

**Almost at the end ...**

***“If you don’t remember anything else,  
remember this !!!!”***

## Who am !?

- Peter Briggs
- CCP4 programmer and ...

## CCP4 has an booth #327 in “Data Alley” in the exhibit

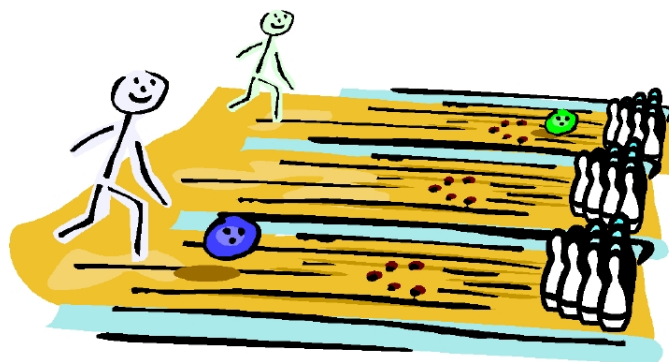
- Come and see us for manuals, demonstrations of software, or a friendly chat 😊
- Gwyndaf, Stuart, Paul ...

## Follow-up for this workshop

- Please fill in and return the questionnaires in the CCP4 packs
- If you have anything missing from the packs or want copies of the slides please let us know

# Please Visit the RCSB PDB Booth #325 in “Data Alley”

- Demonstrations
  - pdb\_extract
  - validation
  - ADIT
  - reengineered PDB site demos during coffee breaks
- Questions answered
- Tattoos, posters and literature
- Poster session Tuesday night #P142



You can always write to us at [deposit@rcsb.rutgers.edu](mailto:deposit@rcsb.rutgers.edu)  
All information is available from [deposit.pdb.org](http://deposit.pdb.org)

# Take home points from Peter

- **Binary installations** for fast start up
- Use CCP4i **project management** tools
- Add **project**, **crystal** and **dataset** information in MTZ
- Switch on **data harvesting**

# My take home points from Martin's talk ...

- CCP4 package contains a wide range of programs for structure determination “**from cradle to grave**”
- Links well with **external programs** e.g. SHELX, SOLVE, ARP/wARP
- **New programs** coming online e.g. PHASER, BP3, Pirate, Buccaneer
- Improved **Model Building Tools** (CCP4mg & Coot) coming soon
- It *is* possible to solve structures quickly in CCP4 (~10 mins!)

# Take home points from Gwyndaf's talk

- Do the best possible job of your data collection
- Run MOSFLM on your first few images to determine strategy and data collection parameters
- Run SCALA as soon as possible to estimate data quality and presence of any anomalous signal

# Take home points from Roberto's talk

- Collect good data
- If aniso is not possible then always give TLS a go
- Use good starting descriptions on starting material for ligand descriptions
- Try to understand the output and read literature

# Take home points from Stuart & Paul's talks

- Great new tools for viewing and building being developed within CCP4 framework
- Contact Stuart/Paul for more information & availability
- CCP4mg:  
<http://www.ysbl.york.ac.uk/~mcnicholas/ccp4mg/MG-distrib>
- Coot: <http://www.ysbl.york.ac.uk/~emsley/coot/>

# Shuchi and Kyle say...

- Use **pdb\_extract** to prepare your data
- **Validate** your files before deposition
- Use **ADIT** to deposit your files

## And finally ...

- Thanks to the speakers!
- Thanks to the organisers!
- Thanks to you for coming!
- **Please come and visit the PDB and CCP4 booths in the exhibition**
  - #325 and #327 in “Data Alley”