## Jane S Richardson

## List of Publications by Citations

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130 52,159 142 52 h-index g-index citations papers 8.1 60,549 7.16 142 L-index avg, IF ext. citations ext. papers

#	Paper	IF	Citations
130	PHENIX: a comprehensive Python-based system for macromolecular structure solution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2010</b> , 66, 213-21		16067
129	MolProbity: all-atom structure validation for macromolecular crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2010</b> , 66, 12-21		9600
128	Structure validation by Calpha geometry: phi,psi and Cbeta deviation. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2003</b> , 50, 437-50	4.2	3522
127	MolProbity: all-atom contacts and structure validation for proteins and nucleic acids. <i>Nucleic Acids Research</i> , <b>2007</b> , 35, W375-83	20.1	3030
126	The anatomy and taxonomy of protein structure. Advances in Protein Chemistry, 1981, 34, 167-339		2607
125	Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in Phenix. <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2019</b> , 75, 861-877	5.5	1527
124	Amino acid preferences for specific locations at the ends of alpha helices. <i>Science</i> , <b>1988</b> , 240, 1648-52	33.3	1337
123	MolProbity: More and better reference data for improved all-atom structure validation. <i>Protein Science</i> , <b>2018</b> , 27, 293-315	6.3	1169
122	Asparagine and glutamine: using hydrogen atom contacts in the choice of side-chain amide orientation. <i>Journal of Molecular Biology</i> , <b>1999</b> , 285, 1735-47	6.5	1064
121	Determination and analysis of the 2 A-structure of copper, zinc superoxide dismutase. <i>Journal of Molecular Biology</i> , <b>1982</b> , 160, 181-217	6.5	879
120	The penultimate rotamer library. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2000</b> , 40, 389-408	4.2	849
119	MOLPROBITY: structure validation and all-atom contact analysis for nucleic acids and their complexes. <i>Nucleic Acids Research</i> , <b>2004</b> , 32, W615-9	20.1	816
118	Structure and mechanism of copper, zinc superoxide dismutase. <i>Nature</i> , <b>1983</b> , 306, 284-7	50.4	797
117	Natural beta-sheet proteins use negative design to avoid edge-to-edge aggregation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2002</b> , 99, 2754-9	11.5	660
116	The Phenix software for automated determination of macromolecular structures. <i>Methods</i> , <b>2011</b> , 55, 94-106	4.6	580
115	beta-Sheet topology and the relatedness of proteins. <i>Nature</i> , <b>1977</b> , 268, 495-500	50.4	512
114	Electrostatic recognition between superoxide and copper, zinc superoxide dismutase. <i>Nature</i> , <b>1983</b> , 306, 287-90	50.4	498

113	Visualizing and quantifying molecular goodness-of-fit: small-probe contact dots with explicit hydrogen atoms. <i>Journal of Molecular Biology</i> , <b>1999</b> , 285, 1711-33	6.5	445
112	Crystal structure of bovine Cu,Zn superoxide dismutase at 3 A resolution: chain tracing and metal ligands. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>1975</b> , 72, 1349-	·5 <sup>1</sup> 3 <sup>1.5</sup>	381
111	A new generation of crystallographic validation tools for the protein data bank. <i>Structure</i> , <b>2011</b> , 19, 139	95 <del>5.4</del> 12	335
110	Structures of the bacterial ribosome in classical and hybrid states of tRNA binding. <i>Science</i> , <b>2011</b> , 332, 981-4	33.3	285
109	Principles and Patterns of Protein Conformation <b>1989</b> , 1-98		227
108	Three dimensional structure of erabutoxin b neurotoxic protein: inhibitor of acetylcholine receptor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>1976</b> , 73, 2991-4	11.5	225
107	The beta bulge: a common small unit of nonrepetitive protein structure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>1978</b> , 75, 2574-8	11.5	223
106	Alternate states of proteins revealed by detailed energy landscape mapping. <i>Journal of Molecular Biology</i> , <b>2011</b> , 405, 607-18	6.5	207
105	The backrub motion: how protein backbone shrugs when a sidechain dances. Structure, <b>2006</b> , 14, 265-74	45.2	197
104	RNA backbone: consensus all-angle conformers and modular string nomenclature (an RNA Ontology Consortium contribution). <i>Rna</i> , <b>2008</b> , 14, 465-81	5.8	188
103	The kinemage: a tool for scientific communication. <i>Protein Science</i> , <b>1992</b> , 1, 3-9	6.3	175
102	The de novo design of protein structures. <i>Trends in Biochemical Sciences</i> , <b>1989</b> , 14, 304-9	10.3	170
101	Scientific benchmarks for guiding macromolecular energy function improvement. <i>Methods in Enzymology</i> , <b>2013</b> , 523, 109-43	1.7	164
100	Handedness of crossover connections in beta sheets. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>1976</b> , 73, 2619-23	11.5	160
99	Use of knowledge-based restraints in phenix.refine to improve macromolecular refinement at low resolution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2012</b> , 68, 381-90		156
98	RNA backbone is rotameric. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2003</b> , 100, 13904-9	11.5	154
97	Similarity of three-dimensional structure between the immunoglobulin domain and the copper, zinc superoxide dismutase subunit. <i>Journal of Molecular Biology</i> , <b>1976</b> , 102, 221-35	6.5	145
96	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, 8747-51	11.5	138

95	Recommendations of the wwPDB NMR Validation Task Force. Structure, 2013, 21, 1563-70	5.2	117
94	Simultaneous comparison of three protein sequences. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>1985</b> , 82, 3073-7	11.5	117
93	The Alacoil: a very tight, antiparallel coiled-coil of helices. <i>Protein Science</i> , <b>1995</b> , 4, 2252-60	6.3	102
92	The tyrosine corner: a feature of most Greek key beta-barrel proteins. <i>Protein Science</i> , <b>1994</b> , 3, 1927-37	6.3	102
91	Graphical tools for macromolecular crystallography in PHENIX. <i>Journal of Applied Crystallography</i> , <b>2012</b> , 45, 581-586	3.8	95
90	OSPREY: protein design with ensembles, flexibility, and provable algorithms. <i>Methods in Enzymology</i> , <b>2013</b> , 523, 87-107	1.7	94
89	phenix.model_vs_data: a high-level tool for the calculation of crystallographic model and data statistics. <i>Journal of Applied Crystallography</i> , <b>2010</b> , 43, 669-676	3.8	91
88	Molecular conformation of erabutoxin b; atomic coordinates at 2.5 A resolution. <i>Biochemical and Biophysical Research Communications</i> , <b>1979</b> , 88, 950-9	3.4	81
87	Advances, interactions, and future developments in the CNS, Phenix, and Rosetta structural biology software systems. <i>Annual Review of Biophysics</i> , <b>2013</b> , 42, 265-87	21.1	76
86	The other 90% of the protein: assessment beyond the Calphas for CASP8 template-based and high-accuracy models. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2009</b> , 77 Suppl 9, 29-49	4.2	70
85	Molprobity's ultimate rotamer-library distributions for model validation. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2016</b> , 84, 1177-89	4.2	69
84	Schematic drawings of protein structures. <i>Methods in Enzymology</i> , <b>1985</b> , 115, 359-80	1.7	67
83	Sculpting proteins interactively: continual energy minimization embedded in a graphical modeling system. <i>Protein Science</i> , <b>1994</b> , 3, 198-210	6.3	66
82	Alpha-carbon coordinates for bovine Cu,Zn superoxide dismutase. <i>Biochemical and Biophysical Research Communications</i> , <b>1975</b> , 63, 986-92	3.4	64
81	The extracellular nuclease of Staphylococcus aureus: structures of the native enzyme and an enzyme-inhibitor complex at 4 A resolution. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>1969</b> , 64, 420-7	11.5	64
80	Algorithm for backrub motions in protein design. <i>Bioinformatics</i> , <b>2008</b> , 24, i196-204	7.2	63
79	Kinemagessimple macromolecular graphics for interactive teaching and publication. <i>Trends in Biochemical Sciences</i> , <b>1994</b> , 19, 135-8	10.3	52
78	Teaching molecular 3-D literacy. <i>Biochemistry and Molecular Biology Education</i> , <b>2002</b> , 30, 21-26	1.3	50

77	Folding kinetics of a fluorescent variant of monomeric lambda repressor. <i>Biochemistry</i> , <b>1998</b> , 37, 9179-8	<b>5</b> .2	49	
76	The RNA Ontology Consortium: an open invitation to the RNA community. <i>Rna</i> , <b>2006</b> , 12, 533-41	5.8	49	
75	New insights into Hoogsteen base pairs in DNA duplexes from a structure-based survey. <i>Nucleic Acids Research</i> , <b>2015</b> , 43, 3420-33	20.1	48	•
74	A test of enhancing model accuracy in high-throughput crystallography. <i>Journal of Structural and Functional Genomics</i> , <b>2005</b> , 6, 1-11		43	
73	Asparagine and glutamine rotamers: B-factor cutoff and correction of amide flips yield distinct clustering. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>1999</b> , 96, 400-5	11.5	41	•
72	Describing patterns of protein tertiary structure. <i>Methods in Enzymology</i> , <b>1985</b> , 115, 341-58	1.7	40	
71	New tools in MolProbity validation: CaBLAM for CryoEM backbone, UnDowser to rethink "waters," and NGL Viewer to recapture online 3D graphics. <i>Protein Science</i> , <b>2020</b> , 29, 315-329	6.3	39	
70	Autofix for backward-fit sidechains: using MolProbity and real-space refinement to put misfits in their place. <i>Journal of Structural and Functional Genomics</i> , <b>2009</b> , 10, 83-93		33	
69	"Active" conformation of an inactive semi-synthetic ribonuclease-S. <i>Journal of Molecular Biology</i> , <b>1981</b> , 149, 313-7	6.5	33	
68	Multiscale conformational heterogeneity in staphylococcal protein a: possible determinant of functional plasticity. <i>Structure</i> , <b>2014</b> , 22, 1467-77	5.2	31	
67	Two Crystal Forms of Bovine Superoxide Dismutase. <i>Journal of Biological Chemistry</i> , <b>1972</b> , 247, 6368-636	6 <del>9</del> .4	31	
66	Target domain definition and classification in CASP8. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2009</b> , 77 Suppl 9, 10-7	4.2	30	
65	Helix lap-joints as ion-binding sites: DNA-binding motifs and Ca-binding "EF hands" are related by charge and sequence reversal. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1988</b> , 4, 229-39	4.2	30	
64	Early ribbon drawings of proteins. <i>Nature Structural Biology</i> , <b>2000</b> , 7, 624-5		29	
63	Automated identification of elemental ions in macromolecular crystal structures. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2014</b> , 70, 1104-14		27	
62	New tools provide a second look at HDV ribozyme structure, dynamics and cleavage. <i>Nucleic Acids Research</i> , <b>2014</b> , 42, 12833-46	20.1	26	
61	Teaching and Assessing Three-Dimensional Molecular Literacy in Undergraduate Biochemistry. Journal of Chemical Education, <b>2002</b> , 79, 551	2.4	24	
60	The role of local backrub motions in evolved and designed mutations. <i>PLoS Computational Biology</i> , <b>2012</b> , 8, e1002629	5	24	

59	Broad Analysis of Vicinal Disulfides: Occurrences, Conformations with Cis or with Trans Peptides, and Functional Roles Including Sugar Binding. <i>Journal of Molecular Biology</i> , <b>2017</b> , 429, 1321-1335	6.5	23
58	The simple construction of protein alpha-carbon models. <i>Biopolymers</i> , <b>1972</b> , 11, 2381-5	2.2	23
57	The Crystal Structure of Bovine Cu2+,Zn2+ Superoxide Dismutase at 5.5-A Resolution. <i>Journal of Biological Chemistry</i> , <b>1974</b> , 249, 5677-5683	5.4	23
56	The high-throughput protein-to-structure pipeline at SECSG. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2005</b> , 61, 679-84		22
55	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. <i>Nature Methods</i> , <b>2021</b> , 18, 156-164	21.6	22
54	Recent developments in phasing and structure refinement for macromolecular crystallography. <i>Current Opinion in Structural Biology</i> , <b>2009</b> , 19, 566-72	8.1	21
53	RNABC: forward kinematics to reduce all-atom steric clashes in RNA backbone. <i>Journal of Mathematical Biology</i> , <b>2008</b> , 56, 253-78	2	21
52	The cis-Pro touch-turn: a rare motif preferred at functional sites. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2004</b> , 56, 298-309	4.2	21
51	Manganese superoxide dismutases from Escherichia coli and from yeast mitochondria: preliminary x-ray crystallographic studies. <i>Journal of Molecular Biology</i> , <b>1976</b> , 105, 327-32	6.5	21
50	The RNA Ontology (RNAO): An ontology for integrating RNA sequence and structure data. <i>Applied Ontology</i> , <b>2011</b> , 6, 53-89	1.4	20
49	Computational Methods for RNA Structure Validation and Improvement. <i>Methods in Enzymology</i> , <b>2015</b> , 558, 181-212	1.7	19
48	New tools and data for improving structures, using all-atom contacts. <i>Methods in Enzymology</i> , <b>2003</b> , 374, 385-412	1.7	19
47	Model validation: local diagnosis, correction and when to quit. <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2018</b> , 74, 132-142	5.5	18
46	Doing molecular biophysics: finding, naming, and picturing signal within complexity. <i>Annual Review of Biophysics</i> , <b>2013</b> , 42, 1-28	21.1	17
45	THE PLOTOTHICKENS: MORE DATA, MORE DIMENSIONS, MORE USES <b>2013</b> , 46-61		17
44	KinImmerse: Macromolecular VR for NMR ensembles. Source Code for Biology and Medicine, 2009, 4, 3	1.9	17
43	Structural genomics of Pyrococcus furiosus: X-ray crystallography reveals 3D domain swapping in rubrerythrin. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2004</b> , 57, 878-82	4.2	17
42	Kinetic role of helix caps in protein folding is context-dependent. <i>Biochemistry</i> , <b>2004</b> , 43, 3814-23	3.2	17

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41	Interpretation of electron density maps. <i>Methods in Enzymology</i> , <b>1985</b> , 115, 189-206	1.7	16
40	Improved chemistry restraints for crystallographic refinement by integrating the Amber force field into Phenix. <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2020</b> , 76, 51-62	5.5	16
39	Protein imperfections: separating intrinsic from extrinsic variation of torsion angles. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2005</b> , 61, 88-98		14
38	The penultimate rotamer library <b>2000</b> , 40, 389		14
37	Protein design and folding: template trapping of self-assembled helical bundles. <i>Journal of Peptide Science</i> , <b>2001</b> , 7, 146-51	2.1	13
36	Crystallographic model validation: from diagnosis to healing. <i>Current Opinion in Structural Biology</i> , <b>2013</b> , 23, 707-14	8.1	12
35	Assessment of Molecular Construction in Undergraduate Biochemistry. <i>Journal of Chemical Education</i> , <b>2005</b> , 82, 1854	2.4	12
34	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. <i>Journal of Structural Biology</i> , <b>2018</b> , 204, 301-312	3.4	10
33	Away from the edge II: in-house Se-SAS phasing with chromium radiation. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2005</b> , 61, 960-6		10
32	Studying and polishing the PDB's macromolecules. <i>Biopolymers</i> , <b>2013</b> , 99, 170-82	2.2	9
32	Studying and polishing the PDB's macromolecules. <i>Biopolymers</i> , <b>2013</b> , 99, 170-82  Biophysical highlights from 54 years of macromolecular crystallography. <i>Biophysical Journal</i> , <b>2014</b> , 106, 510-25	2.2	9
	Biophysical highlights from 54 years of macromolecular crystallography. <i>Biophysical Journal</i> , <b>2014</b> ,		
31	Biophysical highlights from 54 years of macromolecular crystallography. <i>Biophysical Journal</i> , <b>2014</b> , 106, 510-25  RNA backbone rotamersfinding your way in seven dimensions. <i>Biochemical Society Transactions</i> ,	2.9	
31	Biophysical highlights from 54 years of macromolecular crystallography. <i>Biophysical Journal</i> , <b>2014</b> , 106, 510-25  RNA backbone rotamersfinding your way in seven dimensions. <i>Biochemical Society Transactions</i> , <b>2005</b> , 33, 485-7	2.9	9
31 30 29	Biophysical highlights from 54 years of macromolecular crystallography. <i>Biophysical Journal</i> , <b>2014</b> , 106, 510-25  RNA backbone rotamersfinding your way in seven dimensions. <i>Biochemical Society Transactions</i> , <b>2005</b> , 33, 485-7  VIEW <b>1993</b> ,  Preliminary X-ray diffraction studies of acyl carrier protein from Escherichia coli. <i>Journal of</i>	2.9	9 9
31 30 29 28	Biophysical highlights from 54 years of macromolecular crystallography. <i>Biophysical Journal</i> , <b>2014</b> , 106, 510-25  RNA backbone rotamersfinding your way in seven dimensions. <i>Biochemical Society Transactions</i> , <b>2005</b> , 33, 485-7  VIEW <b>1993</b> ,  Preliminary X-ray diffraction studies of acyl carrier protein from Escherichia coli. <i>Journal of Molecular Biology</i> , <b>1985</b> , 182, 467-8  The singly-wound parallel beta barrel: a proposed structure for 2-keto-3-deoxy-6-phosphogluconate aldolase. <i>Biochemical and Biophysical Research</i>	2.9 5.1 6.5	9 9 9
31 30 29 28	Biophysical highlights from 54 years of macromolecular crystallography. <i>Biophysical Journal</i> , <b>2014</b> , 106, 510-25  RNA backbone rotamersfinding your way in seven dimensions. <i>Biochemical Society Transactions</i> , <b>2005</b> , 33, 485-7  VIEW <b>1993</b> ,  Preliminary X-ray diffraction studies of acyl carrier protein from Escherichia coli. <i>Journal of Molecular Biology</i> , <b>1985</b> , 182, 467-8  The singly-wound parallel beta barrel: a proposed structure for 2-keto-3-deoxy-6-phosphogluconate aldolase. <i>Biochemical and Biophysical Research Communications</i> , <b>1979</b> , 90, 285-90  Improving SARS-CoV-2 structures: Peer review by early coordinate release. <i>Biophysical Journal</i> ,	<ul><li>2.9</li><li>5.1</li><li>6.5</li><li>3.4</li></ul>	9 9 9 9

23	Constructing atomic structural models into cryo-EM densities using molecular dynamics - Pros and cons. <i>Journal of Structural Biology</i> , <b>2018</b> , 204, 319-328	3.4	6
22	Structure of the hypothetical protein PF0899 from Pyrococcus furiosus at 1.85 A resolution. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , <b>2007</b> , 63, 549-52		5
21	Making the invisible enemy visible. <i>Nature Structural and Molecular Biology</i> , <b>2021</b> , 28, 404-408	17.6	5
20	Introduction: protein motifs. <i>FASEB Journal</i> , <b>1994</b> , 8, 1237-9	0.9	4
19	Seeing the PDB. Journal of Biological Chemistry, 2021, 296, 100742	5.4	4
18	SymROP: ROP protein with identical helices redesigned by all-atom contact analysis and molecular dynamics. <i>Journal of Molecular Graphics and Modelling</i> , <b>2000</b> , 18, 290-8, 309-10	2.8	3
17	Making the invisible enemy visible <b>2020</b> ,		3
16	All-atom contacts: a new approach to structure validation. <i>Methods of Biochemical Analysis</i> , <b>2003</b> , 44, 305-20		3
15	The RNA Ontology (RNAO): An ontology for integrating RNA sequence and structure data. <i>Nature Precedings</i> , <b>2009</b> ,		2
14	An illustrated museum of protein structures. <i>Biophysical Journal</i> , <b>1980</b> , 32, 211-3	2.9	2
13	The importance of residue-level filtering and the Top2018 best-parts dataset of high-quality		
	protein residues. <i>Protein Science</i> , <b>2021</b> ,	6.3	2
12		6.3	2
12	protein residues. <i>Protein Science</i> , <b>2021</b> ,	21.6	2
	Improving AlphaFold modeling using implicit information from experimental density maps		2
11	Improving AlphaFold modeling using implicit information from experimental density maps  A new way to see RNAs. <i>Nature Methods</i> , <b>2020</b> , 17, 663-664	21.6	1
11	Improving AlphaFold modeling using implicit information from experimental density maps  A new way to see RNAs. <i>Nature Methods</i> , <b>2020</b> , 17, 663-664  The protein surface is a moving target. <i>Structure</i> , <b>2004</b> , 12, 912-3	21.6	1
11 10 9	Improving AlphaFold modeling using implicit information from experimental density maps  A new way to see RNAs. Nature Methods, 2020, 17, 663-664  The protein surface is a moving target. Structure, 2004, 12, 912-3  All-Atom Contacts: A New Approach to Structure Validation. Methods of Biochemical Analysis, 2005, 305	21.6	2 1 1

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- An algorithm for smoothly tessellating beta-sheet structures in proteins. *Journal of Molecular Graphics*, **1995**, 13, 36-45, 58
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- THE DE NOVO DESIGN OF PROTEIN STRUCTURES **1990**, 173-182