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## General Reference List (Annotated)

1. M. P. Allen and D. J. Tildesley. *Computer Simulation of Liquids*. Oxford University Press, New York, 1987.  
[Good advanced reference book for molecular simulations.]
2. A. D. Bates and A. Maxwell. *DNA Topology*, In Focus series, Oxford University Press, New York, 1993.  
[Beautiful paperback on the higher organizational forms of DNA.]
3. V. A. Bloomfield, D. M. Crothers, and I. Tinoco, Jr. *Nucleic Acids: Structures, Properties, and Functions*. University Science Press, New York, 2000.  
[Comprehensive account of nucleic acids at an advanced level, with emphasis on biological function and experimental techniques. The first part describes nucleic acid properties on the atomic and molecular levels as deduced by various experimental techniques. The second part presents macromolecular features of nucleic acids in solution (e.g., dynamics behavior, DNA supercoiling). The third part covers noncovalent interactions of nucleic acids and other molecules (ions, drugs, proteins) and higher-order structures due to cellular packing.]
4. C. Branden and J. Tooze. *Introduction to Protein Structure*, second edition, Garland Publishing Inc., New York, 1999.  
([www.proteinstructure.com/](http://www.proteinstructure.com/)).  
[A modern and nicely illustrated protein structure textbook dealing with basic structural principles (part 1) and other topics (part 2, broadly grouped under the heading of relationships among structure, function, and engineering). Part 2 includes chapters on transcription regulation, signal transduction, immune regulation, membrane and fibrous proteins, and virus structures.]

5. P. Bratley, B. L. Fox, and L. E. Schrage. *A Guide to Simulation*. Springer-Verlag, New York, 1987.  
[Good introduction to Monte Carlo simulations.]
6. C. L. Brooks, III, M. Karplus, and B. M. Pettitt. *Proteins: A Theoretical Perspective of Dynamics, Structure, and Thermodynamics*. Wiley Interscience, New York, 1988.  
[Nice collection on protein simulations.]
7. U. Burkert and N. L. Allinger. *Molecular Mechanics*. American Chemical Society, Washington D.C., 1982.  
[Basic introductory monograph on molecular mechanics.]
8. C. R. Cantor and P.R. Schimmel. *Biophysical Chemistry*. Vol. 1,2,3. W.H. Freeman and Company, San Francisco, 1980.  
[Excellent text and reference book on many aspects of biophysical chemistry.]
9. N. R. Cohen, Editor. *Guidebook on Molecular Modeling in Drug Design*. Academic Press, San Diego, 1996.  
[Modern reference for molecular modeling as applied to drug design problems, containing contributed chapters by industrial and academic scientists, on problem formulation (database analysis, docking), modeling tools, and medicinal chemistry applications.]
10. P. Deuffhard, J. Hermans, B. Leimkuhler, A. E. Mark, S. Reich, R. D. Skeel, Editors. *Computational Molecular Dynamics: Challenges, Methods, Ideas – Proceedings of the 2nd International Symposium on Algorithms for Macromolecular Modelling, Berlin, May 21-24, 1997*, Lecture Notes in Computational Science and Engineering, Vol. 4 (Series Editors M. Griebel, D.E. Keyes, R. M. Nieminen, D. Roose, and T. Schlick), Springer-Verlag, Berlin and New York, 1999.  
[Collection of articles from invited presentations to the May 1997 Berlin workshop on methods for macromolecular modeling. The book contains sections on the following topics: conformational dynamics, thermodynamic modeling, enhanced time-stepping algorithms, quantum-classical simulations, and parallel force field evaluation.]
11. T. E. Creighton, Editor. *Protein Folding*. W.H. Freeman & Company, New York, 1992.  
[Nice collection with general topics regarding proteins covered.]
12. D. Eisenberg and D. Crothers. *Physical Chemistry with Applications to the Life Sciences*. Benjamin Cummings, Menlo Park, CA, 1979.  
[Wonderful physical chemistry textbook, with useful biomolecular information.]
13. A. Fersht. *Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding*. W. H. Freeman and Company, New York, 1999.  
[A comprehensive perspective of both enzyme catalysis and protein folding by a pioneer researcher, an updated version of the author's 1995 text on Enzyme Structure and Mechanism; the text reviews protein structure, emphasizing general principles, as well as mentioning recent advances and insights from theoretical approaches.]

14. D. Frenkel and B. Smit. *Understanding Molecular Simulations. From Algorithms to Applications*. second edition, Academic Press, San Diego, CA, 2001.  
[Excellent introduction to computer simulation of molecular systems, containing a nice mix of mathematical details and more informal, descriptive text. The focus is on Monte Carlo and molecular dynamics methodologies, through comparison and contrast analyses, including simple algorithms and numerical illustrations. Some important recent methodological advances are also included.]
15. L. M. Gierasch and J. King, Editors. *Protein Folding, Deciphering the Second Half of the Genetic Code*. AAAS, Washington D.C., 1990.  
[Interesting and beautifully illustrated collection of articles; best bet: Jane Richardson's origami analogues of protein folding motifs!]
16. H. Gould and J. Tobochnik. *An Introduction to Computer Simulation Methods: Applications to Physical Systems. Parts 1 and 2*. Addison-Wesley, Reading, MA, 1988.  
[A good introduction to computer simulations, with a focus on classical mechanics in Part 1 and statistical physics in Part 2. The material is made highly accessible to undergraduates by the inclusion of many simple numerical examples, useful illustrations, and programming segments.]
17. A. Y. Grosberg and A. R. Khokhlov. *Giant Molecules. Here, There, and Everywhere...* Academic Press, San Diego, CA, 1997.  
[A lively introduction to polymer physics, with nice illustrations and enticing color plates, aptly fitting a beautiful subject. In the format of a coffee-table book, the authors cover important subjects like the wide range of polymeric subjects, ideal chain models and their properties, Brownian motion, biological polymers, and polymer dynamics. An accompanying CD-ROM animates polymer motion, including reptation and coil collapse.]
18. J. M. Haile. *Molecular Dynamics Simulations: Elementary Methods*. Wiley, New York, 1992.  
[Elementary text on molecular dynamics.]
19. M. Kalos and P. A. Whitlock. *Monte Carlo Methods*. John Wiley & Sons, New York, 1986.  
[Good introduction to Monte Carlo techniques.]
20. A. R. Leach. *Molecular Modelling. Principles and Applications*. Pearson Education Limited, Harlow, England, 2001.  
[Broad introduction to many aspects of molecular modeling and computational chemistry techniques, covering basic concepts, quantum and molecular mechanics models, techniques for energy minimization, molecular dynamics, Monte Carlo sampling, protein structure prediction, free energies, solvation, and drug design applications.]
21. K. B. Lipkowitz and D. B. Boyd, Editors *Reviews in Computational Chemistry*. VCH Publishers, New York, 1990 –  
[Nice series of books, with volumes appearing annually with comprehensive reviews and tutorials on many aspects of computational chemistry.]

22. J. A. McCammon and S. C. Harvey. *Dynamics of Proteins and Nucleic Acids*. Cambridge University Press, Cambridge, 1987.  
[First book on biomolecular dynamics simulations.]
23. D. A. McQuarrie. *Statistical Mechanics*. Harper Collins Publishers, New York, 1976.  
[Good reference text.]
24. National Research Council report. *Mathematical Challenges from Theoretical / Computational Chemistry*, National Academy Press, Washington D.C., 1995.  
([www.nap.edu/readingroom/books/mctcc/](http://www.nap.edu/readingroom/books/mctcc/)).  
[Panel report on the opportunities for collaboration, past achievements, and future possibilities between mathematical and chemical scientists.]
25. P. A. Pevzner. *Computational Molecular Biology. An Algorithmic Approach*. MIT Press, Cambridge, MA, 2000.  
[Modern text in computational molecular biology mainly addressed to computer scientists and mathematicians interested in discrete algorithms but accessible to biologists with mathematical grounding. Topics covered include gene hunting, sequencing and mapping, DNA microarray analysis, sequence comparison and alignment, genome evolution, and proteomics.]
26. P. von Ragué Schleyer, Editor-in-Chief, and N. L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, H. F. Schaefer, III, and P. R. Schreiner, Editors. *Encyclopedia of Computational Chemistry* John Wiley & Sons, West Sussex, UK, 1998.  
[Comprehensive reference series (five large volumes) written by experts in the field.]
27. D. C. Rapaport. *The Art of Molecular Dynamics Simulation*. Cambridge University Press, Cambridge, England., 1995.  
[Elementary text on molecular dynamics focusing on software details.]
28. W. Saenger. *Principles of Nucleic Acid Structure*. Springer Advanced Texts in Chemistry, Springer-Verlag, New York, 1984.  
[Wonderful guide to the richness of DNA structure, with an amazing breadth of topics.]
29. T. Schlick and H. H. Gan, Editors. *Computational Methods for Macromolecules: Challenges, Methods, and Applications – Proceedings of the 3rd International Workshop on Algorithms for Macromolecular Modelling, New York, October 12–14, 2000*, Lecture Notes in Computational Science and Engineering, Vol. 24 (Series Editors M. Griebel, D.E. Keyes, R. M. Nieminen, D. Roose, and T. Schlick), Springer-Verlag, Berlin and New York, 2002.  
[Collection of articles from presentations at the 2000 international workshop on macromolecular modeling, covering biomolecular simulation methods and applications. The contributions are grouped under the following subjects: field perspective (preface), biomolecular dynamics applications, molecular dynamics methods, Monte Carlo methods, other conformational sampling approaches, free energy methods, long-range interactions and fast electrostatics, and statistical approaches to protein structures.]
30. R. R. Sinden. *DNA Structure and Function*. Academic Press, San Diego, CA, 1994.  
[Nice modern textbook on DNA structure.]

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31. G. E. Schulz and R. H. Schirmer. *Principles of Protein Structure*. Springer Advanced Texts in Chemistry, Springer-Verlag, New York, 1990.  
[Nice advanced text on the rapidly-changing field of protein folding.]
32. L. Stryer, *Biochemistry*. W.H. Freeman, New York, latest edition (fifth in December 2001).  
[Wonderful biochemistry textbook, up to date.]
33. W. Van Gunsteren and P. Weiner, Editors (1989) and W. Van Gunsteren, P. Weiner, and A.T. Wilkinson, Editors (1993, 1996): *Computer Simulation of Biomolecular Systems: Theoretical and Experimental Applications*. Vol. 1,2,3. ESCOM, Leiden, The Netherlands, 1989, 1993, 1996.  
[Good series on biomolecular simulations, covering both algorithms and applications.]