Innovations and Enhancements in the Upcoming CCP4 Release 10

Ville Uski, Charles Ballard, Maria Fando, Ronan Keegan,
Eugene Krissinel, Andrey Lebedev, David Waterman, Jools Wills
Research Complex at Harwell, Science and Technology Facilities Council, Didcot, UK

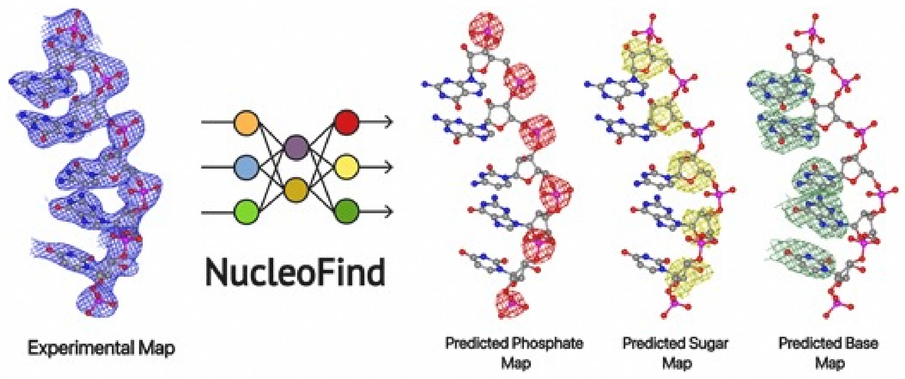
Science and Technology Facilities Council
Scientific Computing
Research Complex at Harwell

CCP4 Software Suite for Macromolecular X-Ray Crystallography - Version 10

The upcoming CCP4 [1] version 10 introduces major infrastructural and functional upgrades for macromolecular structure determination, including Python 3.11 support and enhancements to both the ccp4i2 desktop interface and CCP4 Cloud [3], which now integrates the Moorhen [2] browser-based model builder. Notable new tools include NucleoFind [4], a deep-learning solution for nucleic acid map segmentation, and an update/rewrite of PanDDA (Pan-Dataset Density Analysis) [6–7]. CCP4 maintains a comprehensive pipeline for structure solution, including tools for data processing, molecular replacement, experimental phasing, model building, and validation with ongoing development at the forefront of crystallographic software innovation.

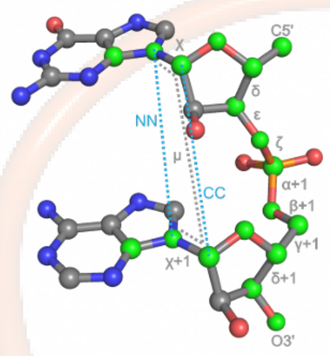
NucleoFind

NucleoFind [4] is a deep-learning-based program for interpreting and segmenting nucleic acid electron-density maps. It predicts the positions of the phosphate group, sugar ring, and nitrogenous base group, significantly enhancing model-building speed and quality compared to traditional methods, even in challenging, noisy datasets. It will be available through CCP4i2 and CCP4 Cloud interfaces as a standalone prediction tool for predicting nucleic acid features in both X-ray and cryo-EM density maps, and in ModelCraft as an automated model-building tool.



DNATCO nucleic acid processing

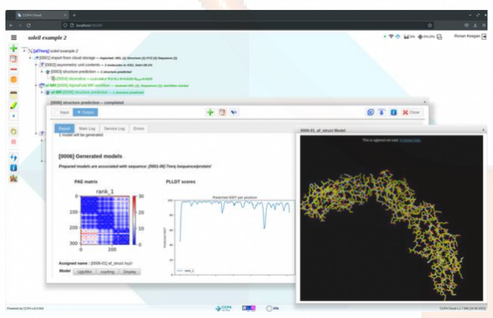
The DNATCO [8] web application provides conformational analysis and validation of nucleic acid structures using the NtC (diNucleotide Conformer) structural alphabet. By assigning NtC labels to dinucleotide steps, DNATCO elucidates backbone geometry and aids structure validation. It is built upon libLLKA, a C++ library for nucleic acid structure annotation.



CCP4 Cloud Updates

Predicted models

CCP4 Cloud enables protein structure prediction using ColabFold, or can search the entire AFDB for search models in molecular replacement.

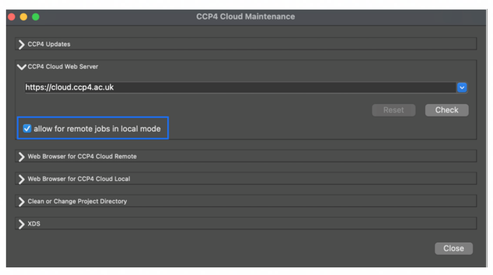


Custom Workflows

Custom workflows automate repetitive tasks.

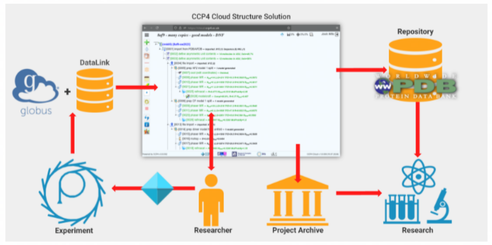
Remote Task Execution

Run tasks from your local instance on a remote CCP4 Cloud server when you need third-party tools, large databases, or significant computational resources.



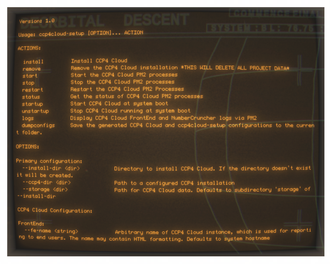
Data fetch from SynchWeb/ISPyB

The Data Fetch feature now includes integration with SynchWeb/ISPyB information management system [10].

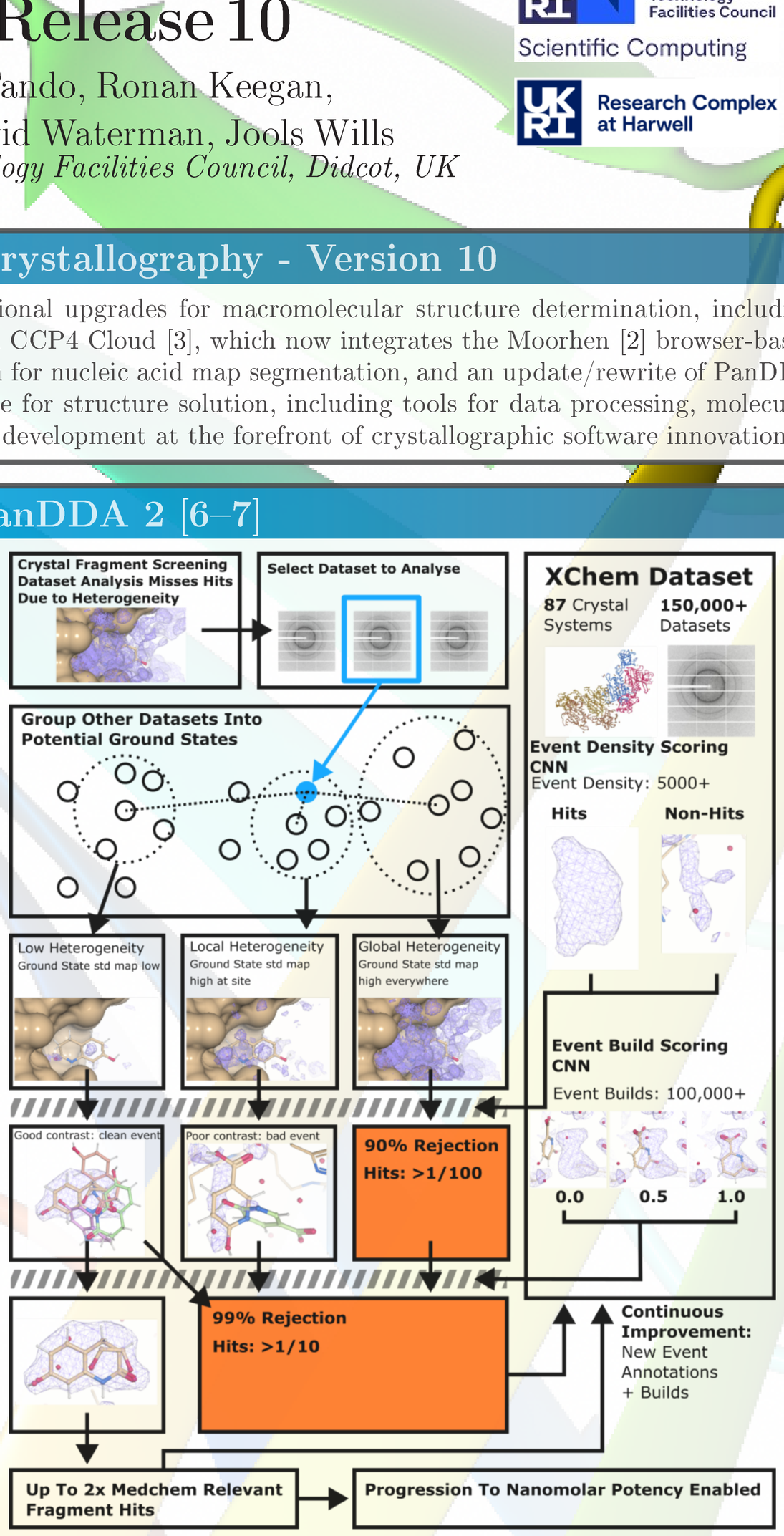


CCP4 Cloud Installer

Installing CCP4 Cloud has become much easier! See `https://ccp4forge.rc-harwell.ac.uk/ccp4/ccp4cloud-setup` for more information.



PanDDA 2 [6–7]



CCP4 Training

CCP4 provides and funds many training events covering the use of the suite for MX structure determination. Events can be from a 1 day introduction to a week or more long workshop. If you are interested in hosting a CCP4 training event, please ask for more details or contact ccp4@ccp4.ac.uk.

Upcoming CCP4 workshops in Europe

- DLS/CCP4 workshop, 24–28 November 2025, Diamond Light Source, UK
- Nordic course on macromolecular X-ray, neutron and electron diffraction, 21–23 October 2025, Oulu, Finland
- CCP4 Study Weekend, January 2026, Nottingham, UK
- CCP4 Central European Workshop on computational structural biology, 26 April – 2 May 2026, Nové Hrady, Czechia
- Structural Biology Course, May/June 2026, Erice, Italy
- CCP4 Summer School, July 2026, UK

References

[1] J. Agirre *et al* (2023). Acta Cryst. D79, 449–461.
[2] P. Emsley, F. Sanchez, S. McNicholas, M. Noble. `https://moorhen.org`
[3] E. Krissinel *et al* (2018). Acta Cryst. D74, 143–151.
[4] J. S. Dialpuri *et al* (2024). Nucleic Acids Research 52, e84.
[5] P. Bond, K. D. Cowtan (2024). Acta Cryst. D78, 1090.
[6] N. Pearce *et al* (2017). Nat. Commun. 8, 15123.
[7] C. Wild. `https://github.com/ConorFWild/pandda_2_gemmi`.
[8] J. Černý *et al* (2020). Acta Cryst. D76, 805–813.
[10] S. J. Fisher *et al* (2015). J. Appl. Crystallogr. 48(3): 927–932.