

N6: A Protein Crystallographic Toolbox: The CCP4 Software Suite and RCSB PDB Deposition Tools

**IUCr 2005 Florence Italy
August 23rd**

About this workshop ...

The objective of this one-day workshop is not to teach crystallography but to teach people how to use some of the programs distributed with the CCP4 package to do protein crystallography, and how to get the best from the RCSB PDB when they deposit their structures.

Thanks to ...

Maeri Howard & Judy Flippen-Anderson (co-organisers)

Helen Berman

CCP4 and RCSB PDB

The IUCr (Annalisa Guerri)

... and all the workshop speakers

About CCP4 ...

CCP4 is the Collaborative Computational Project no.4

- UK-based initiative
- Provides software for Macromolecular X-ray Crystallography
- Educational remit to promote “good practice”
- Core funding from BBSRC
- Additional income from industrial receipts

Core staff based at CCLRC Daresbury Laboratory in UK

- Maintain, develop and release core software
- Make releases of the software suite
- Coordinate other activities including:
 - Annual study weekend
 - Newsletters
 - Maintain website, bulletin board, problems pages
 - Conferences, workshops (like this one!)



CCP4 funds other staff working on CCP4-related projects and programs across the UK

Software is also provided by developers not funded by CCP4

CCP4-related software developments

- CCP4 Molecular Graphics (CCP4mg, Coot)
- Refmac5
- Mosflm
- Phaser, Pirate, BP3, Chooch ...

Other projects

- CCP4 Automation effort
- Involvement in various European projects:
 - e-HTPX, SPINE, BIOXHIT, PIMS ...

Some general CCP4 resources ...

CCP4 website

- <http://www.ccp4.ac.uk/>
- Links to lots of useful information (downloads, documentation...)

Bulletin Board `ccp4bb`

- lively forum for discussing all aspects of protein crystallography
- “Sorry for the non-CCP4 related query...”
- To (un)subscribe: <http://www.ccp4.ac.uk/ccp4bb.php>

Newsletters

- *news@ccp4*
- “Journal style” newsletters
- Current and past issues:
<http://www.ccp4.ac.uk/newsletters.php>



The Protein Data Bank is the single worldwide repository for the processing and distribution of 3-D biological macromolecular structure data.

The RCSB PDB's mission is provide the most accurate, well-annotated data in the most timely and efficient way possible to facilitate new discoveries and advances in science.

As of August 1, 2005 there are more than 31,500 structures available in the archive.



www.pdb.org/ • info@rcsb.org

- Tools available for deposition and validation
 - ADIT (deposit.rcsb.org/adit/)
 - pdb_extract (pdb-extract.rutgers.edu/)
also available through CCP4i
 - Ligand Depot (ligand-depot.rutgers.edu/)
 - Validation suite (deposit.rcsb.org/validate/)
- The RCSB PDB's new and improved search engine is available for beta testing at pdbbeta.rcsb.org

Exhibit Booths

CCP4 is at stand 11

- Meet CCP4 staff and developers
- Software demos, questions, manuals



wwPDB is at booths 28-29

- wwPDB members are exhibiting jointly at IUCr XX
 - RCSB PDB
 - MSD/EBI
 - PDBj
- Staff from all three sites will be available
 - Website/software demos

Please stop by for a visit!

Workshop Timetable		
8:30am	Introduction and Welcome	
Morning session: General		
8:45	An Introduction to the CCP4 Package: Utilities, Tricks and Tips	Peter Briggs
9:30	Overview of using CCP4 for PX	Martin Noble
10:30	Coffee	
11:00	Data Processing and Reduction using MOSFLM & SCALA	Gwyndaf Evans
12:30	Lunch	
Afternoon session		
13:30	TLS Refinement with REFMAC5	Martyn Winn
14:30	CCP4 Molecular Graphics: Pictures & Movies With CCP4MG	Liz Potterton
15:00	Coffee	
15:30	Coot And Graphical Model Building Tools	Paul Emsley
16:00	Data Deposition And Validation Using RCSB PDB Tools	Kyle Burkhardt
Summing Up		
16:45	Summary, or: "if you don't remember anything else from today, remember this..." Questions and Answers	
17:00	Close	

Practical points ...

- Coffee breaks at **10:30am** and **3:00pm** 
- Lunch is provided by the IUCr as part of the workshop fee
- Packs contain copies of all the talks
 - Please let us know if there are missing documents/other problems
 - There are also questionnaires in the packs
 - **please give us feedback!**
- Speakers
 - Please please please stick to time 
 - Mr Timer will assist you ...
 - Gather for photo at morning coffee 