# Gerard J Kleywegt

## List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/4631256/publications.pdf

Version: 2024-02-01

| | | | |
|---|---|---|---|
| 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. Nucleic Acids Research, 2022, 50, D439-D444. | 6.5 | 3,692 |
| 2 | 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. | 5.1 | 3 |
| 3 | A paradigm shift in structural biology. Nature Methods, 2022, 19, 20-23. | 9.0 | 27 |
| 4 | The BioImage Archive â€“ Building a Home for Life-Sciences Microscopy Data. Journal of Molecular Biology, 2022, 434, 167505. | 2.0 | 45 |
| 5 | Validation analysis of EMDB entries. Acta Crystallographica Section D: Structural Biology, 2022, 78, 542-552. | 1.1 | 9 |
| 6 | Three-dimensional Structure Databases of Biological Macromolecules. Methods in Molecular Biology, 2022, 2449, 43-91. | 0.4 | 2 |
| 7 | Whither structural biologists?. IUCrJ, 2022, 9, 399-400. | 1.0 | 6 |
| 8 | Correlative multimodal imaging: Building a community. Methods in Cell Biology, 2021, 162, 417-430. | 0.5 | 6 |
| 9 | Data-deposition protocols for correlative soft X-ray tomography and super-resolution structured illumination microscopy applications. STAR Protocols, 2021, 2, 100253. | 0.5 | 7 |
| 10 | REMBI: Recommended Metadata for Biological Imagesâ€”enabling reuse of microscopy data in biology. Nature Methods, 2021, 18, 1418-1422. | 9.0 | 63 |
| 11 | Image archiving at EMBL-EBI - EMPIAR and the BioImage Archive. Microscopy and Microanalysis, 2021, 27, 2836-2837. | 0.2 | 0 |
| 12 | Highly accurate protein structure prediction for the human proteome. Nature, 2021, 596, 590-596. | 13.7 | 1,773 |
| 13 | PDBe: improved findability of macromolecular structure data in the PDB. Nucleic Acids Research, 2020, 48, D335-D343. | 6.5 | 86 |
| 14 | Protein Data Bank: the single global archive for 3D macromolecular structure data. Nucleic Acids Research, 2019, 47, D520-D528. | 6.5 | 671 |
| 15 | 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, . | 1.4 | 45 |
| 16 | PDBe: towards reusable data delivery infrastructure at protein data bank in Europe. Nucleic Acids Research, 2018, 46, D486-D492. | 6.5 | 76 |
| 17 | Structural biology data archiving â€“ where we are and what lies ahead. FEBS Letters, 2018, 592, 2153-2167. | 1.3 | 11 |
| 18 | Validation of ligands in macromolecular structures determined by X-ray crystallography. Acta Crystallographica Section D: Structural Biology, 2018, 74, 228-236. | 1.1 | 45 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Worldwide Protein Data Bank validation information: usage and trends. Acta Crystallographica Section D: Structural Biology, 2018, 74, 237-244. | 1.1 | 15 |
| 20 | OneDep: Unified wwPDB System for Deposition, Biocuration, and Validation of Macromolecular Structures in the PDB Archive. Structure, 2017, 25, 536-545. | 1.6 | 130 |
| 21 | Protein Data Bank (PDB): The Single Global Macromolecular Structure Archive. Methods in Molecular Biology, 2017, 1607, 627-641. | 0.4 | 592 |
| 22 | Validation of Structures in the Protein Data Bank. Structure, 2017, 25, 1916-1927. | 1.6 | 210 |
| 23 | Resolution ofab initioshapes determined from small-angle scattering. IUCrJ, 2016, 3, 440-447. | 1.0 | 88 |
| 24 | The archiving and dissemination of biological structure data. Current Opinion in Structural Biology, 2016, 40, 17-22. | 2.6 | 28 |
| 25 | Web-based volume slicer for 3D electron-microscopy data from EMDB. Journal of Structural Biology, 2016, 194, 164-170. | 1.3 | 13 |
| 26 | EMDataBank unified data resource for 3DEM. Nucleic Acids Research, 2016, 44, D396-D403. | 6.5 | 230 |
| 27 | PDBe: improved accessibility of macromolecular structure data from PDB and EMDB. Nucleic Acids Research, 2016, 44, D385-D395. | 6.5 | 131 |
| 28 | EMPIAR: a public archive for raw electron microscopy image data. Nature Methods, 2016, 13, 387-388. | 9.0 | 298 |
| 29 | Genome3D: exploiting structure to help users understand their sequences. Nucleic Acids Research, 2015, 43, D382-D386. | 6.5 | 42 |
| 30 | NMR Exchange Format: a unified and open standard for representation of NMR restraint data. Nature Structural and Molecular Biology, 2015, 22, 433-434. | 3.6 | 40 |
| 31 | Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. Structure, 2015, 23, 1156-1167. | 1.6 | 159 |
| 32 | The Protein Data Bank archive as an open data resource. Journal of Computer-Aided Molecular Design, 2014, 28, 1009-1014. | 1.3 | 114 |
| 33 | A 3D cellular context for the macromolecular world. Nature Structural and Molecular Biology, 2014, 21, 841-845. | 3.6 | 47 |
| 34 | Improving the representation of peptideâ€like inhibitor and antibiotic molecules in the Protein Data Bank. Biopolymers, 2014, 101, 659-668. | 1.2 | 31 |
| 35 | PDBe: Protein Data Bank in Europe. Nucleic Acids Research, 2014, 42, D285-D291. | 6.5 | 133 |
| 36 | Vivaldi: Visualization and validation of biomacromolecular NMR structures from the PDB. Proteins: Structure, Function and Bioinformatics, 2013, 81, 583-591. | 1.5 | 13 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | How Community Has Shaped the Protein Data Bank. Structure, 2013, 21, 1485-1491. | 1.6 | 33 |
| 38 | The future of the protein data bank. Biopolymers, 2013, 99, 218-222. | 1.2 | 65 |
| 39 | Web-based visualisation and analysis of 3D electron-microscopy data from EMDB and PDB. Journal of Structural Biology, 2013, 184, 173-181. | 1.3 | 34 |
| 40 | Recommendations of the wwPDB NMR Validation Task Force. Structure, 2013, 21, 1563-1570. | 1.6 | 151 |
| 41 | The role of structural bioinformatics resources in the era of integrative structural biology. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 710-721. | 2.5 | 17 |
| 42 | Report of the wwPDB Small-Angle Scattering Task Force: Data Requirements for Biomolecular Modeling and the PDB. Structure, 2013, 21, 875-881. | 1.6 | 77 |
| 43 | The EBI enzyme portal. Nucleic Acids Research, 2013, 41, D773-D780. | 6.5 | 19 |
| 44 | Comment onTimely deposition of macromolecular structures is necessary for peer reviewby Joostenet al.(2013). Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 2296-2296. | 2.5 | 1 |
| 45 | SIFTS: Structure Integration with Function, Taxonomy and Sequences resource. Nucleic Acids Research, 2012, 41, D483-D489. | 6.5 | 238 |
| 46 | Data management challenges in three-dimensional EM. Nature Structural and Molecular Biology, 2012, 19, 1203-1207. | 3.6 | 49 |
| 47 | PDBe: Protein Data Bank in Europe. Nucleic Acids Research, 2012, 40, D445-D452. | 6.5 | 166 |
| 48 | Genome3D: a UK collaborative project to annotate genomic sequences with predicted 3D structures based on SCOP and CATH domains. Nucleic Acids Research, 2012, 41, D499-D507. | 6.5 | 53 |
| 49 | OMERO: flexible, model-driven data management for experimental biology. Nature Methods, 2012, 9, 245-253. | 9.0 | 478 |
| 50 | The 2010 cryoâ€em modeling challenge. Biopolymers, 2012, 97, 651-654. | 1.2 | 22 |
| 51 | The Protein Data Bank at 40: Reflecting on the Past to Prepare for the Future. Structure, 2012, 20, 391-396. | 1.6 | 120 |
| 52 | Implementing an X-ray validation pipeline for the Protein Data Bank. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 478-483. | 2.5 | 88 |
| 53 | PSICQUIC and PSISCORE: accessing and scoring molecular interactions. Nature Methods, 2011, 8, 528-529. | 9.0 | 274 |
| 54 | A New Generation of Crystallographic Validation Tools for the Protein Data Bank. Structure, 2011, 19, 1395-1412. | 1.6 | 405 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | The Protein Data Bank in Europe (PDBe): bringing structure to biology. Acta Crystallographica Section D: Biological Crystallography, 2011, 67, 324-330. | 2.5 | 27 |
| 56 | EMDataBank.org: unified data resource for CryoEM. Nucleic Acids Research, 2011, 39, D456-D464. | 6.5 | 246 |
| 57 | PDBe: Protein Data Bank in Europe. Nucleic Acids Research, 2011, 39, D402-D410. | 6.5 | 64 |
| 58 | Towards Proteomeâ€“Wide Interaction Models Using the Proteochemometrics Approach. Molecular Informatics, 2010, 29, 499-508. | 1.4 | 15 |
| 59 | Straightforward and complete deposition of NMR data to the PDBe. Journal of Biomolecular NMR, 2010, 48, 85-92. | 1.6 | 7 |
| 60 | Practical application of bioinformatics by the multidisciplinary VIZIER consortium. Antiviral Research, 2010, 87, 95-110. | 1.9 | 39 |
| 61 | Safeguarding the integrity of protein archive. Nature, 2010, 463, 425-425. | 13.7 | 7 |
| 62 | A chemogenomics view on protein-ligand spaces. BMC Bioinformatics, 2009, 10, S13. | 1.2 | 26 |
| 63 | Case-controlled structure validation. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 140-147. | 2.5 | 17 |
| 64 | On vital aid: the why, what and how of validation. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 134-139. | 2.5 | 39 |
| 65 | Limitations and lessons in the use of X-ray structural information in drug design. Drug Discovery Today, 2008, 13, 831-841. | 3.2 | 146 |
| 66 | An Alternative Method for the Evaluation of Docking Performance: RSR vs RMSD. Journal of Chemical Information and Modeling, 2008, 48, 1411-1422. | 2.5 | 166 |
| 67 | Interaction Model Based on Local Protein Substructures Generalizes to the Entire Structural Enzyme-Ligand Space. Journal of Chemical Information and Modeling, 2008, 48, 2278-2288. | 2.5 | 33 |
| 68 | Quality Control and Validation. , 2007, 364, 255-272. | | 10 |
| 69 | Experimental Data for Structure Papers. Science, 2007, 317, 194-195. | 6.0 | 8 |
| 70 | Crystallographic refinement of ligand complexes. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 94-100. | 2.5 | 153 |
| 71 | On the precision of calculated solvent-accessible surface areas. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 270-274. | 2.5 | 17 |
| 72 | ValLigURL: a server for ligand-structure comparison and validation. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 935-938. | 2.5 | 28 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Separating model optimization and model validation in statistical cross-validation as applied to crystallography. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 939-940. | 2.5 | 16 |
| 74 | Chapter 4. Application and Limitations of X-Ray Crystallographic Data in Structure-Guided Ligand and Drug Design. RSC Biomolecular Sciences, 2007, , 73-94. | 0.4 | 2 |
| 75 | 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. | 2.0 | 36 |
| 76 | 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. | 2.5 | 55 |
| 77 | Retrieval and Validation of Structural Information. , 2005, , 185-222. | | 2 |
| 78 | Structure of human semicarbazide-sensitive amine oxidase/vascular adhesion protein-1. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 1550-1562. | 2.5 | 65 |
| 79 | A Survey of Left-handed Helices in Protein Structures. Journal of Molecular Biology, 2005, 347, 231-241. | 2.0 | 83 |
| 80 | DÃ©jÃ Vu All Over Again. Structure, 2004, 12, 2103-2111. | 1.6 | 36 |
| 81 | The Uppsala Electron-Density Server. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 2240-2249. | 2.5 | 324 |
| 82 | Towards complete validated models in the next generation ofARP/wARP. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 2222-2229. | 2.5 | 140 |
| 83 | 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, 13163-13167. | 3.3 | 29 |
| 84 | Pound-Wise but Penny-Foolish. Structure, 2003, 11, 1051-1059. | 1.6 | 90 |
| 85 | Anwendung und Grenzen kristallographischer Daten im strukturbezogenen Liganden- und Wirkstoff-Design. Angewandte Chemie, 2003, 115, 2822-2841. | 1.6 | 23 |
| 86 | Application and Limitations of X-Ray Crystallographic Data in Structure-Based Ligand and Drug Design.. ChemInform, 2003, 34, no. | 0.1 | 1 |
| 87 | Application and Limitations of X-ray Crystallographic Data in Structure-Based Ligand and Drug Design. Angewandte Chemie - International Edition, 2003, 42, 2718-2736. | 7.2 | 331 |
| 88 | The crystal structure of Echinococcus granulosus fatty-acid-binding protein 1. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2003, 1649, 40-50. | 1.1 | 27 |
| 89 | Evaluation of protein fold comparison servers. Proteins: Structure, Function and Bioinformatics, 2003, 54, 260-270. | 1.5 | 97 |
| 90 | The Active Site of Cellobiohydrolase Cel6A fromTrichoderma reesei:Â The Roles of Aspartic Acids D221 and D175. Journal of the American Chemical Society, 2002, 124, 10015-10024. | 6.6 | 133 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | Homo Crystallographicusâ€"Quo Vadis?. Structure, 2002, 10, 465-472. | 1.6 | 55 |
| 92 | Interactive motif and fold recognition in protein structures. Journal of Applied Crystallography, 2002, 35, 137-139. | 1.9 | 35 |
| 93 | 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. | 1.7 | 59 |
| 94 | 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. | 1.7 | 29 |
| 95 | Validation of protein crystal structures. Acta Crystallographica Section D: Biological Crystallography, 2000, 56, 249-265. | 2.5 | 161 |
| 96 | Does NMR Mean â€œNot for Molecular Replacementâ€? Using NMR-Based Search Models to Solve Protein Crystal Structures. Structure, 2000, 8, R213-R220. | 1.6 | 31 |
| 97 | The structures of Î±2u-globulin and its complex with a hyaline droplet inducer. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 753-762. | 2.5 | 50 |
| 98 | Experimental assessment of differences between related protein crystal structures. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 1878-1884. | 2.5 | 104 |
| 99 | Structures of cellular retinoic acid binding proteins I and II in complex with synthetic retinoids. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 1850-1857. | 2.5 | 11 |
| 100 | Crystallographic evidence for substrate ring distortion and protein conformational changes during catalysis in cellobiohydrolase Ce16A from Trichoderma reesei. Structure, 1999, 7, 1035-1045. | 1.6 | 164 |
| 101 | CASP3 comparative modeling evaluation. , 1999, 37, 30-46. | | 48 |
| 102 | Recognition of spatial motifs in protein structures 1 1Edited by J. Thornton. Journal of Molecular Biology, 1999, 285, 1887-1897. | 2.0 | 303 |
| 103 | CASP3 comparative modeling evaluation. Proteins: Structure, Function and Bioinformatics, 1999, 37, 30-46. | 1.5 | 16 |
| 104 | Databases in Protein Crystallography. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 1119-1131. | 2.5 | 412 |
| 105 | [11] Model building and refinement practice. Methods in Enzymology, 1997, 277, 208-230. | 0.4 | 278 |
| 106 | The crystal structure of the catalytic core domain of endoglucanase I from Trichoderma reesei at 3.6 Ã... resolution, and a comparison with related enzymes 1 1Edited by K.Nagai. Journal of Molecular Biology, 1997, 272, 383-397. | 2.0 | 238 |
| 107 | Validation of protein models from Cî± coordinates alone. Journal of Molecular Biology, 1997, 273, 371-376. | 2.0 | 154 |
| 108 | [27] Detecting folding motifs and similarities in protein structures. Methods in Enzymology, 1997, 277, 525-545. | 0.4 | 291 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | Not your average density. Structure, 1997, 5, 1557-1569. | 1.6 | 147 |
| 110 | Checking your imagination: applications of the free R value. Structure, 1996, 4, 897-904. | 1.6 | 379 |
| 111 | Phi/Psi-chology: Ramachandran revisited. Structure, 1996, 4, 1395-1400. | 1.6 | 525 |
| 112 | Storing diffraction data. Nature, 1996, 383, 18-19. | 13.7 | 19 |
| 113 | The active site of Trichoderma reesei cellobiohydrolase II: the role of tyrosine 169. Protein Engineering, Design and Selection, 1996, 9, 691-699. | 1.0 | 75 |
| 114 | Crystal structure of the C2 fragment of streptococcal protein G in complex with the Fc domain of human IgG. Structure, 1995, 3, 265-278. | 1.6 | 340 |
| 115 | Where freedom is given, liberties are taken. Structure, 1995, 3, 535-540. | 1.6 | 244 |
| 116 | Crystal structure of an acetylcholinesteraseâ€“fasciculin complex: interaction of a three-fingered toxin from snake venom with its target. Structure, 1995, 3, 1355-1366. | 1.6 | 232 |
| 117 | Crystallographic and molecular-modeling studies of lipase B from Candida antarctica reveal a stereospecificity pocket for secondary alcohols. Biochemistry, 1995, 34, 16838-16851. | 1.2 | 466 |
| 118 | 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, 1241-1258. | 1.6 | 219 |
| 119 | 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. | 2.0 | 453 |
| 120 | Computer-assisted assignment of 2D1H NMR spectra of proteins: Basic algorithms and application to phoratoxin B. Journal of Biomolecular NMR, 1991, 1, 23-47. | 1.6 | 40 |
| 121 | STELLA and CLAIRE: A Seraglio of Programs for Human-Aided Assignment of 2D 1H NMR Spectra of Proteins. , 1991, , 427-437. | | 0 |
| 122 | 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. | 0.5 | 16 |
| 123 | Toward automatic assignment of protein 1H NMR spectra. Journal of Magnetic Resonance, 1989, 85, 186-197. | 0.5 | 11 |