

Frank DiMaio

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

133 papers	9,474 citations	50 h-index	96 g-index
157 ext. papers	13,663 ext. citations	16.1 avg, IF	6.31 L-index

#	Paper	IF	Citations
133	High-resolution comparative modeling with RosettaCM. <i>Structure</i> , 2013 , 21, 1735-42	5.2	649
132	EMRinger: side chain-directed model and map validation for 3D cryo-electron microscopy. <i>Nature Methods</i> , 2015 , 12, 943-6	21.6	523
131	Accurate prediction of protein structures and interactions using a three-track neural network. <i>Science</i> , 2021 , 373, 871-876	33.3	522
130	Cryo-electron microscopy structure of a coronavirus spike glycoprotein trimer. <i>Nature</i> , 2016 , 531, 114-117	50.4	354
129	Crystal structure of a monomeric retroviral protease solved by protein folding game players. <i>Nature Structural and Molecular Biology</i> , 2011 , 18, 1175-7	17.6	316
128	Glycan shield and epitope masking of a coronavirus spike protein observed by cryo-electron microscopy. <i>Nature Structural and Molecular Biology</i> , 2016 , 23, 899-905	17.6	252
127	Atomic-accuracy models from 4.5-Å cryo-electron microscopy data with density-guided iterative local refinement. <i>Nature Methods</i> , 2015 , 12, 361-365	21.6	245
126	Refinement of protein structures into low-resolution density maps using rosetta. <i>Journal of Molecular Biology</i> , 2009 , 392, 181-90	6.5	230
125	Automated structure refinement of macromolecular assemblies from cryo-EM maps using Rosetta. <i>ELife</i> , 2016 , 5,	8.9	227
124	Alternate states of proteins revealed by detailed energy landscape mapping. <i>Journal of Molecular Biology</i> , 2011 , 405, 607-18	6.5	207
123	Simultaneous Optimization of Biomolecular Energy Functions on Features from Small Molecules and Macromolecules. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 6201-6212	6.4	199
122	High thermodynamic stability of parametrically designed helical bundles. <i>Science</i> , 2014 , 346, 481-485	33.3	196
121	Improved molecular replacement by density- and energy-guided protein structure optimization. <i>Nature</i> , 2011 , 473, 540-3	50.4	196
120	De novo design of protein homo-oligomers with modular hydrogen-bond network-mediated specificity. <i>Science</i> , 2016 , 352, 680-7	33.3	194
119	Relaxation of backbone bond geometry improves protein energy landscape modeling. <i>Protein Science</i> , 2014 , 23, 47-55	6.3	192
118	Near-atomic model of microtubule-tau interactions. <i>Science</i> , 2018 , 360, 1242-1246	33.3	175
117	Design of ordered two-dimensional arrays mediated by noncovalent protein-protein interfaces. <i>Science</i> , 2015 , 348, 1365-8	33.3	173

116	Structure of the type VI secretion system contractile sheath. <i>Cell</i> , 2015 , 160, 952-962	56.2	172
115	Macromolecular modeling and design in Rosetta: recent methods and frameworks. <i>Nature Methods</i> , 2020 , 17, 665-680	21.6	165
114	Combined covalent-electrostatic model of hydrogen bonding improves structure prediction with Rosetta. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 609-22	6.4	163
113	Structural basis for scaffolding-mediated assembly and maturation of a dsDNA virus. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011 , 108, 1355-60	11.5	162
112	Structures of MERS-CoV spike glycoprotein in complex with sialoside attachment receptors. <i>Nature Structural and Molecular Biology</i> , 2019 , 26, 1151-1157	17.6	161
111	Modeling symmetric macromolecular structures in Rosetta3. <i>PLoS ONE</i> , 2011 , 6, e20450	3.7	142
110	Improved low-resolution crystallographic refinement with Phenix and Rosetta. <i>Nature Methods</i> , 2013 , 10, 1102-4	21.6	137
109	De novo protein structure determination from near-atomic-resolution cryo-EM maps. <i>Nature Methods</i> , 2015 , 12, 335-8	21.6	131
108	Protocols for Molecular Modeling with Rosetta3 and RosettaScripts. <i>Biochemistry</i> , 2016 , 55, 4748-63	3.2	118
107	Cryo-EM structure of the protein-conducting ERAD channel Hrd1 in complex with Hrd3. <i>Nature</i> , 2017 , 548, 352-355	50.4	117
106	phenix.mr_rosetta: molecular replacement and model rebuilding with Phenix and Rosetta. <i>Journal of Structural and Functional Genomics</i> , 2012 , 13, 81-90		109
105	Crystal structure of Toll-like receptor adaptor MAL/TIRAP reveals the molecular basis for signal transduction and disease protection. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011 , 108, 14879-84	11.5	105
104	Cryo-electron microscopy structure of the lipid droplet-formation protein seipin. <i>Journal of Cell Biology</i> , 2018 , 217, 4080-4091	7.3	97
103	Structural basis for the initiation of eukaryotic transcription-coupled DNA repair. <i>Nature</i> , 2017 , 551, 653-657	50.4	94
102	Accurate computational design of multipass transmembrane proteins. <i>Science</i> , 2018 , 359, 1042-1046	33.3	93
101	Cryo-EM Structure of Caspase-8 Tandem DED Filament Reveals Assembly and Regulation Mechanisms of the Death-Inducing Signaling Complex. <i>Molecular Cell</i> , 2016 , 64, 236-250	17.6	89
100	Programmable design of orthogonal protein heterodimers. <i>Nature</i> , 2019 , 565, 106-111	50.4	87
99	RosettaES: a sampling strategy enabling automated interpretation of difficult cryo-EM maps. <i>Nature Methods</i> , 2017 , 14, 797-800	21.6	84

98	Structural basis of TIR-domain-assembly formation in MAL- and MyD88-dependent TLR4 signaling. <i>Nature Structural and Molecular Biology</i> , 2017 , 24, 743-751	17.6	82
97	Improved de novo structure prediction in CASP11 by incorporating coevolution information into Rosetta. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016 , 84 Suppl 1, 67-75	4.2	82
96	Anti-diabetic drug binding site in a mammalian K channel revealed by Cryo-EM. <i>ELife</i> , 2017 , 6,	8.9	81
95	Virology. A virus that infects a hyperthermophile encapsidates A-form DNA. <i>Science</i> , 2015 , 348, 914-7	33.3	79
94	Advances, interactions, and future developments in the CNS, Phenix, and Rosetta structural biology software systems. <i>Annual Review of Biophysics</i> , 2013 , 42, 265-87	21.1	76
93	One contact for every twelve residues allows robust and accurate topology-level protein structure modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014 , 82 Suppl 2, 208-18	4.2	70
92	Cryo-EM model validation using independent map reconstructions. <i>Protein Science</i> , 2013 , 22, 865-8	6.3	64
91	De novo protein design by citizen scientists. <i>Nature</i> , 2019 , 570, 390-394	50.4	63
90	Protein structure prediction using Rosetta in CASP12. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018 , 86 Suppl 1, 113-121	4.2	63
89	A refined model of the prototypical Salmonella SPI-1 T3SS basal body reveals the molecular basis for its assembly. <i>PLoS Pathogens</i> , 2013 , 9, e1003307	7.6	63
88	The dynamic disulphide relay of quiescin sulphydryl oxidase. <i>Nature</i> , 2012 , 488, 414-8	50.4	62
87	Automatically Fixing Errors in Glycoprotein Structures with Rosetta. <i>Structure</i> , 2019 , 27, 134-139.e3	5.2	59
86	Structure of EspB from the ESX-1 type VII secretion system and insights into its export mechanism. <i>Structure</i> , 2015 , 23, 571-583	5.2	57
85	Computational design of transmembrane pores. <i>Nature</i> , 2020 , 585, 129-134	50.4	56
84	Determination of the structures of symmetric protein oligomers from NMR chemical shifts and residual dipolar couplings. <i>Journal of the American Chemical Society</i> , 2011 , 133, 6288-98	16.4	55
83	Structural basis for substrate gripping and translocation by the ClpB AAA+ disaggregase. <i>Nature Communications</i> , 2019 , 10, 2393	17.4	50
82	Unique double-ring structure of the peroxisomal Pex1/Pex6 ATPase complex revealed by cryo-electron microscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, E4017-25	11.5	50
81	Structure of the C-terminal region of an ERG channel and functional implications. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 11648-53	11.5	50

80	Protein homology model refinement by large-scale energy optimization. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 3054-3059	11.5	49
79	The molecular basis for flexibility in the flexible filamentous plant viruses. <i>Nature Structural and Molecular Biology</i> , 2015 , 22, 642-4	17.6	45
78	Cryo-EM structure of a group II chaperonin in the prehydrolysis ATP-bound state leading to lid closure. <i>Structure</i> , 2011 , 19, 633-9	5.2	45
77	Structure of a Chaperone-Usher Pilus Reveals the Molecular Basis of Rod Uncoiling. <i>Cell</i> , 2016 , 164, 269-278	37.8	41
76	Structure and stoichiometry of an accessory subunit TRIP8b interaction with hyperpolarization-activated cyclic nucleotide-gated channels. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 7899-904	11.5	40
75	CryoEM structure of a prokaryotic cyclic nucleotide-gated ion channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 4430-4435	11.5	35
74	Designing Two-Dimensional Protein Arrays through Fusion of Multimers and Interface Mutations. <i>Nano Letters</i> , 2015 , 15, 5235-9	11.5	35
73	The Molecular Architecture of Native BBSome Obtained by an Integrated Structural Approach. <i>Structure</i> , 2019 , 27, 1384-1394.e4	5.2	33
72	De novo protein design by deep network hallucination. <i>Nature</i> , 2021 ,	50.4	33
71	Phase separation of Polo-like kinase 4 by autoactivation and clustering drives centriole biogenesis. <i>Nature Communications</i> , 2019 , 10, 4959	17.4	32
70	Model for a novel membrane envelope in a filamentous hyperthermophilic virus. <i>ELife</i> , 2017 , 6,	8.9	32
69	A Structural Model of the Endogenous Human BAF Complex Informs Disease Mechanisms. <i>Cell</i> , 2020 , 183, 802-817.e24	56.2	31
68	Multiple liquid crystalline geometries of highly compacted nucleic acid in a dsRNA virus. <i>Nature</i> , 2019 , 570, 252-256	50.4	30
67	Automatic structure prediction of oligomeric assemblies using Robetta in CASP12. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018 , 86 Suppl 1, 283-291	4.2	29
66	Crucial steps in the structure determination of a coronavirus spike glycoprotein using cryo-electron microscopy. <i>Protein Science</i> , 2017 , 26, 113-121	6.3	28
65	An enumerative algorithm for de novo design of proteins with diverse pocket structures. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 22135-22145	11.5	28
64	Crystal structure of the transport unit of the autotransporter adhesin involved in diffuse adherence from Escherichia coli. <i>Journal of Structural Biology</i> , 2014 , 187, 20-29	3.4	26
63	Crystal structure of XMRV protease differs from the structures of other retropepsins. <i>Nature Structural and Molecular Biology</i> , 2011 , 18, 227-9	17.6	26

62	Self-Assembling 2D Arrays with de Novo Protein Building Blocks. <i>Journal of the American Chemical Society</i> , 2019 , 141, 8891-8895	16.4	24
61	Structural Insights into Mdn1, an Essential AAA Protein Required for Ribosome Biogenesis. <i>Cell</i> , 2018 , 175, 822-834.e18	56.2	24
60	Tools for Model Building and Optimization into Near-Atomic Resolution Electron Cryo-Microscopy Density Maps. <i>Methods in Enzymology</i> , 2016 , 579, 255-76	1.7	23
59	The HCN channel voltage sensor undergoes a large downward motion during hyperpolarization. <i>Nature Structural and Molecular Biology</i> , 2019 , 26, 686-694	17.6	22
58	Perturbing the energy landscape for improved packing during computational protein design. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021 , 89, 436-449	4.2	22
57	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. <i>Nature Methods</i> , 2021 , 18, 156-164	21.6	22
56	An extensively glycosylated archaeal pilus survives extreme conditions. <i>Nature Microbiology</i> , 2019 , 4, 1401-1410	26.6	21
55	BRCA1/BARD1 site-specific ubiquitylation of nucleosomal H2A is directed by BARD1. <i>Nature Structural and Molecular Biology</i> , 2021 , 28, 268-277	17.6	21
54	The Therapeutic Antibody LM609 Selectively Inhibits Ligand Binding to Human α Integrin via Steric Hindrance. <i>Structure</i> , 2017 , 25, 1732-1739.e5	5.2	20
53	Analyses of subnanometer resolution cryo-EM density maps. <i>Methods in Enzymology</i> , 2010 , 483, 1-29	1.7	20
52	Structure of the type VI secretion system TssK-TssF-TssG baseplate subcomplex revealed by cryo-electron microscopy. <i>Nature Communications</i> , 2018 , 9, 5385	17.4	20
51	Germline VRC01 antibody recognition of a modified clade C HIV-1 envelope trimer and a glycosylated HIV-1 gp120 core. <i>ELife</i> , 2018 , 7,	8.9	19
50	Efficient consideration of coordinated water molecules improves computational protein-protein and protein-ligand docking discrimination. <i>PLoS Computational Biology</i> , 2020 , 16, e1008103	5	19
49	Advances in Rosetta structure prediction for difficult molecular-replacement problems. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2202-8		18
48	CASP11 refinement experiments with ROSETTA. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016 , 84 Suppl 1, 314-22	4.2	18
47	Allosteric conformational change of a cyclic nucleotide-gated ion channel revealed by DEER spectroscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 10839-10847	11.5	15
46	COMBINES-CID: An Efficient Method for De Novo Engineering of Highly Specific Chemically Induced Protein Dimerization Systems. <i>Journal of the American Chemical Society</i> , 2019 , 141, 10948-10952	16.4	15
45	High-resolution structure of a retroviral protease folded as a monomer. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 907-14		15

44	Modeling oblong proteins and water-mediated interfaces with RosettaDock in CAPRI rounds 28-35. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017 , 85, 479-486	4.2	14
43	The origin of consistent protein structure refinement from structural averaging. <i>Structure</i> , 2015 , 23, 1123-8	5.2	14
42	Polymerization in the actin ATPase clan regulates hexokinase activity in yeast. <i>Science</i> , 2020 , 367, 1039-1042	10.4	13
41	Crystal structure analysis of EstA from <i>Arthrobacter</i> sp. Rue61a--an insight into catalytic promiscuity. <i>FEBS Letters</i> , 2014 , 588, 1154-60	3.8	13
40	3.1 Å structure of yeast RNA polymerase II elongation complex stalled at a cyclobutane pyrimidine dimer lesion solved using streptavidin affinity grids. <i>Journal of Structural Biology</i> , 2019 , 207, 270-278	3.4	12
39	cryoem-cloud-tools: A software platform to deploy and manage cryo-EM jobs in the cloud. <i>Journal of Structural Biology</i> , 2018 , 203, 230-235	3.4	12
38	Force Field Optimization Guided by Small Molecule Crystal Lattice Data Enables Consistent Sub-Angstrom Protein-Ligand Docking. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 2000-2010	6.4	12
37	Prediction of Protein Mutational Free Energy: Benchmark and Sampling Improvements Increase Classification Accuracy. <i>Frontiers in Bioengineering and Biotechnology</i> , 2020 , 8, 558247	5.8	11
36	The cryo-EM structure of the bacterial flagellum cap complex suggests a molecular mechanism for filament elongation. <i>Nature Communications</i> , 2020 , 11, 3210	17.4	9
35	Computational design of mixed chirality peptide macrocycles with internal symmetry. <i>Protein Science</i> , 2020 , 29, 2433-2445	6.3	9
34	Structural basis for autophagy inhibition by the human Rubicon-Rab7 complex. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 17003-17010	11.5	9
33	Cryo-electron Microscopy Imaging of Alzheimer's Amyloid-beta 42 Oligomer Displayed on a Functionally and Structurally Relevant Scaffold. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 18680-18687	16.4	9
32	Computational design of a synthetic PD-1 agonist. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021 , 118,	11.5	9
31	Discovery and Characterization of Spike N-Terminal Domain-Binding Aptamers for Rapid SARS-CoV-2 Detection. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 21211-21215	16.4	9
30	Structural and functional insight into regulation of kinesin-1 by microtubule-associated protein MAP7.. <i>Science</i> , 2022 , 375, 326-331	33.3	8
29	Rosetta Structure Prediction as a Tool for Solving Difficult Molecular Replacement Problems. <i>Methods in Molecular Biology</i> , 2017 , 1607, 455-466	1.4	6
28	Deep learning enables the atomic structure determination of the Fanconi Anemia core complex from cryoEM. <i>IUCrJ</i> , 2020 , 7, 881-892	4.7	5
27	Cryo-EM structures of CTP synthase filaments reveal mechanism of pH-sensitive assembly during budding yeast starvation. <i>ELife</i> , 2021 , 10,	8.9	5

26	Author response: Automated structure refinement of macromolecular assemblies from cryo-EM maps using Rosetta 2016 ,		5
25	Phospho-regulation, nucleotide binding and ion access control in potassium-chloride cotransporters. <i>EMBO Journal</i> , 2021 , 40, e107294	13	5
24	Improving hybrid statistical and physical forcefields through local structure enumeration. <i>Protein Science</i> , 2016 , 25, 1525-34	6.3	5
23	Cryo-EM structure of the bacterial actin Alfa reveals unique assembly and ATP-binding interactions and the absence of a conserved subdomain. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 3356-3361	11.5	4
22	Spherical-harmonic decomposition for molecular recognition in electron-density maps. <i>International Journal of Data Mining and Bioinformatics</i> , 2009 , 3, 205-27	0.5	4
21	Electromechanical coupling mechanism for activation and inactivation of an HCN channel. <i>Nature Communications</i> , 2021 , 12, 2802	17.4	4
20	Structure and lipid dynamics in the maintenance of lipid asymmetry inner membrane complex of A. baumannii. <i>Communications Biology</i> , 2021 , 4, 817	6.7	4
19	Structural Studies of Coronavirus Fusion Proteins. <i>Microscopy and Microanalysis</i> , 2019 , 25, 1300-1301	0.5	3
18	Atomic model of microtubule-bound tau		3
17	Structure of the phosphoinositide 3-kinase (PI3K) p110 β p101 complex reveals molecular mechanism of GPCR activation. <i>Science Advances</i> , 2021 , 7,	14.3	3
16	Treponema pallidum genome sequencing from six continents reveals variability in vaccine candidate genes and dominance of Nichols clade strains in Madagascar.. <i>PLoS Neglected Tropical Diseases</i> , 2021 , 15, e0010063	4.8	2
15	Crystal Structure and Mechanistic Molecular Modeling Studies of Diterpene Cyclase Rv3377c. <i>Biochemistry</i> , 2020 , 59, 4507-4515	3.2	2
14	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks		2
13	Growing Glycans in Rosetta: Accurate de novo glycan modeling, density fitting, and rational sequon design		2
12	Seipin forms a flexible cage at lipid droplet formation sites.. <i>Nature Structural and Molecular Biology</i> , 2022 ,	17.6	2
11	Architecture and antigenicity of the Nipah virus attachment glycoprotein.. <i>Science</i> , 2022 , eabm5561	33.3	2
10	Independent evolution of polymerization in the Actin ATPase clan regulates hexokinase activity		1
9	Prediction of protein mutational free energy: benchmark and sampling improvements increase classification accuracy		1

8	Deep learning enables the atomic structure determination of the Fanconi Anemia core complex from cryoEM		1
7	Cryo-electron Microscopy Imaging of Alzheimer's Amyloid-beta 42 Oligomer Displayed on a Functionally and Structurally Relevant Scaffold. <i>Angewandte Chemie</i> , 2021 , 133, 18828-18835	3.6	1
6	Discovery and Characterization of Spike N-Terminal Domain-Binding Aptamers for Rapid SARS-CoV-2 Detection. <i>Angewandte Chemie</i> , 2021 , 133, 21381-21385	3.6	1
5	Cryo-EM Structures of CTP Synthase Filaments Reveal Mechanism of pH-Sensitive Assembly During Budding Yeast Starvation		1
4	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. <i>Nature Communications</i> , 2021 , 12, 6947	17.4	0
3	Large-scale design and refinement of stable proteins using sequence-only models.. <i>PLoS ONE</i> , 2022 , 17, e0265020	3.7	0
2	Processing Structurally Heterogeneous Cryo-EM Data Using Atomic Models. <i>Microscopy and Microanalysis</i> , 2019 , 25, 228-229	0.5	
1	Protein Structure Modeling with Rosetta: Case Studies in Structure Prediction and Enzyme Repurposing. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2013 , 353-362	0.1	