

# Paul Langan

## List of Publications by Year in descending order

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155  
papers

13,517  
citations

57758

44  
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21540

114  
g-index

183  
all docs

183  
docs citations

183  
times ranked

12725  
citing authors

#	ARTICLE	IF	CITATIONS
1	Lignin Valorization: Improving Lignin Processing in the Biorefinery. <i>Science</i> , 2014, 344, 1246843.	12.6	2,994
2	Crystal Structure and Hydrogen-Bonding System in Cellulose I $\beta$ from Synchrotron X-ray and Neutron Fiber Diffraction. <i>Journal of the American Chemical Society</i> , 2002, 124, 9074-9082.	13.7	2,231
3	Crystal Structure and Hydrogen Bonding System in Cellulose I $\beta$ from Synchrotron X-ray and Neutron Fiber Diffraction. <i>Journal of the American Chemical Society</i> , 2003, 125, 14300-14306.	13.7	1,274
4	X-ray Structure of Mercerized Cellulose II at 1 Å $\dots$ Resolution. <i>Biomacromolecules</i> , 2001, 2, 410-416.	5.4	457
5	A Revised Structure and Hydrogen-Bonding System in Cellulose II from a Neutron Fiber Diffraction Analysis. <i>Journal of the American Chemical Society</i> , 1999, 121, 9940-9946.	13.7	328
6	Restructuring the Crystalline Cellulose Hydrogen Bond Network Enhances Its Depolymerization Rate. <i>Journal of the American Chemical Society</i> , 2011, 133, 11163-11174.	13.7	321
7	Cellulose III $\beta$ Crystal Structure and Hydrogen Bonding by Synchrotron X-ray and Neutron Fiber Diffraction. <i>Macromolecules</i> , 2004, 37, 8548-8555.	4.8	267
8	Joint X-ray and neutron refinement with <i>phenix.refine</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1153-1163.	2.5	259
9	Periodic Disorder along Ramie Cellulose Microfibrils. <i>Biomacromolecules</i> , 2003, 4, 1013-1017.	5.4	216
10	Neutron Crystallography, Molecular Dynamics, and Quantum Mechanics Studies of the Nature of Hydrogen Bonding in Cellulose I $\beta$ . <i>Biomacromolecules</i> , 2008, 9, 3133-3140.	5.4	215
11	Common processes drive the thermochemical pretreatment of lignocellulosic biomass. <i>Green Chemistry</i> , 2014, 16, 63-68.	9.0	198
12	Metal Ion Roles and the Movement of Hydrogen during Reaction Catalyzed by D-Xylose Isomerase: A Joint X-Ray and Neutron Diffraction Study. <i>Structure</i> , 2010, 18, 688-699.	3.3	139
13	Generalized X-ray and neutron crystallographic analysis: more accurate and complete structures for biological macromolecules. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2009, 65, 567-573.	2.5	137
14	Neutron crystallography: opportunities, challenges, and limitations. <i>Current Opinion in Structural Biology</i> , 2008, 18, 593-600.	5.7	136
15	Insights into Hydrogen Bonding and Stacking Interactions in Cellulose. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14191-14202.	2.5	122
16	Ionic-Liquid Induced Changes in Cellulose Structure Associated with Enhanced Biomass Hydrolysis. <i>Biomacromolecules</i> , 2011, 12, 3091-3098.	5.4	113
17	Effect of lignin content on changes occurring in poplar cellulose ultrastructure during dilute acid pretreatment. <i>Biotechnology for Biofuels</i> , 2014, 7, 150.	6.2	113
18	A Structural Study of CESA1 Catalytic Domain of Arabidopsis Cellulose Synthesis Complex: Evidence for CESA Trimers. <i>Plant Physiology</i> , 2016, 170, 123-135.	4.8	104

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19	Synchrotron X-ray structures of cellulose I <sup>2</sup> and regenerated cellulose II at ambient temperature and 100ÅK. <i>Cellulose</i> , 2005, 12, 551-562.	4.9	102
20	Conformational Flexibility of Soluble Cellulose Oligomers: Chain Length and Temperature Dependence. <i>Journal of the American Chemical Society</i> , 2009, 131, 14786-14794.	13.7	102
21	X-ray Structure of Ammonia <sup>+</sup> Cellulose I: A New Insights into the Conversion of Cellulose I to Cellulose III. <i>Macromolecules</i> , 2006, 39, 2947-2952.	4.8	94
22	Nature and Kinetic Analysis of Carbon <sup>+</sup> Carbon Bond Fragmentation Reactions of Cation Radicals Derived from SET-Oxidation of Lignin Model Compounds. <i>Journal of Organic Chemistry</i> , 2010, 75, 6549-6562.	3.2	88
23	Neutron Structure of Human Carbonic Anhydrase II: Implications for Proton Transfer. <i>Biochemistry</i> , 2010, 49, 415-421.	2.5	82
24	Dynamics of water bound to crystalline cellulose. <i>Scientific Reports</i> , 2017, 7, 11840.	3.3	82
25	Exploring new strategies for cellulosic biofuels production. <i>Energy and Environmental Science</i> , 2011, 4, 3820.	30.8	79
26	Rapid determination of hydrogen positions and protonation states of diisopropyl fluorophosphatase by joint neutron and X-ray diffraction refinement. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 713-718.	7.1	77
27	Toward resolving the catalytic mechanism of dihydrofolate reductase using neutron and ultrahigh-resolution X-ray crystallography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 18225-18230.	7.1	72
28	Structural characterization of crystals of $\beta$ -glycine during anomalous electrical behaviour. <i>Acta Crystallographica Section B: Structural Science</i> , 2002, 58, 728-733.	1.8	70
29	Neutron diffraction studies of Escherichia coli dihydrofolate reductase complexed with methotrexate. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 18493-18498.	7.1	68
30	Protein crystallography with spallation neutrons: the user facility at Los Alamos Neutron Science Center. <i>Journal of Applied Crystallography</i> , 2004, 37, 24-31.	4.5	66
31	The Macromolecular Neutron Diffractometer MaNDi at the Spallation Neutron Source. <i>Journal of Applied Crystallography</i> , 2015, 48, 1302-1306.	4.5	64
32	X-ray Crystallographic, Scanning Microprobe X-ray Diffraction, and Cross-Polarized/Magic Angle Spinning <sup>13</sup> C NMR Studies of the Structure of Cellulose III. <i>Biomacromolecules</i> , 2009, 10, 302-309.	5.4	63
33	Identification of the Elusive Hydronium Ion Exchanging Roles with a Proton in an Enzyme at Lower pH <sup>+</sup> Values. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 7520-7523.	13.8	62
34	Joint X-ray/Neutron Crystallographic Study of HIV-1 Protease with Clinical Inhibitor Amprenavir: Insights for Drug Design. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 5631-5635.	6.4	61
35	Locating active-site hydrogen atoms in D-xylose isomerase: Time-of-flight neutron diffraction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 8342-8347.	7.1	60
36	Structural coarsening of aspen wood by hydrothermal pretreatment monitored by small- and wide-angle scattering of X-rays and neutrons on oriented specimens. <i>Cellulose</i> , 2014, 21, 1015-1024.	4.9	56

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37	Water in Crystalline Fibers of Dihydrate $\beta$ -D-Glucopyranosyl-2-Deoxy-2-Amino-D-Glucopyranoside Results in Unexpected Absence of Intramolecular Hydrogen Bonding. <i>PLoS ONE</i> , 2012, 7, e39376.	2.5	55
38	MARTINI Coarse-Grained Model for Crystalline Cellulose Microfibers. <i>Journal of Physical Chemistry B</i> , 2015, 119, 465-473.	2.6	54
39	New sources and instrumentation for neutrons in biology. <i>Chemical Physics</i> , 2008, 345, 133-151.	1.9	53
40	Reversible swelling of the cell wall of poplar biomass by ionic liquid at room temperature. <i>Bioresource Technology</i> , 2011, 102, 4518-4523.	9.6	53
41	Neutron Structure of Human Carbonic Anhydrase II: A Hydrogen-Bonded Water Network Observed between pH 7.8 and 10.0. <i>Biochemistry</i> , 2011, 50, 9421-9423.	2.5	52
42	Direct observation of hydrogen atom dynamics and interactions by ultrahigh resolution neutron protein crystallography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 15301-15306.	7.1	51
43	Looking at hydrogen bonds in cellulose. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1172-1177.	2.5	48
44	Comparison of changes in cellulose ultrastructure during different pretreatments of poplar. <i>Cellulose</i> , 2014, 21, 2419-2431.	4.9	47
45	Neutron scattering in the biological sciences: progress and prospects. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 1129-1168.	2.3	47
46	Protein crystallography with spallation neutrons: collecting and processing wavelength-resolved Laue protein data. <i>Journal of Applied Crystallography</i> , 2004, 37, 253-257.	4.5	45
47	A high-angle neutron fibre diffraction study of the hydration of deuterated A-DNA. <i>Biophysical Chemistry</i> , 1997, 69, 85-96.	2.8	44
48	Hydration Control of the Mechanical and Dynamical Properties of Cellulose. <i>Biomacromolecules</i> , 2014, 15, 4152-4159.	5.4	44
49	The effect of deuteration on protein structure: a high-resolution comparison of hydrogenous and perdeuterated haloalkane dehalogenase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2007, 63, 1000-1008.	2.5	42
50	Neutron and X-ray structural studies of short hydrogen bonds in photoactive yellow protein (PYP). <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2007, 63, 1178-1184.	2.5	42
51	Hydrogen Location in Stages of an Enzyme-Catalyzed Reaction: Time-of-Flight Neutron Structure of d-Xylose Isomerase with Bound d-Xylose. <i>Biochemistry</i> , 2008, 47, 7595-7597.	2.5	42
52	The structure of the complex of cellulose I with ethylenediamine by X-ray crystallography and cross-polarization/magic angle spinning $^{13}\text{C}$ nuclear magnetic resonance. <i>Cellulose</i> , 2009, 16, 943-957.	4.9	42
53	Hydrolysis of DFP and the Nerve Agent ( <i>Sarin</i> ) by DFPase Proceeds along Two Different Reaction Pathways: Implications for Engineering Bioscavengers. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4479-4489.	2.6	42
54	Long-Range Electrostatics-Induced Two-Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 4924-4927.	13.8	42

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55	Regioselectivity of Enzymatic and Photochemical Single Electron Transfer Promoted Carbon <sup>13</sup> Carbon Bond Fragmentation Reactions of Tetrameric Lignin Model Compounds. <i>Journal of Organic Chemistry</i> , 2011, 76, 2840-2852.	3.2	40
56	Neutron crystallographic and molecular dynamics studies of the structure of ammonia-cellulose I: rearrangement of hydrogen bonding during the treatment of cellulose with ammonia. <i>Cellulose</i> , 2011, 18, 191-206.	4.9	39
57	A coarse-grained model for synergistic action of multiple enzymes on cellulose. <i>Biotechnology for Biofuels</i> , 2012, 5, 55.	6.2	39
58	Direct Determination of the Hydrogen Bonding Arrangement in Anhydrous $\beta$ -D-Glucopyranose by Neutron Fiber Diffraction. <i>Biomacromolecules</i> , 2012, 13, 288-291.	5.4	39
59	Why genetic modification of lignin leads to low-recalcitrance biomass. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 358-364.	2.8	38
60	Morphological changes in the cellulose and lignin components of biomass occur at different stages during steam pretreatment. <i>Cellulose</i> , 2014, 21, 873-878.	4.9	37
61	A joint x-ray and neutron study on amicyanin reveals the role of protein dynamics in electron transfer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 6817-6822.	7.1	36
62	Reintroducing Electrostatics into Macromolecular Crystallographic Refinement: Application to Neutron Crystallography and DNA Hydration. <i>Structure</i> , 2011, 19, 523-533.	3.3	36
63	High resolution neutron fibre diffraction data on hydrogenated and deuterated cellulose. <i>International Journal of Biological Macromolecules</i> , 1999, 26, 279-283.	7.5	35
64	Protein structures by spallation neutron crystallography. <i>Journal of Synchrotron Radiation</i> , 2008, 15, 215-218.	2.4	35
65	Direct Determination of Protonation States of Histidine Residues in a 2.2 Å Neutron Structure of Deoxy-Human Normal Adult Hemoglobin and Implications for the Bohr Effect. <i>Journal of Molecular Biology</i> , 2010, 398, 276-291.	4.2	35
66	Direct determination of protonation states and visualization of hydrogen bonding in a glycoside hydrolase with neutron crystallography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 12384-12389.	7.1	35
67	X-ray crystallographic studies of family 11 xylanase Michaelis and product complexes: implications for the catalytic mechanism. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 11-23.	2.5	34
68	The structure of celluloses. <i>Powder Diffraction</i> , 2008, 23, 92-95.	0.2	33
69	Probing the Early Events Associated with Liquid Ammonia Pretreatment of Native Crystalline Cellulose. <i>Journal of Physical Chemistry B</i> , 2011, 115, 9782-9788.	2.6	33
70	Evidence for Complex Molecular Architectures for Solvent-Extracted Lignins. <i>ACS Macro Letters</i> , 2012, 1, 568-573.	4.8	33
71	Neutron Laue diffraction in macromolecular crystallography. <i>Physica B: Condensed Matter</i> , 1997, 241-243, 1122-1130.	2.7	32
72	Conceptual design of a macromolecular neutron diffractometer (MaNDi) for the SNS. <i>Journal of Applied Crystallography</i> , 2005, 38, 964-974.	4.5	31

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73	Time-resolved X-ray diffraction microprobe studies of the conversion of cellulose I to ethylenediamine-cellulose I. <i>Cellulose</i> , 2010, 17, 735-745.	4.9	30
74	High-resolution neutron crystallographic studies of the hydration of the coenzyme cob(II)alamin. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011, 67, 584-591.	2.5	30
75	Controlled incorporation of deuterium into bacterial cellulose. <i>Cellulose</i> , 2014, 21, 927-936.	4.9	30
76	Tailored instrumentation for long-pulse neutron spallation sources. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2008, 589, 34-46.	1.6	29
77	Understanding Multiscale Structural Changes During Dilute Acid Pretreatment of Switchgrass and Poplar. <i>ACS Sustainable Chemistry and Engineering</i> , 2017, 5, 426-435.	6.7	29
78	Coarse-Grained Model for the Interconversion between Native and Liquid Ammonia-Treated Crystalline Cellulose. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8031-8037.	2.6	27
79	Improving the accuracy and resolution of neutron crystallographic data by three-dimensional profile fitting of Bragg peaks in reciprocal space. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 1085-1095.	2.3	27
80	Low- and room-temperature X-ray structures of protein kinase A ternary complexes shed new light on its activity. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 854-860.	2.5	26
81	Tension wood structure and morphology conducive for better enzymatic digestion. <i>Biotechnology for Biofuels</i> , 2018, 11, 44.	6.2	26
82	X-ray structure of the ternary MTX $\hat{A}$ -NADPH complex of the anthrax dihydrofolate reductase: A pharmacophore for dual-site inhibitor design. <i>Journal of Structural Biology</i> , 2009, 166, 162-171.	2.8	25
83	In silicostudies of crystalline cellulose and its degradation by enzymes. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1184-1188.	2.5	25
84	BraggNet: integrating Bragg peaks using neural networks. <i>Journal of Applied Crystallography</i> , 2019, 52, 854-863.	4.5	25
85	Insights into the Phosphoryl Transfer Catalyzed by cAMP-Dependent Protein Kinase: An X-ray Crystallographic Study of Complexes with Various Metals and Peptide Substrate SP20. <i>Biochemistry</i> , 2013, 52, 3721-3727.	2.5	24
86	Protein crystallography with spallation neutrons. <i>Journal of Synchrotron Radiation</i> , 2004, 11, 80-82.	2.4	23
87	L-Arabinose Binding, Isomerization, and Epimerization by D-Xylose Isomerase: X-Ray/Neutron Crystallographic and Molecular Simulation Study. <i>Structure</i> , 2014, 22, 1287-1300.	3.3	22
88	Phosphoryl Transfer Reaction Snapshots in Crystals. <i>Journal of Biological Chemistry</i> , 2015, 290, 15538-15548.	3.4	22
89	Protein Kinase A Catalytic Subunit Primed for Action: Time-Lapse Crystallography of Michaelis Complex Formation. <i>Structure</i> , 2015, 23, 2331-2340.	3.3	22
90	Preliminary time-of-flight neutron diffraction study on diisopropyl fluorophosphatase (DFPase) from <i>Loligo vulgaris</i> . <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2007, 63, 42-45.	0.7	21

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91	Seeing the chemistry in biology with neutron crystallography. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13705.	2.8	21
92	A preliminary time-of-flight neutron diffraction study of <i>Streptomyces rubiginosus</i> D-xylose isomerase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2004, 60, 241-249.	2.5	20
93	Collecting and Processing Neutron Fibre Diffraction Data from a Single-Crystal Diffractometer. <i>Journal of Applied Crystallography</i> , 1996, 29, 383-389.	4.5	19
94	Inorganic pyrophosphatase crystals from <i>Thermococcus thio-reducens</i> for X-ray and neutron diffraction. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2012, 68, 1482-1487.	0.7	19
95	Engineering acidic <i>Streptomyces rubiginosus</i> D-xylose isomerase by rational enzyme design. <i>Protein Engineering, Design and Selection</i> , 2014, 27, 59-64.	2.1	19
96	The location of water around the DNA double-helix. <i>Physica B: Condensed Matter</i> , 1989, 156-157, 468-470.	2.7	18
97	Neutron structure and mechanistic studies of diisopropyl fluorophosphatase (DFPase). <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1131-1138.	2.5	18
98	Inhibition of D-xylose isomerase by polyols: atomic details by joint X-ray/neutron crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 1201-1206.	2.5	18
99	Structure and dynamics of a complex of cellulose with EDA: insights into the action of amines on cellulose. <i>Cellulose</i> , 2013, 20, 1563-1571.	4.9	18
100	The crystal structure of mono-ethylenediamine $\beta$ -chitin from synchrotron X-ray fiber diffraction. <i>Carbohydrate Polymers</i> , 2013, 92, 1737-1742.	10.2	18
101	Metal-Free cAMP-Dependent Protein Kinase Can Catalyze Phosphoryl Transfer. <i>Biochemistry</i> , 2014, 53, 3179-3186.	2.5	18
102	Thermal green protein, an extremely stable, nonaggregating fluorescent protein created by structure-guided surface engineering. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 1225-1237.	2.6	18
103	New Developments in Instrumentation for X-ray and Neutron Fibre Diffraction Experiments. <i>Journal of Applied Crystallography</i> , 1998, 31, 758-766.	4.5	17
104	Neutron Laue diffraction studies of coenzyme cob(II)alamin. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 51-59.	2.5	17
105	Neutron Technologies for Bioenergy Research. <i>Industrial Biotechnology</i> , 2012, 8, 209-216.	0.8	17
106	X-ray structure of perdeuterated diisopropyl fluorophosphatase (DFPase): perdeuteration of proteins for neutron diffraction. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2010, 66, 379-385.	0.7	16
107	Determination of cellulose crystallinity from powder diffraction diagrams. <i>Biopolymers</i> , 2015, 103, 67-73.	2.4	15
108	Evaluation of models determined by neutron diffraction and proposed improvements to their validation and deposition. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 800-813.	2.3	15

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109	A preliminary time-of-flight neutron diffraction study on amicyanin from <i>Paracoccus denitrificans</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2005, 61, 640-642.	2.5	14
110	The initial structure of cellulose during ammonia pretreatment. <i>Cellulose</i> , 2014, 21, 1117-1126.	4.9	14
111	Preliminary joint neutron and X-ray crystallographic study of human carbonic anhydrase II. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2009, 65, 495-498.	0.7	13
112	Synthesis, capillary crystallization and preliminary joint X-ray and neutron crystallographic study of Z-DNA without polyamine at low pH. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2006, 62, 453-456.	0.7	11
113	Macromolecular neutron crystallography at the Protein Crystallography Station (PCS). <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1206-1212.	2.5	11
114	Production of Bacterial Cellulose with Controlled Deuterium-Hydrogen Substitution for Neutron Scattering Studies. <i>Methods in Enzymology</i> , 2015, 565, 123-146.	1.0	11
115	Preliminary neutron and ultrahigh-resolution X-ray diffraction studies of the aspartic proteinase endothiapepsin cocrystallized with a gem-diol inhibitor. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2007, 63, 1080-1083.	0.7	10
116	Enzymes for carbon sequestration: neutron crystallographic studies of carbonic anhydrase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1178-1183.	2.5	10
117	Neutron diffraction from fibers. <i>Crystallography Reviews</i> , 2005, 11, 125-147.	1.5	9
118	Preliminary time-of-flight neutron diffraction study of human deoxyhemoglobin. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2008, 64, 270-273.	0.7	9
119	Room-temperature ultrahigh-resolution time-of-flight neutron and X-ray diffraction studies of H/D-exchanged crambin. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2012, 68, 119-123.	0.7	9
120	Neutron diffraction studies of the structure of PEEK. <i>Physica B: Condensed Matter</i> , 1992, 180-181, 528-530.	2.7	8
121	W3Y single mutant of rubredoxin from <i>Pyrococcus furiosus</i> : a preliminary time-of-flight neutron study. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2004, 60, 200-202.	2.5	8
122	Capturing the Catalytic Proton of Dihydrofolate Reductase: Implications for General Acid-Base Catalysis. <i>ACS Catalysis</i> , 2021, 11, 5873-5884.	11.2	8
123	A neutron diffraction study of the distribution of water in the A form of the DNA double helix. <i>Physica B: Condensed Matter</i> , 1992, 180-181, 759-761.	2.7	7
124	A low-temperature neutron diffraction study of Mn12-acetate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2001, 57, 909-910.	0.4	7
125	Preliminary joint X-ray and neutron protein crystallographic studies of ecDHFR complexed with folate and NADP <sup>+</sup> . <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2014, 70, 814-818.	0.8	7
126	Visualizing the Bohr effect in hemoglobin: neutron structure of equine cyanomethemoglobin in the R state and comparison with human deoxyhemoglobin in the T state. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 892-903.	2.3	7



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127	Responses to 'Atomic resolution': a badly abused term in structural biology. <i>Acta Crystallographica Section D: Structural Biology</i> , 2017, 73, 381-383.	2.3	7
128	Neutron fibre diffraction studies of DNA hydration. <i>Physica B: Condensed Matter</i> , 1995, 213-214, 783-785.	2.7	6
129	Protonation states of histidine and other key residues in deoxy normal human adult hemoglobin by neutron protein crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1144-1152.	2.5	6
130	Preliminary joint X-ray and neutron protein crystallographic studies of endoxylanase II from the fungus <i>Trichoderma longibrachiatum</i> . <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2011, 67, 283-286.	0.7	6
131	Long-Range Electrostatics-Induced Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. <i>Angewandte Chemie</i> , 2016, 128, 5008-5011.	2.0	6
132	Molecular Interactions in an $\beta$ -Chitin/Hydrazine Complex: Dynamic Hydrogen Bonds and Improvement of Polymeric Crystallinity. <i>Crystal Growth and Design</i> , 2016, 16, 3345-3352.	3.0	6
133	Using neutron protein crystallography to understand enzyme mechanisms. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1257-1261.	2.5	5
134	Opportunities and challenges with the growth of neutron crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1121-1123.	2.5	5
135	Solvent molecular interactions observed in crystal structures of $\beta$ -chitin complexes. <i>Cellulose</i> , 2014, 21, 1007-1014.	4.9	5
136	A high-angle neutron fibre diffraction study of the hydration of B-DNA. <i>Physica B: Condensed Matter</i> , 1997, 241-243, 1166-1168.	2.7	4
137	Preliminary neutron and X-ray crystallographic studies of equine cyanomethemoglobin. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2010, 66, 474-477.	0.7	4
138	Preliminary joint neutron time-of-flight and X-ray crystallographic study of human ABO(H) blood group A glycosyltransferase. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2011, 67, 258-262.	0.7	4
139	High angle neutron fibre diffraction studies of the distribution of water around the D form of DNA. <i>Physica B: Condensed Matter</i> , 1992, 180-181, 737-739.	2.7	3
140	Neutron fibre diffraction: Recent advances at the ILL. <i>Physica B: Condensed Matter</i> , 1997, 234-236, 213-214.	2.7	3
141	The distribution of water in highly ordered fibres of hyaluronic acid. <i>Physica B: Condensed Matter</i> , 1997, 234-236, 215-216.	2.7	3
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