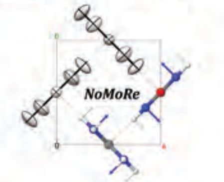
Refinement methods

Acta Cryst. (2016). A72, 206–214
https://doi.org/10.1107/S2053273315024699

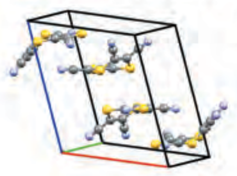


Dynamic quantum crystallography: lattice-dynamical models refined against diffraction data. I. Theory

A. A. Hoser and A. Ø. Madsen

A new refinement approach based on lattice dynamics derived from periodic *ab initio* calculations is described. The approach is tested on high-resolution diffraction data for urea.

Acta Cryst. (2016). B72, 439–459
https://doi.org/10.1107/S2052520616007447

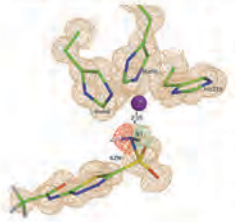


Report on the sixth blind test of organic crystal structure prediction methods

A. M. Reilly *et al.*

The results of the sixth blind test of organic crystal structure prediction methods are presented and discussed, highlighting progress for salts, hydrates and bulky flexible molecules, as well as on-going challenges.

Acta Cryst. (2016). D72, 586–598
https://doi.org/10.1107/S2059798316002837



XModeScore: a novel method for accurate protonation/tautomer-state determination using quantum-mechanically driven macromolecular X-ray crystallographic refinement

O. Borbulevych, R. I. Martin, I. J. Tickle and L. M. Westerhoff

XModeScore determines the correct protomeric/tautomeric state or mode of active-site residues along with any bound ligand(s) using quantum-mechanics-based X-ray refinement followed by post-refinement scoring based on a combination of energetic strain (or ligand strain) and rigorous difference electron-density analysis.

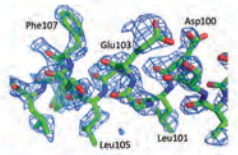
Acta Cryst. (2017). D73, 469–477
https://doi.org/10.1107/S2059798317007859

Recent developments in the *CCP-EM* software suite

T. Burnley, C. M. Palmer and M. Winn

An overview is given of the new *CCP-EM* software suite, including the underpinning framework, the current functionality and the distribution procedure. This first version of the suite has a focus on building and refining atomic models.

Acta Cryst. (2016). F72, 188–197
https://doi.org/10.1107/S2053230X16000923

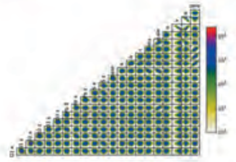


The use of noncrystallographic symmetry averaging to solve structures from data affected by perfect hemihedral twinning

C. Sabin and P. Plevka

Molecular replacement and noncrystallographic symmetry averaging were used to detwin a data set affected by perfect hemihedral twinning. The noncrystallographic symmetry averaging of the electron-density map corrected errors in the detwinning introduced by the differences between the molecular-replacement model and the crystallized structure.

J. Appl. Cryst. (2016). 49, 2201–2209
https://doi.org/10.1107/S1600576716016423



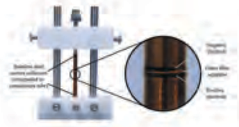
Bayesian method for the analysis of diffraction patterns using *BLAND*

J. E. Lesniewski, S. M. Disseler, D. J. Quintana, P. A. Kienzle and W. D. Ratcliff

The implementation of Bayesian data analysis techniques for refinement of diffraction patterns is presented. The effectiveness of the method is shown through example refinements of a variety of neutron diffraction patterns from real materials.

Sampling

J. Appl. Cryst. (2016). 49, 1665–1673
https://doi.org/10.1107/S1600576716012632



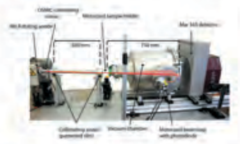
A radially accessible tubular *in situ* X-ray cell for spatially resolved *operando* scattering and spectroscopic studies of electrochemical energy storage devices

H. Liu, P. K. Allan, O. J. Borkiewicz, C. Kurtz, C. P. Grey, K. W. Chapman and P. J. Chupas

Spatially resolved X-ray scattering and spectroscopy measurements, to separately probe and map reactions of individual components and regions within an operating electrochemical device, are enabled by the development of a tubular *in situ* cell.

SAXS/WAXS

J. Appl. Cryst. (2016). 49, 1624–1631
https://doi.org/10.1107/S1600576716012127



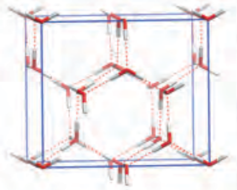
MOMAC: a SAXS/WAXS laboratory instrument dedicated to nanomaterials

O. Taché, S. Rouzière, P. Joly, M. Amara, B. Fleury, A. Thill, P. Launois, O. Spalla and B. Abécassis

An in-house-constructed SAXS/WAXS instrument dedicated to the study of a wide range of nanomaterials is described. The different parts of the instrument are described in detail, along with several calibration standards and examples from recent research.

Temperature effects

Acta Cryst. (2016). B72, 514–529
https://doi.org/10.1107/S2052520616005382



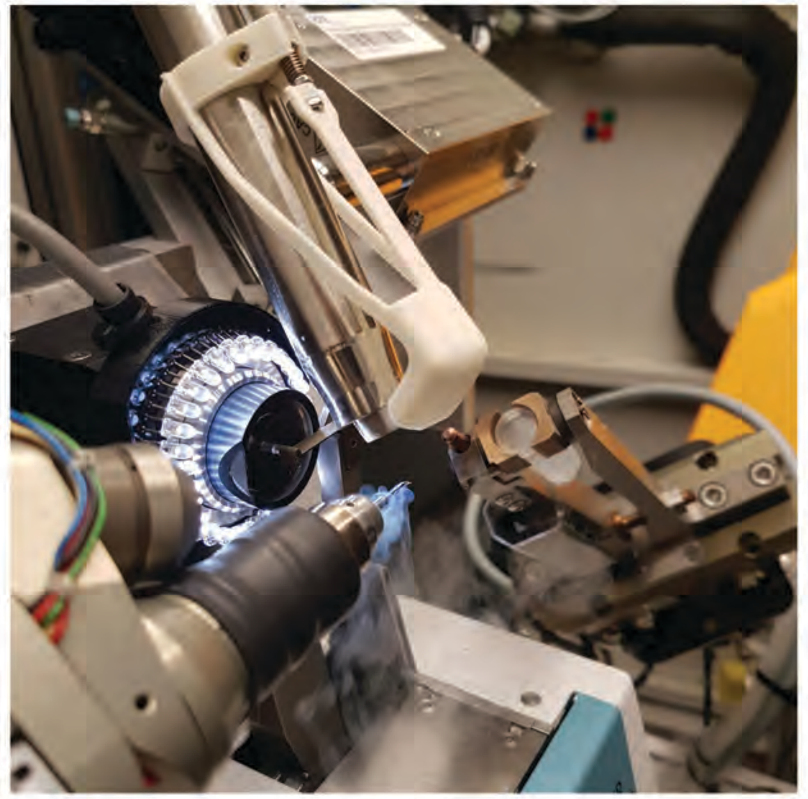
How important is thermal expansion for predicting molecular crystal structures and thermochemistry at finite temperatures?

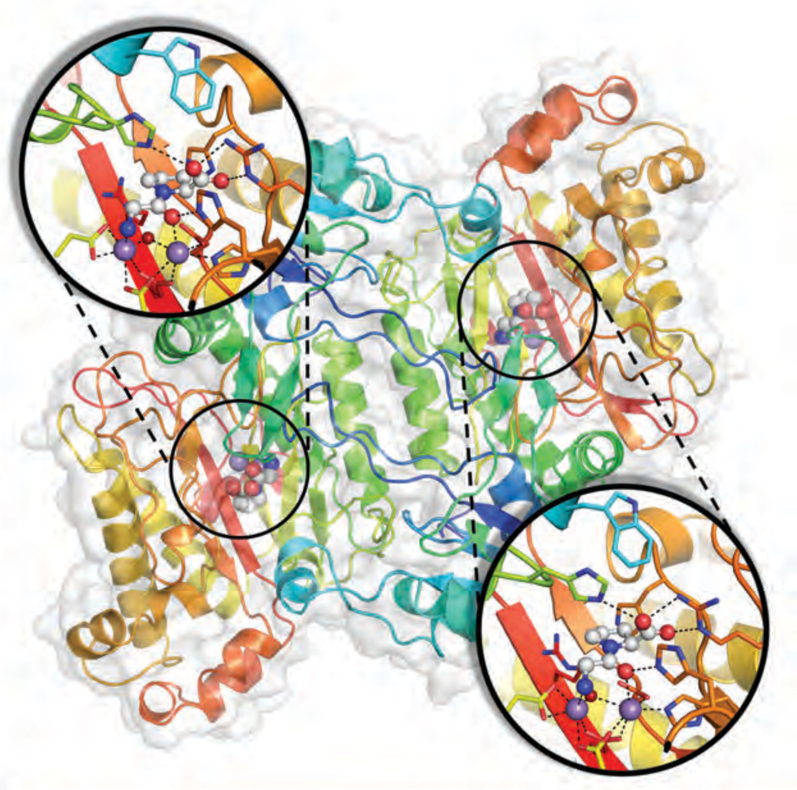
Y. N. Heit and G. J. O. Beran

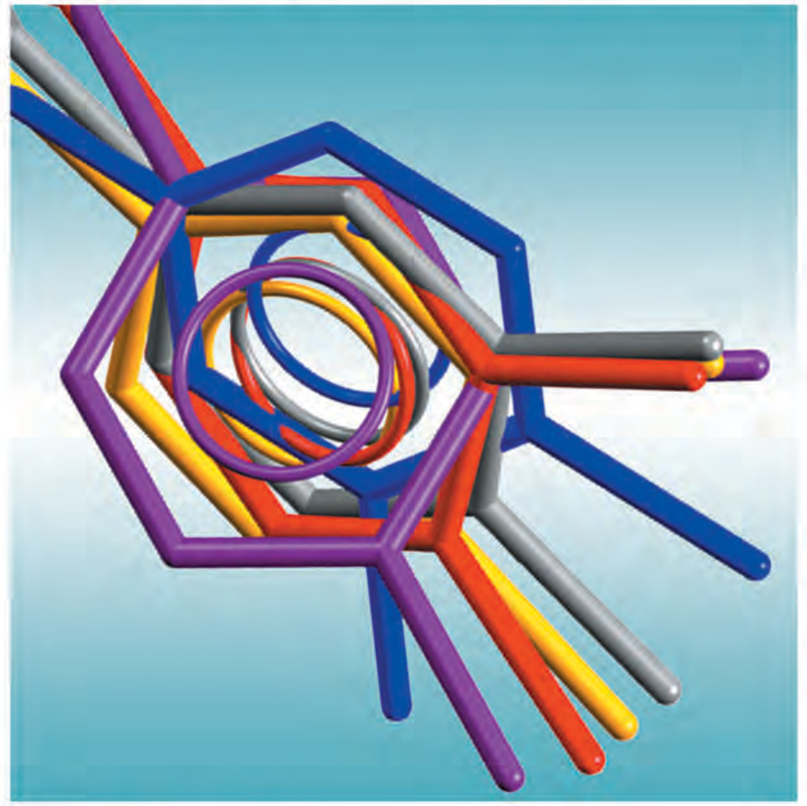
Molecular crystals expand at finite temperatures, which can have appreciable impacts on crystal structure and thermochemical properties. The ability to model thermal expansion using high-level electronic structure methods in the quasi-harmonic approximation and the importance of including thermal expansion effects is assessed for several small molecule crystals.

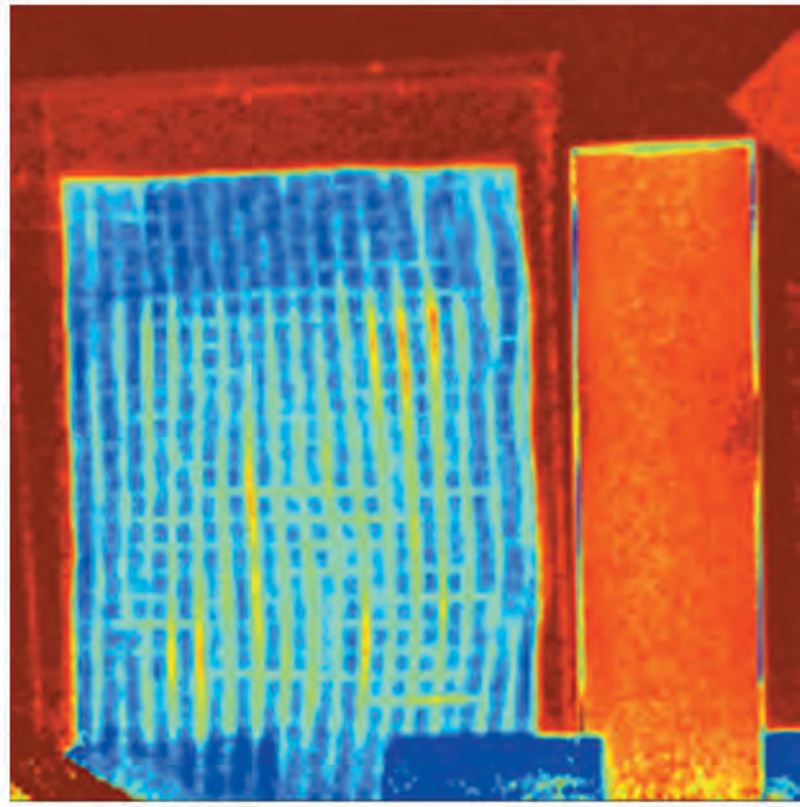
IUCr Instrumentation and methods

Selected articles from IUCr journals







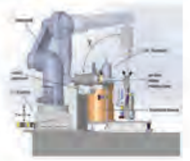


journals.iucr.org

Instrumentation and tool making are fundamentally important for scientific progress, enabling exploration at the frontiers of the micro- and macro-world. As Galilei's telescope opened up the Cosmos, Stelluti's compound microscope, built by Galilei, revealed the micro-world. Subsequent discoveries by Röntgen, Laue and Bragg relied on new instrumentation to revolutionise structural sciences. Rightly, the IUCr and its various journals place significant weight on instrument development, ranging from tiny cryo-loops to neutron facilities, synchrotrons and free-electron lasers. – Janos Hajdu

Automation

Acta Cryst. (2016). D72, 966–975
https://doi.org/10.1107/S205979831601158X



RoboDiff: combining a sample changer and goniometer for highly automated macromolecular crystallography experiments

D. Nurizzo *et al.*

An industrial six-axis robot has been combined with a high-accuracy air-bearing rotation axis to create a single device with the capabilities of both transferring cryocooled protein crystals from a sample-containing dewar and collecting complete X-ray diffraction data sets.

Acta Cryst. (2016). D72, 454–466
https://doi.org/10.1107/S2059798316000954

Automated harvesting and processing of protein crystals through laser photoablation

U. Zander *et al.*

New methods for crystal mounting, soaking and cryocooling contribute to bridging the automation gap between crystallization and X-ray data collection.

Synchrotron beamlines

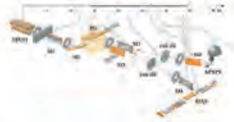
J. Appl. Cryst. (2016). **49**, 1428–1432
https://doi.org/10.1107/S160057671601195X

The new NCPSS BL19U2 beamline at the SSRF for small-angle X-ray scattering from biological macromolecules in solution

N. Li, X. Li, Y. Wang, G. Liu, P. Zhou, H. Wu, C. Hong, F. Bian and R. Zhang

A new biological small-angle X-ray scattering beamline (BioSAXS, BL19U2) at the Shanghai Synchrotron Radiation Facility (SSRF) is dedicated exclusively to small-angle scattering experiments from biological macromolecules in solution. As part of the important facilities in the National Center for Protein Sciences Shanghai (NCPSS), this BioSAXS beamline is the first in China to serve the rapidly increasing biology communities.

J. Synchrotron Rad. (2017). **24**, 344–353
https://doi.org/10.1107/S1600577516019056



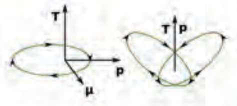
The SPECIES beamline at the MAX IV Laboratory: a facility for soft X-ray RIXS and APXPS

S. Urpelainen *et al.*

SPECIES, the soft X-ray beamline for resonant inelastic scattering and ambient-pressure photoelectron spectroscopy at MAX IV, is described.

Compton scattering

Acta Cryst. (2016). A72, 197–205
https://doi.org/10.1107/S2053273316000863



On the possibility of using X-ray Compton scattering to study magnetoelectrical properties of crystals

S. P. Collins *et al.*

The possibility of using X-ray Compton scattering to reveal antisymmetric components of the electron momentum density, as a fingerprint of magnetoelectric sample properties, is investigated experimentally and theoretically by studying the polar ferromagnet $GaFeO_3$.

On the cover of this leaflet (clockwise from top left): robot-assisted sample mounting allows for high-throughput data collection of protein crystals at the HZB-MX beamlines at BESSY II (credit: HZB-MX group); crystal structure of pathological prolidase mutant shown in cartoon representation. Insets represent the bimetallic catalytic center with bound GlyPro ligand (credit: HZB-MX group); directional dark-field imaging at the ANTARES beamline [*J. Appl. Cryst.* (2016). **49**, 1488–1500]; overlay of the conformations of 2-{[4-(3,4-dichlorophenethyl)phenyl]amino}benzoic acid in forms *A*–*D* [*Acta Cryst.* (2016). B72, 514–529].

Cryo-EM

Acta Cryst. (2015). D71, 136–153
https://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.

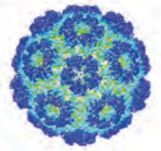
Acta Cryst. (2017). F73, 174–183
https://doi.org/10.1107/S2053230X17003740

Cryo-electron microscopy and X-ray crystallography: complementary approaches to structural biology and drug discovery

C. Vénien-Bryan, Z. Li, L. Vuillard and J. A. Boutin

Single-particle cryo-electron microscopy (cryo-EM) has gained its '*lettres de noblesse*' in structural biology. The synergistic convergence of technological and computational advances now make this a feasible method for determining structures at near-atomic to atomic resolution (~5–2 Å). The potential impact of cryo-EM on drug discovery is discussed, together with how the method can provide information on conformational variability connected to the function of macromolecular complexes.

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



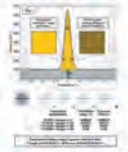
CryoEM at IUCrJ: a new era

S. Subramaniam, W. Kühlbrandt and R. Henderson

In this overview, we 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.

Detectors

Acta Cryst. (2016). D72, 1036–1048
https://doi.org/10.1107/S2059798316012304



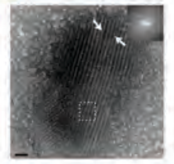
EIGER detector: application in macromolecular crystallography

A. Casanas *et al.*

The application of the EIGER hybrid photon-counting pixel detector in macromolecular crystallography is presented. Data-collection strategies exploiting the unique features of EIGER are discussed.

Electron microscopy

Acta Cryst. (2016). D72, 603–615
https://doi.org/10.1107/S2059798316001546

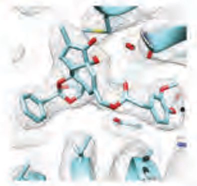


Transmission electron microscopy for the evaluation and optimization of crystal growth

H. P. Stevenson *et al.*

In this article, the potential of transmission electron microscopy to assist in the process of generating well diffracting crystals for conventional crystallography, as well as for free-electron laser and micro-electron diffraction applications, is demonstrated.

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



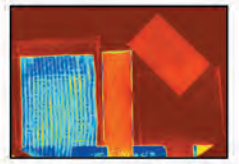
The potential use of single-particle electron microscopy as a tool for structure-based inhibitor design

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.

Neutron instruments

J. Appl. Cryst. (2016). **49**, 1488–1500
https://doi.org/10.1107/S1600576716011080

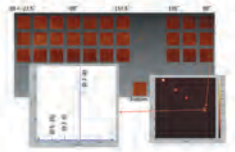


The new neutron grating interferometer at the ANTARES beamline: design, principles and applications

T. Reimann, S. Mühlbauer, M. Horisberger, B. Betz, P. Böni and M. Schulz

In this paper the principles, design and applications of the new neutron grating interferometry (nGI) setup at the Heinz Maier-Leibnitz Zentrum are presented. The dark-field contrast modality of the setup allows one to obtain spatially resolved information about the microstructure of a sample. In this way, nGI closes the gap between neutron imaging and small-angle neutron scattering.

J. Appl. Cryst. (2016). **49**, 120–127
https://doi.org/10.1107/S1600576715022943



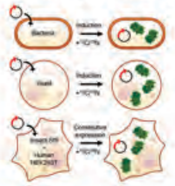
SENJU: a new time-of-flight single-crystal neutron diffractometer at J-PARC

T. Ohhara *et al.*

SENJU, a time-of-flight Laue-type single-crystal neutron diffractometer, was developed at the Materials and Life Science Experimental Facility of the Japan Accelerator Research Complex (J-PARC). Molecular structure analysis of a sub-millimetre taurine crystal and magnetic structure analysis of an MnF_2 crystal were performed to evaluate its performance.

NMR

IUCrJ (2017). **4**, 108–118
https://doi.org/10.1107/S2052252516020625



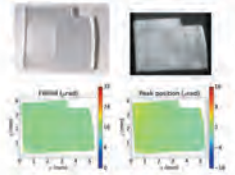
In-cell NMR: a topical review

E. Luchinat and L. Banci

In-cell NMR has emerged in the past decade as a unique approach to obtain structural and functional information on biological macromolecules within living cells at atomic resolution. In this review, the major advances of in-cell NMR are discussed, with a special focus on recent developments and applications in eukaryotic and mammalian cells.

Optics

J. Appl. Cryst. (2016). **49**, 1240–1244
https://doi.org/10.1107/S160057671600917



Diamond drumhead crystals for X-ray optics applications

T. Kolodziej, P. Vodnala, S. Terentyev, V. Blank and Y. Shvyd'ko

Numerous applications in X-ray crystal optics and instrumentation require ultra-thin perfect diamond single crystals, just a few micrometres to a few tens of micrometres thick, properly functioning under Bragg diffraction conditions. Reported here are the successful manufacture and characterization of diamond drumhead crystals using picosecond laser milling.

Programs

J. Appl. Cryst. (2016). **49**, 646–652
https://doi.org/10.1107/S1600576716000455

FIT2D: a multi-purpose data reduction, analysis and visualization program

A. P. Hammersley

FIT2D, a general-purpose and specialist one- and two-dimensional data reduction and analysis program, is described.

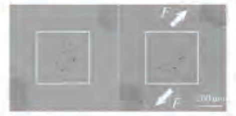
J. Appl. Cryst. (2016). **49**, 1245–1252
https://doi.org/10.1107/S1600576716008074

SHARP: a distributed GPU-based ptychographic solver

S. Marchesini, H. Krishnan, B. J. Daurer, D. A. Shapiro, T. Perciano, J. A. Sethian and F. R. N. C. Maia

The *SHARP* framework provides fast images from high-throughput ptychographic datasets and a corner stone for demanding higher-dimensional analysis such as spectro-ptychography or tomo-ptychography.

J. Synchrotron Rad. (2016). **23**, 1254–1263
https://doi.org/10.1107/S1600577516010195



Real-time image-content-based beamline control for smart 4D X-ray imaging

M. Vogelgesang, T. Farago, T. F. Morgeneyer, L. Helfen, T. dos Santos Rolo, A. Myagotin and T. Baumbach

A flexible experiment workflow system based on high-throughput data acquisition and processsing for feedback-driven and online imaging experiments is presented.

IUCrJ (2017). **4**, 50–64
https://doi.org/10.1107/S2052252516018017

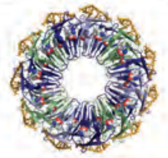
CADEE: Computer-Aided Directed Evolution of Enzymes

B. A. Amrein, F. Steffen-Munsberg, I. Szeler, M. Purg, Y. Kulkarni and S. C. L. Kamerlin

A new computational tool, *CADEE* (Computer-Aided Directed Evolution of Enzymes), is presented.

Radiation damage

Acta Cryst. (2016). D72, 648–657
https://doi.org/10.1107/S2059798316003351



RNA protects a nucleoprotein complex against radiation damage

C. S. Bury, J. E. McGeehan, A. A. Antson, I. Carmichael, M. Gerstel, M. B. Shevtsov and E. F. Garman

Systematic analysis of radiation damage within a protein–RNA complex over a large dose range (1.3–25 MGy) reveals significant differential susceptibility of RNA and protein. A new method of difference electron-density quantification is presented.