Matthew P Blakeley

List of Publications by Year
in descending order

95	2,526	186265	214800
papers	citations	28 h-index	47 g-index

98	98	98	2323
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Metal Ion Roles and the Movement of Hydrogen during Reaction Catalyzed by D-Xylose Isomerase: A Joint X-Ray and Neutron Diffraction Study. Structure, 2010, 18, 688-699.	3.3	139
2	Neutron crystallography: opportunities, challenges, and limitations. Current Opinion in Structural Biology, 2008, 18, 593-600.	5.7	136
3	Neutron cryo-crystallography captures the protonation state of ferryl heme in a peroxidase. Science, 2014, 345, 193-197.	12.6	136
4	Sub-atomic resolution X-ray crystallography and neutron crystallography: promise, challenges and potential. IUCrJ, 2015, 2, 464-474.	2.2	104
5	Neutron macromolecular crystallography. Crystallography Reviews, 2009, 15, 157-218.	1.5	92
6	A molecular mechanism for transthyretin amyloidogenesis. Nature Communications, 2019, 10, 925.	12.8	92
7	Neutron macromolecular crystallography with LADI-III. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 1198-1205.	2.5	76
8	Quantum model of catalysis based on a mobile proton revealed by subatomic x-ray and neutron diffraction studies of h-aldose reductase. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 1844-1848.	7.1	74
9	Covalent narlaprevir- and boceprevir-derived hybrid inhibitors of SARS-CoV-2 main protease. Nature Communications, 2022, 13, 2268.	12.8	69
10	The 15-K neutron structure of saccharide-free concanavalin A. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 16405-16410.	7.1	68
11	The determination of protonation states in proteins. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 906-922.	2.5	66
12	Neutron structure of typeâ€II antifreeze protein allows the reconstruction of AFPâ€“ice interface. Journal of Molecular Recognition, 2011, 24, 724-732.	2.1	64
13	Identification of the Elusive Hydronium Ion Exchanging Roles with a Proton in an Enzyme at Lower pHâ€...Values. Angewandte Chemie - International Edition, 2011, 50, 7520-7523.	13.8	62
14	High-resolution neutron protein crystallography with radically small crystal volumes: application of perdeuteration to human aldose reductase. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 1413-1417.	2.5	61
15	Joint X-ray/Neutron Crystallographic Study of HIV-1 Protease with Clinical Inhibitor Amprenavir: Insights for Drug Design. Journal of Medicinal Chemistry, 2013, 56, 5631-5635.	6.4	61
16	Direct visualization of a Fe(IV)â€“OH intermediate in a heme enzyme. Nature Communications, 2016, 7, 13445.	12.8	60
17	Nearâ€Atomic Resolution Neutron Crystallography on Perdeuterated Pyrococcus furiosus Rubredoxin: Implication of Hydronium Ions and Protonation State Equilibria in Redox Changes. Angewandte Chemie - International Edition, 2013, 52, 1022-1025.	13.8	56
18	Direct visualization of critical hydrogen atoms in a pyridoxal 5â€²-phosphate enzyme. Nature Communications, 2017, 8, 955.	12.8	55

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19	New sources and instrumentation for neutrons in biology. Chemical Physics, 2008, 345, 133-151.	1.9	53
20	Longâ€Range Electrostaticsâ€Induced Twoâ€Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. Angewandte Chemie - International Edition, 2016, 55, 4924-4927.	13.8	42
21	Unambiguous determination of H-atom positions: comparing results from neutron and high-resolution X-ray crystallography. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 558-567.	2.5	40
22	"To Be or Not to Be" Protonated: Atomic Details of Human Carbonic Anhydrase-Clinical Drug Complexes by Neutron Crystallography and Simulation. Structure, 2018, 26, 383-390.e3.	3.3	40
23	Protonation-state determination in proteins using high-resolution X-ray crystallography: effects of resolution and completeness. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 800-809.	2.5	39
24	Neutron Diffraction Studies of a Class A Î²-Lactamase Toho-1 E166A/R274N/R276N Triple Mutant. Journal of Molecular Biology, 2010, 396, 1070-1080.	4.2	34
25	The active site protonation states of perdeuterated Toho-1 Î²-lactamase determined by neutron diffraction support a role for Glu166 as the general base in acylation. FEBS Letters, 2011, 585, 364-368.	2.8	32
26	Elucidation of Hydrogen Bonding Patterns in Ligand-Free, Lactose- and Glycerol-Bound Galectin-3C by Neutron Crystallography to Guide Drug Design. Journal of Medicinal Chemistry, 2018, 61, 4412-4420.	6.4	32
27	Neutron Diffraction Reveals Hydrogen Bonds Critical for cGMP-Selective Activation: Insights for cGMP-Dependent Protein Kinase Agonist Design. Biochemistry, 2014, 53, 6725-6727.	2.5	31
28	High-resolution neutron and X-ray diffraction room-temperature studies of an H-FABPâ€“oleic acid complex: study of the internal water cluster and ligand binding by a transferred multipolar electron-density distribution. IUCrJ, 2016, 3, 115-126.	2.2	31
29	Synchrotron and neutron techniques in biological crystallography. Chemical Society Reviews, 2004, 33, 548.	38.1	30
30	Binding site asymmetry in human transthyretin: insights from a joint neutron and X-ray crystallographic analysis using perdeuterated protein. IUCrJ, 2014, 1, 429-438.	2.2	28
31	Comparison of hydrogen determination with X-ray and neutron crystallography in a human aldose reductaseâ€“inhibitor complex. European Biophysics Journal, 2006, 35, 577-583.	2.2	27
32	The Neutron Structure of Urate Oxidase Resolves a Long-Standing Mechanistic Conundrum and Reveals Unexpected Changes in Protonation. PLoS ONE, 2014, 9, e86651.	2.5	27
33	Rapid visualization of hydrogen positions in protein neutron crystallographic structures. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 35-41.	2.5	26
34	Zooming in on protons: Neutron structure of protein kinase A trapped in a product complex. Science Advances, 2019, 5, eaav0482.	10.3	26
35	Neutron Laue macromolecular crystallography. European Biophysics Journal, 2006, 35, 611-620.	2.2	25
36	Room Temperature Neutron Crystallography of Drug Resistant HIV-1 Protease Uncovers Limitations of X-ray Structural Analysis at 100 K. Journal of Medicinal Chemistry, 2017, 60, 2018-2025.	6.4	25

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37	Catalytically important damage-free structures of a copper nitrite reductase obtained by femtosecond X-ray laser and room-temperature neutron crystallography. IUCrJ, 2019, 6, 761-772.	2.2	24
38	Neutron protein crystallography at ultra-low (<15â€…K) temperatures. Journal of Applied Crystallography, 2012, 45, 686-692.	4.5	23
39	L-Arabinose Binding, Isomerization, and Epimerization by D-Xylose Isomerase: X-Ray/Neutron Crystallographic and Molecular Simulation Study. Structure, 2014, 22, 1287-1300.	3.3	22
40	Visualizing the protons in a metalloenzyme electron proton transfer pathway. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 6484-6490.	7.1	22
41	Perdeuteration: improved visualization of solvent structure in neutron macromolecular crystallography. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 3266-3272.	2.5	20
42	Neutron macromolecular crystallography. Emerging Topics in Life Sciences, 2018, 2, 39-55.	2.6	20
43	Large crystal growth by thermal control allows combined X-ray and neutron crystallographic studies to elucidate the protonation states inAspergillus flavusurate oxidase. Journal of the Royal Society Interface, 2009, 6, S599-610.	3.4	19
44	Characterization of image plates for neutron diffraction. Journal of Applied Crystallography, 2009, 42, 749-757.	4.5	19
45	Inorganic pyrophosphatase crystals fromThermococcus thioreducensfor X-ray and neutron diffraction. Acta Crystallographica Section F: Structural Biology Communications, 2012, 68, 1482-1487.	0.7	19
46	Perdeuteration, purification, crystallization and preliminary neutron diffraction of an ocean pout type III antifreeze protein. Acta Crystallographica Section F: Structural Biology Communications, 2009, 65, 406-409.	0.7	18
47	Inhibition of<scp>D</scp>-xylose isomerase by polyols: atomic details by joint X-ray/neutron crystallography. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 1201-1206.	2.5	18
48	A preliminary neutron diffraction study of rasburicase, a recombinant urate oxidase enzyme, complexed with 8-azaxanthin. Acta Crystallographica Section F: Structural Biology Communications, 2006, 62, 306-309.	0.7	16
49	Perdeuteration, crystallization, data collection and comparison of five neutron diffraction data sets of complexes of human galectin-3C. Acta Crystallographica Section D: Structural Biology, 2016, 72, 1194-1202.	2.3	15
50	An extended N-H bond, driven by a conserved second-order interaction, orients the flavin N5 orbital in cholesterol oxidase. Scientific Reports, 2017, 7, 40517.	3.3	14
51	Preliminary neutron crystallographic analysis of selectively CH₃-protonated deuterated rubredoxin fromPyrococcus furiosus. Acta Crystallographica Section F: Structural Biology Communications, 2008, 64, 537-540.	0.7	13
52	Using neutron crystallography to elucidate the basis of selective inhibition of carbonic anhydrase by saccharin and a derivative. Journal of Structural Biology, 2019, 205, 147-154.	2.8	13
53	Neutron crystallography reveals mechanisms used by Pseudomonas aeruginosa for host-cell binding. Nature Communications, 2022, 13, 194.	12.8	13
54	A preliminary neutron crystallographic study of thaumatin. Acta Crystallographica Section F: Structural Biology Communications, 2008, 64, 378-381.	0.7	12

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55	Production, crystallization and neutron diffraction of fully deuterated human myelin peripheral membrane protein P2. Acta Crystallographica Section F, Structural Biology Communications, 2015, 71, 1391-1395.	0.8	11
56	Combined neutron and X-ray diffraction studies of DNA in crystals and solutions. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 1244-1248.	2.5	10
57	Human myelin protein P2: from crystallography to timeâ€lapse membrane imaging and neuropathyâ€associated variants. FEBS Journal, 2021, 288, 6716-6735.	4.7	10
58	Perdeuteration, large crystal growth and neutron data collection ofLeishmania mexicanatriose-phosphate isomerase E65Q variant. Acta Crystallographica Section F, Structural Biology Communications, 2019, 75, 260-269.	0.8	9
59	Visualization of hydrogen atoms in a perdeuterated lectin-fucose complex reveals key details of protein-carbohydrate interactions. Structure, 2021, 29, 1003-1013.e4.	3.3	8
60	Back-exchange of deuterium in neutron crystallography: characterization by IR spectroscopy. Journal of Applied Crystallography, 2017, 50, 660-664.	4.5	8
61	A preliminary neutron crystallographic study of an A-DNA crystal. Acta Crystallographica Section F: Structural Biology Communications, 2009, 65, 232-235.	0.7	7
62	Incorporation of methyl-protonated valine and leucine residues into deuterated ocean pout type III antifreeze protein: expression, crystallization and preliminary neutron diffraction studies. Acta Crystallographica Section F: Structural Biology Communications, 2010, 66, 665-669.	0.7	7
63	Longâ€Range Electrostaticsâ€Induced Twoâ€Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. Angewandte Chemie, 2016, 128, 5008-5011.	2.0	6
64	Visualizing Tetrahedral Oxyanion Bound in HIV-1 Protease Using Neutrons: Implications for the Catalytic Mechanism and Drug Design. ACS Omega, 2020, 5, 11605-11617.	3.5	6
65	Production of perdeuterated fucose from glyco-engineered bacteria. Glycobiology, 2021, 31, 151-158.	2.5	6
66	Joint neutron/X-ray crystal structure of a mechanistically relevant complex of perdeuterated urate oxidase and simulations provide insight into the hydration step of catalysis. IUCrJ, 2021, 8, 46-59.	2.2	6
67	Room temperature crystallography of human acetylcholinesterase bound to a substrate analogue 4K-TMA: Towards a neutron structure. Current Research in Structural Biology, 2021, 3, 206-215.	2.2	6
68	Neutron structures of Leishmania mexicana triosephosphate isomerase in complex with reaction-intermediate mimics shed light on the proton-shuttling steps. IUCrJ, 2021, 8, 633-643.	2.2	6
69	Sweet neutron crystallography. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 1139-1143.	2.5	5
70	Neutron crystallography aids in drug design. IUCrJ, 2016, 3, 296-297.	2.2	5
71	Microgravity crystallization of perdeuterated tryptophan synthase for neutron diffraction. Npj Microgravity, 2022, 8, 13.	3.7	5
72	Preliminary neutron crystallographic study of human transthyretin. Acta Crystallographica Section F: Structural Biology Communications, 2011, 67, 1428-1431.	0.7	4

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73	Temperature-Induced Replacement of Phosphate Proton with Metal Ion Captured in Neutron Structures of A-DNA. Structure, 2018, 26, 1645-1650.e3.	3.3	4
74	Proton transfer and drug binding details revealed in neutron diffraction studies of wild-type and drug resistant HIV-1 protease. Methods in Enzymology, 2020, 634, 257-279.	1.0	4
75	Heme peroxidaseâ€"Trapping intermediates by cryo neutron crystallography. Methods in Enzymology, 2020, 634, 379-389.	1.0	3
76	A preliminary neutron crystallographic study of proteinase K at pD 6.5. Acta Crystallographica Section F: Structural Biology Communications, 2009, 65, 184-187.	0.7	2
77	A preliminary neutron diffraction study of Î³-chymotrypsin. Acta Crystallographica Section F: Structural Biology Communications, 2009, 65, 317-320.	0.7	2
78	Neutron Crystallography Detects Differences in Protein Dynamics: Structure of the PKG II Cyclic Nucleotide Binding Domain in Complex with an Activator. Biochemistry, 2018, 57, 1833-1837.	2.5	1
79	Protonation state determination in proteins using high-resolution protein X-ray crystallography: effects of resolution and completeness. Acta Crystallographica Section A: Foundations and Advances, 2009, 65, s43-s44.	0.3	1
80	Direct observation of protonation states in a PLP-dependent enzyme by neutron crystallography. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, a26-a26.	0.1	1
81	Use of neutron scattering techniques for Antifreeze Protein mechanistic studies. Neutron News, 2014, 25, 24-27.	0.2	0
82	Protein kinase A in the neutron beam: Insights for catalysis from directly observing protons. Methods in Enzymology, 2020, 634, 311-331.	1.0	0
83	What is so sweet about neutron crystallography?. Acta Crystallographica Section A: Foundations and Advances, 2009, 65, s167-s167.	0.3	0
84	High-resolution X-ray and neutron data collection on antifreeze protein. Acta Crystallographica Section A: Foundations and Advances, 2009, 65, s172-s172.	0.3	0
85	Mechanism of IPPase shown by high resolution Neutron and X-ray crystallography. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1211-C1211.	0.1	0
86	UHR PX and NPC studies of H-FABP water network with tiny perdeuterated crystals. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1200-C1200.	0.1	0
87	Perdeuteration: Vital to visualising solvent in neutron crystallography?. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1208-C1208.	0.1	0
88	Neutron macromolecular crystallography at the Institut Laue-Langevin. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s146-s146.	0.1	0
89	High resolution neutron and X-ray diffraction RT studies of an H-FABP â€“ Oleic acid complex: study of the internal water cluster and the ligand binding by a transferred multipolar electron density distribution. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s43-s43.	0.1	0
90	An ab initio fully deuterated tiny crystal (1x0.25x0.20mm) allows neutron data collection at room temperature up to 1.90Ã…. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s231-s231.	0.1	0

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91	Targeting transthyretin amyloidosis: joint neutron and X-ray diffraction analysis of a pathogenic protein. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s44-s44.	0.1	0
92	Neutron crystallographic and scattering studies of function and inhibition of HIV-1 protease. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, a36-a36.	0.1	0
93	Unravelling transthyretin amyloidosis by neutron crystallography. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C646-C646.	0.1	0
94	Neutron crystallography of insulin using a radically small-volume crystal. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C446-C446.	0.1	0
95	Joint X-ray and neutron protein crystallography for the study of enzyme-isoform selectivity by small-molecule inhibitors. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e41-e41.	0.1	0