# CCP4 6.1 and beyond: Tools for Macromolecular Crystallography

**The Collaborative Computational Project No.4 (CCP4) provides a widely-used suite of software for the determination of macromolecular structures from X-ray crystallography data to the international structural biology community.**

The next release of the suite is version 6.1 which contains a number of new and updated programs to meet the challenges of both high-throughput and difficult structure determinations, including: improved methods for phasing, refinement and model building; automated pipelines; molecular graphics packages; and improved graphical interfaces.

Further information and downloads of trial versions of CCP4 6.1 can be found via http://www.ccp4.ac.uk, or by contacting CCP4 staff at ccp4@stfc.ac.uk.

## New and improved programs

**Significant new and updated programs incorporating improved methods for various stages of the structure determination process include:**

• **Refmac** (Murshudov et al) couples increased automation with many improvements, including twin refinement and SAD likelihood target

• **Buccaneer** (Cowtan) provides statistical model building, using a likelihood-based target to identify connected C-alpha positions in electron density maps to trace protein structures

• **Phaser** (McCoy et al) now incorporates functions for experimental phasing for SAD and combined MR/SAD, complementing the existing molecular replacement capabilities

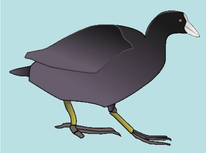
• **Rapper** (Furnham et al) generates protein conformers by sampling likely conformers within a given set of restraints and can be used as a building tool in various situations

• **Ctruncate** (Stein, Ballard et al) gives improved handling of anisotropy and twinning detection in reflection data

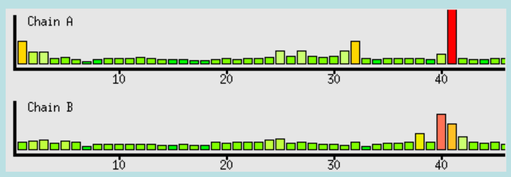
• **Pointless** (Evans) determines Laue and Patterson group from unmerged reflection data, as well as providing many other useful subsidiary functions

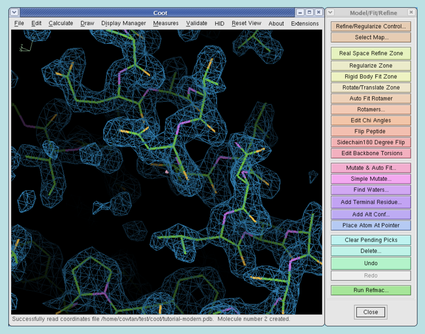
## Molecular Graphics Tools

**CCP4 includes two complementary molecular graphics programs:**



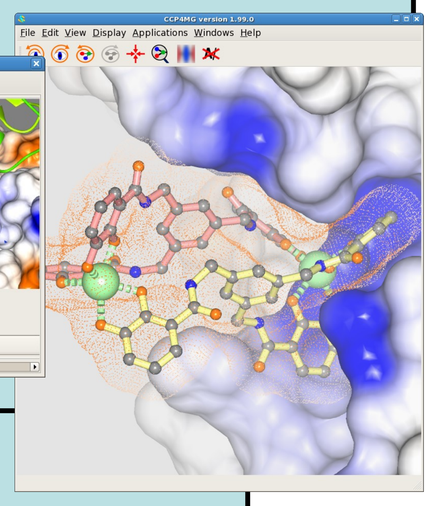
• **Coot** (below) (Cowtan, Emsley & Lohkamp) is a tool for building 3D atomic models of biological macromolecules into electron density maps, and for validating these models against electron density maps. It is highly interactive, intuitive and easy to use, making a range of powerful tools and functions readily available to both novices and experts.




• **CCP4mg** (below) (Potterton and McNicholas) provides easy tools for creating presentation molecular graphics and movies. It will draw all the popular representation styles for models including surfaces with electrostatic potential and also electron density, text annotation and vectors. The program also has many tools for structure analysis and model superposition.

CCP4mg version 2.0 will use the Qt library to provide a much improved user interface and better program performance. It will be available shortly after CCP4 6.1.


## Automated Pipelines in CCP4

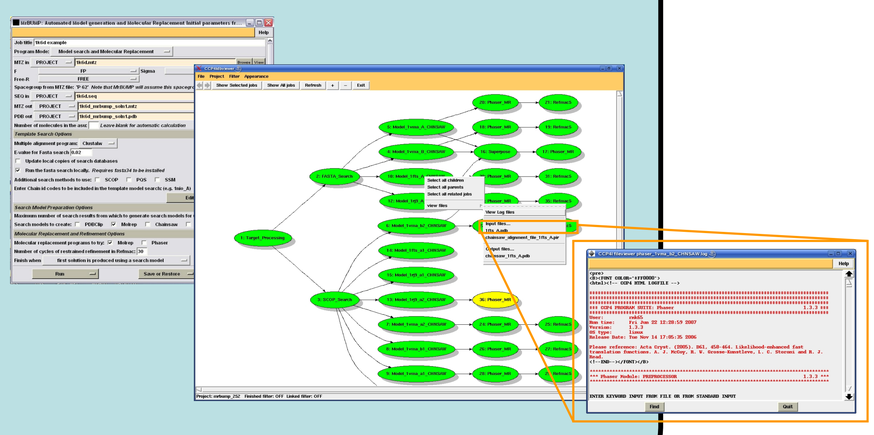
**CCP4 6.1 contains a number of automated pipelines covering various stages of the structure determination process. These combine existing programs with built-in expert knowledge in order to operate with minimal user input.**

• **MrBUMP** – (right) (Keegan and Winn) automated molecular replacement including search model discovery and preparation. MrBUMP uses a brute-force approach to find and prepare a large number of search models before carrying out molecular replacement for each against the target data.

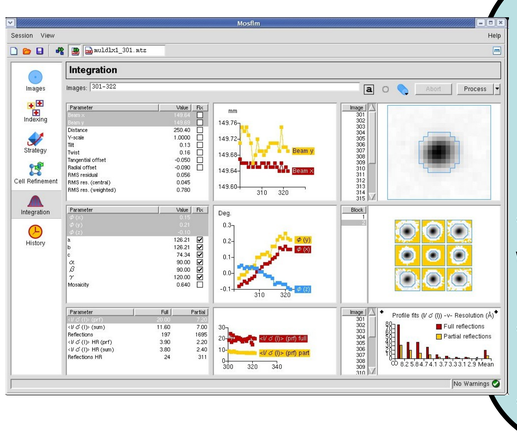
• **Balbes** – (Murshudov et al) automated molecular replacement against a database of protein domains.

• **xia2** – (Winter) automated data reduction and analysis, aimed at both novice users with little expertise, and experts wishing to process high volumes of data.

• **CRANK** – (Pannu et al) a suite for automated macromolecular structure solution. CRANK combines substructure detection and phasing with existing crystallographic programs for density modification and model building.



## Graphical Interfaces and Tools




**New tools and interfaces facilitate running the underlying software, inspecting data and reviewing progress:**

• **iMosflm** (left) (Leslie et al) is the new interface for the MOSFLM data processing and integration program, improving over the old X-windows based interface by combining more intuitive access to MOSFLM's functions with better graphical feedback.

• **idiffdisp** (Remacle & Winter) is a lightweight viewer for diffraction images which helps with rapid analysis and inspection.

• **dbviewer** (Yang & Briggs) gives a graphical view of CCP4i projects, for reviewing the progress of the structure solution process.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