

# Bernhard Rupp

## List of Publications by Year in descending order

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Version: 2024-02-01

81  
papers

3,878  
citations

147566

31  
h-index

128067

60  
g-index

83  
all docs

83  
docs citations

83  
times ranked

4909  
citing authors

#	ARTICLE	IF	CITATIONS
1	Group depositions to the Protein Data Bank need adequate presentation and different archiving protocol. <i>Protein Science</i> , 2022, 31, 784-786.	3.1	6
2	A VSV-based assay quantifies coronavirus Mpro/3CLpro/Nsp5 main protease activity and chemical inhibition. <i>Communications Biology</i> , 2022, 5, 391.	2.0	9
3	Covid-19.bioreproducibility.org: A web resource for <scp>SARS-CoV</scp>-related structural models. <i>Protein Science</i> , 2021, 30, 115-124.	3.1	15
4	Crystallographic models of SARS-CoV-2 3CL <sup>pro</sup> : in-depth assessment of structure quality and validation. <i>IUCr</i> , 2021, 8, 238-256.	1.0	21
5	Rapid response to emerging biomedical challenges and threats. <i>IUCr</i> , 2021, 8, 395-407.	1.0	5
6	Correcting cis-transgressions in macromolecular structure models. <i>FEBS Journal</i> , 2021, , .	2.2	1
7	The structure of neurofibromin isoform 2 reveals different functional states. <i>Nature</i> , 2021, 599, 315-319.	13.7	22
8	Ligand-centered assessment of SARS-CoV-2 drug target models in the Protein Data Bank. <i>FEBS Journal</i> , 2020, 287, 3703-3718.	2.2	35
9	Structural and functional comparison of fumarylacetoacetate domain containing protein 1 in human and mouse. <i>Bioscience Reports</i> , 2020, 40, .	1.1	2
10	Enzymatic Route toward 6-Methylated Baeocystin and Psilocybin. <i>ChemBioChem</i> , 2019, 20, 2824-2829.	1.3	17
11	Controlled dehydration, structural flexibility and gadolinium MRI contrast compound binding in the human plasma glycoprotein afamin. <i>Acta Crystallographica Section D: Structural Biology</i> , 2019, 75, 1071-1083.	1.1	2
12	Expression, Purification, and Biochemical Characterization of Human Afamin. <i>Journal of Proteome Research</i> , 2018, 17, 1269-1277.	1.8	8
13	Detect, correct, retract: How to manage incorrect structural models. <i>FEBS Journal</i> , 2018, 285, 444-466.	2.2	49
14	Against Method: Table 1 "Cui Bono?". <i>Structure</i> , 2018, 26, 919-923.	1.6	9
15	Validation of Protein-Ligand Crystal Structure Models: Small Molecule and Peptide Ligands. <i>Methods in Molecular Biology</i> , 2017, 1607, 611-625.	0.4	7
16	<i>Twilight</i>reloaded: the peptide experience. <i>Acta Crystallographica Section D: Structural Biology</i> , 2017, 73, 211-222.	1.1	9
17	Structural Evidence for a Role of the Multi-functional Human Glycoprotein Afamin in Wnt Transport. <i>Structure</i> , 2017, 25, 1907-1915.e5.	1.6	29
18	Correcting the record of structural publications requires joint effort of the community and journal editors. <i>FEBS Journal</i> , 2016, 283, 4452-4457.	2.2	31

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19	The N14 anti-afamin antibody Fab: a rare VL1 CDR glycosylation, crystallographic re-sequencing, molecular plasticity and conservativeversusenthusiastic modelling. Acta Crystallographica Section D: Structural Biology, 2016, 72, 1267-1280.	1.1	11
20	Comment on Three X-ray Crystal Structure Papers. Journal of Immunology, 2016, 196, 521-524.	0.4	11
21	Additional Comment on Three X-ray Crystal Structure Papers. Journal of Immunology, 2016, 196, 528-530.	0.4	7
22	Only seeing is believing - the power of evidence and reason. Postepy Biochemii, 2016, 62, 250-256.	0.5	3
23	Reviewing biomolecular crystallography proposals: time for a paradigm change. Trends in Biochemical Sciences, 2015, 40, 419-421.	3.7	4
24	Models of proteinâ€“ligand crystal structures: trust, but verify. Journal of Computer-Aided Molecular Design, 2015, 29, 817-836.	1.3	70
25	Cleaning protocols for crystallization robots: preventing protease contamination. Acta Crystallographica Section F, Structural Biology Communications, 2015, 71, 100-102.	0.4	1
26	The solvent component of macromolecular crystals. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 1023-1038.	2.5	47
27	Approaches to automated protein crystal harvesting. Acta Crystallographica Section F, Structural Biology Communications, 2014, 70, 133-155.	0.4	41
28	Ten years of probabilistic estimates of biocrystal solvent content: new insights <i>via</i> nonparametric kernel density estimate. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 1579-1588.	2.5	57
29	Avoidable errors in deposited macromolecular structures: an impediment to efficient data mining. IUCr, 2014, 1, 179-193.	1.0	58
30	Techniques, tools and best practices for ligand electron-density analysis and results from their application to deposited crystal structures. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 150-167.	2.5	94
31	Visualizing ligand molecules in twilight electron density. Acta Crystallographica Section F: Structural Biology Communications, 2013, 69, 195-200.	0.7	63
32	Model building, refinement and validation. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 325-327.	2.5	1
33	Detection and analysis of unusual features in the structural model and structure-factor data of a birch pollen allergen. Acta Crystallographica Section F: Structural Biology Communications, 2012, 68, 366-376.	0.7	18
34	Protein structure reports in JIMD â€“an important enhancement of journal scope. Journal of Inherited Metabolic Disease, 2011, 34, 563-564.	1.7	0
35	First experiences with semi-autonomous robotic harvesting of protein crystals. Journal of Structural and Functional Genomics, 2011, 12, 77-82.	1.2	15
36	Scientific inquiry, inference and critical reasoning in the macromolecular crystallography curriculum. Journal of Applied Crystallography, 2010, 43, 1242-1249.	1.9	11

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37	Structural basis for abrogated binding between staphylococcal enterotoxin A superantigen vaccine and MHC-III $\beta$ . <i>Protein Science</i> , 2009, 11, 642-651.	3.1	9
38	Performance Evaluation of Shake&#x0026;wARP, A Cluster Enabled Application for Macromolecular Crystallography. , 2009, , .		0
39	Macromolecular Crystallography. <i>Springer Protocols</i> , 2008, , 821-849.	0.1	1
40	Operator-assisted harvesting of protein crystals using a universal micromanipulation robot. <i>Journal of Applied Crystallography</i> , 2007, 40, 539-545.	1.9	26
41	Automated robotic harvesting of protein crystalsâ€”addressing a critical bottleneck or instrumentation overkill?. <i>Journal of Structural and Functional Genomics</i> , 2007, 8, 145-152.	1.2	12
42	Mass spectrometric identification of serine hydrolase OVCA2 in the medulloblastoma cell line DAOY. <i>Cancer Letters</i> , 2006, 241, 235-249.	3.2	11
43	Antibody Elbow Angles are Influenced by their Light Chain Class. <i>Journal of Molecular Biology</i> , 2006, 357, 1566-1574.	2.0	229
44	Real-space solution to the problem of full disclosure. <i>Nature</i> , 2006, 444, 817-817.	13.7	10
45	High Throughput Protein Crystallography. , 2005, , 61-104.		1
46	Structure of pyrR (Rv1379) from <i>Mycobacterium tuberculosis</i> : a persistence gene and protein drug target. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2005, 61, 355-364.	2.5	17
47	The Crystal Structure of Rv1347c, a Putative Antibiotic Resistance Protein from <i>Mycobacterium tuberculosis</i> , Reveals a GCN5-related Fold and Suggests an Alternative Function in Siderophore Biosynthesis. <i>Journal of Biological Chemistry</i> , 2005, 280, 13978-13986.	1.6	42
48	Cocrystal Structures of NC6.8 Fab Identify Key Interactions for High Potency Sweetener Recognition:â€” Implications for the Design of Synthetic Sweeteners. <i>Biochemistry</i> , 2005, 44, 9889-9898.	1.2	9
49	Crystal structure of <i>Clostridium botulinum</i> neurotoxin protease in a product-bound state: Evidence for noncanonical zinc protease activity. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 6888-6893.	3.3	99
50	Distributions of pI versus pH provide prior information for the design of crystallization screening experiments: response to comment on 'Protein isoelectric point as a predictor for increased crystallization screening efficiency'. <i>Bioinformatics</i> , 2004, 20, 2171-2174.	1.8	18
51	Protein isoelectric point as a predictor for increased crystallization screening efficiency. <i>Bioinformatics</i> , 2004, 20, 2162-2168.	1.8	113
52	Laboratory scale structural genomics. <i>Journal of Structural and Functional Genomics</i> , 2004, 5, 147-157.	1.2	17
53	<i>Mycobacterium tuberculosis</i> RmlC epimerase (Rv3465): a promising drug-target structure in the rhamnose pathway. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2004, 60, 895-902.	2.5	34
54	Predictive models for protein crystallization. <i>Methods</i> , 2004, 34, 390-407.	1.9	63

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55	Structural Bioinformatic Approaches to the Discovery of New Antimycobacterial Drugs. <i>Current Pharmaceutical Design</i> , 2004, 10, 3195-3211.	0.9	31
56	Matthews coefficient probabilities: Improved estimates for unit cell contents of proteins, DNA, and protein-nucleic acid complex crystals. <i>Protein Science</i> , 2003, 12, 1865-1871.	3.1	672
57	High-Throughput Crystallography at an Affordable Cost: The TB Structural Genomics Consortium Crystallization Facility. <i>ChemInform</i> , 2003, 34, no.	0.1	0
58	Effective electron-density map improvement and structure validation on a Linux multi-CPU web cluster: The TB Structural Genomics Consortium Bias Removal Web Service. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2003, 59, 2200-2210.	2.5	39
59	Maximum-likelihood crystallization. <i>Journal of Structural Biology</i> , 2003, 142, 162-169.	1.3	41
60	High-Throughput Crystallography at an Affordable Cost: The TB Structural Genomics Consortium Crystallization Facility. <i>Accounts of Chemical Research</i> , 2003, 36, 173-181.	7.6	64
61	Crystal Structure of Mycobacterium tuberculosis Diaminopimelate Decarboxylase, an Essential Enzyme in Bacterial Lysine Biosynthesis. <i>Journal of Biological Chemistry</i> , 2003, 278, 18588-18596.	1.6	72
62	Apolipoprotein E4 Forms a Molten Globule. <i>Journal of Biological Chemistry</i> , 2002, 277, 50380-50385.	1.6	184
63	The TB Structural Genomics Consortium: Providing a Structural Foundation for Drug Discovery. <i>Current Drug Targets Infectious Disorders</i> , 2002, 2, 121-141.	2.1	66
64	Concanavalin A in a dimeric crystal form: revisiting structural accuracy and molecular flexibility. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 735-743.	2.5	35
65	The TB structural genomics consortium crystallization facility: towards automation from protein to electron density. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 1514-1518.	2.5	46
66	The high-speed Hydra-Plus-One system for automated high-throughput protein crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 1523-1526.	2.5	36
67	Two divalent metal ions in the active site of a new crystal form of human apurinic/aprimidinic endonuclease, ape1: implications for the catalytic mechanism 1 Edited by I. A. Wilson. <i>Journal of Molecular Biology</i> , 2001, 307, 1023-1034.	2.0	173
68	Interaction of the N-Terminal Domain of Apolipoprotein E4 with Heparin. <i>Biochemistry</i> , 2001, 40, 2826-2834.	1.2	98
69	Questions about the structure of the botulinum neurotoxin B light chain in complex with a target peptide. , 2001, 8, 663-664.		35
70	Conformational flexibility in the apolipoprotein E amino-terminal domain structure determined from three new crystal forms: Implications for lipid binding. <i>Protein Science</i> , 2000, 9, 886-897.	3.1	47
71	Binding of an Antibody Mimetic of the Human Low Density Lipoprotein Receptor to Apolipoprotein E Is Governed through Electrostatic Forces. <i>Journal of Biological Chemistry</i> , 2000, 275, 7109-7116.	1.6	16
72	Cloning, Expression, and One-Step Purification of the Minimal Essential Domain of the Light Chain of Botulinum Neurotoxin Type A. <i>Protein Expression and Purification</i> , 2000, 19, 125-130.	0.6	28

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73	Structure of polyglutamine. FEBS Letters, 2000, 472, 166-167.	1.3	16
74	Differences in Stability among the Human Apolipoprotein E Isoforms Determined by the Amino-Terminal Domain. Biochemistry, 2000, 39, 11657-11666.	1.2	289
75	Structure of a monoclonal 2E8 Fab antibody fragment specific for the low-density lipoprotein-receptor binding region of apolipoprotein E refined at 1.9. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 122-128.	2.5	13
76	Purification, Characterization, and Crystallization of the Distal BRCT Domain of the Human XRCC1 DNA Repair Protein. Protein Expression and Purification, 1999, 16, 236-242.	0.6	7
77	Carboxyl-Terminal Domain of Human Apolipoprotein E: Expression, Purification, and Crystallization. Protein Expression and Purification, 1999, 17, 267-272.	0.6	26
78	Cadmium-induced crystallization of proteins: II. Crystallization of the Salmonella typhimuri histidine-binding protein in complex with histidine, arginine, or lysine. Protein Science, 1998, 7, 600-604.	3.1	30
79	Random coil conformation for extended polyglutamine stretches in aqueous soluble monomeric peptides. Chemical Biology and Drug Design, 1997, 50, 73-75.	1.2	99
80	Novel mechanism for defective receptor binding of apolipoprotein E2 in type III hyperlipoproteinemia. Nature Structural and Molecular Biology, 1996, 3, 718-722.	3.6	115
81	Biomolecular Crystallography. , 0, , .		98