## **Barry Honig**

## List of Publications by Year in Descending Order

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62 24,393 92 95 g-index h-index citations papers 8.8 26,190 6.7 95 L-index avg, IF ext. citations ext. papers

#	Paper	IF	Citations
92	Intrinsic DNA Shape Accounts for Affinity Differences between Hox-Cofactor Binding Sites. <i>Cell Reports</i> , <b>2018</b> , 24, 2221-2230	10.6	21
91	Free Energy Perturbation Calculation of Relative Binding Free Energy between Broadly Neutralizing Antibodies and the gp120 Glycoprotein of HIV-1. <i>Journal of Molecular Biology</i> , <b>2017</b> , 429, 930-947	6.5	47
90	Genome-wide prediction of minor-groove electrostatic potential enables biophysical modeling of protein-DNA binding. <i>Nucleic Acids Research</i> , <b>2017</b> , 45, 12565-12576	20.1	38
89	A hybrid method for protein-protein interface prediction. <i>Protein Science</i> , <b>2016</b> , 25, 159-65	6.3	25
88	Predicting peptide-mediated interactions on a genome-wide scale. <i>PLoS Computational Biology</i> , <b>2015</b> , 11, e1004248	5	13
87	OnTheFly: a database of Drosophila melanogaster transcription factors and their binding sites. <i>Nucleic Acids Research</i> , <b>2014</b> , 42, D167-71	20.1	31
86	Using systems and structure biology tools to dissect cellular phenotypes. <i>Journal of the American Medical Informatics Association: JAMIA</i> , <b>2012</b> , 19, 171-5	8.6	2
85	Cofactor binding evokes latent differences in DNA binding specificity between Hox proteins. <i>Cell</i> , <b>2011</b> , 147, 1270-82	56.2	330
84	A map of minor groove shape and electrostatic potential from hydroxyl radical cleavage patterns of DNA. <i>ACS Chemical Biology</i> , <b>2011</b> , 6, 1314-20	4.9	71
83	MarkUs: a server to navigate sequence-structure-function space. <i>Nucleic Acids Research</i> , <b>2011</b> , 39, W357	<b>'-£</b> 3.1	15
82	Diversity in DNA recognition by p53 revealed by crystal structures with Hoogsteen base pairs. <i>Nature Structural and Molecular Biology</i> , <b>2010</b> , 17, 423-9	17.6	171
81	VASP: a volumetric analysis of surface properties yields insights into protein-ligand binding specificity. <i>PLoS Computational Biology</i> , <b>2010</b> , 6, e1000881	5	36
80	PUDGE: a flexible, interactive server for protein structure prediction. <i>Nucleic Acids Research</i> , <b>2010</b> , 38, W550-4	20.1	9
79	Origins of specificity in protein-DNA recognition. <i>Annual Review of Biochemistry</i> , <b>2010</b> , 79, 233-69	29.1	606
78	Electrostatic interactions between arginines and the minor groove in the nucleosome. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2010</b> , 27, 861-6	3.6	62
77	High-throughput computational structure-based characterization of protein families: START domains and implications for structural genomics. <i>Journal of Structural and Functional Genomics</i> , <b>2010</b> , 11, 51-9		8
76	Solution NMR structures of proteins VPA0419 from Vibrio parahaemolyticus and yiiS from Shigella flexneri provide structural coverage for protein domain family PFAM 04175. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2010</b> , 78, 779-84	4.2	

## (2005-2009)

75	Structural relationships among proteins with different global topologies and their implications for function annotation strategies. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2009</b> , 106, 17377-82	11.5	72	
74	Nuance in the double-helix and its role in protein-DNA recognition. <i>Current Opinion in Structural Biology</i> , <b>2009</b> , 19, 171-7	8.1	84	
73	Structural elucidation of the Cys-His-Glu-Asn proteolytic relay in the secreted CHAP domain enzyme from the human pathogen Staphylococcus saprophyticus. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2009</b> , 74, 515-9	4.2	27	
72	The role of DNA shape in protein-DNA recognition. <i>Nature</i> , <b>2009</b> , 461, 1248-53	50.4	696	
71	Loop modeling: Sampling, filtering, and scoring. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2008</b> , 70, 834-43	4.2	120	
70	Poisson-Boltzmann calculations of nonspecific salt effects on protein-protein binding free energies. <i>Biophysical Journal</i> , <b>2007</b> , 92, 1891-9	2.9	83	
69	Prediction of side-chain conformations on protein surfaces. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2007</b> , 66, 814-23	4.2	27	
68	Identification of a chloride ion binding site in Na+/Cl -dependent transporters. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2007</b> , 104, 12761-6	11.5	171	
67	Functional specificity of a Hox protein mediated by the recognition of minor groove structure. <i>Cell</i> , <b>2007</b> , 131, 530-43	56.2	254	
66	Calculation of pKas in RNA: on the structural origins and functional roles of protonated nucleotides. <i>Journal of Molecular Biology</i> , <b>2007</b> , 366, 1475-96	6.5	115	
65	On the nature of cavities on protein surfaces: application to the identification of drug-binding sites. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2006</b> , 63, 892-906	4.2	209	
64	Structural refinement of protein segments containing secondary structure elements: Local sampling, knowledge-based potentials, and clustering. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2006</b> , 65, 463-79	4.2	33	
63	Structural alignment of proteinDNA interfaces: insights into the determinants of binding specificity. <i>Journal of Molecular Biology</i> , <b>2005</b> , 345, 1027-45	6.5	64	
62	Protein structure prediction: inroads to biology. <i>Molecular Cell</i> , <b>2005</b> , 20, 811-9	17.6	130	
61	Comparative study of generalized born models: Born radii and peptide folding. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 3008-22	3.4	78	
60	Solution structure of Archaeglobus fulgidis peptidyl-tRNA hydrolase (Pth2) provides evidence for an extensive conserved family of Pth2 enzymes in archea, bacteria, and eukaryotes. <i>Protein Science</i> , <b>2005</b> , 14, 2849-61	6.3	23	
59	Retroviral matrix domains share electrostatic homology: models for membrane binding function throughout the viral life cycle. <i>Structure</i> , <b>2005</b> , 13, 1521-31	5.2	77	
58	An assessment of the accuracy of methods for predicting hydrogen positions in protein structures. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2005</b> , 61, 296-309	4.2	32	

57	Comparative study of generalized Born models: protein dynamics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2005</b> , 102, 6760-4	11.5	63
56	A hierarchical approach to all-atom protein loop prediction. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2004</b> , 55, 351-67	4.2	1329
55	The SufE sulfur-acceptor protein contains a conserved core structure that mediates interdomain interactions in a variety of redox protein complexes. <i>Journal of Molecular Biology</i> , <b>2004</b> , 344, 549-65	6.5	51
54	Structural genomics: computational methods for structure analysis. <i>Protein Science</i> , <b>2003</b> , 12, 1813-21	6.3	88
53	Using multiple structure alignments, fast model building, and energetic analysis in fold recognition and homology modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2003</b> , 53 Suppl 6, 430-5	4.2	276
52	Solution structure of Vibrio cholerae protein VC0424: a variation of the ferredoxin-like fold. <i>Protein Science</i> , <b>2003</b> , 12, 1556-61	6.3	9
51	Solution NMR structure of the 30S ribosomal protein S28E from Pyrococcus horikoshii. <i>Protein Science</i> , <b>2003</b> , 12, 2823-30	6.3	19
50	Sequence, structure and energetic determinants of phosphopeptide selectivity of SH2 domains. <i>Journal of Molecular Biology</i> , <b>2003</b> , 334, 823-41	6.5	41
49	GRASP2: visualization, surface properties, and electrostatics of macromolecular structures and sequences. <i>Methods in Enzymology</i> , <b>2003</b> , 374, 492-509	1.7	187
48	Rapid grid-based construction of the molecular surface and the use of induced surface charge to calculate reaction field energies: applications to the molecular systems and geometric objects. Journal of Computational Chemistry, <b>2002</b> , 23, 128-37	3.5	573
47	Evaluating conformational free energies: the colony energy and its application to the problem of loop prediction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2002</b> , 99, 7432-7	11.5	311
46	The role of electrostatic and nonpolar interactions in the association of peripheral proteins with membranes. <i>Current Topics in Membranes</i> , <b>2002</b> , 277-307	2.2	51
45	On the role of electrostatic interactions in the design of protein-protein interfaces. <i>Journal of Molecular Biology</i> , <b>2002</b> , 318, 161-77	6.5	210
44	On the role of the crystal environment in determining protein side-chain conformations. <i>Journal of Molecular Biology</i> , <b>2002</b> , 320, 597-608	6.5	691
43	Electrostatic control of the membrane targeting of C2 domains. <i>Molecular Cell</i> , <b>2002</b> , 9, 145-54	17.6	195
42	Electrostatic contributions to protein-protein interactions: fast energetic filters for docking and their physical basis. <i>Protein Science</i> , <b>2001</b> , 10, 2147-61	6.3	87
41	The role of electrostatic interactions in the regulation of the membrane association of G protein beta gamma heterodimers. <i>Journal of Biological Chemistry</i> , <b>2001</b> , 276, 45153-9	5.4	51
40	Extending the accuracy limits of prediction for side-chain conformations. <i>Journal of Molecular Biology</i> , <b>2001</b> , 311, 421-30	6.5	354

39	Electrostatic aspects of protein-protein interactions. Current Opinion in Structural Biology, 2000, 10, 153-9.1	Ĺ	612
38	Free energy determinants of tertiary structure and the evaluation of protein models. <i>Protein Science</i> , <b>2000</b> , 9, 2181-91	3	92
37	Structural determinants of trypsin affinity and specificity for cationic inhibitors. <i>Protein Science</i> , <b>1999</b> , 8, 2621-9	3	24
36	GRASS: a server for the graphical representation and analysis of structures. <i>Protein Science</i> , <b>1999</b> , 8, 676&3	3	29
35	Calculating the electrostatic properties of RNA provides new insights into molecular interactions and function. <i>Nature Structural Biology</i> , <b>1999</b> , 6, 1055-61		176
34	Electrostatic contributions to the stability of hyperthermophilic proteins. <i>Journal of Molecular Biology</i> , <b>1999</b> , 289, 1435-44	5	292
33	Protein folding: from the levinthal paradox to structure prediction. <i>Journal of Molecular Biology</i> , <b>1999</b> , 293, 283-93	5	129
32	Electrostatics and the membrane association of Src: theory and experiment. <i>Biochemistry</i> , <b>1998</b> , 37, 2145, 5	9	159
31	Electrostatic contributions to the binding free energy of the lambdacl repressor to DNA.  Biophysical Journal, 1998, 75, 2262-73	)	96
30	Free Energy of Amide Hydrogen Bond Formation in Vacuum, in Water, and in Liquid Alkane Solution. <i>Journal of Physical Chemistry B</i> , <b>1997</b> , 101, 450-457	1	134
29	Monovalent and Divalent Salt Effects on Electrostatic Free Energies Defined by the Nonlinear Poisson <b>B</b> oltzmann Equation: Application to DNA Binding Reactions. <i>Journal of Physical Chemistry B</i> , <b>1997</b> , 101, 9113-9118	1	55
28	On the calculation of binding free energies using continuum methods: application to MHC class I protein-peptide interactions. <i>Protein Science</i> , <b>1997</b> , 6, 1293-301	3	164
27	Electrostatic Potentials in Rhodopseudomonas viridis Reaction Centers: Implications for the Driving Force and Directionality of Electron Transfer <i>The Journal of Physical Chemistry</i> , <b>1996</b> , 100, 4277-42	91	184
26	New Model for Calculation of Solvation Free Energies: Correction of Self-Consistent Reaction Field Continuum Dielectric Theory for Short-Range Hydrogen-Bonding Effects. <i>The Journal of Physical Chemistry</i> , <b>1996</b> , 100, 11775-11788		852
25	Calculation of Alkane to Water Solvation Free Energies Using Continuum Solvent Models. <i>The Journal of Physical Chemistry</i> , <b>1996</b> , 100, 2744-2752		106
24	Salt effects on polyelectrolyte-ligand binding: comparison of Poisson-Boltzmann, and limiting law/counterion binding models. <i>Biopolymers</i> , <b>1995</b> , 36, 245-62	2	108
23	The fast multipole boundary element method for molecular electrostatics: An optimal approach for large systems. <i>Journal of Computational Chemistry</i> , <b>1995</b> , 16, 898-913	5	131
22	Evaluation of the conformational free energies of loops in proteins. <i>Proteins: Structure, Function</i> 4.2	2	106

21	Correlating solvation free energies and surface tensions of hydrocarbon solutes. <i>Biophysical Chemistry</i> , <b>1994</b> , 51, 397-403; discussion 404-9	3.5	102
20	Accurate First Principles Calculation of Molecular Charge Distributions and Solvation Energies from Ab Initio Quantum Mechanics and Continuum Dielectric Theory. <i>Journal of the American Chemical Society</i> , <b>1994</b> , 116, 11875-11882	16.4	953
19	Accurate Calculation of Hydration Free Energies Using Macroscopic Solvent Models. <i>The Journal of Physical Chemistry</i> , <b>1994</b> , 98, 1978-1988		1798
18	On the calculation of pKas in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1993</b> , 15, 252-65	4.2	489
17	Perturbing the polar environment of Asp102 in trypsin: consequences of replacing conserved Ser214. <i>Biochemistry</i> , <b>1992</b> , 31, 3059-64	3.2	78
16	Analysis of the heat capacity dependence of protein folding. <i>Journal of Molecular Biology</i> , <b>1992</b> , 227, 889-900	6.5	99
15	The electrostatic contribution to DNA base-stacking interactions. <i>Biopolymers</i> , <b>1992</b> , 32, 145-59	2.2	84
14	Calculations of Proton Uptake in Rhodobacter Sphaeroides Reaction Centers <b>1992</b> , 403-410		14
13	A rapid finite difference algorithm, utilizing successive over-relaxation to solve the Poisson <b>B</b> oltzmann equation. <i>Journal of Computational Chemistry</i> , <b>1991</b> , 12, 435-445	3.5	1088
12	Protein folding and association: insights from the interfacial and thermodynamic properties of hydrocarbons. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1991</b> , 11, 281-96	4.2	5087
11	The inclusion of electrostatic hydration energies in molecular mechanics calculations. <i>Journal of Computer-Aided Molecular Design</i> , <b>1991</b> , 5, 5-20	4.2	88
10	Electrical potential of transfer RNAs: codon-anticodon recognition. <i>Biochemistry</i> , <b>1990</b> , 29, 340-6	3.2	46
9	Electrostatic Analysis of the Midpoints of the Four Hemes in the Bound Cytochrome of the Reaction Center of RP. Viridis. <i>Jerusalem Symposia on Quantum Chemistry and Biochemistry</i> , <b>1990</b> , 53-60		4
8	Electrostatic Analysis of the Midpoints of the Cofactors in the Reaction Center Protein of Rp.viridis <b>1990</b> , 47-52		1
7	The electrostatic potential of B-DNA. <i>Biopolymers</i> , <b>1989</b> , 28, 975-93	2.2	250
6	Electrical potentials in trypsin isozymes. <i>Biochemistry</i> , <b>1989</b> , 28, 9918-26	3.2	72
5	Calculation of the total electrostatic energy of a macromolecular system: solvation energies, binding energies, and conformational analysis. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1988</b> , 4, 7-18	4.2	724
4	Focusing of electric fields in the active site of Cu-Zn superoxide dismutase: effects of ionic strength and amino-acid modification. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1986</b> , 1, 47-59	4.2	681

## LIST OF PUBLICATIONS

173, 515-21

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2	On the calculation of electrostatic interactions in proteins. <i>Journal of Molecular Biology</i> , <b>1985</b> , 184, 503-169	5	273
1	On the environment of ionizable groups in globular proteins. <i>Journal of Molecular Biology</i> , <b>1984</b> ,	5	140

Reevaluation of the Born model of ion hydration. *The Journal of Physical Chemistry*, **1985**, 89, 5588-5593

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