

## CCP4 8.1 - the next major release of the CCP4 suite

Autumn 2023 will see the next major release of the CCP4 software suite. Following the, largely, successful update from python2 to python3 for the 8.0 series, 8.1 will use a python 3.9 base. Among the step changes is the move to DIALS 3.13+ [1] with an updated graphical user interface, DUI2, greater coot scripting from Paul Emsley [2], the introduction of webCoot (code name moorhen) [3], plus developments from the Phaser team in Cambridge, and finally native M series processor support on Macs. In the meantime the planned monthly update schedule [4] to 8.0 will see further developments on the use of predicted models, CCP4cloud [5] and CCP4i2 [6].

The suit provides automated pipelines and tools for the macromolecular structure solution process, including for example XIA2 for data-processing, MRBump and ARCIMBOLDO for molecular replacement, CRANK2 for experimental phasing, Modelcraft for model building. There is continued development of tools to use predicted models in phasing (MRParse, SliceNDice), model building and validation (Conkit). The CCP4cloud interface can be integrated into a facilities services to offer more fine grained control, and provide a “one stop shop” for the structure solution.

[1] <http://dials.github.io>

[2] <https://github.com/pemsley>

[3] <http://moorhen.org>

[4] [http://www.ccp4.ac.uk/?page\\_id=3088](http://www.ccp4.ac.uk/?page_id=3088)

[5] <https://cloud.ccp4.ac.uk>

[6] <https://ccp4i2.gitlab.io/rstdocs/updatelog/index.html>

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