & Viewing Utilities



Program List



‘External’ Programs

- Arp/warp
- Shelx
- Mosflm
- Xtalview

Example 1 Lyase

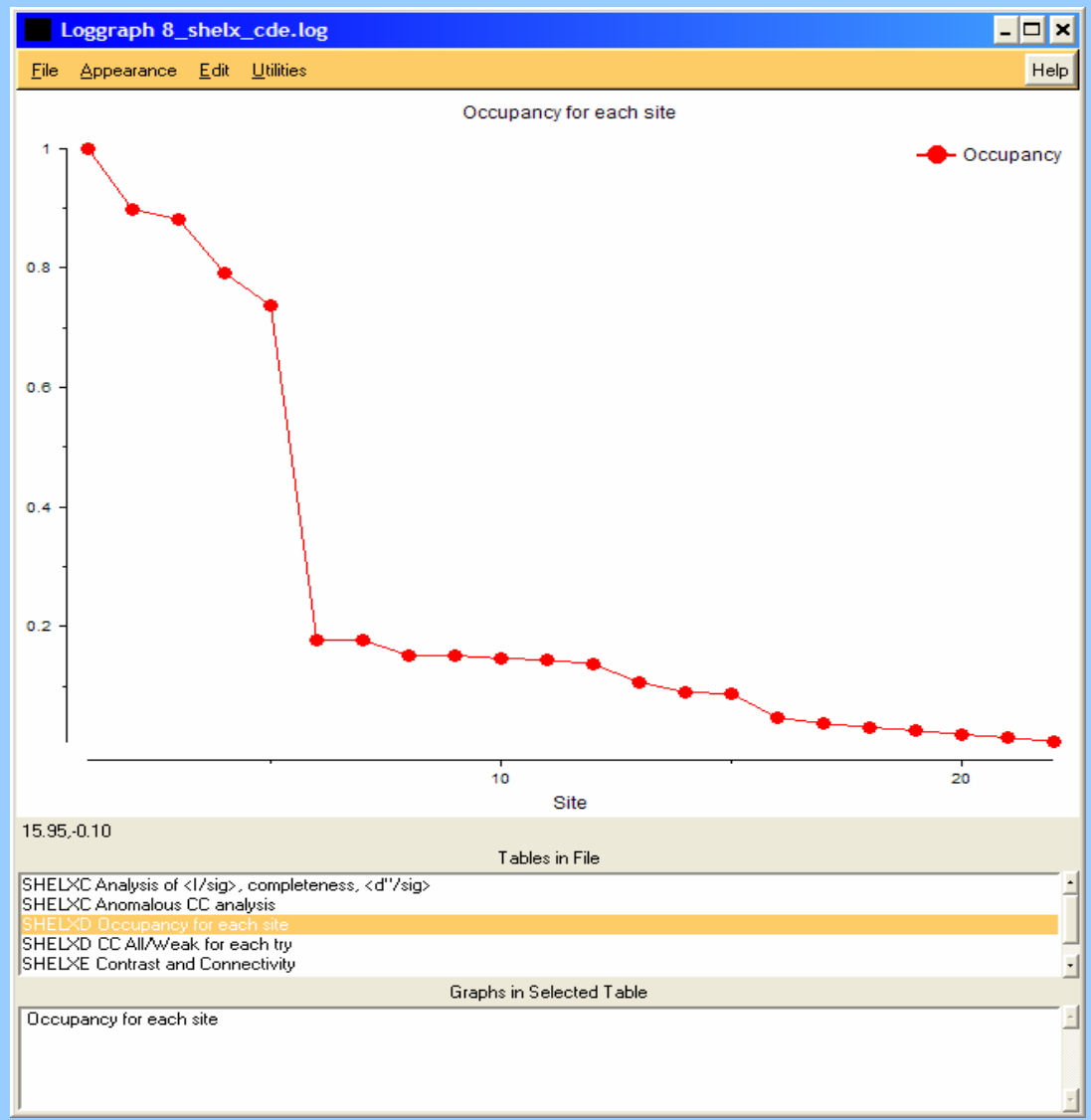
- Space group H32, unit cell 58.8 58.8 588.5

- All programs used are runnable from interface

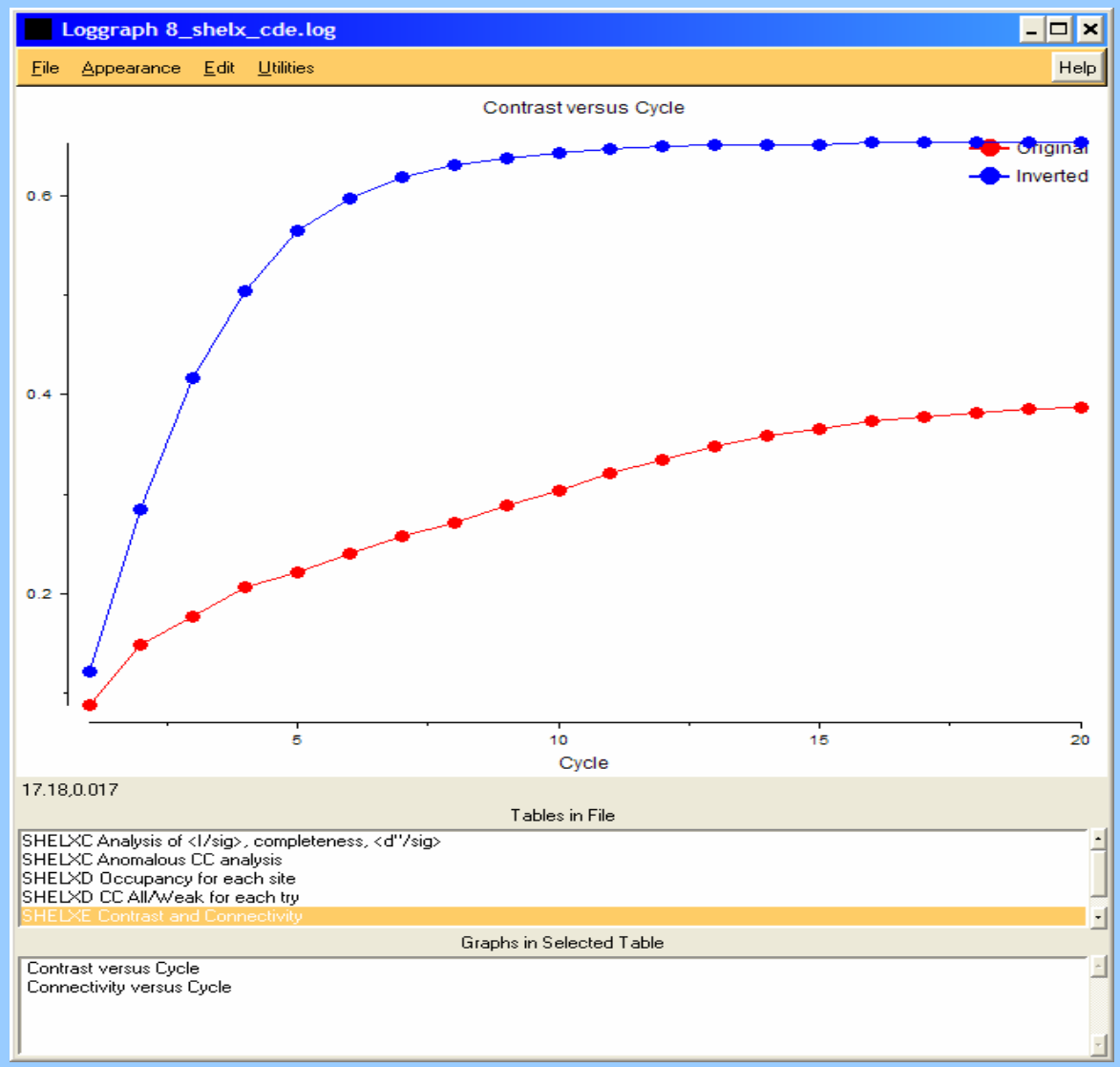
- Se MAD Shelxd to find sites
- MLPHARE, DM phasing/phase improvement
- ARP/wARP, REFMAC model building/refinement

- Input/output ‘chaining’ trivial (but not automatic)

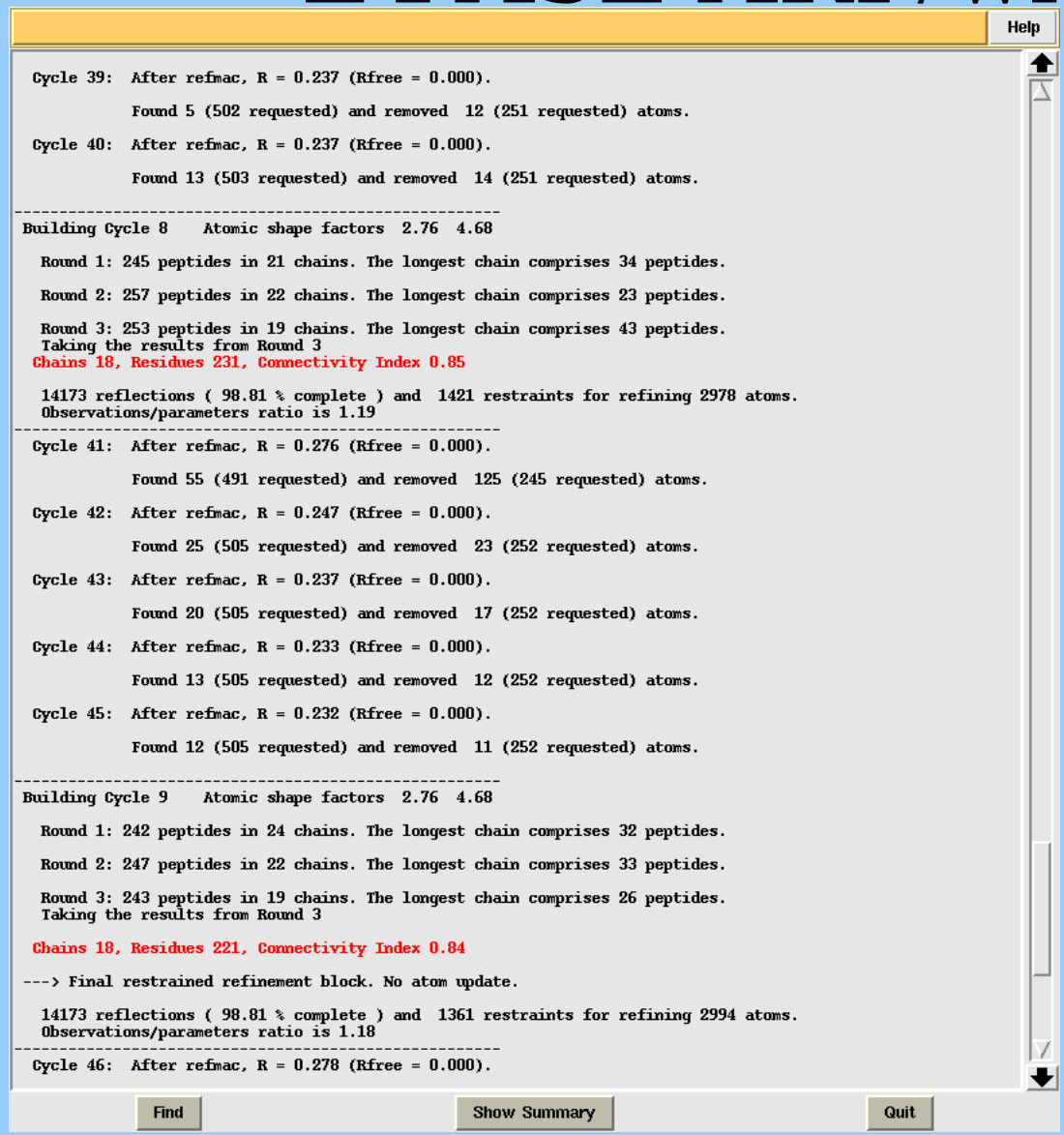
LYASE SHELXD



LYASE SHELXE



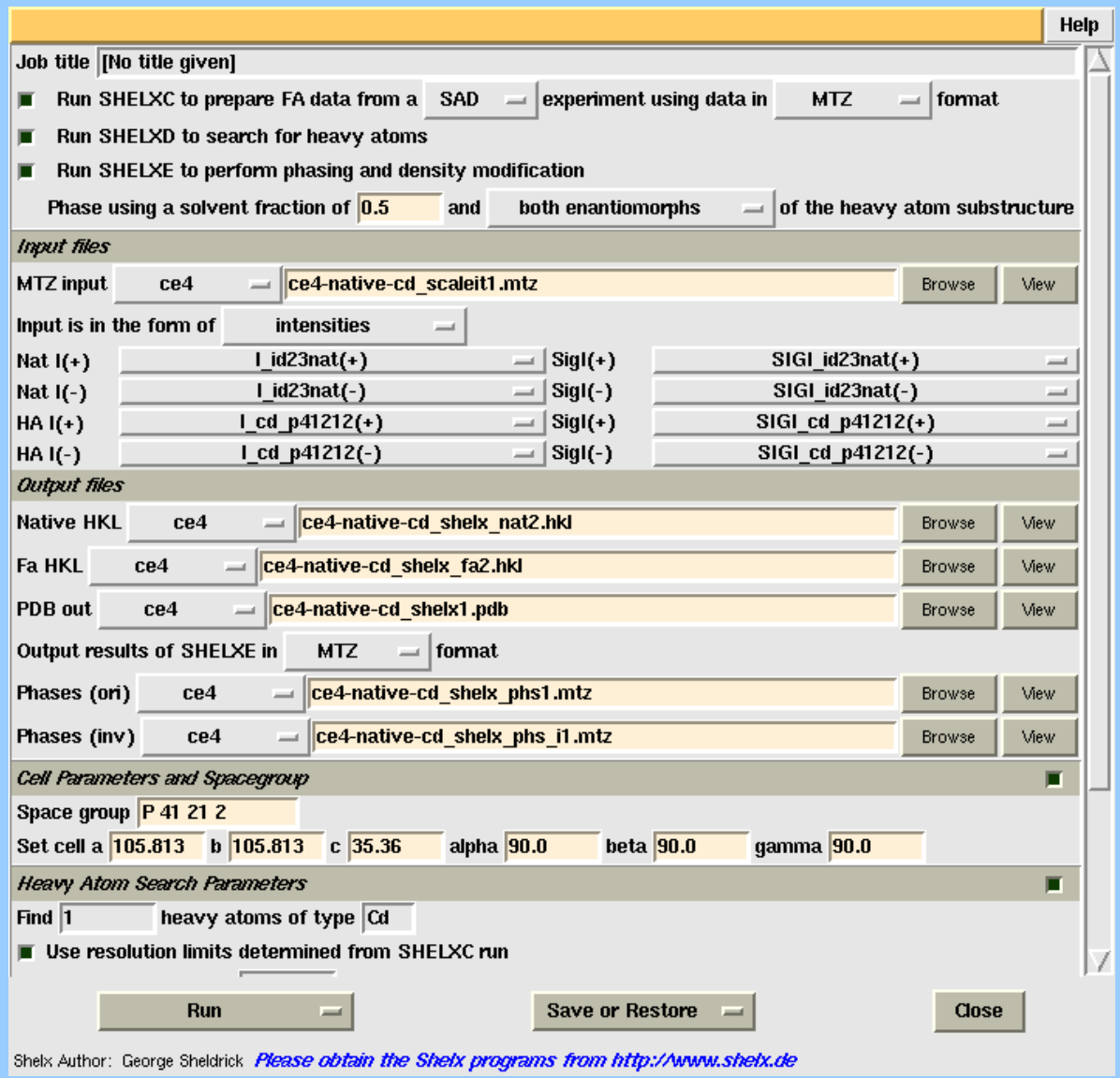
LYASE ARP/wARP



Example 2 Two esterases

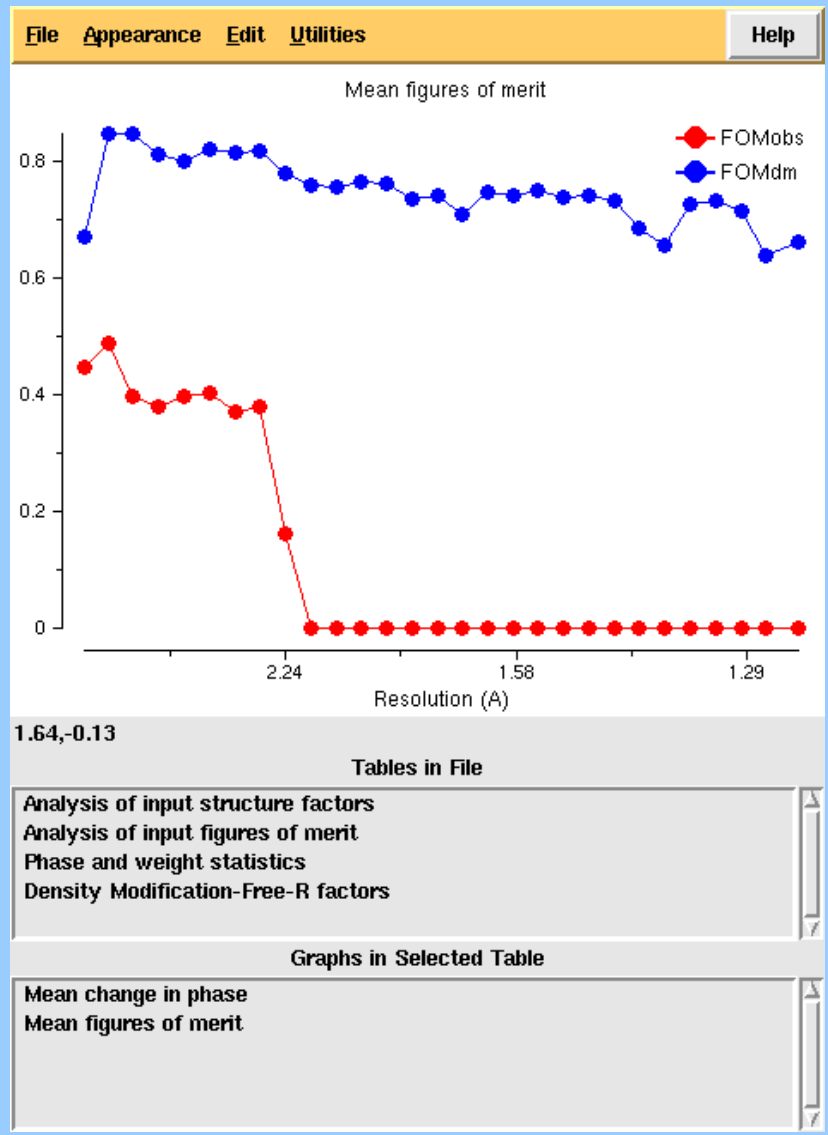
- CE4 one crystal form ($P4_12_12$ / $P4_32_12$)
- Cd SIRAS
- SHELXD, MLPHARE, DM, ARP/WARP, REFMAC
- AXA with 2 crystal forms ($P2_1$ / $P2_12_12_1$)
- Molecular Replacement

CE4 SHELX C/D/E



CE4 Phasing & Phase Improvement

- MLPhare with site from SHELXD
- DM



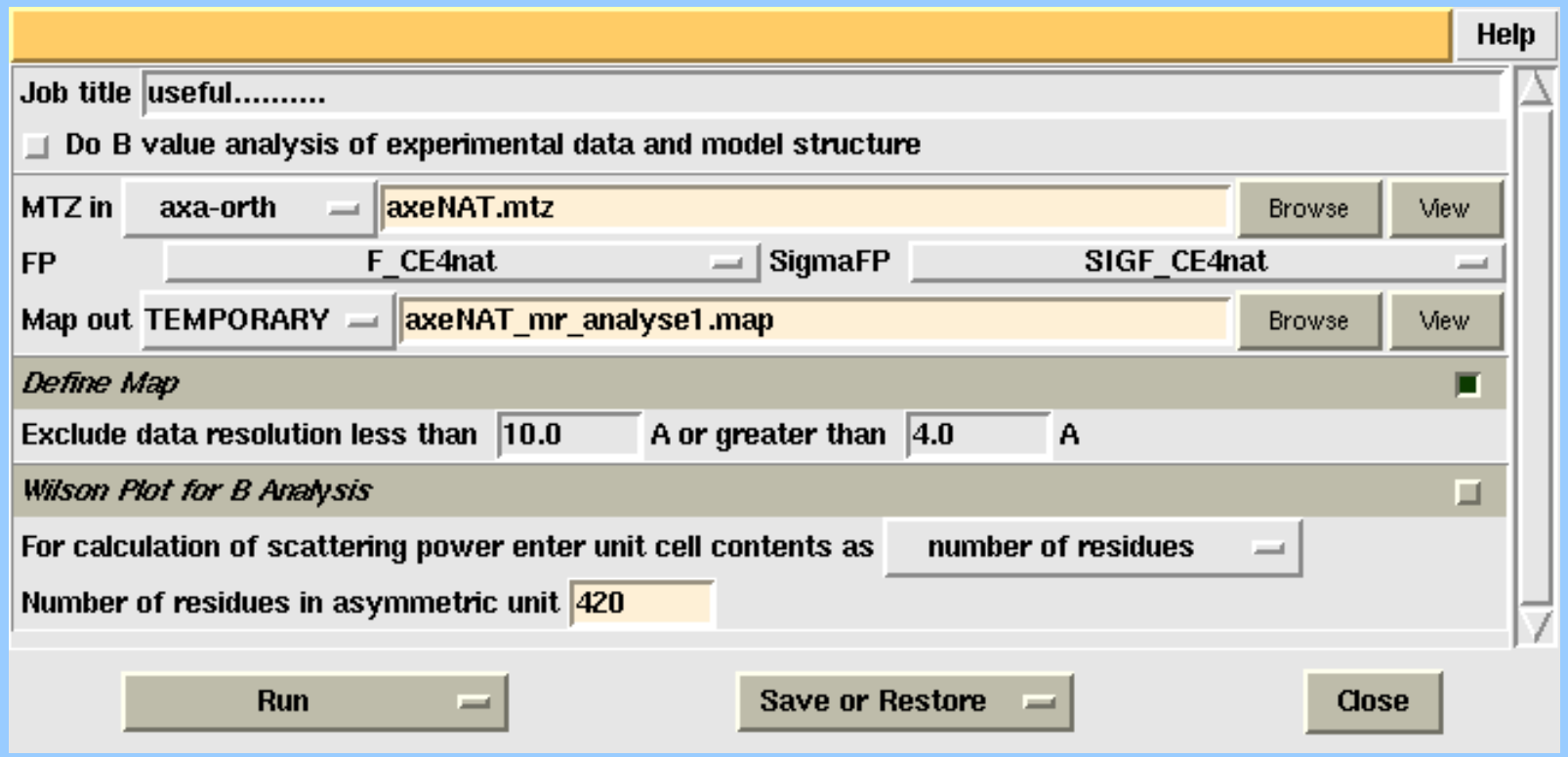
AXA $P2_1$ AMoRe Rotation function

Help

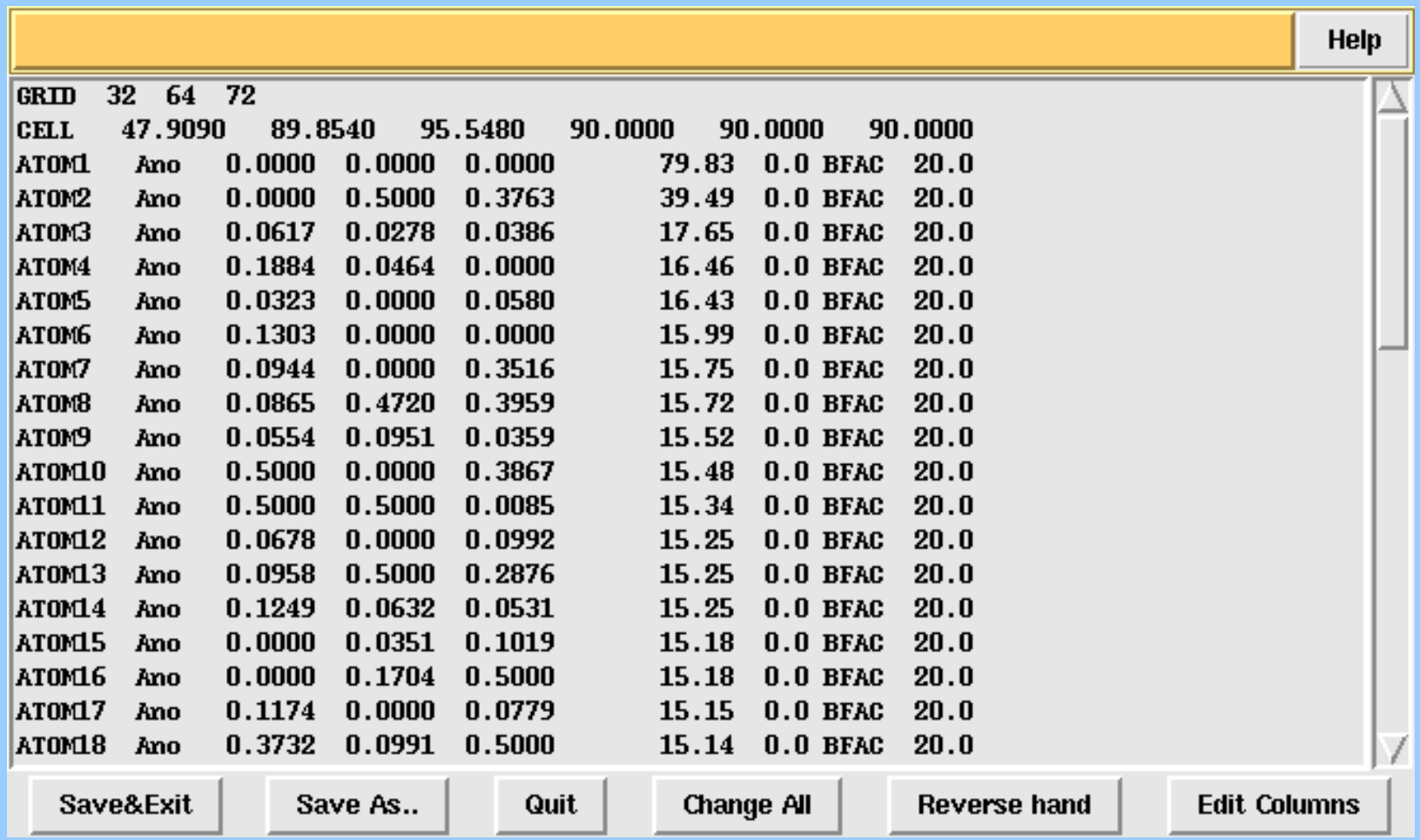
```
#CCP4I VERSION CCP4Interface 1.3.20
#CCP4I SCRIPT MR tran ce4model
#CCP4I DATE 24 Mar 2005  22:15:41
#CCP4I USER jpt
#CCP4I PROJECT axa
#CCP4I JOB_ID 17
#CCP4I SYMMETRY P21
#CCP4I CELL 57.4200 47.9670 75.0210 90.0000 92.0170 90.0000
#CCP4I RESOLUTION 3.0 14.0
SOLUTIONTF1_3   1  269.74   82.79  302.05  0.0500  0.0000  0.3654 14.6 56.6 14.7   1   32.0
SOLUTIONTF1_1   1   97.68   90.00  225.00  0.1625  0.0000  0.4327 13.6 57.0 13.8   2   32.2
SOLUTIONTF1_2   1   82.38   90.00   45.28  0.4375  0.0000  0.2404 13.5 56.8 12.6  11   44.1
SOLUTIONTF1_4   1   83.02   88.02   46.50  0.3250  0.0000  0.2692 13.4 57.0 12.2  15   46.1
SOLUTIONTF1_5   1   96.51   90.00  226.27  0.1625  0.0000  0.4231 13.4 57.2 12.9   3   32.7
SOLUTIONTF1_12  1  302.48   30.09  285.33  0.0875  0.0000  0.3846 11.7 57.3 10.1   2   31.4
SOLUTIONTF1_6   1  103.57   78.79  207.31  0.4750  0.0000  0.2692 11.4 57.8  9.4   2   42.1
SOLUTIONTF1_9   1   25.41   85.88   49.84  0.1250  0.0000  0.2692 11.4 57.1  9.4  12   44.9
SOLUTIONTF1_15  1  268.73   65.78  293.62  0.3625  0.0000  0.3269 11.4 57.8 11.7   2   38.3
SOLUTIONTF1_7   1  261.64   77.10  290.20  0.4750  0.0000  0.2885 11.3 57.4 10.1   3   39.8
SOLUTIONTF1_25  1  104.00   46.67   81.90  0.0750  0.0000  0.1827 11.3 57.3  8.8   1   37.2
SOLUTIONTF1_16  1   25.73   85.77   51.15  0.2125  0.0000  0.4327 11.2 57.0  9.7   3   35.9
SOLUTIONTF1_13  1  268.93   90.00  120.60  0.1250  0.0000  0.3942 11.1 57.4  9.8  11   32.4
SOLUTIONTF1_14  1  311.45   54.36  135.69  0.0500  0.0000  0.4135 11.1 57.4  9.6  12   28.0
SOLUTIONTF1_18  1  302.49   30.47  287.14  0.0875  0.0000  0.3846 11.1 57.4  9.8   1   31.4
SOLUTIONTF1_8   1  260.51   77.02  289.00  0.1625  0.0000  0.0865 10.9 57.5  9.7   2   32.8
SOLUTIONTF1_10  1  104.10   77.73  205.29  0.1500  0.0000  0.2500 10.9 57.6  9.3   4   48.2
SOLUTIONTF1_11  1  309.86   54.27  136.76  0.0500  0.0000  0.4135 10.9 57.2  9.5  13   28.0
SOLUTIONTF1_17  1   72.68   90.00   24.00  0.2500  0.0000  0.0192 10.9 57.4 10.5   1   37.6
SOLUTIONTF1_26  1  246.00   15.04  266.50  0.4250  0.0000  0.4519 10.8 57.4  8.6  12   26.4
SOLUTIONTF1_22  1  249.00   13.50  263.50  0.4000  0.0000  0.1154 10.7 57.8  8.6  20   32.0
SOLUTIONTF1_33  1   19.09   85.81  273.08  0.3125  0.0000  0.0000 10.6 57.6  8.3   4   32.2
SOLUTIONTF1_24  1  119.42   21.79  330.80  0.3000  0.0000  0.4135 10.5 57.8  8.4   3   35.4
SOLUTIONTF1_21  1    9.85   54.79  226.31  0.2250  0.0000  0.0096 10.4 57.4  9.7   5   35.2
```

Save&Exit | Save As.. | Quit | Change All

AXA $P2_12_12_1$ Analyse data



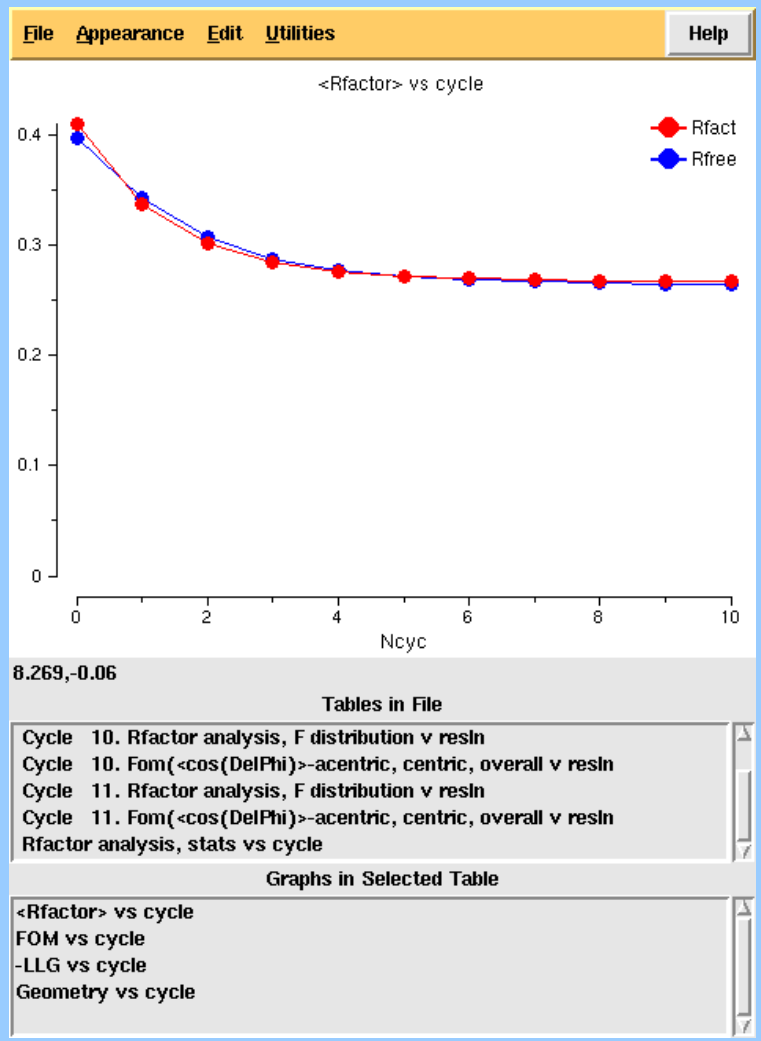
AXA $P2_12_12_1$ Analyse data Results



AXA $P2_12_12_1$ Solution

MOLREP, two molecules

Initial refinement REFMAC



Acknowledgements

- Eleanor Dodson
- Keith Wilson
- Gideon Davies
- Ed Taylor
- Sam Hart

- Everyone else in YSBL