

# Thomas R Schneider

## List of Publications by Citations

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83  
papers

8,360  
citations

34  
h-index

88  
g-index

88  
ext. papers

9,002  
ext. citations

10.4  
avg, IF

6.03  
L-index

| #  | Paper   | IF   | Citations |
|----|---|------|-----------|
| 83 | [16] SHELXL: High-resolution refinement. <i>Methods in Enzymology</i> , <b>1997</b> , 319-343   | 1.7  | 1940      |
| 82 | Substructure solution with SHELXD. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2002</b> , 58, 1772-9   |      | 1408      |
| 81 | HKL2MAP: a graphical user interface for macromolecular phasing with SHELX programs. <i>Journal of Applied Crystallography</i> , <b>2004</b> , 37, 843-844   | 3.8  | 599       |
| 80 | Structural basis for the autoinhibition and STI-571 inhibition of c-Kit tyrosine kinase. <i>Journal of Biological Chemistry</i> , <b>2004</b> , 279, 31655-63   | 5.4  | 470       |
| 79 | Mechanism of Aurora B activation by INCENP and inhibition by hesperadin. <i>Molecular Cell</i> , <b>2005</b> , 18, 379-386  | 4.6  | 321       |
| 78 | Crystal structure of the ubiquitin binding domains of rabex-5 reveals two modes of interaction with ubiquitin. <i>Cell</i> , <b>2006</b> , 124, 1183-95   | 56.2 | 233       |
| 77 | 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> , <b>2004</b> , 55, 792-804                      | 4.2  | 232       |
| 76 | Macromolecular Cryocrystallography. <i>Journal of Applied Crystallography</i> , <b>1997</b> , 30, 211-237   | 3.8  | 220       |
| 75 | Crystal structure of the endosomal SNARE complex reveals common structural principles of all SNAREs. <i>Nature Structural Biology</i> , <b>2002</b> , 9, 107-11   |      | 207       |
| 74 | Serial crystallography on in vivo grown microcrystals using synchrotron radiation. <i>IUCrJ</i> , <b>2014</b> , 1, 87-94  | 4.7  | 164       |
| 73 | Crystal structure of vancomycin. <i>Structure</i> , <b>1996</b> , 4, 1509-15  | 5.2  | 150       |
| 72 | Loop closure and intersubunit communication in tryptophan synthase. <i>Biochemistry</i> , <b>1998</b> , 37, 5394-406  | 3.2  | 135       |
| 71 | X-ray structure determination of a metastable state of carbon monoxide myoglobin after photodissociation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>1996</b> , 93, 7013-6 | 11.5 | 131       |
| 70 | The inhibition mechanism of human 20S proteasomes enables next-generation inhibitor design. <i>Science</i> , <b>2016</b> , 353, 594-8   | 33.3 | 123       |
| 69 | A genetic algorithm for the identification of conformationally invariant regions in protein molecules. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2002</b> , 58, 195-208                      |      | 113       |
| 68 | X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease. <i>Science</i> , <b>2021</b> , 372, 642-646   | 33.3 | 95        |
| 67 | Evolution of feedback-inhibited beta /alpha barrel isoenzymes by gene duplication and a single mutation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2003</b> , 100, 862-7  | 11.5 | 94        |

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| 66 | RAPIDO: a web server for the alignment of protein structures in the presence of conformational changes. <i>Nucleic Acids Research</i> , <b>2008</b> , 36, W42-6  | 20.1 | 91 |
| 65 | X-ray snapshots of serine protease catalysis reveal a tetrahedral intermediate. <i>Nature Structural Biology</i> , <b>2001</b> , 8, 689-94   |      | 89 |
| 64 | Refinement of triclinic hen egg-white lysozyme at atomic resolution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1998</b> , 54, 522-46  |      | 85 |
| 63 | 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> , <b>2017</b> , 24, 323-332  | 2.4  | 84 |
| 62 | Core Mediator structure at 3.4 Å extends model of transcription initiation complex. <i>Nature</i> , <b>2017</b> , 545, 248-251   | 50.4 | 74 |
| 61 | Objective comparison of protein structures: error-scaled difference distance matrices. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2000</b> , 56, 714-21  |      | 74 |
| 60 | 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> , <b>2004</b> , 55, 805-13 | 4.2  | 66 |
| 59 | Contribution of the intramolecular disulfide bridge to the folding stability of REIV, the variable domain of a human immunoglobulin kappa light chain. <i>Folding &amp; Design</i> , <b>1996</b> , 1, 431-40   |      | 59 |
| 58 | Protein-protein recognition, hydride transfer and proton pumping in the transhydrogenase complex. <i>Structure</i> , <b>2000</b> , 8, 809-15   | 5.2  | 53 |
| 57 | Crystal structure of domain A of <i>Thermus flavus</i> 5S rRNA and the contribution of water molecules to its structure. <i>FEBS Letters</i> , <b>1994</b> , 351, 159-64   | 3.8  | 53 |
| 56 | Structure of catalase HPII from <i>Escherichia coli</i> at 1.9 Å resolution. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1999</b> , 34, 155-66  | 4.2  | 51 |
| 55 | Liquid application method for time-resolved analyses by serial synchrotron crystallography. <i>Nature Methods</i> , <b>2019</b> , 16, 979-982  | 21.6 | 41 |
| 54 | Alignment of protein structures in the presence of domain motions. <i>BMC Bioinformatics</i> , <b>2008</b> , 9, 352  | 3.6  | 41 |
| 53 | Terahertz radiation induces non-thermal structural changes associated with Fröhlich condensation in a protein crystal. <i>Structural Dynamics</i> , <b>2015</b> , 2, 054702  | 3.2  | 37 |
| 52 | 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> , <b>2004</b> , 337, 675-90  | 6.5  | 37 |
| 51 | The structural bases for agonist diversity in an glutamate receptor-like channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2020</b> , 117, 752-760  | 11.5 | 37 |
| 50 | An NAD Phosphorylase Toxin Triggers Mycobacterium tuberculosis Cell Death. <i>Molecular Cell</i> , <b>2019</b> , 73, 1282-1291.e8  | 17.6 | 37 |
| 49 | Stereoselective synthesis of some novel heterocyclic estrone derivatives by intramolecular 1,3-dipolar cycloaddition. <i>Tetrahedron</i> , <b>2002</b> , 58, 6843-6849   | 2.4  | 34 |

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|----|--|------|----|
| 48 | Structure of Ecballium elaterium trypsin inhibitor II (EETI-II): a rigid molecular scaffold. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2005</b> , 61, 1255-62   |      | 33 |
| 47 | Influence of internal dynamics on accuracy of protein NMR structures: derivation of realistic model distance data from a long molecular dynamics trajectory. <i>Journal of Molecular Biology</i> , <b>1999</b> , 285, 727-40 <sup>6.5</sup>  |      | 33 |
| 46 | Alumoxane Hydride and Aluminum Chalcogenide Hydride Compounds with Pyrazolato Ligands. <i>Angewandte Chemie - International Edition</i> , <b>2000</b> , 39, 4276-4279  | 16.4 | 32 |
| 45 | Automatic solution of heavy-atom substructures. <i>Methods in Enzymology</i> , <b>2003</b> , 374, 37-83  | 1.7  | 31 |
| 44 | Domain identification by iterative analysis of error-scaled difference distance matrices. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2004</b> , 60, 2269-75  |      | 31 |
| 43 | The First Structurally Characterized Aluminum Compounds with Terminal Acetylide Groups This work was supported by the Deutsche Forschungsgemeinschaft. N.C.M.-Z. thanks the Schweizerischer Nationalfonds for a fellowship. <i>Angewandte Chemie - International Edition</i> , <b>2000</b> , 39, 3000-3101         | 16.4 | 31 |
| 42 | Subatomic and atomic crystallographic studies of aldose reductase: implications for inhibitor binding. <i>Cellular and Molecular Life Sciences</i> , <b>2004</b> , 61, 763-73  | 10.3 | 28 |
| 41 | Crystal structure of the gamma-2 herpesvirus LANA DNA binding domain identifies charged surface residues which impact viral latency. <i>PLoS Pathogens</i> , <b>2013</b> , 9, e1003673   | 7.6  | 25 |
| 40 | The crystallographic structure of the aldose reductase-IDD552 complex shows direct proton donation from tyrosine 48. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2004</b> , 60, 1347-54   |      | 25 |
| 39 | Ab initio structure determination of the lantibiotic mersacidin. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2000</b> , 56, 705-13  |      | 25 |
| 38 | Asymmetric Tris- and Cyclic Silylhydroxylamines from Trimeric and Tetrameric Lithium N,N-Bis(silyl)hydroxylamides. <i>Organometallics</i> , <b>2000</b> , 19, 5376-5383  | 3.8  | 25 |
| 37 | 1.7 Å structure of the stabilized REIv mutant T39K. Application of local NCS restraints. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1999</b> , 55, 1158-67   |      | 25 |
| 36 | Structural and Functional Characterization of the BcsG Subunit of the Cellulose Synthase in <i>Salmonella typhimurium</i> . <i>Journal of Molecular Biology</i> , <b>2018</b> , 430, 3170-3189   | 6.5  | 19 |
| 35 | X-ray crystallography reveals stringent conservation of protein fold after removal of the only disulfide bridge from a stabilized immunoglobulin variable domain. <i>Folding &amp; Design</i> , <b>1997</b> , 2, 357-61  |      | 18 |
| 34 | Structural insights into the inhibition of glycine reuptake. <i>Nature</i> , <b>2021</b> , 591, 677-681  | 50.4 | 18 |
| 33 | Structure of balhimycin and its complex with solvent molecules. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1998</b> , 54, 175-83   |      | 17 |
| 32 | 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> , <b>2004</b> , 54, 135-52 | 4.2  | 17 |
| 31 | 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> , <b>2018</b> , 86, 912-923  | 4.2  | 16 |

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|----|--|------|----|
| 30 | Profiling cellular diversity in sponges informs animal cell type and nervous system evolution. <i>Science</i> , <b>2021</b> , 374, 717-723   | 33.3 | 15 |
| 29 | MXCuBE2: the dawn of MXCuBE Collaboration. <i>Journal of Synchrotron Radiation</i> , <b>2019</b> , 26, 393-405   | 2.4  | 14 |
| 28 | A novel Glycosidase 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> , <b>2014</b> , 70, 1366-74 |      | 14 |
| 27 | Ultrahigh-resolution study of protein atomic displacement parameters at cryotemperatures obtained with a helium cryostat. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2006</b> , 62, 1535-44  |      | 14 |
| 26 | A multocrystal diffraction data-collection approach for studying structural dynamics with millisecond temporal resolution. <i>IUCrJ</i> , <b>2016</b> , 3, 393-401   | 4.7  | 14 |
| 25 | Microfluidic Chips for In Situ Crystal X-ray Diffraction and In Situ Dynamic Light Scattering for Serial Crystallography. <i>Journal of Visualized Experiments</i> , <b>2018</b> ,   | 1.6  | 14 |
| 24 | Rat ceruloplasmin: a new labile copper binding site and zinc/copper mosaic. <i>Metallomics</i> , <b>2017</b> , 9, 1828-1838  | 4.3  | 13 |
| 23 | Use of multiple anomalous dispersion to phase highly merohedrally twinned crystals of interleukin-1beta. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2003</b> , 59, 290-8   |      | 13 |
| 22 | SCEDS: protein fragments for molecular replacement in Phaser. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2013</b> , 69, 2216-25  |      | 12 |
| 21 | Silylhydrazine und dimere N,N'-Dilithium-N,N'-bis(silyl)hydrazide [Synthesen, Reaktionen, Isomerisierungen. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2001</b> , 627, 2581-2588   | 1.3  | 12 |
| 20 | Synchrotron radiation: micrometer-sized x-ray beams as fine tools for macromolecular crystallography. <i>HFSP Journal</i> , <b>2008</b> , 2, 302-6   |      | 11 |
| 19 | Visualization of protein crystals by high-energy phase-contrast X-ray imaging. <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2019</b> , 75, 947-958   | 5.5  | 11 |
| 18 | SITCOM: a program for comparing sites in macromolecular substructures. <i>Journal of Applied Crystallography</i> , <b>2006</b> , 39, 618-619   | 3.8  | 9  |
| 17 | Data collection with a tailored X-ray beam size at 2.69 Å wavelength (4.6 keV): sulfur SAD phasing of Cdc23(Nterm). <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2016</b> , 72, 403-12   | 5.5  | 8  |
| 16 | Optical performance and radiation stability of polymer X-ray refractive nano-lenses. <i>Journal of Synchrotron Radiation</i> , <b>2019</b> , 26, 714-719   | 2.4  | 6  |
| 15 | Optimization of selenium substructures as obtained from SHELXD. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2003</b> , 59, 1987-94  |      | 6  |
| 14 | A steroidal phenyldihydro-1,3-oxazine derivative. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2000</b> , 56, e363-e364  |      | 6  |
| 13 | Stereoselective Synthesis of the Two trans-(16-Hydroxymethyl)-3-methoxy-13β-estra-1,3,5(10)-trien-17-ol Isomers. <i>Collection of Czechoslovak Chemical Communications</i> , <b>2003</b> , 68, 1141-1148   |      | 5  |

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|----|---|------|---|
| 12 | Structure of the alpha-amylase inhibitor tendamistat at 0.93 Å. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2003</b> , 59, 1737-43   |      | 5 |
| 11 | Long-wavelength Mesh&Collect native SAD phasing from microcrystals. <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2019</b> , 75, 192-199   | 5.5  | 5 |
| 10 | Identification of the point of diminishing returns in high-multiplicity data collection for sulfur SAD phasing. <i>Journal of Synchrotron Radiation</i> , <b>2017</b> , 24, 19-28   | 2.4  | 4 |
| 9  | 3-Sulfino-propionyl-coenzyme A (3SP-CoA) desulfonase from <i>Advenella mimigardefordensis</i> DPN7(T): crystal structure and function of a desulfonase with an acyl-CoA dehydrogenase fold. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2015</b> , 71, 1360-72 |      | 4 |
| 8  | Clustering of atomic displacement parameters in bovine trypsin reveals a distributed lattice of atoms with shared chemical properties. <i>Scientific Reports</i> , <b>2019</b> , 9, 19281   | 4.9  | 4 |
| 7  | Structural information content at high resolution: MAD versus native. <i>Methods in Enzymology</i> , <b>2003</b> , 374, 321-41  | 1.7  | 3 |
| 6  | Comparison of different X-ray data-collection systems using the crystal structure of octreotide. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1995</b> , 51, 60-8   |      | 3 |
| 5  | 3-Methoxy-1 $\beta$ -phenyl-4 $\beta$ -dihydro-1H-pyrazolo[4,3-f]estra-1,3,5(10)-triene. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2002</b> , 58, o810-o811  |      | 2 |
| 4  | 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> , <b>1999</b> , 55, 1586-8                         |      | 2 |
| 3  | Structural insights into glycine reuptake inhibition  |      | 1 |
| 2  | Ground-state destabilization by electrostatic repulsion is not a driving force in orotidine-5 $\beta$ -monophosphate decarboxylase catalysis. <i>Nature Catalysis</i> , <b>2022</b> , 5, 332-341  | 36.5 | 1 |
| 1  | Advances in experimental phasing. <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2016</b> , 72, 291-2   | 5.5  |   |