Jane S Richardson

List of Publications by Year in descending order

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132 papers 67,517 citations

53 h-index 117 g-index

142 all docs

142 docs citations

times ranked

142

60716 citing authors

#	Article	IF	Citations
1	<i>PHENIX</i> : a comprehensive Python-based system for macromolecular structure solution. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 213-221.	2.5	20,564
2	<i>MolProbity</i> : all-atom structure validation for macromolecular crystallography. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 12-21.	2.5	12,318
3	Structure validation by Cα geometry: ï•,ï^ and Cβ deviation. Proteins: Structure, Function and Bioinformatics, 2003, 50, 437-450.	1.5	4,134
4	Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in <i>Phenix</i> . Acta Crystallographica Section D: Structural Biology, 2019, 75, 861-877.	1.1	4,060
5	MolProbity: all-atom contacts and structure validation for proteins and nucleic acids. Nucleic Acids Research, 2007, 35, W375-W383.	6.5	3,443
6	The Anatomy and Taxonomy of Protein Structure. Advances in Protein Chemistry, 1981, 34, 167-339.	4.4	3,057
7	MolProbity: More and better reference data for improved allâ€atom structure validation. Protein Science, 2018, 27, 293-315.	3.1	2,776
8	Amino acid preferences for specific locations at the ends of alpha helices. Science, 1988, 240, 1648-1652.	6.0	1,458
9	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.	2.0	1,264
10	The penultimate rotamer library. Proteins: Structure, Function and Bioinformatics, 2000, 40, 389-408.	1.5	977
11	Determination and analysis of the 2 Ã structure of copper, zinc superoxide dismutase. Journal of Molecular Biology, 1982, 160, 181-217.	2.0	952
12	MOLPROBITY: structure validation and all-atom contact analysis for nucleic acids and their complexes. Nucleic Acids Research, 2004, 32, W615-W619.	6.5	938
13	Structure and mechanism of copper, zinc superoxide dismutase. Nature, 1983, 306, 284-287.	13.7	905
14	The Phenix software for automated determination of macromolecular structures. Methods, 2011, 55, 94-106.	1.9	764
15	Natural Â-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.	3.3	744
16	\hat{l}^2 -Sheet topology and the relatedness of proteins. Nature, 1977, 268, 495-500.	13.7	568
17	Electrostatic recognition between superoxide and copper, zinc superoxide dismutase. Nature, 1983, 306, 287-290.	13.7	541

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19	Crystal structure of bovine Cu,Zn superoxide dismutase at 3 A resolution: chain tracing and metal ligands Proceedings of the National Academy of Sciences of the United States of America, 1975, 72, 1349-1353.	3.3	411
20	A New Generation of Crystallographic Validation Tools for the Protein Data Bank. Structure, 2011, 19, 1395-1412.	1.6	405
21	Structures of the Bacterial Ribosome in Classical and Hybrid States of tRNA Binding. Science, 2011, 332, 981-984.	6.0	343
22	Alternate States of Proteins Revealed by Detailed Energy Landscape Mapping. Journal of Molecular Biology, 2011, 405, 607-618.	2.0	324
23	Principles and Patterns of Protein Conformation. , 1989, , 1-98.		260
24	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.	3.3	249
25	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.	3.3	249
26	The Backrub Motion: How Protein Backbone Shrugs When a Sidechain Dances. Structure, 2006, 14, 265-274.	1.6	237
27	Use of knowledge-based restraints in <i>phenix.refine</i> to improve macromolecular refinement at low resolution. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 381-390.	2.5	230
28	RNA backbone: Consensus all-angle conformers and modular string nomenclature (an RNA Ontology) Tj ETQq0	0 0 rgBT /0	Overlock 10 Ti 216
29	The kinemage: A tool for scientific communication. Protein Science, 1992, 1, 3-9.	3.1	208
30	Scientific Benchmarks for Guiding Macromolecular Energy Function Improvement. Methods in Enzymology, 2013, 523, 109-143.	0.4	195
31	The de novo design of protein structures. Trends in Biochemical Sciences, 1989, 14, 304-309.	3.7	192
32	RNA backbone is rotameric. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 13904-13909.	3.3	184
33	Handedness of crossover connections in beta sheets Proceedings of the National Academy of Sciences of the United States of America, 1976, 73, 2619-2623.	3.3	174
34	Similarity of three-dimensional structure between the immunoglobulin domain and the copper, zinc superoxide dismutase subunit. Journal of Molecular Biology, 1976, 102, 221-235.	2.0	160
35	Recommendations of the wwPDB NMR Validation Task Force. Structure, 2013, 21, 1563-1570.	1.6	151
36	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.	3.3	150

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37	Graphical tools for macromolecular crystallography in <i>PHENIX</i> . Journal of Applied Crystallography, 2012, 45, 581-586.	1.9	139
38	Simultaneous comparison of three protein sequences Proceedings of the National Academy of Sciences of the United States of America, 1985, 82, 3073-3077.	3.3	137
39	The tyrosine corner: A feature of most greek key βâ€barrel proteins. Protein Science, 1994, 3, 1927-1937.	3.1	116
40	The Alacoil: A very tight, antiparallel coiledâ€coil of helices. Protein Science, 1995, 4, 2252-2260.	3.1	114
41	<i>phenix.model_vs_data</i> : a high-level tool for the calculation of crystallographic model and data statistics. Journal of Applied Crystallography, 2010, 43, 669-676.	1.9	112
42	osprey. Methods in Enzymology, 2013, 523, 87-107.	0.4	105
43	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.	3.1	104
44	Molecular conformation of erabutoxin b; Atomic coordinates at 2.5 \tilde{A} resolution. Biochemical and Biophysical Research Communications, 1979, 88, 950-959.	1.0	91
45	Molprobity's ultimate rotamer-library distributions for model validation. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1177-1189.	1.5	90
46	Advances, Interactions, and Future Developments in the CNS, Phenix, and Rosetta Structural Biology Software Systems. Annual Review of Biophysics, 2013, 42, 265-287.	4.5	88
47	Sculpting proteins interactively: Continual energy minimization embedded in a graphical modeling system. Protein Science, 1994, 3, 198-210.	3.1	84
48	Schematic drawings of protein structures. Methods in Enzymology, 1985, 115, 359-380.	0.4	82
49	The other 90% of the protein: Assessment beyond the Cαs for CASP8 templateâ€based and highâ€accuracy models. Proteins: Structure, Function and Bioinformatics, 2009, 77, 29-49.	1.5	79
50	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. Nature Methods, 2021, 18, 156-164.	9.0	73
51	Algorithm for backrub motions in protein design. Bioinformatics, 2008, 24, i196-i204.	1.8	72
52	Alpha-carbon coordinates for bovine Cu, Zn superoxide dismutase. Biochemical and Biophysical Research Communications, 1975, 63, 986-992.	1.0	70
53	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.	3.3	67
54	New insights into Hoogsteen base pairs in DNA duplexes from a structure-based survey. Nucleic Acids Research, 2015, 43, 3420-3433.	6.5	66

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55	The RNA Ontology Consortium: An open invitation to the RNA community. Rna, 2006, 12, 533-541.	1.6	59
56	Teaching molecular 3-D literacy. Biochemistry and Molecular Biology Education, 2002, 30, 21-26.	0.5	56
57	Kinemages - simple macromolecular graphics for interactive teaching and publication. Trends in Biochemical Sciences, 1994, 19, 135-138.	3.7	54
58	Folding Kinetics of a Fluorescent Variant of Monomeric λ Repressorâ€. Biochemistry, 1998, 37, 9179-9185.	1.2	50
59	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.	3.3	46
60	Describing patterns of protein tertiary structure. Methods in Enzymology, 1985, 115, 341-358.	0.4	45
61	A test of enhancing model accuracy in high-throughput crystallography. Journal of Structural and Functional Genomics, 2005, 6, 1-11.	1.2	45
62	Early ribbon drawings of proteins., 2000, 7, 624-625.		44
63	Automated identification of elemental ions in macromolecular crystal structures. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 1104-1114.	2.5	40
64	Multiscale Conformational Heterogeneity in Staphylococcal Protein A: Possible Determinant of Functional Plasticity. Structure, 2014, 22, 1467-1477.	1.6	40
65	New tools provide a second look at HDV ribozyme structure, dynamics and cleavage. Nucleic Acids Research, 2014, 42, 12833-12846.	6.5	38
66	"Active―conformation of an inactive semi-synthetic ribonuclease-S. Journal of Molecular Biology, 1981, 149, 313-317.	2.0	35
67	Autofix for backward-fit sidechains: using MolProbity and real-space refinement to put misfits in their place. Journal of Structural and Functional Genomics, 2009, 10, 83-93.	1.2	35
68	Target domain definition and classification in CASP8. Proteins: Structure, Function and Bioinformatics, 2009, 77, 10-17.	1.5	33
69	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.	2.0	32
70	Two Crystal Forms of Bovine Superoxide Dismutase. Journal of Biological Chemistry, 1972, 247, 6368-6369.	1.6	32
71	The Role of Local Backrub Motions in Evolved and Designed Mutations. PLoS Computational Biology, 2012, 8, e1002629.	1.5	32
72	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.	1.5	31

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73	Model validation: local diagnosis, correction and when to quit. Acta Crystallographica Section D: Structural Biology, 2018, 74, 132-142.	1.1	29
74	Improved chemistry restraints for crystallographic refinement by integrating the Amber force field into <i>Phenix</i> . Acta Crystallographica Section D: Structural Biology, 2020, 76, 51-62.	1.1	29
75	The Crystal Structure of Bovine Cu2+,Zn2+ Superoxide Dismutase at 5.5-A Resolution. Journal of Biological Chemistry, 1974, 249, 5677-5683.	1.6	28
76	Teaching and Assessing Three-Dimensional Molecular Literacy in Undergraduate Biochemistry. Journal of Chemical Education, 2002, 79, 551.	1.1	27
77	The simple construction of protein alpha-Carbon models. Biopolymers, 1972, 11, 2381-2385.	1.2	26
78	Computational Methods for RNA Structure Validation and Improvement. Methods in Enzymology, 2015, 558, 181-212.	0.4	25
79	New Tools and Data for Improving Structures, Using All-Atom Contacts. Methods in Enzymology, 2003, 374, 385-412.	0.4	24
80	RNABC: forward kinematics to reduce all-atom steric clashes in RNA backbone. Journal of Mathematical Biology, 2007, 56, 253-278.	0.8	24
81	Recent developments in phasing and structure refinement for macromolecular crystallography. Current Opinion in Structural Biology, 2009, 19, 566-572.	2.6	23
82	The RNA Ontology (RNAO): An ontology for integrating RNA sequence and structure data. Applied Ontology, 2011, 6, 53-89.	1.0	23
83	Manganese superoxide dismutases from Escherichia coli and from yeast mitochondria: Preliminary X-ray crystallographic studies. Journal of Molecular Biology, 1976, 105, 327-332.	2.0	22
84	The cis-pro touch-turn: A rare motif preferred at functional sites. Proteins: Structure, Function and Bioinformatics, 2004, 56, 298-309.	1.5	22
85	The high-throughput protein-to-structure pipeline at SECSG. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 679-684.	2.5	22
86	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.	1.3	22
87	Interpretation of electron density maps. Methods in Enzymology, 1985, 115, 189-206.	0.4	21
88	Doing Molecular Biophysics: Finding, Naming, and Picturing Signal Within Complexity. Annual Review of Biophysics, 2013, 42, 1-28.	4.5	21
89	Improving SARS-CoV-2 structures: Peer review by early coordinate release. Biophysical Journal, 2021, 120, 1085-1096.	0.2	21
90	KinImmerse: Macromolecular VR for NMR ensembles. Source Code for Biology and Medicine, 2009, 4, 3.	1.7	19

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91	Structural genomics of Pyrococcus furiosus: X-ray crystallography reveals 3D domain swapping in rubrerythrin. Proteins: Structure, Function and Bioinformatics, 2004, 57, 878-882.	1.5	18
92	Kinetic Role of Helix Caps in Protein Folding Is Context-Dependentâ€. Biochemistry, 2004, 43, 3814-3823.	1.2	18
93	"THE PLOT―THICKENS: MORE DATA, MORE DIMENSIONS, MORE USES. , 2013, , 46-61.		18
94	Making the invisible enemy visible. Nature Structural and Molecular Biology, 2021, 28, 404-408.	3.6	18
95	VIEW., 1993,,.		16
96	Protein imperfections: separating intrinsic from extrinsic variation of torsion angles. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 88-98.	2.5	15
97	Protein design and folding: template trapping of self-assembled helical bundles. Journal of Peptide Science, 2001, 7, 146-151.	0.8	14
98	Crystallographic model validation: from diagnosis to healing. Current Opinion in Structural Biology, 2013, 23, 707-714.	2.6	14
99	The penultimate rotamer library. , 2000, 40, 389.		14
100	The singly-wound parallel \hat{l}^2 barrel: A proposed structure for 2-keto-3-deoxy-6-phosphogluconate aldolase. Biochemical and Biophysical Research Communications, 1979, 90, 285-290.	1.0	13
101	Seeing the PDB. Journal of Biological Chemistry, 2021, 296, 100742.	1.6	13
102	Preliminary X-ray diffraction studies of acyl carrier protein from Escherichia coli. Journal of Molecular Biology, 1985, 182, 467-468.	2.0	12
103	Assessment of Molecular Construction in Undergraduate Biochemistry. Journal of Chemical Education, 2005, 82, 1854.	1.1	12
104	Studying and polishing the PDB's macromolecules. Biopolymers, 2013, 99, 170-182.	1.2	12
105	RNA backbone rotamers – finding your way in seven dimensions. Biochemical Society Transactions, 2005, 33, 485-487.	1.6	11
106	Away from the edge II: in-house Se-SAS phasing with chromium radiation. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 960-966.	2.5	10
107	Biophysical Highlights from 54 Years of Macromolecular Crystallography. Biophysical Journal, 2014, 106, 510-525.	0.2	10
108	Mismodeled purines: implicit alternates and hidden Hoogsteens. Acta Crystallographica Section D: Structural Biology, 2017, 73, 852-859.	1.1	9

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109	Constructing atomic structural models into cryo-EM densities using molecular dynamics – Pros and cons. Journal of Structural Biology, 2018, 204, 319-328.	1.3	9
110	Protein structure: A new twist for hairpin turns. Nature, 1985, 316, 102-103.	13.7	8
111	Facile chemical synthesis and equilibrium unfolding properties of CopG. Protein Science, 2004, 13, 1918-1926.	3.1	8
112	Structure of the hypothetical protein PF0899 fromPyrococcus furiosusat 1.85â€Ã resolution. Acta Crystallographica Section F: Structural Biology Communications, 2007, 63, 549-552.	0.7	6
113	The importance of residueâ€level filtering and the Top2018 bestâ€parts dataset of highâ€quality protein residues. Protein Science, 2022, 31, 290-300.	3.1	6
114	Introduction: Protein Motifs. FASEB Journal, 1994, 8, 1237-1239.	0.2	5
115	An illustrated museum of protein structures. Biophysical Journal, 1980, 32, 211-213.	0.2	3
116	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.	1.3	3
117	All-Atom Contacts: A New Approach to Structure Validation. Methods of Biochemical Analysis, 2005, , 305-320.	0.2	3
118	The RNA Ontology (RNAO): An ontology for integrating RNA sequence and structure data. Nature Precedings, 2009, , .	0.1	3
119	All-atom contacts: a new approach to structure validation. Methods of Biochemical Analysis, 2003, 44, 305-20.	0.2	3
120	The Zen of Model Anomalies – Correct Most of Them. Treasure the Meaningful Valid Few. Live Serenely with the Rest!. NATO Science for Peace and Security Series A: Chemistry and Biology, 2013, , 1-10.	0.5	2
121	High-Grade Ore for Data Mining in 3D Structures. , 2003, , 139-161.		2
122	The Protein Surface Is a Moving Target. Structure, 2004, 12, 912-913.	1.6	1
123	A new way to see RNAs. Nature Methods, 2020, 17, 663-664.	9.0	1
124	An algorithm for smoothly tessellating \hat{l}^2 -sheet structures in proteins. Journal of Molecular Graphics, 1995, 13, 36-45.	1.7	0
125	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.	1.2	0
126	Through the Ramachandran Haze: Ca-Parameters Reveal Secondary Structure at Low Resolution. Biophysical Journal, 2013, 104, 19a-20a.	0.2	0

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127	Real Rotamers using Real-Space Correlation Coefficients. Biophysical Journal, 2013, 104, 547a.	0.2	o
128	Crystallography - Energetically Innovative at 100. Biophysical Journal, 2014, 106, 34a.	0.2	0
129	Cover Image, Volume 84, Issue 9. Proteins: Structure, Function and Bioinformatics, 2016, 84, C1-C1.	1.5	O
130	MDFF Error Analysis: A Tool for Determining Stereochemical and Thermodynamic Correct Structures. Biophysical Journal, 2019, 116, 140a-141a.	0.2	0
131	THE DE NOVO DESIGN OF PROTEIN STRUCTURES. , 1990, , 173-182.		0
132	Design of small symmetrical four-helix bundle proteins. , 2002, , 293-294.		0