# Barry Honig

## List of Publications by Citations



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

| # | Paper | IF | Citations |
|---|---|---|---|
| 92 | Protein folding and association: insights from the interfacial and thermodynamic properties of hydrocarbons. *Proteins: Structure, Function and Bioinformatics*, **1991**, 11, 281-96 | 4.2 | 5087 |
| 91 | Accurate Calculation of Hydration Free Energies Using Macroscopic Solvent Models. *The Journal of Physical Chemistry*, **1994**, 98, 1978-1988 | | 1798 |
| 90 | A hierarchical approach to all-atom protein loop prediction. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 351-67 | 4.2 | 1329 |
| 89 | A rapid finite difference algorithm, utilizing successive over-relaxation to solve the PoissonBoltzmann equation. *Journal of Computational Chemistry*, **1991**, 12, 435-445 | 3.5 | 1088 |
| 88 | Accurate First Principles Calculation of Molecular Charge Distributions and Solvation Energies from Ab Initio Quantum Mechanics and Continuum Dielectric Theory. *Journal of the American Chemical Society*, **1994**, 116, 11875-11882 | 16.4 | 953 |
| 87 | New Model for Calculation of Solvation Free Energies: Correction of Self-Consistent Reaction Field Continuum Dielectric Theory for Short-Range Hydrogen-Bonding Effects. *The Journal of Physical Chemistry*, **1996**, 100, 11775-11788 | | 852 |
| 86 | Calculation of the total electrostatic energy of a macromolecular system: solvation energies, binding energies, and conformational analysis. *Proteins: Structure, Function and Bioinformatics*, **1988**, 4, 7-18 | 4.2 | 724 |
| 85 | The role of DNA shape in protein-DNA recognition. *Nature*, **2009**, 461, 1248-53 | 50.4 | 696 |
| 84 | On the role of the crystal environment in determining protein side-chain conformations. *Journal of Molecular Biology*, **2002**, 320, 597-608 | 6.5 | 691 |
| 83 | Focusing of electric fields in the active site of Cu-Zn superoxide dismutase: effects of ionic strength and amino-acid modification. *Proteins: Structure, Function and Bioinformatics*, **1986**, 1, 47-59 | 4.2 | 681 |
| 82 | Electrostatic aspects of protein-protein interactions. *Current Opinion in Structural Biology*, **2000**, 10, 153-9 | 9.1 | 612 |
| 81 | Origins of specificity in protein-DNA recognition. *Annual Review of Biochemistry*, **2010**, 79, 233-69 | 29.1 | 606 |
| 80 | 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*, **2002**, 23, 128-37 | 3.5 | 573 |
| 79 | On the calculation of pKas in proteins. *Proteins: Structure, Function and Bioinformatics*, **1993**, 15, 252-65 | 4.2 | 489 |
| 78 | Reevaluation of the Born model of ion hydration. *The Journal of Physical Chemistry*, **1985**, 89, 5588-5593 | | 488 |
| 77 | Extending the accuracy limits of prediction for side-chain conformations. *Journal of Molecular Biology*, **2001**, 311, 421-30 | 6.5 | 354 |
| 76 | Cofactor binding evokes latent differences in DNA binding specificity between Hox proteins. *Cell*, **2011**, 147, 1270-82 | 56.2 | 330 |

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| 75 | Evaluating conformational free energies: the colony energy and its application to the problem of loop prediction. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 7432-7 | 11.5 | 311 |
| 74 | Electrostatic contributions to the stability of hyperthermophilic proteins. *Journal of Molecular Biology*, **1999**, 289, 1435-44 | 6.5 | 292 |
| 73 | Using multiple structure alignments, fast model building, and energetic analysis in fold recognition and homology modeling. *Proteins: Structure, Function and Bioinformatics*, **2003**, 53 Suppl 6, 430-5 | 4.2 | 276 |
| 72 | On the calculation of electrostatic interactions in proteins. *Journal of Molecular Biology*, **1985**, 184, 503-16 | 6.5 | 273 |
| 71 | Functional specificity of a Hox protein mediated by the recognition of minor groove structure. *Cell*, **2007**, 131, 530-43 | 56.2 | 254 |
| 70 | The electrostatic potential of B-DNA. *Biopolymers*, **1989**, 28, 975-93 | 2.2 | 250 |
| 69 | On the role of electrostatic interactions in the design of protein-protein interfaces. *Journal of Molecular Biology*, **2002**, 318, 161-77 | 6.5 | 210 |
| 68 | On the nature of cavities on protein surfaces: application to the identification of drug-binding sites. *Proteins: Structure, Function and Bioinformatics*, **2006**, 63, 892-906 | 4.2 | 209 |
| 67 | Electrostatic control of the membrane targeting of C2 domains. *Molecular Cell*, **2002**, 9, 145-54 | 17.6 | 195 |
| 66 | GRASP2: visualization, surface properties, and electrostatics of macromolecular structures and sequences. *Methods in Enzymology*, **2003**, 374, 492-509 | 1.7 | 187 |
| 65 | Electrostatic Potentials in Rhodopseudomonas viridis Reaction Centers: Implications for the Driving Force and Directionality of Electron Transfer *The Journal of Physical Chemistry*, **1996**, 100, 4277-4291 | | 184 |
| 64 | Calculating the electrostatic properties of RNA provides new insights into molecular interactions and function. *Nature Structural Biology*, **1999**, 6, 1055-61 | | 176 |
| 63 | Diversity in DNA recognition by p53 revealed by crystal structures with Hoogsteen base pairs. *Nature Structural and Molecular Biology*, **2010**, 17, 423-9 | 17.6 | 171 |
| 62 | Identification of a chloride ion binding site in Na+/Cl -dependent transporters. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 12761-6 | 11.5 | 171 |
| 61 | On the calculation of binding free energies using continuum methods: application to MHC class I protein-peptide interactions. *Protein Science*, **1997**, 6, 1293-301 | 6.3 | 164 |
| 60 | Electrostatics and the membrane association of Src: theory and experiment. *Biochemistry*, **1998**, 37, 2145-59 | 3.2 | 159 |
| 59 | On the environment of ionizable groups in globular proteins. *Journal of Molecular Biology*, **1984**, 173, 515-21 | 6.5 | 140 |
| 58 | Free Energy of Amide Hydrogen Bond Formation in Vacuum, in Water, and in Liquid Alkane Solution. *Journal of Physical Chemistry B*, **1997**, 101, 450-457 | 3.4 | 134 |

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| 57 | The fast multipole boundary element method for molecular electrostatics: An optimal approach for large systems. *Journal of Computational Chemistry*, **1995**, 16, 898-913 | 3.5 | 131 |
| 56 | Protein structure prediction: inroads to biology. *Molecular Cell*, **2005**, 20, 811-9 | 17.6 | 130 |
| 55 | Protein folding: from the levinthal paradox to structure prediction. *Journal of Molecular Biology*, **1999**, 293, 283-93 | 6.5 | 129 |
| 54 | Loop modeling: Sampling, filtering, and scoring. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 834-43 | 4.2 | 120 |
| 53 | Calculation of pKas in RNA: on the structural origins and functional roles of protonated nucleotides. *Journal of Molecular Biology*, **2007**, 366, 1475-96 | 6.5 | 115 |
| 52 | Salt effects on polyelectrolyte-ligand binding: comparison of Poisson-Boltzmann, and limiting law/counterion binding models. *Biopolymers*, **1995**, 36, 245-62 | 2.2 | 108 |
| 51 | Calculation of Alkane to Water Solvation Free Energies Using Continuum Solvent Models. *The Journal of Physical Chemistry*, **1996**, 100, 2744-2752 | | 106 |
| 50 | Evaluation of the conformational free energies of loops in proteins. *Proteins: Structure, Function and Bioinformatics*, **1994**, 18, 119-32 | 4.2 | 106 |
| 49 | Correlating solvation free energies and surface tensions of hydrocarbon solutes. *Biophysical Chemistry*, **1994**, 51, 397-403; discussion 404-9 | 3.5 | 102 |
| 48 | Analysis of the heat capacity dependence of protein folding. *Journal of Molecular Biology*, **1992**, 227, 889-900 | 6.5 | 99 |
| 47 | Electrostatic contributions to the binding free energy of the lambdacI repressor to DNA. *Biophysical Journal*, **1998**, 75, 2262-73 | 2.9 | 96 |
| 46 | Free energy determinants of tertiary structure and the evaluation of protein models. *Protein Science*, **2000**, 9, 2181-91 | 6.3 | 92 |
| 45 | Structural genomics: computational methods for structure analysis. *Protein Science*, **2003**, 12, 1813-21 | 6.3 | 88 |
| 44 | The inclusion of electrostatic hydration energies in molecular mechanics calculations. *Journal of Computer-Aided Molecular Design*, **1991**, 5, 5-20 | 4.2 | 88 |
| 43 | Electrostatic contributions to protein-protein interactions: fast energetic filters for docking and their physical basis. *Protein Science*, **2001**, 10, 2147-61 | 6.3 | 87 |
| 42 | Nuance in the double-helix and its role in protein-DNA recognition. *Current Opinion in Structural Biology*, **2009**, 19, 171-7 | 8.1 | 84 |
| 41 | The electrostatic contribution to DNA base-stacking interactions. *Biopolymers*, **1992**, 32, 145-59 | 2.2 | 84 |
| 40 | Poisson-Boltzmann calculations of nonspecific salt effects on protein-protein binding free energies. *Biophysical Journal*, **2007**, 92, 1891-9 | 2.9 | 83 |

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| 39 | Comparative study of generalized born models: Born radii and peptide folding. *Journal of Physical Chemistry B*, **2005**, 109, 3008-22 | 3.4 | 78 |
| 38 | Perturbing the polar environment of Asp102 in trypsin: consequences of replacing conserved Ser214. *Biochemistry*, **1992**, 31, 3059-64 | 3.2 | 78 |
| 37 | Retroviral matrix domains share electrostatic homology: models for membrane binding function throughout the viral life cycle. *Structure*, **2005**, 13, 1521-31 | 5.2 | 77 |
| 36 | Structural relationships among proteins with different global topologies and their implications for function annotation strategies. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 17377-82 | 11.5 | 72 |
| 35 | Electrical potentials in trypsin isozymes. *Biochemistry*, **1989**, 28, 9918-26 | 3.2 | 72 |
| 34 | A map of minor groove shape and electrostatic potential from hydroxyl radical cleavage patterns of DNA. *ACS Chemical Biology*, **2011**, 6, 1314-20 | 4.9 | 71 |
| 33 | Structural alignment of protein--DNA interfaces: insights into the determinants of binding specificity. *Journal of Molecular Biology*, **2005**, 345, 1027-45 | 6.5 | 64 |
| 32 | Comparative study of generalized Born models: protein dynamics. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6760-4 | 11.5 | 63 |
| 31 | Electrostatic interactions between arginines and the minor groove in the nucleosome. *Journal of Biomolecular Structure and Dynamics*, **2010**, 27, 861-6 | 3.6 | 62 |
| 30 | Monovalent and Divalent Salt Effects on Electrostatic Free Energies Defined by the Nonlinear PoissonBoltzmann Equation: Application to DNA Binding Reactions. *Journal of Physical Chemistry B*, **1997**, 101, 9113-9118 | 3.4 | 55 |
| 29 | The SufE sulfur-acceptor protein contains a conserved core structure that mediates interdomain interactions in a variety of redox protein complexes. *Journal of Molecular Biology*, **2004**, 344, 549-65 | 6.5 | 51 |
| 28 | The role of electrostatic interactions in the regulation of the membrane association of G protein beta gamma heterodimers. *Journal of Biological Chemistry*, **2001**, 276, 45153-9 | 5.4 | 51 |
| 27 | The role of electrostatic and nonpolar interactions in the association of peripheral proteins with membranes. *Current Topics in Membranes*, **2002**, 277-307 | 2.2 | 51 |
| 26 | Free Energy Perturbation Calculation of Relative Binding Free Energy between Broadly Neutralizing Antibodies and the gp120 Glycoprotein of HIV-1. *Journal of Molecular Biology*, **2017**, 429, 930-947 | 6.5 | 47 |
| 25 | Electrical potential of transfer RNAs: codon-anticodon recognition. *Biochemistry*, **1990**, 29, 340-6 | 3.2 | 46 |
| 24 | Sequence, structure and energetic determinants of phosphopeptide selectivity of SH2 domains. *Journal of Molecular Biology*, **2003**, 334, 823-41 | 6.5 | 41 |
| 23 | Genome-wide prediction of minor-groove electrostatic potential enables biophysical modeling of protein-DNA binding. *Nucleic Acids Research*, **2017**, 45, 12565-12576 | 20.1 | 38 |
| 22 | VASP: a volumetric analysis of surface properties yields insights into protein-ligand binding specificity. *PLoS Computational Biology*, **2010**, 6, e1000881 | 5 | 36 |

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| 21 | Structural refinement of protein segments containing secondary structure elements: Local sampling, knowledge-based potentials, and clustering. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 463-79 | 4.2 | 33 |
| 20 | An assessment of the accuracy of methods for predicting hydrogen positions in protein structures. *Proteins: Structure, Function and Bioinformatics*, **2005**, 61, 296-309 | 4.2 | 32 |
| 19 | OnTheFly: a database of Drosophila melanogaster transcription factors and their binding sites. *Nucleic Acids Research*, **2014**, 42, D167-71 | 20.1 | 31 |
| 18 | GRASS: a server for the graphical representation and analysis of structures. *Protein Science*, **1999**, 8, 676-9 | 6.3 | 29 |
| 17 | Structural elucidation of the Cys-His-Glu-Asn proteolytic relay in the secreted CHAP domain enzyme from the human pathogen Staphylococcus saprophyticus. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 515-9 | 4.2 | 27 |
| 16 | Prediction of side-chain conformations on protein surfaces. *Proteins: Structure, Function and Bioinformatics*, **2007**, 66, 814-23 | 4.2 | 27 |
| 15 | A hybrid method for protein-protein interface prediction. *Protein Science*, **2016**, 25, 159-65 | 6.3 | 25 |
| 14 | Structural determinants of trypsin affinity and specificity for cationic inhibitors. *Protein Science*, **1999**, 8, 2621-9 | 6.3 | 24 |
| 13 | Solution structure of Archaeglobus fulgidis peptidyl-tRNA hydrolase (Pth2) provides evidence for an extensive conserved family of Pth2 enzymes in archea, bacteria, and eukaryotes. *Protein Science*, **2005**, 14, 2849-61 | 6.3 | 23 |
| 12 | Intrinsic DNA Shape Accounts for Affinity Differences between Hox-Cofactor Binding Sites. *Cell Reports*, **2018**, 24, 2221-2230 | 10.6 | 21 |
| 11 | Solution NMR structure of the 30S ribosomal protein S28E from Pyrococcus horikoshii. *Protein Science*, **2003**, 12, 2823-30 | 6.3 | 19 |
| 10 | MarkUs: a server to navigate sequence-structure-function space. *Nucleic Acids Research*, **2011**, 39, W357-61 | 20.1 | 15 |
| 9 | Calculations of Proton Uptake in Rhodobacter Sphaeroides Reaction Centers **1992**, 403-410 | | 14 |
| 8 | Predicting peptide-mediated interactions on a genome-wide scale. *PLoS Computational Biology*, **2015**, 11, e1004248 | 5 | 13 |
| 7 | PUDGE: a flexible, interactive server for protein structure prediction. *Nucleic Acids Research*, **2010**, 38, W550-4 | 20.1 | 9 |
| 6 | Solution structure of Vibrio cholerae protein VC0424: a variation of the ferredoxin-like fold. *Protein Science*, **2003**, 12, 1556-61 | 6.3 | 9 |
| 5 | High-throughput computational structure-based characterization of protein families: START domains and implications for structural genomics. *Journal of Structural and Functional Genomics*, **2010**, 11, 51-9 | | 8 |
| 4 | Electrostatic Analysis of the Midpoints of the Four Hemes in the Bound Cytochrome of the Reaction Center of RP. Viridis. *Jerusalem Symposia on Quantum Chemistry and Biochemistry*, **1990**, 53-60 | | 4 |

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| 3 | Using systems and structure biology tools to dissect cellular phenotypes. *Journal of the American Medical Informatics Association: JAMIA*, **2012**, 19, 171-5 | 8.6 | 2 |
| 2 | Electrostatic Analysis of the Midpoints of the Cofactors in the Reaction Center Protein of Rp.viridis **1990**, 47-52 | | 1 |
| 1 | Solution NMR structures of proteins VPA0419 from Vibrio parahaemolyticus and yiiS from Shigella flexneri provide structural coverage for protein domain family PFAM 04175. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 779-84 | 4.2 | |