Roman A Laskowski

List of Publications by Year
in descending order

102 papers	46,281 citations	44069 48 h-index	38395 95 g-index
107 all docs	107 docs citations	107 times ranked	46558 citing authors

#	Article	IF	Citations
1	PROCHECK: a program to check the stereochemical quality of protein structures. Journal of Applied Crystallography, 1993, 26, 283-291.	4.5	21,188
2	AQUA and PROCHECK-NMR: Programs for checking the quality of protein structures solved by NMR. Journal of Biomolecular NMR, 1996, 8, 477-86.	2.8	4,736
3	LIGPLOT: a program to generate schematic diagrams of protein-ligand interactions. Protein Engineering, Design and Selection, 1995, 8, 127-134.	2.1	4,648
4	LigPlot+: Multiple Ligandâ€“Protein Interaction Diagrams for Drug Discovery. Journal of Chemical Information and Modeling, 2011, 51, 2778-2786.	5.4	4,148
5	Main-chain Bond Lengths and Bond Angles in Protein Structures. Journal of Molecular Biology, 1993, 231, 1049-1067.	4.2	1,142
6	PDBsum: Structural summaries of PDB entries. Protein Science, 2018, 27, 129-134.	7.6	910
7	SURFNET: A program for visualizing molecular surfaces, cavities, and intermolecular interactions. Journal of Molecular Graphics, 1995, 13, 323-330.	1.1	870
8	ProFunc: a server for predicting protein function from 3D structure. Nucleic Acids Research, 2005, 33, W89-W93.	14.5	576
9	PDBsum: a web-based database of summaries and analyses of all PDB structures. Trends in Biochemical Sciences, 1997, 22, 488-490.	7.5	536
10	PDBsum new things. Nucleic Acids Research, 2009, 37, D355-D359.	14.5	526
11	A genome-wide meta-analysis identifies 22 loci associated with eight hematological parameters in the HaemGen consortium. Nature Genetics, 2009, 41, 1182-1190.	21.4	481
12	CATH: comprehensive structural and functional annotations for genome sequences. Nucleic Acids Research, 2015, 43, D376-D381.	14.5	399
13	PDBsum more: new summaries and analyses of the known 3D structures of proteins and nucleic acids. Nucleic Acids Research, 2004, 33, D266-D268.	14.5	373
14	Predicting Protein Ligand Binding Sites by Combining Evolutionary Sequence Conservation and 3D Structure. PLoS Computational Biology, 2009, 5, e1000585.	3.2	356
15	Predicting protein function from sequence and structural data. Current Opinion in Structural Biology, 2005, 15, 275-284.	5.7	280
16	PDBsum additions. Nucleic Acids Research, 2014, 42, D292-D296.	14.5	279
17	Derivation of 3D coordinate templates for searching structural databases: Application to serâ€Hisâ€Asp catalytic triads in the serine proteinases and lipases. Protein Science, 1996, 5, 1001-1013.	7.6	229
18	Protein folds and functions. Structure, 1998, 6, 875-884.	3.3	207

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19	The implications of alternative splicing in the ENCODE protein complement. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 5495-5500.	7.1	206
20	NUCPLOT: a program to generate schematic diagrams of protein-nucleic acid interactions. Nucleic Acids Research, 1997, 25, 4940-4945.	14.5	203
21	Protein Function Prediction Using Local 3D Templates. Journal of Molecular Biology, 2005, 351, 614-626.	4.2	195
22	BLEEP?potential of mean force describing protein-ligand interactions: I. Generating potential. Journal of Computational Chemistry, 1999, 20, 1165-1176.	3.3	194
23	Shape Variation in Protein Binding Pockets and their Ligands. Journal of Molecular Biology, 2007, 368, 283-301.	4.2	188
24	The structural basis of allosteric regulation in proteins. FEBS Letters, 2009, 583, 1692-1698.	2.8	187
25	A method for localizing ligand binding pockets in protein structures. Proteins: Structure, Function and Bioinformatics, 2005, 62, 479-488.	2.6	181
26	Validation of protein models derived from experiment. Current Opinion in Structural Biology, 1998, 8, 631-639.	5.7	172
27	Visualization of macromolecular structures. Nature Methods, 2010, 7, S42-S55.	19.0	137
28	Integrating Structure, Bioinformatics, and Enzymology to Discover Function. Journal of Biological Chemistry, 2003, 278, 26039-26045.	3.4	115
29	Who checks the checkers? four validation tools applied to eight atomic resolution structures 1 1Edited by I. A. Wilson. Journal of Molecular Biology, 1998, 276, 417-436.	4.2	114
30	AlphaFold heralds a data-driven revolution in biology and medicine. Nature Medicine, 2021, 27, 1666-1669.	30.7	108
31	Knowledge-based validation of protein structure coordinates derived by X-ray crystallography and NMR spectroscopy. Current Opinion in Structural Biology, 1994, 4, 731-737.	5.7	100
32	Molecular basis of inherited diseases: a structural perspective. Trends in Genetics, 2003, 19, 505-513.	6.7	92
33	X-SITE: Use of Empirically Derived Atomic Packing Preferences to Identify Favourable Interaction Regions in the Binding Sites of Proteins. Journal of Molecular Biology, 1996, 259, 175-201.	4.2	89
34	Representative Amino Acid Side Chain Interactions in Proteins. A Comparison of Highly Accurate Correlatedab InitioQuantum Chemical and Empirical Potential Procedures. Journal of Chemical Theory and Computation, 2009, 5, 982-992.	5.3	89
35	Anatomy of enzyme channels. BMC Bioinformatics, 2014, 15, 379.	2.6	89
36	Exploring the Evolution of Novel Enzyme Functions within Structurally Defined Protein Superfamilies. PLoS Computational Biology, 2012, 8, e1002403.	3.2	80

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37	Towards Fully Automated Structure-based Function Prediction in Structural Genomics: A Case Study. Journal of Molecular Biology, 2007, 367, 1511-1522.	4.2	79
38	Error Estimates of Protein Structure Coordinates and Deviations from Standard Geometry by Full-Matrix Refinement ofÎ³B- andÎ²B2-Crystallin. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 243-252.	2.5	78
39	VarSite: Disease variants and protein structure. Protein Science, 2020, 29, 111-119.	7.6	77
40	Chopping and Changing: the Evolution of the Flavin-dependent Monooxygenases. Journal of Molecular Biology, 2016, 428, 3131-3146.	4.2	75
41	From protein structure to biochemical function?. Journal of Structural and Functional Genomics, 2003, 4, 167-177.	1.2	72
42	Understanding the molecular machinery of genetics through 3D structures. Nature Reviews Genetics, 2008, 9, 141-151.	16.3	69
43	Crystal Structure of Enterococcus faecalis SlyA-like Transcriptional Factor. Journal of Biological Chemistry, 2003, 278, 20240-20244.	3.4	65
44	Enhancing the functional annotation of PDB structures in PDBsum using key figures extracted from the literature. Bioinformatics, 2007, 23, 1824-1827.	4.1	64
45	Crystal Structure of Thermotoga maritima 0065, a Member of the IclR Transcriptional Factor Family. Journal of Biological Chemistry, 2002, 277, 19183-19190.	3.4	63
46	On the diversity of physicochemical environments experienced by identical ligands in binding pockets of unrelated proteins. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1120-1136.	2.6	59
47	Dihydrofolate reductase: a potential drug target in trypanosomes and leishmania. Journal of Computer-Aided Molecular Design, 1998, 12, 241-257.	2.9	55
48	Amino Acid Changes in Disease-Associated Variants Differ Radically from Variants Observed in the 1000 Genomes Project Dataset. PLoS Computational Biology, 2013, 9, e1003382.	3.2	54
49	Rising levels of atmospheric oxygen and evolution of Nrf2. Scientific Reports, 2016, 6, 27740.	3.3	52
50	VarMap: a web tool for mapping genomic coordinates to protein sequence and structure and retrieving protein structural annotations. Bioinformatics, 2019, 35, 4854-4856.	4.1	46
51	FunTree: a resource for exploring the functional evolution of structurally defined enzyme superfamilies. Nucleic Acids Research, 2012, 40, D776-D782.	14.5	44
52	BetaCavityWeb: a webserver for molecular voids and channels. Nucleic Acids Research, 2015, 43, W413-W418.	14.5	43
53	Rfreeand theRfreeRatio. I. Derivation of Expected Values of Cross-Validation Residuals Used in Macromolecular Least-Squares Refinement. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 547-557.	2.5	42
54	<scp>PDBsum</scp> extras: <scp>SARSâ€CoV</scp>â€2 and <scp>AlphaFold</scp> models. Protein Science, 2022, 31, 283-289.	7.6	42

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55	Rfreeand theRfreeratio. II. Calculation of the expected values and variances of cross-validation statistics in macromolecular least-squares refinement. Acta Crystallographica Section D: Biological Crystallography, 2000, 56, 442-450.	2.5	41
56	Non-randomness in side-chain packing: the distribution of interplanar angles. , 1997, 29, 370-380.		37
57	Energy Matrix of Structurally Important Side-Chain/Side-Chain Interactions in Proteins. Journal of Chemical Theory and Computation, 2010, 6, 2191-2203.	5.3	33
58	Chemical Fragments that Hydrogen Bond to Asp, Glu, Arg, and His Side Chains in Protein Binding Sites. Journal of Medicinal Chemistry, 2010, 53, 3086-3094.	6.4	33
59	Structural analysis of pathogenic mutations in theDYRK1Agene in patients with developmental disorders. Human Molecular Genetics, 2017, 26, ddw409.	2.9	33
60	Structural Annotation of Mycobacterium tuberculosis Proteome. PLoS ONE, 2011, 6, e27044.	2.5	33
61	BetaSCPWeb: side-chain prediction for protein structures using Voronoi diagrams and geometry prioritization. Nucleic Acids Research, 2016, 44, W416-W423.	14.5	31
62	Protein structure and phenotypic analysis of pathogenic and population missense variants inSTXBP1. Molecular Genetics & Genomic Medicine, 2017, 5, 495-507.	1.2	29
63	Integrating population variation and protein structural analysis to improve clinical interpretation of missense variation: application to the WD40 domain. Human Molecular Genetics, 2016, 25, 927-935.	2.9	26
64	Streptococcus pneumoniaYlxR at 1.35â€…Ã… shows a putative new fold. Acta Crystallographica Section D: Biological Crystallography, 2001, 57, 1747-1751.	2.5	23
65	Structural Quality Assurance. Methods of Biochemical Analysis, 2005, , 273-303.	0.2	23
66	Target Selection and Determination of Function in Structural Genomics. IUBMB Life, 2003, 55, 249-255.	3.4	22
67	Exome sequencing identifies a missense mutation in Isl1 associated with low penetrance otitis media in dearisch mice. Genome Biology, 2011, 12, R90.	9.6	22
68	Representative Amino Acid Side-Chain Interactions in Proteinâ€“DNA Complexes: A Comparison of Highly Accurate Correlated Ab Initio Quantum Mechanical Calculations and Efficient Approaches for Applications to Large Systems. Journal of Chemical Theory and Computation, 2015, 11, 4086-4092.	5.3	22
69	The ProFunc Function Prediction Server. Methods in Molecular Biology, 2017, 1611, 75-95.	0.9	22
70	ArchSchema: a tool for interactive graphing of related Pfam domain architectures. Bioinformatics, 2010, 26, 1260-1261.	4.1	21
71	Structural quality assurance. Methods of Biochemical Analysis, 2003, 44, 273-303.	0.2	21
72	New Tools and Resources for Analysing Protein Structures and Their Interactions. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 1132-1138.	2.5	19

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73	SPINE bioinformatics and data-management aspects of high-throughput structural biology. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 1184-1195.	2.5	19
74	THE RAMACHANDRAN PLOT AND PROTEIN STRUCTURE VALIDATION. , 2013, , 62-75.		19
75	WSsas: a web service for the annotation of functional residues through structural homologues. Bioinformatics, 2009, 25, 1192-1194.	4.1	17
76	Structure of SAICAR synthase fromThermotoga maritimaat 2.2â€…Ã… reveals an unusual covalent dimer. Acta Crystallographica Section F: Structural Biology Communications, 2006, 62, 335-339.	0.7	16
77	BetaVoid: Molecular voids via beta-complexes and Voronoi diagrams. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1829-1849.	2.6	16
78	X-ray crystal structure of CutA from Thermotoga maritima at 1.4 Ã… resolution. Proteins: Structure, Function and Bioinformatics, 2003, 54, 162-165.	2.6	14
79	1,000 structures and more from the MCSG. BMC Structural Biology, 2011, 11, 2.	2.3	14
80	Large-Scale Quantitative Assessment of Binding Preferences in Proteinâ€“Nucleic Acid Complexes. Journal of Chemical Theory and Computation, 2015, 11, 1939-1948.	5.3	12
81	Sequence-Specific Recognition of DNA by Proteins: Binding Motifs Discovered Using a Novel Statistical/Computational Analysis. PLoS ONE, 2016, 11, e0158704.	2.5	10
82	An automated protocol for modelling peptide substrates to proteases. BMC Bioinformatics, 2020, 21, 586.	2.6	7
83	Use of parallel processing in the study of protein. Ligand binding. Journal of Computational Chemistry, 1990, 11, 314-325.	3.3	6
84	Protein Structure Databases. Molecular Biotechnology, 2011, 48, 183-198.	2.4	6
85	Abstracting knowledge from the protein data bank. Biopolymers, 2013, 99, 183-188.	2.4	6
86	Conserved protein YecM fromEscherichia coli shows structural homology to metal-binding isomerases and oxygenases. Proteins: Structure, Function and Bioinformatics, 2003, 51, 311-314.	2.6	4
87	Variation of geometrical and physicochemical properties in protein binding pockets and their ligands. BMC Bioinformatics, 2007, 8, .	2.6	4
88	A computational and structural analysis of germline and somatic variants affecting the DDR mechanism, and their impact on human diseases. Scientific Reports, 2021, 11, 14268.	3.3	4
89	Conformational analysis of pentapeptide sequences matching a proposed recognition motif for lysosomal degradation. BBA - Proteins and Proteomics, 1996, 1293, 243-253.	2.1	3
90	The fine details of evolution. Biochemical Society Transactions, 2009, 37, 723-726.	3.4	3

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91	Protein Structure Databases. Methods in Molecular Biology, 2016, 1415, 31-53.	0.9	3
92	Impact of Structural Observables From Simulations to Predict the Effect of Single-Point Mutations in MHC Class II Peptide Binders. Frontiers in Molecular Biosciences, 2021, 8, 636562.	3.5	3
93	LigSearch: a knowledge-based web server to identify likely ligands for a protein target. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 2395-2402.	2.5	2
94	MGOS: A library for molecular geometry and its operating system. Computer Physics Communications, 2020, 251, 107101.	7.5	2
95	Proteins: interaction at a distance. IUCrJ, 2015, 2, 609-610.	2.2	2
96	Estimation of weights and validation: a marginal likelihood approach. Acta Crystallographica Section D: Biological Crystallography, 2003, 59, 1557-1566.	2.5	1
97	Protein Structure Databases. Methods in Molecular Biology, 2010, 609, 59-82.	0.9	1
98	Determining Function from Structure. , 2005, , 163-184.		0
99	Structural bioinformatics: from protein structure to function. NATO Science Series Series II, Mathematics, Physics and Chemistry, 2007, , 165-179.	0.1	0
100	Integrated Servers for Structure-Informed Function Prediction. , 2017, , 427-448.		0
101	Bioinformatics and Protein Design. Current Pharmaceutical Biotechnology, 2002, 3, 317-327.	1.6	0
102	Integrated Servers for Structure-Informed Function Prediction. , 2009, , 251-272.		0