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List of Articles by Year
in descending order

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Version: 2025-02-01

111 peer-reviewed articles	56,525 peer-reviewed citations	51021 47 peer-reviewed h-index	81142 6.39 score
138 documents	71027 doc citations	35916 56 h-index	97427 citing authors

#	Article	IF	Citations
1	Cis-nonProline peptides: Genuine occurrences and their functional roles. Protein Science, 2025, 34, .	3.5	2
2	Outcomes of the EMDataResource cryo-EM Ligand Modeling Challenge. Nature Methods, 2024, 21, 1340-1348.	13.1	16
3	The bad and the good of trends in model building and refinement for sparse-data regions: pernicious forms of overfitting versus good new tools and predictions. Acta Crystallographica Section D: Structural Biology, 2023, 79, 1071-1078.	2.8	6
4	AlphaFold predictions are valuable hypotheses and accelerate but do not replace experimental structure determination. Nature Methods, 2023, 21, 110-116.	13.1	368
5	The importance of residue-level filtering and the Top2018 best-parts dataset of high-quality protein residues. Protein Science, 2022, 31, 290-300.	3.5	19
6	Improved AlphaFold modeling with implicit experimental information. Nature Methods, 2022, 19, 1376-1382.	13.1	133
7	Seeing the PDB. Journal of Biological Chemistry, 2021, 296, 100742.	1.3	21
8	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. Nature Methods, 2021, 18, 156-164.	13.1	119
9	Improving SARS-CoV-2 structures: Peer review by early coordinate release. Biophysical Journal, 2021, 120, 1085-1096.	1.5	27
10	New tools in MolProbity validation: CaBLAM for CryoEM backbone, UnDowser to rethink “waters,” and NGL Viewer to recapture online 3D graphics. Protein Science, 2020, 29, 315-329.	3.5	182
11	Improved chemistry restraints for crystallographic refinement by integrating the Amber force field into Phenix. Acta Crystallographica Section D: Structural Biology, 2020, 76, 51-62.	2.8	46
12	A database of high-quality protein residues for reference data, library construction and motif analysis. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, a437-a437.	0.0	0
13	Model validation: local diagnosis, correction and when to quit. Acta Crystallographica Section D: Structural Biology, 2018, 74, 132-142.	2.8	41
14	MolProbity: More and better reference data for improved all-atom structure validation. Protein Science, 2018, 27, 293-315.	3.5	4,986
15	Constructing atomic structural models into cryo-EM densities using molecular dynamics – Pros and cons. Journal of Structural Biology, 2018, 204, 319-328.	1.5	10
16	Assessment of detailed conformations suggests strategies for improving cryoEM models: Helix at lower resolution, ensembles, pre-refinement fixups, and validation at multi-residue length scale. Journal of Structural Biology, 2018, 204, 301-312.	1.5	24
17	Broad Analysis of Vicinal Disulfides: Occurrences, Conformations with Cis or with Trans Peptides, and Functional Roles Including Sugar Binding. Journal of Molecular Biology, 2017, 429, 1321-1335.	2.9	45
18	Mismodeled purines: implicit alternates and hidden Hoogsteens. Acta Crystallographica Section D: Structural Biology, 2017, 73, 852-859.	2.8	11

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19	Molprobity's ultimate rotamer-library distributions for model validation. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1177-1189.	1.9	118
20	New insights into Hoogsteen base pairs in DNA duplexes from a structure-based survey. Nucleic Acids Research, 2015, 43, 3420-3433.	10.7	85
21	New tools provide a second look at HDV ribozyme structure, dynamics and cleavage. Nucleic Acids Research, 2014, 42, 12833-12846.	10.7	44
22	Biophysical Highlights from 54 Years of Macromolecular Crystallography. Biophysical Journal, 2014, 106, 510-525.	1.5	12
23	Automated identification of elemental ions in macromolecular crystal structures. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 1104-1114.	3.1	46
24	Multiscale Conformational Heterogeneity in Staphylococcal Protein A: Possible Determinant of Functional Plasticity. Structure, 2014, 22, 1467-1477.	2.4	53
25	Studying and polishing the PDB's macromolecules. Biopolymers, 2013, 99, 170-182.	1.5	12
26	Crystallographic model validation: from diagnosis to healing. Current Opinion in Structural Biology, 2013, 23, 707-714.	4.6	14
27	Recommendations of the wwPDB NMR Validation Task Force. Structure, 2013, 21, 1563-1570.	2.4	164
28	Advances, Interactions, and Future Developments in the CNS, Phenix, and Rosetta Structural Biology Software Systems. Annual Review of Biophysics, 2013, 42, 265-287.	7.4	101
29	Doing Molecular Biophysics: Finding, Naming, and Picturing Signal Within Complexity. Annual Review of Biophysics, 2013, 42, 1-28.	7.4	22
30	Graphical tools for macromolecular crystallography inPHENIX. Journal of Applied Crystallography, 2012, 45, 581-586.	1.7	170
31	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.	3.1	281
32	The Role of Local Backrub Motions in Evolved and Designed Mutations. PLoS Computational Biology, 2012, 8, e1002629.	1.9	34
33	Alternate States of Proteins Revealed by Detailed Energy Landscape Mapping. Journal of Molecular Biology, 2011, 405, 607-618.	2.9	460
34	The Phenix software for automated determination of macromolecular structures. Methods, 2011, 55, 94-106.	2.0	936
35	A New Generation of Crystallographic Validation Tools for the Protein Data Bank. Structure, 2011, 19, 1395-1412.	2.4	474
36	The RNA Ontology (RNAO): An ontology for integrating RNA sequence and structure data. Applied Ontology, 2011, 6, 53-89.	0.5	23

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37	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.	1.7	128
38	MolProbity: all-atom structure validation for macromolecular crystallography. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 12-21.	3.1	14,617
39	PHENIX: a comprehensive Python-based system for macromolecular structure solution. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 213-221.	3.1	24,808
40	The RNA Ontology (RNAO): An ontology for integrating RNA sequence and structure data. Nature Precedings, 2009, , .	0.0	3
41	Recent developments in phasing and structure refinement for macromolecular crystallography. Current Opinion in Structural Biology, 2009, 19, 566-572.	4.6	25
42	Target domain definition and classification in CASP8. Proteins: Structure, Function and Bioinformatics, 2009, 77, 10-17.	1.9	34
43	The other 90% of the protein: Assessment beyond the Cαs for CASP8 template-based and high-accuracy models. Proteins: Structure, Function and Bioinformatics, 2009, 77, 29-49.	1.9	82
44	KinImmerse: Macromolecular VR for NMR ensembles. Source Code for Biology and Medicine, 2009, 4, .	0.5	20
45	RNA backbone: Consensus all-angle conformers and modular string nomenclature (an RNA Ontology Consortium contribution). Rna, 2008, 14, 465-481.	2.5	251
46	Algorithm for backrub motions in protein design. Bioinformatics, 2008, 24, i196-i204.	3.2	78
47	Autofix for backward-fit sidechains: using MolProbity and real-space refinement to put misfits in their place. Journal of Structural and Functional Genomics, 2008, 10, 83-93.	0.0	38
48	MolProbity: all-atom contacts and structure validation for proteins and nucleic acids. Nucleic Acids Research, 2007, 35, W375-W383.	10.7	3,892
49	Structure of the hypothetical protein PF0899 fromPyrococcus furiosusat 1.85 Å resolution. Acta Crystallographica Section F: Structural Biology Communications, 2007, 63, 549-552.	0.7	8
50	RNABC: forward kinematics to reduce all-atom steric clashes in RNA backbone. Journal of Mathematical Biology, 2007, 56, 253-278.	1.7	26
51	Structural and transcriptional analyses of a purine nucleotide-binding protein from Pyrococcus furiosus: a component of a novel, membrane-bound multiprotein complex unique to this hyperthermophilic archaeon. Journal of Structural and Functional Genomics, 2007, 8, 1-10.	0.0	0
52	The Backrub Motion: How Protein Backbone Shrugs When a Sidechain Dances. Structure, 2006, 14, 265-274.	2.4	252
53	The RNA Ontology Consortium: An open invitation to the RNA community. Rna, 2006, 12, 533-541.	2.5	61
54	A test of enhancing model accuracy in high-throughput crystallography. Journal of Structural and Functional Genomics, 2005, 6, 1-11.	0.0	46

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55	Protein imperfections: separating intrinsic from extrinsic variation of torsion angles. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 88-98.	3.1	15
56	Away from the edge II: in-house Se-SAS phasing with chromium radiation. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 960-966.	3.1	10
57	The high-throughput protein-to-structure pipeline at SECSG. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 679-684.	3.1	22
58	Assessment of Molecular Construction in Undergraduate Biochemistry. Journal of Chemical Education, 2005, 82, 1854.	1.7	14
59	MOLPROBITY: structure validation and all-atom contact analysis for nucleic acids and their complexes. Nucleic Acids Research, 2004, 32, W615-W619.	10.7	1,024
60	The cis-pro touch-turn: A rare motif preferred at functional sites. Proteins: Structure, Function and Bioinformatics, 2004, 56, 298-309.	1.9	24
61	Structural genomics ofPyrococcus furiosus: X-ray crystallography reveals 3D domain swapping in rubrerythrin. Proteins: Structure, Function and Bioinformatics, 2004, 57, 878-882.	1.9	20
62	Kinetic Role of Helix Caps in Protein Folding Is Context-Dependent†. Biochemistry, 2004, 43, 3814-3823.	1.5	18
63	Facile chemical synthesis and equilibrium unfolding properties of CopG. Protein Science, 2004, 13, 1918-1926.	3.5	8
64	Structure validation by Cα geometry: ϕ,ψ and Cβ deviation. Proteins: Structure, Function and Bioinformatics, 2003, 50, 437-450.	1.9	4,516
65	RNA backbone is rotameric. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 13904-13909.	5.2	206
66	Natural -sheet proteins use negative design to avoid edge-to-edge aggregation. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 2754-2759.	5.2	795
67	Teaching and Assessing Three-Dimensional Molecular Literacy in Undergraduate Biochemistry. Journal of Chemical Education, 2002, 79, 551.	1.7	27
68	Teaching molecular 3-D literacy. Biochemistry and Molecular Biology Education, 2002, 30, 21-26.	0.5	58
69	Protein design and folding: template trapping of self-assembled helical bundles. Journal of Peptide Science, 2001, 7, 146-151.	1.6	14
70	The penultimate rotamer library. Proteins: Structure, Function and Bioinformatics, 2000, 40, 389-408.	1.9	1,029
71	SymROP: ROP protein with identical helices redesigned by all-atom contact analysis and molecular dynamics. Journal of Molecular Graphics and Modelling, 2000, 18, 290-298.	2.1	4
72	Asparagine and glutamine rotamers: B-factor cutoff and correction of amide flips yield distinct clustering. Proceedings of the National Academy of Sciences of the United States of America, 1999, 96, 400-405.	5.2	50

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73	Visualizing and quantifying molecular goodness-of-fit: small-probe contact dots with explicit hydrogen atoms 1 1Edited by J. Thornton. Journal of Molecular Biology, 1999, 285, 1711-1733.	2.9	542
74	Asparagine and glutamine: using hydrogen atom contacts in the choice of side-chain amide orientation 1 1Edited by J. Thornton. Journal of Molecular Biology, 1999, 285, 1735-1747.	2.9	1,448
75	Folding Kinetics of a Fluorescent Variant of Monomeric λ Repressor†. Biochemistry, 1998, 37, 9179-9185.	1.5	50
76	The Alacoil: A very tight, antiparallel coiled-coil of helices. Protein Science, 1995, 4, 2252-2260.	3.5	121
77	An algorithm for smoothly tessellating β-sheet structures in proteins. Journal of Molecular Graphics, 1995, 13, 36-45.	2.7	0
78	Sculpting proteins interactively: Continual energy minimization embedded in a graphical modeling system. Protein Science, 1994, 3, 198-210.	3.5	86
79	The tyrosine corner: A feature of most greek key β-barrel proteins. Protein Science, 1994, 3, 1927-1937.	3.5	131
80	Kinemages - simple macromolecular graphics for interactive teaching and publication. Trends in Biochemical Sciences, 1994, 19, 135-138.	5.8	54
81	Betadoublet: de novo design, synthesis, and characterization of a beta-sandwich protein.. Proceedings of the National Academy of Sciences of the United States of America, 1994, 91, 8747-8751.	5.2	155
82	A Common Arch Structure in Beta Sandwich Proteins: the Tyrosine Turn. Protein Engineering, Design and Selection, 1993, , .	2.2	0
83	The kinemage: A tool for scientific communication. Protein Science, 1992, 1, 3-9.	3.5	212
84	Using appropriate nomenclature. Trends in Biochemical Sciences, 1991, 16, 11.	5.8	9
85	Role of Arginine 180 and Glutamic Acid 177 of Ricin Toxin A Chain in Enzymatic Inactivation of Ribosomes. Molecular and Cellular Biology, 1990, 10, 6257-6263.	1.5	34
86	The de novo design of protein structures. Trends in Biochemical Sciences, 1989, 14, 304-309.	5.8	199
87	Helix lap-joints as ion-binding sites: DNA-binding motifs and Ca-binding “EF hands” are related by charge and sequence reversal. Proteins: Structure, Function and Bioinformatics, 1988, 4, 229-239.	1.9	31
88	The heme and Fe4S4 cluster in the crystallographic structure of Escherichia coli sulfite reductase.. Journal of Biological Chemistry, 1986, 261, 10277-10281.	1.3	93
89	Simultaneous comparison of three protein sequences.. Proceedings of the National Academy of Sciences of the United States of America, 1985, 82, 3073-3077.	5.2	139
90	Preliminary X-ray diffraction studies of acyl carrier protein from Escherichia coli. Journal of Molecular Biology, 1985, 182, 467-468.	2.9	12

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91	Structure and mechanism of copper, zinc superoxide dismutase. Nature, 1983, 306, 284-287.	30.7	986
92	Electrostatic recognition between superoxide and copper, zinc superoxide dismutase. Nature, 1983, 306, 287-290.	30.7	567
93	Determination and analysis of the 2 Å structure of copper, zinc superoxide dismutase. Journal of Molecular Biology, 1982, 160, 181-217.	2.9	974
94	"Active" conformation of an inactive semi-synthetic ribonuclease-S. Journal of Molecular Biology, 1981, 149, 313-317.	2.9	35
95	An illustrated museum of protein structures. Biophysical Journal, 1980, 32, 211-213.	1.5	3
96	Molecular conformation of erabutoxin b; Atomic coordinates at 2.5 Å resolution. Biochemical and Biophysical Research Communications, 1979, 88, 950-959.	1.5	91
97	The singly-wound parallel β barrel: A proposed structure for 2-keto-3-deoxy-6-phosphogluconate aldolase. Biochemical and Biophysical Research Communications, 1979, 90, 285-290.	1.5	13
98	The beta bulge: a common small unit of nonrepetitive protein structure.. Proceedings of the National Academy of Sciences of the United States of America, 1978, 75, 2574-2578.	5.2	259
99	β-Sheet topology and the relatedness of proteins. Nature, 1977, 268, 495-500.	30.7	596
100	Similarity of three-dimensional structure between the immunoglobulin domain and the copper, zinc superoxide dismutase subunit. Journal of Molecular Biology, 1976, 102, 221-235.	2.9	164
101	Manganese superoxide dismutases from Escherichia coli and from yeast mitochondria: Preliminary X-ray crystallographic studies. Journal of Molecular Biology, 1976, 105, 327-332.	2.9	22
102	Three dimensional structure of erabutoxin b neurotoxic protein: inhibitor of acetylcholine receptor.. Proceedings of the National Academy of Sciences of the United States of America, 1976, 73, 2991-2994.	5.2	252
103	Handedness of crossover connections in beta sheets.. Proceedings of the National Academy of Sciences of the United States of America, 1976, 73, 2619-2623.	5.2	183
104	Alpha-carbon coordinates for bovine Cu, Zn superoxide dismutase. Biochemical and Biophysical Research Communications, 1975, 63, 986-992.	1.5	70
105	The Crystal Structure of Bovine Cu2+,Zn2+ Superoxide Dismutase at 5.5-A Resolution. Journal of Biological Chemistry, 1974, 249, 5677-5683.	1.3	32
106	The simple construction of protein alpha-Carbon models. Biopolymers, 1972, 11, 2381-2385.	1.5	26
107	Two Crystal Forms of Bovine Superoxide Dismutase. Journal of Biological Chemistry, 1972, 247, 6368-6369.	1.3	32
108	THE EXTRACELLULAR NUCLEASE OF Staphylococcus aureus: STRUCTURES OF THE NATIVE ENZYME AND AN ENZYME-INHIBITOR COMPLEX AT 4 A RESOLUTION. Proceedings of the National Academy of Sciences of the United States of America, 1969, 64, 420-427.	5.2	67

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109	Categorizing prediction modes within low-pLDDT regions of AlphaFold 2 structures: near-predictive, pseudostructure and barbed wire. Acta Crystallographica Section D: Structural Biology, 0, 81, 558-572.	2.8	9
110	New targets and procedures for validating the valence geometry of nucleic acid structures. Nucleic Acids Research, 0, 54, .	10.7	3
111	RNAprecis: Prediction of full-detail RNA conformation from the experimentally best-observed sparse parameters. PLoS Computational Biology, 0, 22, e1014242.	1.9	0