Metals in biology

Acta Cryst. (2017). D**73**, 223–233
https://doi.org/10.1107/S2059798317001061

CheckMyMetal: a macromolecular metal-binding validation tool

H. Zheng, D. R. Cooper, P. J. Porebski, I. G. Shabalin, K. B. Handing and W. Minor

The metal-site validation tool *CheckMyMetal* is described, with examples to follow.

J. Synchrotron Rad. (2016). **23**, 1490–1497
https://doi.org/10.1107/S1600577516012807

Nuclear incorporation of iron during the eukaryotic cell cycle

I. Robinson, Y. Yang, F. Zhang, C. Lynch, M. Yusuf and P. Cloetens

Scanning X-ray fluorescence microscopy has been used to probe the distribution of S, P and Fe within cell nuclei at the new ID16 beamline. Estimates of P, S and mass signals for the chromosomal matter agree with quantitative X-ray phase contrast projection microscopy images of the same samples, while fluorescence shows Fe incorporation.

Viruses and pathogens

Acta Cryst. (2016). F**72**, 257–262
https://doi.org/10.1107/S2053230X1600217X

Crystal structure of histone-like protein from *Streptococcus mutans* refined to 1.9 Å resolution

P. O'Neil, S. Lovell, N. Mehzabeen, K. Battaile and I. Biswas

Streptococcal histone-like proteins (HLPs) are essential for bacterial survival. Here, the structure of *S. mutans* HLP was determined at 1.9 Å resolution.

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. (2017). F**73**, 116–122
https://doi.org/10.1107/S2053230X17001601

Crystal structure of full-length *Zika virus* NS5 protein reveals a conformation similar to *Japanese encephalitis virus* NS5

A. K. Upadhyay, M. Cyr, K. Longenecker, R. Tripathi, C. Sun and D. J. Kempf

The recent epidemic of *Zika virus* (ZIKV) has created a major global health concern. Here, the crystal structure of the full-length ZIKV NS5 protein at 3.05 Å resolution is presented to facilitate the structure-based design of antiviral agents against ZIKV.

Acta Cryst. (2016). F**72**, 853–862
https://doi.org/10.1107/S2053230X16017854

1.45 Å resolution structure of SRPN18 from the malaria vector *Anopheles gambiae*

D. A. Meekins, X. Zhang, K. P. Battaile, S. Lovell and K. Michel

The structure of the *A. gambiae* serine proteinase inhibitor (serpin) SRPN18 was determined, revealing an unusually short and constricted reactive-center loop.

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New developments in X-ray and neutron crystallography together with the cryo-EM "resolution revolution" play major roles in defining spatial organization of multicomponent assemblies including viruses, membrane channels, DNA-repair systems, drug targets and engineered bio-structures, while femtosecond nano-crystallography and cryo-EM can sample dynamic structures, including protein crystals inside cells and signaling systems. These are communicated brilliantly through the IUCr journals, and crystallography continues to underpin our understanding of the life sciences in both space and time. – Sir Tom Blundell

Drug discovery

IUCrJ (2017). **4**, 308–321
https://doi.org/10.1107/S2052252517009241

Protein crystallography and drug discovery: recollections of knowledge exchange between academia and industry

T. L. Blundell

Structure-guided drug discovery is a story of applications of protein crystallography and knowledge exchange between academia and industry. It has led to new drug approvals by the FDA in the USA and hope for treatment of rare genetic diseases and infectious diseases in the developing world.

Acta Cryst. (2017). **D73**, 534–540
https://doi.org/10.1107/S2059798317004077

The potential use of single-particle electron microscopy as a tool for structure-based inhibitor design

S. Rawson, M. J. McPhillie, R. M. Johnson, C. W. G. Fishwick and S. P. Muench

Recent developments in electron microscopy have provided new opportunities in the field of structure-based drug design. This review looks at the challenges that remain and the future prospects for the use of electron microscopy in this area.

IUCrJ (2016). **3**, 10–19
https://doi.org/10.1107/S2052252515019971

Peptide binding to a bacterial signal peptidase visualized by peptide tethering and carrier-driven crystallization

Y. T. Ting, P. W. R. Harris, G. Batot, M. A. Brimble, E. N. Baker and P. G. Young

Utilizing a peptide-anchoring strategy, transient signal-peptide complexes of a Gram-positive bacterial signal peptidase were trapped, revealing the atomic details of their interaction.

Acta Cryst. (2015). **F71**, 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.

Serial crystallography

IUCrJ (2017). **4**, 322–339
https://doi.org/10.1107/S2052252517005760

XFELs for structure and dynamics in biology

J. C. H. Spence

The use of X-ray lasers to obtain structures and molecular movies in biology is reviewed. Methods include single-particle imaging, serial crystallography and fast solution scattering at room temperature.

Acta Cryst. (2016). **D72**, 520–523
https://doi.org/10.1107/S2059798316001480

Microcrystal delivery by pulsed liquid droplet for serial femtosecond crystallography

F. Mafuné *et al.*

A liquid-droplet injector delivers microcrystals of lysozyme in a pulse-by-pulse manner for conducting serial femtosecond crystallography with an X-ray free-electron laser. The structure was determined at a resolution of 2.3 Å with low sample consumption.

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 *et al.*

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.

Acta Cryst. (2015). **D71**, 2519–2525
http://dx.doi.org/10.1107/S139900471501857X

Native sulfur/chlorine SAD phasing for serial femtosecond crystallography

T. Nakane *et al.*

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

IUCrJ (2016). **3**, 271–281
https://doi.org/10.1107/S205225251600823X

Serial crystallography captures enzyme catalysis in copper nitrite reductase at atomic resolution from one crystal

S. Horrell, S. V. Antonyuk, R. R. Eady, S. S. Hasnain, M. A. Hough and R. W. Strange

Serial crystallography has been used to drive copper nitrite reductase through its enzymatic cycle while sampling the same volume of a single cryogenically maintained crystal. A structural movie of X-ray-driven enzyme catalysis has thus been obtained, revealing the structural changes that occur during the catalytic reaction in unprecedented detail.

Acta Cryst. (2016). **D72**, 93–112
https://doi.org/10.1107/S2059798315021683

In meso in situ serial X-ray crystallography of soluble and membrane proteins at cryogenic temperatures

C.-Y. Huang *et al.*

A method for performing high-throughput *in situ* serial X-ray crystallography with soluble and membrane proteins in the lipid cubic phase at cryogenic temperatures (100 K) is described. It works with nanogram to single-digit microgram quantities of protein and lipid (and ligand when present), and is compatible with both high-resolution native data collection and experimental phasing without the need for crystal harvesting.

Methods and techniques

Acta Cryst. (2016). **A72**, 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.

Acta Cryst. (2015). **D71**, 2079–2088
https://doi.org/10.1107/S1399004715014194

In vacuo X-ray data collection from graphene-wrapped protein crystals

A. J. Warren, A. D. Crawshaw, J. Trincao, P. Aller, S. Alcock, I. Nistea, P. S. Salgado and G. Evans

A method is reported for collecting room-temperature data from protein crystals under vacuum by protecting them with a thin graphene layer.

J. Appl. Cryst. (2016). **49**, 1117–1120
https://doi.org/10.1107/S1600576716011134

CCP-FEL: a collection of computer programs for free-electron laser research

F. R. N. C. Maia, T. A. White, N. D. Loh and J. Hajdu

The latest virtual special issue of *Journal of Applied Crystallography* (http://journals.iucr.org/-special_issues/2016/ccpfel) presents tools for a range of topics in free-electron laser research such as simulation of experiments, online monitoring of data collection, selection of hits, diagnostics of data quality, data management, data analysis and structure determination for both nanocrystallography and single-particle diffractive imaging.

Acta Cryst. (2017). **D73**, 187–194
https://doi.org/10.1107/S2059798316013553

Glycoblocks: a schematic three-dimensional representation for glycans and their interactions

S. McNicholas and J. Agirre

With structural glycoscience finally gaining popularity, the need for a clear way of depicting glycans and their interactions in three dimensions is more pressing than ever. Here the Glycoblocks representation is introduced, which combines a simplified bonding-network depiction with the familiar two-dimensional glycan notation brought into three dimensions.

J. Appl. Cryst. (2016). **49**, 1861–1875
https://doi.org/10.1107/S160057671601517X

Atomistic modelling of scattering data in the Collaborative Computational Project for Small Angle Scattering (CCP-SAS)

S. J. Perkins *et al.*

The CCP-SAS project is currently developing software for the atomistic and coarse-grained molecular modelling of X-ray and neutron small-angle scattering data. Its computational framework is described, alongside applications in biology and soft matter.

Acta Cryst. (2017). **D73**, 131–140
https://doi.org/10.1107/S2059798316020283

Getting the chemistry right: protonation, tautomers and the importance of H atoms in biological chemistry

B. Bax, C. Chung and C. Edge

H atoms are 'hard to see' in X-ray crystal structures of protein–ligand complexes. This paper discusses the problem of identifying the correct tautomeric form(s) of protein-bound ligands.

J. Synchrotron Rad. (2016). **23**, 842–849
https://doi.org/10.1107/S1600577516005658

Integration of TomoPy and the ASTRA toolbox for advanced processing and reconstruction of tomographic synchrotron data

D. M. Pelt, D. Gürsoy, W. J. Palenstijn, J. Sijbers, F. De Carlo and K. J. Batenburg

The integration of two Python toolboxes used for processing tomographic data, TomoPy and the ASTRA toolbox, is presented.

Acta Cryst. (2017). **D73**, 112–122
https://doi.org/10.1107/S2059798317000067

AceDRG: a stereochemical description generator for ligands

F. Long, R. A. Nicholls, P. Emsley, S. Gražulis, A. Merkys, A. Vaitkus and G. N. Murshudov

The program *AceDRG* generates accurate stereochemical descriptions, and one or more conformations, of a given ligand. The program also analyses entries and extracts local environment-dependent atom types, bonds and angles from the Crystallography Open Database.

J. Appl. Cryst. (2016). **49**, 2015–2020
https://doi.org/10.1107/S1600576716016514

SEC-SANS: size exclusion chromatography combined *in situ* with small-angle neutron scattering

A. Jordan, M. Jacques, C. Merrick, J. Devos, V. T. Forsyth, L. Porcar and A. Martel

This publication describes the combination of size exclusion chromatography with small-angle neutron scattering *in situ*. The need for this technique and the progress achieved thanks to it are illustrated by relevant examples.