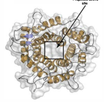
Acta Cryst. (2015). D**71**, 408–415
http://dx.doi.org/10.1107/S1399004714026443



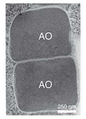
Structure of the GH76 α-mannanase homolog, BT2949, from the gut symbiont *Bacteroides thetaiotaomicron*

A. J. Thompson, F. Cuskin, R. J. Spears, J. Dabin, J. P. Turkenburg, H. J. Gilbert and G. J. Davies

A high-resolution structure of a noncanonical α-mannanase relevant to human health and nutrition has been solved *via* heavy-atom phasing of a selenomethionine derivative.

Serial crystallography

IUCrJ (2016). **3**, 88–95
http://dx.doi.org/10.1107/S2052252515022927

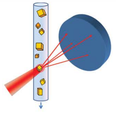


In cellulo serial crystallography of alcohol oxidase crystals inside yeast cells

A. J. Jakobi, D. M. Passon, K. Knoops, F. Stellato, M. Liang, T. A. White, T. Seine, M. Messerschmidt, H. N. Chapman and M. Wilmanns

The application of serial femtosecond crystallography to naturally occurring peroxisomal protein crystals within yeast cells is described. The concept of utilizing peroxisomes for the production of protein nanocrystals is outlined.

IUCrJ (2015). **2**, 246–255
http://dx.doi.org/10.1107/S205225251402702X

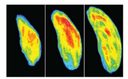


Serial femtosecond crystallography: the first five years

I. Schlichting

The advent of hard X-ray free-electron lasers has opened a new chapter in macromolecular crystallography. Recent results, developments and prospects of serial femtosecond crystallography are described.

IUCrJ (2015). **2**, 575–583
http://dx.doi.org/10.1107/S205225251501235X

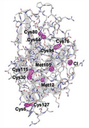


Three-dimensional coherent X-ray diffractive imaging of whole frozen-hydrated cells

J. A. Rodriguez, R. Xu, C.-C. Chen, Z. Huang, H. Jiang, A. L. Chen, K. S. Raines, A. Pryor Jr, D. Nam, L. Wiegart, C. Song, A. Madsen, Y. Chushkin, F. Zontone, P. J. Bradley and J. Miao

Since its first experimental demonstration in 1999, coherent diffractive imaging (CDI) has been applied to image a broad range of samples using advanced synchrotron radiation, X-ray free-electron lasers, high harmonic generation and electrons. Here, the first experimental demonstration of cryogenic CDI for quantitative three-dimensional imaging of whole frozen-hydrated cells is reported. As a proof of principle, the three-dimensional mass density of the sub-cellular organization of a *Neospora caninum* cell is determined based on its natural contrast.

Acta Cryst. (2015). D**71**, 2519–2525
http://dx.doi.org/10.1107/S139900471501857X



Native sulfur/chlorine SAD phasing for serial femtosecond crystallography

T. Nakane, C. Song, M. Suzuki, E. Nango, J. Kobayashi, T. Masuda, S. Inoue, E. Mizohata, T. Nakatsu, T. Tanaka, R. Tanaka, T. Shimamura, K. Tono, Y. Joti, T. Kameshima, T. Hatsui, M. Yabashi, O. Nureki, S. Iwata and M. Sugahara

Sulfur SAD phasing facilitates the structure determination of diverse native proteins using femtosecond X-rays from free-electron lasers *via* serial femtosecond crystallography.

Acta Cryst. (2015). F**71**, 823–830
http://dx.doi.org/10.1107/S2053230X15009061

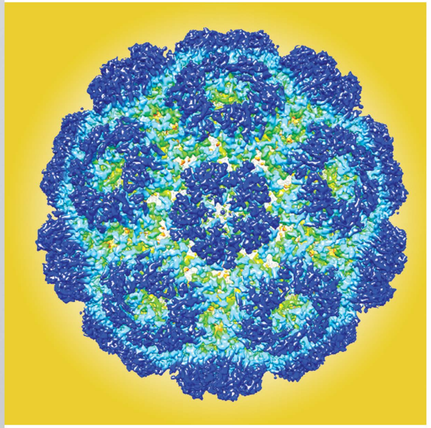
Towards time-resolved serial crystallography in a microfluidic device

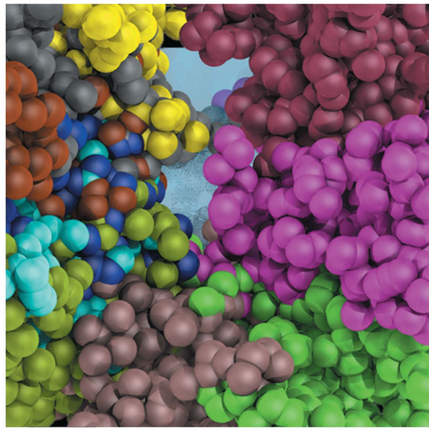
A. S. Pawate, V. Srajer, J. Schieferstein, S. Guha, R. Henning, I. Kosheleva, M. Schmidt, Z. Ren, P. J. A. Kenis and S. L. Perry

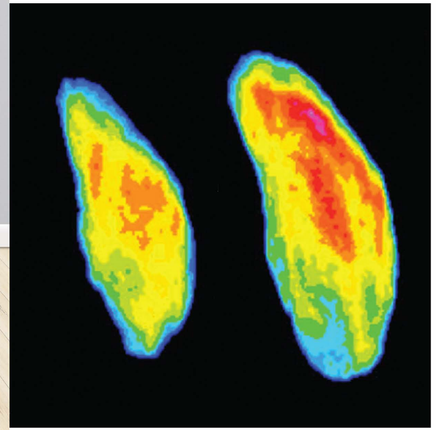
An X-ray compatible microfluidic crystallization platform enables *in situ* time-resolved serial Laue crystallography.

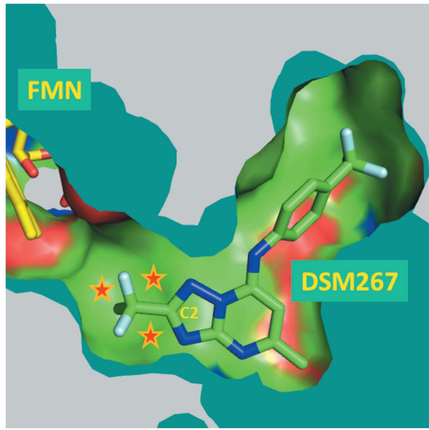
IUCrBio

Structural biology from IUCr journals









journals.iucr.org

IUCrJ (2015). **2**, 602–604
http://dx.doi.org/10.1107/S2052252515017509

Crystallography in the 21st century

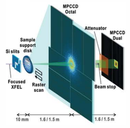
S. S. Hasnain

The field of crystallography, which has had a major impact on the sciences in the last 100 years, is continuing to expand scientific horizons as technical and conceptual boundaries are overcome. Structure–function–dynamics will become an integrated theme for many studies as will obtaining structures without the 'benevolent tyranny' of crystals.

Methods and instrumentation

Acta Cryst. (2016). A**72**, 179–189
http://dx.doi.org/10.1107/S2053273315023980

Cryogenic coherent X-ray diffraction imaging of biological samples at SACLA: a correlative approach with cryo-electron and light microscopy

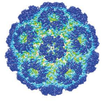


Y. Takayama and K. Yonekura

Cryogenic coherent X-ray diffraction imaging can be used for structural analysis of unstained, non-crystalline, whole biological samples such as cells and cell organelles. This article reports on current and future applications of cryo-coherent diffraction imaging with the X-ray free-electron laser (XFEL) at the Japanese XFEL facility, SACLA, and demonstrates the merit of a correlative approach with cryo-electron and light microscopy.

IUCrJ (2016). **3**, 3–7
http://dx.doi.org/10.1107/S2052252515023738

CryoEM at IUCrJ: a new era



S. Subramaniam, W. Kühlbrandt and R. Henderson

In this overview, the authors briefly outline recent advances in electron cryomicroscopy (cryoEM) and explain why the journal **IUCrJ** can provide a natural home for publications covering many present and future developments in the cryoEM field.

Acta Cryst. (2015). D**71**, 136–153
http://dx.doi.org/10.1107/S1399004714021683

Tools for macromolecular model building and refinement into electron cryo-microscopy reconstructions

A. Brown, F. Long, R. A. Nicholls, J. Toots, P. Emsley and G. Murshudov

A description is given of new tools to facilitate model building and refinement into electron cryo-microscopy reconstructions.

Acta Cryst. (2016). D**72**, 303–318
http://dx.doi.org/10.1107/S2059798316000401

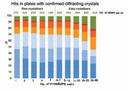
An overview of heavy-atom derivatization of protein crystals

A. C. W. Pike, E. F. Garman, T. Krojer, F. von Delft and E. P. Carpenter

This review summarizes the reasons why the heavy-atom derivatization of protein crystals can be useful, how to select heavy atoms, how to produce a heavy-atom-modified crystal that still diffracts and how to determine whether the protein has been modified.

Acta Cryst. (2016). D**72**, 224–235
http://dx.doi.org/10.1107/S2059798315024687

Lessons from ten years of crystallization experiments at the SGC



J. T. Ng, C. Dekker, P. Reardon and F. von Delft

Observations are presented from retrospective analyses of the crystallization strategies deployed at the Structural Genomics Consortium, Oxford during its first decade of existence, providing practical guidelines for the design of screening experiments.

Acta Cryst. (2015). F**71**, 1228–1234
http://dx.doi.org/10.1107/S2053230X15014892

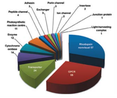
Analysis of crystallization data in the Protein Data Bank

J. Kirkwood, D. Hargreaves, S. O'Keefe and J. Wilson

In a large-scale study using data from the Protein Data Bank, some of the many reported findings regarding the crystallization of proteins were investigated.

Acta Cryst. (2015). F**71**, 3–18
http://dx.doi.org/10.1107/S2053230X14026843

A comprehensive review of the lipid cubic phase or *in meso* method for crystallizing membrane and soluble proteins and complexes



M. Caffrey

Recent applications of this method for *in situ* serial crystallography at X-ray free-electron lasers and synchrotrons are described.

J. Appl. Cryst. (2015). **48**, 1302–1306
http://dx.doi.org/10.1107/S1600576715011243

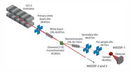
The Macromolecular Neutron Diffractometer MaNDi at the Spallation Neutron Source

L. Coates *et al.*

After several years in construction and commissioning the Macromolecular Neutron Diffractometer (MaNDi) is now operational and accepting general user proposals.

J. Synchrotron Rad. (2015). **22**, 1540–1547
http://dx.doi.org/10.1107/S1600577515016604

MASSIF-1: a beamline dedicated to the fully automatic characterization and data collection from crystals of biological macromolecules

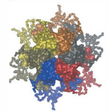


M. W. Bowler *et al.*

MASSIF-1 (ID30A-1) is a new beamline dedicated to the completely automatic characterization and data collection from crystals of biological macromolecules.

IUCrJ (2015). **2**, 207–217
http://dx.doi.org/10.1107/S205225251500202X

Advanced ensemble modelling of flexible macromolecules using X-ray solution scattering

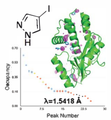


G. Tria, H. D. T. Mertens, M. Kachala and D. I. Svergun

New developments in the modelling of flexible biological macromolecules from SAXS data offer extended possibilities of using high-resolution models and provide metrics for quantitative characterization of the reconstructed ensembles.

IUCrJ (2016). **3**, 51–60
http://dx.doi.org/10.1107/S2052252515021259

Rapid experimental SAD phasing and hot-spot identification with halogenated fragments



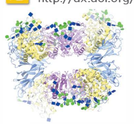
J. D. Bauman, J. J. E. K. Harrison and E. Arnold

4-Bromopyrazole and 4-iodopyrazole bind to many small molecule binding hot spots in target proteins. This promiscuous binding enables the use of these compounds for experimental phase determination by single-wavelength anomalous dispersion (SAD). The low cost and safety of the compounds make them excellent choices for addition to the protein crystallographer's toolkit.

Proteins and complexes

Acta Cryst. (2016). D**72**, 254–265
http://dx.doi.org/10.1107/S2059798315024237

Three-dimensional structures of two heavily N-glycosylated *Aspergillus* sp. family GH3 β-D-glucosidases

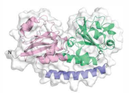


J. Agirre *et al.*

The 3D structures of two industrially important family GH3 β-D-glucosidases from *A. fumigatus* and *A. oryzae* are reported at 1.95 Å resolution. The extensive glycans pose special problems for crystallographic refinement, and new techniques and protocols were developed especially for this work.

Acta Cryst. (2016). F**72**, 214–219
http://dx.doi.org/10.1107/S2053230X16002272

Crystal structure of FhuD at 1.6 Å resolution: a ferrichrome-binding protein from the animal and human pathogen *Staphylococcus pseudintermedius*

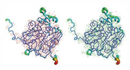


F. Abate, R. Cozzi, M. Maritan, P. Lo Surdo, D. Maione, E. Malito and M. J. Bottomley

The structure displays a canonical class III solute-binding protein fold in a closed conformation, revealing a ligand-binding site suitable for the accommodation of siderophore ligands, here occupied by a polyethylene glycol molecule.

IUCrJ (2015). **2**, 464–474
http://dx.doi.org/10.1107/S2052252515011239

Sub-atomic resolution X-ray crystallography and neutron crystallography: promise, challenges and potential

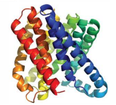


M. P. Blakeley, S. S. Hasnain and S. V. Antonyuk

Neutron crystallography and sub-atomic X-ray crystallography complement each other in defining hydrogen positions in macromolecules. Significant advances have been made but much effort is still required if neutron crystallography is to become a mainstream activity.

Acta Cryst. (2015). D**71**, 1228–1237
http://dx.doi.org/10.1107/S139900471500423X

Structure determination of an integral membrane protein at room temperature from crystals *in situ*

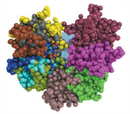


D. Axford, J. Foadi, N.-J. Hu, H. G. Choudhury, S. Iwata, K. Beis, G. Evans and Y. Alguel

The X-ray structure determination of an integral membrane protein using synchrotron diffraction data measured *in situ* at room temperature is demonstrated.

Acta Cryst. (2015). D**71**, 2412–2421
http://dx.doi.org/10.1107/S1399004715018702

Small-angle scattering determination of the shape and localization of human cytochrome P450 embedded in a phospholipid nanodisc environment



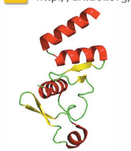
N. Skar-Gislinge, S. A. R. Kynde, I. G. Denisov, X. Ye, I. Lenov, S. G. Sligar and L. Arleth

A combined *ab initio* and rigid-body approach has been developed for small-angle scattering analysis. This provides a previously inaccessible insight into the low-resolution structure of the human cytochrome P450 CYP3A4 when embedded in nanodiscs mimicking a native membrane.

Viruses and pathogens

Acta Cryst. (2016). D**72**, 49–58
http://dx.doi.org/10.1107/S2059798315021439

Molecular architecture of the nucleoprotein C-terminal domain from the Ebola and Marburg viruses

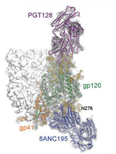


L. E. Baker, J. F. Ellena, K. B. Handing, U. Derewenda, D. Utepbergenov, D. A. Engel and Z. S. Derewenda

Crystal structures of the C-terminal domains of the *Ebolavirus* nucleoproteins (NP^{CT}) from the Bundibugyo and Taï Forest species (BDBV and TAFV, respectively) have been determined. The structures show high similarity to that reported for the Zaire *Ebolavirus* NP^{CT}. However, NMR data revealed that the corresponding domain from the NP of the related MARV species of *Marburgvirus* is distinctly different.

Acta Cryst. (2015). D**71**, 2099–2108
http://dx.doi.org/10.1107/S1399004715013917

Complete epitopes for vaccine design derived from a crystal structure of the broadly neutralizing antibodies PGT128 and 8ANC195 in complex with an HIV-1 Env trimer

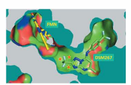


L. Kong, A. Torrents de la Peña, M. C. Deller, F. Garces, K. Sliepen, Y. Hua, R. L. Stanfield, R. W. Sanders and I. A. Wilson

The crystal structure of the broadly neutralizing antibodies 8ANC195 and PGT128 bound to an HIV-1 envelope trimer has been determined. Structural and binding analyses have elucidated the full epitopes for these antibodies in the context of the intact viral glycoprotein, providing improved templates for HIV-1 vaccine design.

Acta Cryst. (2015). F**71**, 485–499
http://dx.doi.org/10.1107/S2053230X15004987

Three-dimensional structures in the design of therapeutics targeting parasitic protozoa: reflections on the past, present and future



W. G. J. Hol

A review and historical perspective covering the many different aspects of antiparasitic drug discovery, in particular targeting protists, is presented. The key role of structural studies in the process is highlighted and specific high-profile examples are given.