Pavel V Afonine

List of Publications by Year
in descending order

73	39,240	93792 39	90395 73
papers	citations	h-index	g-index

83	83	83	47519
all docs	docs citations	times ranked	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.	1.1	4,060
4	Real-space refinement inPHENIXfor cryo-EM and crystallography. Acta Crystallographica Section D: Structural Biology, 2018, 74, 531-544.	1.1	2,065
5	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
6	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
7	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
8	Polder maps: improving OMIT maps by excluding bulk solvent. Acta Crystallographica Section D: Structural Biology, 2017, 73, 148-157.	1.1	500
9	Structure of photosystem II and substrate binding at room temperature. Nature, 2016, 540, 453-457.	13.7	323
10	Joint X-ray and neutron refinement withphenix.refine. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 1153-1163.	2.5	259
11	Modelling dynamics in protein crystal structures by ensemble refinement. ELife, 2012, 1, e00311.	2.8	248
12	Improvement of cryo-EM maps by density modification. Nature Methods, 2020, 17, 923-927.	9.0	243
13	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
14	Structure and membrane remodeling activity of ESCRT-III helical polymers. Science, 2015, 350, 1548-1551.	6.0	230
15	Automated map sharpening by maximization of detail and connectivity. Acta Crystallographica Section D: Structural Biology, 2018, 74, 545-559.	1.1	218
16	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
17	FEM: feature-enhanced map. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 646-666.	2.5	157
18	A robust bulk-solvent correction and anisotropic scaling procedure. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 850-855.	2.5	153

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19	Graphical tools for macromolecular crystallography inPHENIX. Journal of Applied Crystallography, 2012, 45, 581-586.	1.9	139
20	Generalized X-ray and neutron crystallographic analysis: more accurate and complete structures for biological macromolecules. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 567-573.	2.5	137
21	A fully automatic method yielding initial models from high-resolution cryo-electron microscopy maps. Nature Methods, 2018, 15, 905-908.	9.0	137
22	phenix.mr_rosetta: molecular replacement and model rebuilding with Phenix and Rosetta. Journal of Structural and Functional Genomics, 2012, 13, 81-90.	1.2	131
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.	1.9	112
24	Accurate model annotation of a near-atomic resolution cryo-EM map. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3103-3108.	3.3	111
25	An atomic model of brome mosaic virus using direct electron detection and real-space optimization. Nature Communications, 2014, 5, 4808.	5.8	105
26	Crystallographic model quality at a glance. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 297-300.	2.5	95
27	Portal protein functions akin to a DNA-sensor that couples genome-packaging to icosahedral capsid maturation. Nature Communications, 2017, 8, 14310.	5.8	90
28	The cryo-electron microscopy structure of human transcription factor IIH. Nature, 2017, 549, 414-417.	13.7	89
29	A Global Ramachandran Score Identifies Protein Structures with Unlikely Stereochemistry. Structure, 2020, 28, 1249-1258.e2.	1.6	86
30	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. Nature Methods, 2021, 18, 156-164.	9.0	73
31	Validated near-atomic resolution structure of bacteriophage epsilon15 derived from cryo-EM and modeling. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 12301-12306.	3.3	68
32	Interpretation of ensembles created by multiple iterative rebuilding of macromolecular models. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 597-610.	2.5	60
33	On macromolecular refinement at subatomic resolution with interatomic scatterers. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 1194-1197.	2.5	59
34	Averaged kick maps: less noise, more signalâ€¦and probably less bias. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 921-931.	2.5	59
35	Visualizing chaperone-assisted protein folding. Nature Structural and Molecular Biology, 2016, 23, 691-697.	3.6	52
36	Automatic multiple-zone rigid-body refinement with a large convergence radius. Journal of Applied Crystallography, 2009, 42, 607-615.	1.9	49

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37	The solvent component of macromolecular crystals. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 1023-1038.	2.5	47
38	TLSfrom fundamentals to practice. Crystallography Reviews, 2013, 19, 230-270.	0.4	46
39	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
40	Automating crystallographic structure solution and refinement of proteinâ€“ligand complexes. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 144-154.	2.5	43
41	Anomalous X-ray diffraction studies of ion transport in K+ channels. Nature Communications, 2018, 9, 4540.	5.8	42
42	Automated identification of elemental ions in macromolecular crystal structures. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 1104-1114.	2.5	40
43	On the application of the expected log-likelihood gain to decision making in molecular replacement. Acta Crystallographica Section D: Structural Biology, 2018, 74, 245-255.	1.1	40
44	Improved crystallographic models through iterated local density-guided model deformation and reciprocal-space refinement. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 861-870.	2.5	37
45	Model morphing and sequence assignment after molecular replacement. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 2244-2250.	2.5	37
46	On the possibility of the observation of valence electron density for individual bonds in proteins in conventional difference maps. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 260-274.	2.5	35
47	Cryo_fit: Democratization of flexible fitting for cryo-EM. Journal of Structural Biology, 2019, 208, 1-6.	1.3	30
48	Metrics for comparison of crystallographic maps. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 2593-2606.	2.5	29
49	Density modification of cryo-EM maps. Acta Crystallographica Section D: Structural Biology, 2020, 76, 912-925.	1.1	28
50	Cryoâ€EM map interpretation and protein modelâ€building using iterative map segmentation. Protein Science, 2020, 29, 87-99.	3.1	27
51	Q|R: quantum-based refinement. Acta Crystallographica Section D: Structural Biology, 2017, 73, 45-52.	1.1	24
52	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
53	Recent developments in phasing and structure refinement for macromolecular crystallography. Current Opinion in Structural Biology, 2009, 19, 566-572.	2.6	23
54	Solving the scalability issue in quantum-based refinement: Q|R#1. Acta Crystallographica Section D: Structural Biology, 2017, 73, 1020-1028.	1.1	20

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55	Flexible torsion-angle noncrystallographic symmetry restraints for improved macromolecular structure refinement. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 1346-1356.	2.5	19
56	On the use of logarithmic scales for analysis of diffraction data. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 1283-1291.	2.5	18
57	Improved Crystallographic Structures Using Extensive Combinatorial Refinement. Structure, 2013, 21, 1923-1930.	1.6	18
58	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
59	Predicting X-ray diffuse scattering from translationâ€“librationâ€“screw structural ensembles. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 1657-1667.	2.5	14
60	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
61	From deep TLS validation to ensembles of atomic models built from elemental motions. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 1668-1683.	2.5	14
62	Programming new geometry restraints: parallelity of atomic groups. Journal of Applied Crystallography, 2015, 48, 1130-1141.	1.9	13
63	Interactive comparison and remediation of collections of macromolecular structures. Protein Science, 2018, 27, 182-194.	3.1	13
64	Including crystallographic symmetry in quantum-based refinement: Q | R#2. Acta Crystallographica Section D: Structural Biology, 2020, 76, 41-50.	1.1	13
65	Protein identification from electron cryomicroscopy maps by automated model building and side-chain matching. Acta Crystallographica Section D: Structural Biology, 2021, 77, 457-462.	1.1	9
66	Implementation of the riding hydrogen model in CCTBX to support the next generation of X-ray and neutron joint refinement in Phenix. Methods in Enzymology, 2020, 634, 177-199.	0.4	8
67	From deep TLS validation to ensembles of atomic models built from elemental motions. II. Analysis of TLS refinement results by explicit interpretation. Acta Crystallographica Section D: Structural Biology, 2018, 74, 621-631.	1.1	7
68	Real-space quantum-based refinement for cryo-EM: Q | R#3. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1184-1191.	1.1	7
69	Map segmentation, automated model-building and their application to the Cryo-EM Model Challenge. Journal of Structural Biology, 2018, 204, 338-343.	1.3	6
70	Detection of translational noncrystallographic symmetry in Patterson functions. Acta Crystallographica Section D: Structural Biology, 2021, 77, 131-141.	1.1	5
71	Macromolecular crystallographic estructure refinement. Arbor, 2015, 191, a219.	0.1	3
72	Crystallographic Structure Refinement in a Nutshell. NATO Science for Peace and Security Series A: Chemistry and Biology, 2013, , 211-219.	0.5	1

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73	What are the current limits on determination of protonation state using neutron macromolecular crystallography?. Methods in Enzymology, 2020, 634, 225-255.	0.4	0