Nicholas K Sauter

List of Publications by Year
in descending order

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72 papers	11,164 citations	109321 35 h-index	85541 71 g-index
75 all docs	75 docs citations	75 times ranked	14866 citing authors

#	Article	IF	Citations
1	PHENIX: building new software for automated crystallographic structure determination. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 1948-1954.	2.5	3,979
2	Blu-Iceand theDistributed Control System: software for data acquisition and instrument control at macromolecular crystallography beamlines. Journal of Synchrotron Radiation, 2002, 9, 401-406.	2.4	1,018
3	<i>DIALS</i>: implementation and evaluation of a new integration package. Acta Crystallographica Section D: Structural Biology, 2018, 74, 85-97.	2.3	811
4	Structure of the toxic core of Î±-synuclein from invisible crystals. Nature, 2015, 525, 486-490.	27.8	528
5	Structures of the intermediates of Kokâ€™s photosynthetic water oxidation clock. Nature, 2018, 563, 421-425.	27.8	386
6	Simultaneous Femtosecond X-ray Spectroscopy and Diffraction of Photosystem II at Room Temperature. Science, 2013, 340, 491-495.	12.6	378
7	Structure of photosystem II and substrate binding at room temperature. Nature, 2016, 540, 453-457.	27.8	323
8	Architecture of the synaptotagminâ€“SNARE machinery for neuronal exocytosis. Nature, 2015, 525, 62-67.	27.8	268
9	TheComputational Crystallography Toolbox: crystallographic algorithms in a reusable software framework. Journal of Applied Crystallography, 2002, 35, 126-136.	4.5	262
10	Taking snapshots of photosynthetic water oxidation using femtosecond X-ray diffraction and spectroscopy. Nature Communications, 2014, 5, 4371.	12.8	206
11	Nanoflow electrospinning serial femtosecond crystallography. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 1584-1587.	2.5	167
12	Diffraction-geometry refinement in the<i>DIALS</i>framework. Acta Crystallographica Section D: Structural Biology, 2016, 72, 558-575.	2.3	158
13	Drop-on-demand sample delivery for studying biocatalysts in action at X-ray free-electron lasers. Nature Methods, 2017, 14, 443-449.	19.0	150
14	Robust indexing for automatic data collection. Journal of Applied Crystallography, 2004, 37, 399-409.	4.5	149
15	Untangling the sequence of events during the S ₂ â†’ S ₃ 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
16	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
17	Accurate macromolecular structures using minimal measurements from X-ray free-electron lasers. Nature Methods, 2014, 11, 545-548.	19.0	140
18	Protein crystal structure obtained at 2.9 Ã… resolution from injecting bacterial cells into an X-ray free-electron laser beam. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 12769-12774.	7.1	111

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19	Automated diffraction image analysis and spot searching for high-throughput crystal screening. Journal of Applied Crystallography, 2006, 39, 112-119.	4.5	106
20	High-speed fixed-target serial virus crystallography. Nature Methods, 2017, 14, 805-810.	19.0	106
21	Enabling X-ray free electron laser crystallography for challenging biological systems from a limited number of crystals. ELife, 2015, 4, .	6.0	106
22	De novo phasing with X-ray laser reveals mosquito larvicide BinAB structure. Nature, 2016, 539, 43-47.	27.8	98
23	New Python-based methods for data processing. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 1274-1282.	2.5	95
24	XFEL diffraction: developing processing methods toÂoptimize data quality. Journal of Synchrotron Radiation, 2015, 22, 239-248.	2.4	85
25	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
26	XFEL structures of the influenza M2 proton channel: Room temperature water networks and insights into proton conduction. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13357-13362.	7.1	64
27	A revised partiality model and post-refinement algorithm for X-ray free-electron laser data. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 1400-1410.	2.5	60
28	New methods for indexing multi-lattice diffraction data. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 2652-2666.	2.5	56
29	Structure of CPV17 polyhedrin determined by the improved analysis of serial femtosecond crystallographic data. Nature Communications, 2015, 6, 6435.	12.8	56
30	Mix-and-inject XFEL crystallography reveals gated conformational dynamics during enzyme catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 25634-25640.	7.1	56
31	Improving signal strength in serial crystallography with <i>DIALS</i> geometry refinement. Acta Crystallographica Section D: Structural Biology, 2018, 74, 877-894.	2.3	49
32	Measuring and modeling diffuse scattering in protein X-ray crystallography. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 4069-4074.	7.1	48
33	A convolutional neural network-based screening tool for X-ray serial crystallography. Journal of Synchrotron Radiation, 2018, 25, 655-670.	2.4	41
34	High-Resolution XFEL Structure of the Soluble Methane Monooxygenase Hydroxylase Complex with its Regulatory Component at Ambient Temperature in Two Oxidation States. Journal of the American Chemical Society, 2020, 142, 14249-14266.	13.7	41
35	No observable conformational changes in PSII. Nature, 2016, 533, E1-E2.	27.8	40
36	Improved crystal orientation and physical properties from single-shot XFEL stills. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 3299-3309.	2.5	38

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37	<i>TakeTwo</i>: an indexing algorithm suited to still images with known crystal parameters. Acta Crystallographica Section D: Structural Biology, 2016, 72, 956-965.	2.3	35
38	An on-demand, drop-on-drop method for studying enzyme catalysis by serial crystallography. Nature Communications, 2021, 12, 4461.	12.8	34
39	Chemical crystallography by serial femtosecond X-ray diffraction. Nature, 2022, 601, 360-365.	27.8	33
40	Comparing serial X-ray crystallography and microcrystal electron diffraction (MicroED) as methods for routine structure determination from small macromolecular crystals. IUCrJ, 2020, 7, 306-323.	2.2	32
41	Serial femtosecond crystallography on in vivo-grown crystals drives elucidation of mosquitocidal Cyt1Aa bioactivation cascade. Nature Communications, 2020, 11, 1153.	12.8	31
42	<i>dxtbx</i>: the diffraction experiment toolbox. Journal of Applied Crystallography, 2014, 47, 1459-1465.	4.5	29
43	<i>Data Exploration Toolkit</i>for serial diffraction experiments. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 352-356.	2.5	28
44	On the release of<i>cppxfel</i>for processing X-ray free-electron laser images. Journal of Applied Crystallography, 2016, 49, 1065-1072.	4.5	28
45	Advances in X-ray free electron laser (XFEL) diffraction data processing applied to the crystal structure of the synaptotagmin-1 / SNARE complex. ELife, 2016, 5, .	6.0	28
46	Autoindexing with outlier rejection and identification of superimposed lattices. Journal of Applied Crystallography, 2010, 43, 611-616.	4.5	24
47	Methods development for diffraction and spectroscopy studies of metalloenzymes at X-ray free-electron lasers. Philosophical Transactions of the Royal Society B: Biological Sciences, 2014, 369, 20130590.	4.0	23
48	X-ray free-electron laser studies reveal correlated motion during isopenicillin <i>N</i> synthase catalysis. Science Advances, 2021, 7, .	10.3	23
49	Improved statistics for determining the Patterson symmetry from unmerged diffraction intensities. Journal of Applied Crystallography, 2006, 39, 158-168.	4.5	20
50	Photoreversible interconversion of a phytochrome photosensory module in the crystalline state. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 300-307.	7.1	19
51	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
52	The Mn ₄ Ca photosynthetic water-oxidation catalyst studied by simultaneous X-ray spectroscopy and crystallography using an X-ray free-electron laser. Philosophical Transactions of the Royal Society B: Biological Sciences, 2014, 369, 20130324.	4.0	17
53	IOTA: integration optimization, triage and analysis tool for the processing of XFEL diffraction images. Journal of Applied Crystallography, 2016, 49, 1057-1064.	4.5	17
54	SAD phasing of XFEL data depends critically on the error model. Acta Crystallographica Section D: Structural Biology, 2019, 75, 959-968.	2.3	15

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55	Selling reduction versus Niggli reduction for crystallographic lattices. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 115-120.	0.1	14
56	Towards the spatial resolution of metalloprotein charge states by detailed modeling of XFEL crystallographic diffraction. Acta Crystallographica Section D: Structural Biology, 2020, 76, 176-192.	2.3	14
57	Autoindexing the diffraction patterns from crystals with a pseudotranslation. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 553-559.	2.5	13
58	Detection and correction of underassigned rotational symmetry prior to structure deposition. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 503-513.	2.5	13
59	Tightly integrated single- and multi-crystal data collection strategy calculation and parallelized data processing in<i>JBluIce</i>beamline control system. Journal of Applied Crystallography, 2014, 47, 1992-1999.	4.5	12
60	The crystal structure of dGTPase reveals the molecular basis of dGTP selectivity. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 9333-9339.	7.1	12
61	Towards in cellulo virus crystallography. Scientific Reports, 2018, 8, 3771.	3.3	11
62	Room temperature XFEL crystallography reveals asymmetry in the vicinity of the two phylloquinones in photosystem I. Scientific Reports, 2021, 11, 21787.	3.3	11
63	Best practices for high data-rate macromolecular crystallography (HDRMX). Structural Dynamics, 2020, 7, 014302.	2.3	10
64	Artificial Iron Proteins: Modeling the Active Sites in Non-Heme Dioxygenases. Inorganic Chemistry, 2020, 59, 6000-6009.	4.0	10
65	Beyond integration: modeling every pixel to obtain better structure factors from stills. IUCrJ, 2020, 7, 1151-1167.	2.2	8
66	Responses to<i>`Atomic resolution': a badly abused term in structural biology</i>. Acta Crystallographica Section D: Structural Biology, 2017, 73, 381-383.	2.3	7
67	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
68	A space for lattice representation and clustering. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 593-599.	0.1	7
69	Free-electron laser data for multiple-particle fluctuation scattering analysis. Scientific Data, 2018, 5, 180201.	5.3	6
70	XFEL serial crystallography reveals the room temperature structure of methyl-coenzyme M reductase. Journal of Inorganic Biochemistry, 2022, 230, 111768.	3.5	6
71	Transactions from the 69th Annual Meeting of the American Crystallographic Association: Data best practicesâ€"current state and future needs. Structural Dynamics, 2020, 7, 021301.	2.3	1
72	Challenges in solving structures from radiation-damaged tomograms of protein nanocrystals assessed by simulation. Acta Crystallographica Section D: Structural Biology, 2021, 77, 572-586.	2.3	0