Nigel W Moriarty

List of Publications by Year
in descending order

76 papers	45,342 citations	101384 36 h-index	98622 67 g-index
82 all docs	82 docs citations	82 times ranked	47385 citing authors

#	Article	IF	Citations
1	A radical approach to radicals. Acta Crystallographica Section D: Structural Biology, 2022, 78, 43-51.	1.1	0
2	XFEL serial crystallography reveals the room temperature structure of methyl-coenzyme M reductase. Journal of Inorganic Biochemistry, 2022, 230, 111768.	1.5	6
3	PDBx/mmCIF Ecosystem: Foundational Semantic Tools for Structural Biology. Journal of Molecular Biology, 2022, 434, 167599.	2.0	39
4	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.	3.3	7
5	Macromolecular refinement of X-ray and cryoelectron microscopy structures with Phenix/OPLS3e for improved structure and ligand quality. Structure, 2021, 29, 913-921.e4.	1.6	29
6	Cryo-EM structure of the Rhodospirillum rubrum RCâ€“LH1 complex at 2.5â€…Ã…. Biochemical Journal, 2021, 478, 3253-3263.	1.7	23
7	CERES: a cryo-EM re-refinement system for continuous improvement of deposited models. Acta Crystallographica Section D: Structural Biology, 2021, 77, 48-61.	1.1	14
8	Room temperature XFEL crystallography reveals asymmetry in the vicinity of the two phylloquinones in photosystem I. Scientific Reports, 2021, 11, 21787.	1.6	11
9	Structural dynamics in the water and proton channels of photosystem II during the S2 to S3 transition. Nature Communications, 2021, 12, 6531.	5.8	73
10	A Global Ramachandran Score Identifies Protein Structures with Unlikely Stereochemistry. Structure, 2020, 28, 1249-1258.e2.	1.6	86
11	What are the current limits on determination of protonation state using neutron macromolecular crystallography?. Methods in Enzymology, 2020, 634, 225-255.	0.4	0
12	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.	3.3	149
13	Including crystallographic symmetry in quantum-based refinement: Q | R#2. Acta Crystallographica Section D: Structural Biology, 2020, 76, 41-50.	1.1	13
14	Improved chemistry restraints for crystallographic refinement by integrating the Amber force field into Phenix. Acta Crystallographica Section D: Structural Biology, 2020, 76, 51-62.	1.1	29
15	Real-space quantum-based refinement for cryo-EM: Q | R#3. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1184-1191.	1.1	7
16	Arginine off-kilter: guanidinium is not as planar as restraints denote. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1159-1166.	1.1	7
17	Cryo_fit: Democratization of flexible fitting for cryo-EM. Journal of Structural Biology, 2019, 208, 1-6.	1.3	30
18	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.	1.1	46

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19	Ironâ€“sulfur clusters have no right angles. Acta Crystallographica Section D: Structural Biology, 2019, 75, 16-20.	1.1	16
20	Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in Phenix. Acta Crystallographica Section D: Structural Biology, 2019, 75, 861-877.	1.1	4,060
21	Updated validation and deposition tools in the Phenix GUI. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, a339-a339.	0.0	0
22	Accurate geometries for â€œMountain passâ€•regions of the Ramachandran plot using quantum chemical calculations. Proteins: Structure, Function and Bioinformatics, 2018, 86, 273-278.	1.5	7
23	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.	1.9	24
24	Interactive comparison and remediation of collections of macromolecular structures. Protein Science, 2018, 27, 182-194.	3.1	13
25	MolProbity: More and better reference data for improved allâ€atom structure validation. Protein Science, 2018, 27, 293-315.	3.1	2,776
26	Structures of the intermediates of Kokâ€™s photosynthetic water oxidation clock. Nature, 2018, 563, 421-425.	13.7	386
27	Improved chemistry restraints for crystallographic refinement by integrating Amber molecular mechanics in Phenix. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, a145-a145.	0.0	2
28	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.	1.1	15
29	New tools for the analysis and validation of cryo-EM maps and atomic models. Acta Crystallographica Section D: Structural Biology, 2018, 74, 814-840.	1.1	575
30	Polder maps: improving OMIT maps for ligand building and validation. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, a308-a308.	0.0	0
31	High-throughput proteinâ€“ligand complex structure solution with Phenix. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, a445-a445.	0.0	0
32	Polder maps: improving OMIT maps for ligand building and validation. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C48-C48.	0.0	0
33	Polder maps: improving OMIT maps by excluding bulk solvent. Acta Crystallographica Section D: Structural Biology, 2017, 73, 148-157.	1.1	500
34	Solving the scalability issue in quantum-based refinement: Q|R#1. Acta Crystallographica Section D: Structural Biology, 2017, 73, 1020-1028.	1.1	20
35	An editor for the generation and customization of geometry restraints. Acta Crystallographica Section D: Structural Biology, 2017, 73, 123-130.	1.1	27
36	Video tutorials for the Phenix software suite. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1134-C1134.	0.0	0

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37	Structure of photosystem II and substrate binding at room temperature. Nature, 2016, 540, 453-457.	13.7	323
38	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.	1.1	39
39	Improved ligand geometries in crystallographic refinement usingAFITTinPHENIX. Acta Crystallographica Section D: Structural Biology, 2016, 72, 1062-1072.	1.1	29
40	FEM: feature-enhanced map. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 646-666.	2.5	157
41	Azasugar inhibitors as pharmacological chaperones for Krabbe disease. Chemical Science, 2015, 6, 3075-3086.	3.7	42
42	Structural and Biochemical Studies of Actin in Complex with Synthetic Macrolide Tail Analogues. ChemMedChem, 2014, 9, 2286-2293.	1.6	20
43	Conformationâ€dependent backbone geometry restraints set a new standard for protein crystallographic refinement. FEBS Journal, 2014, 281, 4061-4071.	2.2	36
44	Automating crystallographic structure solution and refinement of proteinâ€“ligand complexes. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 144-154.	2.5	43
45	Ligand placement based on prior structures: the guided ligand-replacement method. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 134-143.	2.5	11
46	Flexible torsion-angle noncrystallographic symmetry restraints for improved macromolecular structure refinement. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 1346-1356.	2.5	19
47	New tools for automated model completion and refinement. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C327-C327.	0.0	0
48	Graphical tools for macromolecular crystallography inPHENIX. Journal of Applied Crystallography, 2012, 45, 581-586.	1.9	139
49	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
50	Towards automated crystallographic structure refinement with phenix.refine. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 352-367.	2.5	4,573
51	The Phenix software for automated determination of macromolecular structures. Methods, 2011, 55, 94-106.	1.9	764
52	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.	1.9	112
53	PHENIX: a comprehensive Python-based system for macromolecular structure solution. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 213-221.	2.5	20,564
54	Joint X-ray and neutron refinement withphenix.refine. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 1153-1163.	2.5	259

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55	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
56	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
57	Torsion Angle Refinement and Dynamics as a Tool to Aid Crystallographic Structure Determination. , 2009, , .		1
58	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
59	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
60	Automated Structure Solution with the PHENIX Suite. Methods in Molecular Biology, 2008, 426, 419-435.	0.4	492
61	Ligand identification using electron-density map correlations. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 101-107.	2.5	57
62	Interpretation of ensembles created by multiple iterative rebuilding of macromolecular models. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 597-610.	2.5	60
63	Automated structure determination with phenix. NATO Science Series Series II, Mathematics, Physics and Chemistry, 2007, , 101-109.	0.1	4
64	Automated ligand fitting by core-fragment fitting and extension into density. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 915-922.	2.5	98
65	Recent developments in thePHENIXsoftware for automated crystallographic structure determination. Journal of Synchrotron Radiation, 2004, 11, 53-55.	1.0	319
66	Computational economy improvements in PRISM. International Journal of Chemical Kinetics, 2003, 35, 438-452.	1.0	32
67	TheComputational Crystallography Toolbox: crystallographic algorithms in a reusable software framework. Journal of Applied Crystallography, 2002, 35, 126-136.	1.9	262
68	PHENIX: building new software for automated crystallographic structure determination. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 1948-1954.	2.5	3,979
69	A quantum Monte Carlo study of energy differences in C4H3 and C4H5 isomers. International Journal of Chemical Kinetics, 2001, 33, 808-820.	1.0	18
70	On unimolecular decomposition of phenyl radical. Proceedings of the Combustion Institute, 2000, 28, 1545-1555.	2.4	45
71	AB initio study of naphthalene formation by addition of vinylacetylene to phenyl. Proceedings of the Combustion Institute, 2000, 28, 2563-2568.	2.4	35
72	Propargyl radical: an electron localization function study. Chemical Physics Letters, 1999, 314, 534-542.	1.2	38

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73	Hydrogen Migration in the Phenylethen-2-yl Radical. Journal of Physical Chemistry A, 1999, 103, 7127-7135.	1.1	48
74	PRISM: Piecewise Reusable Implementation of Solution Mapping. An Economical Strategy for Chemical Kinetics. Israel Journal of Chemistry, 1999, 39, 97-106.	1.0	95
75	Hydrogen migration in polyaromatic growth. Proceedings of the Combustion Institute, 1998, 27, 1655-1661.	0.3	51
76	Computational convergence of electronic structure calculations of transition metal ligand complexes. Journal of Computational Chemistry, 1993, 14, 961-969.	1.5	18