

# CCP4 from a user perspective

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04/07/2005

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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

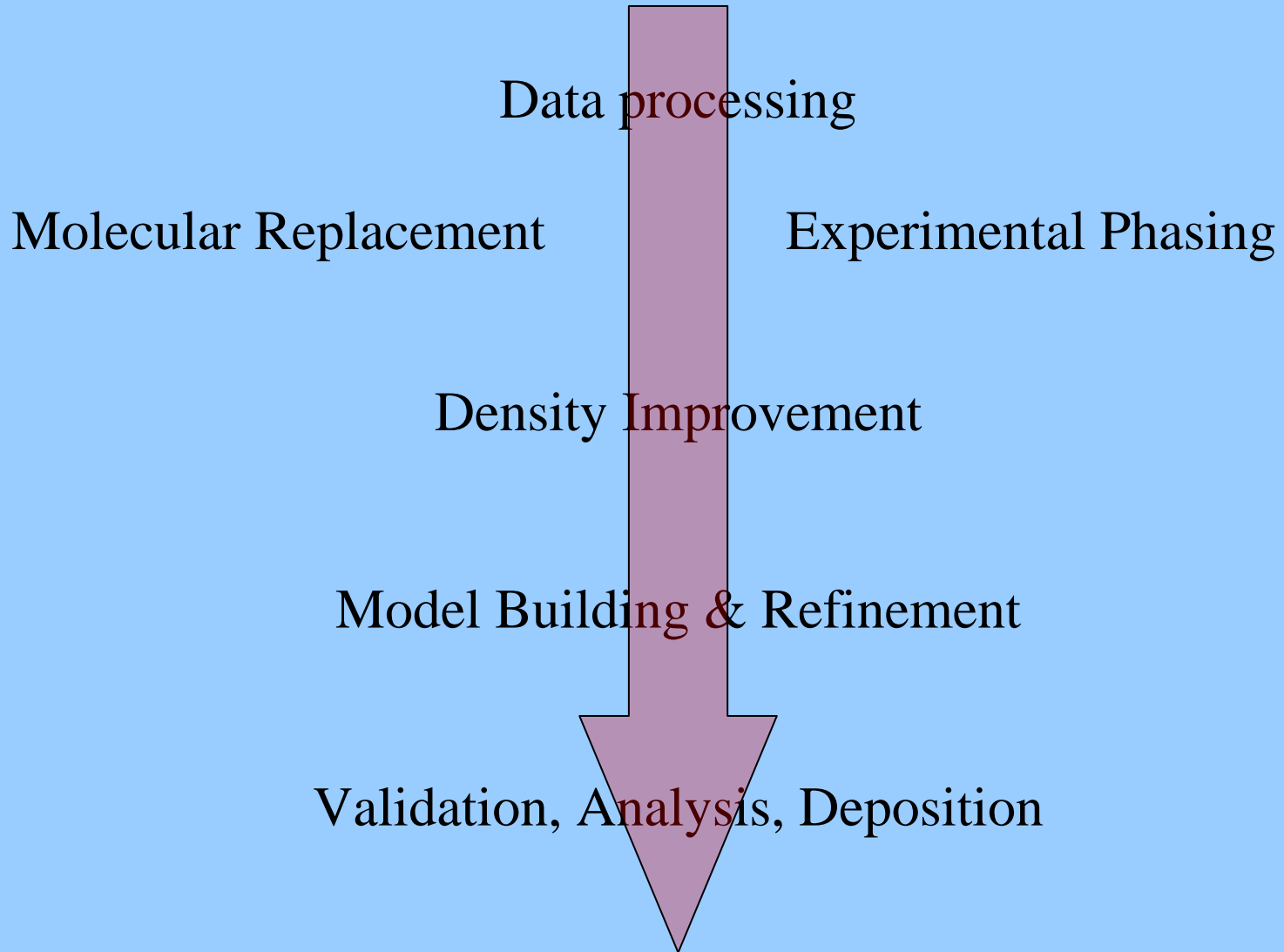
- Members from all over the world
- Fast, expert help from colleagues
- Useful tips
- Non-CCP4 topics
- Heated (entertaining) discussions



# CCP4 Program Suite

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

# Overview



# Interface

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

## 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&amp;ProjectDir

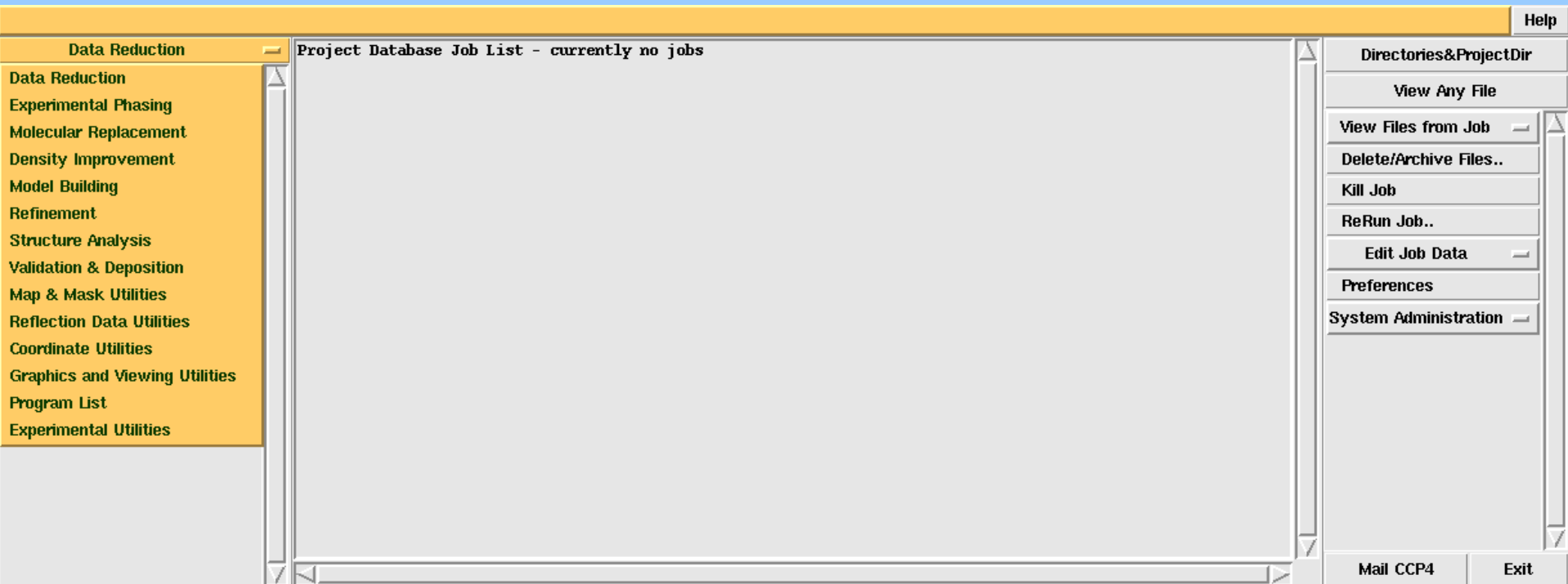
View Any File

- View Files from Job
- Delete/Archive Files..
- Kill Job
- ReRun Job..
- Edit Job Data
- Preferences
- System Administration

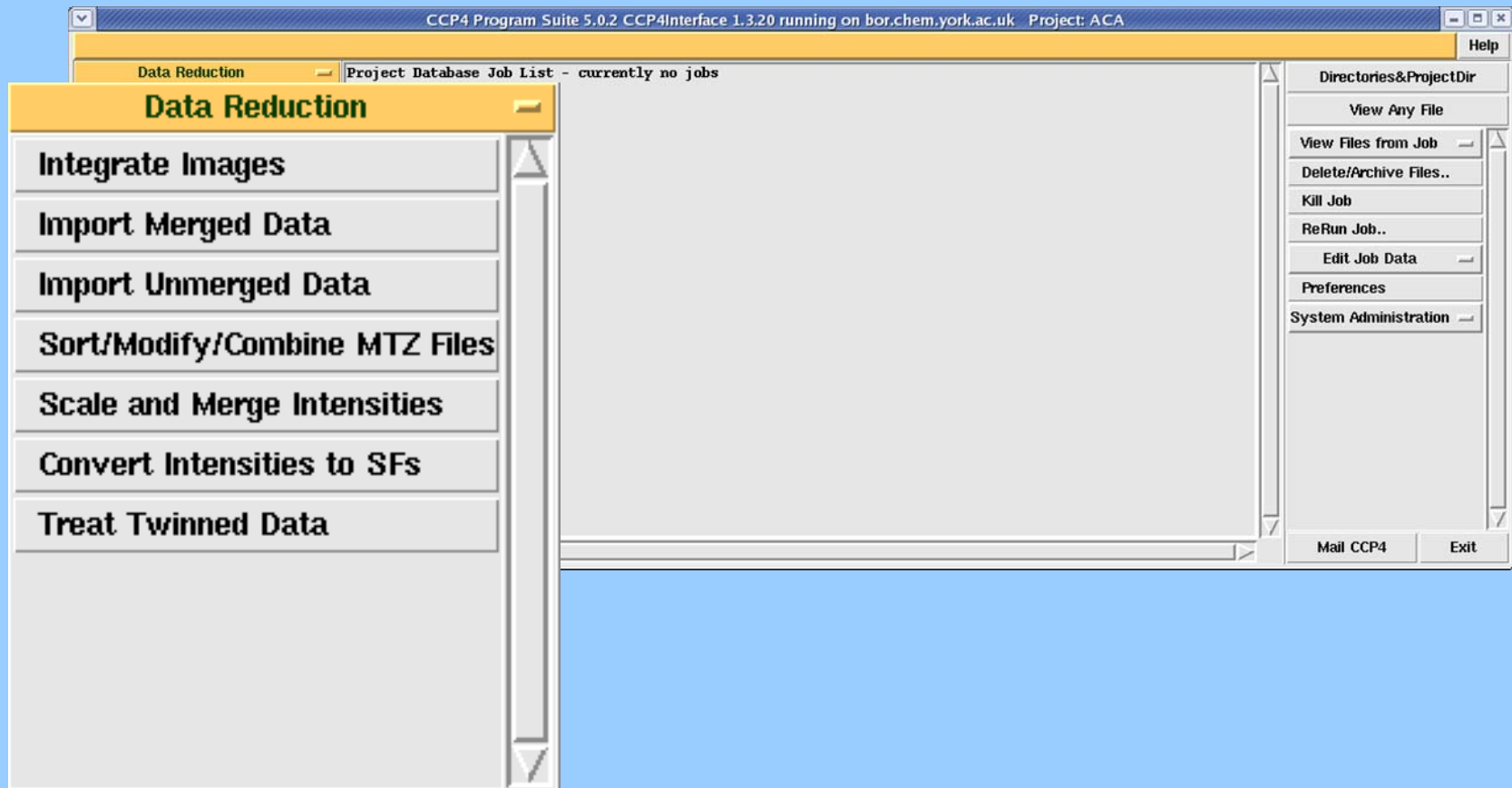
Mail CCP4

Exit

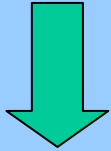
# Modules



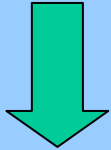
# Data Reduction



MOSFLM

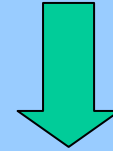


SCALA

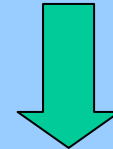


TRUNCATE

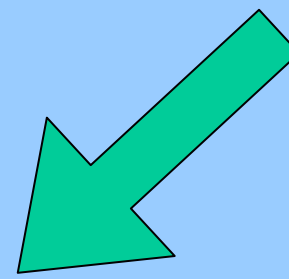
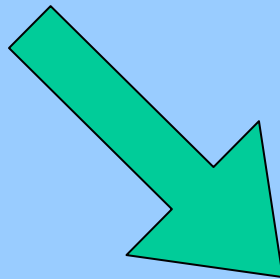
DENZO



SCALEPACK

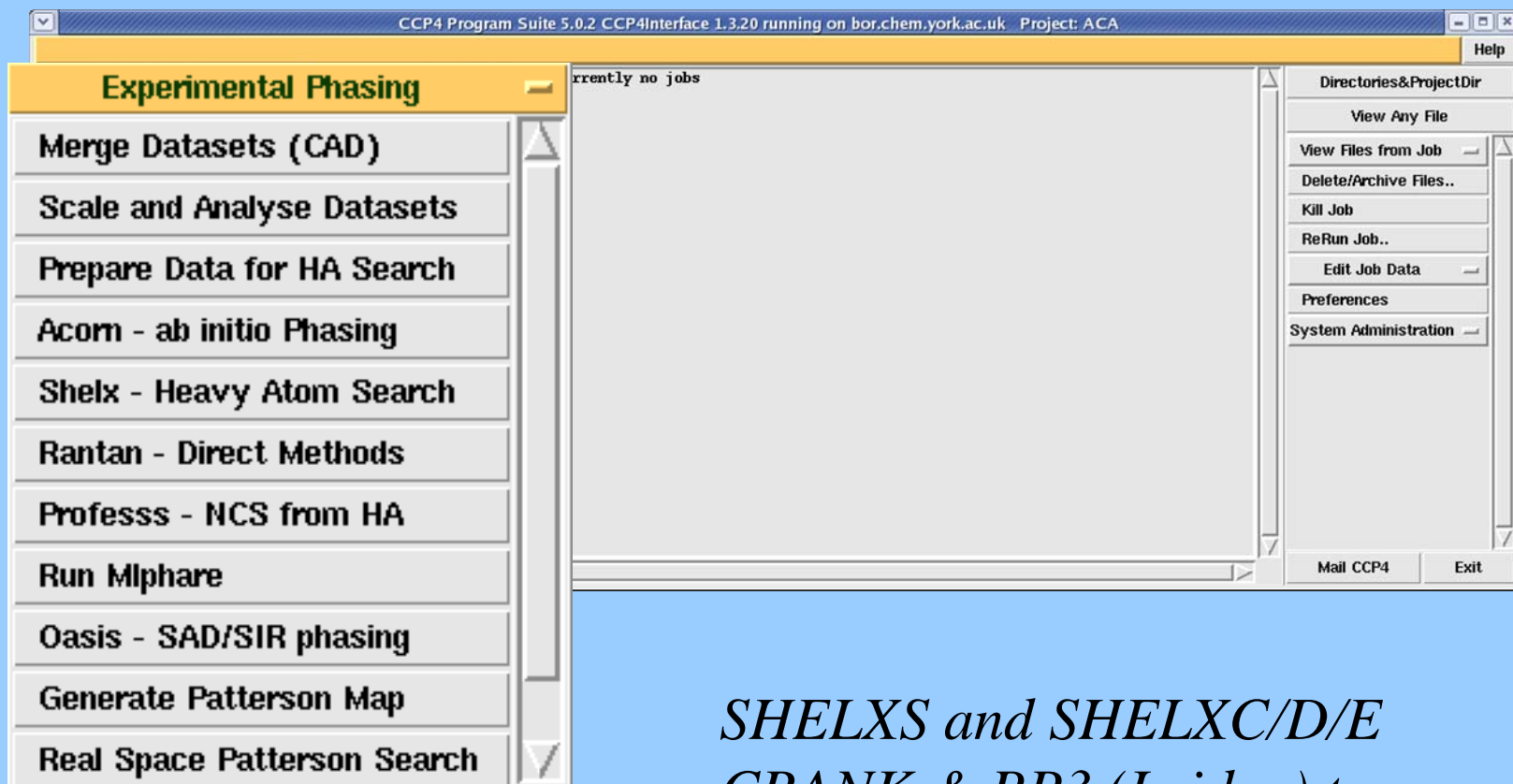


TRUNCATE



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 1.0Å on Se form at  $\lambda = 0.87\text{\AA}$  (SRS)
- Patterson shows Se very clearly
- ACORN gave excellent map in 18 min on SGI

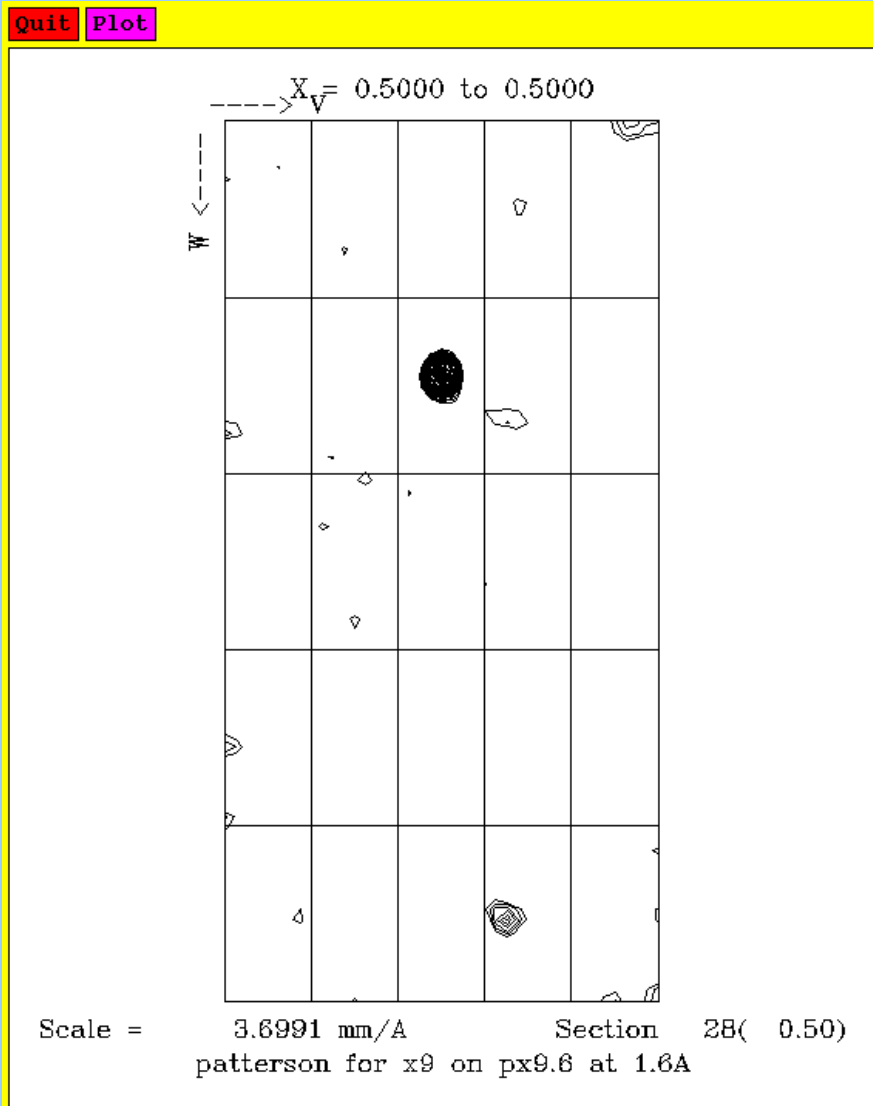
**Ab initio structure determination and functional characterization of CBM36: A new family of calcium-dependent carbohydrate binding modules**

Jamal-Talabani S, Boraston AB, Turkenburg JP, Tarbouriech N, **Ducros VMA**, Davies GJ

**STRUCTURE**

12 (7): 1177-1187 JUL 2004

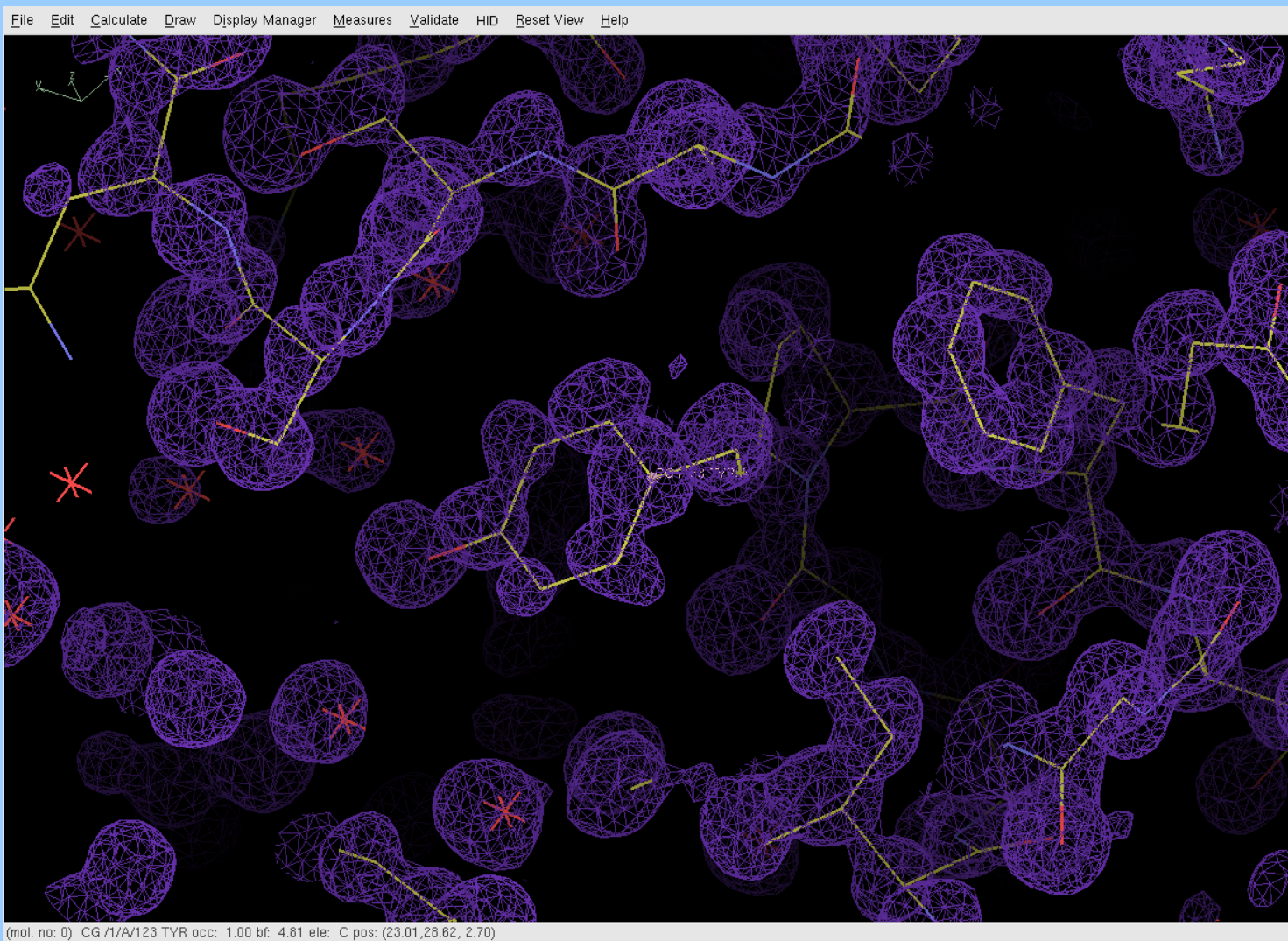
# Patterson



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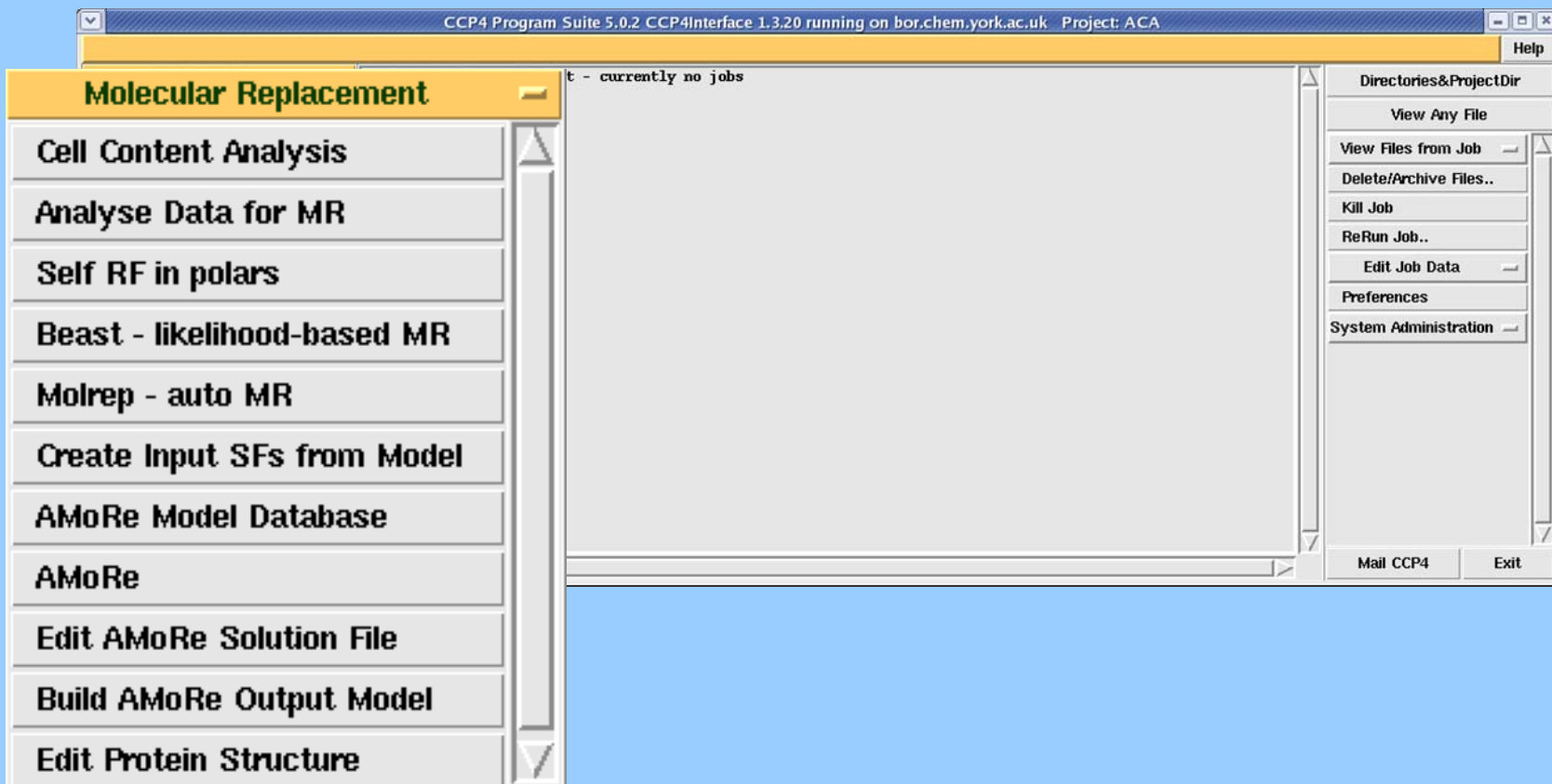
# CBM ACORN map & final model



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# Molecular Replacement



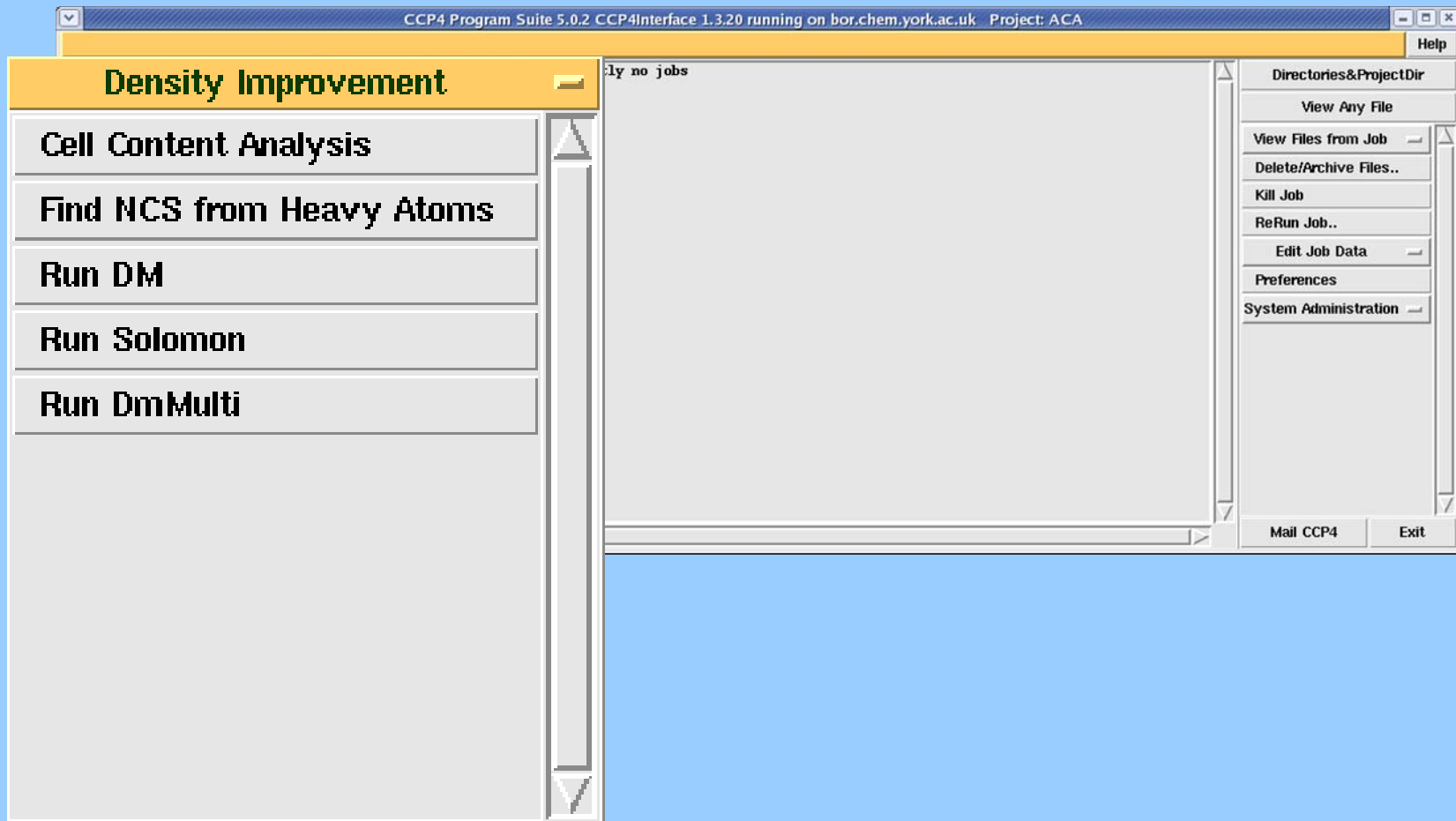
# MR programs

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

# MR Utilities



# Density Improvement

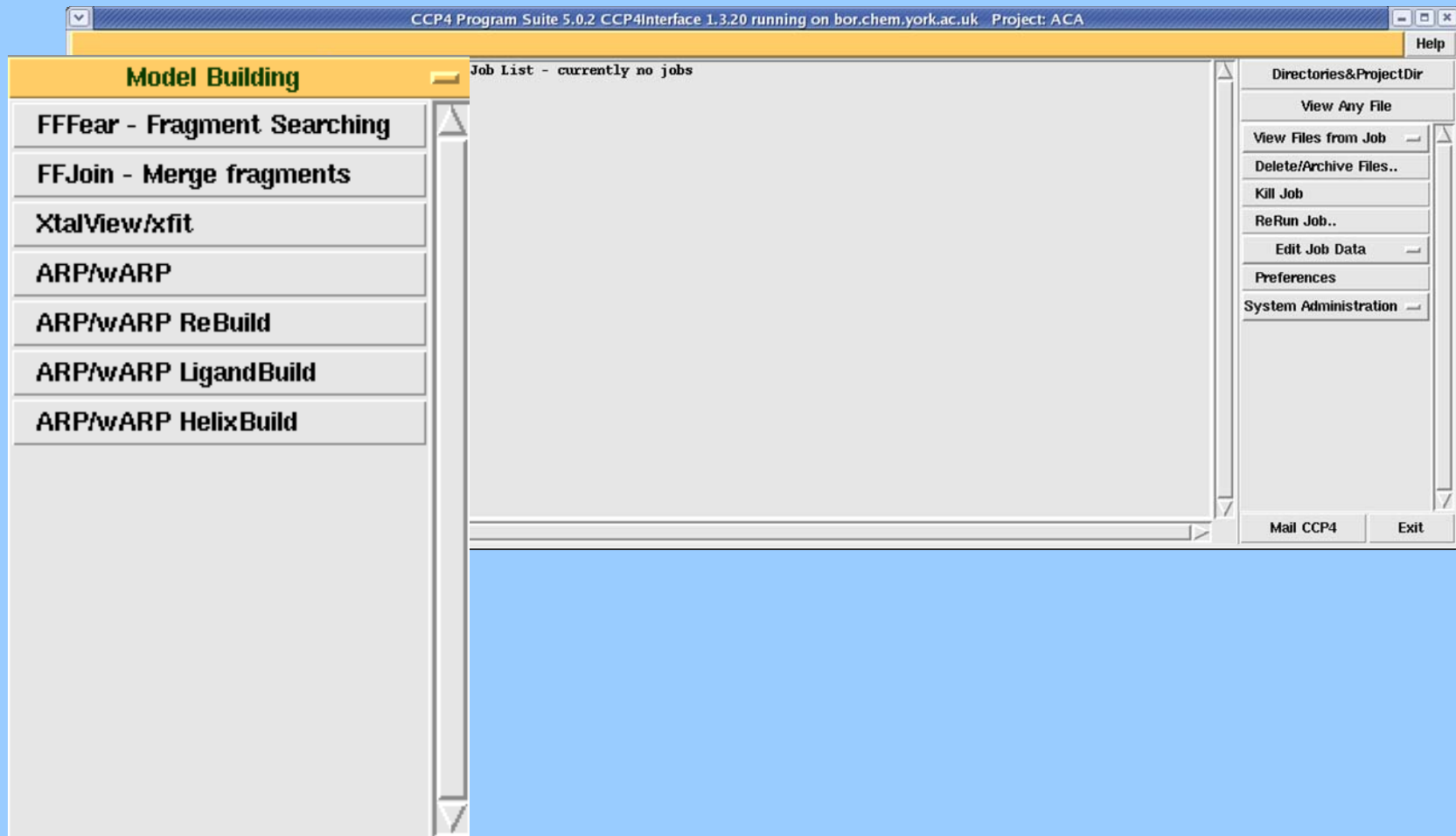


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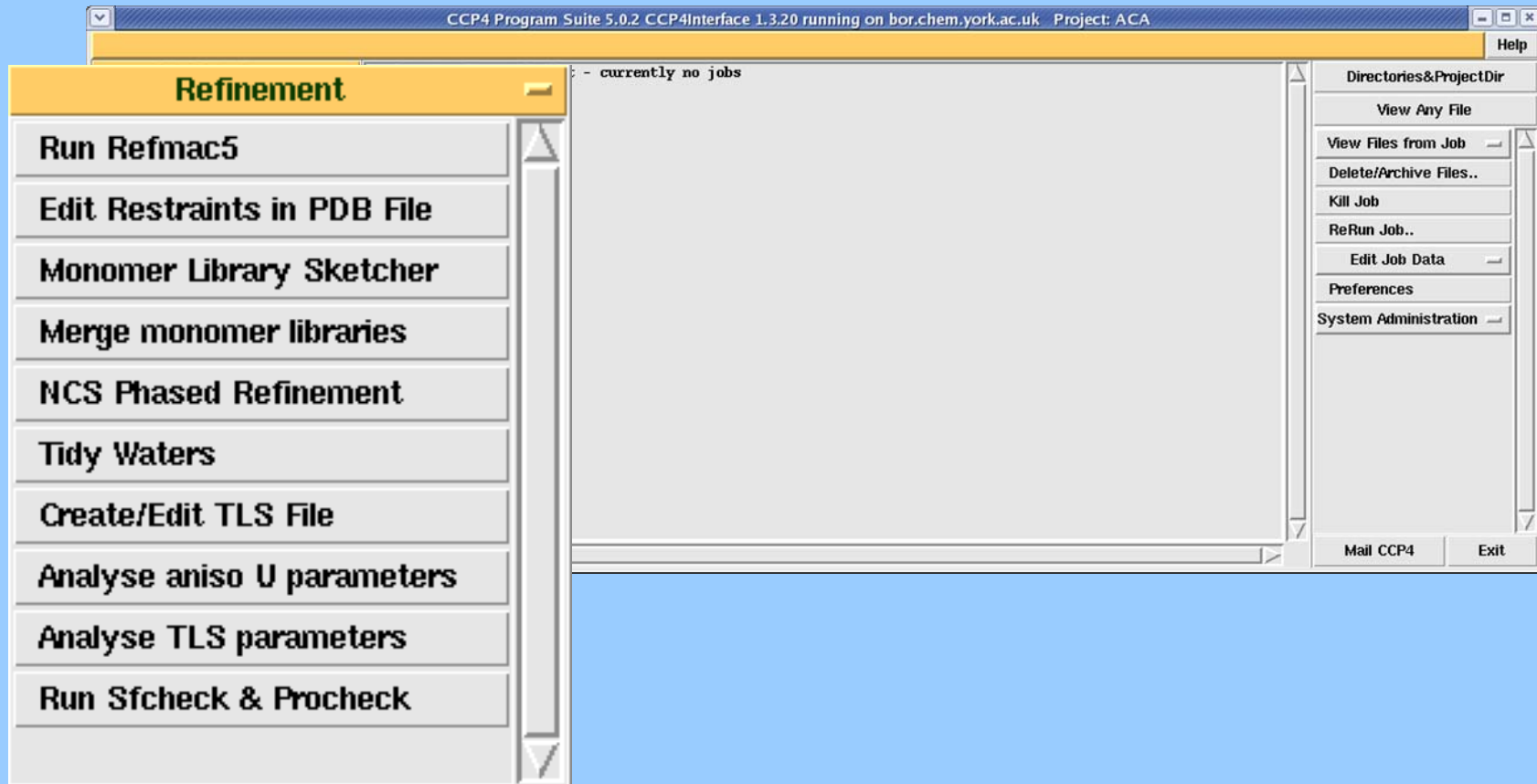
# Model Building



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# Refinement



# REFMAC

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

# Monomer library sketcher

File Edit Help

MOUSE BUTTONS Left:rotate Right:drag Control-left:zoom Control-right:Select active atom  
Shift-left:Click on atom to bond to active atom Shift-right:Click bond to change bond type

Do nothing

Undo last edit

Recentre View

Mouse mode

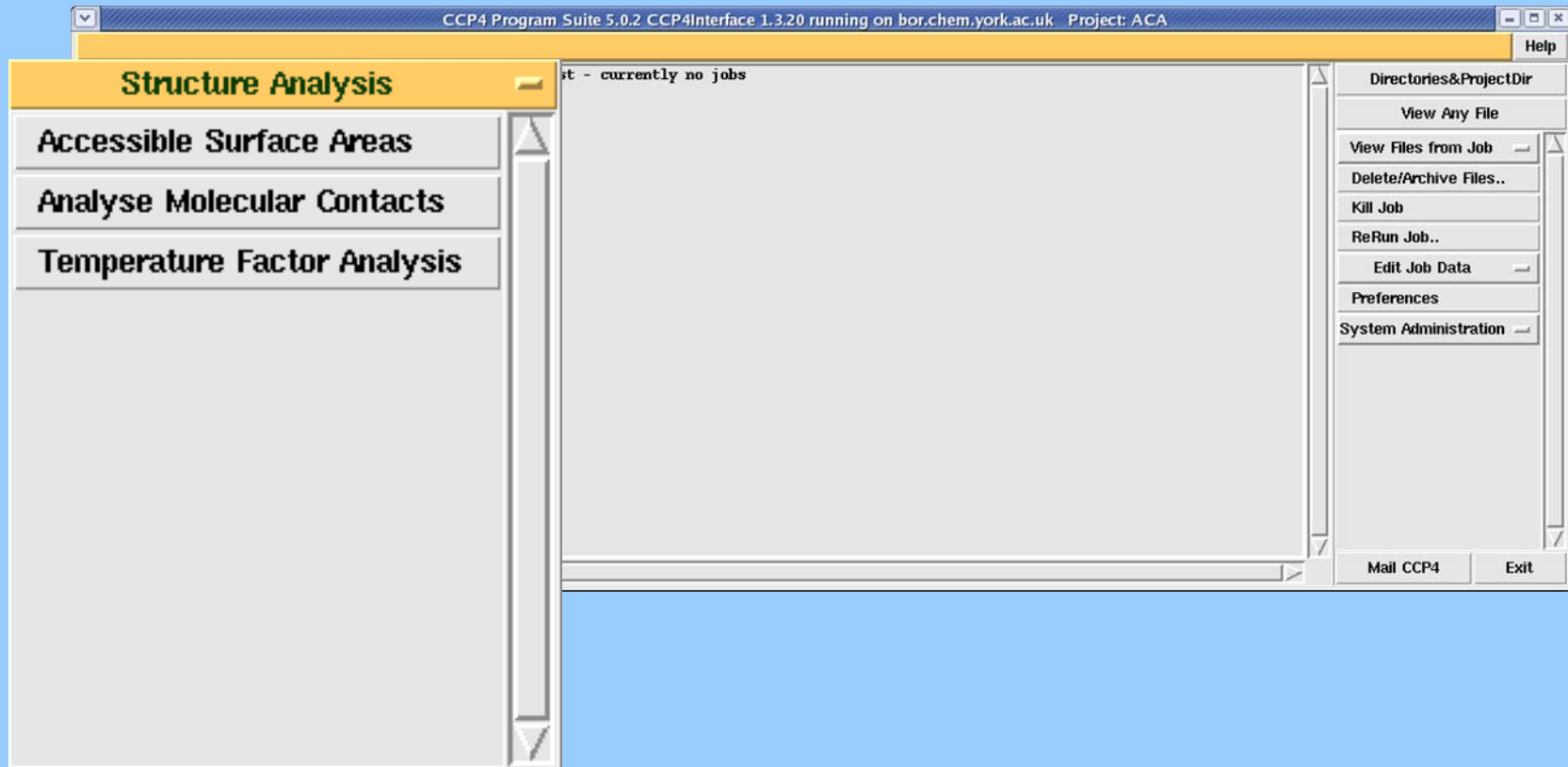
- ◆ Edit Monomer
- ▼ Move Fragment

Element	Name	Ox
O	O2B	0
P	PB	0
O	O1B	0
O	O3B	0
C	C1'	0
O	O5'	0
C	C5'	0
C	C6'	0
O	O6'	0
C	C4'	0
O	O4'	0
C	C3'	0
O	O3'	0

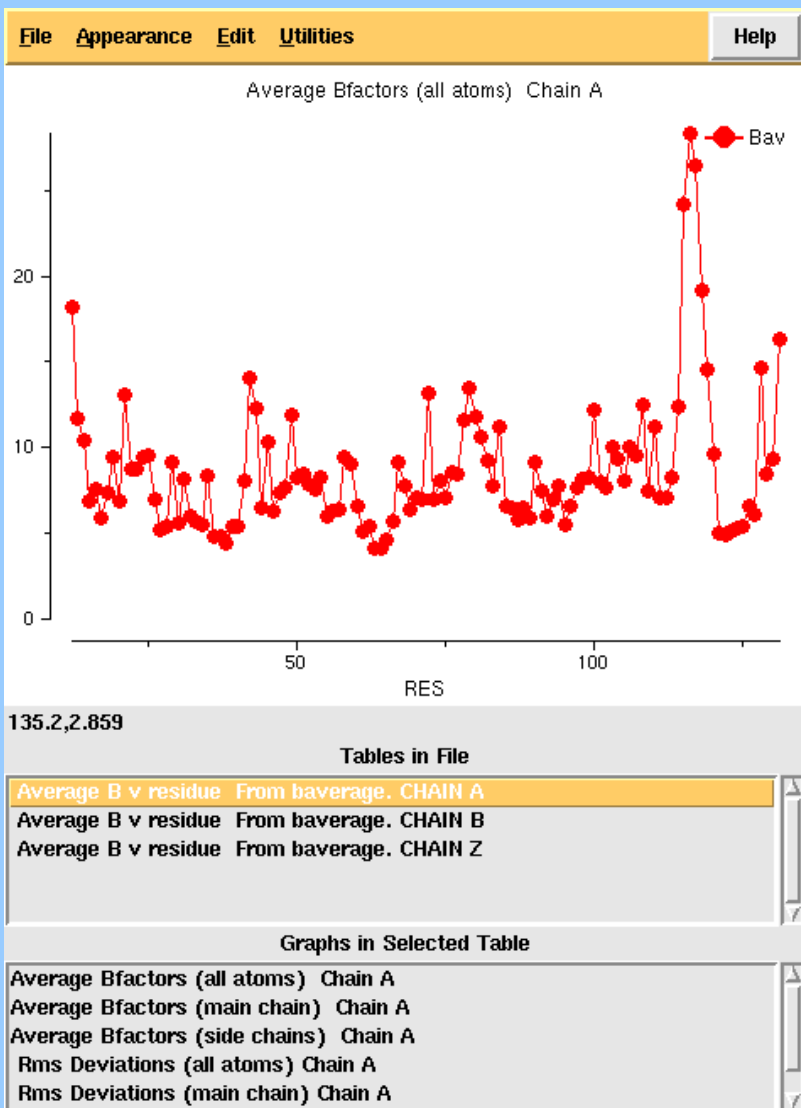
Centre	Sign	B/3	F/4	1/5	2/6
1	C1*	both	N1	C2*	O4*
2	C2*	both	C1*	O2*	C3*
3	C3*	both	C2*	C4*	O3*
4	C4*	both	C3*	O4*	C5*
5	C1'	both	O3B	C2'	O5'
6	C2'	both	C1'	C3'	O2'
7	C3'	both	C2'	C4'	O3'
8	C4'	both	C3'	C5'	O4'
9	C5'	both	C4'	C6'	O5'

Edit Table Add Row

# Structure Analysis



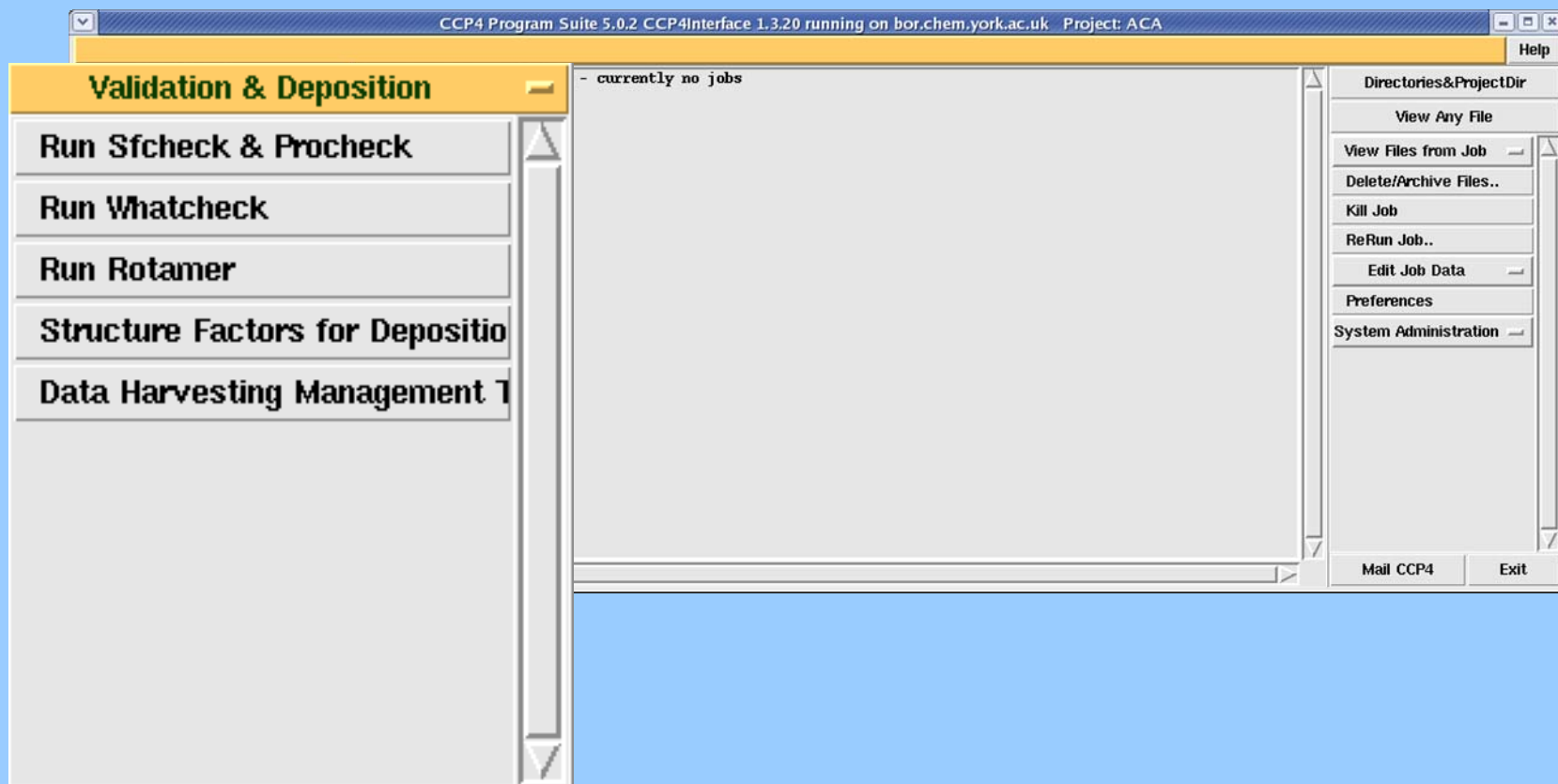
# Temperature factor analysis



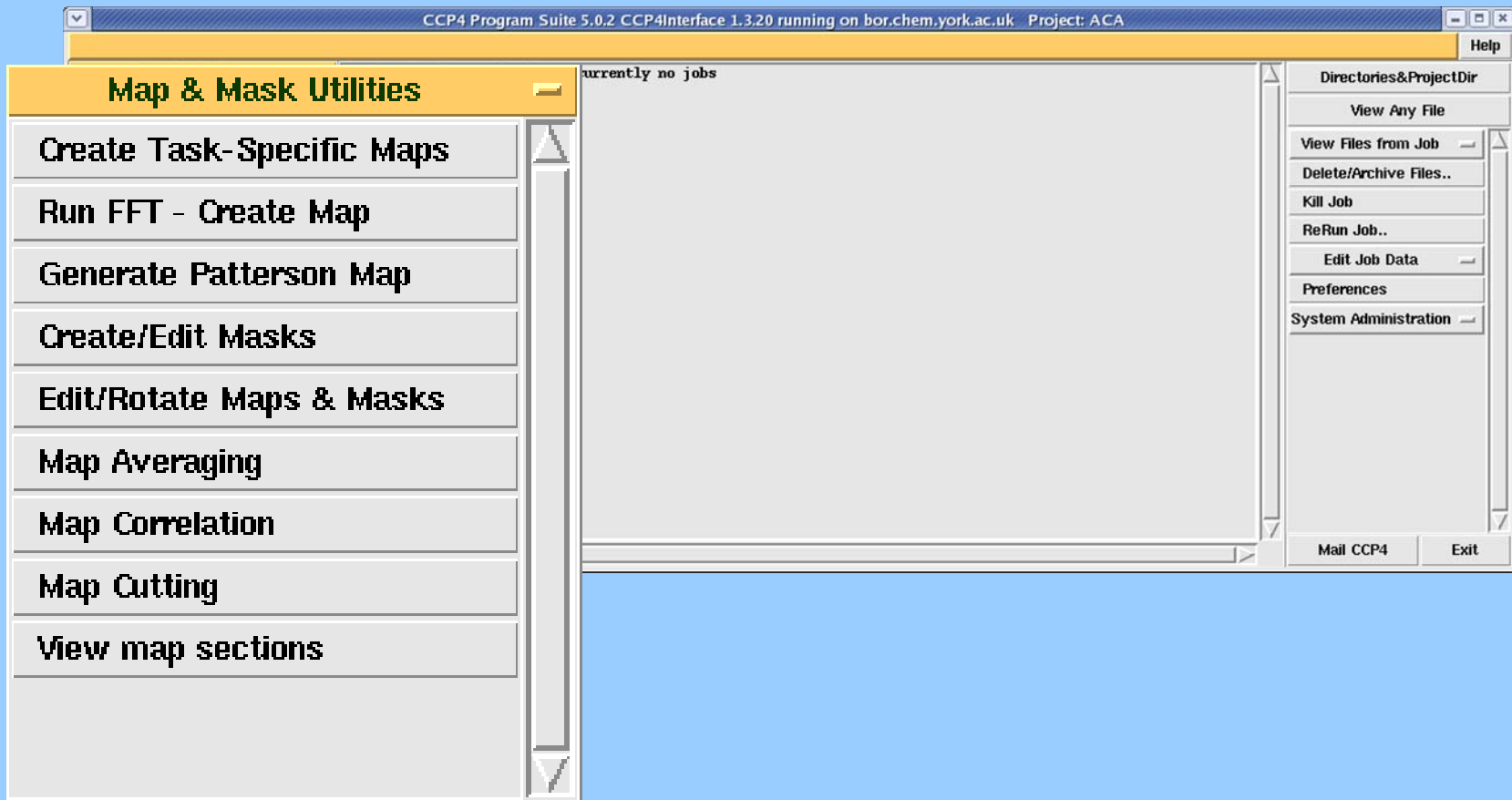
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# Validation & Deposition

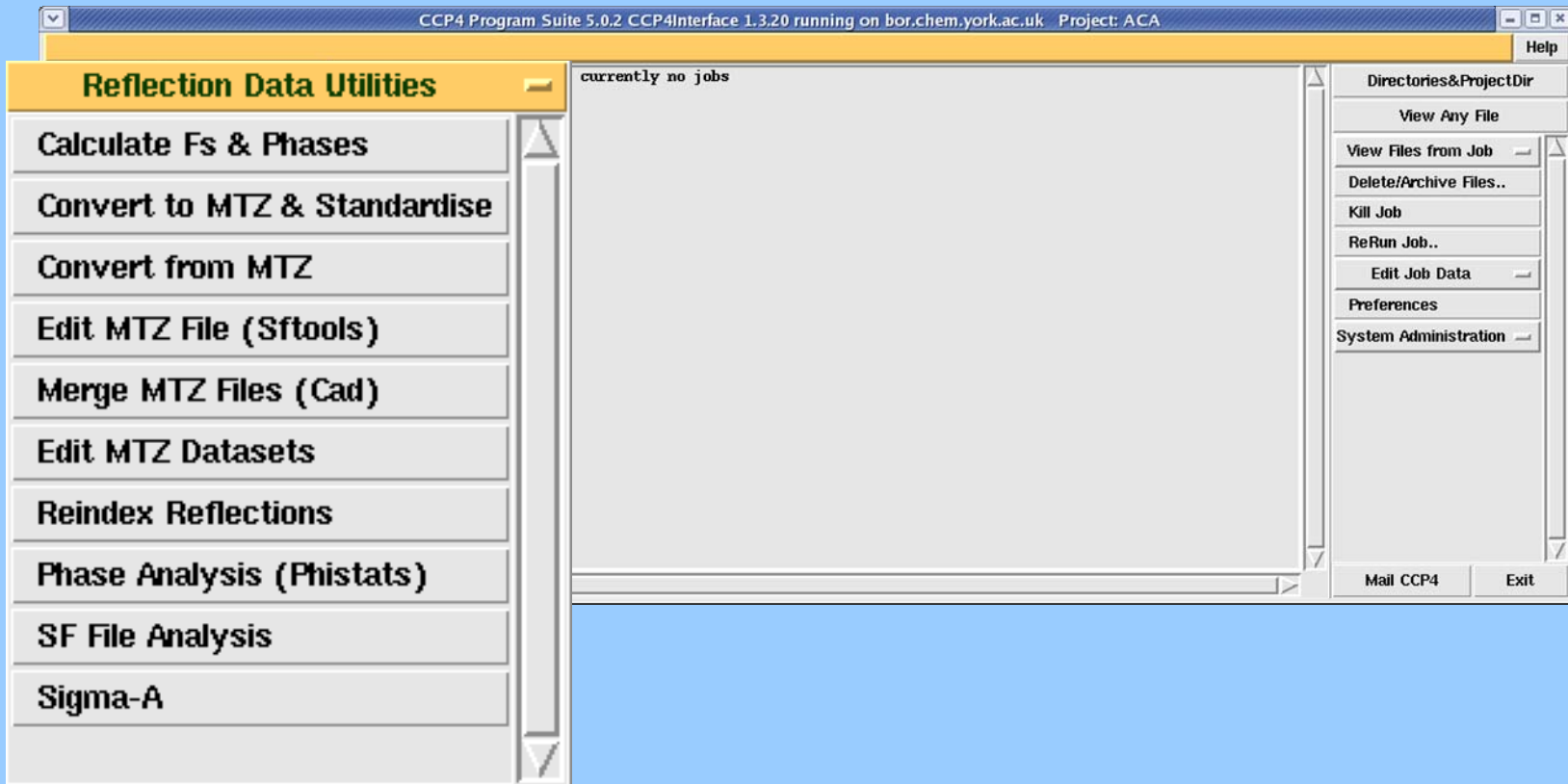


# Map & Mask Utilities





# Reflection Data Utilities



# Convert from MTZ

Select file format (OUTPUT) Help

Job title

Convert MTZ to **CIF** format

MTZ in	x9	CIF	<input type="text"/>	Browse	View
HKL out	x9	XPLOR	<input type="text"/>	Browse	View
		CNS	<input type="text"/>		
<i>MTZ File Labels</i>		MULTAN			<input checked="" type="checkbox"/>
FP		SHELX	<input type="text"/>	Sigma	<input type="text"/>
FC		TNT	<input type="text"/>	FOM	<input type="text"/>
DP		MAIN	<input type="text"/>	SIGDP	<input type="text"/>
I(+)		SCALEPACK	<input type="text"/>	SIGI(+)	<input type="text"/>
I(-)		USER	<input type="text"/>	SIGI(-)	<input type="text"/>
PHIC			<input type="text"/>	Weight	<input type="text"/>
FreeR			<input type="text"/>		

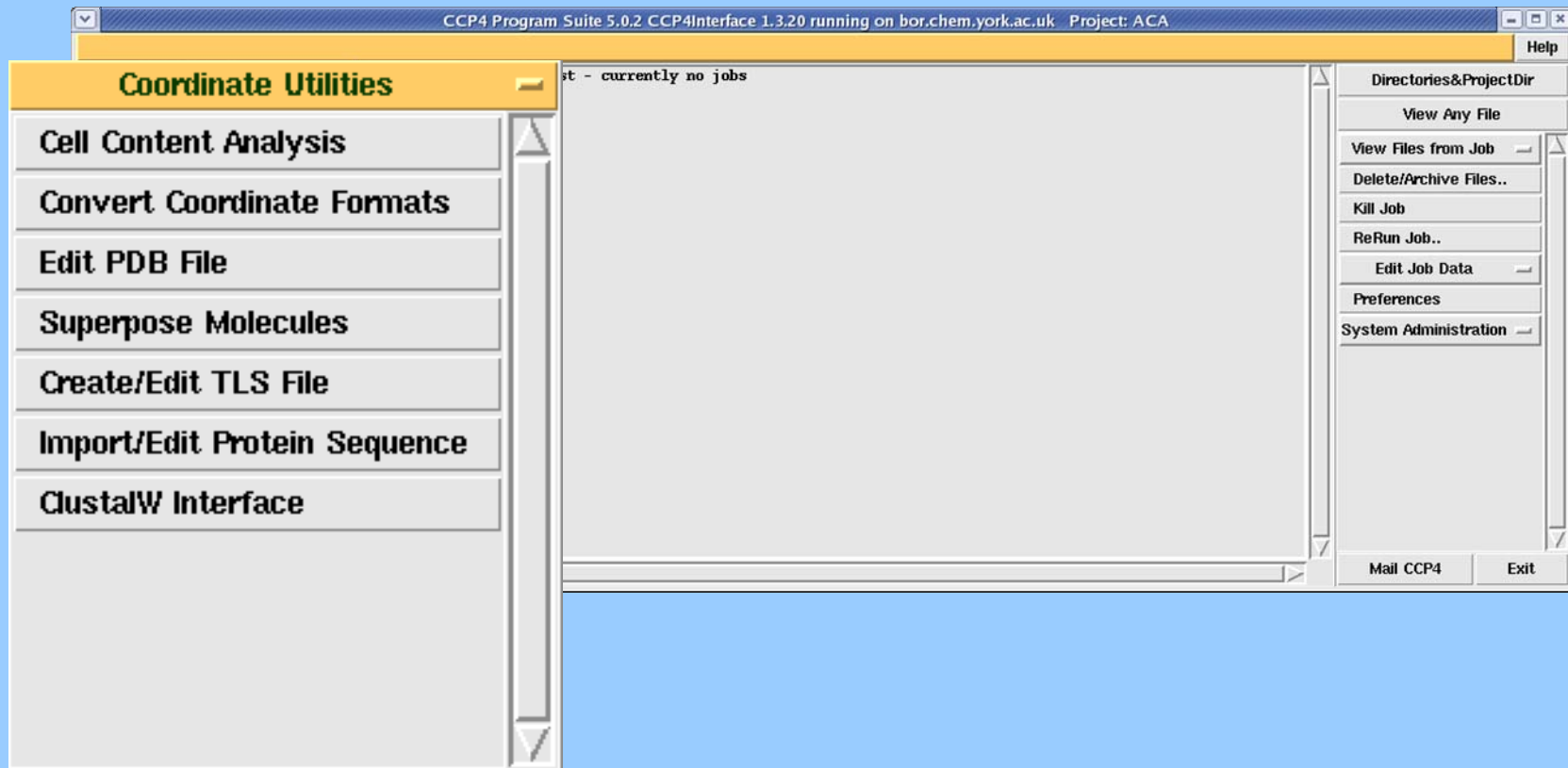
*CIF Format Details*

CIF file data block name

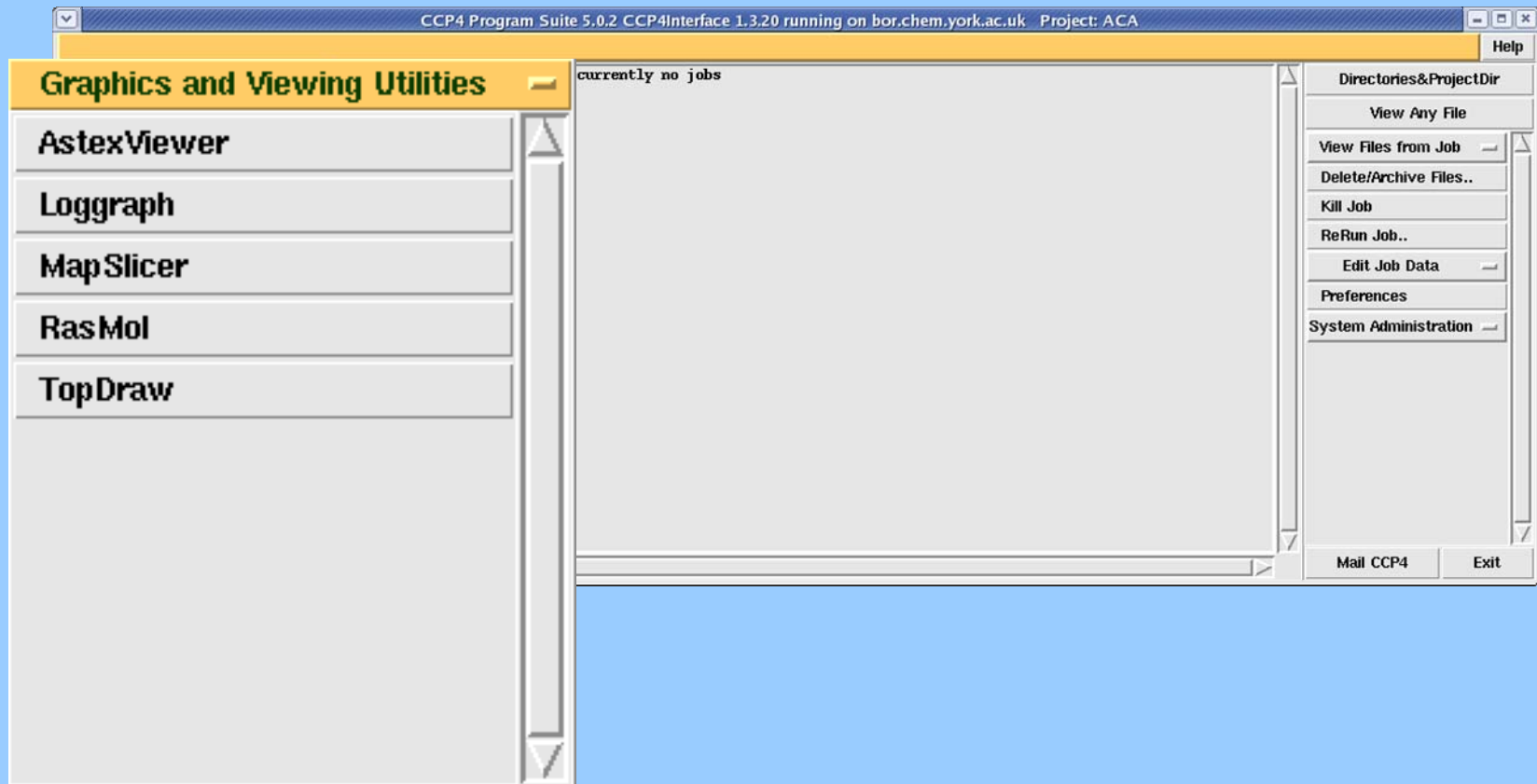
*Exclude Reflections*

*Infrequently Used Options*

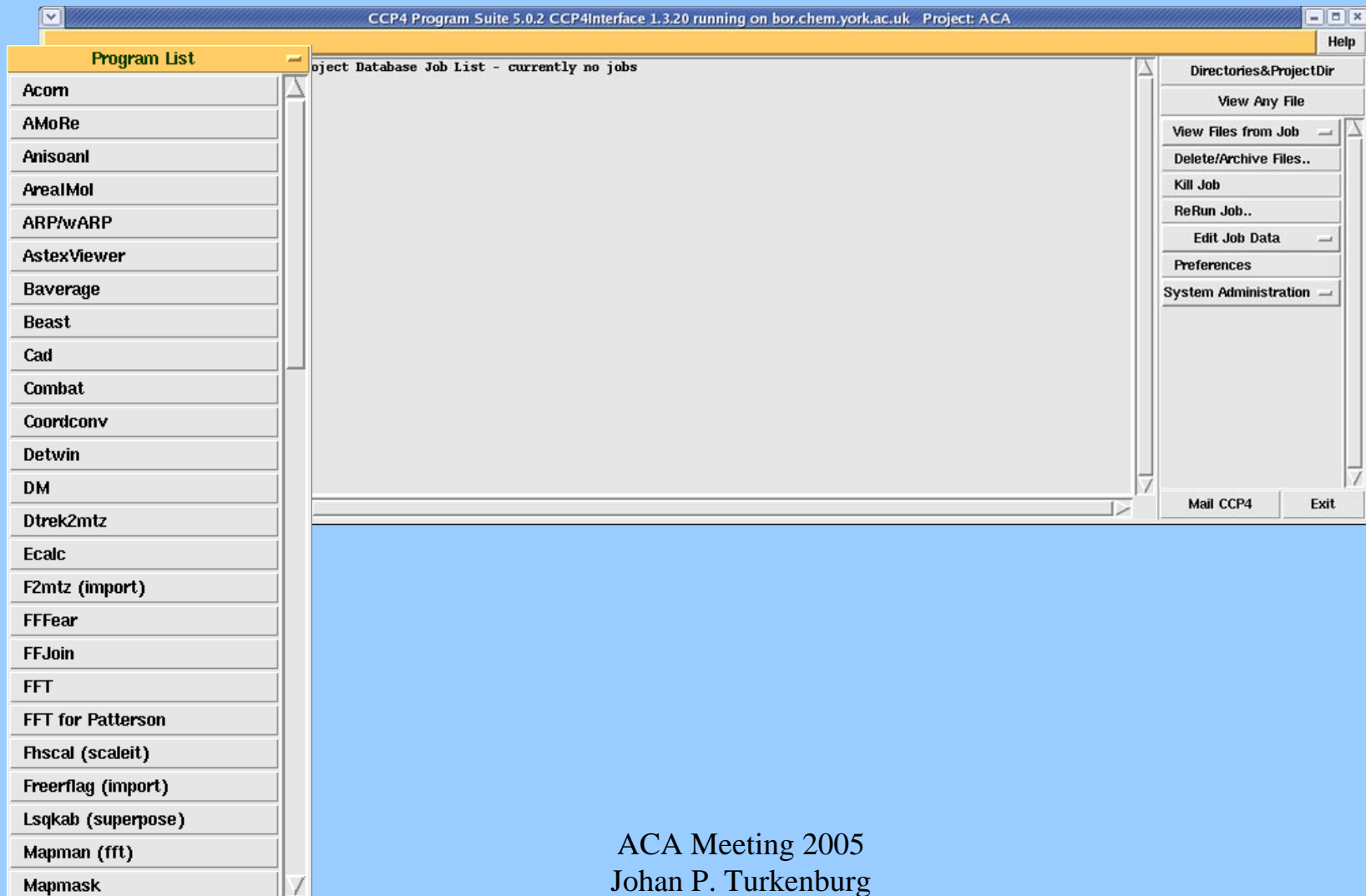
# Coordinate Utilities



# Graphics & Viewing Utilities



# Program List



# 'External' Programs

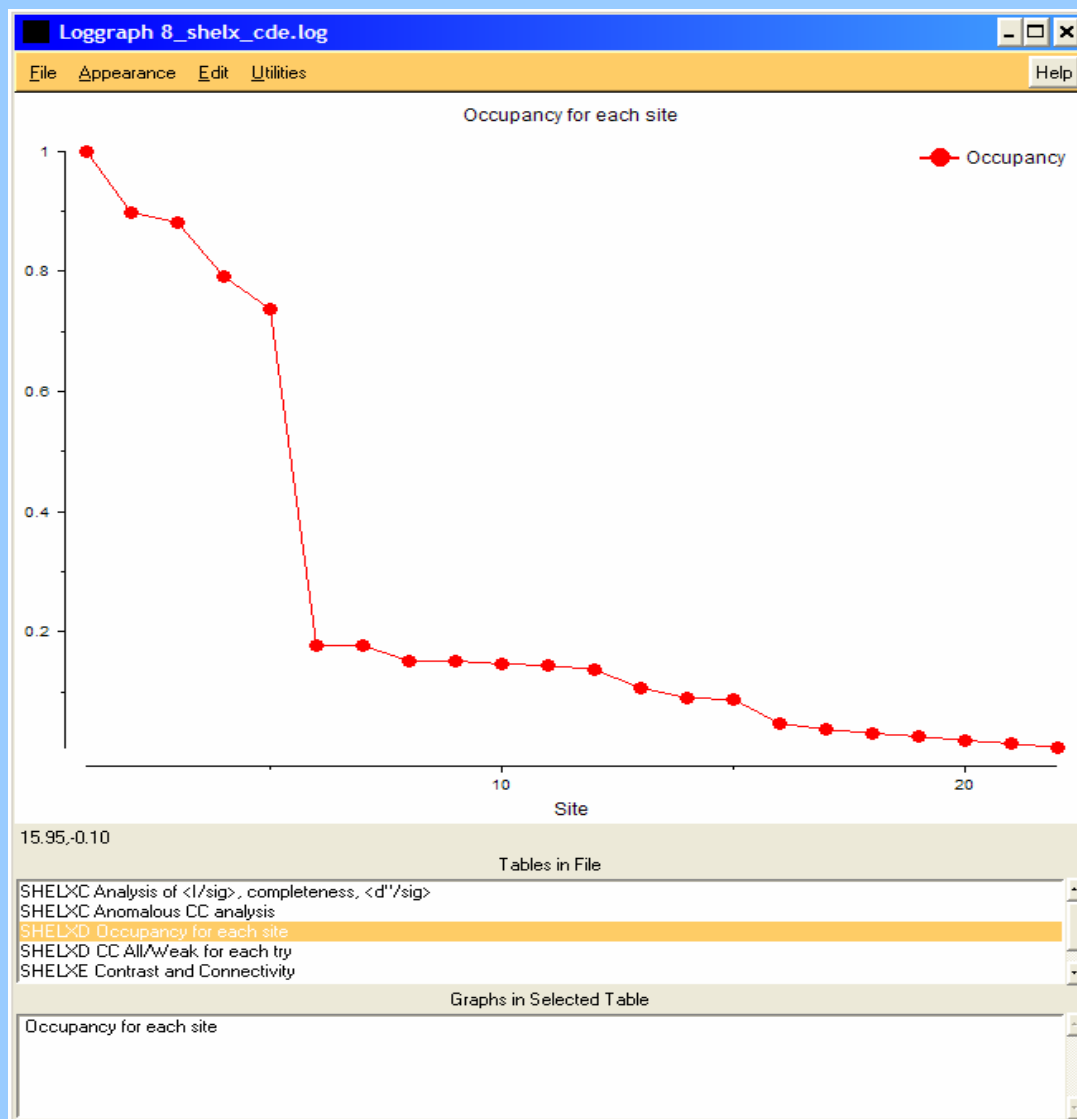
- Arp/warp
- Shelx
- Mosflm
- Xtalview

# 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

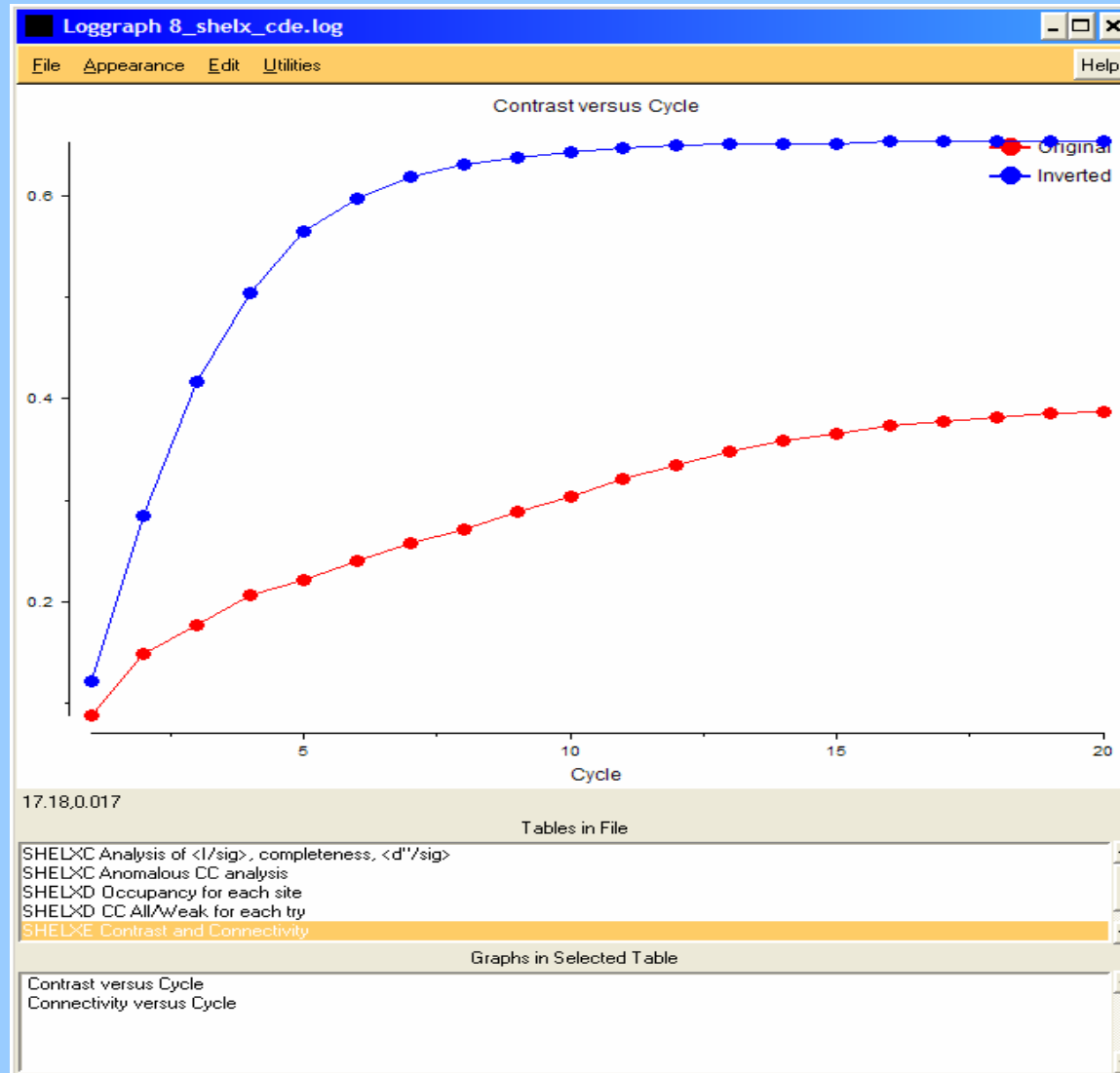


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# LYASE SHELXE



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# LYASE ARP/wARP

Help

Cycle 39: After refmac, R = 0.237 (Rfree = 0.000).  
Found 5 (502 requested) and removed 12 (251 requested) atoms.

Cycle 40: After refmac, R = 0.237 (Rfree = 0.000).  
Found 13 (503 requested) and removed 14 (251 requested) atoms.

-----

Building Cycle 8 Atomic shape factors 2.76 4.68

Round 1: 245 peptides in 21 chains. The longest chain comprises 34 peptides.  
Round 2: 257 peptides in 22 chains. The longest chain comprises 23 peptides.  
Round 3: 253 peptides in 19 chains. The longest chain comprises 43 peptides.  
Taking the results from Round 3  
**Chains 18, Residues 231, Connectivity Index 0.85**

14173 reflections ( 98.81 % complete ) and 1421 restraints for refining 2978 atoms.  
Observations/parameters ratio is 1.19

-----

Cycle 41: After refmac, R = 0.276 (Rfree = 0.000).  
Found 55 (491 requested) and removed 125 (245 requested) atoms.

Cycle 42: After refmac, R = 0.247 (Rfree = 0.000).  
Found 25 (505 requested) and removed 23 (252 requested) atoms.

Cycle 43: After refmac, R = 0.237 (Rfree = 0.000).  
Found 20 (505 requested) and removed 17 (252 requested) atoms.

Cycle 44: After refmac, R = 0.233 (Rfree = 0.000).  
Found 13 (505 requested) and removed 12 (252 requested) atoms.

Cycle 45: After refmac, R = 0.232 (Rfree = 0.000).  
Found 12 (505 requested) and removed 11 (252 requested) atoms.

-----

Building Cycle 9 Atomic shape factors 2.76 4.68

Round 1: 242 peptides in 24 chains. The longest chain comprises 32 peptides.  
Round 2: 247 peptides in 22 chains. The longest chain comprises 33 peptides.  
Round 3: 243 peptides in 19 chains. The longest chain comprises 26 peptides.  
Taking the results from Round 3  
**Chains 18, Residues 221, Connectivity Index 0.84**

---> Final restrained refinement block. No atom update.

14173 reflections ( 98.81 % complete ) and 1361 restraints for refining 2994 atoms.  
Observations/parameters ratio is 1.18

-----

Cycle 46: After refmac, R = 0.278 (Rfree = 0.000).

Find Show Summary Quit

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# 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

Help

Job title [No title given]

Run SHELXC to prepare FA data from a  experiment using data in  format

Run SHELXD to search for heavy atoms

Run SHELXE to perform phasing and density modification

Phase using a solvent fraction of  and  of the heavy atom substructure

**Input files**

MTZ input

Input is in the form of

Nat I(+)	<input type="text" value="I_id23nat(+)"/>	<input type="text" value="SigI(+)"/>	<input type="text" value="SIGI_id23nat(+)"/>
Nat I(-)	<input type="text" value="I_id23nat(-)"/>	<input type="text" value="SigI(-)"/>	<input type="text" value="SIGI_id23nat(-)"/>
HA I(+)	<input type="text" value="I_cd_p41212(+)"/>	<input type="text" value="SigI(+)"/>	<input type="text" value="SIGI_cd_p41212(+)"/>
HA I(-)	<input type="text" value="I_cd_p41212(-)"/>	<input type="text" value="SigI(-)"/>	<input type="text" value="SIGI_cd_p41212(-)"/>

**Output files**

Native HKL

Fa HKL

PDB out

Output results of SHELXE in  format

Phases (ori)

Phases (inv)

**Cell Parameters and Spacegroup**

Space group

Set cell a  b  c  alpha  beta  gamma

**Heavy Atom Search Parameters**

Find  heavy atoms of type

Use resolution limits determined from SHELXC run

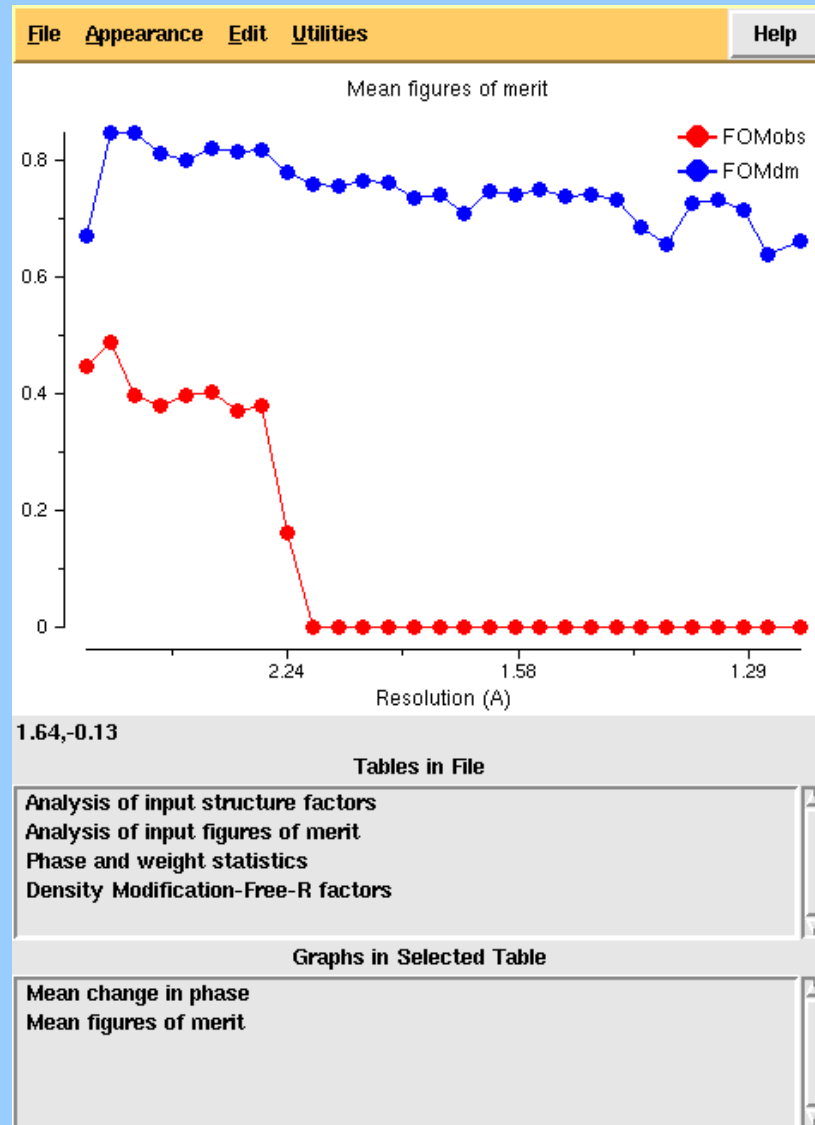
Shelx Author: George Sheldrick [Please obtain the Shelx programs from http://www.shelx.de](http://www.shelx.de)

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# CE4 Phasing & Phase Improvement

- MLPhare with site from SHELXD
- DM



# AXA P2<sub>1</sub> 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<sub>1</sub>2<sub>1</sub>2<sub>1</sub> Analyse data

Help

Job title

Do B value analysis of experimental data and model structure

MTZ in   Browse View

FP  SigmaFP

Map out   Browse View

*Define Map*

Exclude data resolution less than  A or greater than  A

*Wilson Plot for B Analysis*

For calculation of scattering power enter unit cell contents as

Number of residues in asymmetric unit

Run Save or Restore Close

# AXA P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub> Analyse data Results

GRID	32	64	72						
CELL	47.9090	89.8540	95.5480	90.0000	90.0000	90.0000			
ATOM1	Ano	0.0000	0.0000	0.0000	79.83	0.0	BFAC	20.0	
ATOM2	Ano	0.0000	0.5000	0.3763	39.49	0.0	BFAC	20.0	
ATOM3	Ano	0.0617	0.0278	0.0386	17.65	0.0	BFAC	20.0	
ATOM4	Ano	0.1884	0.0464	0.0000	16.46	0.0	BFAC	20.0	
ATOM5	Ano	0.0323	0.0000	0.0580	16.43	0.0	BFAC	20.0	
ATOM6	Ano	0.1303	0.0000	0.0000	15.99	0.0	BFAC	20.0	
ATOM7	Ano	0.0944	0.0000	0.3516	15.75	0.0	BFAC	20.0	
ATOM8	Ano	0.0865	0.4720	0.3959	15.72	0.0	BFAC	20.0	
ATOM9	Ano	0.0554	0.0951	0.0359	15.52	0.0	BFAC	20.0	
ATOM10	Ano	0.5000	0.0000	0.3867	15.48	0.0	BFAC	20.0	
ATOM11	Ano	0.5000	0.5000	0.0085	15.34	0.0	BFAC	20.0	
ATOM12	Ano	0.0678	0.0000	0.0992	15.25	0.0	BFAC	20.0	
ATOM13	Ano	0.0958	0.5000	0.2876	15.25	0.0	BFAC	20.0	
ATOM14	Ano	0.1249	0.0632	0.0531	15.25	0.0	BFAC	20.0	
ATOM15	Ano	0.0000	0.0351	0.1019	15.18	0.0	BFAC	20.0	
ATOM16	Ano	0.0000	0.1704	0.5000	15.18	0.0	BFAC	20.0	
ATOM17	Ano	0.1174	0.0000	0.0779	15.15	0.0	BFAC	20.0	
ATOM18	Ano	0.3732	0.0991	0.5000	15.14	0.0	BFAC	20.0	

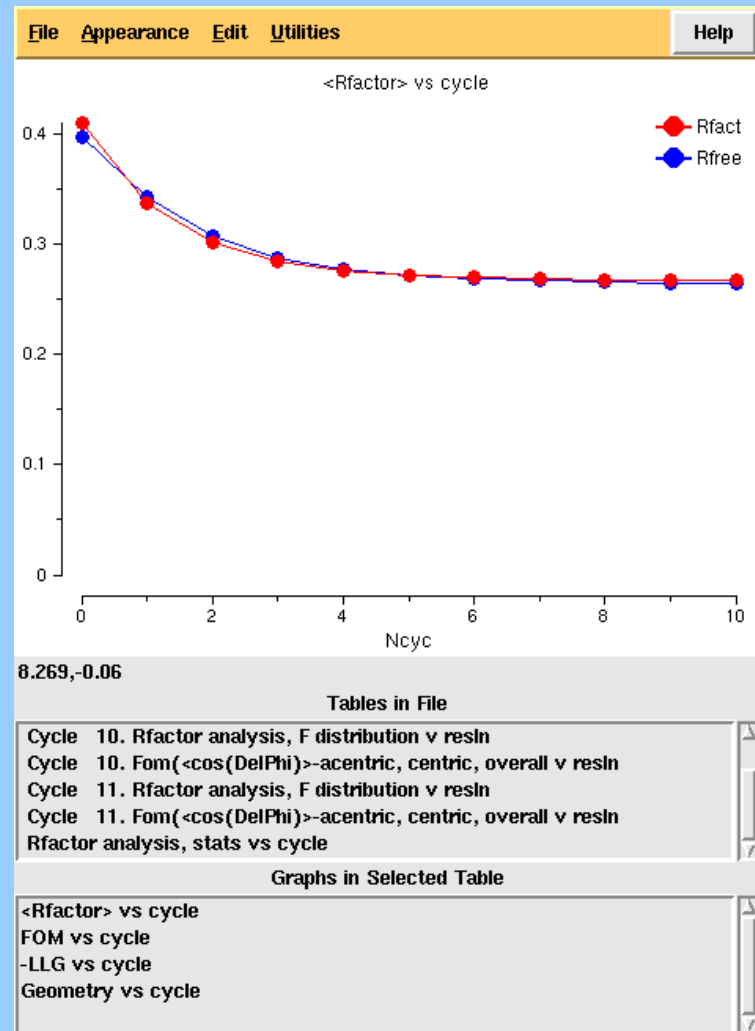
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# AXA $P2_12_12_1$ Solution

MOLREP, two molecules

Initial refinement REFMAC



# Acknowledgements

- Eleanor Dodson
- Keith Wilson
- Gideon Davies
- Ed Taylor
- Sam Hart
  
- Everyone else in YSBL