

James S Fraser

List of Publications by Year in descending order

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Version: 2024-02-01

86
papers

12,659
citations

53794

45
h-index

49909

87
g-index

139
all docs

139
docs citations

139
times ranked

21508
citing authors

#	ARTICLE	IF	CITATIONS
1	Directed evolution of the rRNA methylating enzyme Cfr reveals molecular basis of antibiotic resistance. <i>ELife</i> , 2022, 11, .	6.0	10
2	Integration of software tools for integrative modeling of biomolecular systems. <i>Journal of Structural Biology</i> , 2022, 214, 107841.	2.8	7
3	A counter-enzyme complex regulates glutamate metabolism in <i>Bacillus subtilis</i> . <i>Nature Chemical Biology</i> , 2022, 18, 161-170.	8.0	14
4	Structural basis for context-specific inhibition of translation by oxazolidinone antibiotics. <i>Nature Structural and Molecular Biology</i> , 2022, 29, 162-171.	8.2	31
5	Accurate positioning of functional residues with robotics-inspired computational protein design. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2115480119.	7.1	6
6	Ligand binding remodels protein side-chain conformational heterogeneity. <i>ELife</i> , 2022, 11, .	6.0	33
7	The mechanisms of catalysis and ligand binding for the SARS-CoV-2 NSP3 macrodomain from neutron and x-ray diffraction at room temperature. <i>Science Advances</i> , 2022, 8, .	10.3	24
8	qFit: 3: Protein and ligand multiconformer modeling for X-ray crystallographic and single-particle cryo-EM density maps. <i>Protein Science</i> , 2021, 30, 270-285.	7.6	34
9	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDDataResource challenge. <i>Nature Methods</i> , 2021, 18, 156-164.	19.0	73
10	ORACLE reveals a bright future to fight bacteria. <i>ELife</i> , 2021, 10, .	6.0	0
11	State of the structure address on MET receptor activation by HGF. <i>Biochemical Society Transactions</i> , 2021, 49, 645-661.	3.4	5
12	Fragment binding to the Nsp3 macrodomain of SARS-CoV-2 identified through crystallographic screening and computational docking. <i>Science Advances</i> , 2021, 7, .	10.3	100
13	Co-occurring Alterations in the RAS-MAPK Pathway Limit Response to MET Inhibitor Treatment in MET Exon 14 Skipping Mutation-Positive Lung Cancer. <i>Clinical Cancer Research</i> , 2020, 26, 439-449.	7.0	64
14	Comparative host-coronavirus protein interaction networks reveal pan-viral disease mechanisms. <i>Science</i> , 2020, 370, .	12.6	508
15	Discovery of allosteric binding sites by crystallographic fragment screening. <i>Current Opinion in Structural Biology</i> , 2020, 65, 209-216.	5.7	16
16	Synthetic group A streptogramin antibiotics that overcome Vat resistance. <i>Nature</i> , 2020, 586, 145-150.	27.8	63
17	Ensemble-based enzyme design can recapitulate the effects of laboratory directed evolution in silico. <i>Nature Communications</i> , 2020, 11, 4808.	12.8	67
18	Expanding the space of protein geometries by computational design of de novo fold families. <i>Science</i> , 2020, 369, 1132-1136.	12.6	57

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19	Genetic interaction mapping informs integrative structure determination of protein complexes. <i>Science</i> , 2020, 370, .	12.6	24
20	An ultrapotent synthetic nanobody neutralizes SARS-CoV-2 by stabilizing inactive Spike. <i>Science</i> , 2020, 370, 1473-1479.	12.6	336
21	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. <i>Nature</i> , 2020, 583, 459-468.	27.8	3,542
22	Assessment of the nucleotide modifications in the high-resolution cryo-electron microscopy structure of the <i>Escherichia coli</i> 50S subunit. <i>Nucleic Acids Research</i> , 2020, 48, 2723-2732.	14.5	22
23	What Will Computational Modeling Approaches Have to Say in the Era of Atomistic Cryo-EM Data?. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2410-2412.	5.4	15
24	Differences in the chitinolytic activity of mammalian chitinases on soluble and insoluble substrates. <i>Protein Science</i> , 2020, 29, 952-963.	7.6	15
25	Assessment of enzyme active site positioning and tests of catalytic mechanisms through X-ray-derived conformational ensembles. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 33204-33215.	7.1	39
26	Comparing serial X-ray crystallography and microcrystal electron diffraction (MicroED) as methods for routine structure determination from small macromolecular crystals. <i>IUCr</i> , 2020, 7, 306-323.	2.2	32
27	Synthetic Essentiality of Metabolic Regulator PDHK1 in PTEN-Deficient Cells and Cancers. <i>Cell Reports</i> , 2019, 28, 2317-2330.e8.	6.4	12
28	Temperature-jump solution X-ray scattering reveals distinct motions in a dynamic enzyme. <i>Nature Chemistry</i> , 2019, 11, 1058-1066.	13.6	67
29	Biomaterials in non-integer dimensions. <i>Nature Chemistry</i> , 2019, 11, 599-600.	13.6	5
30	Effects of α -tubulin acetylation on microtubule structure and stability. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 10366-10371.	7.1	216
31	Liquid-like and rigid-body motions in molecular-dynamics simulations of a crystalline protein. <i>Structural Dynamics</i> , 2019, 6, 064704.	2.3	14
32	Computational design of a modular protein sense-response system. <i>Science</i> , 2019, 366, 1024-1028.	12.6	91
33	Mix-and-inject XFEL crystallography reveals gated conformational dynamics during enzyme catalysis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 25634-25640.	7.1	56
34	A Multi-model Approach to Assessing Local and Global Cryo-EM Map Quality. <i>Structure</i> , 2019, 27, 344-358.e3.	3.3	55
35	Biophysical Characterization of a Disabled Double Mutant of Soybean Lipoxygenase: The α -of Precise Substrate Positioning Relative to Metal Cofactor and an Identified Dynamical Network. <i>Journal of the American Chemical Society</i> , 2019, 141, 1555-1567.	13.7	19
36	Bringing diffuse X-ray scattering into focus. <i>Current Opinion in Structural Biology</i> , 2018, 50, 109-116.	5.7	29

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37	Rescue of conformational dynamics in enzyme catalysis by directed evolution. <i>Nature Communications</i> , 2018, 9, 1314.	12.8	97
38	Fit-ligand Reveals Widespread Conformational Heterogeneity of Drug-Like Molecules in X-Ray Electron Density Maps. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 11183-11198.	6.4	44
39	Extending chemical perturbations of the ubiquitin fitness landscape in a classroom setting reveals new constraints on sequence tolerance. <i>Biology Open</i> , 2018, 7, .	1.2	17
40	An expanded allosteric network in PTP1B by multitemperature crystallography, fragment screening, and covalent tethering. <i>ELife</i> , 2018, 7, .	6.0	120
41	Conformational variation of proteins at room temperature is not dominated by radiation damage. <i>Journal of Synchrotron Radiation</i> , 2017, 24, 73-82.	2.4	50
42	Flexibility and Design: Conformational Heterogeneity along the Evolutionary Trajectory of a Redesigned Ubiquitin. <i>Structure</i> , 2017, 25, 739-749.e3.	3.3	22
43	Cytidine deaminase efficiency of the lentiviral viral restriction factor APOBEC3C correlates with dimerization. <i>Nucleic Acids Research</i> , 2017, 45, 3378-3394.	14.5	38
44	Hydrogen-Deuterium Exchange of Lipoxygenase Uncovers a Relationship between Distal, Solvent Exposed Protein Motions and the Thermal Activation Barrier for Catalytic Proton-Coupled Electron Tunneling. <i>ACS Central Science</i> , 2017, 3, 570-579.	11.3	55
45	XFEL structures of the influenza M2 proton channel: Room temperature water networks and insights into proton conduction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 13357-13362.	7.1	64
46	Allosteric Inhibitors, Crystallography, and Comparative Analysis Reveal Network of Coordinated Movement across Human Herpesvirus Proteases. <i>Journal of the American Chemical Society</i> , 2017, 139, 11650-11653.	13.7	13
47	Measuring and modeling diffuse scattering in protein X-ray crystallography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 4069-4074.	7.1	48
48	Preprints for the life sciences. <i>Science</i> , 2016, 352, 899-901.	12.6	119
49	Data publication with the structural biology data grid supports live analysis. <i>Nature Communications</i> , 2016, 7, 10882.	12.8	113
50	High-density grids for efficient data collection from multiple crystals. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 2-11.	2.3	62
51	CryptoSite: Expanding the Druggable Proteome by Characterization and Prediction of Cryptic Binding Sites. <i>Journal of Molecular Biology</i> , 2016, 428, 709-719.	4.2	190
52	Determination of ubiquitin fitness landscapes under different chemical stresses in a classroom setting. <i>ELife</i> , 2016, 5, .	6.0	71
53	Automated structure refinement of macromolecular assemblies from cryo-EM maps using Rosetta. <i>ELife</i> , 2016, 5, .	6.0	407
54	One Crystal, Two Temperatures: Cryocooling Penalties Alter Ligand Binding to Transient Protein Sites. <i>ChemBioChem</i> , 2015, 16, 1560-1564.	2.6	76

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55	Predicting X-ray diffuse scattering from translationâ€librationâ€screw structural ensembles. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 1657-1667.	2.5	14
56	Exposing Hidden Alternative Backbone Conformations in X-ray Crystallography Using qFit. <i>PLoS Computational Biology</i> , 2015, 11, e1004507.	3.2	81
57	Negative Epistasis and Evolvability in TEM-1 β -Lactamaseâ€The Thin Line between an Enzyme's Conformational Freedom and Disorder. <i>Journal of Molecular Biology</i> , 2015, 427, 2396-2409.	4.2	102
58	High-resolution structures of the M2 channel from influenza A virus reveal dynamic pathways for proton stabilization and transduction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 14260-14265.	7.1	92
59	Integrative, dynamic structural biology at atomic resolutionâ€it's about time. <i>Nature Methods</i> , 2015, 12, 307-318.	19.0	220
60	Lineage-Specific Viral Hijacking of Non-canonical E3 Ubiquitin Ligase Cofactors in the Evolution of Vif Anti-APOBEC3 Activity. <i>Cell Reports</i> , 2015, 11, 1236-1250.	6.4	42
61	EMRinger: side chainâ€directed model and map validation for 3D cryo-electron microscopy. <i>Nature Methods</i> , 2015, 12, 943-946.	19.0	799
62	Keep on Moving: Discovering and Perturbing the Conformational Dynamics of Enzymes. <i>Accounts of Chemical Research</i> , 2015, 48, 423-430.	15.6	84
63	From deep TLS validation to ensembles of atomic models built from elemental motions. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 1668-1683.	2.5	14
64	Mapping the conformational landscape of a dynamic enzyme by multitemperature and XFEL crystallography. <i>ELife</i> , 2015, 4, .	6.0	143
65	Conformational dynamics of a crystalline protein from microsecond-scale molecular dynamics simulations and diffuse X-ray scattering. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 17887-17892.	7.1	55
66	Incorporation of protein flexibility and conformational energy penalties in docking screens to improve ligand discovery. <i>Nature Chemistry</i> , 2014, 6, 575-583.	13.6	124
67	Protein structural ensembles are revealed by redefining X-ray electron density noise. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 237-242.	7.1	79
68	Integrated description of protein dynamics from room-temperature X-ray crystallography and NMR. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, E445-54.	7.1	142
69	E pluribus unum, no more: from one crystal, many conformations. <i>Current Opinion in Structural Biology</i> , 2014, 28, 56-62.	5.7	53
70	Discovery and Characterization of Gut Microbiota Decarboxylases that Can Produce the Neurotransmitter Tryptamine. <i>Cell Host and Microbe</i> , 2014, 16, 495-503.	11.0	473
71	Crystal Cryocooling Distorts Conformational Heterogeneity in a Model Michaelis Complex of DHFR. <i>Structure</i> , 2014, 22, 899-910.	3.3	131
72	Automated identification of functional dynamic contact networks from X-ray crystallography. <i>Nature Methods</i> , 2013, 10, 896-902.	19.0	130

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73	From Structure to Systems: High-Resolution, Quantitative Genetic Analysis of RNA Polymerase II. <i>Cell</i> , 2013, 154, 775-788.	28.9	132
74	Flexible Backbone Sampling Methods to Model and Design Protein Alternative Conformations. <i>Methods in Enzymology</i> , 2013, 523, 61-85.	1.0	44
75	From Systems to Structure: Bridging Networks and Mechanism. <i>Molecular Cell</i> , 2013, 49, 222-231.	9.7	46
76	Control of protein signaling using a computationally designed GTPase/GEF orthogonal pair. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 5277-5282.	7.1	73
77	CheShift-2 resolves a local inconsistency between two X-ray crystal structures. <i>Journal of Biomolecular NMR</i> , 2012, 54, 193-198.	2.8	4
78	Systematic Functional Prioritization of Protein Posttranslational Modifications. <i>Cell</i> , 2012, 150, 413-425.	28.9	375
79	Mining electron density for functionally relevant protein polymorphism in crystal structures. <i>Cellular and Molecular Life Sciences</i> , 2011, 68, 1829-1841.	5.4	23
80	Accessing protein conformational ensembles using room-temperature X-ray crystallography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 16247-16252.	7.1	511
81	Automated electron density sampling reveals widespread conformational polymorphism in proteins. <i>Protein Science</i> , 2010, 19, 1420-1431.	7.6	155
82	The tumor-associated EpCAM regulates morphogenetic movements through intracellular signaling. <i>Journal of Cell Biology</i> , 2010, 191, 645-659.	5.2	58
83	Hidden alternative structures of proline isomerase essential for catalysis. <i>Nature</i> , 2009, 462, 669-673.	27.8	447
84	Immunoglobulin-like domains on bacteriophage: weapons of modest damage?. <i>Current Opinion in Microbiology</i> , 2007, 10, 382-387.	5.1	86
85	An atypical receiver domain controls the dynamic polar localization of the <i>Myxococcus xanthus</i> social motility protein FrzS. <i>Molecular Microbiology</i> , 2007, 65, 319-332.	2.5	32
86	Ig-Like Domains on Bacteriophages: A Tale of Promiscuity and Deceit. <i>Journal of Molecular Biology</i> , 2006, 359, 496-507.	4.2	169