

# Report on the Joint CCP4-RCSB PDB Workshop at the IUCr XX

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In a previous CCP4 newsletter (see [Newsletter 42](#)) we reported on the one-day CCP4 workshop held at the ACA meeting in Orlando Florida at the start of the summer. We were pleased to be able to bookend the summer conference season with a second one-day satellite workshop - this time a joint effort between CCP4 and the RCSB PDB, at the XX IUCr Congress in Florence, Italy. This workshop - entitled "*A Protein Crystallographic Toolbox: CCP4 Software Suite and PDB Deposition Tools*" - continues a tradition of collaboration between the two projects. The workshop attracted around sixty registered participants ranging from graduate students through to experienced crystallographers, bringing with them a broad range of familiarity with the CCP4 and RCSB software. The workshop followed our familiar format, with the speakers (generally a mixture of software developers and expert users) giving detailed user-focused presentations on the software in their area of expertise. The presentations were intended to help novice users get started while at the same time surprising more expert users with new or less-well known aspects of the software.

After a brief joint introduction from **Peter Briggs** of CCP4 and **Helen Berman** of the RCSB-PDB, the first session concentrated on giving a broad overview intended to lay the foundations for the later talks. This included an introduction to the non-crystallographic "technical" aspects of using the CCP4 suite and an excellent overview from **Martin Noble** of the range of crystallographic functions in the suite. His tour of the suite emphasised CCP4's "cradle to grave" coverage of the structure determination process and its close integration with other non-CCP4 software packages.

The remaining presentations focused on practical aspects of the software for key stages of structure determination and deposition. **Gwyndaf Evans** covered data processing, integration and scaling using MOSFLM and SCALA, including tell-tale signs which indicate whether data processing is working (*hint*: look for sudden deviations from otherwise smoothly-varying behaviours) and how to address various problem cases. **Martyn Winn** talked about refinement with REFMAC5, focusing particularly on the use of TLS parameters. He made a good case for trying TLS, as at worst it will make no difference to your refinement while at best it can give a big improvement. Analysis of TLS values may also be a useful tool in suggesting biologically significant protein domain motions.

This was followed by impressive demonstrations by **Liz Potterton** and **Paul Emsley** of two faces of CCP4's molecular graphics project, CCP4MG and Coot respectively: the former currently focuses on providing presentation-quality representations of molecular models, while the latter is a platform for powerful model building tools. Both packages are now becoming widely used and are already key tools in many macromolecular crystallographers' toolkits (they will also both be available as part of the forthcoming CCP4 v6.0 release). **Kyle Burkhardt** of the RCSB-PDB closed appropriately by focusing on the deposition of refined protein structures. She emphasised a number of issues, including the

existence of software tools to help make deposition easier and the importance of validation prior to and during the deposition process, and reminded the audience that the deposition sites want to work with the authors to ensure the best possible representation of their data in the archive.

The workshop closed with a summary of the most interesting "bullet points" from each of the talks. Although the audience response was muted (possibly due to the vastness of the Cimabue Room!) the feedback provided via the questionnaires was very positive, and we were also pleased to see a large percentage of younger crystallographers in attendance. Many people reported that they found the presentations helpful and that they would be trying out the software afterwards. As always there were also requests for a longer workshop with more hands-on demonstrations and more examples of real-life problems - we are of course interested in addressing these issues in future (and in this regard CCP4 would also welcome any offers of help in organising such workshops).

Next year we hope to be back at the [ACA in Hawai'i](#) and at the [ECM in Leuven, Belgium](#). The materials from this IUCr workshop can be found online via <http://www.ccp4.ac.uk/courses/IUCr2005/>. More information about CCP4 can be found at <http://www.ccp4.ac.uk> and about the RCSB PDB at <http://www.rcsb.org/pdb/>.



## Acknowledgements

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*From back to front, left to right: Gwyndaf Evans, Martin Noble, Peter Briggs, Maeri Howard, Paul Emsley, Liz Potterton, Kyle Burkhardt, Martyn Winn*