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Book review

Water and Biological Macromolecules, Topics in Molecular and Structural Biology, Volume 17. Edited by Eric Westhof, Macmillan Press 1993. ISBN 0-333-55116-8, 459 pages plus index, £65.

I approached this book as a computer graphics molecular modeler interested in achieving the most accurate simulations of water behaviour and knowing of the unease with which many physicists view our present simple concepts of the complex entity that is water. I doubt wether the book would make physicists feel more comfortable, as it is much more involved in the water–macromolecule interface than that of water–water interactions.

Introductory information is provided on water structure (Ch 1 by H.F.J. Savage) and its dynamic properties (Ch 2 by H.-D. Lüdemann) and a good deal of detail supplied in the last two chapters discussing hydration forces (Ch 13 by C.J. van Oss) and solvation thermodynamics (Ch 14 by A. Ben-Naim). The impressive author list continues for the bulk of the book which concentrates on particular macromolecular interactions (proteins, nucleic acids, polysaccharides, and lipids; each being represented by several well known experts in their fields). The chapters are all extensively referenced with titles for further reading and there are many useful tables and figures. Each section is refreshingly illustrated with a modern artist drawing which "tries to convey the tension between geometry and dynamics so strongly inherent to the nature of water" (Editor's Preface). From my particular bias I also enjoyed the following representative vignettes: the consideration of water in X-ray crystallography and neutron scattering (Ch 1); the ubiqutious states of water at different temperatures and pressures (Ch 2); the H-bonding network within water (Ch 2); molecular dynamics simulations for proteins and their comparison with X-ray solutions (Ch 3); molecular dynamics simulations for DNA including a comparison of the CHARMm and AMBER forcefields (Ch 6); structural water bridges in and around nucleic acids (Chs 7 and 8); Raman and Brillouin approaches and a discussion of the dielectric constant (Ch 9); a comprehensive summary of the X-ray data on saccharide interactions with water and proteins (Chs 10 and 11); and, an additionally useful reference chapter on lipids (Ch 12). As discussed above, Chs 13 and 14 provided the more theoretical approach to water thermodynamics which I particularly appreciated and were very readable despite the requirement to introduce the basic equations. In general the

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book could be read easily by the non-specialist, although a glossary of terms and eponymous forces/theories/equations would have been useful.

My major criticism remains that, with the exceptions quoted above, the applicability of the various commercially available molecular modeling software to the treatment of water and forecefield development were not discussed at length. Perhaps more important, there was no feeling about the way the subject was going to progress in the future to answer the difficult problems which remain in considering water structure.

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