Gerard J Kleywegt

List of Publications by Year in Descending Order

121 papers	12,059 citations	56 h-index	109 g-index
132 ext. papers	15,549 ext. citations	9.7 avg, IF	6.24 L-index

#	Paper	IF	Citations
121	A paradigm shift in structural biology.. *Nature Methods*, **2022**, 19, 20-23	21.6	3
120	Glucomannan and beta-glucan degradation by Mytilus edulis Cel45A: Crystal structure and activity comparison with GH45 subfamily A, B and C. *Carbohydrate Polymers*, **2022**, 277, 118771	10.3	1
119	The BioImage Archive - building a home for life-sciences microscopy data.. *Journal of Molecular Biology*, **2022**, 167505	6.5	3
118	Validation analysis of EMDB entries.. *Acta Crystallographica Section D: Structural Biology*, **2022**, 78, 542-552	3.5	0
117	Three-dimensional Structure Databases of Biological Macromolecules.. *Methods in Molecular Biology*, **2022**, 2449, 43-91	1.4	
116	AlphaFold Protein Structure Database: massively expanding the structural coverage of protein-sequence space with high-accuracy models. *Nucleic Acids Research*, **2021**,	20.1	285
115	Data-deposition protocols for correlative soft X-ray tomography and super-resolution structured illumination microscopy applications. *STAR Protocols*, **2021**, 2, 100253	1.4	3
114	REMBI: Recommended Metadata for Biological Images-enabling reuse of microscopy data in biology. *Nature Methods*, **2021**, 18, 1418-1422	21.6	16
113	Correlative multimodal imaging: Building a community. *Methods in Cell Biology*, **2021**, 162, 417-430	1.8	1
112	Image archiving at EMBL-EBI - EMPIAR and the BioImage Archive. *Microscopy and Microanalysis*, **2021**, 27, 2836-2837	0.5	
111	Highly accurate protein structure prediction for the human proteome. *Nature*, **2021**, 596, 590-596	50.4	399
110	PDBe: improved findability of macromolecular structure data in the PDB. *Nucleic Acids Research*, **2020**, 48, D335-D343	20.1	50
109	Protein Data Bank: the single global archive for 3D macromolecular structure data. *Nucleic Acids Research*, **2019**, 47, D520-D528	20.1	308
108	Structural biology data archiving - where we are and what lies ahead. *FEBS Letters*, **2018**, 592, 2153-2167	3.8	8
107	Validation of ligands in macromolecular structures determined by X-ray crystallography. *Acta Crystallographica Section D: Structural Biology*, **2018**, 74, 228-236	5.5	29
106	Worldwide Protein Data Bank validation information: usage and trends. *Acta Crystallographica Section D: Structural Biology*, **2018**, 74, 237-244	5.5	11
105	Worldwide Protein Data Bank biocuration supporting open access to high-quality 3D structural biology data. *Database: the Journal of Biological Databases and Curation*, **2018**, 2018,	5	31

104	PDBe: towards reusable data delivery infrastructure at protein data bank in Europe. *Nucleic Acids Research*, **2018**, 46, D486-D492	20.1	57
103	OneDep: Unified wwPDB System for Deposition, Biocuration, and Validation of Macromolecular Structures in the PDB Archive. *Structure*, **2017**, 25, 536-545	5.2	86
102	Protein Data Bank (PDB): The Single Global Macromolecular Structure Archive. *Methods in Molecular Biology*, **2017**, 1607, 627-641	1.4	271
101	Validation of Structures in the Protein Data Bank. *Structure*, **2017**, 25, 1916-1927	5.2	130
100	Web-based volume slicer for 3D electron-microscopy data from EMDB. *Journal of Structural Biology*, **2016**, 194, 164-70	3.4	9
99	EMDataBank unified data resource for 3DEM. *Nucleic Acids Research*, **2016**, 44, D396-403	20.1	113
98	PDBe: improved accessibility of macromolecular structure data from PDB and EMDB. *Nucleic Acids Research*, **2016**, 44, D385-95	20.1	111
97	EMPIAR: a public archive for raw electron microscopy image data. *Nature Methods*, **2016**, 13, 387-8	21.6	206
96	Resolution of shapes determined from small-angle scattering. *IUCrJ*, **2016**, 3, 440-447	4.7	69
95	The archiving and dissemination of biological structure data. *Current Opinion in Structural Biology*, **2016**, 40, 17-22	8.1	23
94	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. *Structure*, **2015**, 23, 1156-67	5.2	131
93	Genome3D: exploiting structure to help users understand their sequences. *Nucleic Acids Research*, **2015**, 43, D382-6	20.1	33
92	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. *Nature Structural and Molecular Biology*, **2015**, 22, 433-4	17.6	26
91	The Protein Data Bank archive as an open data resource. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 1009-14	4.2	85
90	A 3D cellular context for the macromolecular world. *Nature Structural and Molecular Biology*, **2014**, 21, 841-5	17.6	33
89	Improving the representation of peptide-like inhibitor and antibiotic molecules in the Protein Data Bank. *Biopolymers*, **2014**, 101, 659-68	2.2	26
88	PDBe: Protein Data Bank in Europe. *Nucleic Acids Research*, **2014**, 42, D285-91	20.1	109
87	Vivaldi: visualization and validation of biomacromolecular NMR structures from the PDB. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 583-91	4.2	12

86	How community has shaped the Protein Data Bank. *Structure*, **2013**, 21, 1485-91	5.2	27
85	The future of the Protein Data Bank. *Biopolymers*, **2013**, 99, 218-22	2.2	61
84	Web-based visualisation and analysis of 3D electron-microscopy data from EMDB and PDB. *Journal of Structural Biology*, **2013**, 184, 173-81	3.4	23
83	Recommendations of the wwPDB NMR Validation Task Force. *Structure*, **2013**, 21, 1563-70	5.2	117
82	The role of structural bioinformatics resources in the era of integrative structural biology. *Acta Crystallographica Section D: Biological Crystallography*, **2013**, 69, 710-21		14
81	Report of the wwPDB Small-Angle Scattering Task Force: data requirements for biomolecular modeling and the PDB. *Structure*, **2013**, 21, 875-81	5.2	65
80	The EBI enzyme portal. *Nucleic Acids Research*, **2013**, 41, D773-80	20.1	13
79	Comment on timely deposition of macromolecular structures is necessary for peer review by Joosten et al. (2013). *Acta Crystallographica Section D: Biological Crystallography*, **2013**, 69, 2296		1
78	SIFTS: Structure Integration with Function, Taxonomy and Sequences resource. *Nucleic Acids Research*, **2013**, 41, D483-9	20.1	181
77	Genome3D: a UK collaborative project to annotate genomic sequences with predicted 3D structures based on SCOP and CATH domains. *Nucleic Acids Research*, **2013**, 41, D499-507	20.1	48
76	The Protein Data Bank at 40: reflecting on the past to prepare for the future. *Structure*, **2012**, 20, 391-6	5.2	93
75	Implementing an X-ray validation pipeline for the Protein Data Bank. *Acta Crystallographica Section D: Biological Crystallography*, **2012**, 68, 478-83		73
74	OMERO: flexible, model-driven data management for experimental biology. *Nature Methods*, **2012**, 9, 245-53	21.6	313
73	Data management challenges in three-dimensional EM. *Nature Structural and Molecular Biology*, **2012**, 19, 1203-7	17.6	34
72	PDBe: Protein Data Bank in Europe. *Nucleic Acids Research*, **2012**, 40, D445-52	20.1	75
71	PSICQUIC and PSISCORE: accessing and scoring molecular interactions. *Nature Methods*, **2011**, 8, 528-9	21.6	227
70	A new generation of crystallographic validation tools for the protein data bank. *Structure*, **2011**, 19, 1395-412	5.2	335
69	The Protein Data Bank in Europe (PDBe): bringing structure to biology. *Acta Crystallographica Section D: Biological Crystallography*, **2011**, 67, 324-30		25

68	EMDataBank.org: unified data resource for CryoEM. *Nucleic Acids Research*, **2011**, 39, D456-64	20.1	209
67	PDBe: Protein Data Bank in Europe. *Nucleic Acids Research*, **2011**, 39, D402-10	20.1	48
66	Safeguarding the integrity of protein archive. *Nature*, **2010**, 463, 425	50.4	7
65	Towards Proteome-Wide Interaction Models Using the Proteochemometrics Approach. *Molecular Informatics*, **2010**, 29, 499-508	3.8	14
64	Straightforward and complete deposition of NMR data to the PDBe. *Journal of Biomolecular NMR*, **2010**, 48, 85-92	3	7
63	Practical application of bioinformatics by the multidisciplinary VIZIER consortium. *Antiviral Research* , **2010**, 87, 95-110	10.8	38
62	A chemogenomics view on protein-ligand spaces. *BMC Bioinformatics*, **2009**, 10 Suppl 6, S13	3.6	24
61	Case-controlled structure validation. *Acta Crystallographica Section D: Biological Crystallography*, **2009**, 65, 140-7		15
60	On vital aid: the why, what and how of validation. *Acta Crystallographica Section D: Biological Crystallography*, **2009**, 65, 134-9		34
59	Limitations and lessons in the use of X-ray structural information in drug design. *Drug Discovery Today*, **2008**, 13, 831-41	8.8	133
58	An alternative method for the evaluation of docking performance: RSR vs RMSD. *Journal of Chemical Information and Modeling*, **2008**, 48, 1411-22	6.1	89
57	Interaction model based on local protein substructures generalizes to the entire structural enzyme-ligand space. *Journal of Chemical Information and Modeling*, **2008**, 48, 2278-88	6.1	30
56	Crystallographic refinement of ligand complexes. *Acta Crystallographica Section D: Biological Crystallography*, **2007**, 63, 94-100		149
55	On the precision of calculated solvent-accessible surface areas. *Acta Crystallographica Section D: Biological Crystallography*, **2007**, 63, 270-4		15
54	ValLigURL: a server for ligand-structure comparison and validation. *Acta Crystallographica Section D: Biological Crystallography*, **2007**, 63, 935-8		25
53	Separating model optimization and model validation in statistical cross-validation as applied to crystallography. *Acta Crystallographica Section D: Biological Crystallography*, **2007**, 63, 939-40		13
52	Chapter 4:Application and Limitations of X-Ray Crystallographic Data in Structure-Guided Ligand and Drug Design. *RSC Biomolecular Sciences*, **2007**, 73-94		2
51	Quality control and validation. *Methods in Molecular Biology*, **2007**, 364, 255-72	1.4	9

50	Experimental data for structure papers. *Science*, **2007**, 317, 194-5	33.3	6
49	Structural basis of the suppressed catalytic activity of wild-type human glutathione transferase T1-1 compared to its W234R mutant. *Journal of Molecular Biology*, **2006**, 355, 96-105	6.5	32
48	New crystal structures of human glutathione transferase A1-1 shed light on glutathione binding and the conformation of the C-terminal helix. *Acta Crystallographica Section D: Biological Crystallography*, **2006**, 62, 197-207		45
47	A survey of left-handed helices in protein structures. *Journal of Molecular Biology*, **2005**, 347, 231-41	6.5	67
46	Retrieval and Validation of Structural Information **2005**, 185-222		
45	Structure of human semicarbazide-sensitive amine oxidase/vascular adhesion protein-1. *Acta Crystallographica Section D: Biological Crystallography*, **2005**, 61, 1550-62		60
44	D□vu all over again: finding and analyzing protein structure similarities. *Structure*, **2004**, 12, 2103-11	5.2	16
43	The Uppsala Electron-Density Server. *Acta Crystallographica Section D: Biological Crystallography*, **2004**, 60, 2240-9		285
42	Towards complete validated models in the next generation of ARP/wARP. *Acta Crystallographica Section D: Biological Crystallography*, **2004**, 60, 2222-9		137
41	Incorporation of a single His residue by rational design enables thiol-ester hydrolysis by human glutathione transferase A1-1. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 13163-7	11.5	25
40	Evaluation of protein fold comparison servers. *Proteins: Structure, Function and Bioinformatics*, **2004** , 54, 260-70	4.2	84
39	Pound-wise but penny-foolish: How well do micromolecules fare in macromolecular refinement?. *Structure*, **2003**, 11, 1051-9	5.2	85
38	Anwendung und Grenzen kristallographischer Daten im strukturbezogenen Liganden- und Wirkstoff-Design. *Angewandte Chemie*, **2003**, 115, 2822-2841	3.6	16
37	Application and Limitations of X-Ray Crystallographic Data in Structure-Based Ligand and Drug Design.. *ChemInform*, **2003**, 34, no		1
36	Application and limitations of X-ray crystallographic data in structure-based ligand and drug design. *Angewandte Chemie - International Edition*, **2003**, 42, 2718-36	16.4	285
35	The crystal structure of Echinococcus granulosus fatty-acid-binding protein 1. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2003**, 1649, 40-50	4	25
34	Homo crystallographicus--quo vadis?. *Structure*, **2002**, 10, 465-72	5.2	45
33	Interactive motif and fold recognition in protein structures. *Journal of Applied Crystallography*, **2002**, 35, 137-139	3.8	27

32	The active site of cellobiohydrolase Cel6A from Trichoderma reesei: the roles of aspartic acids D221 and D175. *Journal of the American Chemical Society*, **2002**, 124, 10015-24	16.4	116
31	Engineering of a glycosidase Family 7 cellobiohydrolase to more alkaline pH optimum: the pH behaviour of Trichoderma reesei Cel7A and its E223S/ A224H/L225V/T226A/D262G mutant. *Biochemical Journal*, **2001**, 356, 19-30	3.8	53
30	Engineering of a glycosidase Family 7 cellobiohydrolase to more alkaline pH optimum: the pH behaviour of Trichoderma reesei Cel7A and its E223S/ A224H/L225V/T226A/D262G mutant. *Biochemical Journal*, **2001**, 356, 19-30	3.8	22
29	Validation of protein crystal structures. *Acta Crystallographica Section D: Biological Crystallography*, **2000**, 56, 249-65		145
28	Does NMR mean "not for molecular replacement"? Using NMR-based search models to solve protein crystal structures. *Structure*, **2000**, 8, R213-20	5.2	29
27	The structures of alpha 2u-globulin and its complex with a hyaline droplet inducer. *Acta Crystallographica Section D: Biological Crystallography*, **1999**, 55, 753-62		43
26	Experimental assessment of differences between related protein crystal structures. *Acta Crystallographica Section D: Biological Crystallography*, **1999**, 55, 1878-84		103
25	Structures of cellular retinoic acid binding proteins I and II in complex with synthetic retinoids. *Acta Crystallographica Section D: Biological Crystallography*, **1999**, 55, 1850-7		11
24	Crystallographic evidence for substrate ring distortion and protein conformational changes during catalysis in cellobiohydrolase Ce16A from trichoderma reesei. *Structure*, **1999**, 7, 1035-45	5.2	150
23	CASP3 comparative modeling evaluation. *Proteins: Structure, Function and Bioinformatics*, **1999**, Suppl 3, 30-46	4.2	43
22	Recognition of spatial motifs in protein structures. *Journal of Molecular Biology*, **1999**, 285, 1887-97	6.5	272
21	CASP3 comparative modeling evaluation. *Proteins: Structure, Function and Bioinformatics*, **1999**, 37, 30-46	4.2	15
20	Databases in protein crystallography. *Acta Crystallographica Section D: Biological Crystallography*, **1998**, 54, 1119-31		387
19	Model building and refinement practice. *Methods in Enzymology*, **1997**, 277, 208-30	1.7	232
18	The crystal structure of the catalytic core domain of endoglucanase I from Trichoderma reesei at 3.6 A resolution, and a comparison with related enzymes. *Journal of Molecular Biology*, **1997**, 272, 383-97	6.5	215
17	Validation of protein models from Calpha coordinates alone. *Journal of Molecular Biology*, **1997**, 273, 371-6	6.5	135
16	Detecting folding motifs and similarities in protein structures. *Methods in Enzymology*, **1997**, 277, 525-45	1.7	255
15	Not your average density. *Structure*, **1997**, 5, 1557-69	5.2	142

14	The active site of Trichoderma reesei cellobiohydrolase II: the role of tyrosine 169. *Protein Engineering, Design and Selection*, **1996**, 9, 691-9	1.9	68
13	Checking your imagination: applications of the free R value. *Structure*, **1996**, 4, 897-904	5.2	360
12	Phi/psi-chology: Ramachandran revisited. *Structure*, **1996**, 4, 1395-400	5.2	478
11	Storing diffraction data. *Nature*, **1996**, 383, 18-9	50.4	16
10	Crystallographic and molecular-modeling studies of lipase B from Candida antarctica reveal a stereospecificity pocket for secondary alcohols. *Biochemistry*, **1995**, 34, 16838-51	3.2	418
9	Crystal structure of the C2 fragment of streptococcal protein G in complex with the Fc domain of human IgG. *Structure*, **1995**, 3, 265-78	5.2	311
8	Where freedom is given, liberties are taken. *Structure*, **1995**, 3, 535-40	5.2	217
7	Crystal structure of an acetylcholinesterase-fasciculin complex: interaction of a three-fingered toxin from snake venom with its target. *Structure*, **1995**, 3, 1355-66	5.2	217
6	Crystal structures of cellular retinoic acid binding proteins I and II in complex with all-trans-retinoic acid and a synthetic retinoid. *Structure*, **1994**, 2, 1241-58	5.2	208
5	Structure determination and refinement of human alpha class glutathione transferase A1-1, and a comparison with the Mu and Pi class enzymes. *Journal of Molecular Biology*, **1993**, 232, 192-212	6.5	428
4	Computer-assisted assignment of 2D 1H NMR spectra of proteins: basic algorithms and application to phoratoxin B. *Journal of Biomolecular NMR*, **1991**, 1, 23-47	3	39
3	STELLA and CLAIRE: A Seraglio of Programs for Human-Aided Assignment of 2D 1H NMR Spectra of Proteins **1991**, 427-437		
2	A versatile approach toward the partially automatic recognition of cross peaks in 2D 1 H NMR spectra. *Journal of Magnetic Resonance*, **1990**, 88, 601-608		8
1	Toward automatic assignment of protein 1H NMR spectra. *Journal of Magnetic Resonance*, **1989**, 85, 186-197		6