John D Westbrook

List of Publications by Year
in descending order

108 papers	46,283 citations	34076 52 h-index	28275 105 g-index
116 all docs	116 docs citations	116 times ranked	46425 citing authors

#	Article	IF	Citations
1	Evolution of the <scp>SARSâ€CoV</scp>â€2 proteome in three dimensions (3D) during the first 6 months of the <scp>COVID</scp>â€19 pandemic. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1054-1080.	1.5	31
2	<scp>RCSB</scp> Protein Data Bank: Celebrating 50â€‰years of the <scp>PDB</scp> with new tools for understanding and visualizing biological macromolecules in <scp>3D</scp>. Protein Science, 2022, 31, 187-208.	3.1	84
3	Simplified quality assessment for small-molecule ligands in the Protein Data Bank. Structure, 2022, 30, 252-262.e4.	1.6	12
4	RCSB Protein Data Bank: improved annotation, search and visualization of membrane protein structures archived in the PDB. Bioinformatics, 2022, 38, 1452-1454.	1.8	41
5	PDBx/mmCIF Ecosystem: Foundational Semantic Tools for Structural Biology. Journal of Molecular Biology, 2022, 434, 167599.	2.0	39
6	RCSB Protein Data Bank: Architectural Advances Towards Integrated Searching and Efficient Access to Macromolecular Structure Data from the PDB Archive. Journal of Molecular Biology, 2021, 433, 166704.	2.0	106
7	Enhanced validation of small-molecule ligands and carbohydrates in the Protein Data Bank. Structure, 2021, 29, 393-400.e1.	1.6	28
8	Modernized uniform representation of carbohydrate molecules in the Protein Data Bank. Glycobiology, 2021, 31, 1204-1218.	1.3	17
9	RCSB Protein Data Bank 1D tools and services. Bioinformatics, 2021, 36, 5526-5527.	1.8	15
10	RCSB Protein Data Bank: powerful new tools for exploring 3D structures of biological macromolecules for basic and applied research and education in fundamental biology, biomedicine, biotechnology, bioengineering and energy sciences. Nucleic Acids Research, 2021, 49, D437-D451.	6.5	918
11	New system for archiving integrative structures. Acta Crystallographica Section D: Structural Biology, 2021, 77, 1486-1496.	1.1	22
12	RCSB Protein Data Bank: Enabling biomedical research and drug discovery. Protein Science, 2020, 29, 52-65.	3.1	223
13	The TRUST Principles for digital repositories. Scientific Data, 2020, 7, 144.	2.4	158
14	Impact of the Protein Data Bank on antineoplastic approvals. Drug Discovery Today, 2020, 25, 837-850.	3.2	24
15	Impact of the Protein Data Bank Across Scientific Disciplines. Data Science Journal, 2020, 19, 25.	0.6	17
16	Archiving and disseminating integrative structure models. Journal of Biomolecular NMR, 2019, 73, 385-398.	1.6	20
17	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
18	How Structural Biologists and the Protein Data Bank Contributed to Recent FDA New Drug Approvals. Structure, 2019, 27, 211-217.	1.6	65

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19	Protein Data Bank: the single global archive for 3D macromolecular structure data. Nucleic Acids Research, 2019, 47, D520-D528.	6.5	671
20	RCSB Protein Data Bank: biological macromolecular structures enabling research and education in fundamental biology, biomedicine, biotechnology and energy. Nucleic Acids Research, 2019, 47, D464-D474.	6.5	918
21	Development of a Prototype System for Archiving Integrative/Hybrid Structure Models of Biological Macromolecules. Structure, 2018, 26, 894-904.e2.	1.6	81
22	RCSB Protein Data Bank: Sustaining a living digital data resource that enables breakthroughs in scientific research and biomedical education. Protein Science, 2018, 27, 316-330.	3.1	219
23	Worldwide Protein Data Bank biocuration supporting open access to high-quality 3D structural biology data. Database: the Journal of Biological Databases and Curation, 2018, 2018, .	1.4	45
24	OUP accepted manuscript. Nucleic Acids Research, 2017, 45, D271-D281.	6.5	619
25	Multivariate Analyses of Quality Metrics for Crystal Structures in the PDB Archive. Structure, 2017, 25, 458-468.	1.6	28
26	OneDep: Unified wwPDB System for Deposition, Biocuration, and Validation of Macromolecular Structures in the PDB Archive. Structure, 2017, 25, 536-545.	1.6	130
27	Validation of Structures in the Protein Data Bank. Structure, 2017, 25, 1916-1927.	1.6	210
28	2017 publication guidelines for structural modelling of small-angle scattering data from biomolecules in solution: an update. Acta Crystallographica Section D: Structural Biology, 2017, 73, 710-728.	1.1	205
29	Crystallography and Databases. Data Science Journal, 2017, 16, .	0.6	28
30	DCC: a Swiss army knife for structure factor analysis and validation. Journal of Applied Crystallography, 2016, 49, 1081-1084.	1.9	22
31	Specification of the Crystallographic Information File format, version 2.0. Journal of Applied Crystallography, 2016, 49, 277-284.	1.9	37
32	Extension of the sasCIF format and its applications for data processing and deposition. Journal of Applied Crystallography, 2016, 49, 302-310.	1.9	18
33	EMDataBank unified data resource for 3DEM. Nucleic Acids Research, 2016, 44, D396-D403.	6.5	230
34	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. Nature Structural and Molecular Biology, 2015, 22, 433-434.	3.6	40
35	Data to knowledge: how to get meaning from your result. IUCrJ, 2015, 2, 45-58.	1.0	12
36	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. Structure, 2015, 23, 1156-1167.	1.6	159

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37	The chemical component dictionary: complete descriptions of constituent molecules in experimentally determined 3D macromolecules in the Protein Data Bank. Bioinformatics, 2015, 31, 1274-1278.	1.8	110
38	The RCSB Protein Data Bank: views of structural biology for basic and applied research and education. Nucleic Acids Research, 2015, 43, D345-D356.	6.5	461
39	Improving the representation of peptideâ€like inhibitor and antibiotic molecules in the Protein Data Bank. Biopolymers, 2014, 101, 659-668.	1.2	31
40	The Nucleic Acid Database: new features and capabilities. Nucleic Acids Research, 2014, 42, D114-D122.	6.5	194
41	Report of the wwPDB Small-Angle Scattering Task Force: Data Requirements for Biomolecular Modeling and the PDB. Structure, 2013, 21, 875-881.	1.6	77
42	Chemical annotation of small and peptide-like molecules at the Protein Data Bank. Database: the Journal of Biological Databases and Curation, 2013, 2013, bat079.	1.4	14
43	The RCSB Protein Data Bank: new resources for research and education. Nucleic Acids Research, 2012, 41, D475-D482.	6.5	418
44	Data management challenges in three-dimensional EM. Nature Structural and Molecular Biology, 2012, 19, 1203-1207.	3.6	49
45	Structural Biology Knowledgebase: a biologists resource for protein structure and sample information. FASEB Journal, 2012, 26, lb194.	0.2	0
46	The Structural Biology Knowledgebase - search Online for Protein Sequences, Structures, Functions, Methods and More. Biophysical Journal, 2011, 100, 319a.	0.2	0
47	The evolution of the RCSB Protein Data Bank website. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 782-789.	6.2	7
48	The Structural Biology Knowledgebase: a portal to protein structures, sequences, functions, and methods. Journal of Structural and Functional Genomics, 2011, 12, 45-54.	1.2	65
49	The RCSB Protein Data Bank: redesigned web site and web services. Nucleic Acids Research, 2011, 39, D392-D401.	6.5	549
50	EMDataBank.org: unified data resource for CryoEM. Nucleic Acids Research, 2011, 39, D456-D464.	6.5	246
51	How to use the PSI Structural Genomics Knowledgebase to Enable Research. Biophysical Journal, 2010, 98, 250a.	0.2	0
52	HOW TO USE THE PSI STRUCTURAL GENOMICS KNOWLEDGEBASE TO ENABLE RESEARCH. FASEB Journal, 2010, 24, 902.2.	0.2	0
53	The protein structure initiative structural genomics knowledgebase. Nucleic Acids Research, 2009, 37, D365-D368.	6.5	94
54	The Protein Model Portal. Journal of Structural and Functional Genomics, 2009, 10, 1-8.	1.2	130

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55	The Protein Structure Initiative Structural Genomics Knowledgebase. FASEB Journal, 2009, 23, 858.10.	0.2	0
56	Representation of viruses in the remediated PDB archive. Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 874-882.	2.5	35
57	Solid-State Changes in Ligand-to-Metal Charge-Transfer Spectra of (NH₃)₅Ru^{III}(2,4-dihydroxybenzoate) and (NH₃)₅Ru^{III}(xanthine) Chromophores. Inorganic Chemistry, 2008, 47, 9813-9827.	1.9	6
58	RNA backbone: Consensus all-angle conformers and modular string nomenclature (an RNA Ontology) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.6	216
59	Remediation of the protein data bank archive. Nucleic Acids Research, 2007, 36, D426-D433.	6.5	136
60	Realism about PDB. Nature Biotechnology, 2007, 25, 845-846.	9.4	17
61	Outcome of a Workshop on Archiving Structural Models of Biological Macromolecules. Structure, 2006, 14, 1211-1217.	1.6	60
62	The RCSB PDB information portal for structural genomics. Nucleic Acids Research, 2006, 34, D302-D305.	6.5	334
63	Report of the Working Group on Crystal Phase Identifiers. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, 575-580.	0.3	9
64	A framework for scientific data modeling and automated software development. Bioinformatics, 2005, 21, 1678-1684.	1.8	42
65	PDBML: the representation of archival macromolecular structure data in XML. Bioinformatics, 2005, 21, 988-992.	1.8	154
66	The PDB Format, mmCIF Formats, and Other Data Formats. Methods of Biochemical Analysis, 2005, , 159-179.	0.2	20
67	The Nucleic Acid Database. Methods of Biochemical Analysis, 2005, , 199-216.	0.2	4
68	TargetDB: a target registration database for structural genomics projects. Bioinformatics, 2004, 20, 2860-2862.	1.8	182
69	The distribution and query systems of the RCSB Protein Data Bank. Nucleic Acids Research, 2004, 32, 223D-225.	6.5	108
70	Design of a data model for developing laboratory information management and analysis systems for protein production. Proteins: Structure, Function and Bioinformatics, 2004, 58, 278-284.	1.5	27
71	Automated and accurate deposition of structures solved by X-ray diffraction to the Protein Data Bank. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 1833-1839.	2.5	236
72	The Impact of Structural Genomics on the Protein Data Bank. Molecular Diagnosis and Therapy, 2004, 4, 247-252.	3.3	26

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73	The Protein Data Bank: A Case Study in Management of Community Data. Current Proteomics, 2004, 1, 49-57.	0.1	16
74	The RCSB Protein Data Bank: a redesigned query system and relational database based on the mmCIF schema. Nucleic Acids Research, 2004, 33, D233-D237.	6.5	303
75	Tools for the automatic identification and classification of RNA base pairs. Nucleic Acids Research, 2003, 31, 3450-3460.	6.5	240
76	The Protein Data Bank and structural genomics. Nucleic Acids Research, 2003, 31, 489-491.	6.5	331
77	The Need for Dictionaries, Ontologies, and Controlled Vocabularies. OMICS A Journal of Integrative Biology, 2003, 7, 9-10.	1.0	2
78	Validation of Protein Structures for Protein Data Bank. Methods in Enzymology, 2003, 374, 370-385.	0.4	43
79	The Protein Data Bank. , 2003, , 389-405.		29
80	The PDB format, mmCIF, and other data formats. Methods of Biochemical Analysis, 2003, 44, 161-79.	0.2	32
81	An ontology driven architecture for derived representations of macromolecular structure. Bioinformatics, 2002, 18, 1280-1281.	1.8	16
82	The Protein Data Bank: unifying the archive. Nucleic Acids Research, 2002, 30, 245-248.	6.5	261
83	RNAML: A standard syntax for exchanging RNA information. Rna, 2002, 8, 707-717.	1.6	91
84	A biologist's guide to synchrotron facilities: the BioSync web resource. Trends in Biochemical Sciences, 2002, 27, 213-215.	3.7	10
85	The Protein Data Bank. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 899-907.	2.5	2,023
86	The Nucleic Acid Database. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 889-898.	2.5	57
87	Announcement of the BioSync web site. Nature Structural Biology, 2001, 8, 663-663.	9.7	9
88	The Protein Data Bank and the challenge of structural genomics. Nature Structural Biology, 2000, 7, 957-959.	9.7	511
89	STAR/mmCIF: An ontology for macromolecular structure. Bioinformatics, 2000, 16, 159-168.	1.8	78
90	The Protein Data Bank. Nucleic Acids Research, 2000, 28, 235-242.	6.5	31,087

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91	CIF Applications. XI.A La Mode: a ligand and monomer object data environment. I. Automated construction of mmCIF monomer and ligand models. Journal of Applied Crystallography, 1999, 32, 125-133.	1.9	6
92	The Nucleic Acid Database: A Resource for Nucleic Acid Science. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 1095-1104.	2.5	13
93	[30] Macromolecular crystallographic information file. Methods in Enzymology, 1997, 277, 571-590.	0.4	148
94	Geometric Parameters in Nucleic Acids:Â Nitrogenous Bases. Journal of the American Chemical Society, 1996, 118, 509-518.	6.6	191
95	Nucleic acid crystallography: A view from the nucleic acid database. Progress in Biophysics and Molecular Biology, 1996, 66, 255-288.	1.4	29
96	The Nucleic Acid Database: Present and future. Journal of Research of the National Institute of Standards and Technology, 1996, 101, 243.	0.4	2
97	<title>Simulation of photophysical processes of indoles in solution</title>. , 1992, , .		1
98	Molecular and electronic structures of pentaammineruthenium(II)-thioether complexes. The nature of Ru(II)-S back bonding elucidated by structural, electronic spectral, and molecular orbital studies. Journal of the American Chemical Society, 1992, 114, 4345-4353.	6.6	28
99	An interactive FORTRAN program for three-dimensional molecular visualization. Computers & Chemistry, 1992, 16, 265-266.	1.2	0
100	Molecular electrostatic potentials and partial atomic charges from correlated wave functions: Applications to the electronic ground and excited states of 3-methylindole. Journal of Computational Chemistry, 1992, 13, 979-989.	1.5	17
101	Solvent effects on the adiabatic free energy difference between the ground and excited states of methylindole in water. The Journal of Physical Chemistry, 1991, 95, 6756-6758.	2.9	18
102	Conserving energy during molecular dynamics simulations of water, proteins, and proteins in water. Journal of Computational Chemistry, 1990, 11, 1169-1180.	1.5	86
103	Simple models for solvation effects on electronic transition energies: Formaldehyde and water. Chemical Physics Letters, 1989, 154, 531-535.	1.2	35
104	Synthesis and properties of the valence tautomer of cis-iodosocyclopropanecarboxylic acid: 4,5-methano-1-hydroxyiodoxol-3(1H)-one. Journal of the American Chemical Society, 1989, 111, 6729-6734.	6.6	33
105	Organoiodinane reagents for phosphate cleavage: experimental and computational studies. Journal of the American Chemical Society, 1989, 111, 250-258.	6.6	44
106	Crystal, molecular, and electronic structures of pentaammineruthenium(III)-thioether complexes. Journal of the American Chemical Society, 1989, 111, 4082-4091.	6.6	19
107	Ab initio all-electron and effective core potential calculations on CuCl2?4. International Journal of Quantum Chemistry, 1988, 34, 245-255.	1.0	4
108	Molecular and electronic structure of (L-histidinato)pentammineruthenium(III) chloride monohydrate, (H3N)5RuIII(his)Cl3Â·H2O. X-ray structure, single-crystal polarized charge-transfer spectra, and ab initio and semiempirical molecular orbital calculations. Journal of the American Chemical Society, 1987, 109, 7025-7031.	6.6	56