

# Thomas R Schneider

## List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Ground-state destabilization by electrostatic repulsion is not a driving force in orotidine-5- $\alpha$ -monophosphate decarboxylase catalysis. <i>Nature Catalysis</i> , 2022, 5, 332-341.	34.4	12
2	Structural insights into the inhibition of glycine reuptake. <i>Nature</i> , 2021, 591, 677-681.	27.8	69
3	X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease. <i>Science</i> , 2021, 372, 642-646.	12.6	240
4	Profiling cellular diversity in sponges informs animal cell type and nervous system evolution. <i>Science</i> , 2021, 374, 717-723.	12.6	111
5	The structural bases for agonist diversity in an <i>Arabidopsis thaliana</i> glutamate receptor-like channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 752-760.	7.1	70
6	<i>MXCuBE2</i> : the dawn of <i>MXCuBE</i> Collaboration. <i>Journal of Synchrotron Radiation</i> , 2019, 26, 393-405.	2.4	30
7	Liquid application method for time-resolved analyses by serial synchrotron crystallography. <i>Nature Methods</i> , 2019, 16, 979-982.	19.0	74
8	Optical performance and radiation stability of polymer X-ray refractive nano-lenses. <i>Journal of Synchrotron Radiation</i> , 2019, 26, 714-719.	2.4	12
9	An NAD <sup>+</sup> Phosphorylase Toxin Triggers <i>Mycobacterium tuberculosis</i> Cell Death. <i>Molecular Cell</i> , 2019, 73, 1282-1291.e8.	9.7	58
10	Clustering of atomic displacement parameters in bovine trypsin reveals a distributed lattice of atoms with shared chemical properties. <i>Scientific Reports</i> , 2019, 9, 19281.	3.3	7
11	Long-wavelength <i>Mesh&amp;Collect</i> native SAD phasing from microcrystals. <i>Acta Crystallographica Section D: Structural Biology</i> , 2019, 75, 192-199.	2.3	8
12	Visualization of protein crystals by high-energy phase-contrast X-ray imaging. <i>Acta Crystallographica Section D: Structural Biology</i> , 2019, 75, 947-958.	2.3	16
13	The structure of the N-terminal module of the cell wall hydrolase RipA and its role in regulating catalytic activity. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 912-923.	2.6	26
14	Microfluidic Chips for <i>In Situ</i> Crystal X-ray Diffraction and <i>In Situ</i> Dynamic Light Scattering for Serial Crystallography. <i>Journal of Visualized Experiments</i> , 2018, , .	0.3	16
15	Structural and Functional Characterization of the BcsG Subunit of the Cellulose Synthase in <i>Salmonella typhimurium</i> . <i>Journal of Molecular Biology</i> , 2018, 430, 3170-3189.	4.2	29
16	Identification of the point of diminishing returns in high-multiplicity data collection for sulfur SAD phasing. <i>Journal of Synchrotron Radiation</i> , 2017, 24, 19-28.	2.4	4
17	Core Mediator structure at 3.4 Å... extends model of transcription initiation complex. <i>Nature</i> , 2017, 545, 248-251.	27.8	100
18	Rat ceruloplasmin: a new labile copper binding site and zinc/copper mosaic. <i>Metallomics</i> , 2017, 9, 1828-1838.	2.4	14

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19	P13, the EMBL macromolecular crystallography beamline at the low-emittance PETRA III ring for high- and low-energy phasing with variable beam focusing. <i>Journal of Synchrotron Radiation</i> , 2017, 24, 323-332.	2.4	155
20	Bayesian analysis of non-thermal structural changes induced by terahertz radiation in protein crystals. , 2016, , .		0
21	A multicrystal diffraction data-collection approach for studying structural dynamics with millisecond temporal resolution. <i>IUCr</i> , 2016, 3, 393-401.	2.2	19
22	Data collection with a tailored X-ray beam size at 2.69 Å wavelength (4.6 keV): sulfur SAD phasing of Cdc23Nterm. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 403-412.	2.3	10
23	Advances in experimental phasing. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 291-292.	2.3	0
24	The inhibition mechanism of human 20 S proteasomes enables next-generation inhibitor design. <i>Science</i> , 2016, 353, 594-598.	12.6	170
25	Terahertz radiation induces non-thermal structural changes associated with Frhlich condensation in a protein crystal. <i>Structural Dynamics</i> , 2015, 2, 054702.	2.3	56
26	3-Sulfino-propionyl-coenzyme A (3SP-CoA) desulfonase from <i>Advenella mimigardefordensis</i> DPN7 <sup>T</sup> : crystal structure and function of a desulfonase with an acyl-CoA dehydrogenase fold. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 1360-1372.	2.5	6
27	A novel Î <sup>2</sup> -xylosidase structure from <i>Geobacillus thermoglucosidasius</i> : the first crystal structure of a glycoside hydrolase family GH52 enzyme reveals unpredicted similarity to other glycoside hydrolase folds. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 1366-1374.	2.5	17
28	Serial crystallography on <i>in vivo</i> grown microcrystals using synchrotron radiation. <i>IUCr</i> , 2014, 1, 87-94.	2.2	204
29	Crystal Structure of the Gamma-2 Herpesvirus LANA DNA Binding Domain Identifies Charged Surface Residues Which Impact Viral Latency. <i>PLoS Pathogens</i> , 2013, 9, e1003673.	4.7	33
30	SCEDS: protein fragments for molecular replacement in <i>Phaser</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 2216-2225.	2.5	16
31	Alignment of protein structures in the presence of domain motions. <i>BMC Bioinformatics</i> , 2008, 9, 352.	2.6	44
32	RAPIDO: a web server for the alignment of protein structures in the presence of conformational changes. <i>Nucleic Acids Research</i> , 2008, 36, W42-W46.	14.5	99
33	Synchrotron radiation: Micrometer-sized x-ray beams as fine tools for macromolecular crystallography. <i>HFSP Journal</i> , 2008, 2, 302-306.	2.5	11
34	Crystal Structure of the Ubiquitin Binding Domains of Rabex-5 Reveals Two Modes of Interaction with Ubiquitin. <i>Cell</i> , 2006, 124, 1183-1195.	28.9	259
35	Ultrahigh-resolution study of protein atomic displacement parameters at cryotemperatures obtained with a helium cryostat. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2006, 62, 1535-1544.	2.5	16
36	SITCOM: a program for comparing sites in macromolecular substructures. <i>Journal of Applied Crystallography</i> , 2006, 39, 618-619.	4.5	10

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37	Structure of Ecalactin, a trypsin inhibitor II (EETI-II): a rigid molecular scaffold. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2005, 61, 1255-1262.	2.5	38
38	Mechanism of Aurora B Activation by INCENP and Inhibition by Hesperadin. <i>Molecular Cell</i> , 2005, 18, 379-391.	9.7	354
39	Structural Basis for the Autoinhibition and STI-571 Inhibition of c-Kit Tyrosine Kinase. <i>Journal of Biological Chemistry</i> , 2004, 279, 31655-31663.	3.4	533
40	Subatomic and atomic crystallographic studies of aldose reductase: implications for inhibitor binding. <i>Cellular and Molecular Life Sciences</i> , 2004, 61, 763-773.	5.4	29
41	Ultrahigh resolution drug design. II. Atomic resolution structures of human aldose reductase holoenzyme complexed with fidarestat and minalrestat: Implications for the binding of cyclic imide inhibitors. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 55, 805-813.	2.6	83
42	Ultrahigh resolution drug design I: Details of interactions in human aldose reductase-inhibitor complex at 0.66 Å... <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 55, 792-804.	2.6	280
43	The crystallographic structure of the aldose reductase-IDD552 complex shows direct proton donation from tyrosine 48. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2004, 60, 1347-1354.	2.5	29
44	Domain identification by iterative analysis of error-scaled difference distance matrices. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2004, 60, 2269-2275.	2.5	31
45	<i>HKL2MAP</i>; a graphical user interface for macromolecular phasing with <i>SHELX</i> programs. <i>Journal of Applied Crystallography</i> , 2004, 37, 843-844.	4.5	681
46	Substrate and Metal Complexes of 3-Deoxy-d-arabino-heptulosonate-7-phosphate Synthase from <i>Saccharomyces cerevisiae</i> Provide New Insights into the Catalytic Mechanism. <i>Journal of Molecular Biology</i> , 2004, 337, 675-690.	4.2	45
47	Use of multiple anomalous dispersion to phase highly merohedrally twinned crystals of interleukin-1 $\beta$ . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2003, 59, 290-298.	2.5	14
48	Structure of the $\alpha$ -amylase inhibitor tendamistat at 0.93 Å... <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2003, 59, 1737-1743.	2.5	6
49	Optimization of selenium substructures as obtained from SHELXD. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2003, 59, 1987-1994.	2.5	8
50	Molecular basis for redox-Bohr and cooperative effects in cytochrome c3 from <i>Desulfovibrio desulfuricans</i> ATCC 27774: Crystallographic and modeling studies of oxidized and reduced high-resolution structures at pH 7.6. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 54, 135-152.	2.6	20
51	Structural Information Content at High Resolution: MAD versus Native. <i>Methods in Enzymology</i> , 2003, 374, 321-341.	1.0	7
52	Evolution of feedback-inhibited $\alpha$ / $\beta$ barrel isoenzymes by gene duplication and a single mutation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003, 100, 862-867.	7.1	114
53	Automatic Solution of Heavy-Atom Substructures. <i>Methods in Enzymology</i> , 2003, 374, 37-83.	1.0	34
54	Stereoselective Synthesis of the Two trans-(16-Hydroxymethyl)-3-methoxy-13 $\beta$ -estra-1,3,5(10)-trien-17-ol Isomers. <i>Collection of Czechoslovak Chemical Communications</i> , 2003, 68, 1141-1148.	1.0	6

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55	A genetic algorithm for the identification of conformationally invariant regions in protein molecules. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 195-208.	2.5	118
56	Substructure solution with SHELXD. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 1772-1779.	2.5	1,481
57	3-Methoxy-1-phenyl-4,5-dihydro-1H-pyrazolo[4,3-b]estra-1,3,5(10)-triene. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2002, 58, o810-o811.	0.2	2
58	Stereoselective synthesis of some novel heterocyclic estrone derivatives by intramolecular 1,3-dipolar cycloaddition. <i>Tetrahedron</i> , 2002, 58, 6843-6849.	1.9	37
59	Crystal structure of the endosomal SNARE complex reveals common structural principles of all SNAREs. <i>Nature Structural Biology</i> , 2002, 9, 107-111.	9.7	239
60	Silylhydrazine und dimere N,N-Dilithium-N,N-bis(silyl)hydrazide - Synthesen, Reaktionen, Isomerisierungen. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2001, 627, 2581-2588.	1.2	15
61	X-ray snapshots of serine protease catalysis reveal a tetrahedral intermediate. <i>Nature Structural Biology</i> , 2001, 8, 689-694.	9.7	96
62	The First Structurally Characterized Aluminum Compounds with Terminal Acetylide Groups. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 3099-3101.	13.8	36
63	Alumoxane Hydride and Aluminum Chalcogenide Hydride Compounds with Pyrazolato Ligands. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 4276-4279.	13.8	36
64	A steroidal phenyldihydro-1,3-oxazine derivative. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2000, 56, e363-e364.	0.4	6
65	Ab initio structure determination of the lantibiotic mersacidin. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2000, 56, 705-713.	2.5	27
66	Objective comparison of protein structures: error-scaled difference distance matrices. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2000, 56, 714-721.	2.5	79
67	Protein-protein recognition, hydride transfer and proton pumping in the transhydrogenase complex I. Because Structure with Folding & Design operates a "Continuous Publication System" for Research Papers, this paper has been published on the internet before being printed (accessed from) <a href="http://www.structure.org/structure/2000/8/000-015">http://www.structure.org/structure/2000/8/000-015</a>	13.8	45
68	Asymmetric Tris- and Cyclic Silylhydroxylamines from Trimeric and Tetrameric Lithium N,N-Bis(silyl)hydroxylamides. <i>Organometallics</i> , 2000, 19, 5376-5383.	2.3	31
69	1.7 Å structure of the stabilized REIv mutant T39K. Application of local NCS restraints. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 1158-1167.	2.5	29
70	Crystallization and preliminary X-ray analysis of 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase (tyrosine inhibitable) from <i>Saccharomyces cerevisiae</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 1586-1588.	2.5	5
71	Structure of catalase HPII from <i>Escherichia coli</i> at 1.9 Å resolution. , 1999, 34, 155-166.		60
72	Influence of internal dynamics on accuracy of protein NMR structures: derivation of realistic model distance data from a long molecular dynamics trajectory. Edited by G. Von Heijne. <i>Journal of Molecular Biology</i> , 1999, 285, 727-740.	4.2	38

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73	Structure of Balhimycin and its Complex with Solvent Molecules. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 175-183.	2.5	19
74	Refinement of Triclinic Hen Egg-White Lysozyme at Atomic Resolution. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 522-546.	2.5	100
75	Loop Closure and Intersubunit Communication in Tryptophan Synthase., Biochemistry, 1998, 37, 5394-5406.	2.5	146
76	[16] SHELXL: High-resolution refinement. Methods in Enzymology, 1997, , 319-343.	1.0	2,318
77	X-ray crystallography reveals stringent conservation of protein fold after removal of the only disulfide bridge from a stabilized immunoglobulin variable domain. Folding & Design, 1997, 2, 357-361.	4.5	18
78	Macromolecular Cryocrystallography. Journal of Applied Crystallography, 1997, 30, 211-237.	4.5	242
79	X-ray structure determination of a metastable state of carbonmonoxy myoglobin after photodissociation.. Proceedings of the National Academy of Sciences of the United States of America, 1996, 93, 7013-7016.	7.1	135
80	Refinement of 2-Amino-6-(4-methyl-1-piperazinyl)-4-(tricyclo[3.3.1.1 <sup>3,7</sup> ]dec-1-yl)-1,3,5-triazine at Three Different Temperatures using Image-Plate Data. Journal of Applied Crystallography, 1996, 29, 261-264.	4.5	1
81	Crystal structure of vancomycin. Structure, 1996, 4, 1509-1515.	3.3	179
82	Contribution of the intramolecular disulfide bridge to the folding stability of REIv, the variable domain of a human immunoglobulin Î <sup>l</sup> light chain. Folding & Design, 1996, 1, 431-440.	4.5	61
83	Comparison of different X-ray data-collection systems using the crystal structure of octreotide. Acta Crystallographica Section D: Biological Crystallography, 1995, 51, 60-68.	2.5	5
84	Crystal structure of domain A ofThermus flavus5S rRNA and the contribution of water molecules to its structure. FEBS Letters, 1994, 351, 159-164.	2.8	59