

# Matthew P Blakeley

## List of Publications by Year in descending order

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95  
papers

2,526  
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docs citations

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#	ARTICLE	IF	CITATIONS
1	Neutron crystallography reveals mechanisms used by <i>Pseudomonas aeruginosa</i> for host-cell binding. <i>Nature Communications</i> , 2022, 13, 194.	5.8	13
2	Covalent narpaprevir- and boceprevir-derived hybrid inhibitors of SARS-CoV-2 main protease. <i>Nature Communications</i> , 2022, 13, 2268.	5.8	69
3	Microgravity crystallization of perdeuterated tryptophan synthase for neutron diffraction. <i>Npj Microgravity</i> , 2022, 8, 13.	1.9	5
4	Production of perdeuterated fucose from glyco-engineered bacteria. <i>Glycobiology</i> , 2021, 31, 151-158.	1.3	6
5	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. <i>IUCr</i> , 2021, 8, 46-59.	1.0	6
6	Room temperature crystallography of human acetylcholinesterase bound to a substrate analogue 4K-TMA: Towards a neutron structure. <i>Current Research in Structural Biology</i> , 2021, 3, 206-215.	1.1	6
7	Neutron structures of <i>Leishmania mexicana</i> triosephosphate isomerase in complex with reaction-intermediate mimics shed light on the proton-shuttling steps. <i>IUCr</i> , 2021, 8, 633-643.	1.0	6
8	Human myelin protein P2: from crystallography to time-resolved membrane imaging and neuropathology-associated variants. <i>FEBS Journal</i> , 2021, 288, 6716-6735.	2.2	10
9	Visualization of hydrogen atoms in a perdeuterated lectin-fucose complex reveals key details of protein-carbohydrate interactions. <i>Structure</i> , 2021, 29, 1003-1013.e4.	1.6	8
10	Visualizing Tetrahedral Oxyanion Bound in HIV-1 Protease Using Neutrons: Implications for the Catalytic Mechanism and Drug Design. <i>ACS Omega</i> , 2020, 5, 11605-11617.	1.6	6
11	Visualizing the protons in a metalloenzyme electron proton transfer pathway. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 6484-6490.	3.3	22
12	Protein kinase A in the neutron beam: Insights for catalysis from directly observing protons. <i>Methods in Enzymology</i> , 2020, 634, 311-331.	0.4	0
13	Heme peroxidase trapping intermediates by cryo neutron crystallography. <i>Methods in Enzymology</i> , 2020, 634, 379-389.	0.4	3
14	Proton transfer and drug binding details revealed in neutron diffraction studies of wild-type and drug resistant HIV-1 protease. <i>Methods in Enzymology</i> , 2020, 634, 257-279.	0.4	4
15	Catalytically important damage-free structures of a copper nitrite reductase obtained by femtosecond X-ray laser and room-temperature neutron crystallography. <i>IUCr</i> , 2019, 6, 761-772.	1.0	24
16	Zooming in on protons: Neutron structure of protein kinase A trapped in a product complex. <i>Science Advances</i> , 2019, 5, eaav0482.	4.7	26
17	A molecular mechanism for transthyretin amyloidogenesis. <i>Nature Communications</i> , 2019, 10, 925.	5.8	92
18	Using neutron crystallography to elucidate the basis of selective inhibition of carbonic anhydrase by saccharin and a derivative. <i>Journal of Structural Biology</i> , 2019, 205, 147-154.	1.3	13

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19	Perdeuteration, large crystal growth and neutron data collection of <i>Leishmania mexicana</i> triose-phosphate isomerase E65Q variant. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2019, 75, 260-269.	0.4	9
20	Neutron Crystallography Detects Differences in Protein Dynamics: Structure of the PKG II Cyclic Nucleotide Binding Domain in Complex with an Activator. <i>Biochemistry</i> , 2018, 57, 1833-1837.	1.2	1
21	Elucidation of Hydrogen Bonding Patterns in Ligand-Free, Lactose- and Glycerol-Bound Galectin-3C by Neutron Crystallography to Guide Drug Design. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 4412-4420.	2.9	32
22	"To Be or Not to Be" Protonated: Atomic Details of Human Carbonic Anhydrase-Clinical Drug Complexes by Neutron Crystallography and Simulation. <i>Structure</i> , 2018, 26, 383-390.e3.	1.6	40
23	Neutron macromolecular crystallography. <i>Emerging Topics in Life Sciences</i> , 2018, 2, 39-55.	1.1	20
24	Temperature-Induced Replacement of Phosphate Proton with Metal Ion Captured in Neutron Structures of A-DNA. <i>Structure</i> , 2018, 26, 1645-1650.e3.	1.6	4
25	Joint X-ray and neutron protein crystallography for the study of enzyme-isoform selectivity by small-molecule inhibitors. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2018, 74, e41-e41.	0.0	0
26	Room Temperature Neutron Crystallography of Drug Resistant HIV-1 Protease Uncovers Limitations of X-ray Structural Analysis at 100 K. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 2018-2025.	2.9	25
27	An extended N-H bond, driven by a conserved second-order interaction, orients the flavin N5 orbital in cholesterol oxidase. <i>Scientific Reports</i> , 2017, 7, 40517.	1.6	14
28	Direct visualization of critical hydrogen atoms in a pyridoxal 5'-phosphate enzyme. <i>Nature Communications</i> , 2017, 8, 955.	5.8	55
29	Direct observation of protonation states in a PLP-dependent enzyme by neutron crystallography. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, a26-a26.	0.0	1
30	Back-exchange of deuterium in neutron crystallography: characterization by IR spectroscopy. <i>Journal of Applied Crystallography</i> , 2017, 50, 660-664.	1.9	8
31	Neutron crystallographic and scattering studies of function and inhibition of HIV-1 protease. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, a36-a36.	0.0	0
32	Unravelling transthyretin amyloidosis by neutron crystallography. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, C646-C646.	0.0	0
33	Neutron crystallography of insulin using a radically small-volume crystal. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, C446-C446.	0.0	0
34	Long-Range Electrostatics-Induced Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. <i>Angewandte Chemie</i> , 2016, 128, 5008-5011.	1.6	6
35	Long-Range Electrostatics-Induced Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 4924-4927.	7.2	42
36	Direct visualization of a Fe(IV)-OH intermediate in a heme enzyme. <i>Nature Communications</i> , 2016, 7, 13445.	5.8	60

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37	High-resolution neutron and X-ray diffraction room-temperature studies of an H-FABP-oleic acid complex: study of the internal water cluster and ligand binding by a transferred multipolar electron-density distribution. <i>IUCr</i> , 2016, 3, 115-126.	1.0	31
38	Neutron crystallography aids in drug design. <i>IUCr</i> , 2016, 3, 296-297.	1.0	5
39	Perdeuteration, crystallization, data collection and comparison of five neutron diffraction data sets of complexes of human galectin-3C. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 1194-1202.	1.1	15
40	High resolution neutron and X-ray diffraction RT studies of an H-FABP-oleic acid complex: study of the internal water cluster and the ligand binding by a transferred multipolar electron density distribution. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2016, 72, s43-s43.	0.0	0
41	An ab initio fully deuterated tiny crystal (1x0.25x0.20mm) allows neutron data collection at room temperature up to 1.90Å... <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2016, 72, s231-s231.	0.0	0
42	Targeting transthyretin amyloidosis: joint neutron and X-ray diffraction analysis of a pathogenic protein. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2016, 72, s44-s44.	0.0	0
43	Production, crystallization and neutron diffraction of fully deuterated human myelin peripheral membrane protein P2. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2015, 71, 1391-1395.	0.4	11
44	Sub-atomic resolution X-ray crystallography and neutron crystallography: promise, challenges and potential. <i>IUCr</i> , 2015, 2, 464-474.	1.0	104
45	Neutron macromolecular crystallography at the Institut Laue-Langevin. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2015, 71, s146-s146.	0.0	0
46	The Neutron Structure of Urate Oxidase Resolves a Long-Standing Mechanistic Conundrum and Reveals Unexpected Changes in Protonation. <i>PLoS ONE</i> , 2014, 9, e86651.	1.1	27
47	Use of neutron scattering techniques for Antifreeze Protein mechanistic studies. <i>Neutron News</i> , 2014, 25, 24-27.	0.1	0
48	Perdeuteration: improved visualization of solvent structure in neutron macromolecular crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 3266-3272.	2.5	20
49	Neutron Diffraction Reveals Hydrogen Bonds Critical for cGMP-Selective Activation: Insights for cGMP-Dependent Protein Kinase Agonist Design. <i>Biochemistry</i> , 2014, 53, 6725-6727.	1.2	31
50	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.	1.6	22
51	Neutron cryo-crystallography captures the protonation state of ferryl heme in a peroxidase. <i>Science</i> , 2014, 345, 193-197.	6.0	136
52	Binding site asymmetry in human transthyretin: insights from a joint neutron and X-ray crystallographic analysis using perdeuterated protein. <i>IUCr</i> , 2014, 1, 429-438.	1.0	28
53	Mechanism of IPPase shown by high resolution Neutron and X-ray crystallography. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2014, 70, C1211-C1211.	0.0	0
54	UHR PX and NPC studies of H-FABP water network with tiny perdeuterated crystals. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2014, 70, C1200-C1200.	0.0	0

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55	Perdeuteration: Vital to visualising solvent in neutron crystallography?. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1208-C1208.	0.0	0
56	Near-Atomic Resolution Neutron Crystallography on Perdeuterated <i>Pyrococcus furiosus</i> Rubredoxin: Implication of Hydronium Ions and Protonation State Equilibria in Redox Changes. Angewandte Chemie - International Edition, 2013, 52, 1022-1025.	7.2	56
57	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.	2.9	61
58	Inhibition of D-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
59	Inorganic pyrophosphatase crystals from <i>Thermococcus thioreducens</i> for X-ray and neutron diffraction. Acta Crystallographica Section F: Structural Biology Communications, 2012, 68, 1482-1487.	0.7	19
60	Rapid visualization of hydrogen positions in protein neutron crystallographic structures. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 35-41.	2.5	26
61	Neutron protein crystallography at ultra-low (<math>15\text{ K}</math>) temperatures. Journal of Applied Crystallography, 2012, 45, 686-692.	1.9	23
62	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
63	The active site protonation states of perdeuterated Toho-1 $\beta$ -lactamase determined by neutron diffraction support a role for Glu166 as the general base in acylation. FEBS Letters, 2011, 585, 364-368.	1.3	32
64	Preliminary neutron crystallographic study of human transthyretin. Acta Crystallographica Section F: Structural Biology Communications, 2011, 67, 1428-1431.	0.7	4
65	Neutron structure of type III antifreeze protein allows the reconstruction of AFP-ice interface. Journal of Molecular Recognition, 2011, 24, 724-732.	1.1	64
66	Identification of the Elusive Hydronium Ion Exchanging Roles with a Proton in an Enzyme at Lower pH-Values. Angewandte Chemie - International Edition, 2011, 50, 7520-7523.	7.2	62
67	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.	1.6	139
68	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
69	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
70	Sweet neutron crystallography. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 1139-1143.	2.5	5
71	Neutron macromolecular crystallography with LADI-III. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 1198-1205.	2.5	76
72	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

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73	Neutron Diffraction Studies of a Class A $\beta$ -Lactamase Toho-1 E166A/R274N/R276N Triple Mutant. <i>Journal of Molecular Biology</i> , 2010, 396, 1070-1080.	2.0	34
74	Large crystal growth by thermal control allows combined X-ray and neutron crystallographic studies to elucidate the protonation states in <i>Aspergillus flavus</i> urate oxidase. <i>Journal of the Royal Society Interface</i> , 2009, 6, S599-610.	1.5	19
75	A preliminary neutron crystallographic study of proteinase K at pD 6.5. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2009, 65, 184-187.	0.7	2
76	A preliminary neutron crystallographic study of an A-DNA crystal. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2009, 65, 232-235.	0.7	7
77	A preliminary neutron diffraction study of $\beta$ -chymotrypsin. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2009, 65, 317-320.	0.7	2
78	Perdeuteration, purification, crystallization and preliminary neutron diffraction of an ocean pout type III antifreeze protein. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2009, 65, 406-409.	0.7	18
79	Characterization of image plates for neutron diffraction. <i>Journal of Applied Crystallography</i> , 2009, 42, 749-757.	1.9	19
80	Neutron macromolecular crystallography. <i>Crystallography Reviews</i> , 2009, 15, 157-218.	0.4	92
81	Protonation state determination in proteins using high-resolution protein X-ray crystallography: effects of resolution and completeness. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, s43-s44.	0.3	1
82	What is so sweet about neutron crystallography?. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, s167-s167.	0.3	0
83	High-resolution X-ray and neutron data collection on antifreeze protein. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, s172-s172.	0.3	0
84	A preliminary neutron crystallographic study of thaumatin. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2008, 64, 378-381.	0.7	12
85	Preliminary neutron crystallographic analysis of selectively $\text{CH}_3$ -protonated deuterated rubredoxin from <i>Pyrococcus furiosus</i> . <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2008, 64, 537-540.	0.7	13
86	New sources and instrumentation for neutrons in biology. <i>Chemical Physics</i> , 2008, 345, 133-151.	0.9	53
87	Neutron crystallography: opportunities, challenges, and limitations. <i>Current Opinion in Structural Biology</i> , 2008, 18, 593-600.	2.6	136
88	Quantum model of catalysis based on a mobile proton revealed by subatomic x-ray and neutron diffraction studies of h-aldose reductase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 1844-1848.	3.3	74
89	The determination of protonation states in proteins. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2007, 63, 906-922.	2.5	66
90	A preliminary neutron diffraction study of rasburicase, a recombinant urate oxidase enzyme, complexed with 8-azaxanthin. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2006, 62, 306-309.	0.7	16

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91	Comparison of hydrogen determination with X-ray and neutron crystallography in a human aldose reductase inhibitor complex. <i>European Biophysics Journal</i> , 2006, 35, 577-583.	1.2	27
92	Neutron Laue macromolecular crystallography. <i>European Biophysics Journal</i> , 2006, 35, 611-620.	1.2	25
93	High-resolution neutron protein crystallography with radically small crystal volumes: application of perdeuteration to human aldose reductase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2005, 61, 1413-1417.	2.5	61
94	The 15-K neutron structure of saccharide-free concanavalin A. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 16405-16410.	3.3	68
95	Synchrotron and neutron techniques in biological crystallography. <i>Chemical Society Reviews</i> , 2004, 33, 548.	18.7	30