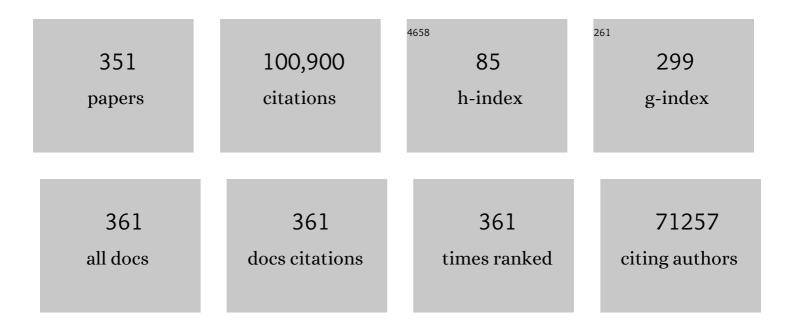
## Paul D. Adams

List of Publications by Year in descending order

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PALLE D ADAMS

| #  | Article   | IF   | CITATIONS |
|----|---|------|-----------|
| 1  | Integration of software tools for integrative modeling of biomolecular systems. Journal of<br>Structural Biology, 2022, 214, 107841.  | 2.8  | 7         |
| 2  | Modular automated bottom-up proteomic sample preparation for high-throughput applications. PLoS ONE, 2022, 17, e0264467.  | 2.5  | 3         |
| 3  | A Synthetic Gene Library Yields a Previously Unknown Clycoside Phosphorylase That Degrades and<br>Assembles Poly-β-1,3-GlcNAc, Completing the Suite of β-Linked GlcNAc Polysaccharides. ACS Central<br>Science, 2022, 8, 430-440.                 | 11.3 | 7         |
| 4  | <i>O</i> -/ <i>N</i> -/ <i>S</i> -Specificity in Glycosyltransferase Catalysis: From Mechanistic<br>Understanding to Engineering. ACS Catalysis, 2021, 11, 1810-1815.   | 11.2 | 42        |
| 5  | Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. Nature Methods, 2021, 18, 156-164.   | 19.0 | 73        |
| 6  | Protein identification from electron cryomicroscopy maps by automated model building and side-chain matching. Acta Crystallographica Section D: Structural Biology, 2021, 77, 457-462.  | 2.3  | 9         |
| 7  | Mechanism Across Scales: A Holistic Modeling Framework Integrating Laboratory and Field Studies for Microbial Ecology. Frontiers in Microbiology, 2021, 12, 642422.   | 3.5  | 12        |
| 8  | Efficient production of oxidized terpenoids via engineering fusion proteins of terpene synthase and cytochrome P450. Metabolic Engineering, 2021, 64, 41-51.  | 7.0  | 33        |
| 9  | Engineering Saccharomyces cerevisiae for isoprenol production. Metabolic Engineering, 2021, 64, 154-166.  | 7.0  | 34        |
| 10 | Experimental and theoretical insights into the effects of pH on catalysis of bond-cleavage by the<br>lignin peroxidase isozyme H8 from Phanerochaete chrysosporium. Biotechnology for Biofuels, 2021,<br>14, 108.                                 | 6.2  | 10        |
| 11 | A multiplexed nanostructure-initiator mass spectrometry (NIMS) assay for simultaneously detecting glycosyl hydrolase and lignin modifying enzyme activities. Scientific Reports, 2021, 11, 11803.   | 3.3  | 7         |
| 12 | 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. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, e2102342118. | 7.1  | 7         |
| 13 | Accurate prediction of protein structures and interactions using a three-track neural network.<br>Science, 2021, 373, 871-876.  | 12.6 | 2,843     |
| 14 | Macromolecular refinement of X-ray and cryoelectron microscopy structures with Phenix/OPLS3e for improved structure and ligand quality. Structure, 2021, 29, 913-921.e4.  | 3.3  | 29        |
| 15 | <i>CERES</i> : a cryo-EM re-refinement system for continuous improvement of deposited models. Acta<br>Crystallographica Section D: Structural Biology, 2021, 77, 48-61.   | 2.3  | 14        |
| 16 | Structural dynamics in the water and proton channels of photosystem II during the S2 to S3 transition. Nature Communications, 2021, 12, 6531.   | 12.8 | 73        |
| 17 | Cryoâ€EM map interpretation and protein modelâ€building using iterative map segmentation. Protein<br>Science, 2020, 29, 87-99.  | 7.6  | 27        |
| 18 | Structural Mechanism of Regioselectivity in an Unusual Bacterial Acyl-CoA Dehydrogenase. Journal of the American Chemical Society, 2020, 142, 835-846.  | 13.7 | 9         |

| #  | Article  | IF   | CITATIONS |
|----|--|------|-----------|
| 19 | Characterization of a Metal-Resistant Bacillus Strain With a High Molybdate Affinity ModA From<br>Contaminated Sediments at the Oak Ridge Reservation. Frontiers in Microbiology, 2020, 11, 587127.  | 3.5  | 11        |
| 20 | Novel bacterial clade reveals origin of form I Rubisco. Nature Plants, 2020, 6, 1158-1166.   | 9.3  | 46        |
| 21 | Improvement of cryo-EM maps by density modification. Nature Methods, 2020, 17, 923-927.  | 19.0 | 243       |
| 22 | Draft Genome Sequence of <i>Bacillus</i> sp. Strain EB106-08-02-XG196, Isolated from<br>High-Nitrate-Contaminated Sediment. Microbiology Resource Announcements, 2020, 9, .  | 0.6  | 0         |
| 23 | A Global Ramachandran Score Identifies Protein Structures with Unlikely Stereochemistry. Structure, 2020, 28, 1249-1258.e2.  | 3.3  | 86        |
| 24 | Implementation of the riding hydrogen model in CCTBX to support the next generation of X-ray and neutron joint refinement in Phenix. Methods in Enzymology, 2020, 634, 177-199.  | 1.0  | 8         |
| 25 | An iron (II) dependent oxygenase performs the last missing step of plant lysine catabolism. Nature<br>Communications, 2020, 11, 2931.  | 12.8 | 11        |
| 26 | Response of <i>Pseudomonas putida</i> to Complex, Aromaticâ€Rich Fractions from Biomass.<br>ChemSusChem, 2020, 13, 4455-4467.  | 6.8  | 23        |
| 27 | What are the current limits on determination of protonation state using neutron macromolecular crystallography?. Methods in Enzymology, 2020, 634, 225-255.  | 1.0  | 0         |
| 28 | Structure and Function of BorB, the Type II Thioesterase from the Borrelidin Biosynthetic Gene<br>Cluster. Biochemistry, 2020, 59, 1630-1639.  | 2.5  | 10        |
| 29 | Untangling the sequence of events during the S <sub>2</sub> → S <sub>3</sub> transition in photosystem II and implications for the water oxidation mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 12624-12635. | 7.1  | 149       |
| 30 | Improved chemistry restraints for crystallographic refinement by integrating the Amber force field into <i>Phenix</i> . Acta Crystallographica Section D: Structural Biology, 2020, 76, 51-62.   | 2.3  | 29        |
| 31 | Density modification of cryo-EM maps. Acta Crystallographica Section D: Structural Biology, 2020, 76, 912-925.   | 2.3  | 28        |
| 32 | Arginine off-kilter: guanidinium is not as planar as restraints denote. Acta Crystallographica Section<br>D: Structural Biology, 2020, 76, 1159-1166.  | 2.3  | 7         |
| 33 | Cryo_fit: Democratization of flexible fitting for cryo-EM. Journal of Structural Biology, 2019, 208, 1-6.  | 2.8  | 30        |
| 34 | Automated "Cells-To-Peptides―Sample Preparation Workflow for High-Throughput, Quantitative<br>Proteomic Assays of Microbes. Journal of Proteome Research, 2019, 18, 3752-3761.   | 3.7  | 32        |
| 35 | Optimization of the IPP-bypass mevalonate pathway and fed-batch fermentation for the production of isoprenol in Escherichia coli. Metabolic Engineering, 2019, 56, 85-96.  | 7.0  | 46        |
| 36 | Structural insights into dehydratase substrate selection for the borrelidin and fluvirucin polyketide synthases. Journal of Industrial Microbiology and Biotechnology, 2019, 46, 1225-1235.  | 3.0  | 7         |

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|----|---|-----|-----------|
| 37 | Massively Parallel Fitness Profiling Reveals Multiple Novel Enzymes in <i>Pseudomonas putida</i> Lysine Metabolism. MBio, 2019, 10, .   | 4.1 | 60        |
| 38 | Methyl ketone production by <i>Pseudomonas putida</i> is enhanced by plantâ€derived amino acids.<br>Biotechnology and Bioengineering, 2019, 116, 1909-1922.   | 3.3 | 29        |
| 39 | A rapid methods development workflow for high-throughput quantitative proteomic applications.<br>PLoS ONE, 2019, 14, e0211582.  | 2.5 | 17        |
| 40 | Announcing mandatory submission of PDBx/mmCIF format files for crystallographic depositions to the Protein Data Bank (PDB). Acta Crystallographica Section D: Structural Biology, 2019, 75, 451-454.  | 2.3 | 46        |
| 41 | Iron―and aluminium―nduced depletion of molybdenum in acidic environments impedes the nitrogen<br>cycle. Environmental Microbiology, 2019, 21, 152-163.  | 3.8 | 22        |
| 42 | Iron–sulfur clusters have no right angles. Acta Crystallographica Section D: Structural Biology,<br>2019, 75, 16-20.  | 2.3 | 16        |
| 43 | Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in <i>Phenix</i> . Acta Crystallographica Section D: Structural Biology, 2019, 75, 861-877.  | 2.3 | 4,060     |
| 44 | Updated validation and deposition tools in the <i>Phenix</i> GUI. Acta Crystallographica Section A:<br>Foundations and Advances, 2019, 75, a339-a339.   | 0.1 | 0         |
| 45 | Developing a shared computing and networking infrastructure for the ALS-ENABLE structural biology program at the Advanced Light Source. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, a248-a248.                      | 0.1 | 0         |
| 46 | Efficient real-space refinement for cryo-EM and crystallography. Acta Crystallographica Section A:<br>Foundations and Advances, 2019, 75, e86-e86.  | 0.1 | 0         |
| 47 | Microbial Functional Gene Diversity Predicts Groundwater Contamination and Ecosystem Functioning. MBio, 2018, 9, .  | 4.1 | 57        |
| 48 | Integrated analysis of isopentenyl pyrophosphate (IPP) toxicity in isoprenoid-producing Escherichia coli. Metabolic Engineering, 2018, 47, 60-72.   | 7.0 | 106       |
| 49 | Toward industrial production of isoprenoids in <i>Escherichia coli</i> : Lessons learned from<br>CRISPRâ€Cas9 based optimization of a chromosomally integrated mevalonate pathway. Biotechnology<br>and Bioengineering, 2018, 115, 1000-1013. | 3.3 | 39        |
| 50 | Employing a biochemical protecting group for a sustainable indigo dyeing strategy. Nature Chemical<br>Biology, 2018, 14, 256-261.   | 8.0 | 143       |
| 51 | <i>DiSCaMB</i> : a software library for aspherical atom model X-ray scattering factor calculations<br>with CPUs and GPUs. Journal of Applied Crystallography, 2018, 51, 193-199.  | 4.5 | 24        |
| 52 | Discovery of enzymes for toluene synthesis from anoxic microbial communities. Nature Chemical<br>Biology, 2018, 14, 451-457.  | 8.0 | 47        |
| 53 | Interactive comparison and remediation of collections of macromolecular structures. Protein Science, 2018, 27, 182-194.   | 7.6 | 13        |
| 54 | MolProbity: More and better reference data for improved allâ€atom structure validation. Protein<br>Science, 2018, 27, 293-315.  | 7.6 | 2,776     |

| #  | Article  | IF   | CITATIONS |
|----|--|------|-----------|
| 55 | A bacterial pioneer produces cellulase complexes that persist through community succession. Nature<br>Microbiology, 2018, 3, 99-107.   | 13.3 | 38        |
| 56 | Structures of the intermediates of Kok's photosynthetic water oxidation clock. Nature, 2018, 563, 421-425.   | 27.8 | 386       |
| 57 | Distribution of evaluation scores for the models submitted to the second cryo-EM model challenge.<br>Data in Brief, 2018, 20, 1629-1638.   | 1.0  | 5         |
| 58 | Rapid characterization of the activities of lignin-modifying enzymes based on nanostructure-initiator mass spectrometry (NIMS). Biotechnology for Biofuels, 2018, 11, 266.   | 6.2  | 14        |
| 59 | Renewable production of high density jet fuel precursor sesquiterpenes from Escherichia coli.<br>Biotechnology for Biofuels, 2018, 11, 285.  | 6.2  | 43        |
| 60 | Engineering glycoside hydrolase stability by the introduction of zinc binding. Acta Crystallographica<br>Section D: Structural Biology, 2018, 74, 702-710.   | 2.3  | 1         |
| 61 | A fully automatic method yielding initial models from high-resolution cryo-electron microscopy maps. Nature Methods, 2018, 15, 905-908.  | 19.0 | 137       |
| 62 | Jungle Express is a versatile repressor system for tight transcriptional control. Nature<br>Communications, 2018, 9, 3617.   | 12.8 | 33        |
| 63 | Automated flow-based/digital microfluidic platform integrated with onsite electroporation process for multiplex genetic engineering applications. , 2018, , .  |      | 5         |
| 64 | Map segmentation, automated model-building and their application to the Cryo-EM Model Challenge.<br>Journal of Structural Biology, 2018, 204, 338-343.   | 2.8  | 6         |
| 65 | Evaluation system and web infrastructure for the second cryo-EM model challenge. Journal of Structural Biology, 2018, 204, 96-108.   | 2.8  | 11        |
| 66 | From deep TLS validation to ensembles of atomic models built from elemental motions. II. Analysis of<br>TLS refinement results by explicit interpretation. Acta Crystallographica Section D: Structural<br>Biology, 2018, 74, 621-631. | 2.3  | 7         |
| 67 | Improved chemistry restraints for crystallographic refinement by integrating Amber molecular<br>mechanics in Phenix. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, a145-a145.                                  | 0.1  | 2         |
| 68 | Evaluation of models determined by neutron diffraction and proposed improvements to their validation and deposition. Acta Crystallographica Section D: Structural Biology, 2018, 74, 800-813.  | 2.3  | 15        |
| 69 | Automated map sharpening by maximization of detail and connectivity. Acta Crystallographica Section<br>D: Structural Biology, 2018, 74, 545-559.   | 2.3  | 218       |
| 70 | Real-space refinement in <i>PHENIX</i> for cryo-EM and crystallography. Acta Crystallographica<br>Section D: Structural Biology, 2018, 74, 531-544.  | 2.3  | 2,065     |
| 71 | New tools for the analysis and validation of cryo-EM maps and atomic models. Acta Crystallographica<br>Section D: Structural Biology, 2018, 74, 814-840.   | 2.3  | 575       |
| 72 | Polder maps: improving OMIT maps for ligand building and validation. Acta Crystallographica Section<br>A: Foundations and Advances, 2018, 74, a308-a308.   | 0.1  | 0         |

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|----|--|------|-----------|
| 73 | The collaborative crystallography program at the Advanced Light Source. Acta Crystallographica<br>Section A: Foundations and Advances, 2018, 74, a431-a431.  | 0.1  | 0         |
| 74 | High-throughput protein–ligand complex structure solution with Phenix. Acta Crystallographica<br>Section A: Foundations and Advances, 2018, 74, a445-a445.   | 0.1  | 0         |
| 75 | Self-assembled gold nanoparticle film for nanostructure-initiator mass spectrometry with passive on-line salt fractionation. , 2017, , .   |      | 0         |
| 76 | Parallel microarraying of microfluidic droplets for high-throughput integration with matrix-assisted laser desorption ionization mass spectrometry. , 2017, , .  |      | 0         |
| 77 | Accurate model annotation of a near-atomic resolution cryo-EM map. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3103-3108.  | 7.1  | 111       |
| 78 | Structure of the human TRiC/CCT Subunit 5 associated with hereditary sensory neuropathy. Scientific Reports, 2017, 7, 3673.  | 3.3  | 31        |
| 79 | Structure of aryl O-demethylase offers molecular insight into a catalytic tyrosine-dependent<br>mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114,<br>E3205-E3214. | 7.1  | 24        |
| 80 | Production of jet fuel precursor monoterpenoids from engineered <i>Escherichia coli</i> .<br>Biotechnology and Bioengineering, 2017, 114, 1703-1712.   | 3.3  | 81        |
| 81 | On-chip integration of droplet microfluidics and nanostructure-initiator mass spectrometry for enzyme screening. Lab on A Chip, 2017, 17, 323-331.   | 6.0  | 44        |
| 82 | The Experiment Data Depot: A Web-Based Software Tool for Biological Experimental Data Storage,<br>Sharing, and Visualization. ACS Synthetic Biology, 2017, 6, 2248-2259.   | 3.8  | 45        |
| 83 | The cryo-electron microscopy structure of human transcription factor IIH. Nature, 2017, 549, 414-417.  | 27.8 | 89        |
| 84 | Comprehensive <i>in Vitro</i> Analysis of Acyltransferase Domain Exchanges in Modular Polyketide<br>Synthases and Its Application for Short-Chain Ketone Production. ACS Synthetic Biology, 2017, 6,<br>139-147.       | 3.8  | 100       |
| 85 | Polder maps: improving OMIT maps for ligand building and validation. Acta Crystallographica Section<br>A: Foundations and Advances, 2017, 73, C48-C48.   | 0.1  | 0         |
| 86 | Polder maps: improving OMIT maps by excluding bulk solvent. Acta Crystallographica Section D:<br>Structural Biology, 2017, 73, 148-157.  | 2.3  | 500       |
| 87 | Reply to Kiser: Dioxygen binding in NOV1 crystal structures. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E6029-E6030.  | 7.1  | 4         |
| 88 | Plant cell wall glycosyltransferases: High-throughput recombinant expression screening and general requirements for these challenging enzymes. PLoS ONE, 2017, 12, e0177591.   | 2.5  | 21        |
| 89 | Expression of naturally ionic liquid-tolerant thermophilic cellulases in Aspergillus niger. PLoS ONE, 2017, 12, e0189604.  | 2.5  | 13        |
| 90 | X-ray diffraction analysis and <i>in vitro</i> characterization of the UAM2 protein from <i>Oryza sativa</i> . Acta Crystallographica Section F, Structural Biology Communications, 2017, 73, 241-245.                 | 0.8  | 1         |

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|-----|--|------|-----------|
| 91  | Berkeley Screen: a set of 96 solutions for general macromolecular crystallization. Journal of Applied<br>Crystallography, 2017, 50, 1352-1358.   | 4.5  | 11        |
| 92  | An editor for the generation and customization of geometry restraints. Acta Crystallographica Section D: Structural Biology, 2017, 73, 123-130.  | 2.3  | 27        |
| 93  | Phasing strategies II – molecular replacement. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, a391-a391.  | 0.1  | 0         |
| 94  | Model-building using cryo-EM and crystallographic maps. Acta Crystallographica Section A:<br>Foundations and Advances, 2017, 73, C1327-C1327.  | 0.1  | 0         |
| 95  | Video tutorials for the <i>Phenix</i> software suite. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1134-C1134.   | 0.1  | 0         |
| 96  | Structure and mechanism of NOV1, a resveratrol-cleaving dioxygenase. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 14324-14329.  | 7.1  | 50        |
| 97  | Can I solve my structure by SAD phasing? Planning an experiment, scaling data and evaluating the useful anomalous correlation and anomalous signal. Acta Crystallographica Section D: Structural Biology, 2016, 72, 359-374. | 2.3  | 29        |
| 98  | No observable conformational changes in PSII. Nature, 2016, 533, E1-E2.  | 27.8 | 40        |
| 99  | Nonâ€invasive imaging of cellulose microfibril orientation within plant cell walls by polarized Raman microspectroscopy. Biotechnology and Bioengineering, 2016, 113, 82-90.   | 3.3  | 21        |
| 100 | Structural and Biochemical Characterization of the Early and Late Enzymes in the Lignin β-Aryl Ether<br>Cleavage Pathway from Sphingobium sp. SYK-6. Journal of Biological Chemistry, 2016, 291, 10228-10238.                | 3.4  | 44        |
| 101 | Characterizing Strain Variation in Engineered E.Âcoli Using a Multi-Omics-Based Workflow. Cell<br>Systems, 2016, 2, 335-346.   | 6.2  | 73        |
| 102 | Comparative Community Proteomics Demonstrates the Unexpected Importance of Actinobacterial<br>Glycoside Hydrolase Family 12 Protein for Crystalline Cellulose Hydrolysis. MBio, 2016, 7, .                                   | 4.1  | 17        |
| 103 | Structure of photosystem II and substrate binding at room temperature. Nature, 2016, 540, 453-457.   | 27.8 | 323       |
| 104 | Can I solve my structure by SAD phasing? Anomalous signal in SAD phasing. Acta Crystallographica<br>Section D: Structural Biology, 2016, 72, 346-358.  | 2.3  | 31        |
| 105 | A second-generation expression system for tyrosine-sulfated proteins and its application in crop protection. Integrative Biology (United Kingdom), 2016, 8, 542-545.   | 1.3  | 23        |
| 106 | A Droplet Microfluidic Platform for Automating Genetic Engineering. ACS Synthetic Biology, 2016, 5, 426-433.   | 3.8  | 63        |
| 107 | Exploiting the Substrate Promiscuity of Hydroxycinnamoyl-CoA:Shikimate Hydroxycinnamoyl<br>Transferase to Reduce Lignin. Plant and Cell Physiology, 2016, 57, 568-579.   | 3.1  | 78        |
| 108 | Structural Basis of Stereospecificity in the Bacterial Enzymatic Cleavage of β-Aryl Ether Bonds in<br>Lignin. Journal of Biological Chemistry, 2016, 291, 5234-5246.   | 3.4  | 40        |

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|-----|--|-----|-----------|
| 109 | A new default restraint library for the protein backbone in <i>Phenix</i> : a conformation-dependent<br>geometry goes mainstream. Acta Crystallographica Section D: Structural Biology, 2016, 72, 176-179. | 2.3 | 39        |
| 110 | Improved ligand geometries in crystallographic refinement using <i>AFITT</i> in <i>PHENIX</i> . Acta<br>Crystallographica Section D: Structural Biology, 2016, 72, 1062-1072.                              | 2.3 | 29        |
| 111 | New bulk-solvent model improves model-to-data fit and facilitates map interpretation. Acta<br>Crystallographica Section A: Foundations and Advances, 2016, 72, s22-s22.                                    | 0.1 | Ο         |
| 112 | Predicting X-ray diffuse scattering from translation–libration–screw structural ensembles. Acta<br>Crystallographica Section D: Biological Crystallography, 2015, 71, 1657-1667.                           | 2.5 | 14        |
| 113 | Analytics for Metabolic Engineering. Frontiers in Bioengineering and Biotechnology, 2015, 3, 135.  | 4.1 | 79        |
| 114 | Development of a High Throughput Platform for Screening Glycoside Hydrolases Based on Oxime-NIMS. Frontiers in Bioengineering and Biotechnology, 2015, 3, 153.   | 4.1 | 14        |
| 115 | Use of Nanostructure-Initiator Mass Spectrometry to Deduce Selectivity of Reaction in Glycoside Hydrolases. Frontiers in Bioengineering and Biotechnology, 2015, 3, 165.                                   | 4.1 | 6         |
| 116 | Natural Bacterial Communities Serve as Quantitative Geochemical Biosensors. MBio, 2015, 6, e00326-15.  | 4.1 | 173       |
| 117 | The Berkeley Center for Structural Biology at the Advanced Light Source. Synchrotron Radiation News, 2015, 28, 22-27.  | 0.8 | 2         |
| 118 | NMR Exchange Format: a unified and open standard for representation of NMR restraint data. Nature Structural and Molecular Biology, 2015, 22, 433-434.   | 8.2 | 40        |
| 119 | Multifunctional cellulase catalysis targeted by fusion to different carbohydrate-binding modules.<br>Biotechnology for Biofuels, 2015, 8, 220.   | 6.2 | 49        |
| 120 | Programming new geometry restraints: parallelity of atomic groups. Journal of Applied<br>Crystallography, 2015, 48, 1130-1141.   | 4.5 | 13        |
| 121 | Principal component analysis of proteomics (PCAP) as a tool to direct metabolic engineering.<br>Metabolic Engineering, 2015, 28, 123-133.  | 7.0 | 140       |
| 122 | Metabolic engineering for the high-yield production of isoprenoid-based C5 alcohols in E. coli.<br>Scientific Reports, 2015, 5, 11128.   | 3.3 | 125       |
| 123 | Identification and Characterization of a Golgi-Localized UDP-Xylose Transporter Family from Arabidopsis. Plant Cell, 2015, 27, 1218-1227.  | 6.6 | 61        |
| 124 | FEM: feature-enhanced map. Acta Crystallographica Section D: Biological Crystallography, 2015, 71,<br>646-666.   | 2.5 | 157       |
| 125 | A Versatile Microfluidic Device for Automating Synthetic Biology. ACS Synthetic Biology, 2015, 4, 1151-1164.   | 3.8 | 81        |
| 126 | Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. Structure, 2015, 23, 1156-1167.   | 3.3 | 159       |

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| #   | Article   | IF   | CITATIONS |
|-----|---|------|-----------|
| 127 | Indexing amyloid peptide diffraction from serial femtosecond crystallography: new algorithms for sparse patterns. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 357-366.  | 2.5  | 18        |
| 128 | Using support vector machines to improve elemental ion identification in macromolecular crystal structures. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 1147-1158.  | 2.5  | 4         |
| 129 | Standard Flow Liquid Chromatography for Shotgun Proteomics in Bioenergy Research. Frontiers in Bioengineering and Biotechnology, 2015, 3, 44.   | 4.1  | 44        |
| 130 | EMRinger: side chain–directed model and map validation for 3D cryo-electron microscopy. Nature<br>Methods, 2015, 12, 943-946.   | 19.0 | 799       |
| 131 | Macromolecular X-ray structure determination using weak, single-wavelength anomalous data.<br>Nature Methods, 2015, 12, 127-130.  | 19.0 | 31        |
| 132 | A droplet-to-digital (D2D) microfluidic device for single cell assays. Lab on A Chip, 2015, 15, 225-236.  | 6.0  | 70        |
| 133 | From deep TLS validation to ensembles of atomic models built from elemental motions. Acta<br>Crystallographica Section D: Biological Crystallography, 2015, 71, 1668-1683.  | 2.5  | 14        |
| 134 | Macromolecular crystallographic estructure refinement. Arbor, 2015, 191, a219.  | 0.3  | 3         |
| 135 | Cellulosic Biomass Pretreatment and Sugar Yields as a Function of Biomass Particle Size. PLoS ONE, 2014, 9, e100836.  | 2.5  | 19        |
| 136 | Development of a Native Escherichia coli Induction System for Ionic Liquid Tolerance. PLoS ONE, 2014,<br>9, e101115.  | 2.5  | 31        |
| 137 | Understanding the Role of Histidine in the GHSxG Acyltransferase Active Site Motif: Evidence for<br>Histidine Stabilization of the Malonyl-Enzyme Intermediate. PLoS ONE, 2014, 9, e109421.   | 2.5  | 10        |
| 138 | Pressure stabilizer for reproducible picoinjection in droplet microfluidic systems. Lab on A Chip, 2014, 14, 4533-4539.   | 6.0  | 34        |
| 139 | A Peptide-Based Method for 13C Metabolic Flux Analysis in Microbial Communities. PLoS Computational Biology, 2014, 10, e1003827.  | 3.2  | 56        |
| 140 | An atomic model of brome mosaic virus using direct electron detection and real-space optimization.<br>Nature Communications, 2014, 5, 4808.   | 12.8 | 105       |
| 141 | Structural and Biochemical Studies of Actin in Complex with Synthetic Macrolide Tail Analogues.<br>ChemMedChem, 2014, 9, 2286-2293.   | 3.2  | 20        |
| 142 | Conformationâ€dependent backbone geometry restraints set a new standard for protein<br>crystallographic refinement. FEBS Journal, 2014, 281, 4061-4071.   | 4.7  | 36        |
| 143 | Conformational dynamics of a crystalline protein from microsecond-scale molecular dynamics simulations and diffuse X-ray scattering. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 17887-17892. | 7.1  | 55        |
| 144 | Error Rate Comparison during Polymerase Chain Reaction by DNA Polymerase. Molecular Biology<br>International, 2014, 2014, 1-8.  | 1.7  | 160       |

| #   | Article   | IF   | CITATIONS |
|-----|---|------|-----------|
| 145 | Improved crystal orientation and physical properties from single-shot XFEL stills. Acta<br>Crystallographica Section D: Biological Crystallography, 2014, 70, 3299-3309.  | 2.5  | 38        |
| 146 | Metrics for comparison of crystallographic maps. Acta Crystallographica Section D: Biological<br>Crystallography, 2014, 70, 2593-2606.  | 2.5  | 29        |
| 147 | Structure of the OsSERK2 leucine-rich repeat extracellular domain. Acta Crystallographica Section D:<br>Biological Crystallography, 2014, 70, 3080-3086.  | 2.5  | 16        |
| 148 | Accurate macromolecular structures using minimal measurements from X-ray free-electron lasers.<br>Nature Methods, 2014, 11, 545-548.  | 19.0 | 140       |
| 149 | Correlation analysis of targeted proteins and metabolites to assess and engineer microbial isopentenol production. Biotechnology and Bioengineering, 2014, 111, 1648-1658.                                      | 3.3  | 89        |
| 150 | Rapid Kinetic Characterization of Glycosyl Hydrolases Based on Oxime Derivatization and<br>Nanostructure-Initiator Mass Spectrometry (NIMS). ACS Chemical Biology, 2014, 9, 1470-1479.                          | 3.4  | 36        |
| 151 | CRYO-EM Atomic Model of Brome Mosaic Virus Derived from Direct Electron Detection Images and a Real-Space Model Optimization Protocol. Biophysical Journal, 2014, 106, 600a.                                    | 0.5  | 2         |
| 152 | Analysis of plant nucleotide sugars by hydrophilic interaction liquid chromatography and tandem mass spectrometry. Analytical Biochemistry, 2014, 448, 14-22.   | 2.4  | 49        |
| 153 | Production of anteiso-branched fatty acids in Escherichia coli; next generation biofuels with improved cold-flow properties. Metabolic Engineering, 2014, 26, 111-118.  | 7.0  | 55        |
| 154 | <i>In Vitro</i> Analysis of Carboxyacyl Substrate Tolerance in the Loading and First Extension<br>Modules of Borrelidin Polyketide Synthase. Biochemistry, 2014, 53, 5975-5977.                                 | 2.5  | 21        |
| 155 | Identification of a Sphingolipid α-Glucuronosyltransferase That Is Essential for Pollen Function<br>in <i>Arabidopsis</i> Â Â Â. Plant Cell, 2014, 26, 3314-3325.   | 6.6  | 80        |
| 156 | Automated identification of elemental ions in macromolecular crystal structures. Acta<br>Crystallographica Section D: Biological Crystallography, 2014, 70, 1104-1114.  | 2.5  | 40        |
| 157 | Phylogenomically Guided Identification of Industrially Relevant GH1 β-Glucosidases through DNA<br>Synthesis and Nanostructure-Initiator Mass Spectrometry. ACS Chemical Biology, 2014, 9, 2082-2091.            | 3.4  | 78        |
| 158 | Constructing Tailored Isoprenoid Products by Structure-Guided Modification of Geranylgeranyl<br>Reductase. Structure, 2014, 22, 1028-1036.  | 3.3  | 28        |
| 159 | A targeted proteomics toolkit for high-throughput absolute quantification of Escherichia coli<br>proteins. Metabolic Engineering, 2014, 26, 48-56.  | 7.0  | 45        |
| 160 | Taking snapshots of photosynthetic water oxidation using femtosecond X-ray diffraction and spectroscopy. Nature Communications, 2014, 5, 4371.  | 12.8 | 206       |
| 161 | Biochemical and Structural Studies of NADH-Dependent FabG Used To Increase the Bacterial<br>Production of Fatty Acids under Anaerobic Conditions. Applied and Environmental Microbiology, 2014,<br>80, 497-505. | 3.1  | 42        |
| 162 | Combining Crystallographic and Structure-Modeling Approaches in Macromolecular<br>Crystallography. Biophysical Journal, 2014, 106, 34a.   | 0.5  | 0         |

| #   | Article  | IF   | CITATIONS |
|-----|--|------|-----------|
| 163 | The plant glycosyltransferase clone collection for functional genomics. Plant Journal, 2014, 79, 517-529.  | 5.7  | 67        |
| 164 | Diffuse X-Ray Scattering for Ensemble Modeling of Crystalline Proteins. Biophysical Journal, 2014, 106, 384a.  | 0.5  | 0         |
| 165 | Automating crystallographic structure solution and refinement of protein–ligand complexes. Acta<br>Crystallographica Section D: Biological Crystallography, 2014, 70, 144-154.                                   | 2.5  | 43        |
| 166 | Ligand placement based on prior structures: the guided ligand-replacement method. Acta<br>Crystallographica Section D: Biological Crystallography, 2014, 70, 134-143.  | 2.5  | 11        |
| 167 | Flexible torsion-angle noncrystallographic symmetry restraints for improved macromolecular<br>structure refinement. Acta Crystallographica Section D: Biological Crystallography, 2014, 70,<br>1346-1356.        | 2.5  | 19        |
| 168 | Addition of a carbohydrate-binding module enhances cellulase penetration into cellulose substrates.<br>Biotechnology for Biofuels, 2013, 6, 93.  | 6.2  | 63        |
| 169 | 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. Chemical Engineering Science, 2013, 103, 21-28. | 3.8  | 14        |
| 170 | Understanding the impact of ionic liquid pretreatment on cellulose and lignin via thermochemical analysis. Biomass and Bioenergy, 2013, 54, 276-283.   | 5.7  | 55        |
| 171 | Metabolic engineering of Escherichia coli for limonene and perillyl alcohol production. Metabolic<br>Engineering, 2013, 19, 33-41.   | 7.0  | 343       |
| 172 | Engineering dynamic pathway regulation using stress-response promoters. Nature Biotechnology, 2013, 31, 1039-1046.   | 17.5 | 411       |
| 173 | <i>TLS</i> from fundamentals to practice. Crystallography Reviews, 2013, 19, 230-270.  | 1.5  | 46        |
| 174 | A universal flow cytometry assay for screening carbohydrate-active enzymes using glycan microspheres. Chemical Communications, 2013, 49, 5441.   | 4.1  | 5         |
| 175 | Improved low-resolution crystallographic refinement with Phenix and Rosetta. Nature Methods, 2013, 10, 1102-1104.  | 19.0 | 175       |
| 176 | Improved Crystallographic Structures Using Extensive Combinatorial Refinement. Structure, 2013, 21, 1923-1930.   | 3.3  | 18        |
| 177 | Simultaneous Femtosecond X-ray Spectroscopy and Diffraction of Photosystem II at Room Temperature. Science, 2013, 340, 491-495.  | 12.6 | 378       |
| 178 | Utilizing a highly responsive gene, yhjX, in E. coli based production of 1,4-butanediol. Chemical<br>Engineering Science, 2013, 103, 68-73.  | 3.8  | 13        |
| 179 | Advances, Interactions, and Future Developments in the CNS, Phenix, and Rosetta Structural Biology<br>Software Systems. Annual Review of Biophysics, 2013, 42, 265-287.  | 10.0 | 88        |
| 180 | Survey of renewable chemicals produced from lignocellulosic biomass during ionic liquid pretreatment. Biotechnology for Biofuels, 2013, 6, 14.   | 6.2  | 151       |

| #   | Article   | IF   | CITATIONS |
|-----|---|------|-----------|
| 181 | Droplet-based microfluidic platform for heterogeneous enzymatic assays. Lab on A Chip, 2013, 13, 1817.  | 6.0  | 42        |
| 182 | Three Novel Rice Genes Closely Related to the ArabidopsisIRX9, IRX9L, and IRX14 Genes and Their Roles in Xylan Biosynthesis. Frontiers in Plant Science, 2013, 4, 83.   | 3.6  | 83        |
| 183 | From Soil to Structure, a Novel Dimeric β-Glucosidase Belonging to Glycoside Hydrolase Family 3<br>Isolated from Compost Using Metagenomic Analysis. Journal of Biological Chemistry, 2013, 288,<br>14985-14992.        | 3.4  | 42        |
| 184 | High throughput nanostructure-initiator mass spectrometry screening of microbial growth conditions for maximal Î <sup>2</sup> -glucosidase production. Frontiers in Microbiology, 2013, 4, 365.                         | 3.5  | 11        |
| 185 | Intensity statistics in the presence of translational noncrystallographic symmetry. Acta<br>Crystallographica Section D: Biological Crystallography, 2013, 69, 176-183.   | 2.5  | 43        |
| 186 | Bulk-solvent and overall scaling revisited: faster calculations, improved results. Acta<br>Crystallographica Section D: Biological Crystallography, 2013, 69, 625-634.  | 2.5  | 79        |
| 187 | Model morphing and sequence assignment after molecular replacement. Acta Crystallographica<br>Section D: Biological Crystallography, 2013, 69, 2244-2250.   | 2.5  | 37        |
| 188 | <i>Phaser.MRage</i> : automated molecular replacement. Acta Crystallographica Section D: Biological<br>Crystallography, 2013, 69, 2276-2286.  | 2.5  | 216       |
| 189 | Validated near-atomic resolution structure of bacteriophage epsilon15 derived from cryo-EM and modeling. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 12301-12306.       | 7.1  | 68        |
| 190 | Improved Activity of a Thermophilic Cellulase, Cel5A, from Thermotoga maritima on Ionic Liquid<br>Pretreated Switchgrass. PLoS ONE, 2013, 8, e79725.  | 2.5  | 20        |
| 191 | Golgi Enrichment and Proteomic Analysis of Developing Pinus radiata Xylem by Free-Flow<br>Electrophoresis. PLoS ONE, 2013, 8, e84669.   | 2.5  | 11        |
| 192 | Mechanism of nucleotide sensing in group II chaperonins. EMBO Journal, 2012, 31, 3949-3950.   | 7.8  | 2         |
| 193 | Mechanism of nucleotide sensing in group II chaperonins. EMBO Journal, 2012, 31, 731-740.   | 7.8  | 32        |
| 194 | Supplementation of Intracellular XylR Leads to Coutilization of Hemicellulose Sugars. Applied and Environmental Microbiology, 2012, 78, 2221-2229.  | 3.1  | 27        |
| 195 | Mechanical Stress Analysis as a Method to Understand the Impact of Genetically Engineered Rice and<br>Arabidopsis Plants. Industrial Biotechnology, 2012, 8, 238-244.   | 0.8  | 6         |
| 196 | Shining Light into Black Boxes. Science, 2012, 336, 159-160.  | 12.6 | 154       |
| 197 | Energy-dispersive X-ray emission spectroscopy using an X-ray free-electron laser in a shot-by-shot<br>mode. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109,<br>19103-19107. | 7.1  | 113       |
| 198 | Tracing Determinants of Dual Substrate Specificity in Glycoside Hydrolase Family 5. Journal of Biological Chemistry, 2012, 287, 25335-25343.  | 3.4  | 39        |

| #   | Article   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 199 | Nanoflow electrospinning serial femtosecond crystallography. Acta Crystallographica Section D:<br>Biological Crystallography, 2012, 68, 1584-1587.  | 2.5 | 167       |
| 200 | Enhancing fatty acid production by the expression of the regulatory transcription factor FadR.<br>Metabolic Engineering, 2012, 14, 653-660.   | 7.0 | 173       |
| 201 | Glycoside Hydrolases from a targeted Compost Metagenome, activity-screening and functional characterization. BMC Biotechnology, 2012, 12, 38.   | 3.3 | 48        |
| 202 | Manipulation of the carbon storage regulator system for metabolite remodeling and biofuel production in Escherichia coli. Microbial Cell Factories, 2012, 11, 79.                                     | 4.0 | 53        |
| 203 | Automatic Fortran to C++ conversion with FABLE. Source Code for Biology and Medicine, 2012, 7, 5.   | 1.7 | 15        |
| 204 | Thermoascus aurantiacus is a promising source of enzymes for biomass deconstruction under thermophilic conditions. Biotechnology for Biofuels, 2012, 5, 54.   | 6.2 | 88        |
| 205 | Structure of FabH and factors affecting the distribution of branched fatty acids in <i>Micrococcus luteus</i> . Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 1320-1328.    | 2.5 | 9         |
| 206 | Understanding changes in lignin of Panicum virgatum and Eucalyptus globulus as a function of ionic<br>liquid pretreatment. Bioresource Technology, 2012, 126, 156-161.                                | 9.6 | 60        |
| 207 | 1.7 Refinement of X-ray Crystal Structures. , 2012, , 105-115.  |     | 3         |
| 208 | Encoding substrates with mass tags to resolve stereospecific reactions using Nimzyme. Rapid<br>Communications in Mass Spectrometry, 2012, 26, 611-615.  | 1.5 | 20        |
| 209 | Application of targeted proteomics to metabolically engineered <i><scp>E</scp>scherichia coli</i> .<br>Proteomics, 2012, 12, 1289-1299.   | 2.2 | 21        |
| 210 | Improving the Accuracy of Macromolecular Structure Refinement at 7ÂÃ Resolution. Structure, 2012,<br>20, 957-966.   | 3.3 | 37        |
| 211 | Room temperature femtosecond X-ray diffraction of photosystem II microcrystals. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 9721-9726.                | 7.1 | 144       |
| 212 | The Protein Structure Initiative Structural Biology Knowledgebase Technology Portal: a structural biology web resource. Journal of Structural and Functional Genomics, 2012, 13, 57-62.               | 1.2 | 20        |
| 213 | phenix.mr_rosetta: molecular replacement and model rebuilding with Phenix and Rosetta. Journal of<br>Structural and Functional Genomics, 2012, 13, 81-90.   | 1.2 | 131       |
| 214 | Acoustic deposition with NIMS as a high-throughput enzyme activity assay. Analytical and Bioanalytical Chemistry, 2012, 403, 707-711.   | 3.7 | 33        |
| 215 | Graphical tools for macromolecular crystallography in <i>PHENIX</i> . Journal of Applied Crystallography, 2012, 45, 581-586.  | 4.5 | 139       |
| 216 | Use of knowledge-based restraints in <i>phenix.refine</i> to improve macromolecular refinement at<br>low resolution. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 381-390. | 2.5 | 230       |

| #   | Article   | IF   | CITATIONS |
|-----|---|------|-----------|
| 217 | 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 <i>Corynebacterium glutamicum</i> . Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 391-403. | 2.5  | 26        |
| 218 | Towards automated crystallographic structure refinement with <i>phenix.refine</i> . Acta<br>Crystallographica Section D: Biological Crystallography, 2012, 68, 352-367.   | 2.5  | 4,573     |
| 219 | Improved crystallographic models through iterated local density-guided model deformation and<br>reciprocal-space refinement. Acta Crystallographica Section D: Biological Crystallography, 2012, 68,<br>861-870.  | 2.5  | 37        |
| 220 | Raman-spectroscopy-based noninvasive microanalysis of native lignin structure. Analytical and Bioanalytical Chemistry, 2012, 402, 983-987.  | 3.7  | 22        |
| 221 | Molecular replacement and model-building using distant homology models as templates. Acta<br>Crystallographica Section A: Foundations and Advances, 2012, 68, s17-s18.  | 0.3  | 1         |
| 222 | Modelling dynamics in protein crystal structures by ensemble refinement. ELife, 2012, 1, e00311.  | 6.0  | 248       |
| 223 | Colloid-based multiplexed screening for plant biomass-degrading glycoside hydrolase activities in microbial communities. Energy and Environmental Science, 2011, 4, 2884.   | 30.8 | 29        |
| 224 | The Structural Biology Knowledgebase - search Online for Protein Sequences, Structures, Functions,<br>Methods and More. Biophysical Journal, 2011, 100, 319a.   | 0.5  | 0         |
| 225 | Impact of ionic liquid pretreated plant biomass on Saccharomyces cerevisiae growth and biofuel production. Green Chemistry, 2011, 13, 2743.   | 9.0  | 139       |
| 226 | Blind image analysis for the compositional and structural characterization of plant cell walls.<br>Analytica Chimica Acta, 2011, 702, 172-177.  | 5.4  | 26        |
| 227 | The Phenix software for automated determination of macromolecular structures. Methods, 2011, 55, 94-106.  | 3.8  | 764       |
| 228 | A New Generation of Crystallographic Validation Tools for the Protein Data Bank. Structure, 2011, 19, 1395-1412.  | 3.3  | 405       |
| 229 | Structure of a Three-Domain Sesquiterpene Synthase: A Prospective Target for Advanced Biofuels<br>Production. Structure, 2011, 19, 1876-1884.   | 3.3  | 76        |
| 230 | The Structural Biology Knowledgebase: a portal to protein structures, sequences, functions, and methods. Journal of Structural and Functional Genomics, 2011, 12, 45-54.  | 1.2  | 65        |
| 231 | <i>iotbx.cif</i> : a comprehensive CIF toolbox. Journal of Applied Crystallography, 2011, 44, 1259-1263.  | 4.5  | 487       |
| 232 | Exact direct-space asymmetric units for the 230 crystallographic space groups. Acta Crystallographica<br>Section A: Foundations and Advances, 2011, 67, 269-275.  | 0.3  | 11        |
| 233 | High-throughput enzymatic hydrolysis of lignocellulosic biomass via in-situ regeneration.<br>Bioresource Technology, 2011, 102, 1329-1337.  | 9.6  | 26        |
| 234 | Targeted proteomics for metabolic pathway optimization: Application to terpene production.<br>Metabolic Engineering, 2011, 13, 194-203.   | 7.0  | 169       |

| #   | Article  | IF  | CITATIONS |
|-----|--|-----|-----------|
| 235 | The Structural Biology Knowledgebase – structures, functions, methods and more. Acta<br>Crystallographica Section A: Foundations and Advances, 2011, 67, C555-C555.  | 0.3 | 0         |
| 236 | Graphical tools for structure determination and refinement inPHENIX. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C161-C162.  | 0.3 | 0         |
| 237 | Ensemble refinement of protein crystal structures in <i>PHENIX</i> . Acta Crystallographica Section A:<br>Foundations and Advances, 2011, 67, C133-C134.   | 0.3 | 1         |
| 238 | A trigonometric minimum model for refinement. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C597-C597.   | 0.3 | 0         |
| 239 | Supramolecular Self-Assembled Chaos: Polyphenolic Lignin's Barrier to Cost-Effective Lignocellulosic<br>Biofuels. Molecules, 2010, 15, 8641-8688.  | 3.8 | 151       |
| 240 | Crystal structure of the transcriptional activator HlyU from <i>Vibrio vulnificus</i> CMCP6. FEBS<br>Letters, 2010, 584, 1097-1102.  | 2.8 | 18        |
| 241 | Molecular simulations provide new insights into the role of the accessory immunoglobulinâ€ike<br>domain of Cel9A. FEBS Letters, 2010, 584, 3431-3435.  | 2.8 | 17        |
| 242 | Corrigendum to "Molecular simulations provide new insights into the role of the accessory<br>immunoglobulin-like domain of Cel9A―[FEBS Lett. 584 (2010) 3432-3436]. FEBS Letters, 2010, 584,<br>3672-3672. | 2.8 | 0         |
| 243 | <i>phenix.model_vs_data</i> : a high-level tool for the calculation of crystallographic model and<br>data statistics. Journal of Applied Crystallography, 2010, 43, 669-676.                               | 4.5 | 112       |
| 244 | <i>PHENIX</i> : a comprehensive Python-based system for macromolecular structure solution. Acta<br>Crystallographica Section D: Biological Crystallography, 2010, 66, 213-221.                             | 2.5 | 20,564    |
| 245 | Joint X-ray and neutron refinement with <i>phenix.refine</i> . Acta Crystallographica Section D:<br>Biological Crystallography, 2010, 66, 1153-1163.   | 2.5 | 259       |
| 246 | Opportunities and challenges with the growth of neutron crystallography. Acta Crystallographica<br>Section D: Biological Crystallography, 2010, 66, 1121-1123.   | 2.5 | 5         |
| 247 | Coupling of receptor conformation and ligand orientation determine graded activity. Nature Chemical Biology, 2010, 6, 837-843.   | 8.0 | 121       |
| 248 | Hitherto Unrecognized Fluorescence Properties of Coniferyl Alcohol. Molecules, 2010, 15, 1645-1667.  | 3.8 | 6         |
| 249 | Crystal Structures of a Group II Chaperonin Reveal the Open and Closed States Associated with the<br>Protein Folding Cycle. Journal of Biological Chemistry, 2010, 285, 27958-27966.                       | 3.4 | 66        |
| 250 | Evidence of Functional Protein Dynamics from X-Ray Crystallographic Ensembles. PLoS Computational<br>Biology, 2010, 6, e1000911.   | 3.2 | 32        |
| 251 | The PSI SGKB Technology Portal - An Online Database of Structural Genomics Technologies.<br>Biophysical Journal, 2010, 98, 250a.   | 0.5 | 0         |
| 252 | How to use the PSI Structural Genomics Knowledgebase to Enable Research. Biophysical Journal, 2010,<br>98, 250a.   | 0.5 | 0         |

| #   | Article   | IF   | CITATIONS |
|-----|---|------|-----------|
| 253 | A Microscale Platform for Integrated Cell-Free Expression and Activity Screening of Cellulases.<br>Journal of Proteome Research, 2010, 9, 5677-5683.  | 3.7  | 10        |
| 254 | Microfluidic Glycosyl Hydrolase Screening for Biomass-to-Biofuel Conversion. Analytical Chemistry, 2010, 82, 9513-9520.   | 6.5  | 14        |
| 255 | Photon Science at the ALS for Sustainable Energy. Synchrotron Radiation News, 2010, 23, 8-15.   | 0.8  | Ο         |
| 256 | Biochemical characterization and crystal structure of endoglucanase Cel5A from the<br>hyperthermophilic Thermotoga maritima. Journal of Structural Biology, 2010, 172, 372-379.   | 2.8  | 65        |
| 257 | Raman imaging of cell wall polymers in Arabidopsis thaliana. Biochemical and Biophysical Research<br>Communications, 2010, 395, 521-523.  | 2.1  | 42        |
| 258 | New tools for structure refinement in <i>PHENIX</i> . Acta Crystallographica Section A: Foundations and Advances, 2010, 66, s15-s15.  | 0.3  | 205       |
| 259 | POLYGONand other tools: model validation at a glance. Acta Crystallographica Section A:<br>Foundations and Advances, 2010, 66, s311-s312.   | 0.3  | 1         |
| 260 | Spectroscopic Analyses of the Biofuels-Critical Phytochemical Coniferyl Alcohol and Its Enzyme-Catalyzed Oxidation Products. Molecules, 2009, 14, 4758-4778.  | 3.8  | 4         |
| 261 | The protein structure initiative structural genomics knowledgebase. Nucleic Acids Research, 2009, 37, D365-D368.  | 14.5 | 94        |
| 262 | Recent developments in phasing and structure refinement for macromolecular crystallography.<br>Current Opinion in Structural Biology, 2009, 19, 566-572.  | 5.7  | 23        |
| 263 | Label-free in situ imaging of lignification in the cell wall of low lignin transgenic Populus<br>trichocarpa. Planta, 2009, 230, 589-597.   | 3.2  | 80        |
| 264 | Crystallographic model quality at a glance. Acta Crystallographica Section D: Biological<br>Crystallography, 2009, 65, 297-300.   | 2.5  | 95        |
| 265 | Generalized X-ray and neutron crystallographic analysis: more accurate and complete structures for<br>biological macromolecules. Acta Crystallographica Section D: Biological Crystallography, 2009, 65,<br>567-573.          | 2.5  | 137       |
| 266 | Decision-making in structure solution using Bayesian estimates of map quality: the <i>PHENIX<br/>AutoSol</i> wizard. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 582-601.                         | 2.5  | 804       |
| 267 | Structure of endoglucanase Cel9A from the thermoacidophilic <i>Alicyclobacillus acidocaldarius</i> .<br>Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 744-750.                                      | 2.5  | 29        |
| 268 | Averaged kick maps: less noise, more signal…and probably less bias. Acta Crystallographica Section D:<br>Biological Crystallography, 2009, 65, 921-931.   | 2.5  | 59        |
| 269 | <i>electronic Ligand Builder and Optimization Workbench</i> ( <i>eLBOW</i> ): a tool for ligand<br>coordinate and restraint generation. Acta Crystallographica Section D: Biological Crystallography,<br>2009, 65, 1074-1080. | 2.5  | 1,035     |
| 270 | On the use of logarithmic scales for analysis of diffraction data. Acta Crystallographica Section D:<br>Biological Crystallography, 2009, 65, 1283-1291.  | 2.5  | 18        |

| #   | Article   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 271 | Automatic multiple-zone rigid-body refinement with a large convergence radius. Journal of Applied<br>Crystallography, 2009, 42, 607-615.  | 4.5 | 49        |
| 272 | A rapid and inexpensive labeling method for microarray gene expression analysis. BMC Biotechnology, 2009, 9, 97.  | 3.3 | 24        |
| 273 | Transmembrane signal transduction of the αllbβ3 integrin. Protein Science, 2009, 11, 1800-1812.   | 7.6 | 78        |
| 274 | Torsion Angle Refinement and Dynamics as a Tool to Aid Crystallographic Structure Determination. , 2009, , .  |     | 1         |
| 275 | Iterative model building, structure refinement and density modification with the <i>PHENIX<br/>AutoBuild</i> wizard. Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 61-69. | 2.5 | 1,319     |
| 276 | Surprises and pitfalls arising from (pseudo)symmetry. Acta Crystallographica Section D: Biological<br>Crystallography, 2008, 64, 99-107.  | 2.5 | 81        |
| 277 | Iterative-build OMIT maps: map improvement by iterative model building and refinement without model bias. Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 515-524.          | 2.5 | 165       |
| 278 | Protein structures by spallation neutron crystallography. Journal of Synchrotron Radiation, 2008, 15, 215-218.  | 2.4 | 35        |
| 279 | <i>Web-Ice</i> : integrated data collection and analysis for macromolecular crystallography. Journal of Applied Crystallography, 2008, 41, 176-184.   | 4.5 | 81        |
| 280 | Addressing the Need for Alternative Transportation Fuels: The Joint BioEnergy Institute. ACS Chemical Biology, 2008, 3, 17-20.  | 3.4 | 44        |
| 281 | 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.                         | 1.2 | 2         |
| 282 | Structural Genomics of Minimal Organisms: Pipeline and Results. Methods in Molecular Biology, 2008, 426, 475-496.   | 0.9 | 3         |
| 283 | Macromolecular refinement at subatomic resolution with interatomic scatterers. Acta<br>Crystallographica Section A: Foundations and Advances, 2008, 64, C22-C23.                                    | 0.3 | 1         |
| 284 | Cctbx architecture and algorithms. Acta Crystallographica Section A: Foundations and Advances, 2008, 64, C44-C45.   | 0.3 | 0         |
| 285 | The PSI structural genomics knowledgebase. Acta Crystallographica Section A: Foundations and Advances, 2008, 64, C364-C364.   | 0.3 | 0         |
| 286 | SPARX, a new environment for Cryo-EM image processing. Journal of Structural Biology, 2007, 157, 47-55.   | 2.8 | 356       |
| 287 | Technical Report: Recent Major Improvements to the ALS Sector 5 Macromolecular Crystallography<br>Beamlines. Synchrotron Radiation News, 2007, 20, 23-30.   | 0.8 | 2         |
| 288 | <i>Phaser</i> crystallographic software. Journal of Applied Crystallography, 2007, 40, 658-674.   | 4.5 | 17,782    |

| #   | Article   | IF   | CITATIONS |
|-----|---|------|-----------|
| 289 | Ligand identification using electron-density map correlations. Acta Crystallographica Section D:<br>Biological Crystallography, 2007, 63, 101-107.  | 2.5  | 57        |
| 290 | Interpretation of ensembles created by multiple iterative rebuilding of macromolecular models. Acta<br>Crystallographica Section D: Biological Crystallography, 2007, 63, 597-610.  | 2.5  | 60        |
| 291 | On macromolecular refinement at subatomic resolution with interatomic scatterers. Acta<br>Crystallographica Section D: Biological Crystallography, 2007, 63, 1194-1197.   | 2.5  | 59        |
| 292 | Structure of O67745_AQUAE, a hypothetical protein fromAquifex aeolicus. Acta Crystallographica<br>Section F: Structural Biology Communications, 2007, 63, 369-374.  | 0.7  | 7         |
| 293 | Phenix refine developments. Acta Crystallographica Section A: Foundations and Advances, 2007, 63, s80-s80.  | 0.3  | 0         |
| 294 | Automated ligand fitting by core-fragment fitting and extension into density. Acta Crystallographica<br>Section D: Biological Crystallography, 2006, 62, 915-922.   | 2.5  | 98        |
| 295 | Improved statistics for determining the Patterson symmetry from unmerged diffraction intensities.<br>Journal of Applied Crystallography, 2006, 39, 158-168.   | 4.5  | 20        |
| 296 | Structural Basis for Double-Stranded RNA Processing by Dicer. Science, 2006, 311, 195-198.  | 12.6 | 860       |
| 297 | Crystal structures of a phosphotransacetylase from Bacillus subtilis and its complex with acetyl phosphate. Journal of Structural and Functional Genomics, 2006, 6, 269-279.  | 1.2  | 20        |
| 298 | Automated structure determination with PHENIX. Acta Crystallographica Section A: Foundations and Advances, 2006, 62, s85-s85.   | 0.3  | 2         |
| 299 | Structural Genomics of Minimal Organisms and Protein Fold Space. Journal of Structural and Functional Genomics, 2005, 6, 63-70.   | 1.2  | 29        |
| 300 | A robust bulk-solvent correction and anisotropic scaling procedure. Acta Crystallographica Section<br>D: Biological Crystallography, 2005, 61, 850-855.   | 2.5  | 153       |
| 301 | Automated crystallographic ligand building using the medial axis transform of an electron-density isosurface. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 1354-1363.  | 2.5  | 13        |
| 302 | FINDMOL: automated identification of macromolecules in electron-density maps. Acta<br>Crystallographica Section D: Biological Crystallography, 2005, 61, 1514-1520.   | 2.5  | 3         |
| 303 | Structure of a NAD kinase fromThermotoga maritimaat 2.3â€Ã resolution. Acta Crystallographica<br>Section F: Structural Biology Communications, 2005, 61, 640-646.   | 0.7  | 10        |
| 304 | Crystal structure of DNA sequence specificity subunit of a type I restriction-modification enzyme and its functional implications. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 3248-3253. | 7.1  | 66        |
| 305 | Crystal Structure of a PhoU Protein Homologue. Journal of Biological Chemistry, 2005, 280, 15960-15966.   | 3.4  | 33        |
| 306 | Crystal Structure of the "PhoU-Like―Phosphate Uptake Regulator from Aquifex aeolicus. Journal of<br>Bacteriology, 2005, 187, 4238-4244.   | 2.2  | 29        |

| #   | Article   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 307 | Crystal structure of a bacterial ribonuclease P RNA. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 13392-13397.   | 7.1 | 206       |
| 308 | Crystal Structure of a Heat-inducible Transcriptional Repressor HrcA from Thermotoga maritima:<br>Structural Insight into DNA Binding and Dimerization. Journal of Molecular Biology, 2005, 350,<br>987-996.                            | 4.2 | 24        |
| 309 | Crystal Structures of an NAD Kinase from Archaeoglobus fulgidus in Complex with ATP, NAD, or NADP.<br>Journal of Molecular Biology, 2005, 354, 289-303.   | 4.2 | 35        |
| 310 | Computational Aspects of High-Throughput Crystallographic Macromolecular Structure<br>Determination. Methods of Biochemical Analysis, 2005, 44, 75-87.  | 0.2 | 0         |
| 311 | A robust bulk solvent correction and anisotropic scaling procedure in the CCTBX. Acta<br>Crystallographica Section A: Foundations and Advances, 2005, 61, c160-c160.  | 0.3 | 4         |
| 312 | Hybrid programming in crystallography: Phenix.refine and Phenix.hyss. Acta Crystallographica Section<br>A: Foundations and Advances, 2005, 61, c81-c82.   | 0.3 | 0         |
| 313 | mmCIF and modern macromolecular structure determination software: status and perspectives. Acta<br>Crystallographica Section A: Foundations and Advances, 2005, 61, c127-c127.  | 0.3 | 0         |
| 314 | Recent developments in thePHENIXsoftware for automated crystallographic structure determination.<br>Journal of Synchrotron Radiation, 2004, 11, 53-55.  | 2.4 | 319       |
| 315 | Numerically stable algorithms for the computation of reduced unit cells. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, 1-6.   | 0.3 | 47        |
| 316 | Robust indexing for automatic data collection. Journal of Applied Crystallography, 2004, 37, 399-409.   | 4.5 | 149       |
| 317 | Structural basis of light chain amyloidogenicity: comparison of the thermodynamic properties,<br>fibrillogenic potential and tertiary structural features of four Vλ6 proteins. Journal of Molecular<br>Recognition, 2004, 17, 323-331. | 2.1 | 73        |
| 318 | 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.                              | 4.2 | 80        |
| 319 | Exploring the Structural Dynamics of the E.coli Chaperonin GroEL Using Translation-libration-screw<br>Crystallographic Refinement of Intermediate States. Journal of Molecular Biology, 2004, 342, 229-245.                             | 4.2 | 109       |
| 320 | Role of the Â-phosphate of ATP in triggering protein folding by GroEL-GroES: function, structure and energetics. EMBO Journal, 2003, 22, 4877-4887.   | 7.8 | 130       |
| 321 | X-Ray Crystallographic and Kinetic Studies of Human Sorbitol Dehydrogenase. Structure, 2003, 11, 1071-1085.   | 3.3 | 83        |
| 322 | Substructure search procedures for macromolecular structures. Acta Crystallographica Section D:<br>Biological Crystallography, 2003, 59, 1966-1973.   | 2.5 | 214       |
| 323 | On symmetries of substructures. Acta Crystallographica Section D: Biological Crystallography, 2003, 59, 1974-1977.  | 2.5 | 8         |
| 324 | High-resolution structure of RNase P protein from Thermotoga maritima. Proceedings of the National<br>Academy of Sciences of the United States of America, 2003, 100, 7497-7502.  | 7.1 | 87        |

| #   | Article   | IF   | CITATIONS |
|-----|---|------|-----------|
| 325 | Automatic Solution of Heavy-Atom Substructures. Methods in Enzymology, 2003, 374, 37-83.  | 1.0  | 34        |
| 326 | Molecular Dynamics Applied to X-ray Structure Refinement. Accounts of Chemical Research, 2002, 35, 404-412.   | 15.6 | 68        |
| 327 | TheComputational Crystallography Toolbox: crystallographic algorithms in a reusable software framework. Journal of Applied Crystallography, 2002, 35, 126-136.  | 4.5  | 262       |
| 328 | On the handling of atomic anisotropic displacement parameters. Journal of Applied Crystallography, 2002, 35, 477-480.   | 4.5  | 48        |
| 329 | Algorithms for deriving crystallographic space-group information. II. Treatment of special positions.<br>Acta Crystallographica Section A: Foundations and Advances, 2002, 58, 60-65.   | 0.3  | 24        |
| 330 | PHENIX: building new software for automated crystallographic structure determination. Acta<br>Crystallographica Section D: Biological Crystallography, 2002, 58, 1948-1954.   | 2.5  | 3,979     |
| 331 | Patterson correlation methods: a review of molecular replacement withCNS. Acta Crystallographica<br>Section D: Biological Crystallography, 2001, 57, 1390-1396.   | 2.5  | 11        |
| 332 | Recent developments in software for the automation of crystallographic macromolecular structure determination. Current Opinion in Structural Biology, 2000, 10, 564-568.  | 5.7  | 16        |
| 333 | Use of a New Label, 13Cî—»18O, in the Determination of a Structural Model of Phospholamban in a Lipid<br>Bilayer. Spatial Restraints Resolve the Ambiguity Arising from Interpretations of Mutagenesis Data.<br>Journal of Molecular Biology, 2000, 300, 677-685. | 4.2  | 92        |
| 334 | Extending the limits of molecular replacement through combined simulated annealing and<br>maximum-likelihood refinement. Acta Crystallographica Section D: Biological Crystallography, 1999,<br>55, 181-190.  | 2.5  | 30        |
| 335 | Annealing in crystallography: a powerful optimization tool. Progress in Biophysics and Molecular<br>Biology, 1999, 72, 135-155.   | 2.9  | 25        |
| 336 | Experimentally based orientational refinement of membrane protein models: a structure for the<br>Influenza A M2 H + channel 1 1Edited by G. von Heijne. Journal of Molecular Biology, 1999, 286, 951-962.   | 4.2  | 141       |
| 337 | Models for the Transmembrane Region of the Phospholamban Pentamer: Which Is Correct? a. Annals of the New York Academy of Sciences, 1998, 853, 178-185.   | 3.8  | 9         |
| 338 | Crystallography & NMR System: A New Software Suite for Macromolecular Structure<br>Determination. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 905-921.  | 2.5  | 14,711    |
| 339 | Recent developments for the efficient crystallographic refinement of macromolecular structures.<br>Current Opinion in Structural Biology, 1998, 8, 606-611.   | 5.7  | 83        |
| 340 | New Applications of Simulated Annealing in Crystallographic Refinement. , 1998, , 143-157.  |      | 2         |
| 341 | STRUCTURAL PERSPECTIVES OF PHOSPHOLAMBAN, A HELICAL TRANSMEMBRANE PENTAMER. Annual Review of Biophysics and Biomolecular Structure, 1997, 26, 157-179.  | 18.3 | 67        |
| 342 | Cross-validated maximum likelihood enhances crystallographic simulated annealing refinement.<br>Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 5018-5023.   | 7.1  | 623       |

| #   | Article  | IF  | CITATIONS |
|-----|--|-----|-----------|
| 343 | New applications of simulated annealing in X-ray crystallography and solution NMR. Structure, 1997, 5, 325-336.  | 3.3 | 197       |
| 344 | Structure of the Transmembrane Cysteine Residues in Phospholamban. Journal of Membrane Biology, 1997, 155, 199-206.  | 2.1 | 25        |
| 345 | Improved prediction for the structure of the dimeric transmembrane domain of glycophorin A obtained through global searching. Proteins: Structure, Function and Bioinformatics, 1996, 26, 257-261.       | 2.6 | 149       |
| 346 | Improved prediction for the structure of the dimeric transmembrane domain of glycophorin A<br>obtained through global searching. Proteins: Structure, Function and Bioinformatics, 1996, 26,<br>257-261. | 2.6 | 6         |
| 347 | Computational searching and mutagenesis suggest a structure for the pentameric transmembrane domain of phospholamban. Nature Structural and Molecular Biology, 1995, 2, 154-162.                         | 8.2 | 198       |
| 348 | Conformational variability in the refined structure of the chaperonin GroEL at 2.8 Ã resolution.<br>Nature Structural and Molecular Biology, 1995, 2, 1083-1094.   | 8.2 | 219       |
| 349 | Structural organization of the pentameric transmembrane alpha-helices of phospholamban, a cardiac<br>ion channel EMBO Journal, 1994, 13, 4757-4764.  | 7.8 | 175       |
| 350 | A dimerization motif for transmembrane α–helices. Nature Structural Biology, 1994, 1, 157-163.   | 9.7 | 294       |
| 351 | Structure of rodent urinary proteins. Biochemical Society Transactions, 1990, 18, 936-937.   | 3.4 | 11        |