James S Fraser

List of Publications by Year
in descending order

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	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. Nature, 2020, 583, 459-468.	27.8	3,542
2	EMRinger: side chainâ€“directed model and map validation for 3D cryo-electron microscopy. Nature Methods, 2015, 12, 943-946.	19.0	799
3	Accessing protein conformational ensembles using room-temperature X-ray crystallography. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 16247-16252.	7.1	511
4	Comparative host-coronavirus protein interaction networks reveal pan-viral disease mechanisms. Science, 2020, 370, .	12.6	508
5	Discovery and Characterization of Gut Microbiota Decarboxylases that Can Produce the Neurotransmitter Tryptamine. Cell Host and Microbe, 2014, 16, 495-503.	11.0	473
6	Hidden alternative structures of proline isomerase essential for catalysis. Nature, 2009, 462, 669-673.	27.8	447
7	Automated structure refinement of macromolecular assemblies from cryo-EM maps using Rosetta. ELife, 2016, 5, .	6.0	407
8	Systematic Functional Prioritization of Protein Posttranslational Modifications. Cell, 2012, 150, 413-425.	28.9	375
9	An ultrapotent synthetic nanobody neutralizes SARS-CoV-2 by stabilizing inactive Spike. Science, 2020, 370, 1473-1479.	12.6	336
10	Integrative, dynamic structural biology at atomic resolutionâ€”it's about time. Nature Methods, 2015, 12, 307-318.	19.0	220
11	Effects of Î±-tubulin acetylation on microtubule structure and stability. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 10366-10371.	7.1	216
12	CryptoSite: Expanding the Druggable Proteome by Characterization and Prediction of Cryptic Binding Sites. Journal of Molecular Biology, 2016, 428, 709-719.	4.2	190
13	Ig-Like Domains on Bacteriophages: A Tale of Promiscuity and Deceit. Journal of Molecular Biology, 2006, 359, 496-507.	4.2	169
14	Automated electronâ€density sampling reveals widespread conformational polymorphism in proteins. Protein Science, 2010, 19, 1420-1431.	7.6	155
15	Mapping the conformational landscape of a dynamic enzyme by multitemperature and XFEL crystallography. ELife, 2015, 4, .	6.0	143
16	Integrated description of protein dynamics from room-temperature X-ray crystallography and NMR. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E445-54.	7.1	142
17	From Structure to Systems: High-Resolution, Quantitative Genetic Analysis of RNA Polymerase II. Cell, 2013, 154, 775-788.	28.9	132
18	Crystal Cryocooling Distorts Conformational Heterogeneity in a Model Michaelis Complex of DHFR. Structure, 2014, 22, 899-910.	3.3	131

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19	Automated identification of functional dynamic contact networks from X-ray crystallography. Nature Methods, 2013, 10, 896-902.	19.0	130
20	Incorporation of protein flexibility and conformational energy penalties in docking screens to improve ligand discovery. Nature Chemistry, 2014, 6, 575-583.	13.6	124
21	An expanded allosteric network in PTP1B by multitemperature crystallography, fragment screening, and covalent tethering. ELife, 2018, 7, .	6.0	120
22	Preprints for the life sciences. Science, 2016, 352, 899-901.	12.6	119
23	Data publication with the structural biology data grid supports live analysis. Nature Communications, 2016, 7, 10882.	12.8	113
24	Negative Epistasis and Evolvability in TEM-1 Î²-Lactamaseâ€”The Thin Line between an Enzyme's Conformational Freedom and Disorder. Journal of Molecular Biology, 2015, 427, 2396-2409.	4.2	102
25	Fragment binding to the Nsp3 macrodomain of SARS-CoV-2 identified through crystallographic screening and computational docking. Science Advances, 2021, 7, .	10.3	100
26	Rescue of conformational dynamics in enzyme catalysis by directed evolution. Nature Communications, 2018, 9, 1314.	12.8	97
27	High-resolution structures of the M2 channel from influenza A virus reveal dynamic pathways for proton stabilization and transduction. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 14260-14265.	7.1	92
28	Computational design of a modular protein sense-response system. Science, 2019, 366, 1024-1028.	12.6	91
29	Immunoglobulin-like domains on bacteriophage: weapons of modest damage?. Current Opinion in Microbiology, 2007, 10, 382-387.	5.1	86
30	Keep on Moving: Discovering and Perturbing the Conformational Dynamics of Enzymes. Accounts of Chemical Research, 2015, 48, 423-430.	15.6	84
31	Exposing Hidden Alternative Backbone Conformations in X-ray Crystallography Using qFit. PLoS Computational Biology, 2015, 11, e1004507.	3.2	81
32	Protein structural ensembles are revealed by redefining X-ray electron density noise. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 237-242.	7.1	79
33	One Crystal, Two Temperatures: Cryocooling Penalties Alter Ligand Binding to Transient Protein Sites. ChemBioChem, 2015, 16, 1560-1564.	2.6	76
34	Control of protein signaling using a computationally designed GTPase/GEF orthogonal pair. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 5277-5282.	7.1	73
35	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. Nature Methods, 2021, 18, 156-164.	19.0	73
36	Determination of ubiquitin fitness landscapes under different chemical stresses in a classroom setting. ELife, 2016, 5, .	6.0	71

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37	Temperature-jump solution X-ray scattering reveals distinct motions in a dynamic enzyme. Nature Chemistry, 2019, 11, 1058-1066.	13.6	67
38	Ensemble-based enzyme design can recapitulate the effects of laboratory directed evolution in silico. Nature Communications, 2020, 11, 4808.	12.8	67
39	XFEL structures of the influenza M2 proton channel: Room temperature water networks and insights into proton conduction. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13357-13362.	7.1	64
40	Co-occurring Alterations in the RASâ€“MAPK Pathway Limit Response to MET Inhibitor Treatment in MET Exon 14 Skipping Mutation-Positive Lung Cancer. Clinical Cancer Research, 2020, 26, 439-449.	7.0	64
41	Synthetic group A streptogramin antibiotics that overcome Vat resistance. Nature, 2020, 586, 145-150.	27.8	63
42	High-density grids for efficient data collection from multiple crystals. Acta Crystallographica Section D: Structural Biology, 2016, 72, 2-11.	2.3	62
43	The tumor-associated EpCAM regulates morphogenetic movements through intracellular signaling. Journal of Cell Biology, 2010, 191, 645-659.	5.2	58
44	Expanding the space of protein geometries by computational design of de novo fold families. Science, 2020, 369, 1132-1136.	12.6	57
45	Mix-and-inject XFEL crystallography reveals gated conformational dynamics during enzyme catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 25634-25640.	7.1	56
46	Conformational dynamics of a crystalline protein from microsecond-scale molecular dynamics simulations and diffuse X-ray scattering. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 17887-17892.	7.1	55
47	Hydrogenâ€“Deuterium Exchange of Lipoxygenase Uncovers a Relationship between Distal, Solvent Exposed Protein Motions and the Thermal Activation Barrier for Catalytic Proton-Coupled Electron Tunneling. ACS Central Science, 2017, 3, 570-579.	11.3	55
48	A Multi-model Approach to Assessing Local and Global Cryo-EM Map Quality. Structure, 2019, 27, 344-358.e3.	3.3	55
49	E pluribus unum, no more: from one crystal, many conformations. Current Opinion in Structural Biology, 2014, 28, 56-62.	5.7	53
50	Conformational variation of proteins at room temperature is not dominated by radiation damage. Journal of Synchrotron Radiation, 2017, 24, 73-82.	2.4	50
51	Measuring and modeling diffuse scattering in protein X-ray crystallography. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 4069-4074.	7.1	48
52	From Systems to Structure: Bridging Networks and Mechanism. Molecular Cell, 2013, 49, 222-231.	9.7	46
53	Flexible Backbone Sampling Methods to Model and Design Protein Alternative Conformations. Methods in Enzymology, 2013, 523, 61-85.	1.0	44
54	qFit-ligand Reveals Widespread Conformational Heterogeneity of Drug-Like Molecules in X-Ray Electron Density Maps. Journal of Medicinal Chemistry, 2018, 61, 11183-11198.	6.4	44

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55	Lineage-Specific Viral Hijacking of Non-canonical E3ÂUbiquitin Ligase Cofactors in the Evolution of Vif Anti-APOBEC3 Activity. Cell Reports, 2015, 11, 1236-1250.	6.4	42
56	Assessment of enzyme active site positioning and tests of catalytic mechanisms through X-rayâ€“derived conformational ensembles. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 33204-33215.	7.1	39
57	Cytidine deaminase efficiency of the lentiviral viral restriction factor APOBEC3C correlates with dimerization. Nucleic Acids Research, 2017, 45, 3378-3394.	14.5	38
58	<scp>qFit</scp> 3: Protein and ligand multiconformer modeling for Xâ€ray crystallographic and singleâ€particle <scp>cryoâ€EM</scp> density maps. Protein Science, 2021, 30, 270-285.	7.6	34
59	Ligand binding remodels protein side-chain conformational heterogeneity. ELife, 2022, 11, .	6.0	33
60	An atypical receiver domain controls the dynamic polar localization of the Myxococcus xanthus social motility protein FrzS. Molecular Microbiology, 2007, 65, 319-332.	2.5	32
61	Comparing serial X-ray crystallography and microcrystal electron diffraction (MicroED) as methods for routine structure determination from small macromolecular crystals. IUCrJ, 2020, 7, 306-323.	2.2	32
62	Structural basis for context-specific inhibition of translation by oxazolidinone antibiotics. Nature Structural and Molecular Biology, 2022, 29, 162-171.	8.2	31
63	Bringing diffuse X-ray scattering into focus. Current Opinion in Structural Biology, 2018, 50, 109-116.	5.7	29
64	Genetic interaction mapping informs integrative structure determination of protein complexes. Science, 2020, 370, .	12.6	24
65	The mechanisms of catalysis and ligand binding for the SARS-CoV-2 NSP3 macrodomain from neutron and x-ray diffraction at room temperature. Science Advances, 2022, 8, .	10.3	24
66	Mining electron density for functionally relevant protein polysterism in crystal structures. Cellular and Molecular Life Sciences, 2011, 68, 1829-1841.	5.4	23
67	Flexibility and Design: Conformational Heterogeneity along the Evolutionary Trajectory of a Redesigned Ubiquitin. Structure, 2017, 25, 739-749.e3.	3.3	22
68	Assessment of the nucleotide modifications in the high-resolution cryo-electron microscopy structure of the Escherichia coli 50S subunit. Nucleic Acids Research, 2020, 48, 2723-2732.	14.5	22
69	Biophysical Characterization of a Disabled Double Mutant of Soybean Lipoxygenase: The â€œUndoingâ€•of Precise Substrate Positioning Relative to Metal Cofactor and an Identified Dynamical Network. Journal of the American Chemical Society, 2019, 141, 1555-1567.	13.7	19
70	Extending chemical perturbations of the ubiquitin fitness landscape in a classroom setting reveals new constraints on sequence tolerance. Biology Open, 2018, 7, .	1.2	17
71	Discovery of allosteric binding sites by crystallographic fragment screening. Current Opinion in Structural Biology, 2020, 65, 209-216.	5.7	16
72	What Will Computational Modeling Approaches Have to Say in the Era of Atomistic Cryo-EM Data?. Journal of Chemical Information and Modeling, 2020, 60, 2410-2412.	5.4	15

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73	Differences in the chitinolytic activity of mammalian chitinases on soluble and insoluble substrates. Protein Science, 2020, 29, 952-963.	7.6	15
74	Predicting X-ray diffuse scattering from translationâ€“librationâ€“screw structural ensembles. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 1657-1667.	2.5	14
75	Liquid-like and rigid-body motions in molecular-dynamics simulations of a crystalline protein. Structural Dynamics, 2019, 6, 064704.	2.3	14
76	From deep TLS validation to ensembles of atomic models built from elemental motions. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 1668-1683.	2.5	14
77	A counter-enzyme complex regulates glutamate metabolism in Bacillus subtilis. Nature Chemical Biology, 2022, 18, 161-170.	8.0	14
78	Allosteric Inhibitors, Crystallography, and Comparative Analysis Reveal Network of Coordinated Movement across Human Herpesvirus Proteases. Journal of the American Chemical Society, 2017, 139, 11650-11653.	13.7	13
79	Synthetic Essentiality of Metabolic Regulator PDHK1 in PTEN-Deficient Cells and Cancers. Cell Reports, 2019, 28, 2317-2330.e8.	6.4	12
80	Directed evolution of the rRNA methylating enzyme Cfr reveals molecular basis of antibiotic resistance. ELife, 2022, 11, .	6.0	10
81	Integration of software tools for integrative modeling of biomolecular systems. Journal of Structural Biology, 2022, 214, 107841.	2.8	7
82	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.	7.1	6
83	Biomaterials in non-integer dimensions. Nature Chemistry, 2019, 11, 599-600.	13.6	5
84	State of the structure address on MET receptor activation by HGF. Biochemical Society Transactions, 2021, 49, 645-661.	3.4	5
85	CheShift-2 resolves a local inconsistency between two X-ray crystal structures. Journal of Biomolecular NMR, 2012, 54, 193-198.	2.8	4
86	ORACLE reveals a bright future to fight bacteria. ELife, 2021, 10, .	6.0	0