

# Gerard J Kleywegt

## List of Publications by Citations

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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	Phi/psi-chology: Ramachandran revisited. <i>Structure</i> , <b>1996</b> , 4, 1395-400	5.2	478
120	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> , <b>1993</b> , 232, 192-212	6.5	428
119	Crystallographic and molecular-modeling studies of lipase B from <i>Candida antarctica</i> reveal a stereospecificity pocket for secondary alcohols. <i>Biochemistry</i> , <b>1995</b> , 34, 16838-51	3.2	418
118	Highly accurate protein structure prediction for the human proteome. <i>Nature</i> , <b>2021</b> , 596, 590-596	50.4	399
117	Databases in protein crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1998</b> , 54, 1119-31		387
116	Checking your imagination: applications of the free R value. <i>Structure</i> , <b>1996</b> , 4, 897-904	5.2	360
115	A new generation of crystallographic validation tools for the protein data bank. <i>Structure</i> , <b>2011</b> , 19, 1395-412	5.4	335
114	OMERO: flexible, model-driven data management for experimental biology. <i>Nature Methods</i> , <b>2012</b> , 9, 245-53	21.6	313
113	Crystal structure of the C2 fragment of streptococcal protein G in complex with the Fc domain of human IgG. <i>Structure</i> , <b>1995</b> , 3, 265-78	5.2	311
112	Protein Data Bank: the single global archive for 3D macromolecular structure data. <i>Nucleic Acids Research</i> , <b>2019</b> , 47, D520-D528	20.1	308
111	The Uppsala Electron-Density Server. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2004</b> , 60, 2240-9		285
110	Application and limitations of X-ray crystallographic data in structure-based ligand and drug design. <i>Angewandte Chemie - International Edition</i> , <b>2003</b> , 42, 2718-36	16.4	285
109	AlphaFold Protein Structure Database: massively expanding the structural coverage of protein-sequence space with high-accuracy models. <i>Nucleic Acids Research</i> , <b>2021</b> ,	20.1	285
108	Recognition of spatial motifs in protein structures. <i>Journal of Molecular Biology</i> , <b>1999</b> , 285, 1887-97	6.5	272
107	Protein Data Bank (PDB): The Single Global Macromolecular Structure Archive. <i>Methods in Molecular Biology</i> , <b>2017</b> , 1607, 627-641	1.4	271
106	Detecting folding motifs and similarities in protein structures. <i>Methods in Enzymology</i> , <b>1997</b> , 277, 525-45	1.7	255
105	Model building and refinement practice. <i>Methods in Enzymology</i> , <b>1997</b> , 277, 208-30	1.7	232

104	PSICQUIC and PSISCORE: accessing and scoring molecular interactions. <i>Nature Methods</i> , <b>2011</b> , 8, 528-9	21.6	227
103	Where freedom is given, liberties are taken. <i>Structure</i> , <b>1995</b> , 3, 535-40	5.2	217
102	Crystal structure of an acetylcholinesterase-fasciculin complex: interaction of a three-fingered toxin from snake venom with its target. <i>Structure</i> , <b>1995</b> , 3, 1355-66	5.2	217
101	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. <i>Journal of Molecular Biology</i> , <b>1997</b> , 272, 383-97	6.5	215
100	EMDataBank.org: unified data resource for CryoEM. <i>Nucleic Acids Research</i> , <b>2011</b> , 39, D456-64	20.1	209
99	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> , <b>1994</b> , 2, 1241-58	5.2	208
98	EMPIAR: a public archive for raw electron microscopy image data. <i>Nature Methods</i> , <b>2016</b> , 13, 387-8	21.6	206
97	SIFTS: Structure Integration with Function, Taxonomy and Sequences resource. <i>Nucleic Acids Research</i> , <b>2013</b> , 41, D483-9	20.1	181
96	Crystallographic evidence for substrate ring distortion and protein conformational changes during catalysis in cellobiohydrolase Ce16A from <i>trichoderma reesei</i> . <i>Structure</i> , <b>1999</b> , 7, 1035-45	5.2	150
95	Crystallographic refinement of ligand complexes. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2007</b> , 63, 94-100		149
94	Validation of protein crystal structures. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2000</b> , 56, 249-65		145
93	Not your average density. <i>Structure</i> , <b>1997</b> , 5, 1557-69	5.2	142
92	Towards complete validated models in the next generation of ARP/wARP. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2004</b> , 60, 2222-9		137
91	Validation of protein models from C $\alpha$ coordinates alone. <i>Journal of Molecular Biology</i> , <b>1997</b> , 273, 371-6	6.5	135
90	Limitations and lessons in the use of X-ray structural information in drug design. <i>Drug Discovery Today</i> , <b>2008</b> , 13, 831-41	8.8	133
89	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. <i>Structure</i> , <b>2015</b> , 23, 1156-67	5.2	131
88	Validation of Structures in the Protein Data Bank. <i>Structure</i> , <b>2017</b> , 25, 1916-1927	5.2	130
87	Recommendations of the wwPDB NMR Validation Task Force. <i>Structure</i> , <b>2013</b> , 21, 1563-70	5.2	117

86	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> , <b>2002</b> , 124, 10015-24	16.4	116
85	EMDataBank unified data resource for 3DEM. <i>Nucleic Acids Research</i> , <b>2016</b> , 44, D396-403	20.1	113
84	PDBe: improved accessibility of macromolecular structure data from PDB and EMDB. <i>Nucleic Acids Research</i> , <b>2016</b> , 44, D385-95	20.1	111
83	PDBe: Protein Data Bank in Europe. <i>Nucleic Acids Research</i> , <b>2014</b> , 42, D285-91	20.1	109
82	Experimental assessment of differences between related protein crystal structures. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1999</b> , 55, 1878-84		103
81	The Protein Data Bank at 40: reflecting on the past to prepare for the future. <i>Structure</i> , <b>2012</b> , 20, 391-6	5.2	93
80	An alternative method for the evaluation of docking performance: RSR vs RMSD. <i>Journal of Chemical Information and Modeling</i> , <b>2008</b> , 48, 1411-22	6.1	89
79	OneDep: Unified wwPDB System for Deposition, Biocuration, and Validation of Macromolecular Structures in the PDB Archive. <i>Structure</i> , <b>2017</b> , 25, 536-545	5.2	86
78	The Protein Data Bank archive as an open data resource. <i>Journal of Computer-Aided Molecular Design</i> , <b>2014</b> , 28, 1009-14	4.2	85
77	Pound-wise but penny-foolish: How well do micromolecules fare in macromolecular refinement?. <i>Structure</i> , <b>2003</b> , 11, 1051-9	5.2	85
76	Evaluation of protein fold comparison servers. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2004</b> , 54, 260-70	4.2	84
75	PDBe: Protein Data Bank in Europe. <i>Nucleic Acids Research</i> , <b>2012</b> , 40, D445-52	20.1	75
74	Implementing an X-ray validation pipeline for the Protein Data Bank. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2012</b> , 68, 478-83		73
73	Resolution of shapes determined from small-angle scattering. <i>IUCrJ</i> , <b>2016</b> , 3, 440-447	4.7	69
72	The active site of <i>Trichoderma reesei</i> cellobiohydrolase II: the role of tyrosine 169. <i>Protein Engineering, Design and Selection</i> , <b>1996</b> , 9, 691-9	1.9	68
71	A survey of left-handed helices in protein structures. <i>Journal of Molecular Biology</i> , <b>2005</b> , 347, 231-41	6.5	67
70	Report of the wwPDB Small-Angle Scattering Task Force: data requirements for biomolecular modeling and the PDB. <i>Structure</i> , <b>2013</b> , 21, 875-81	5.2	65
69	The future of the Protein Data Bank. <i>Biopolymers</i> , <b>2013</b> , 99, 218-22	2.2	61

68	Structure of human semicarbazide-sensitive amine oxidase/vascular adhesion protein-1. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2005</b> , 61, 1550-62		60
67	PDBe: towards reusable data delivery infrastructure at protein data bank in Europe. <i>Nucleic Acids Research</i> , <b>2018</b> , 46, D486-D492	20.1	57
66	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> , <b>2001</b> , 356, 19-30	3.8	53
65	PDBe: improved findability of macromolecular structure data in the PDB. <i>Nucleic Acids Research</i> , <b>2020</b> , 48, D335-D343	20.1	50
64	PDBe: Protein Data Bank in Europe. <i>Nucleic Acids Research</i> , <b>2011</b> , 39, D402-10	20.1	48
63	Genome3D: a UK collaborative project to annotate genomic sequences with predicted 3D structures based on SCOP and CATH domains. <i>Nucleic Acids Research</i> , <b>2013</b> , 41, D499-507	20.1	48
62	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> , <b>2006</b> , 62, 197-207		45
61	Homo crystallographicus--quo vadis?. <i>Structure</i> , <b>2002</b> , 10, 465-72	5.2	45
60	The structures of alpha 2u-globulin and its complex with a hyaline droplet inducer. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1999</b> , 55, 753-62		43
59	CASP3 comparative modeling evaluation. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1999</b> , Suppl 3, 30-46	4.2	43
58	Computer-assisted assignment of 2D 1H NMR spectra of proteins: basic algorithms and application to phoratoxin B. <i>Journal of Biomolecular NMR</i> , <b>1991</b> , 1, 23-47	3	39
57	Practical application of bioinformatics by the multidisciplinary VIZIER consortium. <i>Antiviral Research</i> , <b>2010</b> , 87, 95-110	10.8	38
56	On vital aid: the why, what and how of validation. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2009</b> , 65, 134-9		34
55	Data management challenges in three-dimensional EM. <i>Nature Structural and Molecular Biology</i> , <b>2012</b> , 19, 1203-7	17.6	34
54	Genome3D: exploiting structure to help users understand their sequences. <i>Nucleic Acids Research</i> , <b>2015</b> , 43, D382-6	20.1	33
53	A 3D cellular context for the macromolecular world. <i>Nature Structural and Molecular Biology</i> , <b>2014</b> , 21, 841-5	17.6	33
52	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> , <b>2006</b> , 355, 96-105	6.5	32
51	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> , <b>2018</b> , 2018,	5	31

50	Interaction model based on local protein substructures generalizes to the entire structural enzyme-ligand space. <i>Journal of Chemical Information and Modeling</i> , <b>2008</b> , 48, 2278-88	6.1	30
49	Validation of ligands in macromolecular structures determined by X-ray crystallography. <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2018</b> , 74, 228-236	5.5	29
48	Does NMR mean "not for molecular replacement"? Using NMR-based search models to solve protein crystal structures. <i>Structure</i> , <b>2000</b> , 8, R213-20	5.2	29
47	How community has shaped the Protein Data Bank. <i>Structure</i> , <b>2013</b> , 21, 1485-91	5.2	27
46	Interactive motif and fold recognition in protein structures. <i>Journal of Applied Crystallography</i> , <b>2002</b> , 35, 137-139	3.8	27
45	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. <i>Nature Structural and Molecular Biology</i> , <b>2015</b> , 22, 433-4	17.6	26
44	Improving the representation of peptide-like inhibitor and antibiotic molecules in the Protein Data Bank. <i>Biopolymers</i> , <b>2014</b> , 101, 659-68	2.2	26
43	The Protein Data Bank in Europe (PDBe): bringing structure to biology. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2011</b> , 67, 324-30		25
42	ValligURL: a server for ligand-structure comparison and validation. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2007</b> , 63, 935-8		25
41	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> , <b>2004</b> , 101, 13163-7	11.5	25
40	The crystal structure of Echinococcus granulosus fatty-acid-binding protein 1. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , <b>2003</b> , 1649, 40-50	4	25
39	A chemogenomics view on protein-ligand spaces. <i>BMC Bioinformatics</i> , <b>2009</b> , 10 Suppl 6, S13	3.6	24
38	Web-based visualisation and analysis of 3D electron-microscopy data from EMDB and PDB. <i>Journal of Structural Biology</i> , <b>2013</b> , 184, 173-81	3.4	23
37	The archiving and dissemination of biological structure data. <i>Current Opinion in Structural Biology</i> , <b>2016</b> , 40, 17-22	8.1	23
36	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> , <b>2001</b> , 356, 19-30	3.8	22
35	DJvu all over again: finding and analyzing protein structure similarities. <i>Structure</i> , <b>2004</b> , 12, 2103-11	5.2	16
34	Anwendung und Grenzen kristallographischer Daten im strukturbezogenen Liganden- und Wirkstoff-Design. <i>Angewandte Chemie</i> , <b>2003</b> , 115, 2822-2841	3.6	16
33	Storing diffraction data. <i>Nature</i> , <b>1996</b> , 383, 18-9	50.4	16

32	REMBI: Recommended Metadata for Biological Images-enabling reuse of microscopy data in biology. <i>Nature Methods</i> , <b>2021</b> , 18, 1418-1422	21.6	16
31	Case-controlled structure validation. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2009</b> , 65, 140-7		15
30	On the precision of calculated solvent-accessible surface areas. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2007</b> , 63, 270-4		15
29	CASP3 comparative modeling evaluation. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1999</b> , 37, 30-46.2		15
28	The role of structural bioinformatics resources in the era of integrative structural biology. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2013</b> , 69, 710-21		14
27	Towards Proteome-Wide Interaction Models Using the Proteochemometrics Approach. <i>Molecular Informatics</i> , <b>2010</b> , 29, 499-508	3.8	14
26	The EBI enzyme portal. <i>Nucleic Acids Research</i> , <b>2013</b> , 41, D773-80	20.1	13
25	Separating model optimization and model validation in statistical cross-validation as applied to crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2007</b> , 63, 939-40		13
24	Vivaldi: visualization and validation of biomacromolecular NMR structures from the PDB. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2013</b> , 81, 583-91	4.2	12
23	Worldwide Protein Data Bank validation information: usage and trends. <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2018</b> , 74, 237-244	5.5	11
22	Structures of cellular retinoic acid binding proteins I and II in complex with synthetic retinoids. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1999</b> , 55, 1850-7		11
21	Web-based volume slicer for 3D electron-microscopy data from EMDB. <i>Journal of Structural Biology</i> , <b>2016</b> , 194, 164-70	3.4	9
20	Quality control and validation. <i>Methods in Molecular Biology</i> , <b>2007</b> , 364, 255-72	1.4	9
19	Structural biology data archiving - where we are and what lies ahead. <i>FEBS Letters</i> , <b>2018</b> , 592, 2153-2167.3,8		8
18	A versatile approach toward the partially automatic recognition of cross peaks in 2D 1 H NMR spectra. <i>Journal of Magnetic Resonance</i> , <b>1990</b> , 88, 601-608		8
17	Safeguarding the integrity of protein archive. <i>Nature</i> , <b>2010</b> , 463, 425	50.4	7
16	Straightforward and complete deposition of NMR data to the PDBe. <i>Journal of Biomolecular NMR</i> , <b>2010</b> , 48, 85-92	3	7
15	Experimental data for structure papers. <i>Science</i> , <b>2007</b> , 317, 194-5	33.3	6

14	Toward automatic assignment of protein 1H NMR spectra. <i>Journal of Magnetic Resonance</i> , <b>1989</b> , 85, 186-197	6
13	A paradigm shift in structural biology.. <i>Nature Methods</i> , <b>2022</b> , 19, 20-23	21.6 3
12	Data-deposition protocols for correlative soft X-ray tomography and super-resolution structured illumination microscopy applications. <i>STAR Protocols</i> , <b>2021</b> , 2, 100253	1.4 3
11	The Biolmage Archive - building a home for life-sciences microscopy data.. <i>Journal of Molecular Biology</i> , <b>2022</b> , 167505	6.5 3
10	Chapter 4:Application and Limitations of X-Ray Crystallographic Data in Structure-Guided Ligand and Drug Design. <i>RSC Biomolecular Sciences</i> , <b>2007</b> , 73-94	2
9	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> , <b>2013</b> , 69, 2296	1
8	Application and Limitations of X-Ray Crystallographic Data in Structure-Based Ligand and Drug Design.. <i>ChemInform</i> , <b>2003</b> , 34, no	1
7	Glucomannan 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> , <b>2022</b> , 277, 118771	10.3 1
6	Correlative multimodal imaging: Building a community. <i>Methods in Cell Biology</i> , <b>2021</b> , 162, 417-430	1.8 1
5	Validation analysis of EMDB entries.. <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2022</b> , 78, 542-552	0
4	Retrieval and Validation of Structural Information <b>2005</b> , 185-222	
3	STELLA and CLAIRE: A Seraglio of Programs for Human-Aided Assignment of 2D 1H NMR Spectra of Proteins <b>1991</b> , 427-437	
2	Image archiving at EMBL-EBI - EMPIAR and the Biolmage Archive. <i>Microscopy and Microanalysis</i> , <b>2021</b> , 27, 2836-2837	0.5
1	Three-dimensional Structure Databases of Biological Macromolecules.. <i>Methods in Molecular Biology</i> , <b>2022</b> , 2449, 43-91	1.4