Jeffrey J Gray

List of Publications by Year in Descending Order

148 papers	9,653 citations	47 h-index	97 g-index
191 ext. papers	12,004 ext. citations	5.9 avg, IF	6.42 L-index

#	Paper	IF	Citations
148	Antibody structure prediction using interpretable deep learning.. *Patterns*, **2022**, 3, 100406	5.1	16
147	"How Do We Do This at a Distance?!" A Descriptive Study of Remote Undergraduate Research Programs during COVID-19.. *CBE Life Sciences Education*, **2022**, 21, ar1	3.4	4
146	Accurate positioning of functional residues with robotics-inspired computational protein design.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2115480119	11.5	0
145	Induced fit with replica exchange improves protein complex structure prediction. *PLoS Computational Biology*, **2022**, 18, e1010124	5	
144	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. *Nature Communications*, **2021**, 12, 6947	17.4	0
143	The structural basis of PTEN regulation by multi-site phosphorylation. *Nature Structural and Molecular Biology*, **2021**, 28, 858-868	17.6	5
142	Development of a Broadly Accessible, Computationally Guided Biochemistry Course-Based Undergraduate Research Experience. *Journal of Chemical Education*, **2021**, 98, 400-409	2.4	3
141	Robustification of RosettaAntibody and Rosetta SnugDock. *PLoS ONE*, **2021**, 16, e0234282	3.7	6
140	PyRosetta Jupyter Notebooks Teach Biomolecular Structure Prediction and Design.. *The Biophysicist*, **2021**, 2, 108-122	1	1
139	Development and Evaluation of GlycanDock: A Protein-Glycoligand Docking Refinement Algorithm in Rosetta. *Journal of Physical Chemistry B*, **2021**,	3.4	3
138	An expanded benchmark for antibody-antigen docking and affinity prediction reveals insights into antibody recognition determinants. *Structure*, **2021**, 29, 606-621.e5	5.2	13
137	Advances to tackle backbone flexibility in protein docking. *Current Opinion in Structural Biology*, **2021**, 67, 178-186	8.1	15
136	Membrane Protein Engineering with Rosetta. *Methods in Molecular Biology*, **2021**, 2315, 43-57	1.4	1
135	Structural basis for peptide substrate specificities of glycosyltransferase GalNAc-T2. *ACS Catalysis*, **2021**, 11, 2977-2991	13.1	3
134	Diverse Scientific Benchmarks for Implicit Membrane Energy Functions. *Journal of Chemical Theory and Computation*, **2021**, 17, 5248-5261	6.4	1
133	A high-affinity human TCR-like antibody detects celiac disease gluten peptide-MHC complexes and inhibits T cell activation. *Science Immunology*, **2021**, 6,	28	3
132	Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 1800-1823	4.2	17

131	Colicin-Mediated Transport of DNA through the Iron Transporter FepA. *MBio*, **2021**, 12, e0178721	7.8	1
130	Shotgun scanning glycomutagenesis: A simple and efficient strategy for constructing and characterizing neoglycoproteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	1
129	Better together: Elements of successful scientific software development in a distributed collaborative community. *PLoS Computational Biology*, **2020**, 16, e1007507	5	15
128	Macromolecular modeling and design in Rosetta: recent methods and frameworks. *Nature Methods*, **2020**, 17, 665-680	21.6	165
127	Protein docking and steered molecular dynamics suggest alternative phospholamban-binding sites on the SERCA calcium transporter. *Journal of Biological Chemistry*, **2020**, 295, 11262-11274	5.4	7
126	Protein Structure Prediction and Design in a Biologically Realistic Implicit Membrane. *Biophysical Journal*, **2020**, 118, 2042-2055	2.9	27
125	Computer-based Engineering of Thermostabilized Antibody Fragments. *AICHE Journal*, **2020**, 66, e16864	3.6	4
124	Novel sampling strategies and a coarse-grained score function for docking homomers, flexible heteromers, and oligosaccharides using Rosetta in CAPRI rounds 37-45. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 973-985	4.2	9
123	Deep Learning in Protein Structural Modeling and Design. *Patterns*, **2020**, 1, 100142	5.1	52
122	Geometric potentials from deep learning improve prediction of CDR H3 loop structures. *Bioinformatics*, **2020**, 36, i268-i275	7.2	17
121	Non-H3 CDR template selection in antibody modeling through machine learning. *PeerJ*, **2019**, 7, e6179	3.1	8
120	Hfq structure reveals a conserved mechanism of RNA annealing regulation. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 10978-10987	11.5	14
119	Flexible Backbone Assembly and Refinement of Symmetrical Homomeric Complexes. *Structure*, **2019**, 27, 1041-1051.e8	5.2	8
118	Plasma Cells Are the Most Abundant Gluten Peptide MHC-expressing Cells in Inflamed Intestinal Tissues From Patients With Celiac Disease. *Gastroenterology*, **2019**, 156, 1428-1439.e10	13.3	45
117	Toward the computational design of protein crystals with improved resolution. *Acta Crystallographica Section D: Structural Biology*, **2019**, 75, 1015-1027	5.5	2
116	The structure of the colorectal cancer-associated enzyme GalNAc-T12 reveals how nonconserved residues dictate its function. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 20404-20410	11.5	12
115	A humanized yeast system to analyze cleavage of prelamin A by ZMPSTE24. *Methods*, **2019**, 157, 47-55	4.6	7
114	A Parametric Rosetta Energy Function Analysis with LK Peptides on SAM Surfaces. *Langmuir*, **2018**, 34, 5279-5289	4	2

113	Targeting the CoREST complex with dual histone deacetylase and demethylase inhibitors. *Nature Communications*, **2018**, 9, 53	17.4	116
112	Cover Image, Volume 86, Issue 1. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86, C4-C4	4.2	
111	Efficient flexible backbone protein-protein docking for challenging targets. *Bioinformatics*, **2018**, 34, 3461-3469	7.2	57
110	Nanostructure, osteopontin, and mechanical properties of calcitic avian eggshell. *Science Advances*, **2018**, 4, eaar3219	14.3	47
109	Web-accessible molecular modeling with Rosetta: The Rosetta Online Server that Includes Everyone (ROSIE). *Protein Science*, **2018**, 27, 259-268	6.3	32
108	Comparison of NMR and crystal structures of membrane proteins and computational refinement to improve model quality. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86, 57-74	4.2	3
107	Chiral switching in biomineral suprastructures induced by homochiral l-amino acid. *Science Advances* , **2018**, 4, eaas9819	14.3	28
106	Repertoire Analysis of Antibody CDR-H3 Loops Suggests Affinity Maturation Does Not Typically Result in Rigidification. *Frontiers in Immunology*, **2018**, 9, 413	8.4	26
105	Modulation of calcium oxalate dihydrate growth by phosphorylated osteopontin peptides. *Journal of Structural Biology*, **2018**, 204, 131-144	3.4	9
104	A Benchmarking Study of PeptideBiomineral Interactions. *Crystal Growth and Design*, **2018**, 18, 607-616	3.5	9
103	Modeling and docking of antibody structures with Rosetta. *Nature Protocols*, **2017**, 12, 401-416	18.8	159
102	Glycoengineering of Esterase Activity through Metabolic Flux-Based Modulation of Sialic Acid. *ChemBioChem*, **2017**, 18, 1204-1215	3.8	8
101	Chiral acidic amino acids induce chiral hierarchical structure in calcium carbonate. *Nature Communications*, **2017**, 8, 15066	17.4	99
100	The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design. *Journal of Chemical Theory and Computation*, **2017**, 13, 3031-3048	6.4	486
99	Residue-centric modeling and design of saccharide and glycoconjugate structures. *Journal of Computational Chemistry*, **2017**, 38, 276-287	3.5	31
98	Acidic C-terminal domains autoregulate the RNA chaperone Hfq. *ELife*, **2017**, 6,	8.9	40
97	A cyber-linked undergraduate research experience in computational biomolecular structure prediction and design. *PLoS Computational Biology*, **2017**, 13, e1005837	5	7
96	Structure-based cross-docking analysis of antibody-antigen interactions. *Scientific Reports*, **2017**, 7, 8145	4.9	24

95	Modeling oblong proteins and water-mediated interfaces with RosettaDock in CAPRI rounds 28-35. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 479-486	4.2	14
94	Accurate Structure Prediction of CDR H3 Loops Enabled by a Novel Structure-Based C-Terminal Constraint. *Journal of Immunology*, **2017**, 198, 505-515	5.3	33
93	A high throughput mutagenic analysis of yeast sumo structure and function. *PLoS Genetics*, **2017**, 13, e1006612	6	7
92	Expanding the toolkit for membrane protein modeling in Rosetta. *Bioinformatics*, **2017**, 33, 754-756	7.2	14
91	Pushing the Backbone in Protein-Protein Docking. *Structure*, **2016**, 24, 1821-1829	5.2	33
90	Structural Diversity in the Type IV Pili of Multidrug-resistant Acinetobacter. *Journal of Biological Chemistry*, **2016**, 291, 22924-22935	5.4	31
89	Improved prediction of antibody VL-VH orientation. *Protein Engineering, Design and Selection*, **2016**, 29, 409-418	1.9	32
88	Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84 Suppl 1, 323-48	4.2	111
87	Large-scale sequence and structural comparisons of human naive and antigen-experienced antibody repertoires. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E2636-45	11.5	118
86	Shape complementarity and hydrogen bond preferences in protein-protein interfaces: implications for antibody modeling and protein-protein docking. *Bioinformatics*, **2016**, 32, 2451-6	7.2	43
85	Computational modeling of membrane proteins. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 1-24	4.2	69
84	Rosetta-MPDock: A Novel Computational Tool for Protein-Protein Docking within the Membrane Bilayer. *Biophysical Journal*, **2015**, 108, 250a	2.9	2
83	Interfacial Mineral–Peptide Properties of a Mineral Binding Peptide from Osteonectin and Bone-like Apatite. *Chemistry of Materials*, **2015**, 27, 5562-5569	9.6	18
82	Molecular Determinants for Protein Stabilization by Insertional Fusion to a Thermophilic Host Protein. *ChemBioChem*, **2015**, 16, 2392-402	3.8	9
81	An Integrated Framework Advancing Membrane Protein Modeling and Design. *PLoS Computational Biology*, **2015**, 11, e1004398	5	92
80	Functional loss of semaphorin 3C and/or semaphorin 3D and their epistatic interaction with ret are critical to Hirschsprung disease liability. *American Journal of Human Genetics*, **2015**, 96, 581-96	11	82
79	The origin of CDR H3 structural diversity. *Structure*, **2015**, 23, 302-11	5.2	57
78	Blind prediction performance of RosettaAntibody 3.0: grafting, relaxation, kinematic loop modeling, and full CDR optimization. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 1611-23	4.2	72

77	Structure-based non-canonical amino acid design to covalently crosslink an antibody-antigen complex. *Journal of Structural Biology*, **2014**, 185, 215-22	3.4	18
76	Blind prediction of interfacial water positions in CAPRI. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 620-32	4.2	43
75	A comprehensive, high-resolution map of a gene's fitness landscape. *Molecular Biology and Evolution*, **2014**, 31, 1581-92	8.3	190
74	Protein-protein docking with dynamic residue protonation states. *PLoS Computational Biology*, **2014**, 10, e1004018	5	14
73	Scientific benchmarks for guiding macromolecular energy function improvement. *Methods in Enzymology*, **2013**, 523, 109-43	1.7	164
72	Neutron reflectometry studies of the adsorbed structure of the amelogenin, LRAP. *Journal of Physical Chemistry B*, **2013**, 117, 3098-109	3.4	26
71	Using the RosettaSurface algorithm to predict protein structure at mineral surfaces. *Methods in Enzymology*, **2013**, 532, 343-66	1.7	20
70	Extending RosettaDock with water, sugar, and pH for prediction of complex structures and affinities for CAPRI rounds 20-27. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 2201-9	4.2	20
69	Adding diverse noncanonical backbones to rosetta: enabling peptidomimetic design. *PLoS ONE*, **2013**, 8, e67051	3.7	47
68	Serverification of molecular modeling applications: the Rosetta Online Server that Includes Everyone (ROSIE). *PLoS ONE*, **2013**, 8, e63906	3.7	230
67	Alternative computational protocols for supercharging protein surfaces for reversible unfolding and retention of stability. *PLoS ONE*, **2013**, 8, e64363	3.7	50
66	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 1980-7	4.2	78
65	Solid-State NMR Studies of Biomineralization Peptides and Proteins. *ACS Symposium Series*, **2012**, 77-96	0.4	4
64	Enzymatic excision of uracil residues in nucleosomes depends on the local DNA structure and dynamics. *Biochemistry*, **2012**, 51, 6028-38	3.2	39
63	Rapid calculation of protein pKa values using Rosetta. *Biophysical Journal*, **2012**, 103, 587-595	2.9	51
62	Targeted DNA methylation using an artificially bisected M.HhaI fused to zinc fingers. *PLoS ONE*, **2012**, 7, e44852	3.7	27
61	Structure-based design of supercharged, highly thermoresistant antibodies. *Chemistry and Biology*, **2012**, 19, 449-55		108
60	Prediction of calcite morphology from computational and experimental studies of mutations of a de novo-designed peptide. *Langmuir*, **2011**, 27, 11520-7	4	8

59	ROSETTA3: an object-oriented software suite for the simulation and design of macromolecules. *Methods in Enzymology*, **2011**, 487, 545-74	1.7	1216
58	Community-wide assessment of protein-interface modeling suggests improvements to design methodology. *Journal of Molecular Biology*, **2011**, 414, 289-302	6.5	114
57	Real-time PyMOL visualization for Rosetta and PyRosetta. *PLoS ONE*, **2011**, 6, e21931	3.7	35
56	Computed structures of point deletion mutants and their enzymatic activities. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2844-60	4.2	5
55	Partial high-resolution structure of phosphorylated and non-phosphorylated leucine-rich amelogenin protein adsorbed to hydroxyapatite. *Journal of Physical Chemistry C*, **2011**, 115, 13775-13785	3.8	39
54	Analysis and modeling of the variable region of camelid single-domain antibodies. *Journal of Immunology*, **2011**, 186, 6357-67	5.3	57
53	Enzyme replacement therapy prevents dental defects in a model of hypophosphatasia. *Journal of Dental Research*, **2011**, 90, 470-6	8.1	96
52	Mechanism of polyubiquitin chain recognition by the human ubiquitin conjugating enzyme Ube2g2. *Journal of Biological Chemistry*, **2011**, 286, 3981-91	5.4	11
51	Benchmarking and analysis of protein docking performance in Rosetta v3.2. *PLoS ONE*, **2011**, 6, e22477	3.7	190
50	PyRosetta: a script-based interface for implementing molecular modeling algorithms using Rosetta. *Bioinformatics*, **2010**, 26, 689-91	7.2	333
49	SnugDock: paratope structural optimization during antibody-antigen docking compensates for errors in antibody homology models. *PLoS Computational Biology*, **2010**, 6, e1000644	5	95
48	De novo design of peptide-calcite biomineralization systems. *Journal of the American Chemical Society*, **2010**, 132, 12252-62	16.4	43
47	Computational predictions of the mutant behavior of AraC. *Journal of Molecular Biology*, **2010**, 398, 462-70	6.3	5
46	Phosphorylation-dependent inhibition of mineralization by osteopontin ASARM peptides is regulated by PHEX cleavage. *Journal of Bone and Mineral Research*, **2010**, 25, 695-705	6.3	124
45	Toward a structure determination method for biomineral-associated protein using combined solid-state NMR and computational structure prediction. *Structure*, **2010**, 18, 1678-87	5.2	35
44	Structurally distinct toxicity inhibitors bind at common loci on β-amyloid fibril. *Protein Science*, **2010**, 19, 2291-304	6.3	20
43	A generalized approach to sampling backbone conformations with RosettaDock for CAPRI rounds 13-19. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 3115-23	4.2	39
42	Modulation of calcium oxalate dihydrate growth by selective crystal-face binding of phosphorylated osteopontin and polyaspartate peptide showing occlusion by sectoral (compositional) zoning. *Journal of Biological Chemistry*, **2009**, 284, 23491-501	5.4	53

41	Allosteric communication occurs via networks of tertiary and quaternary motions in proteins. *PLoS Computational Biology*, **2009**, 5, e1000293	5	80
40	Identification of structural mechanisms of HIV-1 protease specificity using computational peptide docking: implications for drug resistance. *Structure*, **2009**, 17, 1636-1648	5.2	28
39	Toward high-resolution homology modeling of antibody Fv regions and application to antibody-antigen docking. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 497-514	4.2	149
38	RosettaAntibody: antibody variable region homology modeling server. *Nucleic Acids Research*, **2009**, 37, W474-9	20.1	123
37	Solution- and adsorbed-state structural ensembles predicted for the statherin-hydroxyapatite system. *Biophysical Journal*, **2009**, 96, 3082-91	2.9	49
36	Structure prediction of domain insertion proteins from structures of individual domains. *Structure*, **2008**, 16, 513-27	5.2	17
35	The RosettaDock server for local protein-protein docking. *Nucleic Acids Research*, **2008**, 36, W233-8	20.1	389
34	Conformer selection and induced fit in flexible backbone protein-protein docking using computational and NMR ensembles. *Journal of Molecular Biology*, **2008**, 381, 1068-87	6.5	128
33	Analysis of protein kinase autophosphorylation using expressed protein ligation and computational modeling. *Journal of the American Chemical Society*, **2008**, 130, 5667-9	16.4	16
32	Modeling the structure of mAb 14B7 bound to the anthrax protective antigen. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 218-30	4.2	28
31	Contact rearrangements form coupled networks from local motions in allosteric proteins. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 455-66	4.2	75
30	Structure prediction of protein-solid surface interactions reveals a molecular recognition motif of statherin for hydroxyapatite. *Journal of the American Chemical Society*, **2007**, 129, 13713-22	16.4	103
29	Local motions in a benchmark of allosteric proteins. *Proteins: Structure, Function and Bioinformatics*, **2007**, 67, 385-99	4.2	90
28	Incorporating biochemical information and backbone flexibility in RosettaDock for CAPRI rounds 6-12. *Proteins: Structure, Function and Bioinformatics*, **2007**, 69, 793-800	4.2	37
27	Truncation of the caspase-related subunit (Gpi8p) of Saccharomyces cerevisiae GPI transamidase: dimerization revealed. *Archives of Biochemistry and Biophysics*, **2007**, 462, 83-93	4.1	10
26	High-resolution protein-protein docking. *Current Opinion in Structural Biology*, **2006**, 16, 183-93	8.1	152
25	Structural model of the mAb 806-EGFR complex using computational docking followed by computational and experimental mutagenesis. *Structure*, **2006**, 14, 401-14	5.2	48
24	Applying linear interaction energy method for rational design of noncompetitive allosteric inhibitors of the sarco- and endoplasmic reticulum calcium-ATPase. *Journal of Medicinal Chemistry*, **2005**, 48, 3005-14	8.3	29

23	CAPRI rounds 3-5 reveal promising successes and future challenges for RosettaDock. *Proteins: Structure, Function and Bioinformatics*, **2005**, 60, 181-6	4.2	49
22	The interaction of proteins with solid surfaces. *Current Opinion in Structural Biology*, **2004**, 14, 110-5	8.1	683
21	Protein-protein docking predictions for the CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2003**, 52, 118-22	4.2	93
20	Protein-protein docking with simultaneous optimization of rigid-body displacement and side-chain conformations. *Journal of Molecular Biology*, **2003**, 331, 281-99	6.5	858
19	Adsorption of colloidal particles by Brownian dynamics simulation: Kinetics and surface structures. *Journal of Chemical Physics*, **2001**, 114, 1366-1381	3.9	39
18	Adsorption of Charge-Bidisperse Mixtures of Colloidal Particles. *Langmuir*, **2001**, 17, 7935-7947	4	11
17	Microstructure Formation and Kinetics in the Random Sequential Adsorption of Polydisperse Tethered Nanoparticles Modeled as Hard Disks. *Langmuir*, **2001**, 17, 2317-2328	4	26
16	Nonequilibrium phase behavior during the random sequential adsorption of tethered hard disks. *Physical Review Letters*, **2000**, 85, 4430-3	7.4	20
15	Origin of anomalous multibody interactions. *Nature*, **1999**, 402, 750-750	50.4	16
14	Rheology and dynamics of sheared arrays of colloidal particles. *Journal of Rheology*, **1998**, 42, 1121-1151	4.1	27
13	Effect of trisodium citrate treatment on hybridoma cell viability. *Biotechnology Letters*, **1991**, 5, 295-298		10
12	An Expanded Benchmark for Antibody-Antigen Docking and Affinity Prediction Reveals Insights into Antibody Recognition Determinants. *SSRN Electronic Journal*,	1	2
11	Efficient Flexible Backbone Protein-Protein Docking for Challenging Targets		3
10	Novel sampling strategies and a coarse-grained score function for docking homomers, flexible heteromers, and oligosaccharides using Rosetta in CAPRI Rounds 37–45		1
9	Protein Docking and Steered Molecular Dynamics Reveal Alternative Regulatory Sites on the SERCA Calcium Transporter		2
8	Shotgun scanning glycomutagenesis: a simple and efficient strategy for constructing and characterizing neoglycoproteins		2
7	The Rosetta all-atom energy function for macromolecular modeling and design		3
6	Geometric Potentials from Deep Learning Improve Prediction of CDR H3 Loop Structures		3

5	Diverse scientific benchmarks for implicit membrane energy functions	1
4	Modeling and docking antibody structures with Rosetta	1
3	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks	2
2	Antibody structure prediction using interpretable deep learning	6
1	Growing Glycans in Rosetta: Accurate de novo glycan modeling, density fitting, and rational sequon design	2