

# Douglas C Rees

## List of Publications by Year in descending order

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109  
papers

15,399  
citations

38660

50  
h-index

27345

106  
g-index

131  
all docs

131  
docs citations

131  
times ranked

10872  
citing authors

#	ARTICLE	IF	CITATIONS
1	ABC transporters: the power to change. <i>Nature Reviews Molecular Cell Biology</i> , 2009, 10, 218-227.	16.1	1,105
2	Nitrogenase MoFe-Protein at 1.16 Å Resolution: A Central Ligand in the FeMo-Cofactor. <i>Science</i> , 2002, 297, 1696-1700.	6.0	1,041
3	The <i>E. coli</i> BtuCD Structure: A Framework for ABC Transporter Architecture and Mechanism. <i>Science</i> , 2002, 296, 1091-1098.	6.0	1,039
4	Structural Basis of Biological Nitrogen Fixation. <i>Chemical Reviews</i> , 1996, 96, 2965-2982.	23.0	1,015
5	Structural basis of biological nitrogen fixation. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2005, 363, 971-984.	1.6	852
6	Evidence for Interstitial Carbon in Nitrogenase FeMo Cofactor. <i>Science</i> , 2011, 334, 940-940.	6.0	774
7	Crystal Structure of <i>Escherichia coli</i> MscS, a Voltage-Modulated and Mechanosensitive Channel. <i>Science</i> , 2002, 298, 1582-1587.	6.0	574
8	Structure of ADP-ATF4-stabilized nitrogenase complex and its implications for signal transduction. <i>Nature</i> , 1997, 387, 370-376.	13.7	517
9	Redox-Dependent Structural Changes in the Nitrogenase P-Cluster. <i>Biochemistry</i> , 1997, 36, 1181-1187.	1.2	498
10	MOLYBDENUM-COFACTOR-CONTAINING ENZYMES: Structure and Mechanism. <i>Annual Review of Biochemistry</i> , 1997, 66, 233-267.	5.0	489
11	Structure of the <i>Escherichia coli</i> Fumarate Reductase Respiratory Complex. <i>Science</i> , 1999, 284, 1961-1966.	6.0	400
12	Ligand binding to the FeMo-cofactor: Structures of CO-bound and reactivated nitrogenase. <i>Science</i> , 2014, 345, 1620-1623.	6.0	343
13	Mechanosensitive Channels: What Can They Do and How Do They Do It?. <i>Structure</i> , 2011, 19, 1356-1369.	1.6	303
14	Nitrogenase: standing at the crossroads. <i>Current Opinion in Chemical Biology</i> , 2000, 4, 559-566.	2.8	287
15	X-ray crystal structures of the oxidized and reduced forms of the rubredoxin from the marine hyperthermophilic archaeobacterium <i>pyrococcus furiosus</i> . <i>Protein Science</i> , 1992, 1, 1494-1507.	3.1	238
16	How many metals does it take to fix N <sub>2</sub> ? A mechanistic overview of biological nitrogen fixation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 17088-17093.	3.3	225
17	Nitrogenase Complexes: Multiple Docking Sites for a Nucleotide Switch Protein. <i>Science</i> , 2005, 309, 1377-1380.	6.0	216
18	The Interface Between the Biological and Inorganic Worlds: Iron-Sulfur Metalloclusters. <i>Science</i> , 2003, 300, 929-931.	6.0	214

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19	The structure of Escherichia coli BtuF and binding to its cognate ATP binding cassette transporter. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 16642-16647.	3.3	209
20	Great Metalloclusters in Enzymology. Annual Review of Biochemistry, 2002, 71, 221-246.	5.0	198
21	Structural Enzymology of Nitrogenase Enzymes. Chemical Reviews, 2020, 120, 4969-5004.	23.0	194
22	The High-Affinity <i>E. coli</i> Methionine ABC Transporter: Structure and Allosteric Regulation. Science, 2008, 321, 250-253.	6.0	187
23	Structure of a Cofactor-Deficient Nitrogenase MoFe Protein. Science, 2002, 296, 352-356.	6.0	176
24	Structures of the Prokaryotic Mechanosensitive Channels MscL and MscS. Current Topics in Membranes, 2007, 58, 1-24.	0.5	176
25	Structures of the Superoxide Reductase from Pyrococcus furiosus in the Oxidized and Reduced States. Biochemistry, 2000, 39, 2499-2508.	1.2	164
26	Conformational variability in structures of the nitrogenase iron proteins from Azotobacter vinelandii and Clostridium pasteurianum. Journal of Molecular Biology, 1998, 280, 669-685.	2.0	152
27	Some thermodynamic implications for the thermostability of proteins. Protein Science, 2001, 10, 1187-1194.	3.1	152
28	Structural Basis for Heavy Metal Detoxification by an Atm1-Type ABC Exporter. Science, 2014, 343, 1133-1136.	6.0	152
29	Structure and mechanism in prokaryotic mechanosensitive channels. Current Opinion in Structural Biology, 2003, 13, 432-442.	2.6	151
30	In Vitro Functional Characterization of BtuCD-F, the Escherichia coli ABC Transporter for Vitamin B12 Uptake. Biochemistry, 2005, 44, 16301-16309.	1.2	146
31	Crystal Structure of the All-Ferrous [4Fe-4S]0 Form of the Nitrogenase Iron Protein from Azotobacter vinelandii. Biochemistry, 2001, 40, 651-656.	1.2	135
32	Nitrogenase FeMoco investigated by spatially resolved anomalous dispersion refinement. Nature Communications, 2016, 7, 10902.	5.8	131
33	Catalysis-dependent selenium incorporation and migration in the nitrogenase active site iron-molybdenum cofactor. ELife, 2015, 4, e11620.	2.8	116
34	Structure of Precursor-Bound NifEN: A Nitrogenase FeMo Cofactor Maturase/Insertase. Science, 2011, 331, 91-94.	6.0	115
35	Structure and mechanism of Zn <sup>2+</sup> -transporting P-type ATPases. Nature, 2014, 514, 518-522.	13.7	107
36	Structure of a tetrameric MscL in an expanded intermediate state. Nature, 2009, 461, 120-124.	13.7	105

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37	A distinct mechanism for the ABC transporter BtuCD-BtuF revealed by the dynamics of complex formation. <i>Nature Structural and Molecular Biology</i> , 2010, 17, 332-338.	3.6	105
38	Heme packing motifs revealed by the crystal structure of the tetra-heme cytochrome c554 from <i>Nitrosomonas europaea</i> . <i>Nature Structural Biology</i> , 1998, 5, 1005-1012.	9.7	102
39	Crystallographic Studies of the <i>Escherichia coli</i> Quinol-Fumarate Reductase with Inhibitors Bound to the Quinol-binding Site. <i>Journal of Biological Chemistry</i> , 2002, 277, 16124-16130.	1.6	98
40	A P-type ATPase importer that discriminates between essential and toxic transition metals. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 4677-4682.	3.3	88
41	The role of MscL amphipathic N terminus indicates a blueprint for bilayer-mediated gating of mechanosensitive channels. <i>Nature Communications</i> , 2016, 7, 11984.	5.8	87
42	MgATP-Bound and Nucleotide-Free Structures of a Nitrogenase Protein Complex between the Leu 1271 <sup>+</sup> -Fe-Protein and the MoFe-Protein. <i>Biochemistry</i> , 2001, 40, 641-650.	1.2	85
43	Biochemical and Structural Characterization of the Cross-Linked Complex of Nitrogenase: A Comparison to the ADP-AlF <sub>4</sub> -Stabilized Structure. <i>Biochemistry</i> , 2002, 41, 15557-15565.	1.2	81
44	Crystal structure of the molybdate binding protein ModA. <i>Nature Structural Biology</i> , 1997, 4, 703-707.	9.7	72
45	The Effect of Detergent, Temperature, and Lipid on the Oligomeric State of MscL Constructs: Insights from Mass Spectrometry. <i>Chemistry and Biology</i> , 2015, 22, 593-603.	6.2	72
46	Crystal structure of the <i>Acidaminococcus fermentans</i> 2-hydroxyglutaryl-CoA dehydratase component A. <i>Journal of Molecular Biology</i> , 2001, 307, 297-308.	2.0	70
47	The $\hat{\pm}$ -Helix and the Organization and Gating of Channels. <i>Annual Review of Biophysics and Biomolecular Structure</i> , 2002, 31, 207-233.	18.3	65
48	Open and shut: Crystal structures of the dodecylmaltoside solubilized mechanosensitive channel of small conductance from <i>Escherichia coli</i> and <i>Helicobacter pylori</i> at 4.4 Å... and 4.1 Å... resolutions. <i>Protein Science</i> , 2013, 22, 502-509.	3.1	63
49	Rethinking the Nitrogenase Mechanism: Activating the Active Site. <i>Joule</i> , 2019, 3, 2662-2678.	11.7	62
50	The Funnel Approach to the Precrystallization Production of Membrane Proteins. <i>Journal of Molecular Biology</i> , 2008, 377, 62-73.	2.0	58
51	Structural bioenergetics and energy transduction mechanisms. <i>Journal of Molecular Biology</i> , 1999, 293, 343-350.	2.0	50
52	A leucine-rich repeat variant with a novel repetitive protein structural motif. <i>Nature Structural Biology</i> , 1996, 3, 991-994.	9.7	49
53	Comparison of the X-ray structure of native rubredoxin from <i>pyrococcus furiosus</i> with the NMR structure of the zinc-substituted protein. <i>Protein Science</i> , 1992, 1, 1522-1525.	3.1	47
54	Assignment of Individual Metal Redox States in a Metalloprotein by Crystallographic Refinement at Multiple X-ray Wavelengths. <i>Journal of the American Chemical Society</i> , 2007, 129, 2210-2211.	6.6	47

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55	Localized Electronic Structure of Nitrogenase FeMoco Revealed by Selenium K-Edge High Resolution X-ray Absorption Spectroscopy. <i>Journal of the American Chemical Society</i> , 2019, 141, 13676-13688.	6.6	47
56	Structural Characterization of Two CO Molecules Bound to the Nitrogenase Active Site. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 5704-5707.	7.2	47
57	High-resolution structures of the oxidized and reduced states of cytochrome c554 from <i>Nitrosomonas europaea</i> . <i>Journal of Biological Inorganic Chemistry</i> , 2001, 6, 390-397.	1.1	44
58	Structural Evidence for Asymmetrical Nucleotide Interactions in Nitrogenase. <i>Journal of the American Chemical Society</i> , 2015, 137, 146-149.	6.6	44
59	“Feeling the pressure”™: structural insights into a gated mechanosensitive channel. <i>Current Opinion in Structural Biology</i> , 1999, 9, 448-454.	2.6	43
60	Crystallographic Analyses of Ion Channels: Lessons and Challenges. <i>Journal of Biological Chemistry</i> , 2000, 275, 713-716.	1.6	41
61	The Structure of a Conserved Piezo Channel Domain Reveals a Topologically Distinct $\hat{I}^2$ Sandwich Fold. <i>Structure</i> , 2014, 22, 1520-1527.	1.6	41
62	A sulfur-based transport pathway in <i>Cu</i> ATPases. <i>EMBO Reports</i> , 2015, 16, 728-740.	2.0	41
63	Substrate Pathways in the Nitrogenase MoFe Protein by Experimental Identification of Small Molecule Binding Sites. <i>Biochemistry</i> , 2015, 54, 2052-2060.	1.2	41
64	Inward facing conformations of the MetNI methionine ABC transporter: Implications for the mechanism of transinhibition. <i>Protein Science</i> , 2012, 21, 84-96.	3.1	39
65	Noncanonical role for the binding protein in substrate uptake by the MetNI methionine ATP Binding Cassette (ABC) transporter. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E10596-E10604.	3.3	36
66	STRUCTURAL BIOLOGY: Enhanced: Breaching the Barrier. <i>Science</i> , 2003, 301, 603-604.	6.0	34
67	Analyzing your complexes: structure of the quinol-fumarate reductase respiratory complex. <i>Current Opinion in Structural Biology</i> , 2000, 10, 448-455.	2.6	32
68	Nitrogenase MoFe protein from <i>Clostridium pasteurianum</i> at 1.08 Å resolution: comparison with the <i>Azotobacter vinelandii</i> MoFe protein. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 274-282.	2.5	32
69	High Resolution Crystal Structures of the Wild Type and Cys-55 Ser and Cys-59 Ser Variants of the Thioredoxin-like [2Fe-2S] Ferredoxin from <i>Aquifex aeolicus</i> . <i>Journal of Biological Chemistry</i> , 2002, 277, 34499-34507.	1.6	31
70	Functional Analysis of Detergent-Solubilized and Membrane-Reconstituted ATP-Binding Cassette Transporters. <i>Methods in Enzymology</i> , 2005, 400, 429-459.	0.4	31
71	Site-Specific Oxidation State Assignments of the Iron Atoms in the [4Fe:4S] <sup>2+/1+/0/</sup> States of the Nitrogenase Fe-Protein. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 3894-3897.	7.2	30
72	Reversible Protonated Resting State of the Nitrogenase Active Site. <i>Journal of the American Chemical Society</i> , 2017, 139, 10856-10862.	6.6	29

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73	The Sixteenth Iron in the Nitrogenase MoFe Protein. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 10529-10532.	7.2	28
74	Prokaryotic mechanosensitive channels. <i>Advances in Protein Chemistry</i> , 2003, 63, 177-209.	4.4	26
75	The Allosteric Regulatory Mechanism of the <i>Escherichia coli</i> MetNI Methionine ATP Binding Cassette (ABC) Transporter. <i>Journal of Biological Chemistry</i> , 2015, 290, 9135-9140.	1.6	24
76	Overexpression, Purification, and Crystallization of the Membrane-Bound Fumarate Reductase from <i>Escherichia coli</i> . <i>Protein Expression and Purification</i> , 2000, 19, 188-196.	0.6	23
77	OCAM: A new tool for studying the oligomeric diversity of MscL channels. <i>Protein Science</i> , 2011, 20, 313-326.	3.1	23
78	Turnover-Dependent Inactivation of the Nitrogenase MoFe-Protein at High pH. <i>Biochemistry</i> , 2014, 53, 333-343.	1.2	23
79	MscL: channeling membrane tension. <i>Pflügers Archiv European Journal of Physiology</i> , 2015, 467, 15-25.	1.3	23
80	Multiple Amino Acid Sequence Alignment Nitrogenase Component 1: Insights into Phylogenetics and Structure-Function Relationships. <i>PLoS ONE</i> , 2013, 8, e72751.	1.1	23
81	The structures of BtuCD and MscS and their implications for transporter and channel function. <i>FEBS Letters</i> , 2003, 555, 111-115.	1.3	22
82	Electrochemical and structural characterization of <i>Azotobacter vinelandii</i> flavodoxin II. <i>Protein Science</i> , 2017, 26, 1984-1993.	3.1	22
83	A structural framework for unidirectional transport by a bacterial ABC exporter. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 19228-19236.	3.3	21
84	Mechanism of molybdate insertion into pterin-based molybdenum cofactors. <i>Nature Chemistry</i> , 2021, 13, 758-765.	6.6	19
85	Turning a reference inside-out: Commentary on an article by Stevens and Arkin entitled: 'Are membrane proteins inside-out?' (Proteins 1999;36:135-143). <i>Proteins: Structure, Function and Bioinformatics</i> , 2000, 38, 121-122.	1.5	18
86	Structure and stability of the C-terminal helical bundle of the <i>E. coli</i> mechanosensitive channel of large conductance. <i>Protein Science</i> , 2013, 22, 1592-1601.	3.1	18
87	The contribution of methionine to the stability of the <i>Escherichia coli</i> MetNIQ ABC transporter-substrate binding protein complex. <i>Biological Chemistry</i> , 2015, 396, 1127-1134.	1.2	15
88	CaMn <sub>3</sub> IV <sub>4</sub> O <sub>4</sub> Cubane Models of the Oxygen-Evolving Complex: Spin Ground States $S=9/2$ and the Effect of Oxo Protonation. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 17671-17679.	7.2	14
89	Fluorescence activation mechanism and imaging of drug permeation with new sensors for smoking-cessation ligands. <i>ELife</i> , 2022, 11, .	2.8	14
90	Comparing crystallographic and solution structures of nitrogenase complexes. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 727-728.	2.5	12

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91	Macromolecular solvation energies derived from small molecule crystal morphology. <i>Protein Science</i> , 1993, 2, 1882-1889.	3.1	11
92	Structures of the <i>Neisseria meningitidis</i> methionine-binding protein MetQ in substrate-free form and bound to methionine isomers. <i>Protein Science</i> , 2019, 28, 1750-1757.	3.1	10
93	Microcrystal Electron Diffraction Elucidates Water-Specific Polymorphism-Induced Emission Enhancement of Bis-arylacylhydrazones. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 7546-7555.	4.0	8
94	Glutathione binding to the plant AtAtm3 transporter and implications for the conformational coupling of ABC transporters. <i>ELife</i> , 2022, 11, .	2.8	8
95	Opening the Molecular Floodgates. <i>Science</i> , 2008, 321, 1166-1167.	6.0	7
96	A reported archaeal mechanosensitive channel is a structural homolog of MarR-like transcriptional regulators. <i>Protein Science</i> , 2010, 19, 808-814.	3.1	7
97	Elucidating a role for the cytoplasmic domain in the <i>Mycobacterium tuberculosis</i> mechanosensitive channel of large conductance. <i>Scientific Reports</i> , 2018, 8, 14566.	1.6	7
98	Structural Characterization of Two CO Molecules Bound to the Nitrogenase Active Site. <i>Angewandte Chemie</i> , 2021, 133, 5768-5771.	1.6	7
99	The "speed limit" for macromolecular crystal growth. <i>Protein Science</i> , 2018, 27, 1837-1841.	3.1	3
100	Crystal structure of the <i>Escherichia coli</i> transcription termination factor Rho. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2020, 76, 398-405.	0.4	3
101	Characterization of the ABC methionine transporter from <i>Neisseria meningitidis</i> reveals that lipidated MetQ is required for interaction. <i>ELife</i> , 2021, 10, .	2.8	2
102	Powering brain power: GLUT1 and the era of structure based human transporter biology. <i>National Science Review</i> , 2015, 2, 3-4.	4.6	1
103	Site-Specific Oxidation State Assignments of the Iron Atoms in the $[4Fe:4S]^{2+/1+0}$ States of the Nitrogenase Fe-Protein. <i>Angewandte Chemie</i> , 2019, 131, 3934-3937.	1.6	1
104	CaMn <sub>3</sub> IVO <sub>4</sub> Cubane Models of the Oxygen-Evolving Complex: Spin Ground States $S < 9/2$ and the Effect of Oxo Protonation. <i>Angewandte Chemie</i> , 2021, 133, 17812-17820.	1.6	1
105	Titrateable transmembrane residues and a hydrophobic plug are essential for manganese import via the <i>Bacillus anthracis</i> ABC transporter MntBC-A. <i>Journal of Biological Chemistry</i> , 2021, 297, 101087.	1.6	1
106	Modeling the stimulation by glutathione of the steady state kinetics of an adenosine triphosphate binding cassette transporter. <i>Protein Science</i> , 2022, 31, 752-757.	3.1	1
107	Metalloproteins to Membrane Proteins: Biological Energy Transduction Mechanisms. <i>ACS Symposium Series</i> , 2002, , 202-215.	0.5	0
108	The Future of Biological X-Ray Analysis. , 2008, , 145-164.		0

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109	Structural and mechanistic diversity of ABC transporters. FASEB Journal, 2010, 24, 405.1.	0.2	0