Nigel W Moriarty

List of Publications by Year
in descending order

76 papers	45,342 citations	101543 36 h-index	98798 67 g-index
82 all docs	82 docs citations	82 times ranked	47385 citing authors

#	Article	IF	Citations
1	PHENIX: a comprehensive Python-based system for macromolecular structure solution. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 213-221.	2.5	20,564
2	Towards automated crystallographic structure refinement with phenix.refine. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 352-367.	2.5	4,573
3	Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in Phenix. Acta Crystallographica Section D: Structural Biology, 2019, 75, 861-877.	2.3	4,060
4	PHENIX: building new software for automated crystallographic structure determination. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 1948-1954.	2.5	3,979
5	MolProbity: More and better reference data for improved allâ€atom structure validation. Protein Science, 2018, 27, 293-315.	7.6	2,776
6	Iterative model building, structure refinement and density modification with thePHENIX AutoBuildwizard. Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 61-69.	2.5	1,319
7	electronic Ligand Builder and Optimization Workbench(eLBOW): a tool for ligand coordinate and restraint generation. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 1074-1080.	2.5	1,035
8	Decision-making in structure solution using Bayesian estimates of map quality: thePHENIX AutoSolwizard. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 582-601.	2.5	804
9	The Phenix software for automated determination of macromolecular structures. Methods, 2011, 55, 94-106.	3.8	764
10	New tools for the analysis and validation of cryo-EM maps and atomic models. Acta Crystallographica Section D: Structural Biology, 2018, 74, 814-840.	2.3	575
11	Polder maps: improving OMIT maps by excluding bulk solvent. Acta Crystallographica Section D: Structural Biology, 2017, 73, 148-157.	2.3	500
12	Automated Structure Solution with the PHENIX Suite. Methods in Molecular Biology, 2008, 426, 419-435.	0.9	492
13	Structures of the intermediates of Kokâ€™s photosynthetic water oxidation clock. Nature, 2018, 563, 421-425.	27.8	386
14	Structure of photosystem II and substrate binding at room temperature. Nature, 2016, 540, 453-457.	27.8	323
15	Recent developments in thePHENIXsoftware for automated crystallographic structure determination. Journal of Synchrotron Radiation, 2004, 11, 53-55.	2.4	319
16	TheComputational Crystallography Toolbox: crystallographic algorithms in a reusable software framework. Journal of Applied Crystallography, 2002, 35, 126-136.	4.5	262
17	Joint X-ray and neutron refinement withphenix.refine. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 1153-1163.	2.5	259
18	Use of knowledge-based restraints in phenix.refine to improve macromolecular refinement at low resolution. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 381-390.	2.5	230

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19	Iterative-build OMIT maps: map improvement by iterative model building and refinement without model bias. Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 515-524.	2.5	165
20	FEM: feature-enhanced map. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 646-666.	2.5	157
21	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
22	Graphical tools for macromolecular crystallography inPHENIX. Journal of Applied Crystallography, 2012, 45, 581-586.	4.5	139
23	phenix.model_vs_data: a high-level tool for the calculation of crystallographic model and data statistics. Journal of Applied Crystallography, 2010, 43, 669-676.	4.5	112
24	Automated ligand fitting by core-fragment fitting and extension into density. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 915-922.	2.5	98
25	PRISM: Piecewise Reusable Implementation of Solution Mapping. An Economical Strategy for Chemical Kinetics. Israel Journal of Chemistry, 1999, 39, 97-106.	2.3	95
26	A Global Ramachandran Score Identifies Protein Structures with Unlikely Stereochemistry. Structure, 2020, 28, 1249-1258.e2.	3.3	86
27	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
28	Interpretation of ensembles created by multiple iterative rebuilding of macromolecular models. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 597-610.	2.5	60
29	Ligand identification using electron-density map correlations. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 101-107.	2.5	57
30	Hydrogen migration in polyaromatic growth. Proceedings of the Combustion Institute, 1998, 27, 1655-1661.	0.3	51
31	Hydrogen Migration in the Phenylethen-2-yl Radical. Journal of Physical Chemistry A, 1999, 103, 7127-7135.	2.5	48
32	Announcing mandatory submission of PDBx/mmCIF format files for crystallographic depositions to the Protein Data Bank (PDB). Acta Crystallographica Section D: Structural Biology, 2019, 75, 451-454.	2.3	46
33	On unimolecular decomposition of phenyl radical. Proceedings of the Combustion Institute, 2000, 28, 1545-1555.	3.9	45
34	Automating crystallographic structure solution and refinement of proteinâ€"ligand complexes. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 144-154.	2.5	43
35	Azasugar inhibitors as pharmacological chaperones for Krabbe disease. Chemical Science, 2015, 6, 3075-3086.	7.4	42
36	A new default restraint library for the protein backbone inPhenix: a conformation-dependent geometry goes mainstream. Acta Crystallographica Section D: Structural Biology, 2016, 72, 176-179.	2.3	39

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37	PDBx/mmCIF Ecosystem: Foundational Semantic Tools for Structural Biology. Journal of Molecular Biology, 2022, 434, 167599.	4.2	39
38	Propargyl radical: an electron localization function study. Chemical Physics Letters, 1999, 314, 534-542.	2.6	38
39	Conformationâ€dependent backbone geometry restraints set a new standard for protein crystallographic refinement. FEBS Journal, 2014, 281, 4061-4071.	4.7	36
40	AB initio study of naphthalene formation by addition of vinylacetylene to phenyl. Proceedings of the Combustion Institute, 2000, 28, 2563-2568.	3.9	35
41	Computational economy improvements in PRISM. International Journal of Chemical Kinetics, 2003, 35, 438-452.	1.6	32
42	Cryo_fit: Democratization of flexible fitting for cryo-EM. Journal of Structural Biology, 2019, 208, 1-6.	2.8	30
43	Macromolecular refinement of X-ray and cryoelectron microscopy structures with Phenix/OPLS3e for improved structure and ligand quality. Structure, 2021, 29, 913-921.e4.	3.3	29
44	Improved ligand geometries in crystallographic refinement usingAFITTinPHENIX. Acta Crystallographica Section D: Structural Biology, 2016, 72, 1062-1072.	2.3	29
45	Improved chemistry restraints for crystallographic refinement by integrating the Amber force field into Phenix. Acta Crystallographica Section D: Structural Biology, 2020, 76, 51-62.	2.3	29
46	An editor for the generation and customization of geometry restraints. Acta Crystallographica Section D: Structural Biology, 2017, 73, 123-130.	2.3	27
47	DiSCaMB: a software library for aspherical atom model X-ray scattering factor calculations with CPUs and GPUs. Journal of Applied Crystallography, 2018, 51, 193-199.	4.5	24
48	Cryo-EM structure of the Rhodospirillum rubrum RCâ€"LH1 complex at 2.5â€…Ã…. Biochemical Journal, 2021, 478, 3253-3263.	3.7	23
49	Structural and Biochemical Studies of Actin in Complex with Synthetic Macrolide Tail Analogues. ChemMedChem, 2014, 9, 2286-2293.	3.2	20
50	Solving the scalability issue in quantum-based refinement: Q|R#1. Acta Crystallographica Section D: Structural Biology, 2017, 73, 1020-1028.	2.3	20
51	Flexible torsion-angle noncrystallographic symmetry restraints for improved macromolecular structure refinement. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 1346-1356.	2.5	19
52	Computational convergence of electronic structure calculations of transition metal ligand complexes. Journal of Computational Chemistry, 1993, 14, 961-969.	3.3	18
53	A quantum Monte Carlo study of energy differences in C4H3 and C4H5 isomers. International Journal of Chemical Kinetics, 2001, 33, 808-820.	1.6	18
54	Ironâ€"sulfur clusters have no right angles. Acta Crystallographica Section D: Structural Biology, 2019, 75, 16-20.	2.3	16

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55	Evaluation of models determined by neutron diffraction and proposed improvements to their validation and deposition. Acta Crystallographica Section D: Structural Biology, 2018, 74, 800-813.	2.3	15
56	CERES: a cryo-EM re-refinement system for continuous improvement of deposited models. Acta Crystallographica Section D: Structural Biology, 2021, 77, 48-61.	2.3	14
57	Interactive comparison and remediation of collections of macromolecular structures. Protein Science, 2018, 27, 182-194.	7.6	13
58	Including crystallographic symmetry in quantum-based refinement: Q | R#2. Acta Crystallographica Section D: Structural Biology, 2020, 76, 41-50.	2.3	13
59	Ligand placement based on prior structures: the guided ligand-replacement method. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 134-143.	2.5	11
60	Room temperature XFEL crystallography reveals asymmetry in the vicinity of the two phylloquinones in photosystem I. Scientific Reports, 2021, 11, 21787.	3.3	11
61	Accurate geometries for â€œMountain passâ€•regions of the Ramachandran plot using quantum chemical calculations. Proteins: Structure, Function and Bioinformatics, 2018, 86, 273-278.	2.6	7
62	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
63	Real-space quantum-based refinement for cryo-EM: Q | R#3. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1184-1191.	2.3	7
64	Arginine off-kilter: guanidinium is not as planar as restraints denote. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1159-1166.	2.3	7
65	XFEL serial crystallography reveals the room temperature structure of methyl-coenzyme M reductase. Journal of Inorganic Biochemistry, 2022, 230, 111768.	3.5	6
66	Automated structure determination with phenix. NATO Science Series Series II, Mathematics, Physics and Chemistry, 2007, , 101-109.	0.1	4
67	Improved chemistry restraints for crystallographic refinement by integrating Amber molecular mechanics in Phenix. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, a145-a145.	0.1	2
68	Torsion Angle Refinement and Dynamics as a Tool to Aid Crystallographic Structure Determination. , 2009, , .		1
69	Polder maps: improving OMIT maps for ligand building and validation. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C48-C48.	0.1	0
70	What are the current limits on determination of protonation state using neutron macromolecular crystallography?. Methods in Enzymology, 2020, 634, 225-255.	1.0	0
71	New tools for automated model completion and refinement. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C327-C327.	0.1	0
72	Video tutorials for the Phenix software suite. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1134-C1134.	0.1	0

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73	Polder maps: improving OMIT maps for ligand building and validation. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, a308-a308.	0.1	0
74	High-throughput proteinâ€“ligand complex structure solution with Phenix. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, a445-a445.	0.1	0
75	Updated validation and deposition tools in the Phenix GUI. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, a339-a339.	0.1	0
76	A radical approach to radicals. Acta Crystallographica Section D: Structural Biology, 2022, 78, 43-51.	2.3	0