

Name: Paul David Adams
Address: Lawrence Berkeley Laboratory, 1 Cyclotron Road, BLDG 33R0345, Berkeley, CA
Title: Senior Scientist & Professor
Telephone: 510-486-4225
Email: PDAdams@lbl.gov Web: <http://cci.lbl.gov/paul>
Publications: 305 peer reviewed, 53 reviews, books and non-peer reviewed
H-index: Publons - 78 (81,000+ citations), Google Scholar - 96 (110,000+ citations)
Outreach: 200+ invited lectures and workshops

Professional Experience

2021-Now Associate Laboratory Director for Biosciences, Lawrence Berkeley Laboratory
2015-2021 Division Director, Molecular Biophysics & Integrated Bioimaging, Lawrence Berkeley Laboratory
2011-2021 Division Deputy for Biosciences, Advanced Light Source, Lawrence Berkeley Laboratory
2009-Now Laboratory Research Manager, Foundational Sciences Focus Area (ENIGMA)
2007-Now Adjunct Professor, Department of Bioengineering, UC Berkeley, Berkeley CA
2007-Now Vice President for Technology, the Joint BioEnergy Institute, Berkeley CA
2005-Now Senior Scientist, Lawrence Berkeley Laboratory, Berkeley CA
2010-2015 Deputy Division Director, Physical Biosciences, Lawrence Berkeley Laboratory
2004-2011 Head, Berkeley Center for Structural Biology, Berkeley CA
2009-2010 Acting Division Director, Physical Biosciences, Lawrence Berkeley Laboratory
2007-2009 Deputy Division Director, Physical Biosciences, Lawrence Berkeley Laboratory
2003-2007 Deputy Principal Investigator, Berkeley Structural Genomics Center, Berkeley CA
1999-2005 Staff Scientist, Lawrence Berkeley Laboratory, Berkeley CA
1998-1999 Senior Associate, Howard Hughes Medical Institute, New Haven CT
1998-1999 Research Scientist, Yale University, New Haven CT
1997-1998 Associate Research Scientist, Yale University, New Haven CT
1992-1997 Postdoctoral Associate, Yale University, New Haven CT
1992 Project Scientist, Edinburgh Parallel Computing Center, Edinburgh, Scotland

Education

1988-1992 Ph.D. (Structural analysis and molecular modelling of α_{2u} -globulin)
Edinburgh University, Edinburgh, Scotland & Imperial Chemical Industries, UK
1985-1988 B.Sc. Biological Sciences (Biochemistry), Edinburgh University, Edinburgh, Scotland
Summa Cum Laude

Awards

- DOE Secretary's Honor Award, Driving U.S. Competitiveness and Innovations Team (2022)
- Director's Technology Transfer Award, Phenix Software Team (2021)
- DOE Secretary's Achievement Award, National Virtual Biotechnology Laboratory COVID-19 Team (2021)
- Department of Energy, Office of Science, Outstanding Mentor Award, Lawrence Berkeley Laboratory, Berkeley CA (2009)
- Outstanding Performance Award, Lawrence Berkeley Laboratory, Berkeley CA (2004)
- Technology Transfer Award, Lawrence Berkeley Laboratory, Berkeley CA (2002)
- Upjohn prize in Biochemistry, Edinburgh University, Edinburgh, Scotland (1988)
- Science Faculty Bursary, Edinburgh University, Edinburgh, Scotland (1986-1987)

Other Professional Activities

Journal reviewer:

- Acta Crystallographica Sections D and F, Biochemistry, Biophysical Journal, Biopolymers, eLife, IUCrJ, J. Chem. Inf. and Modeling, J. Mol. Biol., JACS, J. Applied Crystallography, J. Synchrotron Radiation, Molecular Microbiology, Nature, Nature Communications, Nature Machine Intelligence, Nature Methods, Nature Protocols, Nature Structural and Molecular Biology, Protein Science, Proteins, PNAS, Royal Society Philosophical Transactions B, Science, Scientific Data, Structure

Peer review:

- BioCARS beamline review, Advanced Photon Source (2022)
- Diamond Light Source Beamline Software Architecture Review (2022)
- LCLS Science & Instrumentation Review in Structural Biology (2020)
- EMBL PETRA III beamline review, DESY (2019)
- NIH P30 review panel (2019)
- NIH Early Stage MIRA award review panel (2018)
- Member, LCLS Proposal review panel (2014-2019)
- NCI Intramural Structural Biology Program (2004, 2017)
- LS-CAT beamline review, Advanced Photon Source (2014, 2019)
- Macromolecular Crystallography beamline review, Diamond Synchrotron (2014)
- BioCARS beamline review, Advanced Photon Source (2013)
- EMBL Grenoble Outstation review panel (2013)
- KAUST Office of Competitive Research Funds (2013, 2014)
- Charter Member, NIH Molecular Structure and Function D study section (2011-2015)
- Ad hoc reviewer, NIH R13 grants (2011)
- Singapore National Research Foundation proposals (2011)
- DOE Knowledgebase program (2010)
- NIH Challenge Grants (2009)
- Los Alamos Biofuels LDRD program (2009)
- NCCR P4I special emphasis panel (2008)
- Netherlands Organization for Scientific Research (2008, 2010, 2014)
- Ad hoc member, NIH Molecular Structure and Function D study section (2008-2010, 2020)
- DOE Small Business Innovation Research proposals (2008)
- Biotechnology & Biological Sciences Research Council, UK (2008, 2009)
- Wellcome Trust awards, UK (2008)
- DOE INCITE program (2007)
- IMCA-CAT 17-ID Experiment End Station Upgrade, APS (2007)

Advisory panels:

- Member, Diamond Light Source (UK) Advisory Committee (2021-Present)
- Member, Pacific Northwest Center for Cryo-EM Advisory Committee (2019-Present)
- Chair, RCSB Advisory Committee (2019-Present)
- Member, RBVI Advisory Committee (2016-2017)
- Member, RCSB Advisory Committee (2015-2019)
- Member, wwPDB Advisory Committee (2013-Present)
- Chair, EM Data Bank Advisory Committee (2013-2016)
- Chair, mmCIF/PDBx working group (2012-Present)
- Member, wwPDB X-ray Validation Task Force (2008-Present)
- Member, Oak Ridge National Laboratory Neutron Future Sciences Advisory Panel (2013)
- Member, Argonne National Laboratory Photon Sciences Advisory Committee (2013)
- Member, Diamond Synchrotron Software Advisory Panel (2012)
- Ad hoc member, NAGMS Council (2010)
- Member, Photon Factory International SAC, Life Science Subcommittee (2009)
- Member, UCLA-DOE Institute for Genomics and Proteomics External Advisory Committee (2008)
- Member, NIGMS/NCRR NSLSII advisory panel (2008-2012)
- Member, Protein Information Management System (PIMS) Scientific Advisory Board (2006-2009)
- Chair, NIH Protein Structure Initiative data management committee (2003-2008)

- Member, International structural genomics organization task force on data deposition (2002-2009)

Teaching:

- Instructor, UC Berkeley BioE 225 (Biomolecular Structure Determination) (2017-Present)
- Instructor, UC Berkeley BioE 290D (Biomolecular Structure Analysis) (2009-2016)
- UC Berkeley BioE 24 (2015)
- Guest lecturer, UC Berkeley MCB 206 (2014)
- Guest lecturer Stanford Bio207 (Protein Folding and Disease) (2009, 2010)
- Co-taught UC Berkeley Chem 272A/B (Biomolecular Crystallography) (2006-2008)

Invited Lectures and Workshops

2022

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 19th-25th.

2021

- Keystone Conference, Frontiers in Cryo-Electron Microscopy, online, February 2nd-6th.

2020

- Cryo-EM Validation in the Age of SARS-CoV-2: Methods, Tools and Applications, online, November 20th.
- Structural Biology Seminar Series, University of Colorado Anschutz Medical Campus, Denver, USA, January 28-30th.
- wwPDB Single-particle EM Data-management Workshop, Hinxton, United Kingdom, January 23rd-26th.
- Stanford-SLAC Cryo-EM Center Cryo-EM Modeling Workshop, Stanford, USA, January 15-17th.

2019

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 13th-30th.
- Structural Biology symposium, Zurich University, Zurich, August 21st.
- Phenix Workshop, 32nd European Crystallographic Meeting, Vienna, Austria, August 18th.
- Crystallographic Computing School, Melk, Austria, August 14-17th.
- American Crystallographic Association Annual Meeting, Covington, KY, July 20th.
- University of Michigan International Cryo-EM data processing workshop, Ann Arbor, MI, USA, June 19-21st.
- Stanford-SLAC Cryo-EM Center Modeling Workshop, Stanford, USA, July 10-12th.
- School on 3D CryoEM image analysis, Erice, Italy, May 30th-June 6th.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, April 22nd-26th.
- Single Particle Cryo-EM Course, Cold Spring Harbor Laboratory, USA, March 21st-24th.
- West Coast Structural Biology Workshop, Asilomar, CA, USA, March 17-19th.
- DOE/BER Genomic Sciences Contractors meeting, Tyson's Corner, VA, USA, February 25-27th.
- Frontiers in Cryo-EM Validation, European Bioinformatics Institute, Hinxton, Cambridge, UK, January 14-15th.

2018

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 14th-30th.
- Advanced Light Source User meeting, LBNL, Berkeley CA, October 2nd.
- European Spallation Source Ikon 15 meeting, Lund University, Lund, Sweden, September 10-12th.
- Phenix workshop, Tsinghua University, Beijing, China, September 3-6th.
- APS Upgrade Macromolecular Crystallography Workshop, Argonne National Laboratory, IL, USA, August 19-21st.
- Cryo-EM workshop, Stockholm, Sweden, August 13-17th.
- Phenix Low Resolution Structure Solution Workshop, Technical University of Vienna, Vienna, May 29th.
- Modern Concepts in Structural Biology Seminar, Technical University of Vienna, Vienna, May 28th.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, May 3rd-11th.

- Tsinghua International Symposium of Computational Structural Biology and Biophysics, Beijing, China, April 17th-22nd.
- 3rd International Symposium on Cryo-3D Image Analysis, Lake Tahoe, USA, March 21st-24th.
- Single Particle Cryo-EM Course, Cold Spring Harbor Laboratory, USA, March 9th-12th.

2017

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 26th-31st.
- American Crystallographic Association Annual Meeting, New Orleans, LA, May 27-29th.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, May 3rd-11th.
- CCP-EM Spring Symposium, Diamond Light Source, Harwell, United Kingdom, April 24th-26th.
- DOE/BER Advisory Council meeting, Gaithersburg MD, USA, April 19-21th.
- West Coast Protein Crystallography Workshop, Asilomar, USA, March 14th-16th.

2016

- SBGrid/NE-CAT Phenix workshop, Boston, MA, November 9-11th.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 21st-25th.
- DOE/BER Molecules to Mesoscale workshop, Rockville, MD, September 20th-23rd.
- 12th International Conference on Biology and Synchrotron Radiation, Palo Alto, CA, August 22nd-24th.
- 5th International Symposium on Diffraction Structural Biology, Knoxville, TN, August 7-9th.
- American Crystallographic Association Annual Meeting, Denver, CO, July 25-26th.
- Diffraction Methods in Structural Biology Gordon Conference, Lewiston, ME, July 17th-22nd.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, May 19th-23rd.
- Phenix workshop, Tsinghua University, Beijing, China, May 6-12th.
- Phenix workshop, EPFL, Lausanne, Switzerland, February 19-24th.
- BioStruct-X Workshop on Ensemble Refinement, Lisbon, Portugal, January 29th-February 4th.
- Nanomedicine Symposium on Basic & Translational Sciences, MD Anderson, Houston, USA January 27-28th.
- Phenix workshop, Shanghai University, Shanghai, China, January 12-18th.
- CCP4 Study weekend, Nottingham, UK, January 7-11th.

2015

- Bay Area Cryo-EM meeting, Berkeley, California, USA, December 4th.
- wwwPDB X-ray Validation Task Force Meeting, Cambridge, UK, November 12-18th.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 23-27th.
- Phenix Workshop, Kansas University, Lawrence Kansas, USA, August 5-7th.
- 3D Electron Microscopy Gordon Conference, New London, NH, June 21st-26th.
- Canadian Light Source Crystallography School, Saskatoon, Canada, June 3rd-6th.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, May 19th-23rd.
- Phenix workshop, Rice University, Houston, USA, April 9-10th.

2014

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 24-27th.
- mmCIF developers meeting, European Bioinformatics Institute, Hinxton, UK, October 8th.
- UC Berkeley BioE Departmental Seminar, Berkeley, CA, USA, September 17th.
- BioXFEL workshop, Berkeley, CA, USA, August 21st.
- CCP4/NIH workshop, Argonne National Laboratory, USA, June 27th-July 1st.
- Advanced Methods in Crystallography, Melbourne, Australia June 17-25th.
- Phenix workshop, Harvard University, Boston, USA, June 7th.

- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, May 27th-30th.
- Mid Atlantic Crystallography meeting/SERCAT Phenix Workshop, U. Maryland, Maryland, USA, April 26th.
- University of Lincoln Nebraska Departmental Seminar, Lincoln Nebraska, USA, April 8th.
- Recent trends in Macromolecular Structure and Function, Chennai, India, January 22nd-25th.
- Phenix workshop, Madras University, Chennai, India, January 21st.

2013

- NMR/mmCIF developers meeting, European Bioinformatics Institute, Hinxton, UK, November 18th-21st.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 25th-29th.
- Theoretical Model Validation Symposium, Rutgers University, USA, October 21st-22nd.
- International Conference on Structural Genomics, Sapporo, Japan, July 27th-August 1st.
- CCP4/NIH workshop, Argonne National Laboratory, USA, June 21st-25th.
- Canadian Light Source Crystallography School, Saskatoon, Canada, June 11-15th.
- Joint UCSF/LBNL Imaging Workshop, UCSF, USA, June 7th.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica, Madrid, Spain, May 6-13th.
- Frontiers in Neutron Structural Biology, Oak Ridge National Laboratory, USA, April 16-18th.
- UC Berkeley Structure Supergroup, Berkeley, USA, April 9th.
- European Spallation Source, Neutron Protein Crystallography, Aarhus University, Denmark, March 21st-22nd.

2012

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 26th-November 1st.
- New Developments of Methods and Software for Protein Crystallography, Xi'an, China, August 26th-28th.
- Phenix workshop, Harvard Medical School, Boston, USA, July 27th.
- CCP4/NIH workshop, Argonne National Laboratory, USA, June 23rd-26th.
- Macromolecular Crystallography School, Instituto de Quimica-Fisica "Rocasolano", Madrid, Spain, May 26th-29th
- Phenix workshop, Universidad Nacional Autónoma de México, Mexico City, Mexico, April 17th-22nd
- Phenix workshop, UT Austin, Texas, USA, Feb 22nd
- Macromolecular Crystallography Workshop, Australian Synchrotron, Melbourne, Australia, February 9th-16th.

2011

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 26th-30th.
- Phenix workshop, ILL Grenoble, October 21st.
- Neutrons in Biology, ILL Grenoble, October 19th-20th.
- SBGrid Annual Meeting, Harvard Medical School, Boston, USA, June 23rd-24th.
- CCP4 workshop, Argonne National Laboratory, Illinois, June 12th-15th.
- Phenix workshop, American Crystallographic Association Annual Meeting, New Orleans, USA, May 28th.
- Phenix workshop, Utrecht University, Utrecht, Netherlands, May 22nd.
- Canadian Light Source Crystallography School, Saskatoon, Canada, May 16th-19th.
- Phenix workshop, International Conference on Structural Genomics, Toronto, Canada, May 10th.

2010

- BHT Meeting, Queen's University, Kingston, Canada, November 5th.
- Departmental Seminar, University of Waterloo, Waterloo, Canada, November 4th.
- Departmental Seminar, Sick Children's Hospital, Toronto, Canada, November 3rd.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 22nd-26th.
- SSRL User Meeting, Workshop 8, Stanford, USA, October 20th.

- Phenix workshop, Rockefeller University, New York, USA, October 6th.
- European Crystallography Meeting, Darmstadt, Germany, August 28th-31st.
- Canadian Light Source Annual Users Meeting, Saskatoon, Canada, June 17th.
- CCP4/NIH workshop, Argonne National Laboratory, USA, June 11th-14th.
- Phenix workshop, University of Houston, Texas, USA, May 30th.
- Bio207 (The Life and Death of Proteins), Stanford University, Palo Alto, USA, April 29th.
- Recent trends in Macromolecular Structure and Function, Chennai, India, January 7th-14th.

2009

- NCCR Workshop on Crystallographic Computing with Phenix, ETH, Zurich, Switzerland, December 4th.
- XXX, IGBMC, Strasbourg, France, December 3rd.
- Phenix Workshop, IGBMC, Strasbourg, France, December 2nd.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 23rd-27th.
- SSRL Summer School, Stanford, USA, September 10th.
- American Crystallographic Association Annual Meeting, Toronto, Canada, July 26th-30th.
- CCP4/NIH workshop, Argonne National Laboratory, USA, June 29th-July 2nd.
- Mid Atlantic Structural Biology meeting, University of Maryland, Maryland, USA, May 29th.
- Quantitative Biology Seminar Series, Los Alamos National Laboratory, USA, May 27th.
- Bio207 (The Life and Death of Proteins), Stanford University, Palo Alto, USA, April 29th.
- Teach SG workshop, Prague, Czech Republic, April 1st-5th.
- DOE Genomics:GTL awardees meeting, Bethesda, USA, February 7th-11th.

2008

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 24th-28th.
- International Structural Genomics Conference, Oxford, UK, September 21st-24th.
- International Union of Crystallography Congress, Osaka, Japan, August 23rd-28th.
- Diffraction Methods in Molecular Biology, Gordon Research Conference, Lewiston, Maine, USA, July 13-18th.
- Macromolecular Crystallography Course, Beijing, China, May 10th-15th.
- New Validation Tools for the Macromolecular Crystallography, Cambridge, UK, April 14th-16th.
- Pittsburgh Conference, New Orleans, USA, March 4th-5th.
- Recent trends in Macromolecular Structure and Function, Chennai, India, January 7th-14th.

2007

- 16th CoLuAa meeting, Aarhus, Denmark, November 9th.
- X-ray Crystallography Computing Workshop, Aarhus, Denmark, November 7th-8th.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 26th-30th.
- RapiData course, Brookhaven National Laboratory, Brookhaven, USA, April XXXX.
- CCP4/MAX-INF Workshop on Phasing and Refinement, York University, UK, April XXXX.
- The Molecular Replacement method, CCP4 Study Weekend, University of Reading, UK, January XXXX.

2006

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 26th-31st.
- International Conference on Structural Genomics workshop, Yokohama, Japan, October 19th-20th.
- Distributed Data Analysis for Neutron Scattering Experiments (DANSE) meeting, Caltech, USA, Aug 15th-16th.
- European Crystallography Meeting, Leuven, Belgium, August 9th-10th.
- Neutron Diffraction Workshop, American Crystallographic Association Annual Meeting, Honolulu, Hawaii, USA, August 22nd-26th.

- Canadian Light Source 9th Annual Users Meeting, Saskatoon, Canada, June 15th-17th.
- 8th International School on the Crystallography of Biological Macromolecules, Como, Italy, May 21st-25th.
- CCP4/MAX-INF Workshop on Phasing and Refinement, Barcelona, Spain, March 1st-7th.
- Trends in Macromolecular Structure and Function, Chennai, India, January 18th-20th.

2005

- EMBL M2M Practical Course, EMBL Hamburg, Germany, November 9th-15th.
- Get Phases workshop, Peking University, Beijing, China, October 29th-November 4th.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 20th-24th.
- NCCR Practical Course, Swiss Light Source, Villigen, Switzerland, October 3rd-7th.
- SSRL Summer School, Stanford, USA, September 13-15th.
- 12th Northern Protein Structural Workshop, Galashiels, Scotland, September 7th-9th.
- EMBO Anomalous Diffraction Workshop, ESRF, Grenoble, France, June 15th-22nd.
- American Crystallographic Association Annual Meeting, Orlando, Florida, USA, May 28th-June 1st.
- Evolving Methods in Crystallography, Erice, Italy, May 11th-22nd.
- Data management for high-throughput crystallography, Cambridge University, Cambridge, UK, Feb 9th-11th.

2004

- American Crystallographic Association mmCIF workshop, CARB, Gaithersburg, Maryland, USA, Nov 16th.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 30th-Nov 2nd.
- NIH Protein Structure Initiative Advisory Committee meeting, NIH, Bethesda, USA, October 28th.
- ALS Users Meeting, Macromolecular Crystallography Workshop, USA, October 19th.
- SSRL Summer School, Stanford, USA, August 16-20th.
- EMBO course on Automated Macromolecular Structure Solution, Amsterdam, Netherlands, May 23rd-Jun 2nd.

2003

- UC Berkeley department of Bio-engineering colloquium talk, Berkeley, December 18th.
- NIH Protein Structure Initiative Advisory Committee meeting, NIH, Bethesda, USA, December 2nd.
- Frontiers in Structural Biology – the Western Canadian Structural Biology Workshop, Banff, Canada, November 21st-23rd.
- SSRL Summer School, Stanford, USA, September 16-19th.
- Aminoff Symposium, Royal Swedish Academy of Sciences, Stockholm, Sweden, September 11-12th.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 25th-30th.
- American Crystallographic Association Annual Meeting, Covington, Kentucky, USA, July 26-30th.
- NIH Data Management Workshop, NIH, Bethesda, Maryland, USA, July 10-11th.
- EMBO Anomalous Diffraction Workshop, ESRF, Grenoble, France, June 17-23rd.
- International Symposium on Diffraction Structural Biology, Tsukuba, Japan, May 28th-31st.
- Data management aspects of high-throughput structure determination, European Bioinformatics Institute, Hinxton, UK, March 14th-15th.

2002

- Getting the most from biological data: bridging the gap between experiment, analysis and simulation, LBNL offices, Washington DC, December 13th.
- Automation for High Throughput Structure Determination, Lawrence Berkeley Laboratory, USA, Dec 6th-8th.
- High-throughput Synchrotron Crystallography, Argonne National Laboratory, USA, November 20th-22nd.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 25th-28th.
- Automation of X-ray Structure Determination for Structural Genomics, Berlin, Germany, October 8th-9th.

- Diffraction Methods in Molecular Biology, Gordon Research Conference, New London, Connecticut, USA, July 14-19th.
- Berkeley & Stanford Synchrotron Radiation Summer School, Stanford, USA, July 8-12th.
- Structural Genomics Informatics and Software Integration Workshop, San Antonio, USA, May 22nd-23rd.
- EMBO Course on Automated Macromolecular Structure Solution, Heidelberg, Germany, May 7-16th.
- Interdisciplinary workshop promoting collaboration in high-throughput X-ray structure determination, Santa Fe, USA, March 22-23rd.
- High-throughput structure determination, CCP4 Study Weekend, University of York, UK, January 4-5th.

2001

- Polarizability in Biomolecular Simulations, Utah, USA, December 13th-14th.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 19th-21st.
- ALS Users Meeting, Macromolecular Crystallography Workshop, USA, October 16th.
- EMBO/MAX-INF Anomalous Diffraction Workshop, ESRF, Grenoble, France, June 18-23rd.
- West Coast Protein Crystallography Workshop, Asilomar, USA, March 25th-28th.
- ESRF High-throughput workshop, ESRF, Grenoble, France, February 20-21st.
- CCP4 Workshop on Refinement of Macromolecular Structure, York University, UK, January 3-9th.

2000

- Computational methods in structural biology, Florida State University, Tallahassee, USA, December 5th.
- SCBMB seminar, Baylor College of Medicine, Houston, USA, November 6th.
- RTG Student Seminar, Arizona State University, Tempe, USA, November 16th.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 21-23rd.
- SSRL Summer School, Stanford, USA, September 18-23rd.
- Diffraction Methods in Molecular Biology, Gordon Research Conference, Andover New Hampshire, USA, July 2-7th.
- EMBO workshop for automated macromolecular structure solution, EMBL, Grenoble, France, Mar 15-25th.
- CNS workshop, Uppsala University, Uppsala, Sweden, February 7-8th.

1999

- High-throughput methods for structural genomics, Argonne National Lab, USA, November 15-16th.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 25-27th.
- International School of Crystallography of Biological Macromolecules, Barcelona, Spain, September 9-15th.
- IUCr Crystallographic Computing School, Cambridge, UK, August 14-20th.
- XVIIIth IUCr Congress and General Assembly, Glasgow, UK, August 4-13th.
- ACA Summer Course in Crystallography, University of Georgia, USA July 12-24th.
- Automation of Structure Determination workshop, Brookhaven National Lab, USA, June 20-21st.
- 29th Mid-Atlantic Protein Crystallography Workshop, Rockville, USA, April 28-30th.
- CNS Workshop, University of Georgia, USA, April 21st.

1998

- EC and CCP4 Workshop on Refinement of Macromolecular Structure, York University, UK, Dec 14-20th.
- Advanced School of Macromolecular Crystallography, Sao Carlos, Brazil, November 29th-December 6th.
- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 25-27th.
- Diffraction Methods in Molecular Biology, Gordon Research Conference, Andover New Hampshire, USA, June 21-26th.
- Modelling and membrane proteins, Biochemical Society UK Spring Meeting, Southampton, UK, March 31st.

1997

- CCP4 Refinement and Validation Workshop, York University, UK, September 1-6th.
- Validation and Refinement of Macromolecular Structures, Oporto, Portugal, August 29-30th.
- Modelling of Membrane Proteins, University of Toronto, Canada, May 5th.
- West Coast Crystallography Workshop, Asilomar, USA, March 15-18th.

Prior to 1997

- Macromolecular Refinement, CCP4 Study Weekend, Chester College, Chester, UK, January 5-6th (1996).
- IMA Program on Protein Structure and Dynamics, University of Minnesota, Minnesota, July 18-22nd (1994).
- CECAM Workshop on Simulations of biological macromolecules: improving sampling with parallelism and other techniques. Orsay, Paris, November 15-17th (1993).

Meetings Organized**2022**

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 9th-25th. [*Course co-organizer*]
- Imaging the rhizosphere and cellular organization, online, January 26-27th. [*Workshop co-organizer*]

2021

- Intracellular organization, and material synthesis and decomposition, online, December 15-16th. [*Workshop co-organizer*]
- Molecular structures, online, October 27-28th. [*Workshop co-organizer*]

2019

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 14th-30th. [*Course co-organizer*]

2018

- Macromolecular Crystallography Course, Cold Spring Harbor Laboratory, USA, October 14th-30th. [*Course co-organizer*]

2017

- Cryo-EM model challenge, Stanford, CA, USA, October 6-8th. [*Meeting co-organizer*]
- Understanding Biology through Structure, Santa Fe, NM, USA, May 13-15th. [*Session chair*]
- Joint BSSD/ASCR session at the DOE/BER Genomic Sciences Contractors Meeting, Arlington, VA, February 7th. [*Session co-chair*]

2016

- DOE/BER Molecules to Mesoscale workshop, Rockville, MD, September 20th-23rd. [*Meeting co-chair*]

2015

- wwPDB Ligand Validation Workshop, Rutgers University, July 29-31st. [*Session co-chair*]
- EM Modeling Challenge Advisory meeting, MIT, Boston, June 19th-21st. [*Meeting co-organizer*]

2014

- Hybrid methods workshop, European Bioinformatics Institute, Hinxton, UK, October 6-7th. [*Session co-chair*]
- Soft X-ray sciences workshop, Advanced Light Source, Berkeley, CA, USA, October 1st-3rd. [*Session co-chair*]
- Diffraction Methods in Molecular Biology, Gordon Research Conference, Lewiston, Maine, USA, July 27th August 1st. [*Session chair*]
- Recent trends in Macromolecular Structure and Function, Chennai, India, January 22nd-25th. [*Member, organizing committee*]

2013

- International Conference on Structural Genomics, Sapporo, Japan, July 27th-August 1st. [*Session co-chair*]

2012

- Diffraction Methods in Molecular Biology, Gordon Research Conference, Lewiston, Maine, USA, July 15-20th. [Session chair]

2011

- Computational Methods session, International Union of Crystallography Meeting, Madrid, Spain, August 22-30th. [Session co-chair]
- Phenix Workshop, American Crystallographic Association Annual Meeting, New Orleans, USA, May 28th. [Session organizer]
- Phenix Workshop, International Conference on Structural Genomics, Toronto, Canada, May 10th. [Session co-organizer]

2010

- Diffraction Methods in Molecular Biology, Gordon Research Conference, Lewiston, Maine, USA, July 18-23rd. [Session chair]

2008

- Pittsburgh Diffraction Conference, Pittsburgh, USA, October 30th - November 1st. [Session co-organizer]
- Recent trends in Macromolecular Structure and Function, Chennai, India, January 7th-14th. [Member, organizing committee]

2007

- International Symposium on Diffraction Structural Biology, Tokyo, Japan, September 10th-13th. [Member, international advisory committee]
- Computational Methods Session, American Crystallographic Association Annual Meeting, Salt Lake City, Utah, USA, July 23rd-26th. [Session co-organizer]
- Multiscale Imaging Workshop, Lawrence Berkeley Laboratory, Berkeley USA, May 17th-18th. [Meeting co-organizer]

2006

- International Conference on Structural Genomics workshop, Yokohama, Japan, October 19th-20th. [Meeting co-organizer]
- Neutron Diffraction Workshop, American Crystallographic Association Annual Meeting, Honolulu, Hawaii, USA, August 22-26th. [Session co-organizer]
- Diffraction Methods in Molecular Biology, Gordon Research Conference, Lewiston, Maine, USA, July 11-16th. [Meeting organizer]

2004

- Computational Methods Session, American Crystallographic Association Annual Meeting, Chicago, Illinois, USA, July 17-23rd. [Session co-organizer]
- Diffraction Methods in Molecular Biology, Gordon Research Conference, Lewiston, Maine, USA, July 11-16th. [Meeting co-organizer]

2003

- NIH Data Management Workshop, NIH, Bethesda, Maryland, USA, July 10-11th. [Meeting co-organizer]

2002

- Automation for High Throughput Structure Determination, Lawrence Berkeley Laboratory, USA, December 6th-8th. [Meeting co-organizer]
- Interdisciplinary workshop promoting collaboration in high-throughput X-ray structure determination, Santa Fe, USA, March 22-23rd. [Meeting co-organizer]

Peer reviewed publications (305 total)

- I. Bhowmick A, Hussein R, Bogacz I, Simon PS, Ibrahim M, Chatterjee R, Doyle MD, Cheah MH, Fransson T, Chernev P, Kim IS, Makita H, Dasgupta M, Kaminsky CJ, Zhang M, Gätcke J, Haupt S, Nangca II, Keable SM,

- Aydin AO, Tono K, Owada S, Gee LB, Fuller FD, Batyuk A, Alonso-Mori R, Holton JM, Paley DW, Moriarty NW, Mamedov F, Adams PD, Brewster AS, Dobbek H, Sauter NK, Bergmann U, Zouni A, Messinger J, Kern J, Yano J, Yachandra VK: Structural evidence for intermediates during O₂ formation in photosystem II. *Nature* 2023, **617**:629–636.
2. Huang J, Quest A, Cruz-Morales P, Deng K, Pereira JH, Van Cura D, Kakumanu R, Baidoo EEK, Dan Q, Chen Y, Petzold CJ, Northen TR, Adams PD, Clark DS, Balskus EP, Hartwig JF, Mukhopadhyay A, Keasling JD: Complete integration of carbene-transfer chemistry into biosynthesis. *Nature* 2023, **617**:403-408.
 3. Englund E, Schmidt M, Nava AA, Lechner A, Deng K, Jocić R, Lin Y, Roberts J, Benites VT, Kakumanu R, Gin JW, Chen Y, Liu Y, Petzold CJ, Baidoo EEK, Northen TR, Adams PD, Katz L, Yuzawa S, Keasling JD: Expanding Extender Substrate Selection for Unnatural Polyketide Biosynthesis by Acyltransferase Domain Exchange within a Modular Polyketide Synthase. *J Am Chem Soc.* 2023. **145**:8822-8832.
 4. Sanders BC, Pokhrel S, Labbe AD, Mathews II, Cooper CJ, Davidson RB, Phillips G, Weiss KL, Zhang Q, O'Neill H, Kaur M, Schmidt JG, Reichard W, Surendranathan S, Parvathareddy J, Phillips L, Rainville C, Sterner DE, Kumaran D, Andi B, Babnigg G, Moriarty NW, Adams PD, Joachimiak A, Hurst BL, Kumar S, Butt TR, Jonsson CB, Ferrins L, Wakatsuki S, Galanie S, Head MS, Parks JM: Potent and selective covalent inhibition of the papain-like protease from SARS-CoV-2. *Nat Commun.* 2023 **14**:1733.
 5. Terwilliger TC, Afonine PV, Liebschner D, Croll TI, McCoy AJ, Oeffner RD, Williams CJ, Poon BK, Richardson JS, Read RJ, Adams PD: Accelerating crystal structure determination with iterative AlphaFold prediction. *Acta Cryst.* 2023, **D79**:234-244.
 6. Prabhakar PK, Pereira JH, Taujale R, Shao W, Bharadwaj VS, Chapla D, Yang JY, Bomble YJ, Moremen KW, Kannan N, Hammel M, Adams PD, Scheller HV, Urbanowicz BR: Structural and biochemical insight into a modular β -1,4-galactan synthase in plants. *Nature Plants* 2023, **9**:486-500.
 7. Dai J, Wilhelm KB, Bischoff AJ, Pereira JH, Dedeo MT, García-Almedina DM, Adams PD, Groves JT, Francis MB: A Membrane-Associated Light-Harvesting Model is Enabled by Functionalized Assemblies of Gene-Doubled TMV Proteins. *Small* 2023. Online ahead of print.
 8. Liebschner D, Moriarty NW, Poon BK, Adams PD: In situ ligand restraints from quantum-mechanical methods. *Acta Cryst.* 2023, **D79**:100-110
 9. Bloomer BJ, Natoli SN, Garcia-Borràs M, Pereira JH, Hu DB, Adams PD, Houk KN, Clark DS, Hartwig JF: Mechanistic and structural characterization of an iridium-containing cytochrome reveals kinetically relevant cofactor dynamics. *Nature Catalysis* 2023, **6**:39-51
 10. Deng K, Wang X, Ing N, Opgenorth P, de Raad M, Kim J, Simmons BA, Adams PD, Singh AK, Lee TS, Northen TR: Rapid quantification of alcohol production in microorganisms based on nanostructure-initiator mass spectrometry (NIMS) *Anal. Biochem.* 2023, **662**:114997
 11. Tom LM, Aulitto M, Wu YW, Deng K, Gao Y, Xiao N, Rodriguez BG, Louime C, Northen TR, Eudes A, Mortimer JC, Adams PD, Scheller HV, Simmons BA, Ceja-Navarro JA, Singer SW: Low-abundance populations distinguish microbiome performance in plant cell wall deconstruction. *Microbiome* 2022 **10**:183
 12. Terwilliger TC, Poon BK, Afonine PV, Schlicksup CJ, Croll TI, Millán C, Richardson JS, Read RJ, Adams PD: Improved AlphaFold modeling with implicit experimental information. *Nat Methods* 2022, **19**:1376-1382
 13. Liu AK, Pereira JH, Kehl AJ, Rosenberg DJ, Orr DJ, Chu SKS, Banda DM, Hammel M, Adams PD, Siegel JB, Shih PM: Structural plasticity enables evolution and innovation of RuBisCO assemblies. *Sci. Adv.* 2022, **8**:eadc9440
 14. Andi B, Kumaran D, Kreidler DF, Soares AS, Keereetaweep J, Jakoncic J, Lazo EO, Shi W, Fuchs MR, Sweet RM, Shanklin J, Adams PD, Schmidt JG, Head MS, McSweeney S: Hepatitis C virus NS3/4A inhibitors and other drug-like compounds as covalent binders of SARS-CoV-2 main protease. *Sci. Rep.* 2022, **12**:12197

15. Macdonald SS, Pereira JH, Liu F, Tegl G, DeGiovanni A, Wardman JF, Deutsch S, Yoshikuni Y, Adams PD, Withers SG: A Synthetic Gene Library Yields a Previously Unknown Glycoside Phosphorylase That Degrades and Assembles Poly- β -1,3-GlcNAc, Completing the Suite of β -Linked GlcNAc Polysaccharides. *ACS Central Science* 2022, **8**:430-440.
16. Westbrook JD, Young JY, Shao C, Feng Z, Guranovic V, Lawson CL, Vallat B, Adams PD, Berrisford JM, Bricogne G, Diederichs K, Joosten RP, Keller P, Moriarty NW, Sobolev OV, Velankar S, Vonrhein C, Waterman DG, Kurisu G, Berman HM, Burley SK, Peisach E: PDBx/mmCIF Ecosystem: Foundational Semantic Tools for Structural Biology. *J Mol Biol.* 2022, **434**:167599.
17. Iwai K, Wehrs M, Garber M, Sustarich J, Washburn L, Costello Z, Kim PW, Ando D, Gaillard WR, Hillson NJ, Adams PD, Mukhopadhyay A, Garcia Martin H, Singh AK: Scalable and automated CRISPR-based strain engineering using droplet microfluidics. *Microsyst Nanoeng.* 2022, **8**:31.
18. Chen Y, Kaplan Lease N, Gin JW, Ogorzalek TL, Adams PD, Hillson NJ, Petzold CJ: Modular automated bottom-up proteomic sample preparation for high-throughput applications. *PLoS One* 2022, **17**:e0264467.
19. Hancock M, Peulen TO, Webb B, Poon B, Fraser JS, Adams P, Sali A: Integration of software tools for integrative modeling of biomolecular systems. *J. Struct. Biol.* 2022, **214**:107841.
20. Hussein R, Ibrahim M, Bhowmick A, Simon PS, Chatterjee R, Lassalle L, Doyle M, Bogacz I, Kim IS, Cheah MH, Gul S, de Lichtenberg C, Chernev P, Pham CC, Young ID, Carbajo S, Fuller FD, Alonso-Mori R, Batyuk A, Sutherlin KD, Brewster AS, Bolotovskiy R, Mendez D, Holton JM, Moriarty NW, Adams PD, Bergmann U, Sauter NK, Dobbek H, Messinger J, Zouni A, Kern J, Yachandra VK, Yano J: Structural dynamics in the water and proton channels of photosystem II during the S2 to S3 transition. *Nature Communications* 2021, **12**:6531.
21. Baek M, DiMaio F, Anishchenko I, Dauparas J, Ovchinnikov S, Lee GR, Wang J, Cong Q, Kinch LN, Schaeffer RD, Millán C, Park H, Adams C, Glassman CR, DeGiovanni A, Pereira JH, Rodrigues AV, van Dijk AA, Ebrecht AC, Opperman DJ, Sagmeister T, Buhlheller C, Pavkov-Keller T, Rathinaswamy MK, Dalwadi U, Yip CK, Burke JE, Garcia KC, Grishin NV, Adams PD, Read RJ, Baker D: Accurate prediction of protein structures and interactions using a three-track neural network. *Science* 2021, **373**:871-876
22. Ibrahim M, Moriarty NW, Kern J, Holton JM, Brewster AS, Bhowmick A, Bergmann U, Zouni A, Messinger J, Yachandra VK, Yano J, Dobbek H, Sauter NK, Adams PD: Reply to Wang et al.: Clear evidence of binding of Ox to the oxygen-evolving complex of photosystem II is best observed in the omit map. *Proc Natl Acad Sci U S A.* 2021 **118**:e2102342118
23. Ing N, Deng K, Chen Y, Aulitto M, Gin JW, Pham TLM, Petzold CJ, Singer SW, Bowen B, Sale KL, Simmons BA, Singh AK, Adams PD, Northen TR: A multiplexed nanostructure-initiator mass spectrometry (NIMS) assay for simultaneously detecting glycosyl hydrolase and lignin modifying enzyme activities. *Sci Rep.* 2021 **11**:11803
24. Pham LTM, Deng K, Northen TR, Singer SW, Adams PD, Simmons BA, Sale KL: Experimental and theoretical insights into the effects of pH on catalysis of bond-cleavage by the lignin peroxidase isozyme H8 from *Phanerochaete chrysosporium*. *Biotechnol Biofuels.* 2021, **14**:108
25. Lui LM, Majumder EL, Smith HJ, Carlson HK, von Netzer F, Fields MW, Stahl DA, Zhou J, Hazen TC, Baliga NS, Adams PD, Arkin AP: Mechanism Across Scales: A Holistic Modeling Framework Integrating Laboratory and Field Studies for Microbial Ecology. *Front Microbiol.* 2021, **12**:642422.
26. Terwilliger TC, Sobolev OV, Afonine PV, Adams PD, Ho CM, Li X, Zhou ZH: Protein identification from electron cryomicroscopy maps by automated model building and side-chain matching. *Acta Cryst.* 2021, **D77**:457-462
27. van Zundert GCP, Moriarty NW, Sobolev OV, Adams PD, Borrelli KW: Macromolecular refinement of X-ray and cryoelectron microscopy structures with Phenix/OPLS3e for improved structure and ligand quality. *Structure* 2021, **29**:913-921.e4

28. Teze D, Coines J, Fredslund F, Dubey KD, Bidart GN, Adams PD, Dueber JE, Svensson B, Rovira C, Welner DH: O-/N-/S-Specificity in Glycosyltransferase Catalysis: From Mechanistic Understanding to Engineering. *ACS Catalysis* 2021, **11**:1810-1815.
29. Kim J, Baidoo EEK, Amer B, Mukhopadhyay A, Adams PD, Simmons BA, Lee TS: Engineering *Saccharomyces cerevisiae* for isoprenol production. *Metab Eng.* 2021, **64**:154-166.
30. Lawson CL, Kryshtafovych A, Adams PD, Afonine PV, Baker ML, Barad BA, Bond P, Burnley T, Cao R, Cheng J, Chojnowski G, Cowtan K, Dill KA, DiMaio F, Farrell DP, Fraser JS, Herzik MA Jr, Hoh SW, Hou J, Hung LV, Igaev M, Joseph AP, Kihara D, Kumar D, Mittal S, Monastyrskyy B, Olek M, Palmer CM, Patwardhan A, Perez A, Pfab J, Pintilie GD, Richardson JS, Rosenthal PB, Sarkar D, Schäfer LU, Schmid MF, Schröder GF, Shekhar M, Si D, Singharoy A, Terashi G, Terwilliger TC, Vaiana A, Wang L, Wang Z, Wankowicz SA, Williams CJ, Winn M, Wu T, Yu X, Zhang K, Berman HM, Chiu W: Cryo-EM model validation recommendations based on outcomes of the 2019 EMDDataResource challenge. *Nature Meth.* 2021, **18**:156-164.
31. Wang X, Pereira JH, Tsutakawa S, Fang X, Adams PD, Mukhopadhyay A, Lee TS: Efficient production of oxidized terpenoids via engineering fusion proteins of terpene synthase and cytochrome P450. *Metab. Eng.* 2021, **64**:41-51.
32. Liebschner D, Afonine PV, Moriarty NW, Poon BK, Chen VB, Adams PD: CERES: a cryo-EM re-refinement system for continuous improvement of deposited models. *Acta Cryst.* 2021, **D77**:48-61.
33. Moriarty NW, Liebschner D, Tronrud DE, Adams PD: Arginine off-kilter: guanidinium is not as planar as restraints denote. *Acta Cryst.* 2020, **D76**:1159-1166.
34. Ge X, Thorgersen MP, Poole FL 2nd, Deutschbauer AM, Chandonia JM, Novichkov PS, Gushgari-Doyle S, Lui LM, Nielsen T, Chakraborty R, Adams PD, Arkin AP, Hazen TC, Adams MWW: Characterization of a Metal-Resistant *Bacillus* Strain With a High Molybdate Affinity ModA From Contaminated Sediments at the Oak Ridge Reservation. *Front Microbiol.* 2020, **11**:587127.
35. Ge X, Thorgersen MP, Poole FL 2nd, Deutschbauer AM, Chandonia JM, Novichkov PS, Adams PD, Arkin AP, Hazen TC, Adams MWW: Draft Genome Sequence of *Bacillus* sp. Strain EB106-08-02-XG196, Isolated from High-Nitrate-Contaminated Sediment. *Microbiol Resour Announc.* 2020, **9**:e01149-20.
36. Terwilliger TC, Sobolev OV, Afonine PV, Adams PD, Read RJ: Density modification of cryo-EM maps. *Acta Cryst.* 2020, **D76**:912-925.
37. Banda DM, Pereira JH, Liu AK, Orr DJ, Hammel M, He C, Parry MAJ, Carmo-Silva E, Adams PD, Banfield JF, Shih PM: Novel bacterial clade reveals origin of form I Rubisco. *Nature Plants* 2020, **6**:1158-1166.
38. Sobolev OV, Afonine PV, Moriarty NW, Hekkelman ML, Joosten RP, Perrakis A, Adams PD: A Global Ramachandran Score Identifies Protein Structures with Unlikely Stereochemistry. *Structure* 2020, **28**:1249-1258.e2.
39. Terwilliger TC, Ludtke SJ, Read RJ, Adams PD, Afonine PV: Improvement of cryo-EM maps by density modification. *Nature Methods* 2020, **9**:923-927.
40. Thompson MG, Blake-Hedges JM, Pereira JH, Hangasky JA, Belcher MS, Moore WM, Barajas JF, Cruz-Morales P, Washington LJ, Haushalter RW, Eiben CB, Liu Y, Skyrud W, Benites VT, Barnum TP, Baidoo EEK, Scheller HV, Marletta MA, Shih PM, Adams PD, Keasling JD: An iron (II) dependent oxygenase performs the last missing step of plant lysine catabolism. *Nat Commun.* 2020, **11**:2931.
41. Ibrahim M, Fransson T, Chatterjee R, Cheah MH, Hussein R, Lassalle L, Sutherlin KD, Young ID, Fuller FD, Gul S, Kim IS, Simon PS, de Lichtenberg C, Chernev P, Bogacz I, Pham CC, Orville AM, Saichek N, Northen T, Batyuk A, Carbajo S, Alonso-Mori R, Tono K, Owada S, Bhowmick A, Bolotovskiy R, Mendez D, Moriarty NW, Holton JM, Dobbek H, Brewster AS, Adams PD, Sauter NK, Bergmann U, Zouni A, Messinger J, Kern J, Yachandra VK, Yano J: Untangling the sequence of events during the S2 → S3 transition in photosystem II and implications for the water oxidation mechanism. *Proc Natl Acad Sci U S A.* 2020, **117**:12624-12635.

42. Curran SC, Pereira JH, Baluyot MJ, Lake J, Puetz H, Rosenburg DJ, Adams P, Keasling JD: Structure and Function of BorB, the Type II Thioesterase from the Borrelidin Biosynthetic Gene Cluster. *Biochemistry* 2020, **59**:1630-1639.
43. Park MR, Chen Y, Thompson M, Benites VT, Fong B, Petzold CJ, Baidoo EEK, Gladden JM, Adams PD, Keasling JD, Simmons BA, Singer SW: Response of *Pseudomonas putida* to Complex, Aromatic-Rich Fractions from Biomass. *ChemSusChem*. 2020, **13**:1–14.
44. Moriarty NW, Janowski PA, Swails JM, Nguyen H, Richardson JS, Case DA, Adams PD: Improved chemistry restraints for crystallographic refinement by integrating the Amber force field into Phenix. *Acta Cryst*. 2020, **76**:51-62.
45. Blake-Hedges JM, Pereira JH, Cruz-Morales P, Thompson MG, Barajas JF, Chen J, Krishna RN, Chan LJG, Nimlos D, Alonso-Martinez C, Baidoo EEK, Chen Y, Gin JW, Katz L, Petzold CJ, Adams PD, Keasling JD: Structural mechanism of regioselectivity in an unusual bacterial acyl-CoA dehydrogenase. *J Am Chem Soc*. 2020, **142**:835-846.
46. Terwilliger TC, Adams PD, Afonine PV, Sobolev OV: Cryo-EM map interpretation and protein model-building using iterative map segmentation. *Protein Sci*. 2020, **29**:87-99.
47. Berman HM, Adams PD, Bonvin AA, Burley SK, Carragher B, Chiu W, DiMaio F, Ferrin TE, Gabanyi MJ, Goddard TD, Griffin PR, Haas J, Hanke CA, Hoch JC, Hummer G, Kurisu G, Lawson CL, Leitner A, Markley JL, Meiler J, Montelione GT, Phillips GN Jr, Prisner T, Rappsilber J, Schriemer DC, Schwede T, Seidel CAM, Strutzenberg TS, Svergun DI, Tajkhorshid E, Trewhella J, Vallat B, Velankar S, Vuister GW, Webb B, Westbrook JD, White KL, Sali A: Federating Structural Models and Data: Outcomes from A Workshop on Archiving Integrative Structures. *Structure* 2019, **27**:1745-1759.
48. Liebschner D, Afonine PV, Baker ML, Bunkóczi G, Chen VB, Croll TI, Hintze B, Hung LW, Jain S, McCoy AJ, Moriarty NW, Oeffner RD, Poon BK, Prisant MG, Read RJ, Richardson JS, Richardson DC, Sammito MD, Sobolev OV, Stockwell DH, Terwilliger TC, Urzhumtsev AG, Videau LL, Williams CJ, Adams PD: Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in Phenix. *Acta Cryst*. 2019, **75**:861-877.
49. Kang A, Mendez-Perez D, Goh EB, Baidoo EEK, Benites VT, Beller HR, Keasling JD, Adams PD, Mukhopadhyay A, Lee TS: Optimization of the IPP-bypass mevalonate pathway and fed-batch fermentation for the production of isoprenol in *Escherichia coli*. *Metab Eng*. 2019, **56**:85-96.
50. Chen Y, Guenther JM, Gin JW, Chan LJG, Costello Z, Ogorzalek TL, Tran HM, Blake-Hedges JM, Keasling JD, Adams PD, García Martín H, Hillson NJ, Petzold CJ: Automated "Cells-To-Peptides" Sample Preparation Workflow for High-Throughput, Quantitative Proteomic Assays of Microbes. *J Proteome Res*. 2019, **18**:3752-3761.
51. Kim DN, Moriarty NW, Kirmizialtin S, Afonine PV, Poon B, Sobolev OV, Adams PD, Sanbonmatsu K: Cryo_fit: Democratization of flexible fitting for cryo-EM. *J Struct Biol*. 2019, **208**:1-6.
52. Barajas JF, McAndrew RP, Thompson MG, Backman TWH, Pang B, de Rond T, Pereira JH, Benites VT, Martín HG, Baidoo EEK, Hillson NJ, Adams PD, Keasling JD: Structural insights into dehydratase substrate selection for the borrelidin and fluvirucin polyketide synthases. *J Ind Microbiol Biotechnol*. 2019, **46**:1225-1235.
53. Thompson MG, Blake-Hedges JM, Cruz-Morales P, Barajas JF, Curran SC, Eiben CB, Harris NC, Benites VT, Gin JW, Sharpless WA, Twigg FF, Skyrud W, Krishna RN, Pereira JH, Baidoo EEK, Petzold CJ, Adams PD, Arkin AP, Deutschbauer AM, Keasling JD: Massively Parallel Fitness Profiling Reveals Multiple Novel Enzymes in *Pseudomonas putida* Lysine Metabolism. *MBio* 2019, **10**:e02577-18.
54. Adams PD, Afonine PV, Baskaran K, Berman HM, Berrisford J, Bricogne G, Brown DG, Burley SK, Chen M, Feng Z, Flensburg C, Gutmanas A, Hoch JC, Ikegawa Y, Kengaku Y, Krissinel E, Kurisu G, Liang Y, Liebschner D, Mak L, Markley JL, Moriarty NW, Murshudov GN, Noble M, Peisach E, Persikova I, Poon BK, Sobolev OV,

- Ulrich EL, Velankar S, Vonrhein C, Westbrook J, Wojdyr M, Yokochi M, Young JY: Announcing mandatory submission of PDBx/mmCIF format files for crystallographic depositions to the Protein Data Bank (PDB). *Acta Cryst* 2019, **75**:451-454.
55. Dong J, Chen Y, Benites VT, Baidoo EEK, Petzold CJ, Beller HR, Eudes A, Scheller HV, Adams PD, Mukhopadhyay A, Simmons BA, Singer SW: Methyl ketone production by *Pseudomonas putida* is enhanced by plant-derived amino acids. *Biotechnol Bioeng*. 2019, **116**:1909-1922.
 56. Chen Y, Vu J, Thompson MG, Sharpless WA, Chan LJG, Gin JW, Keasling JD, Adams PD, Petzold CJ: A rapid methods development workflow for high-throughput quantitative proteomic applications. *PLoS One*. 2019 **14**:e0211582.
 57. Moriarty NW, Adams PD: Iron-sulfur clusters have no right angles. *Acta Cryst*. 2019, **D75**:16-20.
 58. Kern J, Chatterjee R, Young ID, Fuller FD, Lassalle L, Ibrahim M, Gul S, Fransson T, Brewster AS, Alonso-Mori R, Hussein R, Zhang M, Douthit L, de Lichtenberg C, Cheah MH, Shevela D, Wersig J, Seuffert I, Sokaras D, Pastor E, Weninger C, Kroll T, Sierra RG, Aller P, Butryn A, Orville AM, Liang M, Batyuk A, Koglin JE, Carbajo S, Boutet S, Moriarty NW, Holton JM, Dobbek H, Adams PD, Bergmann U, Sauter NK, Zouni A, Messinger J, Yano J, Yachandra VK: Structures of the intermediates of Kok's photosynthetic water oxidation clock. *Nature* 2018, **563**:421-425.
 59. Liu CL, Tian T, Alonso-Gutierrez J, Garabedian B, Wang S, Baidoo EEK, Benites V, Chen Y, Petzold CJ, Adams PD, Keasling JD, Tan T, Lee TS: Renewable production of high density jet fuel precursor sesquiterpenes from *Escherichia coli*. *Biotechnol Biofuels* 2018, **11**:285.
 60. Terwilliger TC, Adams PD, Afonine PV, Sobolev OV: A fully automatic method yielding initial models from high-resolution cryo-electron microscopy maps. *Nat Methods* 2018, **15**:905-908.
 61. Ge X, Vaccaro BJ, Thorgersen MP, Poole FL 2nd, Majumder EL, Zane GM, De León KB, Lancaster WA, Moon JW, Paradis CJ, von Netzer F, Stahl DA, Adams PD, Arkin AP, Wall JD, Hazen TC, Adams MWW: Iron- and Aluminum-Induced Depletion of Molybdenum in Acidic Environments Impedes the Nitrogen Cycle. *Environ Microbiol*. 2018, **21**:152-163.
 62. Deng K, Zeng J, Cheng G, Gao J, Sale KL, Simmons BA, Singh AK, Adams PD, Northen TR: Rapid characterization of the activities of lignin-modifying enzymes based on nanostructure-initiator mass spectrometry (NIMS). *Biotechnol Biofuels* 2018, **11**:266.
 63. Kryshtafovych A, Monastyrskyy B, Adams PD, Lawson CL, Chiu W: Distribution of evaluation scores for the models submitted to the second cryo-EM model challenge. *Data Brief* 2018, **20**:1629-1638.
 64. Afonine PV, Klaholz BP, Moriarty NW, Poon BK, Sobolev OV, Terwilliger TC, Adams PD, Urzhumtsev A: New tools for the analysis and validation of cryo-EM maps and atomic models. *Acta Cryst*. 2018, **D74**:814-840.
 65. Rugg TL, Pereira JH, Chen JC, DeGiovanni A, Novichkov P, Mutalik VK, Tomaleri GP, Singer SW, Hillson NJ, Simmons BA, Adams PD, Thelen MP: Jungle Express is a versatile repressor system for tight transcriptional control. *Nature Comm*. 2018, **9**:3617.
 66. Liebschner D, Afonine PV, Moriarty NW, Langan P, Adams PD: Evaluation of models determined by neutron diffraction and proposed improvements to their validation and deposition. *Acta Cryst*. 2018, **D74**:800-813.
 67. Terwilliger TC, Adams PD, Afonine PV, Sobolev OV: Map segmentation, automated model-building and their application to the Cryo-EM Model Challenge. *J. Struct. Biol*. 2018, **204**:338-343.
 68. Kryshtafovych A, Adams PD, Lawson CL, Chiu W: Evaluation system and web infrastructure for the second cryo-EM model challenge. *J. Struct. Biol*. 2018, **204**:96-108.
 69. Ellinghaus TL, Pereira JH, McAndrew RP, Welner DH, DeGiovanni AM, Guenther JM, Tran HM, Feldman T, Simmons BA, Sale KL, Adams PD: Engineering glycoside hydrolase stability by the introduction of zinc binding. *Acta Cryst*. 2018, **D74**:702-710.

70. Afonine PV, Adams PD, Urzhumtsev A: From deep TLS validation to ensembles of atomic models built from elemental motions. II. Analysis of TLS refinement results by explicit interpretation. *Acta Cryst.* 2018, **D74**:621-631.
71. Terwilliger TC, Sobolev OV, Afonine PV, Adams PD: Automated map sharpening by maximization of detail and connectivity. *Acta Cryst.* 2018, **D74**:545-559.
72. Afonine PV, Poon BK, Read RJ, Sobolev OV, Terwilliger TC, Urzhumtsev A, Adams PD: Real-space refinement in PHENIX for cryo-EM and crystallography. *Acta Cryst.* 2018, **D74**:531-544.
73. Beller HR, Rodrigues AV, Zargar K, Wu Y-W, Saini AV, Saville RM, Pereira JH, Adams PD, Tringe SG, Petzold CJ, Keasling JD: Discovery of enzymes for toluene synthesis from anoxic microbial communities. *Nature Chem. Biol.* 2018, **14**:451-457
74. George KW, Thompson M, Kim J, Baidoo EEK, Wang G, Benites VT, Petzold CJ, Chan LJG, Yilmaz S, Turhanen P, Adams PD, Keasling JD, Lee TS: Integrated analysis of isopentenyl pyrophosphate (IPP) toxicity in isoprenoid-producing *Escherichia coli*. *Metab Eng.* 2018, **47**:60-72.
75. Chodkiewicz ML, Migacz S, Rudnicki W, Makal A, Kalinowski JA, Moriarty NW, Grosse-Kunstleve RW, Afonine PV, Adams PD, Dominiak PM: DiSCaMB: a software library for aspherical atom model X-ray scattering factor calculations with CPUs and GPUs. *J. Appl. Cryst.* 2018, **51**:193-199.
76. He Z, Zhang P, Wu L, Rocha AM, Tu Q, Shi Z, Wu B, Qin Y, Wang J, Yan Q, Curtis D, Ning D, Van Nostrand JD, Wu L, Yang Y, Elias DA, Watson DB, Adams MWW, Fields MW, Alm EJ, Hazen TC, Adams PD, Arkin AP, Zhou J: Microbial Functional Gene Diversity Predicts Groundwater Contamination and Ecosystem Functioning. *MBio.* 2018, **9**:e02435-17.
77. Hsu TM, Welner DH, Russ ZN, Cervantes B, Prathuri RL, Adams PD, Dueber JE: Employing a biochemical protecting group for a sustainable indigo dyeing strategy. *Nature Chem. Biol.* 2018, **14**:256-261.
78. Kolinko S, Wu YW, Tachea F, Denzel E, Hiras J, Gabriel R, Bäcker N, Chan LJG, Eichorst SA, Frey D, Chen Q, Azadi P, Adams PD, Pray TR, Tanjore D, Petzold CJ, Gladden JM, Simmons BA, Singer SW: A bacterial pioneer produces cellulase complexes that persist through community succession. *Nature Microbiol.* 2018, **3**:99-107.
79. Williams CJ, Headd JJ, Moriarty NW, Prisant MG, Videau LL, Deis LN, Verma V, Keedy DA, Hintze BJ, Chen VB, Jain S, Lewis SM, Arendall WB 3rd, Snoeyink J, Adams PD, Lovell SC, Richardson JS, Richardson DC: MolProbity: More and better reference data for improved all-atom structure validation. *Protein Sci.* 2018, **27**:293-311.
80. Amaike Campen S, Lynn J, Sibert SJ, Srikrishnan S, Phatale P, Feldman T, Guenther JM, Hiras J, Tran YTA, Singer SW, Adams PD, Sale KL, Simmons BA, Baker SE, Magnuson JK, Gladden JM: Expression of naturally ionic liquid-tolerant thermophilic cellulases in *Aspergillus niger*. *PLoS One* 2017, **12**:e0189604.
81. Alonso-Gutierrez J, Koma D, Hu Q, Yang Y, Chan LJG, Petzold CJ, Adams PD, Vickers CE, Nielsen LK, Keasling JD, Lee TS: Towards industrial production of isoprenoids in *Escherichia coli*: lessons learned from CRISPR-Cas9 based optimization of a chromosomally integrated mevalonate pathway. *Biotechnol Bioeng.* 2017, **115**:1000-1013.
82. Greber BJ, Nguyen THD, Fang J, Afonine PV, Adams PD, Nogales E: The cryo-electron microscopy structure of human transcription factor IIH. *Nature* 2017, **549**:414-417.
83. Moriarty NW, Liebschner D, Klei HE, Echols N, Afonine PV, Headd J, Poon BK, Adams PD: Interactive Comparison and Remediation of Collections of Macromolecular Structures. *Protein Sci.* 2017, **27**:182-194.
84. Pereira JH, McAndrew RP, Tomaleri GP, Adams PD: Berkeley Screen: a set of 96 solutions for general macromolecular crystallization. *J. Appl. Cryst.* 2017, **50**:1352-1358.
85. Morrell W, Birkel G, Forrer M, Lopez T, Backman T, Dussault M, Petzold CJ, Baidoo EEK, Costello Z, Ando D, Alonso Gutierrez J, George K, Mukhopadhyay A, Vaino I, Keasling JD, Adams PD, Hillson NJ, Garcia Martin H:

The Experiment Data Depot: a web-based software tool for biological experimental data storage, sharing, and visualization. *ACS Synth Biol.* 2017, **6**:2248-2259.

86. McAndrew RP, Sathitsuksanoh N, Mbughuni MM, Heins RA, Pereira JH, George A, Sale KL, Fox BG, Simmons BA, Adams PD: Reply to Kiser: Dioxygen binding in NOVI crystal structures. *Proc Natl Acad Sci U S A* 2017, **114**:E6029-E6030.
87. Pereira JH, McAndrew RP, Sergeeva OA, Ralston CY, King JA, Adams PD: Structure of the human TRiC/CCT Subunit 5 associated with hereditary sensory neuropathy. *Sci. Rep.* 2017, **16**:3673.
88. Welner DH, Shin D, Tomaleri GP, DeGiovanni AM, Tsai AY, Tran HM, Hansen SF, Green DT, Scheller HV, Adams PD: Plant cell wall glycosyltransferases: High-throughput recombinant expression screening and general requirements for these challenging enzymes. *PLoS One* 2017, **12**:e0177591.
89. Kohler AC, Mills MJL, Adams PD, Simmons BA, Sale KL: Structure of aryl O-demethylase offers molecular insight into a catalytic tyrosine-dependent mechanism. *Proc Natl Acad Sci U S A* 2017, **114**:E3205-E3214.
90. Mendez-Perez D, Alonso-Gutierrez J, Hu Q, Molinas M, Baidoo EE, Wang G, Chan LJ, Adams PD, Petzold CJ, Keasling JD, Lee TS: Production of jet fuel precursor monoterpenoids from engineered *Escherichia coli*. *Biotechnol Bioeng.* 2017, **114**:1703-1712.
91. Welner DH, Tsai AY, DeGiovanni AM, Scheller HV, Adams PD: X-ray diffraction analysis and in vitro characterization of the UAM2 protein from *Oryza sativa*. *Acta Cryst* 2017, **F73**:241-245.
92. Hryc CF, Chen DH, Afonine PV, Jakana J, Wang Z, Haase-Pettingell C, Jiang W, Adams PD, King JA, Schmid MF, Chiu W: Accurate model annotation of a near-atomic resolution cryo-EM map. *Proc Natl Acad Sci U S A* 2017, **114**:3103-3108.
93. Liebschner D, Afonine PV, Moriarty NW, Poon BK, Sobolev OV, Terwilliger TC, Adams PD: Polder maps: improving OMIT maps by excluding bulk solvent. *Acta Cryst.* 2017, **D73**:148-157
94. Moriarty NW, Draizen EJ, Adams PD: An editor for the generation and customization of geometry restraints. *Acta Cryst.* 2017, **D73**:123-130
95. Heinemann J, Deng K, Shih SC, Gao J, Adams PD, Singh AK, Northen TR: On-chip integration of droplet microfluidics and nanostructure-initiator mass spectrometry for enzyme screening. *Lab Chip* 2017, **17**:323-331
96. Yuzawa S, Deng K, Wang G, Baidoo EE, Northen TR, Adams PD, Katz L, Keasling JD: Comprehensive in Vitro Analysis of Acyltransferase Domain Exchanges in Modular Polyketide Synthases and Its Application for Short-Chain Ketone Production. *ACS Synth. Biol.* 2017, **6**:139-147
97. McAndrew RP, Sathitsuksanoh N, Mbughuni MM, Heins RA, Pereira JH, George A, Sale KL, Fox BG, Simmons BA, Adams PD: Structure and mechanism of NOVI, a resveratrol-cleaving dioxygenase. *Proc Natl Acad Sci U S A* 2016, **113**:14324-14329
98. Young ID, Ibrahim M, Chatterjee R, Gul S, Fuller FD, Koroidov S, Brewster AS, Tran R, Alonso-Mori R, Kroll T, Michels-Clark T, Laksmono H, Sierra RG, Stan CA, Hussein R, Zhang M, Douthit L, Kubin M, de Lichtenberg C, Vo Pham L, Nilsson H, Cheah MH, Shevela D, Saracini C, Bean MA, Seuffert I, Sokaras D, Weng TC, Pastor E, Weninger C, Fransson T, Lassalle L, Bräuer P, Aller P, Docker PT, Andi B, Orville AM, Glowacka JM, Nelson S, Sikorski M, Zhu D, Hunter MS, Lane TJ, Aquila A, Koglin JE, Robinson J, Liang M, Boutet S, Lyubimov AY, Uervirojnangkoorn M, Moriarty NW, Liebschner D, Afonine PV, Waterman DG, Evans G, Wernet P, Dobbek H, Weis WI, Brunger AT, Zwart PH, Adams PD, Zouni A, Messinger J, Bergmann U, Sauter NK, Kern J, Yachandra VK, Yano J: Structure of photosystem II and substrate binding at room temperature. *Nature* 2016, **540**:453-457
99. Urzhumtsev A, Afonine PV, Van Benschoten AH, Fraser JS, Adams PD: From deep TLS validation to ensembles of atomic models built from elemental motions. Addenda and corrigendum. *Acta Cryst.* 2016, **D72**:1073-1075

100. Janowski PA, Moriarty NW, Kelley BP, Case DA, York DM, Adams PD, Warren GL: Improved ligand geometries in crystallographic refinement using AFITT in PHENIX. *Acta Cryst.* 2016, **D72**:1062-7
101. Hiras J, Wu YW, Deng K, Nicora CD, Aldrich JT, Frey D, Kolinko S, Robinson EW, Jacobs JM, Adams PD, Northen TR, Simmons BA, Singer SW: Comparative Community Proteomics Demonstrates the Unexpected Importance of Actinobacterial Glycoside Hydrolase Family 12 Protein for Crystalline Cellulose Hydrolysis. *MBio* 2016, **2**:e01106-16
102. Brunk E, George KW, Alonso-Gutierrez J, Thompson M, Baidoo E, Wang G, Petzold CJ, McCloskey D, Monk J, Yang L, O'Brien EJ, Batth TS, Martin HG, Feist A, Adams PD, Keasling JD, Palsson BO, Lee TS: Characterizing Strain Variation in Engineered E. coli Using a Multi-Omics-Based Workflow. *Cell Syst.* 2016, **2**:335-46
103. Sauter NK, Echols N, Adams PD, Zwart PH, Kern J, Brewster AS, Koroidov S, Alonso-Mori R, Zouni A, Messinger J, Bergmann U, Yano J, Yachandra VK: No observable conformational changes in PSII. *Nature* 2016, **533**:E1-2
104. Adams PD, Aertgeerts K, Bauer C, Bell JA, Berman HM, Bhat TN, Blaney JM, Bolton E, Bricogne G, Brown D, Burley SK, Case DA, Clark KL, Darden T, Emsley P, Feher VA, Feng Z, Groom CR, Harris SF, Hendle J, Holder T, Joachimiak A, Kleywegt GJ, Krojer T, Marcotrigiano J, Mark AE, Markley JL, Miller M, Minor W, Montelione GT, Murshudov G, Nakagawa A, Nakamura H, Nicholls A, Nicklaus M, Nolte RT, Padyana AK, Peishoff CE, Pieniazek S, Read RJ, Shao C, Sheriff S, Smart O, Soisson S, Spurlino J, Stouch T, Svobodova R, Tempel W, Terwilliger TC, Tronrud D, Velankar S, Ward SC, Warren GL, Westbrook JD, Williams P, Yang H, Young J: Outcome of the First wwPDB/CCDC/D3R Ligand Validation Workshop. *Structure* 2016, **24**:502-8
105. Pereira JH, Heins RA, Gall DL, McAndrew RP, Deng K, Holland KC, Donohue TJ, Noguera DR, Simmons BA, Sale KL, Ralph J, Adams PD: Structural and Biochemical Characterization of the Early and Late Enzymes in the Lignin β -aryl Ether Cleavage Pathway from *Sphingobium* sp SYK-6. *J Biol Chem.* 2016, **291**:10228-38
106. Terwilliger TC, Bunkóczi G, Hung L-W, Zwart PH, Smith JL, Akey DL, Adams PD: Can I solve my structure by SAD phasing? Planning an experiment, scaling data and evaluating the useful anomalous correlation and anomalous signal. *Acta Cryst.* 2016, **72**:359-374
107. Terwilliger TC, Bunkóczi G, Hung L-W, Zwart PH, Smith JL, Akey DL, Adams PD: Can I solve my structure by SAD phasing? Anomalous signal in SAD phasing. *Acta Cryst.* 2016, **72**:346-358
108. Moriarty NW, Tronrud DE, Adams PD, Karplus PA: A new default restraint library for the protein backbone in Phenix: a conformation-dependent geometry goes mainstream. *Acta Cryst.* 2016, **72**:176-179
109. Eudes A, Pereira JH, Yogiswara S, Wang G, Teixeira Benites V, Baidoo EE, Lee TS, Adams PD, Keasling JD, Loqué D: Exploiting The Substrate Promiscuity of Hydroxycinnamoyl-CoA:shikimate Hydroxycinnamoyl Transferase to Reduce Lignin. *Plant Cell Physiol.* 2016, **57**:568-79
110. Gach PC, Shih SC, Sustarich J, Keasling JD, Hillson NJ, Adams PD, Singh AK: A Droplet Microfluidic Platform for Automating Genetic Engineering. *ACS Synthetic Biology* 2016, **5**:426-433
111. Sun L, Singh S, Joo M, Vega-Sanchez M, Ronald P, Simmons BA, Adams P, Auer M: Non-invasive imaging of cellulose microfibril orientation within plant cell walls by polarized Raman microspectroscopy. *Biotechnol Bioeng.* 2016, **113**:82-90
112. Walker JA, Takasuka TE, Deng K, Bianchetti CM, Udell HS, Prom BM, Kim H, Adams PD, Northen TR, Fox BG: Multifunctional cellulase catalysis targeted by fusion to different carbohydrate-binding modules. *Biotechnol Biofuels* 2015, **8**:220
113. Helmich KE, Pereira JH, Gall DL, Heins RA, McAndrew RP Jr, Bingman CA, Deng K, Holland KC, Noguera DR, Simmons BA, Sale KL, Ralph J, Donohue TJ, Adams PD, Phillips GN Jr: Structural basis of stereospecificity in the bacterial enzymatic cleavage of β -aryl ether bonds in lignin. *J Biol Chem.* 2015, **291**:5234-46

114. Schwessinger B, Li X, Ellinghaus TL, Chan LJ, Wei T, Joe A, Thomas N, Pruitt R, Adams PD, Chern MS, Petzold CJ, Liu CC, Ronald PC: A second-generation expression system for tyrosine-sulfated proteins and its application in crop protection. *Integrative Biology* 2015, **8**:542-5
115. Deng K, Takasuka TE, Bianchetti CM, Bergeman LF, Adams PD, Northen TR, Fox BG: Use of Nanostructure-Initiator Mass Spectrometry to Deduce Selectivity of Reaction in Glycoside Hydrolases. *Front Bioeng Biotechnol* 2015, **3**:165
116. Deng K, Guenther JM, Gao J, Bowen BP, Tran H, Reyes-Ortiz V, Cheng X, Sathitsuksanoh N, Heins R, Takasuka TE, Bergeman LF, Geertz-Hansen H, Deutsch S, Loqué D, Sale KL, Simmons BA, Adams PD, Singh AK, Fox BG, Northen TR: Development of a High Throughput Platform for Screening Glycoside Hydrolases Based on Oxime-NIMS. *Front Bioeng Biotechnol* 2015, **3**:153
117. Barad BA, Echols N, Wang RY, Cheng Y, DiMaio F, Adams PD, Fraser JS: EMRinger: side chain-directed model and map validation for 3D cryo-electron microscopy. *Nature Methods* 2015, **12**:943-6
118. Urzhumtsev A, Afonine PV, Van Benschoten AH, Fraser JS, Adams PD: From deep TLS validation to ensembles of atomic models built from elemental motions. *Acta Cryst.* 2015, **71**:1668-83.
119. Van Benschoten AH, Afonine PV, Terwilliger TC, Wall ME, Jackson CJ, Sauter NK, Adams PD, Urzhumtsev A, Fraser JS: Predicting X-ray diffuse scattering from translation-libration-screw structural ensembles. *Acta Cryst.* 2015, **71**:1657-67.
120. Sobolev OV, Afonine PV, Adams PD, Urzhumtsev A: Programming new geometry restraints: parallelity of atomic groups. *J. Appl. Cryst.* 2015, **48**:1130-1141.
121. Sali A, Berman HM, Schwede T, Trewhella J, Kleywegt G, Burley SK, Markley J, Nakamura H, Adams P, Bonvin AM, Chiu W, Peraro MD, Di Maio F, Ferrin TE, Grünwald K, Gutmanas A, Henderson R, Hummer G, Iwasaki K, Johnson G, Lawson CL, Meiler J, Marti-Renom MA, Montelione GT, Nilges M, Nussinov R, Patwardhan A, Rappsilber J, Read RJ, Saibil H, Schröder GF, Schwieters CD, Seidel CA, Svergun D, Topf M, Ulrich EL, Velankar S, Westbrook JD: Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. *Structure* 2015, **23**:1156-67
122. Shih SC, Goyal G, Kim PW, Koutsoubelis N, Keasling JD, Adams PD, Hillson NJ, Singh AK: A Versatile Microfluidic Device for Automating Synthetic Biology. *ACS Synth Biol.* 2015, **4**:1151-64.
123. George KW, Thompson MG, Kang A, Baidoo E, Wang G, Chan LJ, Adams PD, Petzold CJ, Keasling JD, Soon Lee T: Metabolic engineering for the high-yield production of isoprenoid-based C5 alcohols in *E. coli*. *Sci Rep.* 2015, **5**:11128.
124. Gutmanas A, Adams PD, Bardiaux B, Berman HM, Case DA, Fogh RH, Güntert P, Hendrickx PM, Herrmann T, Kleywegt GJ, Kobayashi N, Lange OF, Markley JL, Montelione GT, Nilges M, Ragan TJ, Schwieters CD, Tejero R, Ulrich EL, Velankar S, Vranken WF, Wedell JR, Westbrook J, Wishart DS, Vuister GW: NMR Exchange Format: a unified and open standard for representation of NMR restraint data. *Nat. Struct. Mol. Biol.* 2015, **22**:433-4.
125. Smith MB, Rocha AM, Smillie CS, Olesen SW, Paradis C, Wu L, Campbell JH, Fortney JL, Mehlhorn TL, Lowe KA, Earles JE, Phillips J, Techtmann SM, Joyner DC, Elias DA, Bailey KL, Hurt RA Jr, Preheim SP, Sanders MC, Yang J, Mueller MA, Brooks S, Watson DB, Zhang P, He Z, Dubinsky EA, Adams PD, Arkin AP, Fields MW, Zhou J, Alm EJ, Hazen TC: Natural bacterial communities serve as quantitative geochemical biosensors. *MBio.* 2015, **6**:e00326-15.
126. Morshed N, Echols N, Adams PD: Using support vector machines to improve elemental ion identification in macromolecular crystal structures. *Acta Cryst.* 2015, **71**:1147-58
127. González Fernández-Niño SM, Smith-Moritz AM, Chan LJ, Adams PD, Heazlewood JL, Petzold CJ: Standard flow liquid chromatography for shotgun proteomics in bioenergy research. *Front Bioeng Biotechnol.* 2015, **3**:44.

128. Ebert B, Rautengarten C, Guo X, Xiong G, Stonebloom S, Smith-Moritz AM, Herter T, Chan LJ, Adams PD, Petzold CJ, Pauly M, Willats WG, Heazlewood JL, Scheller HV: Identification and Characterization of a Golgi-Localized UDP-Xylose Transporter Family from Arabidopsis. *Plant Cell* 2015, **27**:1218-1227.
129. Afonine PV, Moriarty NW, Mustyakimov M, Sobolev OV, Terwilliger TC, Turk D, Urzhumtsev A, Adams PD: FEM: feature-enhanced map. *Acta Cryst.* 2015, **D71**:646-666.
130. Brewster AS, Sawaya MR, Rodriguez J, Hattne J, Echols N, McFarlane HT, Cascio D, Adams PD, Eisenberg DS, Sauter NK: Indexing amyloid peptide diffraction from serial femtosecond crystallography: new algorithms for sparse patterns. *Acta Cryst.* 2015, **D71**:357-66.
131. Alonso-Gutierrez J, Kim E, Batth TS, Cho N, Hu Q, Chan LJ, Petzold CJ, Hillson NJ, Adams PD, Keasling JD, Garcia-Martin H, Soon Lee T: Principal component analysis of proteomics (PCAP) as a tool to direct metabolic engineering. *Metab Eng.* 2015, **28**:123-133.
132. Bunkóczy G, McCoy AJ, Echols N, Grosse-Kunstleve RW, Adams PD, Holton JM, Read RJ, Terwilliger TC: Macromolecular X-ray structure determination using weak, single-wavelength anomalous data. *Nature Methods* 2015, **12**:127-130.
133. Sauter NK, Hattne J, Brewster AS, Echols N, Zwart PH, Adams PD: Improved crystal orientation and physical properties from single-shot XFEL stills. *Acta Cryst.* 2014, **D70**:3299-3309.
134. Wall ME, Van Benschoten AH, Sauter NK, Adams PD, Fraser JS, Terwilliger TC: Conformational dynamics of a crystalline protein from microsecond-scale molecular dynamics simulations and diffuse X-ray scattering. *Proc Natl Acad Sci U S A* 2014, **111**:17887-92.
135. McAndrew R, Pruitt RN, Kamita SG, Pereira JH, Majumdar D, Hammock BD, Adams PD, Ronald PC: Structure of the OsSERK2 leucine-rich repeat extracellular domain. *Acta Cryst.* 2014, **D70**:3080-3086.
136. Shih SC, Gach PC, Sustarich J, Simmons BA, Adams PD, Singh S, Singh AK: A droplet-to-digital (D2D) microfluidic device for single cell assays. *Lab Chip* 2014, **15**:225-236.
137. Urzhumtsev A, Afonine PV, Lunin VY, Terwilliger TC, Adams PD: Metrics for comparison of crystallographic maps. *Acta Cryst.* 2014, **D70**:2593-2606.
138. Poust S, Yoon I, Adams PD, Katz L, Petzold CJ, Keasling JD: Understanding the Role of Histidine in the GHSxG Acyltransferase Active Site Motif: Evidence for Histidine Stabilization of the Malonyl-Enzyme Intermediate. *PLoS One* 2014, **9**:e109421.
139. Rhee M, Light YK, Yilmaz S, Adams PD, Saxena D, Meagher RJ, Singh AK: Pressure stabilizer for reproducible picoinjection in droplet microfluidic systems. *Lab Chip* 2014, **14**:4533-9.
140. Haushalter RW, Kim W, Chavkin TA, The L, Garber ME, Nhan M, Adams PD, Petzold CJ, Katz L, Keasling JD: Production of anteiso-branched fatty acids in *Escherichia coli*; next generation biofuels with improved cold-flow properties. *Metab Eng.* 2014, **26C**:48-56.
141. Batth TS, Singh P, Ramakrishnan VR, Sousa MM, Chan LJ, Tran HM, Luning EG, Pan EH, Vuu KM, Keasling JD, Adams PD, Petzold CJ: A targeted proteomics toolkit for high-throughput absolute quantification of *Escherichia coli* proteins. *Metab Eng.* 2014, **26**:48-56.
142. McInerney P, Adams P, Hadi MZ: Error Rate Comparison during Polymerase Chain Reaction by DNA Polymerase. *Molecular Biology International* 2014, 287430
143. Hagen A, Poust S, de Rond T, Yuzawa S, Katz L, Adams PD, Petzold CJ, Keasling JD: In vitro analysis of carboxyacyl substrate tolerance in the loading and first extension modules of Borrelidin PKS. *Biochemistry* 2014, **53**:5975-7.
144. Ghosh A, Nilmeier J, Weaver D, Adams PD, Keasling JD, Mukhopadhyay A, Petzold CJ, Martín HG: A Peptide-Based Method for ¹³C Metabolic Flux Analysis in Microbial Communities. *PLoS Comput Biol.* 2014, **10**:e1003827.

145. Wang Z, Hryc CF, Bammes B, Afonine PV, Jakana J, Chen DH, Liu X, Baker ML, Kao C, Ludtke SJ, Schmid MF, Adams PD, Chiu W: An atomic model of bromo mosaic virus using direct electron detection and real-space optimization. *Nature Commun.* 2014, **5**:4808.
146. Rennie EA, Ebert B, Miles GP, Cahoon RE, Christiansen KM, Stonebloom S, Khatab H, Twell D, Petzold CJ, Adams PD, Dupree P, Heazlewood JL, Cahoon EB, Scheller HV: Identification of a Sphingolipid α -Glucuronosyltransferase That Is Essential for Pollen Function in *Arabidopsis*. *Plant Cell.* 2014, **26**:3314-25.
147. Pereira JH, Petchprayoon C, Hoepker AC, Moriarty N, Fink SJ, Cecere G, Paterson I, Adams PD, Marriott G: Structural and Biochemical Studies of Actin in Complex with Synthetic Macrolide Tail Analogues. *ChemMedChem.* 2014, **9**:2286-93.
148. Kern J, Tran R, Alonso-Mori R, Koroidov S, Echols N, Hattne J, Ibrahim M, Gul S, Laksmono H, Sierra RG, Gildea RJ, Han G, Hellmich J, Lassalle-Kaiser B, Chatterjee R, Brewster AS, Stan CA, Glöckner C, Lampe A, DiFiore D, Milathianaki D, Fry AR, Seibert MM, Koglin JE, Gallo E, Uhlig J, Sokaras D, Weng TC, Zwart PH, Skinner DE, Bogan MJ, Messerschmidt M, Glatzel P, Williams GJ, Boutet S, Adams PD, Zouni A, Messinger J, Sauter NK, Bergmann U, Yano J, Yachandra VK: Taking snapshots of photosynthetic water oxidation using femtosecond X-ray diffraction and spectroscopy. *Nature Comm.* 2014, **5**:4371
149. Heins RA, Cheng X, Nath S, Deng K, Bowen BP, Chivian DC, Datta S, Friedland GD, D'Haeseleer P, Wu D, Tran-Gyamfi M, Scullin CS, Singh S, Shi W, Hamilton MG, Bendall ML, Sczyrba A, Thompson J, Feldman T, Guenther JM, Gladden JM, Cheng JF, Adams PD, Rubin EM, Simmons BA, Sale KL, Northen TR, Deutsch S: Phylogenomic Guided Identification of Industrially Relevant GHI β -Glucosidases Through DNA Synthesis and Nanostructure-Initiator Mass Spectrometry. *ACS Chem. Biol.* 2014, **9**:2082-2091.
150. Frederix M, Hütter K, Leu J, Bath TS, Turner WJ, Rüegg TL, Blanch HW, Simmons BA, Adams PD, Keasling JD, Thelen MP, Dunlop MJ, Petzold CJ, Mukhopadhyay A: Development of a Native *Escherichia coli* Induction System for Ionic Liquid Tolerance. *PLoS One* 2014, **9**:e101115
151. Dougherty MJ, Tran HM, Stavila V, Knierim B, George A, Auer M, Adams PD, Hadi MZ: Cellulosic Biomass Pretreatment and Sugar Yields as a Function of Biomass Particle Size. *PLoS One* 2014, **9**:e100836
152. Kung Y, McAndrew RP, Xie X, Liu CC, Pereira JH, Adams PD, Keasling JD: Constructing Tailored Isoprenoid Products by Structure-Guided Modification of Geranylgeranyl Reductase. *Structure* 2014, **22**:1028-36.
153. Lao J, Oikawa A, Bromley JR, McInerney P, Suttangkakul A, Smith-Moritz AM, Plahar H, Chiu TY, González Fernández-Niño SM, Ebert B, Yang F, Christiansen KM, Hansen SF, Stonebloom S, Adams PD, Ronald PC, Hillson NJ, Hadi MZ, Vega-Sánchez ME, Loqué D, Scheller HV, Heazlewood JL: The Plant Glycosyltransferase Clone Collection for Functional Genomics. *Plant J.* 2014, **79**:517-29.
154. Moriarty NW, Tronrud DE, Adams PD, Karplus PA: Conformation-dependent backbone geometry restraints set a new standard for protein crystallographic refinement. *FEBS J.* 2014, **281**:4061-71.
155. Deng K, Takasuka TE, Heins R, Cheng X, Bergeman LF, Shi J, Aschenbrener R, Deutsch S, Singh S, Sale KL, Simmons BA, Adams PD, Singh AK, Fox BG, Northen TR: Rapid Kinetic Characterization of Glycosyl Hydrolases Based on Oxime Derivatization and Nanostructure-Initiator Mass Spectrometry (NIMS). *ACS Chemical Biology.* 2014, **9**:1470-9.
156. Headd JJ, Echols N, Afonine PV, Moriarty NW, Gildea RJ, Adams PD: Flexible torsion-angle noncrystallographic symmetry restraints for improved macromolecular structure refinement. *Acta Cryst.* 2014, **D70**:1346-1356.
157. Echols N, Morshed N, Afonine PV, McCoy AJ, Miller MD, Read RJ, Richardson JS, Terwilliger TC, Adams PD: Automated identification of elemental ions in macromolecular crystal structures. *Acta Cryst.* 2014, **D70**:1104-1114.
158. Hattne J, Echols N, Tran R, Kern J, Gildea RJ, Brewster AS, Alonso-Mori R, Glöckner C, Hellmich J, Laksmono H, Sierra RG, Lassalle-Kaiser B, Lampe A, Han G, Gul S, DiFiore D, Milathianaki D, Fry AR, Miahnahri A, White

- WE, Schafer DW, Seibert MM, Koglin JE, Sokaras D, Weng TC, Sellberg J, Latimer MJ, Glatzel P, Zwart PH, Grosse-Kunstleve RW, Bogan MJ, Messerschmidt M, Williams GJ, Boutet S, Messinger J, Zouni A, Yano J, Bergmann U, Yachandra VK, Adams PD, Sauter NK: Accurate macromolecular structures using minimal measurements from X-ray free-electron lasers. *Nature Methods* 2014, **11**:545-548.
159. George KW, Chen A, Jain A, Batth TS, Baidoo EE, Wang G, Adams PD, Petzold CJ, Keasling JD, Lee TS: Correlation analysis of targeted proteins and metabolites to assess and engineer microbial isopentenol production. *Biotechnol Bioeng.* 2014, **111**:1648-1658.
160. Ito J, Herter T, Baidoo EE, Lao J, Vega-Sánchez ME, Michelle Smith-Moritz A, Adams PD, Keasling JD, Usadel B, Petzold CJ, Heazlewood JL: Analysis of plant nucleotide sugars by hydrophilic interaction liquid chromatography and tandem mass spectrometry. *Anal Biochem.* 2014, **448**:14-22
161. Echols N, Moriarty NW, Klei HE, Afonine PV, Bunkóczi G, Headd JJ, McCoy AJ, Oeffner RD, Read RJ, Terwilliger TC, Adams PD: Automating crystallographic structure solution and refinement of protein-ligand complexes. *Acta Cryst.* 2014, **D70**:144-154.
162. Klei HE, Moriarty NW, Echols N, Terwilliger TC, Baldwin ET, Pokross M, Posy S, Adams PD: Ligand placement based on prior structures: the guided ligand-replacement method. *Acta Cryst.* 2014, **D70**:134-143.
163. Javidpour P, Pereira JH, Goh EB, McAndrew RP, Ma SM, Friedland GD, Keasling JD, Chhabra SR, Adams PD, Beller HR: Biochemical and Structural Studies of NADH-Dependent FabG Used to Increase the Bacterial Production of Fatty Acids under Anaerobic Conditions. *Appl Environ Microbiol.* 2014, **80**:497-505
164. Parsons HT, Weinberg CS, Macdonald LJ, Adams PD, Petzold CJ, Strabala TJ, Wagner A, Heazlewood JL: Golgi Enrichment and Proteomic Analysis of Developing *Pinus radiata* Xylem by Free-Flow Electrophoresis. *PLoS One* 2013, **8**:e84669.
165. Cheng X, Hiras J, Deng K, Bowen B, Simmons BA, Adams PD, Singer SW, Northen TR: High throughput nanostructure-initiator mass spectrometry screening of microbial growth conditions for maximal β -glucosidase production. *Front Microbiol.* 2013, **4**:365
166. Szmidt-Middleton HL, Ouellet M, Adams PD, Keasling JD, Mukhopadhyay A: Utilizing a highly responsive gene, *yhjX*, in *E. coli* based production of 1,4-butanediol. *Chem. Eng. Sci.* 2013, **103**:68-73
167. Woo HM, Murray GW, Batth TS, Prasad N, Adams PD, Keasling JD, Petzold CJ, Lee TS: Application of targeted proteomics and biological parts assembly in *E. coli* to optimize the biosynthesis of an anti-malarial drug precursor, amorpha-4,11-diene. *Chem. Eng. Sci.* 2013, **103**:21-28
168. Chen Z, Pereira JH, Liu H, Tran HM, Hsu NS, Dibble D, Singh S, Adams PD, Sapra R, Hadi MZ, Simmons BA, Sale KL: Improved Activity of a Thermophilic Cellulase, Cel5A, from *Thermotoga maritima* on Ionic Liquid Pretreated Switchgrass. *PLoS One* 2013, **8**:e79725
169. Bunkóczi G, Echols N, McCoy AJ, Oeffner RD, Adams PD, Read RJ: Phaser.MRage: automated molecular replacement. *Acta Cryst.* 2013, **D69**:2276-2286.
170. Terwilliger TC, Read RJ, Adams PD, Brunger AT, Afonine PV, Hung L-W: Model morphing and sequence assignment after molecular replacement. *Acta Cryst.* 2013, **D69**:2244-2250.
171. Dahl RH, Zhang F, Alonso-Gutierrez J, Baidoo E, Batth TS, Redding-Johanson AM, Petzold CJ, Mukhopadhyay A, Lee TS, Adams PD, Keasling JD: Engineering dynamic pathway regulation using stress-response promoters. *Nat Biotechnol.* 2013, **31**:1039-1046.
172. Dimairo F, Echols N, Headd JJ, Terwilliger TC, Adams PD, Baker D: Improved low-resolution crystallographic refinement with Phenix and Rosetta. *Nature Methods* 2013, **10**:1102-1104
173. Nwachukwu JC, Southern MR, Kiefer JR, Afonine PV, Adams PD, Terwilliger TC, Nettles KW: Improved Crystallographic Structures Using Extensive Combinatorial Refinement. *Structure* 2013, **21**:1923-1930.

174. Baker ML, Hryc CF, Zhang Q, Wu W, Jakana J, Haase-Pettingell C, Afonine PV, Adams PD, King JA, Jiang W, Chiu W: Validated near-atomic resolution structure of bacteriophage epsilon15 derived from cryo-EM and modeling. *Proc Natl Acad Sci U S A*. 2013, **110**:12301-12306.
175. Reyes-Ortiz V, Heins RA, Cheng G, Kim EY, Vernon BC, Elandt RB, Adams PD, Sale KL, Hadi MZ, Simmons BA, Kent MS, Tullman-Ercek D: Addition of a carbohydrate-binding module enhances cellulase penetration into cellulose substrates. *Biotechnol. Biofuels* 2013, **6**:93.
176. Alonso-Gutierrez J, Chan R, Batth TS, Adams PD, Keasling JD, Petzold CJ, Lee TS: Metabolic engineering of *Escherichia coli* for limonene and perillyl alcohol production. *Metab. Eng.* 2013, **19C**:33-41
177. Chiniquy D, Varanasi P, Oh T, Harholt J, Katnelson J, Singh S, Auer M, Simmons B, Adams PD, Scheller HV, Ronald PC: Three Novel Rice Genes Closely Related to the Arabidopsis IRX9, IRX9L, and IRX14 Genes and Their Roles in Xylan Biosynthesis. *Front. Plant Sci.* 2013, **4**:83.
178. Singh S, Varanasi P, Singh P, Adams PD, Auer M, Simmons BA: Understanding the impact of ionic liquid pretreatment on cellulose and lignin via thermochemical analysis. *Biomass & Bioenergy* 2013, **54**:276-283.
179. McAndrew RP, Park JI, Heins RA, Reindl W, Friedland GD, D'haeseleer P, Northen T, Sale KL, Simmons BA, Adams PD: From soil to structure: a novel dimeric β -glucosidase belonging to glycoside hydrolase family 3 isolated from compost using metagenomic analysis. *J. Biol. Chem.* 2013, **288**:14985-14992.
180. Chandrasekaran A, Deng K, Koh CY, Takasuka T, Bergeman LF, Fox BG, Adams PD, Singh AK: A universal flow cytometry assay for screening carbohydrate-active enzymes using glycan microspheres. *Chem. Commun.* 2013, **49**:5441-5443.
181. Afonine PV, Grosse-Kunstleve RW, Adams PD, Urzhumtsev A: Bulk-solvent and overall scaling revisited: faster calculations, improved results. *Acta Cryst.* 2013, **D69**:625-634.
182. Chang C, Sustarich J, Bharadwaj R, Chandrasekaran A, Adams PD, Singh AK: Droplet-based microfluidic platform for heterogeneous enzymatic assays. *Lab Chip.* 2013, **13**:1817-1822.
183. Kern J, Alonso-Mori R, Tran R, Hattne J, Gildea RJ, Echols N, Glöckner C, Hellmich J, Laksmono H, Sierra RG, Lassalle-Kaiser B, Koroidov S, Lampe A, Han G, Gul S, Difiore D, Milathianaki D, Fry AR, Miahnahri A, Schafer DW, Messerschmidt M, Seibert MM, Koglin JE, Sokaras D, Weng TC, Sellberg J, Latimer MJ, Grosse-Kunstleve RW, Zwart PH, White WE, Glatzel P, Adams PD, Bogan MJ, Williams GJ, Boutet S, Messinger J, Zouni A, Sauter NK, Yachandra VK, Bergmann U, Yano J: Simultaneous Femtosecond X-ray Spectroscopy and Diffraction of Photosystem II at Room Temperature. *Science* 2013, **340**:491-495.
184. Varanasi P, Singh P, Auer M, Adams PD, Simmons BA, Singh S: Survey of renewable chemicals produced from lignocellulosic biomass during ionic liquid pretreatment. *Biotechnol Biofuels* 2013, **6**:14.
185. Read RJ, Adams PD, McCoy AJ: Intensity statistics in the presence of translational noncrystallographic symmetry. *Acta Cryst.* 2013, **D69**:176-183.
186. Burnley BT, Afonine PV, Adams PD, Gros P: Modelling dynamics in protein crystal structures by ensemble refinement. *eLife* 2012, **1**:e00311.
187. Alonso-Mori R, Kern J, Gildea RJ, Sokaras D, Weng TC, Lassalle-Kaiser B, Tran R, Hattne J, Laksmono H, Hellmich J, Glöckner C, Echols N, Sierra RG, Schafer DW, Sellberg J, Kenney C, Herbst R, Pines J, Hart P, Herrmann S, Grosse-Kunstleve RW, Latimer MJ, Fry AR, Messerschmidt MM, Miahnahri A, Seibert MM, Zwart PH, White WE, Adams PD, Bogan MJ, Boutet S, Williams GJ, Zouni A, Messinger J, Glatzel P, Sauter NK, Yachandra VK, Yano J, Bergmann U: Energy-dispersive X-ray emission spectroscopy using an X-ray free-electron laser in a shot-by-shot mode. *Proc. Natl. Acad. Sci. USA* 2012, **109**:19103-19107.
188. Sierra RG, Laksmono H, Kern J, Tran R, Hattne J, Alonso-Mori R, Lassalle-Kaiser B, Glöckner C, Hellmich J, Schafer DW, Echols N, Gildea RJ, Grosse-Kunstleve RW, Sellberg J, McQueen TA, Fry AR, Messerschmidt MM, Miahnahri A, Seibert MM, Hampton CY, Starodub D, Loh ND, Sokaras D, Weng T-C, Zwart PH, Glatzel P,

- Milathianaki D, White WE, Adams PD, Williams GJ, Boutet S, Zouni A, Messinger J, Sauter NK, Bergmann U, Yano J, Yachandra VK, Bogan MJ: Nanoflow electrospinning serial femtosecond crystallography. *Acta Cryst.* 2012, **D68**:1584-1587
189. Varanasi P, Singh P, Arora R, Adams PD, Auer M, Simmons BA, Singh S: Understanding changes in lignin of *Panicum virgatum* and *Eucalyptus globulus* as a function of ionic liquid pretreatment. *Bioresour. Technol.* 2012, **126C**:156-161
190. Zhang F, Ouellet M, Batth TS, Adams PD, Petzold CJ, Mukhopadhyay A, Keasling J: Enhancing fatty acid production by the expression of the regulatory transcription factor FadR. *Metab. Eng.* 2012, **14**:653-660.
191. Pereira JH, Goh EB, Keasling JD, Beller HR, Adams PD: Structure of FabH and factors affecting the distribution of branched fatty acids in *Micrococcus luteus*. *Acta Cryst.* 2012, **D68**:1320-1328
192. McClendon SD, Baath T, Petzold CJ, Adams PD, Simmons BA, Singer SW: *Thermoascus aurantiacus* is a promising source of enzymes for biomass deconstruction under thermophilic conditions. *Biotechnol Biofuels.* 2012, **5**:54.
193. Dougherty MJ, D'haeseleer P, Simmons BA, Adams PD, Hadi MZ: Glycoside Hydrolases from a targeted Compost Metagenome, activity-screening and functional characterization. *BMC Biotechnol.* 2012, **12**:38.
194. Reindl W, Deng K, Cheng X, Singh AK, Simmons BA, Adams PD, Northen TR: Nanostructure-Initiator Mass Spectrometry (NIMS) for the Analysis of Enzyme Activities. *Curr. Protoc. Chem. Biol.* 2012, **4**:123-142
195. Terwilliger TC, Read RJ, Adams PD, Brunger AT, Afonine PV, Grosse-Kunstleve RW, Hung L-W: Improved crystallographic models through iterated local density-guided model deformation and reciprocal-space refinement. *Acta Cryst.* 2012, **D68**:861-870.
196. McKee AE, Rutherford BJ, Chivian DC, Baidoo EK, Juminaga D, Kuo D, Benke PI, Dietrich JA, Ma SM, Arkin AP, Petzold CJ, Adams PD, Keasling JD, Chhabra SR: Manipulation of the Carbon Storage Regulator System for Metabolite Remodeling and Biofuel Production in *Escherichia coli*. *Microb. Cell Fact.* 2012, **11**:79.
197. Kern J, Alonso-Mori R, Hellmich J, Tran R, Hattne J, Laksmono H, Glöckner C, Echols N, Sierra RG, Sellberg J, Lassalle-Kaiser B, Gildea RJ, Glatzel P, Grosse-Kunstleve RW, Latimer MJ, McQueen TA, Difiore D, Fry AR, Messerschmidt M, Miahnahri A, Schafer DW, Seibert MM, Sokaras D, Weng TC, Zwart PH, White WE, Adams PD, Bogan MJ, Boutet S, Williams GJ, Messinger J, Sauter NK, Zouni A, Bergmann U, Yano J, Yachandra VK: Room temperature femtosecond X-ray diffraction of photosystem II microcrystals. *Proc. Natl. Acad. Sci. U S A* 2012, **109**:9721-9726.
198. Brunger AT, Adams PD, Frommer P, Fromme R, Levitt M, Schröder GF: Improving the Accuracy of Macromolecular Structure Refinement at 7 Å Resolution. *Structure* 2012, **20**:957-966.
199. Chen Z, Friedland GD, Pereira JH, Revoco SA, Chan R, Park JI, Thelen MP, Adams PD, Arkin AP, Keasling JD, Blanch HW, Simmons BA, Sale KL, Chivian D, Chhabra SR: Tracing determinants of dual-substrate specificity in glycoside hydrolase family 5. *J. Biol. Chem.* 2012, **287**:25335-25343.
200. Grosse-Kunstleve RW, Terwilliger TC, Sauter NK, Adams PD: Automatic Fortran to C++ conversion with FABLE. *Source Code for Biology and Medicine* 2012, **7**:5
201. Echols N, Grosse-Kunstleve RW, Afonine PV, Bunkóczi G, Chen VB, Headd JJ, McCoy AJ, Moriarty NW, Read RJ, Richardson DC, Richardson JS, Terwilliger TC, Adams PD: Graphical tools for macromolecular crystallography in PHENIX. *J. Appl. Cryst.* 2012, **45**:581-586
202. Singh P, Batth TS, Juminaga D, Dahl RH, Keasling JD, Adams PD, Petzold CJ: Application of targeted proteomics to metabolically engineered *Escherichia coli*. *Proteomics* 2012, **12**:1289-1299
203. Gifford LK, Carter LG, Gabanyi MJ, Berman HM, Adams PD: The Protein Structure Initiative Structural Biology Knowledgebase Technology Portal: a structural biology web resource. *J. Struct. Funct. Genomics* 2012, **13**:57-62.

204. Greving M, Cheng X, Reindl W, Bowen B, Deng K, Louie K, Nyman M, Cohen J, Singh A, Simmons B, Adams P, Siuzdak G, Northen T: Acoustic deposition with NIMS as a high-throughput enzyme activity assay. *Anal. Bioanal. Chem.* 2012, **403**:707-711
205. Terwilliger TC, Dimaio F, Read RJ, Baker D, Bunkóczi G, Adams PD, Grosse-Kunstleve RW, Afonine PV, Echols N: phenix.mr_rosetta: molecular replacement and model rebuilding with Phenix and Rosetta. *J. Struct. Funct. Genomics* 2012, **13**:81-90.
206. Afonine PV, Grosse-Kunstleve RW, Echols N, Headd JJ, Moriarty NW, Mustyakimov M, Terwilliger TC, Urzhumtsev A, Zwart PH, Adams PD: Towards automated crystallographic structure refinement with *phenix.refine*. *Acta Cryst.* 2012, **D68**:352-367
207. Headd JJ, Echols N, Afonine PV, Grosse-Kunstleve RW, Chen VB, Moriarty NW, Richardson DC, Richardson JS, Adams PD: Use of knowledge-based restraints in *phenix.refine* to improve macromolecular refinement at low resolution. *Acta Cryst.* 2012, **D68**:381-390
208. Brunger AT, Das D, Deacon AM, Grant J, Terwilliger TC, Read RJ, Adams PD, Levitt M, Schröder GF: Application of DEN refinement and automated model building to a difficult case of molecular-replacement phasing: the structure of a putative succinyl-diaminopimelate desuccinylase from *Corynebacterium glutamicum*. *Acta Cryst.* 2012, **D68**:391-403
209. Deng K, George KW, Reindl W, Keasling JD, Adams PD, Lee TS, Singh AK, Northen TR: Encoding substrates with mass tags to resolve stereospecific reactions using Nimzyme. *Rapid Commun. Mass Spectrom.* 2012, **26**:611-615
210. Groff D, Benke PI, Batth TS, Bokinsky G, Petzold CJ, Adams PD, Keasling JD: Supplementation of intracellular XylR leads to co-utilization of hemicellulose sugars. *Appl. Environ. Microbiol.* 2012, **78**:2221-2229
211. Pereira JH, Ralston CY, Douglas NR, Kumar R, Lopez T, McAndrew RP, Knee KM, King JA, Frydman J, Adams PD: Mechanism of nucleotide sensing in group II chaperonins. *EMBO Journal* 2011, **31**:731-740.
212. McAndrew RP, Peralta-Yahya PP, DeGiovanni A, Pereira JH, Hadi MZ, Keasling JD, Adams PD: Structure of a Three-Domain Sesquiterpene Synthase: A Prospective Target for Advanced Biofuels Production. *Structure* 2011, **19**:1876-1884.
213. Perera PN, Schmidt M, Chiang VL, Schuck PJ, Adams PD: Raman-spectroscopy-based noninvasive microanalysis of native lignin structure. *Anal. Bioanal. Chem.* 2011, **402**:983-987
214. Read RJ, Adams PD, Arendall WB, Brunger AT, Emsley P, Joosten RP, Kleywegt GJ, Krissinel EB, Lutteke T, Otwinowski Z, Perrakis A, Richardson JS, Sheffler WH, Smith JL, Tickle IJ, Vriend G, Zwart PH: A New Generation of Crystallographic Validation Tools for the Protein Data Bank. *Structure* 2011, **19**:1395-1412
215. Gildea RJ, Bourhis LJ, Dolomanov OV, Grosse-Kunstleve RW, Puschmann H, Adams PD, Howard JAK: iotbx.cif: a comprehensive CIF toolbox. *J. Appl. Cryst.* 2011, **44**:1259-1263
216. Ouellet M, Datta S, Dibble DC, Tamrakar PR, Benke PI, Li C, Singh S, Sale KL, Adams PD, Keasling JD, Simmons BA, Holmes BM, Mukhopadhyay A: Impact of ionic liquid pretreated plant biomass on *Saccharomyces cerevisiae* growth and biofuel production. *Green Chem.* 2011, **13**:2743-2749
217. Reindl W, Deng K, Gladden JM, Cheng G, Wong A, Singer SW, Singh S, Lee JC, Yao CH, Hazen TC, Singh AK, Simmons BA, Adams PD, Northen TR: Colloid-based multiplexed screening for plant biomass-degrading glycoside hydrolase activities in microbial communities. *Energy & Environmental Science* 2011, **4**:2884-2893
218. Perera PN, Schmidt M, Schuck PJ, Adams PD: Blind image analysis for the compositional and structural characterization of plant cell walls. *Anal. Chim. Acta.* 2011, **702**:172-7
219. Adams PD, Afonine PV, Bunkóczi G, Chen VB, Echols N, Headd JJ, Hung LW, Jain S, Kapral GJ, Grosse Kunstleve RW, McCoy AJ, Moriarty NW, Oeffner RD, Read RJ, Richardson DC, Richardson JS, Terwilliger TC,

- Zwart PH: The Phenix software for automated determination of macromolecular structures. *Methods* 2011, **55**:94-106.
220. Gabanyi MJ, Adams PD, Arnold K, Bordoli L, Carter LG, Flippen-Andersen J, Gifford L, Haas J, Kouranov A, McLaughlin WA, Micallef DI, Minor W, Shah R, Schwede T, Tao YP, Westbrook JD, Zimmerman M, Berman HM: The Structural Biology Knowledgebase: a portal to protein structures, sequences, functions, and methods. *J. Struct. Funct. Genomics*. 2011, **12**:45-54.
221. Grosse-Kunstleve RW, Wong B, Mustyakimov M, Adams PD: Exact direct-space asymmetric units for the 230 crystallographic space groups. *Acta Cryst.* 2011, **A67**:269-275.
222. Redding-Johanson AM, Batth TS, Chan R, Krupa R, Szmidski HL, Adams PD, Keasling JD, Soon Lee T, Mukhopadhyay A, Petzold CJ: Targeted proteomics for metabolic pathway optimization: Application to terpene production. *Metab. Eng.* 2011, **13**:194-203.
223. Achyuthan KE, Achyuthan AM, Adams PD, Dirk SM, Harper JC, Simmons BA, Singh AK: Supramolecular Self-Assembled Chaos: Polyphenolic Lignin's Barrier to Cost-Effective Lignocellulosic Biofuels. *Molecules* 2010, **15**:8641-8688.
224. Schmidt M, Perera P, Schwartzberg AM, Adams PD, Schuck PJ: Label-free in situ imaging of lignification in plant cell walls. *J Vis Exp.* 2010, Issue 45.
225. Bharadwaj R, Chen Z, Datta S, Holmes BM, Sapra R, Simmons BA, Adams PD, Singh AK: Microfluidic glycosyl hydrolase screening for biomass-to-biofuel conversion. *Anal Chem.* 2010, **82**:9513-9520.
226. Afonine PV, Mustyakimov M, Grosse-Kunstleve RW, Moriarty NW, Langan P, Adams PD: Joint X-ray and neutron refinement with phenix.refine. *Acta Cryst.* 2010, **D66**:1153-1163.
227. Bruning JB, Parent AA, Gil G, Zhao M, Nowak J, Pace MC, Smith CL, Afonine PV, Adams PD, Katzenellenbogen JA, Nettles KW: Coupling of receptor conformation and ligand orientation determine graded activity. *Nature Chem. Biol.* 2010, **6**:837-843.
228. Bharadwaj R, Wong A, Knierim B, Singh S, Holmes BM, Auer M, Simmons BA, Adams PD, Singh AK: High-throughput enzymatic hydrolysis of lignocellulosic biomass via in-situ regeneration. *Bioresour Technol.* 2010, **102**:1329-1337.
229. Chandrasekaran A, Bharadwaj R, Park JJ, Sapra R, Adams PD, Singh AK: A microscale platform for integrated cell-free expression and activity screening of cellulases. *J. Proteome Res.* 2010, **9**:5677-5683.
230. Kohn JE, Afonine PV, Ruscio JZ, Adams PD, Head-Gordon T: Evidence of functional protein dynamics from X-ray crystallographic ensembles. *PLoS Computational Biology* 2010, **6**, e1000911.
231. Liu H, Pereira JH, Adams PD, Sapra R, Simmons BA, Sale KL: Molecular simulations provide new insights into the role of the accessory immunoglobulin-like domain of Cel9a. *FEBS Lett.* 2010, **584**:3431-3435.
232. Pereira JH, Chen Z, McAndrew RP, Sapra R, Chhabra SR, Sale KL, Simmons BA, Adams PD: Biochemical characterization and crystal structure of endoglucanase Cel5A from the hyperthermophilic *Thermotoga maritima*. *J. Struct. Biol.* 2010, **172**:372-379.
233. Pereira JH, Ralston CY, Douglas N, Meyer D, Knee KM, Goulet DR, King JA, Frydman J, Adams PD: Crystal structures of a group II chaperonin reveal the open and closed states associated with the protein folding cycle. *J. Biol. Chem.* 2010, **285**:27958-27966.
234. Afonine PV, Grosse-Kunstleve RW, Chen VB, Headd JJ, Moriarty NW, Richardson JS, Richardson DC, Urzhumtsev A, Zwart PH, Adams PD: phenix.model_vs_data: a high-level tool for the calculation of crystallographic model and data statistics. *J. Appl. Cryst.* 2010, **43**:677-685.
235. Schmidt M, Schwartzberg AM, Carroll A, Chaibang A, Adams PD, Schuck PJ: Raman imaging of cell wall polymers in *Arabidopsis thaliana*. *Biochem. and Biophys. Res. Comm.* 2010, **395**:521-523.

236. Achyuthan KE, Adams PD, Datta S, Simmons BA, Singh AK: Hitherto unrecognized fluorescence properties of coniferyl alcohol. *Molecules* 2010, **15**:1645-1667.
237. Nishi K, Lee HJ, Park SY, Bae SJ, Lee SE, Adams PD, Rhee JH, Kim JS: Crystal structure of the transcriptional activator HlyU from *Vibrio vulnificus* CMCP6. *FEBS Lett.* 2010, **584**:1097-1102.
238. Adams PD, Afonine PV, Bunkóczi G, Chen VB, Davis IW, Echols N, Headd JJ, Hung L-W, Kapral GJ, Grosse-Kunstleve RW, McCoy AJ, Moriarty NW, Oeffner R, Read RJ, Richardson DC, Richardson JS, Terwilliger TC, Zwart PH: PHENIX: a comprehensive Python-based system for macromolecular structure solution. *Acta Cryst.* 2010, **D66**:213-221.
239. Ouellet M, Adams PD, Keasling JD, Mukhopadhyay A: A rapid and inexpensive labeling method for microarray gene expression analysis. *BMC Biotechnology* 2009, **9**:97.
240. Achyuthan KE, Adams PD, Simmons BA, Singh AK: Spectroscopic Analyses of the Biofuels-Critical Phytochemical Coniferyl Alcohol and Its Enzyme-Catalyzed Oxidation Products. *Molecules* 2009, **14**:4758-4778.
241. Urzhumtsev A, Afonine PV, Adams PD: On the use of logarithmic scales for analysis of diffraction data. *Acta Cryst.* 2009, **D65**:1283-1291.
242. Moriarty NW, Grosse-Kunstleve RW, Adams PD: electronic Ligand Builder and Optimization Workbench (eLBOW): a tool for ligand coordinate and restraint generation. *Acta Cryst.* 2009, **D65**:1074-1080.
243. Praznikar J, Afonine PV, Guncar G, Adams PD, Turk D: Averaged kick maps: less noise, more signal...and probably less bias. *Acta Cryst.* 2009, **D65**:921-931.
244. Grosse-Kunstleve RW, Moriarty NW, Adams PD: Torsion Angle Refinement and Dynamics as a tool to aid crystallographic Structure Determination. Proceedings of ASME 2009 International Design Engineering Technical Conferences, San Diego, California 2009, August 30 - September 2. Paper #DETC2009-87737. ASME Press.
245. Pereira JH, Sapra R, Volponi JV, Kozina CL, Simmons B, Adams PD: Structure of endoglucanase Cel9A from the thermoacidophilic Alicyclobacillus acidocaldarius. *Acta Cryst.* 2009, **D65**:744-750.
246. Afonine PV, Grosse-Kunstleve RW, Urzhumtsev A, Adams PD: Automatic multiple-zone rigid-body refinement with a large convergence radius. *J. Appl. Cryst.* 2009, **42**:607-615 Schmidt M, Schwartzberg AM, Perera PN, Weber-Bargioni A, Carroll A, Sarkar P, Bosneaga E, Urban JJ, Song J, Balakshin MY, Capanema EA, Auer M, Adams PD, Chiang VL, James Schuck P: Label-free in situ imaging of lignification in the cell wall of low lignin transgenic *Populus trichocarpa*. *Planta* 2009, **230**:589-597
247. Terwilliger TC, Adams PD, Read RJ, McCoy AJ, Moriarty NW, Grosse-Kunstleve RW, Afonine PV, Zwart PH, Hung L-W: Decision-making in structure solution using Bayesian estimates of map quality: the PHENIX AutoSol wizard. *Acta Cryst.* 2009, **D65**:582-601.
248. Adams PD, Mustyakimov M, Afonine PV, Langan P: Generalized X-ray and neutron crystallographic analysis: more accurate and complete structures for biological macromolecules. *Acta Cryst.* 2009, **D65**:567-573.
249. Urzhumtseva L, Afonine PV, Adams PD, Urzhumtsev A: Crystallographic model quality at a glance. *Acta Cryst.* 2009, **D65**:297-300.
250. Berman HM, Westbrook JD, Gabanyi MJ, Tao W, Shah R, Kouranov A, Schwede T, Arnold K, Kiefer F, Bordoli L, Kopp J, Podvinez M, Adams PD, Carter LG, Minor W, Nair R, Baer JL: The protein structure initiative structural genomics knowledgebase. *Nucleic Acids Research* 2009, **37**:D365-D368.
251. Yan J, Adams PD, Angel RJ, Ross NL, Rivers M, Parise JB, Clark SM: The development of an automated data analysis system for high-pressure powder diffraction data collected using an area detector. *High Pressure Research* 2008, **28**:293-298.

252. Terwilliger TC, Grosse-Kunstleve RW, Afonine PV, Moriarty NW, Adams PD, Read RJ, Zwart PH, Hung LW: Iterative-build OMIT maps: map improvement by iterative model building and refinement without model bias. *Acta Cryst.* 2008, **D64**:515-524.
253. Langan P, Fisher Z, Kovalevsky A, Mustyakimov M, Sutcliffe Valone A, Unkefer C, Waltman MJ, Coates L, Adams PD, Afonine PV, Bennett B, Dealwis C, Schoenborn BP: Protein structures by spallation neutron crystallography. *J. Synchrotron Rad.* 2008, **15**:215-218.
254. Blanch HW, Adams PD, Andrews-Cramer KM, Frommer WB, Simmons BA, Keasling JD: Addressing the need for alternative transportation fuels: the Joint BioEnergy Institute. *ACS Chemical Biology* 2008, **3**:17-20.
255. González A, Moorhead P, McPhillips SE, Song J, Sharp K, Taylor JR, Adams PD, Sauter NK, Soltis SM: Web-Ice: integrated data collection and analysis for macromolecular crystallography. *J. Appl. Cryst.* 2008, **41**:176-184.
256. Zwart PH, Grosse-Kunstleve RW, Lebedev AA, Murshudov GN, Adams PD: Surprises and pitfalls arising from (pseudo)symmetry. *Acta Cryst.* 2008, **D64**:99-107.
257. Terwilliger TC, Grosse-Kunstleve RW, Afonine PV, Moriarty NW, Zwart PH, Hung LW, Read RJ, Adams PD: Iterative model building, structure refinement and density modification with the PHENIX AutoBuild wizard. *Acta Cryst.* 2008, **D64**:61-69.
258. Afonine PV, Grosse-Kunstleve RW, Adams PD, Lunin VY, Urzhumtsev A: On macromolecular refinement at subatomic resolution with interatomic scatterers. *Acta Cryst.* 2007, **D63**:1194-1197.
259. McCoy AJ, Grosse-Kunstleve RW, Adams PD, Winn MD, Storoni LC, Read RJ: Phaser crystallographic software. *J. Appl. Cryst.* 2007, **40**:658-674.
260. Oganessian V, Adams PD, Jancarik J, Kim R, Kim SH: Structure of O67745_AQUAE from *Aquifex aeolicus* resolution. *Acta Cryst.* 2007, **F63**:369-374.
261. Terwilliger TC, Grosse-Kunstleve RW, Afonine PV, Adams PD, Moriarty NW, Zwart P, Read RJ, Turk D, Hung LW: Interpretation of ensembles created by multiple iterative rebuilding of macromolecular models. *Acta Cryst.* 2007, **D63**:597-610.
262. Terwilliger TC, Adams PD, Moriarty NW, Cohn JD: Ligand identification using electron-density map correlations. *Acta Cryst.* 2007, **D63**:101-107.
263. Hohn M, Tang G, Goodyear G, Baldwin PR, Huang Z, Penczek PA, Yang C, Glaeser RM, Adams PD, Ludtke SJ: SPARX, a new environment for Cryo-EM image processing. *J Struct Biol.* 2007, **157**:47-55.
264. Terwilliger TC, Adams PD, Moriarty NW, Cohn JD: Ligand identification using electron-density map correlations. *Acta Cryst.* 2007, **D63**:101-107.
265. Sauter NK, Grosse-Kunstleve RW, Adams PD: Improved statistics for determining the Patterson symmetry from unmerged diffraction intensities. *J. Appl. Cryst.* 2006, **39**:158-168.
266. MacRae IJ, Zhou K, Li F, Repic A, Brooks AN, Cande WZ, Adams PD, Doudna JA: Structural Basis for Double-Stranded RNA Processing by Dicer. *Science* 2006, **311**:195-198.
267. Xu QS, Jancarik J, Luo Y, Kuznetsova K, Yakunin AF, Yokota H, Adams P, Kim R, Kim SH: Crystal Structures of a phosphotransacetylase from *Bacillus subtilis* and its complex with acetyl phosphate. *J. Struct. Funct. Genomics.* 2005, **6**:269-279.
268. Liu J, Lou Y, Yokota H, Adams PD, Kim R, Kim SH: Crystal Structures of an NAD Kinase from *Archaeoglobus fulgidus* in Complex with ATP, NAD, or NADP. *Journal of Molecular Biology* 2005, **354**:289-303.
269. McKee EW, Kanbi LD, Childs KL, Grosse-Kunstleve RW, Adams PD, Sacchettini JC, Ioerger TR: FINDMOL: automated identification of macromolecules in electron-density maps *Acta Cryst.* 2005, **D61**:1514-1520.
270. Kim SH, Shin DH, Liu J, Oganessian V, Chen S, Xu QS, Kim JS, Das D, Schulze-Gahmen U, Holbrook SR, Holbrook EL, Martinez BA, Oganessian N, Degiovanni A, Lou Y, Henriquez M, Huang C, Jancarik J, Pufan R,

- Choi IG, Chandonia JM, Hou J, Gold B, Yokota H, Brenner SE, Adams PD, Kim R: Structural genomics of minimal organisms and protein fold space *J. Struct Funct Genomics*. 2005, **6**:63-70.
271. Aishima J, Russel DS, Guibas LJ, Adams PD, Brunger AT: Automated crystallographic ligand building using the medial axis transform of an electron-density isosurface *Acta Cryst*. 2005, **D61**:1354-1363.
272. Kazantsev AV, Krivenko AA, Harrington DJ, Holbrook SR, Adams PD, Pace NR: Crystal structure of a bacterial ribonuclease P RNA. *Proc. Nat. Acad. Sci. USA*. 2005, **102**:13392-13397.
273. Oganessian V, Huang C, Adams PD, Jancarik J, Yokota HA, Kim R, Kim SH: Structure of a NAD kinase from *Thermotoga maritima* at 2.3 Å resolution. *Acta Cryst*. 2005, **F61**:640-646.
274. Afonine PV, Grosse-Kunstleve RW, Adams PD: A robust bulk-solvent correction and anisotropic scaling procedure. *Acta Cryst*. 2005, **D61**:850-855.
275. Liu J, Lou Y, Yokota H, Adams PD, Kim R, Kim SH: A New Class of Metalloprotein Containing Multinuclear Iron Clusters. *J. Biol. Chem*. 2005, **280**:15960-15966
276. Kim JS, DeGiovanni A, Jancarik J, Adams PD, Yokota H, Kim R, Kim SH: Crystal structure of DNA sequence specificity subunit of a type I restriction-modification enzyme and its functional implications. *Proc. Natl. Acad. Sci. USA*. 2005, **102**:3248-3253.
277. Chaudhry C, Horwich AL, Brunger AT, Adams PD: Exploring the structural dynamics of the E. coli chaperonin GroEL using translation-libration-screw crystallographic refinement of intermediate states. *Journal of Molecular Biology* 2004, **342**:229-245.
278. Wall JS, Gupta V, Wilkerson M, Schell M, Loris R, Adams P, Solomon A, Stevens F, Dealwis C: Structural basis of light chain amyloidogenicity: comparison of the thermodynamic properties, fibrillogenic potential and tertiary structural features of four V λ 6 proteins *J. Mol. Recognition* 2004, **17**:323-331.
279. Sauter NK, Grosse-Kunstleve RW, Adams PD: Robust indexing for automatic data collection. *J. Appl. Cryst*. 2004, **37**:399-409.
280. Grosse-Kunstleve RW, Sauter NK, Adams PD: Numerically stable algorithms for the computation of reduced unit cells. *Acta Cryst*. 2004, **A60**:1-6.
281. Kwon YD, Nagy I, Adams PD, Baumeister W, Jap BK: Crystal Structures of the Rhodococcus Proteasome with and without its Pro-peptides: Implications for the Role of the Pro-peptide in Proteasome Assembly. *Journal of Molecular Biology* 2004, **335**:233-245.
282. Adams PD, Gopal K, Grosse-Kunstleve RW, Hung L-W, Ioerger TR, McCoy AJ, Moriarty NW, Pai RK, Read RJ, Romo TD, Sacchettini JC, Sauter NK, Storoni LC, Terwilliger TC: Recent developments in the PHENIX software for automated crystallographic structure determination. *J. Synchrotron Rad*. 2004, **11**:53-55.
283. Grosse-Kunstleve RW, Adams PD: On symmetries of substructures. *Acta Cryst*. 2003, **D59**:1974-1977.
284. Grosse-Kunstleve RW, Adams PD: Substructure search procedures for macromolecular structures. *Acta Cryst*. 2003, **D59**:1966-1973.
285. Chaudhry C, Farr GW, Todd MJ, Rye HS, Brunger AT, Adams PD, Horwich AL, Sigler PB: Role of the γ -phosphate of ATP in triggering protein folding by GroEL-GroES: function, structure and energetics. *EMBO Journal* 2003, **22**:4877-4887.
286. Pauly TA, Ekstrom JL, Beebe DA, Chrnyk B, Cunningham D, Griffor M, Kamath A, Lee SE, Madura R, Mcguire D, Subashi T, Wasilko D, Watts P, Mylari BL, Oates PJ, Adams PD, Rath VL: X-Ray Crystallographic and Kinetic Studies of Human Sorbitol Dehydrogenase. *Structure* 2003, **11**:1071-1085.
287. Kazantsev AV, Krivenko AA, Harrington DJ, Carter RJ, Holbrook SR, Adams PD, Pace NR: High-resolution structure of RNase P protein from *Thermotoga maritima*. *Proc. Nat. Acad. Sci. USA*. 2003, **100**:7497-7502.

288. Adams PD, Grosse-Kunstleve RW, Hung L-W, Ioerger TR, McCoy AJ, Moriarty NW, Read RJ, Sacchettini JC, Sauter NK, Terwilliger TC: PHENIX: building new software for automated crystallographic structure determination. *Acta Cryst.* 2002, **D58**:1948-1954.
289. Grosse-Kunstleve RW, Adams PD: On the handling of atomic anisotropic displacement parameters. *J. Appl. Cryst.* 2002, **35**:477-480.
290. Gottschalk KE, Adams PD, Brunger AT, Kessler H: Transmembrane signal transduction of the $\alpha\text{IIb}\beta\text{3}$ integrin. *Protein Science* 2002, **11**:1800-1812.
291. Brunger AT, Adams PD: Molecular dynamics applied to X-ray structure refinement. *Accounts of Chemical Research* 2002, **35**:404-412.
292. Grosse-Kunstleve RW, Sauter NK, Moriarty NW, Adams PD: The Computational Crystallography Toolbox: crystallographic algorithms in a reusable software framework. *J. Appl. Cryst.* 2002, **35**:126-136.
293. Grosse-Kunstleve RW, Adams PD: Algorithms for deriving crystallographic space-group information. II. Treatment of special positions. *Acta Cryst.* 2002, **A58**:60-65.
294. Grosse-Kunstleve RW, Adams PD: Patterson correlation methods: a review of molecular replacement with CNS. *Acta Cryst.* 2001, **D57**:1390-1396.
295. Torres J, Adams PD, Arkin IT: Use of a new label, $^{13}\text{C}=^{18}\text{O}$, in the determination of a structural model of phospholamban in a lipid bilayer. Spatial restraints resolve the ambiguity arising from the interpretations of mutagenesis data. *Journal of Molecular Biology* 2000, **300**:677-685.
296. Adams PD, Pannu NS, Read RJ, Brunger AT: Extending the limits of molecular replacement through combined simulated annealing and maximum likelihood refinement. *Acta Cryst.* 1999, **D55**:181-190.
297. Kukul A, Adams PD, Rice LM, Brunger AT, Arkin IT: Experimentally based orientational refinement of membrane protein models: A structure for the Influenza A M2 H⁺ channel. *Journal of Molecular Biology* 1999, **286**:951-962.
298. Brunger AT, Adams PD, Clore GM, Gros P, Grosse-Kunstleve RW, Jiang J-S, Kuszewski J, Nilges M, Pannu NS, Read RJ, Rice LM, Simonson T, Warren GL: Crystallography & NMR system (CNS): A new software system for macromolecular structure determination. *Acta Cryst.* 1998, **D54**:905-921.
299. Adams PD, Pannu NS, Read RJ, Brunger AT: Cross-validated maximum likelihood enhances crystallographic simulated annealing refinement. *Proc. Nat. Acad. Sci. USA.* 1997, **94**:5018-5023.
300. Arkin IT, Adams PD, Brunger AT, Aimoto S, Engelman DM, Smith SO: Structure of the Transmembrane Cysteine Residues in Phospholamban. *J. Membrane Biol.* 1997, **155**:199-206.
301. Adams PD, Engelman DM, Brunger AT: An improved prediction for the structure of the dimeric transmembrane domain of Glycophorin A obtained through global searching. *Proteins* 1996, **26**:257-261.
302. Braig K, Adams PD, Brunger AT: Conformational variability in the refined structure of the chaperonin GroEL at 2.8 Å resolution. *Nature Structural Biology* 1995, **2**:1083-1094.
303. Adams PD, Arkin IT, Engelman DM, Brunger AT: Computational searching and mutagenesis suggest a structure for phospholamban, a cardiac ion channel. *Nature Structural Biology* 1995, **2**:154-162.
304. Arkin IT, Adams PD, MacKenzie KR, Lemmon MA, Brunger AT, Engelman DM: Structural organization of the pentameric transmembrane alpha-helices of phospholamban, a cardiac ion channel. *EMBO Journal* 1994, **13**:4757-4764.
305. Lemmon MA, Treutlein HR, Adams PD, Brunger AT, Engelman DM: A dimerization motif for transmembrane alpha-helices. *Nature Structural Biology* 1994, **1**:157-163.

Publications (reviews, comment, book chapters & non-peer reviewed articles, 53 total)

1. Adams PD, Liebschner D, Terwilliger TC, Afonine PV, Richardson JS: How algorithms from crystallography are helping electron cryo-microscopy. Section 6.5 in *Single-particle Cryo-EM of Biological Macromolecules*, editors Glaeser RM, Nogales E, Chiu W. IOP Publishing, 2021.
2. Liebschner D, Afonine PV, Moriarty NW, Adams PD: What Are the Current Limits on Determination of Protonation State Using Neutron Macromolecular Crystallography? *Methods Enzymol.* 2020, **634**:225-255.
3. Liebschner D, Afonine PV, Urzhumtsev AG, Adams PD: Implementation of the Riding Hydrogen Model in CCTBX to Support the Next Generation of X-ray and Neutron Joint Refinement in Phenix. *Methods Enzymol.* 2020, **634**:177-199.
4. Sauter NK, Adams PD: Overcoming Data Processing Challenges for Breakthrough Crystallography. in *X-Ray Free Electron Lasers: Applications in Materials, Chemistry and Biology*. Eds. Bergmann U, Yachandra V, Yano J. The Royal Society of Chemistry. 2017, 70-87.
5. Petzold CJ, Chan LJ, Nhan M, Adams PD: Analytics for Metabolic Engineering. *Front Bioeng Biotechnol.* 2015, **3**:135
6. Zwart P, Taylor J, Morton S, Cayford R, Fontenay G, Allaire M, Sankaran B, Dickert J, Royal K, Rozales A, Dautz A, Bryant D, Smith N, Ortega S, Sauter N, Adams P, Ralston C: The Berkeley Center for Structural Biology at the Advanced Light Source. *Synchrotron Radiation News* 2015, **28**, 2:22-27.
7. Afonine PV, Urzhumtsev A, Adams PD: Macromolecular crystallographic structure refinement. in *Arbor, Celebrating 100 years of modern crystallography* 2015, **191**:a219
8. Schmidt M, Perera PN, Weber-Bargioni A, Adams PD, Schuck PJ: Raman Spectroscopic Imaging of Biological Systems. in *Imaging Life: Biological Systems from Atoms to Tissues*. Eds. Howard GC, Brown WE, Auer M. Oxford University Press. 2014, 339-377.
9. Wall ME, Adams PD, Fraser JS, Sauter NK: Diffuse x-ray scattering to model protein motions. *Structure.* 2014, **22**:182-184.
10. Urzhumtsev A, Afonine PV, Adams PD: TLS from fundamentals to practice. *Crystallography Reviews* 2013, **19**:230-270
11. Afonine PV, Adams PD: Crystallographic Structure Refinement in a Nutshell. in *Advancing Methods for Biomolecular Crystallography, NATO Science for Peace and Security Series A: Chemistry and Biology*. Eds. Read RJ, Urzhumtsev, Lunin VY. Springer Science+Business Media Dordrecht. 2013, 211-219.
12. Adams PD, Baker D, Brunger AT, Das R, Dimaio F, Read RJ, Richardson DC, Richardson JS, Terwilliger TC: Advances, Interactions, and Future Developments in the CNS, Phenix, and Rosetta Structural Biology Software Systems. *Annu. Rev. Biophys.* 2013, **42**:265-287.
13. Brunger AT, Adams PD: Refinement of X-ray Crystal Structures. In *Comprehensive Biophysics*, Edward Egelman, Editor-in-Chief., Academic Press, 2012.
14. Morin A, Urban J, Adams PD, Foster I, Sali A, Baker D, Sliz P: Research priorities. Shining light into black boxes. *Science* 2012, **336**:159-160
15. Brunger AT, Adams PD, Rice LM: Enhanced Macromolecular Refinement by Simulated Annealing. In *International Tables for Crystallography, Volume F: Crystallography of Biological Macromolecules*, E. Arnold, D.M Himmel and M.G. Rossmann, Eds., John Wiley and Sons, Ltd., 2011, 466-473.
16. Brunger AT, Adams PD, DeLano WL, Gros P, Grosse-Kunstleve RW, Jiang JS, Pannu NS, Read RJ, Rice LM, Simonson T: CNS, a program system for structure-determination and refinement. In *International Tables for Crystallography, Volume F: Crystallography of Biological Macromolecules*, E. Arnold, D.M Himmel and M.G. Rossmann, Eds., John Wiley and Sons, Ltd., 2011, 512-519.
17. Adams PD, Afonine PV, Bunkóczi G, Chen VB, Davis IW, Echols N, Headd JJ, Hung L-W, Kapral GJ, Grosse-Kunstleve RW, McCoy AJ, Moriarty NW, Oeffner R, Read RJ, Richardson DC, Richardson JS, Terwilliger TC,

- Zwart PH: PHENIX: a comprehensive Python-based system for macromolecular structure solution. In *International Tables for Crystallography, Volume F: Crystallography of Biological Macromolecules*, E. Arnold, D.M Himmel and M.G. Rossmann, Eds., John Wiley and Sons, Ltd., 2011, 539-547.
18. Adams P, Langan P: Opportunities and challenges with the growth of neutron crystallography. *Acta Cryst.* 2010, **D66**:1121-1123.
 19. Tamura L, Ahmed M, Bailey S, Bluhm H, Guo J, Heske C, Hexemer A, Liu Z, MacDowell A, Marcus M, Padmore H, Schoenlein B, Teat S, Tyliszczak, Yang W, Adams P, Falcone R, Hussain Z: Photon Science at the ALS for Sustainable Energy. *Synchrotron Radiation News* 2010, **23**, 4:8-15.
 20. Adams PD, Afonine PV, Grosse-Kunstleve RW, Read RJ, Richardson JS, Richardson DC, Terwilliger TC: Recent developments in phasing and structure refinement for macromolecular crystallography. *Current Opinion in Structural Biology* 2009, **19**:566-572.
 21. Grosse-Kunstleve RW, Terwilliger TC, Adams PD: Experience converting a large Fortran-77 program to C++. *Newsletter of the IUCr Commission on Crystallographic Computing* 2009, **10**:74-83.
 22. Zwart PH, Afonine PV, Grosse-Kunstleve RW, Hung L-W, Ioerger TR, McCoy AJ, McKee E, Moriarty NW, Read RJ, Sacchettini JC, Sauter NK, Storoni LC, Terwilliger TC, Adams PD: Automated Structure Solution with the PHENIX Suite. *Methods in Molecular Biology* 2008, **426**:419-436.
 23. Kim SH, Shin DH, Kim R, Adams P, Chandonia JM: Structural genomics of minimal organisms: pipeline and results. *Methods in Molecular Biology* 2008, **426**:475-496.
 24. Bourhis LJ, Grosse-Kunstleve RW, Adams PD: cctbx news *Newsletter of the IUCr Commission on Crystallographic Computing* 2007, **7**:74-80.
 25. Adams PD, Afonine PV, Grosse-Kunstleve RW, Moriarty NW, Sauter NK, Zwart PH, Gopal K, Ioerger TR, Kanbi L, McKee E, Pai RK, Hung L-W, Radhakannan T, McCoy AJ, Read RJ, Storoni LC, Romo TD, Sacchettini JC, Terwilliger TC: Automated structure determination with Phenix. In *Evolving Methods for Macromolecular Crystallography*. Read RJ and Sussman JL, Eds., Springer, Dordrecht, The Netherlands. 2007, 101-109.
 26. Morton S, Glossinger J, Smith-Baumann A, McKean JP, Trame C, Dickert J, Rozales A, Daus A, Taylor J, Zwart P, Duarte R, Padmore H, McDermott G, Adams P: Recent Major Improvements to the ALS Sector 5 Macromolecular Crystallography Beamlines. *Synchrotron Radiation News* 2007, **20**, 4:23-30
 27. Zwart PH, Grosse-Kunstleve RW, Adams PD: Exploring Metric Symmetry. *CCP4 newsletter*, Summer 2006; Contribution 8.
 28. Grosse-Kunstleve RW, Zwart PH, Afonine PV, Ioerger TR, Adams PD: cctbx news *Newsletter of the IUCr Commission on Crystallographic Computing* 2006, **7**:92-105.
 29. Zwart PH, Grosse-Kunstleve RW, Adams PD: Xtrriage and Fest: automatic assessment of X-ray data and substructure structure factor estimation. *CCP4 newsletter*, Winter 2005; Contribution 7.
 30. Kim SH, Shin DH, Wang W, Adams PD, Chandonia JM: Overview of Structural Genomics: Landscape, Premises, and Current Direction. In *Structural Genomics and High Throughput Structural Biology* 2005, M. Sundstrom, M. Norin and A. Edwards, Eds., CRC Press, Taylor and Francis Group.
 31. Afonine PV, Grosse-Kunstleve RW, Adams PD: The Phenix refinement framework. *CCP4 newsletter*, July 2005; Contribution 8.
 32. Zwart PH, Grosse-Kunstleve RW, Adams PD: Characterisation of X-ray data sets. *CCP4 newsletter*, July 2005; Contribution 10.
 33. Grosse-Kunstleve RW, Afonine PV, Sauter NK, Adams PD: cctbx news. *IUCr Computing Commission Newsletter* 2005, **5**:69-91.
 34. Grosse-Kunstleve RW, Afonine PV, Adams PD: cctbx news. *IUCr Computing Commission Newsletter* 2004, **4**:19-36.

35. Grosse-Kunstleve RW, Sauter NK, Adams PD: cctbx news. *IUCr Computing Commission Newsletter* 2004, **3**:22-31.
36. Kochva U, Leonov H, Arkin IT, Adams PD: Modeling Membrane Proteins Utilizing Information from Silent Amino Acid Substitutions. In *Current Protocols in Bioinformatics*. 2003, Baxevanis AD, Petsko GA, Stein LD, Stormo GD, Eds., John Wiley & Sons, Inc.
37. Weeks CM, Adams PD, Berendzen J, Brunger AT, Dodson EJ, Grosse-Kunstleve RW, Schneider TR, Sheldrick GM, Terwilliger TC, Turkenburg MG, Uson I: Automatic solution of heavy-atom substructures. *Methods Enzymol.* 2003, **374**:37-83.
38. Grosse-Kunstleve RW, Wong B, Adams PD: cctbx news: Fast triplet generator for direct methods, Gallery of direct-space asymmetric units, et. al. *IUCr Computing Commission Newsletter* 2003, **2**:10-16.
39. Adams PD, Grosse-Kunstleve RW, Brunger AT: Computational aspects of high-throughput crystallographic macromolecular structure determination *Methods Biochem. Anal.* 2003, **44**:75-87.
40. Grosse-Kunstleve RW, Adams PD: State of the Toolbox: an overview of the Crystallography Toolbox (CCTBX) *IUCr Computing Commission Newsletter* 2003, **1**:28-38.
41. Brunger AT, Adams PD: Molecular dynamics applied to X-ray structure refinement *Accounts of Chemical Research* 2002, **35**:404-412.
42. Brunger AT, Adams PD, Rice LM: Enhanced Macromolecular Refinement by Simulated Annealing. In *International Tables for Crystallography, Volume F: Macromolecular crystallography*, M.G. Rossmann and E. Arnold, Eds., Kluwer Academic Publishers (Dordrecht), 2001, 375-381.
43. Brunger AT, Adams PD, DeLano WL, Gros P, Grosse-Kunstleve RW, Jiang JS, Pannu NS, Read RJ, Rice LM, Simonson T: The structure determination language of the Crystallography & NMR System. In *International Tables for Crystallography, Volume F: Macromolecular crystallography*, M.G. Rossmann and E. Arnold, Eds., Kluwer Academic Publishers (Dordrecht), 2001, 710-716.
44. Adams PD, Grosse-Kunstleve RW: Recent developments in software for automation of crystallographic macromolecular structure determination. *Current Opinion in Structural Biology* 2000, **10**:564-568.
45. Brunger AT, Adams PD, Rice LM: Annealing in crystallography: a powerful optimization tool *Progress in Biophysics & Molecular Biology* 1999, **72**:135-155.
46. Brunger AT, Adams PD, Rice LM: Recent developments for the efficient crystallographic refinement of macromolecular structures. *Current Opinion in Structural Biology* 1998, **8**:606-611.
47. Brunger AT, Adams PD, Rice LM: New Applications of simulated annealing in crystallographic refinement. In *Direct Methods for Solving Macromolecular Structures* 1998, S. Fortier, Ed., Kluwer, 143-157.
48. Adams PD, Lee AS, Brunger AT, Engelman DM: Models for the transmembrane region of the phospholamban pentamer: which is correct?. *Annals of the New York Academy of Science* 1998, **853**:178-185.
49. Brunger AT, Adams PD, Rice LM: New applications of simulated annealing in X-ray crystallography and solution NMR. *Structure* 1997, **5**:325-336.
50. Weissman JS, Fenton WA, Braig K, Adams PD, Horwich AL: *Escherichia Coli* GroEL, structure and function. In *Guidebook to Molecular Chaperones and Protein Folding Sequences* 1997, M.-J. Gething, Ed., Oxford University Press, 173-176.
51. Arkin IT, Adams PD, Brunger AT, Smith SO, Engelman DM: Structural perspectives of phospholamban, a helical transmembrane pentamer. *Annual Reviews of Biophysics and Biomolecular Structure* 1997, **26**:157-222.
52. Adams PD, Brunger AT: Towards Prediction of Membrane Protein Structure. In *Membrane Protein Assembly* 1997, G.V. Heijne, Ed., R.G. Landes Co., Austin, TX.

53. Adams PD, Braig K, Rice LM, Brunger AT: Torsion angle dynamics refinement of the Chaperonin GroEL at 2.8 Å resolution. In *Macromolecular refinement*, Proceedings of the CCP4 study weekend at Chester College 1996, January 5-6, S. Bailey and E. Dodson, Eds., Council of the Central Laboratory of the Research Councils.