

Gerard J Kleywegt

List of Publications by Year in descending order

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123
papers

19,848
citations

23500

58
h-index

17055

122
g-index

132
all docs

132
docs citations

132
times ranked

17950
citing authors

#	ARTICLE	IF	CITATIONS
1	AlphaFold Protein Structure Database: massively expanding the structural coverage of protein-sequence space with high-accuracy models. <i>Nucleic Acids Research</i> , 2022, 50, D439-D444.	6.5	3,692
2	Highly accurate protein structure prediction for the human proteome. <i>Nature</i> , 2021, 596, 590-596.	13.7	1,773
3	Protein Data Bank: the single global archive for 3D macromolecular structure data. <i>Nucleic Acids Research</i> , 2019, 47, D520-D528.	6.5	671
4	Protein Data Bank (PDB): The Single Global Macromolecular Structure Archive. <i>Methods in Molecular Biology</i> , 2017, 1607, 627-641.	0.4	592
5	Phi/Psi-chology: Ramachandran revisited. <i>Structure</i> , 1996, 4, 1395-1400.	1.6	525
6	OMERO: flexible, model-driven data management for experimental biology. <i>Nature Methods</i> , 2012, 9, 245-253.	9.0	478
7	Crystallographic and molecular-modeling studies of lipase B from <i>Candida antarctica</i> reveal a stereospecificity pocket for secondary alcohols. <i>Biochemistry</i> , 1995, 34, 16838-16851.	1.2	466
8	Structure Determination and Refinement of Human Alpha Class Glutathione Transferase A1-1, and a Comparison with the Mu and Pi Class Enzymes. <i>Journal of Molecular Biology</i> , 1993, 232, 192-212.	2.0	453
9	Databases in Protein Crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1998, 54, 1119-1131.	2.5	412
10	A New Generation of Crystallographic Validation Tools for the Protein Data Bank. <i>Structure</i> , 2011, 19, 1395-1412.	1.6	405
11	Checking your imagination: applications of the free R value. <i>Structure</i> , 1996, 4, 897-904.	1.6	379
12	Crystal structure of the C2 fragment of streptococcal protein G in complex with the Fc domain of human IgG. <i>Structure</i> , 1995, 3, 265-278.	1.6	340
13	Application and Limitations of X-ray Crystallographic Data in Structure-Based Ligand and Drug Design. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 2718-2736.	7.2	331
14	The Uppsala Electron-Density Server. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2004, 60, 2240-2249.	2.5	324
15	Recognition of spatial motifs in protein structures 1 Edited by J. Thornton. <i>Journal of Molecular Biology</i> , 1999, 285, 1887-1897.	2.0	303
16	EMPIAR: a public archive for raw electron microscopy image data. <i>Nature Methods</i> , 2016, 13, 387-388.	9.0	298
17	[27] Detecting folding motifs and similarities in protein structures. <i>Methods in Enzymology</i> , 1997, 277, 525-545.	0.4	291
18	[11] Model building and refinement practice. <i>Methods in Enzymology</i> , 1997, 277, 208-230.	0.4	278

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19	PSICQUIC and PSIScore: accessing and scoring molecular interactions. <i>Nature Methods</i> , 2011, 8, 528-529.	9.0	274
20	EMDataBank.org: unified data resource for CryoEM. <i>Nucleic Acids Research</i> , 2011, 39, D456-D464.	6.5	246
21	Where freedom is given, liberties are taken. <i>Structure</i> , 1995, 3, 535-540.	1.6	244
22	The crystal structure of the catalytic core domain of endoglucanase I from <i>Trichoderma reesei</i> at 3.6 Å... resolution, and a comparison with related enzymes 1 Edited by K.Nagai. <i>Journal of Molecular Biology</i> , 1997, 272, 383-397.	2.0	238
23	SIFTS: Structure Integration with Function, Taxonomy and Sequences resource. <i>Nucleic Acids Research</i> , 2012, 41, D483-D489.	6.5	238
24	Crystal structure of an acetylcholinesterase- α -fasciculin complex: interaction of a three-fingered toxin from snake venom with its target. <i>Structure</i> , 1995, 3, 1355-1366.	1.6	232
25	EMDataBank unified data resource for 3DEM. <i>Nucleic Acids Research</i> , 2016, 44, D396-D403.	6.5	230
26	Crystal structures of cellular retinoic acid binding proteins I and II in complex with all-trans-retinoic acid and a synthetic retinoid. <i>Structure</i> , 1994, 2, 1241-1258.	1.6	219
27	Validation of Structures in the Protein Data Bank. <i>Structure</i> , 2017, 25, 1916-1927.	1.6	210
28	An Alternative Method for the Evaluation of Docking Performance: RSR vs RMSD. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1411-1422.	2.5	166
29	PDBe: Protein Data Bank in Europe. <i>Nucleic Acids Research</i> , 2012, 40, D445-D452.	6.5	166
30	Crystallographic evidence for substrate ring distortion and protein conformational changes during catalysis in cellobiohydrolase Ce16A from <i>Trichoderma reesei</i> . <i>Structure</i> , 1999, 7, 1035-1045.	1.6	164
31	Validation of protein crystal structures. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2000, 56, 249-265.	2.5	161
32	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. <i>Structure</i> , 2015, 23, 1156-1167.	1.6	159
33	Validation of protein models from C α coordinates alone. <i>Journal of Molecular Biology</i> , 1997, 273, 371-376.	2.0	154
34	Crystallographic refinement of ligand complexes. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2007, 63, 94-100.	2.5	153
35	Recommendations of the wwPDB NMR Validation Task Force. <i>Structure</i> , 2013, 21, 1563-1570.	1.6	151
36	Not your average density. <i>Structure</i> , 1997, 5, 1557-1569.	1.6	147

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37	Limitations and lessons in the use of X-ray structural information in drug design. <i>Drug Discovery Today</i> , 2008, 13, 831-841.	3.2	146
38	Towards complete validated models in the next generation of ARP/wARP. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2004, 60, 2222-2229.	2.5	140
39	The Active Site of Cellobiohydrolase Cel6A from <i>Trichoderma reesei</i> : The Roles of Aspartic Acids D221 and D175. <i>Journal of the American Chemical Society</i> , 2002, 124, 10015-10024.	6.6	133
40	PDBe: Protein Data Bank in Europe. <i>Nucleic Acids Research</i> , 2014, 42, D285-D291.	6.5	133
41	PDBe: improved accessibility of macromolecular structure data from PDB and EMDB. <i>Nucleic Acids Research</i> , 2016, 44, D385-D395.	6.5	131
42	OneDep: Unified wwPDB System for Deposition, Biocuration, and Validation of Macromolecular Structures in the PDB Archive. <i>Structure</i> , 2017, 25, 536-545.	1.6	130
43	The Protein Data Bank at 40: Reflecting on the Past to Prepare for the Future. <i>Structure</i> , 2012, 20, 391-396.	1.6	120
44	The Protein Data Bank archive as an open data resource. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 1009-1014.	1.3	114
45	Experimental assessment of differences between related protein crystal structures. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 1878-1884.	2.5	104
46	Evaluation of protein fold comparison servers. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 54, 260-270.	1.5	97
47	Pound-Wise but Penny-Foolish. <i>Structure</i> , 2003, 11, 1051-1059.	1.6	90
48	Implementing an X-ray validation pipeline for the Protein Data Bank. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 478-483.	2.5	88
49	Resolution of <i>ab initio</i> shapes determined from small-angle scattering. <i>IUCr</i> , 2016, 3, 440-447.	1.0	88
50	PDBe: improved findability of macromolecular structure data in the PDB. <i>Nucleic Acids Research</i> , 2020, 48, D335-D343.	6.5	86
51	A Survey of Left-handed Helices in Protein Structures. <i>Journal of Molecular Biology</i> , 2005, 347, 231-241.	2.0	83
52	Report of the wwPDB Small-Angle Scattering Task Force: Data Requirements for Biomolecular Modeling and the PDB. <i>Structure</i> , 2013, 21, 875-881.	1.6	77
53	PDBe: towards reusable data delivery infrastructure at protein data bank in Europe. <i>Nucleic Acids Research</i> , 2018, 46, D486-D492.	6.5	76
54	The active site of <i>Trichoderma reesei</i> cellobiohydrolase II: the role of tyrosine 169. <i>Protein Engineering, Design and Selection</i> , 1996, 9, 691-699.	1.0	75

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55	Structure of human semicarbazide-sensitive amine oxidase/vascular adhesion protein-1. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2005, 61, 1550-1562.	2.5	65
56	The future of the protein data bank. <i>Biopolymers</i> , 2013, 99, 218-222.	1.2	65
57	PDBe: Protein Data Bank in Europe. <i>Nucleic Acids Research</i> , 2011, 39, D402-D410.	6.5	64
58	REMBI: Recommended Metadata for Biological Images enabling reuse of microscopy data in biology. <i>Nature Methods</i> , 2021, 18, 1418-1422.	9.0	63
59	Engineering of a glycosidase Family 7 cellobiohydrolase to more alkaline pH optimum: the pH behaviour of <i>Trichoderma reesei</i> Cel7A and its E223S/ A224H/L225V/T226A/D262G mutant. <i>Biochemical Journal</i> , 2001, 356, 19-30.	1.7	59
60	Homo Crystallographicus Quo Vadis?. <i>Structure</i> , 2002, 10, 465-472.	1.6	55
61	New crystal structures of human glutathione transferase A1-1 shed light on glutathione binding and the conformation of the C-terminal helix. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2006, 62, 197-207.	2.5	55
62	Genome3D: a UK collaborative project to annotate genomic sequences with predicted 3D structures based on SCOP and CATH domains. <i>Nucleic Acids Research</i> , 2012, 41, D499-D507.	6.5	53
63	The structures of λ 2u-globulin and its complex with a hyaline droplet inducer. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 753-762.	2.5	50
64	Data management challenges in three-dimensional EM. <i>Nature Structural and Molecular Biology</i> , 2012, 19, 1203-1207.	3.6	49
65	CASP3 comparative modeling evaluation. , 1999, 37, 30-46.		48
66	A 3D cellular context for the macromolecular world. <i>Nature Structural and Molecular Biology</i> , 2014, 21, 841-845.	3.6	47
67	Worldwide Protein Data Bank biocuration supporting open access to high-quality 3D structural biology data. <i>Database: the Journal of Biological Databases and Curation</i> , 2018, 2018, .	1.4	45
68	Validation of ligands in macromolecular structures determined by X-ray crystallography. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 228-236.	1.1	45
69	The BiImage Archive Building a Home for Life-Sciences Microscopy Data. <i>Journal of Molecular Biology</i> , 2022, 434, 167505.	2.0	45
70	Genome3D: exploiting structure to help users understand their sequences. <i>Nucleic Acids Research</i> , 2015, 43, D382-D386.	6.5	42
71	Computer-assisted assignment of 2D ¹ H NMR spectra of proteins: Basic algorithms and application to phoratoxin B. <i>Journal of Biomolecular NMR</i> , 1991, 1, 23-47.	1.6	40
72	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. <i>Nature Structural and Molecular Biology</i> , 2015, 22, 433-434.	3.6	40

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73	On vital aid: the why, what and how of validation. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2009, 65, 134-139.	2.5	39
74	Practical application of bioinformatics by the multidisciplinary VIZIER consortium. <i>Antiviral Research</i> , 2010, 87, 95-110.	1.9	39
75	DÃ©jÃ Vu All Over Again. <i>Structure</i> , 2004, 12, 2103-2111.	1.6	36
76	Structural Basis of the Suppressed Catalytic Activity of Wild-type Human Glutathione Transferase T1-1 Compared to its W234R Mutant. <i>Journal of Molecular Biology</i> , 2006, 355, 96-105.	2.0	36
77	Interactive motif and fold recognition in protein structures. <i>Journal of Applied Crystallography</i> , 2002, 35, 137-139.	1.9	35
78	Web-based visualisation and analysis of 3D electron-microscopy data from EMDB and PDB. <i>Journal of Structural Biology</i> , 2013, 184, 173-181.	1.3	34
79	Interaction Model Based on Local Protein Substructures Generalizes to the Entire Structural Enzyme-Ligand Space. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 2278-2288.	2.5	33
80	How Community Has Shaped the Protein Data Bank. <i>Structure</i> , 2013, 21, 1485-1491.	1.6	33
81	Does NMR Mean "Not for Molecular Replacement"? Using NMR-Based Search Models to Solve Protein Crystal Structures. <i>Structure</i> , 2000, 8, R213-R220.	1.6	31
82	Improving the representation of peptide-like inhibitor and antibiotic molecules in the Protein Data Bank. <i>Biopolymers</i> , 2014, 101, 659-668.	1.2	31
83	Incorporation of a single His residue by rational design enables thiol-ester hydrolysis by human glutathione transferase A1-1. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 13163-13167.	3.3	29
84	Engineering of a glycosidase Family 7 cellobiohydrolase to more alkaline pH optimum: the pH behaviour of <i>Trichoderma reesei</i> Cel7A and its E223S/ A224H/L225V/T226A/D262G mutant. <i>Biochemical Journal</i> , 2001, 356, 19.	1.7	29
85	ValLigURL: a server for ligand-structure comparison and validation. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2007, 63, 935-938.	2.5	28
86	The archiving and dissemination of biological structure data. <i>Current Opinion in Structural Biology</i> , 2016, 40, 17-22.	2.6	28
87	The crystal structure of <i>Echinococcus granulosus</i> fatty-acid-binding protein 1. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2003, 1649, 40-50.	1.1	27
88	The Protein Data Bank in Europe (PDBe): bringing structure to biology. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011, 67, 324-330.	2.5	27
89	A paradigm shift in structural biology. <i>Nature Methods</i> , 2022, 19, 20-23.	9.0	27
90	A chemogenomics view on protein-ligand spaces. <i>BMC Bioinformatics</i> , 2009, 10, S13.	1.2	26

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91	Anwendung und Grenzen kristallographischer Daten im strukturbezogenen Liganden- und Wirkstoff-Design. <i>Angewandte Chemie</i> , 2003, 115, 2822-2841.	1.6	23
92	The 2010 cryo-EM modeling challenge. <i>Biopolymers</i> , 2012, 97, 651-654.	1.2	22
93	Storing diffraction data. <i>Nature</i> , 1996, 383, 18-19.	13.7	19
94	The EBI enzyme portal. <i>Nucleic Acids Research</i> , 2013, 41, D773-D780.	6.5	19
95	On the precision of calculated solvent-accessible surface areas. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2007, 63, 270-274.	2.5	17
96	Case-controlled structure validation. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2009, 65, 140-147.	2.5	17
97	The role of structural bioinformatics resources in the era of integrative structural biology. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 710-721.	2.5	17
98	A versatile approach toward the partially automatic recognition of cross peaks in 2D 1 H NMR spectra. <i>Journal of Magnetic Resonance</i> , 1990, 88, 601-608.	0.5	16
99	Separating model optimization and model validation in statistical cross-validation as applied to crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2007, 63, 939-940.	2.5	16
100	CASP3 comparative modeling evaluation. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 37, 30-46.	1.5	16
101	Towards Proteome-Wide Interaction Models Using the Proteochemometrics Approach. <i>Molecular Informatics</i> , 2010, 29, 499-508.	1.4	15
102	Worldwide Protein Data Bank validation information: usage and trends. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 237-244.	1.1	15
103	Vivaldi: Visualization and validation of biomacromolecular NMR structures from the PDB. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 583-591.	1.5	13
104	Web-based volume slicer for 3D electron-microscopy data from EMDB. <i>Journal of Structural Biology</i> , 2016, 194, 164-170.	1.3	13
105	Toward automatic assignment of protein 1H NMR spectra. <i>Journal of Magnetic Resonance</i> , 1989, 85, 186-197.	0.5	11
106	Structures of cellular retinoic acid binding proteins I and II in complex with synthetic retinoids. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 1850-1857.	2.5	11
107	Structural biology data archiving – where we are and what lies ahead. <i>FEBS Letters</i> , 2018, 592, 2153-2167.	1.3	11
108	Quality Control and Validation. , 2007, 364, 255-272.		10

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109	Validation analysis of EMDB entries. <i>Acta Crystallographica Section D: Structural Biology</i> , 2022, 78, 542-552.	1.1	9
110	Experimental Data for Structure Papers. <i>Science</i> , 2007, 317, 194-195.	6.0	8
111	Straightforward and complete deposition of NMR data to the PDBe. <i>Journal of Biomolecular NMR</i> , 2010, 48, 85-92.	1.6	7
112	Safeguarding the integrity of protein archive. <i>Nature</i> , 2010, 463, 425-425.	13.7	7
113	Data-deposition protocols for correlative soft X-ray tomography and super-resolution structured illumination microscopy applications. <i>STAR Protocols</i> , 2021, 2, 100253.	0.5	7
114	Correlative multimodal imaging: Building a community. <i>Methods in Cell Biology</i> , 2021, 162, 417-430.	0.5	6
115	Whither structural biologists?. <i>IUCrj</i> , 2022, 9, 399-400.	1.0	6
116	Glucomanan and beta-glucan degradation by <i>Mytilus edulis</i> Cel45A: Crystal structure and activity comparison with GH45 subfamily A, B and C. <i>Carbohydrate Polymers</i> , 2022, 277, 118771.	5.1	3
117	Retrieval and Validation of Structural Information. , 2005, , 185-222.		2
118	Chapter 4. Application and Limitations of X-Ray Crystallographic Data in Structure-Guided Ligand and Drug Design. <i>RSC Biomolecular Sciences</i> , 2007, , 73-94.	0.4	2
119	Three-dimensional Structure Databases of Biological Macromolecules. <i>Methods in Molecular Biology</i> , 2022, 2449, 43-91.	0.4	2
120	Application and Limitations of X-Ray Crystallographic Data in Structure-Based Ligand and Drug Design.. <i>ChemInform</i> , 2003, 34, no.	0.1	1
121	Comment on Timely deposition of macromolecular structures is necessary for peer review by Joosten et al. (2013). <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 2296-2296.	2.5	1
122	Image archiving at EMBL-EBI - EMPIAR and the BioImage Archive. <i>Microscopy and Microanalysis</i> , 2021, 27, 2836-2837.	0.2	0
123	STELLA and CLAIRE: A Seraglio of Programs for Human-Aided Assignment of 2D 1H NMR Spectra of Proteins. , 1991, , 427-437.		0