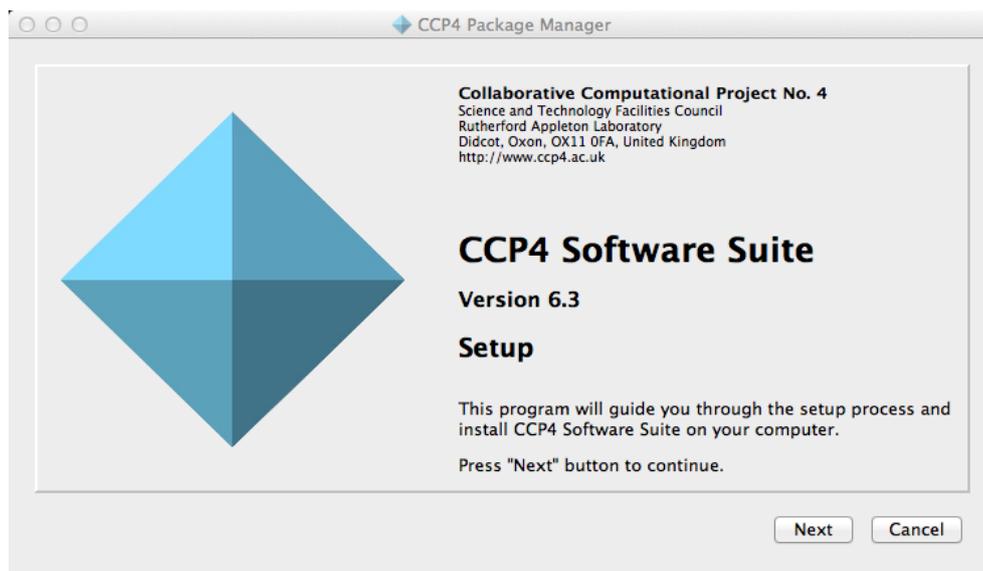


# What's new in CCP4

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The new release of the CCP4 suite is version 6.3.0. This contains the usual compliment of new programs, and updates. One significant change that visitors to the download page <http://www.ccp4.ac.uk/downloads> will notice is the new Package Manager, shown below. This gives a better install experience for Linux and OS X.



*The CCP4 Package Manager.*

The old style packages and ftp site are available as alternatives. Another change is the co-release of Arp/Warp 7.3 from Hamburg. This is a big step for our academic users and those commercial sites that have an Arp/Warp license.

## For CCP4 v6.3.0 “Settle”

### ***New Programs:***

*aimless* (Phil Evans)

*scala* replacement for the scaling and merging of diffraction data. Handles symmetry related reflections together and computes dataset quality statistics on unmerged data.

*prosmart* (Rob Nichols)

*prosmart\_restrain*: external restraint generation for use in the refinement of protein structures.

*prosmart\_align*: alignment, superposition and scoring of protein chains.

*edstats* (Ian Tickle)

electron density map statistic calculation including per residue real space correlation coefficient.

*nautilus* (Kevin Cowtan)

statistical automated building of RNA/DNA in electron density, in the manner of buccaneer.

*zanuda* (Andrey Lebedev)

analysis of refinement results, in particular confirmation of spacegroup.

*phaser.sculptor* (Gabor Bunkoczi)

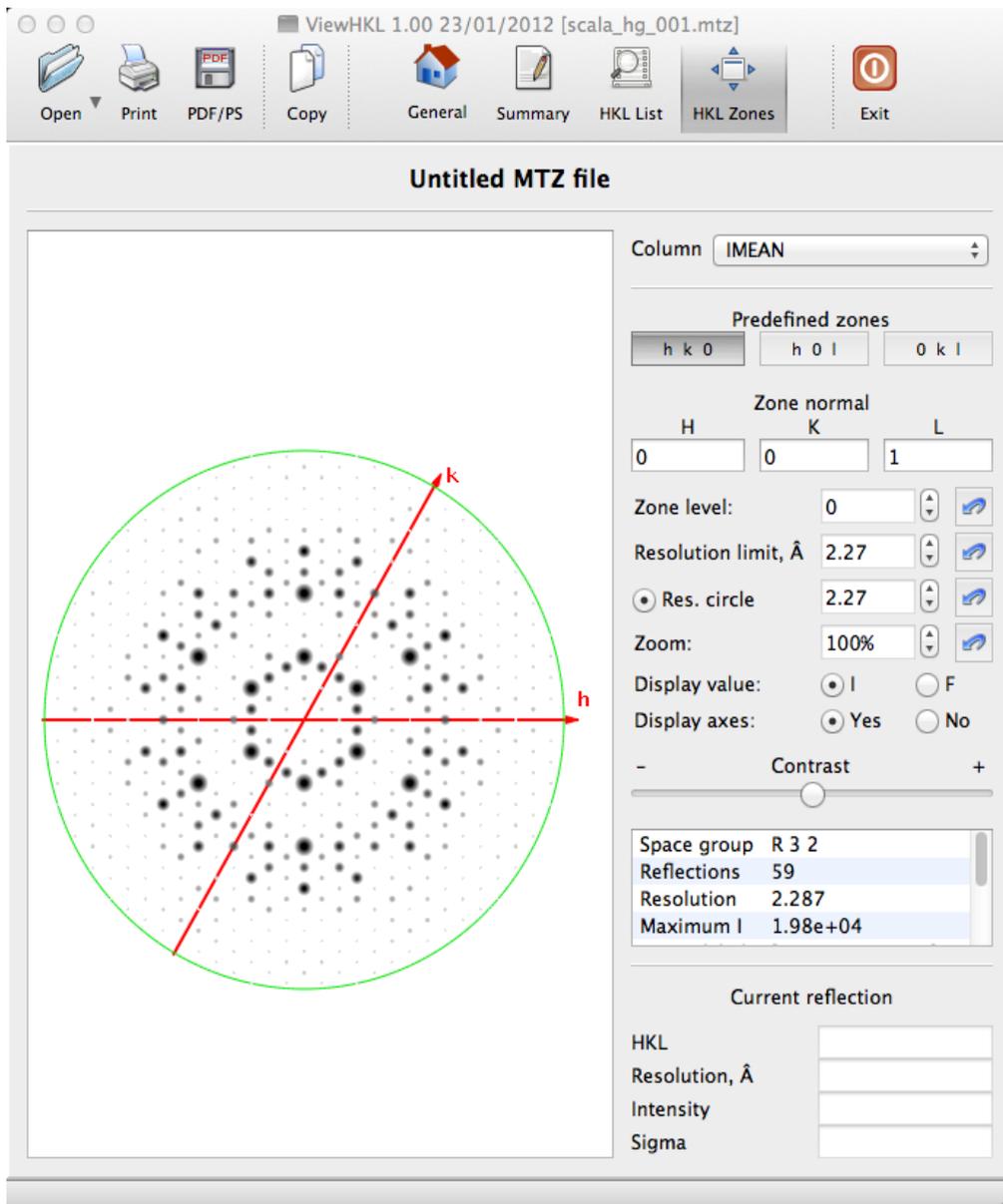
multi-protocol search model preparation including weighted sequence similarity and surface accessibility.

*gesamt* (Eugene Krissinel)

new alignment and superposition program.

*ViewHKL* (Eugene Krissinel)

application for viewing the contents of reflection files, now the default mtz file viewer for the binary distributions.



*Viewhkl display of the contents of an mtz file*

### **Major Updates:**

*Refmac 5.7* (Garib Murshudov)

improved jelly body refinement and use of restraint information.

DNA/RNA and sugar/pucker restraints.

simultaneous refinement and density modification for SAD.

Gibbs sampling of conformational space.

estimation of errors of individual atoms, leading to better electron density.

*Phaser 2.5* (Airlie McCoy, Randy Read)

correction for tNCS in MR.

*imosflm/ipmosflm* (Andrew Leslie, Harry Powell, Owen Johnson)

improved handling of Pilatus Images.

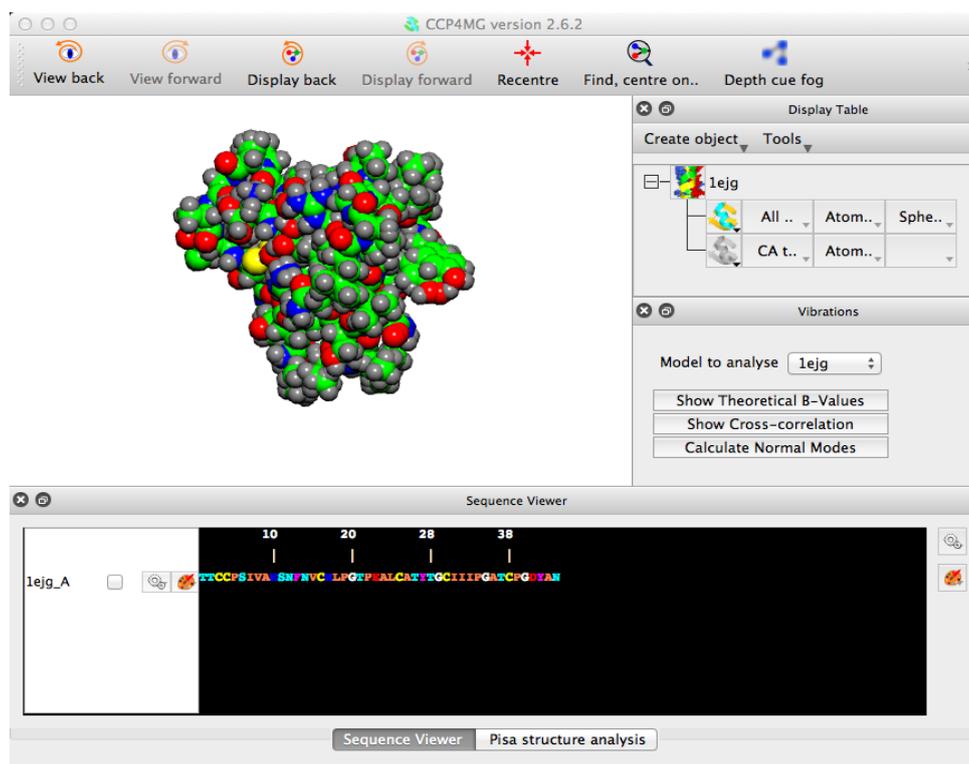
option to use aimless instead of scala in AutoScale.

*PISA* (Eugene Krissinel)

updated database.

*CCP4MG 2.6* (Stuart McNicholas)

improved stability.



*CCP4MG showing the sequence viewer tool*

### ***New Pipelines and interfaces:***

*Dimple* (Ronan Keegan, George Pelios)

ligand density location.

*Ample* (Jaclyn Bidy)

*ab initio* molecular replacement using ROSETTA search models.

Phaser anisotropy calculation and twinning analysis.

new ccp4i interfaces giving access to the anisotropy correction and ML twinning analysis of phaser.

The distributed binaries run across all major platforms, Linux 32/64-bit, OS X 10.4+ and MS Windows. Windows users will be pleased to note that the functionality on Windows is now far closer to the Unix-like systems.

## Other News

### ***Modernisation:***

CCP4 began using the venerated CVS version control system back in 1988. It is not an understatement to say that there is a lot of history in there. Since then the suite has increased in size and complexity, and in the outside world the thinking on version control design has changed markedly. Beginning earlier this year, the core team has begun the task of reorganising the suite and moving to the bazaar version control system. Bazaar is a distributed version control system, in the manner of Git and Mercurial. The ported repositories are hosted on a dedicated server (<http://fg.oisin.rc-harwell.ac.uk>), and are world-readable with the latest versions of the software for the very brave.

The work on the repositories is part of an update of the archiving and distribution of the suite. The other early fruits of this are the Package Manager, and an Updates Manager which will be out in 6.3.1. As a further development the suite will be undergoing further major surgery with the custom configure script being replaced by a more modern system. Much of the build will be made using Cmake. The first pieces of this can be seen in the CmakeList.txt files. Cmake is included with most Linuxes and as a download for OSX. It is an easier to use and more flexible system than the current autotools system.

As part of the move to a quicker release cycle with updates, other plans are in progress. Currently the core group have build and smoke tests running on various platforms via a buildbot herd. As a result of this, nightly builds are available “as is” in an unsupported form. The next twelve months and beyond will see fuller regression tests and even more supported systems, along with automatic bundling. This will give an alternative route to get the latest, but possibly unstable, version of the suite for those who do not want to roll their own.

### ***The Study Weekend:***

The 2012 Study Weekend was on “Data-processing” and took place in Warwick. Some 420 attendees enjoyed talks from the likes of Zbigniew Dauter and Wayne Hendrickson. The Acta D special issue should be available early in the new year. The 2013 Study Weekend will be on “Molecular Replacement” and will take place on the 3-4 January in Nottingham, UK.

As well as the Study Weekend, CCP4 sponsors and organises workshops around the world. The fifth annual CCP4-APS workshop took place in late June 2012 at the Argonne National Laboratory. This was attended by 26 students and lecturers from the US and Europe. This highly successful workshop will be running again next year, so watch the CCP4 website for news of the application dates.

Over the next 12 months there are other planned workshops in Hamburg (Germany), Fukuoka, (Japan) and Brazil.