## Kevin L Weiss

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Cryotrapping peroxide in the active site of human mitochondrial manganese superoxide dismutase crystals for neutron diffraction. Acta Crystallographica Section F, Structural Biology Communications, 2022, 78, 8-16.	0.8	5
2	Covalent narlaprevir- and boceprevir-derived hybrid inhibitors of SARS-CoV-2 main protease. Nature Communications, 2022, 13, 2268.	12.8	69
3	Direct Observation of Protonation State Modulation in SARS-CoV-2 Main Protease upon Inhibitor Binding with Neutron Crystallography. Journal of Medicinal Chemistry, 2021, 64, 4991-5000.	6.4	36
4	Structural plasticity of the selectivity filter in a nonselective ion channel. IUCrJ, 2021, 8, 421-430.	2.2	13
5	Direct detection of coupled proton and electron transfers in human manganese superoxide dismutase. Nature Communications, 2021, 12, 2079.	12.8	23
6	Small-angle neutron scattering solution structures of NADPH-dependent sulfite reductase. Journal of Structural Biology, 2021, 213, 107724.	2.8	10
7	Conformational Dynamics in the Interaction of SARS-CoV-2 Papain-like Protease with Human Interferon-Stimulated Gene 15 Protein. Journal of Physical Chemistry Letters, 2021, 12, 5608-5615.	4.6	14
8	Structural, Electronic, and Electrostatic Determinants for Inhibitor Binding to Subsites S1 and S2 in SARS-CoV-2 Main Protease. Journal of Medicinal Chemistry, 2021, 64, 17366-17383.	6.4	32
9	Pressure and Temperature Effects on the Formation of Aminoacrylate Intermediates of Tyrosine Phenol-lyase Demonstrate Reaction Dynamics. ACS Catalysis, 2020, 10, 1692-1703.	11.2	6
10	Unusual zwitterionic catalytic site of SARS–CoV-2 main protease revealed by neutron crystallography. Journal of Biological Chemistry, 2020, 295, 17365-17373.	3.4	97
11	Probing the role of the conserved residue Clu166 in a class A β-lactamase using neutron and X-ray protein crystallography. Acta Crystallographica Section D: Structural Biology, 2020, 76, 118-123.	2.3	2
12	The structure of a potassium-selective ion channel reveals a hydrophobic gate regulating ion permeation. IUCrJ, 2020, 7, 835-843.	2.2	8
13	A nucleotide-dependent oligomerization of the Escherichia coli replication initiator DnaA requires residue His136 for remodeling of the chromosomal origin. Nucleic Acids Research, 2019, 48, 200-211.	14.5	4
14	Crystallization of a potassium ion channel and X-ray and neutron data collection. Acta Crystallographica Section F, Structural Biology Communications, 2019, 75, 435-438.	0.8	3
15	Zooming in on protons: Neutron structure of protein kinase A trapped in a product complex. Science Advances, 2019, 5, eaav0482.	10.3	26
16	Substrate Binding Induces Conformational Changes in a Class A Î <sup>2</sup> -lactamase That Prime It for Catalysis. ACS Catalysis, 2018, 8, 2428-2437.	11.2	27
17	Neutron scattering in the biological sciences: progress and prospects. Acta Crystallographica Section D: Structural Biology, 2018, 74, 1129-1168.	2.3	47
18	Anomalous X-ray diffraction studies of ion transport in K+ channels. Nature Communications, 2018, 9, 4540.	12.8	42

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19	Redox manipulation of the manganese metal in human manganese superoxide dismutase for neutron diffraction. Acta Crystallographica Section F, Structural Biology Communications, 2018, 74, 677-687.	0.8	10
20	Active-Site Protonation States in an Acyl-Enzyme Intermediate of a Class A β-Lactamase with a Monobactam Substrate. Antimicrobial Agents and Chemotherapy, 2017, 61, .	3.2	26
21	Direct visualization of critical hydrogen atoms in a pyridoxal 5′-phosphate enzyme. Nature Communications, 2017, 8, 955.	12.8	55
22	Neutron diffraction analysis of <i>Pseudomonas aeruginosa</i> peptidyl-tRNA hydrolase 1. Acta Crystallographica Section F, Structural Biology Communications, 2016, 72, 220-223.	0.8	3
23	Exploring the Mechanism of β-Lactam Ring Protonation in the Class A β-lactamase Acylation Mechanism Using Neutron and X-ray Crystallography. Journal of Medicinal Chemistry, 2016, 59, 474-479.	6.4	43
24	The Macromolecular Neutron Diffractometer MaNDi at the Spallation Neutron Source. Journal of Applied Crystallography, 2015, 48, 1302-1306.	4.5	64
25	The Bio-SANS instrument at the High Flux Isotope Reactor of Oak Ridge National Laboratory. Journal of Applied Crystallography, 2014, 47, 1238-1246.	4.5	83
26	X-ray crystallographic studies of family 11 xylanase Michaelis and product complexes: implications for the catalytic mechanism. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 11-23.	2.5	34
27	Cryogenic neutron protein crystallography: routine methods and potential benefits. Journal of Applied Crystallography, 2014, 47, 1431-1434.	4.5	30
28	Neutron and X-ray Crystal Structures of a Perdeuterated Enzyme Inhibitor Complex Reveal the Catalytic Proton Network of the Toho-1 β-Lactamase for the Acylation Reaction. Journal of Biological Chemistry, 2013, 288, 4715-4722.	3.4	41
29	Dynamic Behavior of Oligomeric Inorganic Pyrophosphatase Explored by Quasielastic Neutron Scattering. Journal of Physical Chemistry B, 2012, 116, 9917-9921.	2.6	9
30	The active site protonation states of perdeuterated Toho-1 β-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
31	New sources and instrumentation for neutrons in biology. Chemical Physics, 2008, 345, 133-151.	1.9	53