

MS3-P4 Reaching a new highpoint with crystallography software - APEX3

Martin Adam¹, Eric Hovestreydt¹, Michael Ruf², Joerg Kaercher²

1. Bruker AXS GmbH, Oestliche Rheinbrueckenstrasse 49, 76187 Karlsruhe, GERMANY, info@bruker-axs.com

2. Bruker AXS Inc., 5465 E. Cheryl Parkway, Madison, WI 53711, USA, info@bruker-axs.com

email: martin.adam@bruker.com

In 2004, the APEX2 single crystal suite was first launched and deemed a huge leap forward in terms of functionality and design, compared to previously available software. This suite allowed for complete crystal structure determination, from data collection on the instrument to finalization of a publishable structure, to be completed within one program. Since its launch, the performance of the APEX2 suite has been continuously enhanced by the addition of various features. Today it is one of the most popular software suites used in chemical crystallography. Now, the most extensive revision is available: APEX3. This major new release takes full advantage of important developments in computer hardware and operating systems. Improvements to the new package include a state-of-the-art graphical user interface built with the modern QT4 development framework, updates to faster versions of Python and the PostgreSQL database as well as multi-CPU support for faster data processing, structure solution and reporting. The updated AUTOSTRUCTURE plug-in makes full use of the revolutionary Intrinsic Phasing structure solution engine, increasing the out-of-the-box success rate of structure determinations far beyond 90%. The new Structure Determination plug-in incorporates various structure solution modules, including SHELXT, while ShelXle is fully incorporated as the new default option for fast and convenient structure refinement. Moreover, the efficient twin handling routines known from the APEX2 suite are now fully integrated into the GUI for a new level of seamless twin support. APEX3 extends the ease of use of APEX2, and is readily learned by new users and students alike, keeping the focus on learning the science of crystallography.

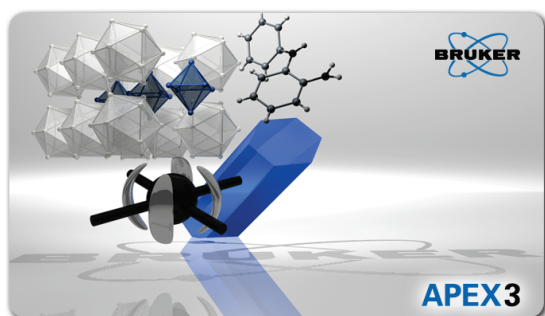


Figure 1. APEX3 Splash screen

Keywords: comprehensive crystallography software, easy-to-use, most popular suite, automated structure solution, SHELXTL

MS4. Advances in phasing, refinement, and autobuilding

Chairs: Navraj Pannu, Eleonor Dodson

MS4-P1 BRICKWORX builds recurrent rna and dna structural motifs into medium and low-resolution electron density maps

Grzegorz Chojnowski^{1,2}, Tomasz Waleń^{1,3}, Paweł Piątkowski¹, Wojciech Potrzebowski¹, Janusz M. Bujnicki^{1,4}

1. International Institute of Molecular and Cell Biology, Warsaw, Poland

2. Present address: European Molecular Biology Laboratory, Hamburg, Germany

3. Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland

4. Institute of Molecular Biology and Biotechnology, Faculty of Biology, Adam Mickiewicz University, Poznań, Poland

email: gchojnowski@gmail.com

BrickworX is a computer program that builds crystal structure models of nucleic acid molecules using recurrent RNA motifs extracted from RNA Bricks database (<http://iimcb.genesilico.pl/rmabricks>) or B-DNA double helices. In a first step, phosphate groups are detected in a user-provided electron-density map. Subsequently, comparing the three-dimensional patterns of the P atoms with a database of nucleic acid fragments, matching positions of the motifs in the unit cell are found. Finally, the matched motifs are merged and refined in real space to find the most likely conformations, including a fit of the sequence to the electron-density map.

The Brickworx program is available for download and as a web server at <http://iimcb.genesilico.pl/brickworx>.

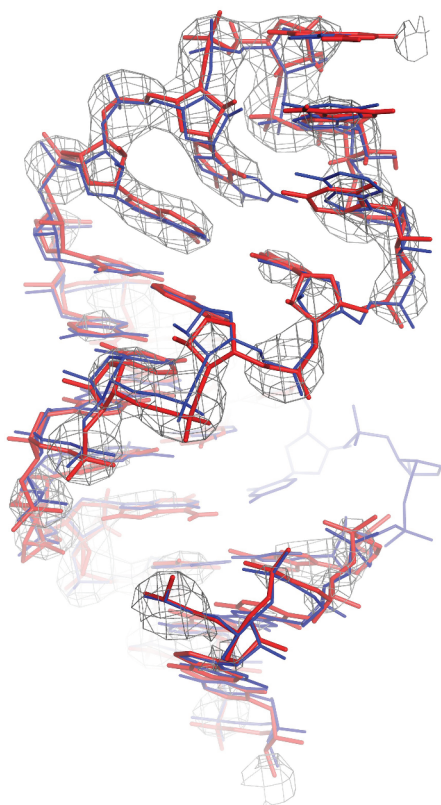


Figure 1. Comparison of published coordinates of the GCGA tetraloop from the group II intron IC subdomain (blue, PDB code 3bwp) and crystal structure model built using Brickworx (red). The model was fitted into the experimentally phased map (3.1 Å resolution) shown contoured at 3.0σ .

Keywords: model building, nucleic acids, macromolecular models

MS4-P2 Advances in CCP4 software suite for macromolecular crystallography

Andrey Lebedev¹, Eugene Krissinel¹, Charles Ballard¹, Ronan Keegan¹, Ville Uski¹, David Waterman¹, Marcin Wojdyr²

1. CCP4, STFC, Research Complex at Harwell, Oxford, OX11 0FA, United Kingdom
2. Diamond Light Source Ltd, Harwell Campus, Oxford, OX11 0DE, United Kingdom

email: andrey.lebedev@stfc.ac.uk

The Collaborative Computational Project Number 4 (CCP4) was set up in the late 1970's in the UK to bring together developers of software for macromolecular crystallography. During the past years many leading software developers in the field of protein crystallography contributed to the CCP4, and the current CCP4 Software Suite provides tools and packages covering all aspects from data collection through to structure deposition [1]. Here we will present details of the latest release series of the Suite, version 6.5.

Release 6.5 brings a few new elements as well as updates and bug fixes to many of the components in the Suite. In particular, this release enforces ligand-related functionalities in CCP4 by introducing new structure and restraint generator Acedrg and carbohydrate validator Privateer-validate. In addition, the new tools enabled to curate and expand the monomer library. Advances in the processing part of the suite comprise processing multi-crystal datasets processing with Blend and multi-lattice datasets with Feckless software. Experimental phasing module has been significantly enforced with new automatic pipeline Crank-2.

In recent years, CCP4 Software Suite has undergone a considerable modernization, which made software building, testing, distribution and updating an automated routine. Yet new challenges arise owing to changing computing environments and concepts, OS updates, thirst for automation, increasing role of graphical front-ends and trends toward remote, web-based computations and hosting projects in the Cloud. We discuss these challenges and general directions for CCP4 development in middle-term perspective.

[1] M. D. Winn, C. C. Ballard, K. D. Cowtan, E. J. Dodson, P. Emsley, P. R. Evans, R. M. Keegan, E. B. Krissinel, A. G. W. Leslie, A. McCoy, S. J. McNicholas, G. N. Murshudov, N. S. Pannu, E. A. Potterton, H. R. Powell, R. J. Read, A. Vagin and K. S. Wilson (2011) Overview of the CCP4 suite and current developments, *Acta Cryst.* **D67** 235-242.

Keywords: Biological Macromolecular X-ray Crystallography, Software for Crystallography, Crystal Structure Determination