Frank DiMaio

List of Publications by Year
in descending order

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132 papers	16,917 citations	26630 56 h-index	20358 116 g-index
157 all docs	157 docs citations	157 times ranked	19804 citing authors

#	Article	IF	Citations
1	Accurate prediction of protein structures and interactions using a three-track neural network. Science, 2021, 373, 871-876.	12.6	2,843
2	High-Resolution Comparative Modeling with RosettaCM. Structure, 2013, 21, 1735-1742.	3.3	1,010
3	EMRinger: side chainâ€“directed model and map validation for 3D cryo-electron microscopy. Nature Methods, 2015, 12, 943-946.	19.0	799
4	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	19.0	513
5	Crystal structure of a monomeric retroviral protease solved by protein folding game players. Nature Structural and Molecular Biology, 2011, 18, 1175-1177.	8.2	463
6	Cryo-electron microscopy structure of a coronavirus spike glycoprotein trimer. Nature, 2016, 531, 114-117.	27.8	453
7	Automated structure refinement of macromolecular assemblies from cryo-EM maps using Rosetta. ELife, 2016, 5, .	6.0	407
8	Simultaneous Optimization of Biomolecular Energy Functions on Features from Small Molecules and Macromolecules. Journal of Chemical Theory and Computation, 2016, 12, 6201-6212.	5.3	382
9	Glycan shield and epitope masking of a coronavirus spike protein observed by cryo-electron microscopy. Nature Structural and Molecular Biology, 2016, 23, 899-905.	8.2	366
10	Alternate States of Proteins Revealed by Detailed Energy Landscape Mapping. Journal of Molecular Biology, 2011, 405, 607-618.	4.2	324
11	Relaxation of backbone bond geometry improves protein energy landscape modeling. Protein Science, 2014, 23, 47-55.	7.6	323
12	Atomic-accuracy models from 4.5-Ã... cryo-electron microscopy data with density-guided iterative local refinement. Nature Methods, 2015, 12, 361-365.	19.0	313
13	Near-atomic model of microtubule-tau interactions. Science, 2018, 360, 1242-1246.	12.6	285
14	De novo protein design by deep network hallucination. Nature, 2021, 600, 547-552.	27.8	280
15	Refinement of Protein Structures into Low-Resolution Density Maps Using Rosetta. Journal of Molecular Biology, 2009, 392, 181-190.	4.2	272
16	High thermodynamic stability of parametrically designed helical bundles. Science, 2014, 346, 481-485.	12.6	264
17	De novo design of protein homo-oligomers with modular hydrogen-bond networkâ€“mediated specificity. Science, 2016, 352, 680-687.	12.6	262
18	Improved molecular replacement by density- and energy-guided protein structure optimization. Nature, 2011, 473, 540-543.	27.8	226

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19	Design of ordered two-dimensional arrays mediated by noncovalent protein-protein interfaces. Science, 2015, 348, 1365-1368.	12.6	219
20	Structures of MERS-CoV spike glycoprotein in complex with sialoside attachment receptors. Nature Structural and Molecular Biology, 2019, 26, 1151-1157.	8.2	218
21	Structure of the Type VI Secretion System Contractile Sheath. Cell, 2015, 160, 952-962.	28.9	216
22	Combined Covalent-Electrostatic Model of Hydrogen Bonding Improves Structure Prediction with Rosetta. Journal of Chemical Theory and Computation, 2015, 11, 609-622.	5.3	204
23	Modeling Symmetric Macromolecular Structures in Rosetta3. PLoS ONE, 2011, 6, e20450.	2.5	197
24	Structural basis for scaffolding-mediated assembly and maturation of a dsDNA virus. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 1355-1360.	7.1	191
25	Protocols for Molecular Modeling with Rosetta3 and RosettaScripts. Biochemistry, 2016, 55, 4748-4763.	2.5	182
26	Improved low-resolution crystallographic refinement with Phenix and Rosetta. Nature Methods, 2013, 10, 1102-1104.	19.0	175
27	De novo protein structure determination from near-atomic-resolution cryo-EM maps. Nature Methods, 2015, 12, 335-338.	19.0	172
28	Cryo-EM structure of the protein-conducting ERAD channel Hrd1 in complex with Hrd3. Nature, 2017, 548, 352-355.	27.8	160
29	Structural basis for the initiation of eukaryotic transcription-coupled DNA repair. Nature, 2017, 551, 653-657.	27.8	151
30	Accurate computational design of multipass transmembrane proteins. Science, 2018, 359, 1042-1046.	12.6	149
31	Cryoâ€“electron microscopy structure of the lipid dropletâ€“formation protein seipin. Journal of Cell Biology, 2018, 217, 4080-4091.	5.2	147
32	Structural basis of TIR-domain-assembly formation in MAL- and MyD88-dependent TLR4 signaling. Nature Structural and Molecular Biology, 2017, 24, 743-751.	8.2	140
33	Programmable design of orthogonal protein heterodimers. Nature, 2019, 565, 106-111.	27.8	139
34	phenix.mr_rosetta: molecular replacement and model rebuilding with Phenix and Rosetta. Journal of Structural and Functional Genomics, 2012, 13, 81-90.	1.2	131
35	Cryo-EM Structure of Caspase-8 Tandem DED Filament Reveals Assembly and Regulation Mechanisms of the Death-Inducing Signaling Complex. Molecular Cell, 2016, 64, 236-250.	9.7	128
36	Crystal structure of Toll-like receptor adaptor MAL/TIRAP reveals the molecular basis for signal transduction and disease protection. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 14879-14884.	7.1	123

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37	Anti-diabetic drug binding site in a mammalian KATP channel revealed by Cryo-EM. ELife, 2017, 6, .	6.0	122
38	Computational design of transmembrane pores. Nature, 2020, 585, 129-134.	27.8	120
39	RosettaES: a sampling strategy enabling automated interpretation of difficult cryo-EM maps. Nature Methods, 2017, 14, 797-800.	19.0	118
40	De novo protein design by citizen scientists. Nature, 2019, 570, 390-394.	27.8	105
41	A Structural Model of the Endogenous Human BAF Complex Informs Disease Mechanisms. Cell, 2020, 183, 802-817.e24.	28.9	100
42	A virus that infects a hyperthermophile encapsidates A-form DNA. Science, 2015, 348, 914-917.	12.6	98
43	Improved de novo structure prediction in <scp>CASP</scp>11 by incorporating coevolution information into Rosetta. Proteins: Structure, Function and Bioinformatics, 2016, 84, 67-75.	2.6	96
44	Automatically Fixing Errors in Glycoprotein Structures with Rosetta. Structure, 2019, 27, 134-139.e3.	3.3	93
45	Advances, Interactions, and Future Developments in the CNS, Phenix, and Rosetta Structural Biology Software Systems. Annual Review of Biophysics, 2013, 42, 265-287.	10.0	88
46	Structural basis for substrate gripping and translocation by the ClpB AAA+ disaggregase. Nature Communications, 2019, 10, 2393.	12.8	88
47	One contact for every twelve residues allows robust and accurate topologyâ€level protein structure modeling. Proteins: Structure, Function and Bioinformatics, 2014, 82, 208-218.	2.6	87
48	Structure of EspB from the ESX-1 Type VII Secretion System and Insights into its Export Mechanism. Structure, 2015, 23, 571-583.	3.3	85
49	Protein structure prediction using Rosetta in CASP12. Proteins: Structure, Function and Bioinformatics, 2018, 86, 113-121.	2.6	85
50	Perturbing the energy landscape for improved packing during computational protein design. Proteins: Structure, Function and Bioinformatics, 2021, 89, 436-449.	2.6	85
51	A Refined Model of the Prototypical Salmonella SPI-1 T3SS Basal Body Reveals the Molecular Basis for Its Assembly. PLoS Pathogens, 2013, 9, e1003307.	4.7	76
52	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. Nature Methods, 2021, 18, 156-164.	19.0	73
53	Cryoâ€EM model validation using independent map reconstructions. Protein Science, 2013, 22, 865-868.	7.6	72
54	The molecular basis for flexibility in the flexible filamentous plant viruses. Nature Structural and Molecular Biology, 2015, 22, 642-644.	8.2	72

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55	Unique double-ring structure of the peroxisomal Pex1/Pex6 ATPase complex revealed by cryo-electron microscopy. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E4017-25.	7.1	72
56	The dynamic disulphide relay of quiescin sulphydryl oxidase. Nature, 2012, 488, 414-418.	27.8	70
57	Determination of the Structures of Symmetric Protein Oligomers from NMR Chemical Shifts and Residual Dipolar Couplings. Journal of the American Chemical Society, 2011, 133, 6288-6298.	13.7	65
58	Protein homology model refinement by large-scale energy optimization. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 3054-3059.	7.1	62
59	An enumerative algorithm for de novo design of proteins with diverse pocket structures. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 22135-22145.	7.1	62
60	Discovery and Characterization of Spike Nâ€Terminal Domainâ€Binding Aptamers for Rapid SARSâ€CoVâ€2 Detection. Angewandte Chemie - International Edition, 2021, 60, 21211-21215.	13.8	62
61	Structure of a Chaperone-Usher Pilus Reveals the Molecular Basis of Rod Uncoiling. Cell, 2016, 164, 269-278.	28.9	61
62	Structure of the C-terminal region of an ERG channel and functional implications. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 11648-11653.	7.1	59
63	Multiple liquid crystalline geometries of highly compacted nucleic acid in a dsRNA virus. Nature, 2019, 570, 252-256.	27.8	59
64	BRCA1/BARD1 site-specific ubiquitylation of nucleosomal H2A is directed by BARD1. Nature Structural and Molecular Biology, 2021, 28, 268-277.	8.2	58
65	Phase separation of Polo-like kinase 4 by autoactivation and clustering drives centriole biogenesis. Nature Communications, 2019, 10, 4959.	12.8	55
66	Prediction of Protein Mutational Free Energy: Benchmark and Sampling Improvements Increase Classification Accuracy. Frontiers in Bioengineering and Biotechnology, 2020, 8, 558247.	4.1	55
67	Structural and functional insight into regulation of kinesin-1 by microtubule-associated protein MAP7. Science, 2022, 375, 326-331.	12.6	53
68	Cryo-EM Structure of a Group II Chaperonin in the Prehydrolysis ATP-Bound State Leading to Lid Closure. Structure, 2011, 19, 633-639.	3.3	52
69	The HCN channel voltage sensor undergoes a large downward motion during hyperpolarization. Nature Structural and Molecular Biology, 2019, 26, 686-694.	8.2	52
70	Force Field Optimization Guided by Small Molecule Crystal Lattice Data Enables Consistent Sub-Angstrom Proteinâ€“Ligand Docking. Journal of Chemical Theory and Computation, 2021, 17, 2000-2010.	5.3	52
71	Structure and stoichiometry of an accessory subunit TRIP8b interaction with hyperpolarization-activated cyclic nucleotide-gated channels. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 7899-7904.	7.1	51
72	CryoEM structure of a prokaryotic cyclic nucleotide-gated ion channel. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 4430-4435.	7.1	51

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73	The Molecular Architecture of Native BBSome Obtained by an Integrated Structural Approach. Structure, 2019, 27, 1384-1394.e4.	3.3	51
74	Automatic structure prediction of oligomeric assemblies using Robetta in CASP12. Proteins: Structure, Function and Bioinformatics, 2018, 86, 283-291.	2.6	49
75	An extensively glycosylated archaeal pilus survives extreme conditions. Nature Microbiology, 2019, 4, 1401-1410.	13.3	46
76	Structural Insights into Mdn1, an Essential AAA Protein Required for Ribosome Biogenesis. Cell, 2018, 175, 822-834.e18.	28.9	42
77	Polymerization in the actin ATPase clan regulates hexokinase activity in yeast. Science, 2020, 367, 1039-1042.	12.6	41
78	Efficient consideration of coordinated water molecules improves computational protein-protein and protein-ligand docking discrimination. PLoS Computational Biology, 2020, 16, e1008103.	3.2	39
79	Cryoâ€electron Microscopy Imaging of Alzheimer's Amyloidâ€beta 42 Oligomer Displayed on a Functionally and Structurally Relevant Scaffold. Angewandte Chemie - International Edition, 2021, 60, 18680-18687.	13.8	39
80	Designing Two-Dimensional Protein Arrays through Fusion of Multimers and Interface Mutations. Nano Letters, 2015, 15, 5235-5239.	9.1	38
81	Allosteric conformational change of a cyclic nucleotide-gated ion channel revealed by DEER spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 10839-10847.	7.1	38
82	Structure of the type VI secretion system TssKâ€“TssFâ€“TssG baseplate subcomplex revealed by cryo-electron microscopy. Nature Communications, 2018, 9, 5385.	12.8	37
83	Self-Assembling 2D Arrays with de Novo Protein Building Blocks. Journal of the American Chemical Society, 2019, 141, 8891-8895.	13.7	37
84	Model for a novel membrane envelope in a filamentous hyperthermophilic virus. ELife, 2017, 6, .	6.0	37
85	COMBINES-CID: An Efficient Method for De Novo Engineering of Highly Specific Chemically Induced Protein Dimerization Systems. Journal of the American Chemical Society, 2019, 141, 10948-10952.	13.7	34
86	Seipin forms a flexible cage at lipid droplet formation sites. Nature Structural and Molecular Biology, 2022, 29, 194-202.	8.2	33
87	Architecture and antigenicity of the Nipah virus attachment glycoprotein. Science, 2022, 375, 1373-1378.	12.6	33
88	Germline VRC01 antibody recognition of a modified clade C HIV-1 envelope trimer and a glycosylated HIV-1 gp120 core. ELife, 2018, 7, .	6.0	32
89	Crucial steps in the structure determination of a coronavirus spike glycoprotein using cryoâ€electron microscopy. Protein Science, 2017, 26, 113-121.	7.6	31
90	Structure and lipid dynamics in the maintenance of lipid asymmetry inner membrane complex of A. baumannii. Communications Biology, 2021, 4, 817.	4.4	31

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91	Crystal structure of the transport unit of the autotransporter adhesin involved in diffuse adherence from Escherichia coli. Journal of Structural Biology, 2014, 187, 20-29.	2.8	30
92	Treponema pallidum genome sequencing from six continents reveals variability in vaccine candidate genes and dominance of Nichols clade strains in Madagascar. PLoS Neglected Tropical Diseases, 2021, 15, e0010063.	3.0	30
93	Tools for Model Building and Optimization into Near-Atomic Resolution Electron Cryo-Microscopy Density Maps. Methods in Enzymology, 2016, 579, 255-276.	1.0	28
94	Computational design of a synthetic PD-1 agonist. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	28
95	Crystal structure of XMRV protease differs from the structures of other retropepsins. Nature Structural and Molecular Biology, 2011, 18, 227-229.	8.2	27
96	3.1â€Ã… structure of yeast RNA polymerase II elongation complex stalled at a cyclobutane pyrimidine dimer lesion solved using streptavidin affinity grids. Journal of Structural Biology, 2019, 207, 270-278.	2.8	27
97	<scp>CASP</scp>11 refinement experiments with <scp>ROSETTA</scp>. Proteins: Structure, Function and Bioinformatics, 2016, 84, 314-322.	2.6	26
98	Structure of the phosphoinositide 3-kinase (PI3K) p110Î³-p101 complex reveals molecular mechanism of GPCR activation. Science Advances, 2021, 7, .	10.3	25
99	Cryo-EM structures of CTP synthase filaments reveal mechanism of pH-sensitive assembly during budding yeast starvation. ELife, 2021, 10, .	6.0	25
100	The Therapeutic Antibody LM609 Selectively Inhibits Ligand Binding to Human Î±VÎ²3 Integrin via Steric Hindrance. Structure, 2017, 25, 1732-1739.e5.	3.3	24
101	Analyses of Subnanometer Resolution Cryo-EM Density Maps. Methods in Enzymology, 2010, 483, 1-29.	1.0	22
102	High-resolution structure of a retroviral protease folded as a monomer. Acta Crystallographica Section D: Biological Crystallography, 2011, 67, 907-914.	2.5	22
103	Advances inRosettastructure prediction for difficult molecular-replacement problems. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 2202-2208.	2.5	20
104	cryoem-cloud-tools: A software platform to deploy and manage cryo-EM jobs in the cloud. Journal of Structural Biology, 2018, 203, 230-235.	2.8	19
105	Phosphoâ€regulation, nucleotide binding and ion access control in potassiumâ€chloride cotransporters. EMBO Journal, 2021, 40, e107294.	7.8	19
106	Modeling oblong proteins and waterâ€mediated interfaces with RosettaDock in CAPRI rounds 28â€“35. Proteins: Structure, Function and Bioinformatics, 2017, 85, 479-486.	2.6	18
107	Structural basis for autophagy inhibition by the human Rubiconâ€“Rab7 complex. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 17003-17010.	7.1	18
108	Electromechanical coupling mechanism for activation and inactivation of an HCN channel. Nature Communications, 2021, 12, 2802.	12.8	17

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109	Large-scale design and refinement of stable proteins using sequence-only models. PLoS ONE, 2022, 17, e0265020.	2.5	17
110	The Origin of Consistent Protein Structure Refinement from Structural Averaging. Structure, 2015, 23, 1123-1128.	3.3	16
111	Computational design of mixed chirality peptide macrocycles with internal symmetry. Protein Science, 2020, 29, 2433-2445.	7.6	16
112	The cryo-EM structure of the bacterial flagellum cap complex suggests a molecular mechanism for filament elongation. Nature Communications, 2020, 11, 3210.	12.8	16
113	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature Communications, 2021, 12, 6947.	12.8	16
114	Crystal structure analysis of EstA from Arthrobacter sp. Rue61a â€“ an insight into catalytic promiscuity. FEBS Letters, 2014, 588, 1154-1160.	2.8	14
115	Discovery and Characterization of Spike Nâ€Terminal Domainâ€Binding Aptamers for Rapid SARSâ€CoVâ€2 Detection. Angewandte Chemie, 2021, 133, 21381-21385.	2.0	14
116	Rosetta Structure Prediction as a Tool for Solving Difficult Molecular Replacement Problems. Methods in Molecular Biology, 2017, 1607, 455-466.	0.9	11
117	Deep learning enables the atomic structure determination of the Fanconi Anemia core complex from cryoEM. IUCrJ, 2020, 7, 881-892.	2.2	10
118	Cryo-EM structure of the bacterial actin AlfA reveals unique assembly and ATP-binding interactions and the absence of a conserved subdomain. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 3356-3361.	7.1	7
119	Spherical-harmonic decomposition for molecular recognition in electron-density maps. International Journal of Data Mining and Bioinformatics, 2009, 3, 205.	0.1	6
120	Improving hybrid statistical and physical forcefields through local structure enumeration. Protein Science, 2016, 25, 1525-1534.	7.6	6
121	Crystal Structure and Mechanistic Molecular Modeling Studies ofMycobacterium tuberculosisDiterpene Cyclase Rv3377c. Biochemistry, 2020, 59, 4507-4515.	2.5	6
122	Cryoâ€electron Microscopy Imaging of Alzheimer's Amyloidâ€beta 42 Oligomer Displayed on a Functionally and Structurally Relevant Scaffold. Angewandte Chemie, 2021, 133, 18828-18835.	2.0	5
123	Structural Studies of Coronavirus Fusion Proteins. Microscopy and Microanalysis, 2019, 25, 1300-1301.	0.4	4
124	Suppressor Mutations in Type II Secretion Mutants of Vibrio cholerae: Inactivation of the VesC Protease. MSphere, 2020, 5, .	2.9	2
125	Protein Structure Modeling with Rosetta: Case Studies in Structure Prediction and Enzyme Repurposing. NATO Science for Peace and Security Series A: Chemistry and Biology, 2013, , 353-362.	0.5	0
126	Processing Structurally Heterogeneous Cryo-EM Data Using Atomic Models. Microscopy and Microanalysis, 2019, 25, 228-229.	0.4	0

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127	Title is missing!. , 2020, 16, e1008103.		0
128	Title is missing!. , 2020, 16, e1008103.		0
129	Title is missing!. , 2020, 16, e1008103.		0
130	Title is missing!. , 2020, 16, e1008103.		0
131	Title is missing!. , 2020, 16, e1008103.		0
132	Title is missing!. , 2020, 16, e1008103.		0