

REFERENCES

23.2 (cont.)

- Otwinowski, Z., Schevitz, R. W., Zhang, R. G., Lawson, C. L., Joachimiak, A., Marmorstein, R. Q., Luisi, B. F. & Sigler, P. B. (1988). Crystal structure of *trp* repressor/operator complex at atomic resolution. *Nature (London)*, **335**, 321–329; erratum (1988), **335**, 837.
- Pabo, C. O. & Sauer, R. T. (1992). Transcription factors: structural families and principles of DNA recognition. *Annu. Rev. Biochem.* **61**, 1053–1095.
- Pardee, A. B. (1966). Purification and properties of a sulfate-binding protein from *Salmonella typhimurium*. *J. Biol. Chem.* **241**, 5886–5892.
- Pavletich, N. P. & Pabo, C. O. (1991). Zinc finger–DNA recognition: crystal structure of a Zif268–DNA complex at 2.1 Å. *Science*, **252**, 809–817.
- Pflugrath, J. W. & Quioco, F. A. (1985). Sulphate sequestered in the sulphate-binding protein of *Salmonella typhimurium* is bound solely by hydrogen bonds. *Nature (London)*, **314**, 257–260.
- Quioco, F. A. (1986). Carbohydrate-binding proteins: tertiary structures and protein–sugar interactions. *Annu. Rev. Biochem.* **55**, 287–315.
- Quioco, F. A., Sack, J. S. & Vyas, N. K. (1989). Substrate specificity and affinity of a protein modulated by bound water molecules. *Nature (London)*, **340**, 404–407.
- Quioco, F. A., Wilson, D. K. & Vyas, N. K. (1987). Stabilization of charges on isolated charged groups sequestered in proteins by polarized peptide units. *Nature (London)*, **329**, 561–564.
- Rademacher, T. W., Parekh, R. B. & Dwek, R. A. (1988). *Glycobiology*. *Annu. Rev. Biochem.* **57**, 785–838.
- Rould, M. A., Perona, J. J. & Steitz, T. A. (1991). Structural basis of anticodon loop recognition by glutamyl-tRNA synthetase. *Nature (London)*, **352**, 213–218.
- Seeman, N. C., Rosenberg, J. M. & Rich, A. (1976). Sequence-specific recognition of double helical nucleic acids by proteins. *Proc. Natl Acad. Sci. USA*, **73**, 804–808.
- Shimon, L. J. & Harrison, S. C. (1993). The phage 434 OR2/R1-69 complex at 2.5 Å resolution. *J. Mol. Biol.* **232**, 826–838.
- Steitz, T. A. (1990). Structural studies of protein–nucleic acid interaction: the sources of sequence-specific binding. *Q. Rev. Biophys.* **23**, 205–280.
- Sutton, R. B., Fasshauer, D., Jan, R. & Brunger, A. T. (1998). Crystal structure of a SNARE complex involved in synaptic exocytosis at 2.4 Å resolution. *Nature (London)*, **395**, 347–353.
- Tucker, P. W., Hazen, E. E. Jr & Cotton, F. A. (1979). Staphylococcal nuclease reviewed: a prototypic study in contemporary enzymology. III. Correlation of the three-dimensional structure with the mechanisms of enzymatic action. *Mol. Cell. Biochem.* **23**, 67–86.
- Ueda, H., Iyo, H., Doi, M., Inoue, M. & Ishida, T. (1991). Cooperative stacking and hydrogen bond pairing interactions of fragment peptide in cap binding protein with mRNA cap structure. *Biochim. Biophys. Acta*, **1075**, 181–186.
- Ueda, H., Iyo, H., Doi, M., Inoue, M., Ishida, T., Morioka, H., Tanaka, T., Nishikawa, S. & Uesugi, S. (1991). Combination of *Trp* and *Glu* residues for recognition of mRNA cap structure. Analysis of m7G base recognition site of human cap binding protein (IF-4E) by site-directed mutagenesis. *FEBS Lett.* **280**, 207–210.
- Varani, G. (1997). A cap for all occasions. *Structure*, **5**, 855–858.
- Volbeda, A., Fontecilla-Camps, J. C. & Frey, M. (1996). Novel metal sites in protein structures. *Curr. Opin. Struct. Biol.* **6**, 804–812.
- Vyas, N. K. (1991). Atomic features of protein–carbohydrate interactions. *Curr. Opin. Struct. Biol.* **1**, 732–740.
- Vyas, N. K., Vyas, M. N. & Quioco, F. A. (1988). Sugar and signal-transducer binding sites of the *Escherichia coli* galactose chemoreceptor protein. *Science*, **242**, 1290–1295.
- Wang, Z., Luecke, H., Yao, N. & Quioco, F. A. (1997). *Nature Struct. Biol.* **4**, 519–522.
- Weis, W. I. & Drickamer, K. (1996). Structural basis of lectin–carbohydrate recognition. *Annu. Rev. Biochem.* **65**, 441–473.
- Werner, M. H., Gronenborn, A. M. & Clore, G. M. (1996). Intercalation, DNA kinking, and the control of transcription. *Science*, **271**, 778–784; erratum (1996), **272**, 19.
- Worm, S. H. van den, Stonehouse, N. J., Valegard, K., Murray, J. B., Walton, C., Fridborg, K., Stockley, P. G. & Liljas, L. (1998). Crystal structures of MS2 coat protein mutants in complex with wild-type RNA operator fragments. *Nucleic Acids Res.* **26**, 1345–1351.
- Yao, N., Ledvina, P. S., Choudhary, A. & Quioco, F. A. (1996). Modulation of a salt link does not affect binding of phosphate to its specific active transport receptor. *Biochemistry*, **35**, 2079–2085.

23.3

- Altona, C., Geise, H. J. & Romers, C. (1968). Conformation of non-aromatic ring compounds, XXIV. On the geometry of the perhydrophenanthrene skeleton in some steroids. *Tetrahedron*, **24**, 13–32.
- Altona, C. & Sundaralingam, M. (1972). Conformational analysis of the sugar ring in nucleosides and nucleotides. *J. Am. Chem. Soc.* **94**, 8205–8212.
- Ansevin, A. T. & Wang, A. H. (1990). Evidence for a new Z-type left-handed DNA helix. *Nucleic Acids Res.* **18**, 6119–6126.
- Arnott, S. (1970). The geometry of nucleic acids. *Prog. Biophys. Mol. Biol.* **21**, 265–319.
- Babcock, M. S. & Olson, W. K. (1994). The effect of mathematics and coordinate system on comparability and ‘dependencies’ of nucleic acid structure parameters. *J. Mol. Biol.* **237**, 98–124.
- Babcock, M. S., Pednault, E. & Olson, W. (1993). Nucleic acid structure analysis: a users guide to a collection of new analysis programs. *J. Biomol. Struct. Dyn.* **11**, 597–628.
- Babcock, M. S., Pednault, E. & Olson, W. (1994). Nucleic acid structure analysis. Mathematics for local Cartesian and helical structure parameters that are truly comparable between structures. *J. Mol. Biol.* **237**, 125–156.
- Basham, B., Eichman, B. F. & Ho, P. S. (1998). The single-crystal structures of Z-DNA. In *Oxford handbook of nucleic acid structure*, edited by S. Neidle, ch. 7, pp. 200–252. Oxford University Press.
- Berman, H. M. (1996). Crystal studies of B-DNA: the answers and the questions. *Biopolymers Nucleic Acid Sci.* **44**, 23–44.
- Bugg, C. E., Thomas, J. M., Sundaralingam, M. & Rao, S. T. (1971). Stereochemistry of nucleic acids and their constituents. X. Solid-state base-stacking patterns in nucleic acid constituents and polynucleotides. *Biopolymers*, **10**, 175–219.
- Crick, F. H. C. & Watson, J. D. (1954). The complementary structure of deoxyribonucleic acid. *Proc. R. Soc. London Ser. A*, **223**, 80–96.
- Crothers, D. M. & Drak, J. (1992). Global features of DNA structure by comparative gel electrophoresis. *Methods Enzymol.* **212**, 46–71.
- Crothers, D. M., Haran, T. E. & Nadeau, J. G. (1990). Intrinsically bent DNA. *J. Biol. Chem.* **265**, 7093–7096.
- Davies, D. B. (1978). Conformations of nucleosides and nucleotides. *Prog. Nucl. Magn. Reson. Spectros.* **12**, 135–186.
- Dickerson, R. E. (1972). The structure and history of an ancient protein. *Sci. Am.* **226** (April), 58–72.
- Dickerson, R. E. (1983). The DNA helix and how it is read. *Sci. Am.* **249** (December), 94–111.
- Dickerson, R. E. (1985). Helix polymorphism and information flow in DNA. In *Proceedings of the Robert A. Welch Foundation conferences on chemical research XXIX: Genetic chemistry; the molecular basis of heredity*, pp. 38–79.
- Dickerson, R. E. (1992). DNA structure from A to Z. *Methods Enzymol.* **211**, 67–111.
- Dickerson, R. E. (1997a). Obituary: Irving Geis, 1908–1997. *Structure*, **5**, 1247–1249.
- Dickerson, R. E. (1997b). Irving Geis, molecular artist, 1908–1997. *Protein Sci.* **6**, 2843–2844.
- Dickerson, R. E. (1997c). Biology in pictures: molecular artistry. *Curr. Biol.* **7**, R720–R741.

23. STRUCTURAL ANALYSIS AND CLASSIFICATION

23.3 (cont.)

- Dickerson, R. E. (1998a). *Sequence-dependent B-DNA conformation in crystals and in protein complexes*. In *Structure, motion, interaction and expression of biological macromolecules*, edited by R. H. Sarma & M. H. Sarma, pp. 17–36. New York: Adenine Press.
- Dickerson, R. E. (1998b). *Helix structure and molecular recognition by B-DNA*. In *Oxford handbook of nucleic acid structure*, edited by S. Neidle, ch. 7, pp. 145–197. Oxford University Press.
- Dickerson, R. E. (1998c). *DNA bending: the prevalence of kinkiness and the virtues of normality*. *Nucleic Acids Res.* **26**, 1906–1926.
- Dickerson, R. E., Bansal, M., Calladine, C. R., Diekmann, S., Hunter, W. N., Kennard, O., Lavery, R., Nelson, H. C. M., Olson, W. K., Saenger, W., Shakked, Z., Sklenar, H., Soumpasis, D. M., Tung, C.-S., von Kitzing, E., Wang, A. H.-J. & Zhurkin, V. B. (1989). *Definitions and nomenclature of nucleic acid structure components*. *EMBO J.* **8**, 1–4; *J. Biomol. Struct. Dyn.* **6**, 627–634; *Nucleic Acids Res.* **17**, 1797–1803; *J. Mol. Biol.* **206**, 787–791.
- Dickerson, R. E. & Chiu, T. K. (1997). *Helix bending as a factor in protein/DNA recognition*. *Biopolymers Nucleic Acid Sci.* **44**, 361–403.
- Dickerson, R. E. & Geis, I. (1969). *The structure and action of proteins*. New York: Harper & Row and Menlo Park: W. A. Benjamin Co.
- Dickerson, R. E. & Geis, I. (1976). *Chemistry, matter and the universe*. Menlo Park: Benjamin/Cummings Co.
- Dickerson, R. E. & Geis, I. (1983). *Hemoglobin: structure, function, evolution, and pathology*. Menlo Park: Benjamin/Cummings Co.
- Dickerson, R. E., Goodsell, D. & Kopka, M. L. (1996). *MPD and DNA bending in crystals and in solution*. *J. Mol. Biol.* **256**, 108–125.
- Dickerson, R. E., Goodsell, D. S., Kopka, M. L. & Pjura, P. E. (1987). *The effect of crystal packing on oligonucleotide double helix structure*. *J. Biomol. Struct. Dyn.* **5**, 557–579.
- Dickerson, R. E., Goodsell, D. S. & Neidle, S. (1994). . . . the tyranny of the lattice. . . . *Proc. Natl Acad. Sci. USA*, **91**, 3579–3583.
- El Hassan, M. A. & Calladine, C. R. (1997). *Conformational characteristics of DNA: empirical classifications and a hypothesis for the conformational behaviour of dinucleotide steps*. *Philos. Trans. R. Soc. London A*, **355**, 43–100.
- Feigon, J. (1996). *DNA triplexes, quadruplexes & aptamers*. In *Encyclopedia of nuclear magnetic resonance*, edited by D. M. Grant & R. K. Harris, pp. 1726–1731. New York: Wiley.
- Franklin, R. E. & Gosling, R. G. (1953). *The structure of sodium thymonucleate fibres. I. The influence of water content*. *Acta Cryst.* **6**, 673–677.
- Haschmeyer, A. E. V. & Rich, A. (1967). *Nucleoside conformation: an analysis of steric barriers to rotation about the glycosidic bond*. *J. Mol. Biol.* **27**, 369–384.
- Herbert, A. & Rich, A. (1996). *The biology of left-handed Z-DNA*. *J. Biol. Chem.* **271**, 11595–11598.
- Ho, P. S. & Mooers, B. H. M. (1996). *Z-DNA crystallography*. *Biopolymers Nucleic Acid Sci.* **44**, 65–90.
- Hoogsteen, K. (1963). *The crystal and molecular structure of a hydrogen-bonded complex between 1-methylthymine and 9-methyladenine*. *Acta Cryst.* **16**, 907–916.
- Hunter, C. A. & Sanders, J. K. M. (1990). *The nature of π - π interactions*. *J. Am. Chem. Soc.* **112**, 5525–5534.
- Juo, Z. S., Chiu, T. K., Leiberman, P. M., Baikalov, I., Berk, A. J. & Dickerson, R. E. (1996). *How proteins recognize the TATA box*. *J. Mol. Biol.* **261**, 239–254.
- Kendrew, J. C. (1961). *The three-dimensional structure of a protein molecule*. *Sci. Am.* **205** (December), 96–110.
- Kim, J. L., Nikolov, D. B. & Burley, S. K. (1993). *Co-crystal structure of TBP recognizing the minor groove of a TATA element*. *Nature (London)*, **365**, 520–527.
- Kim, Y., Geiger, J. H., Hahn, S. & Sigler, P. B. (1993). *Crystal structure of a yeast TBP/TATA-box complex*. *Nature (London)*, **365**, 512–520.
- Koo, H.-S., Drak, J., Rice, J. A. & Crothers, D. M. (1990). *Determination of the extent of DNA bending by an adenine-thymine tract*. *Biochemistry*, **29**, 4227–4234.
- Koo, H.-S., Wu, H.-M. & Crothers, D. M. (1986). *DNA bending at adenine-thymine tracts*. *Nature (London)*, **320**, 501–506.
- Kostrewa, D. & Winkler, F. K. (1995). *Mg²⁺ binding to the active site of EcoRV endonuclease: a crystallographic study of complexes with substrate and product DNA at 2 Å resolution*. *Biochemistry*, **34**, 683–696.
- Langridge, R., Marvin, D. A., Seeds, W. E., Wilson, H. R., Hooper, C. W., Wilkins, M. H. F. & Hamilton, L. D. (1960). *The molecular configurations of deoxyribonucleic acid. II. Molecular models and their Fourier transforms*. *J. Mol. Biol.* **2**, 38–64.
- Lavery, R. & Sklenar, H. (1988). *The definition of generalized helicoidal parameters and of axis curvature for irregular nucleic acids*. *J. Biomol. Struct. Dyn.* **6**, 63–91.
- Lavery, R. & Sklenar, H. (1989). *Defining the structure of irregular nucleic acids: conventions and principles*. *J. Biomol. Struct. Dyn.* **6**, 655–667.
- Leslie, A. G. W., Arnott, S., Chandrasekaran, R. & Ratliff, R. L. (1980). *Polymorphism of DNA double helices*. *J. Mol. Biol.* **143**, 49–72.
- Levitt, M. & Warshel, A. (1978). *Extreme conformational flexibility of the furanose ring in DNA and RNA*. *J. Am. Chem. Soc.* **100**, 2607–2613.
- Lewis, M., Chang, G., Horton, N. C., Kercher, M. A., Pace, H. C., Schumacher, M. A., Brennan, R. G. & Lu, P. (1996). *Crystal structure of the lactose operon repressor and its complexes with DNA and inducer*. *Science*, **271**, 1247–1254.
- Marini, J. C., Levene, S. D., Crothers, D. M. & Englund, P. T. (1982). *Bent helical structures in kinetoplast DNA*. *Proc. Natl Acad. Sci. USA*, **79**, 7664–7668.
- Nikolov, D. B., Chen, H., Halay, E. D., Hoffman, A., Roeder, R. G. & Burley, S. K. (1996). *Crystal structure of a human TATA box-binding protein/TATA element complex*. *Proc. Natl Acad. Sci. USA*, **93**, 4862–4867.
- Parkinson, G., Wilson, C., Gunasekera, A., Ebright, Y. W., Ebright, R. H. & Berman, H. M. (1996). *Structure of the CAP–DNA complex at 2.5 angstroms resolution: a complete picture of the protein–DNA interface*. *J. Mol. Biol.* **260**, 395–408.
- Pelton, J. G. & Wemmer, D. E. (1989). *Structural characterization of a 2:1 distamycin A/d(CGCAAATTGGC) complex by two-dimensional NMR*. *Proc. Natl Acad. Sci. USA*, **86**, 5723–5727.
- Pelton, J. G. & Wemmer, D. E. (1990). *Binding modes of distamycin-A with d(CGCAAATTTGCG)₂ determined by two-dimensional NMR*. *J. Am. Chem. Soc.* **112**, 1393–1399.
- Phillips, D. C. (1966). *The three-dimensional structure of an enzyme molecule*. *Sci. Am.* **215** (November), 78–90.
- Pohl, F. M. (1976). *Polymorphism of a synthetic DNA in solution*. *Nature (London)*, **260**, 365–366.
- Pohl, F. M. & Jovin, T. M. (1972). *Salt-induced co-operative conformational change of a synthetic DNA: equilibrium and kinetic studies with poly(dG-dC)*. *J. Mol. Biol.* **67**, 375–396.
- Rice, P. A., Yang, S.-W., Mizuuchi, K. & Nash, H. A. (1996). *Crystal structure of an IHF–DNA complex: a protein-induced DNA U-turn*. *Cell*, **87**, 1295–1306.
- Saenger, W. (1984). *Principles of nucleic acid structure*. New York, Berlin, Heidelberg and Tokyo: Springer-Verlag.
- Schneider, B., Neidle, S. & Berman, H. M. (1997). *Conformations of the sugar–phosphate backbone in helical DNA crystal structures*. *Biopolymers*, **42**, 113–124.
- Schultz, S. C., Shields, G. C. & Steitz, T. A. (1991). *Crystal structure of a CAP–DNA complex: the DNA is bent by 90 degrees*. *Science*, **253**, 1001–1007.
- Schumacher, M. A., Choi, K. Y., Zalkin, H. & Brennan, R. G. (1994). *Crystal structure of LacI member, PurR, bound to DNA: minor groove binding by alpha helices*. *Science*, **266**, 763–770.
- Schwartz, T., Rould, M. A., Lowenjaunt, K., Herbert, A. & Rich, A. (1999). *Crystal structure of the Z α domain of the human editing enzyme ADAR1 bound to left-handed Z-DNA*. *Science*, **284**, 1841–1845.

23.3 (cont.)

- Seeman, N. C., Rosenberg, J. M. & Rich, A. (1976). Sequence-specific recognition of double helical nucleic acids by proteins. *Proc. Natl Acad. Sci. USA*, **73**, 804–808.
- Sklenár, V. & Feigon, J. (1990). Formation of a stable triplex from a single DNA strand. *Nature (London)*, **345**, 836–838.
- Sprou, D., Young, M. A. & Beveridge, D. L. (1999). Molecular dynamics studies of axis bending in $d(G_5-(GA_4T_4C)_2-C_5)$ and $d(G_5-(GT_4A_4C)_2-C_5)$: effects of sequence polarity on DNA curvature. *J. Mol. Biol.* **285**, 1623–1632.
- Sprou, D., Zacharias, W., Wood, Z. A. & Harvey, S. C. (1995). Dehydrating agents sharply reduce curvature in DNAs containing A-tracts. *Nucleic Acids Res.* **23**, 1816–1821.
- Sundaralingam, M. (1975). Principles governing nucleic acid and polynucleotide conformations. In *Structure and conformation of nucleic acids and protein–nucleic acid interactions*, edited by M. Sundaralingam & S. T. Rao, pp. 487–524. Baltimore: University Park Press.
- Thomas, K. A., Smith, G. M., Thomas, T. B. & Feldmann, R. J. (1982). Electronic distributions within protein phenylalanine aromatic rings are reflected by the three-dimensional oxygen atom environments. *Proc. Natl Acad. Sci. USA*, **79**, 4843–4847.
- Voet, D. & Voet, J. G. (1990). *Biochemistry*. New York: John Wiley & Sons.
- Voet, D. & Voet, J. G. (1995). *Biochemistry*, 2nd edition. New York: John Wiley & Sons.
- Wahl, M. C. & Sundaralingam, M. (1996). Crystal structures of A-DNA duplexes. *Biopolymers Nucleic Acid Sci.* **44**, 45–63.
- Wahl, M. C. & Sundaralingam, M. (1998). A-DNA duplexes in the crystal. In *Oxford handbook of nucleic acid structure*, edited by S. Neidle, ch. 5, pp. 117–144. Oxford University Press.
- Watson, J. D. & Crick, F. H. C. (1953). Molecular structure of nucleic acids: a structure for deoxyribose nucleic acid. *Nature (London)*, **171**, 737–738.
- Winkler, F. K., Banner, D. W., Oefner, C., Tsernoglou, D., Brown, R. S., Heathman, S. P., Bryan, R. K., Martin, P. D., Petratos, K. & Wilson, K. S. (1993). The crystal structure of EcoRV endonuclease and of its complexes with cognate and non-cognate DNA fragments. *EMBO J.* **12**, 1781–1795.
- Wu, H.-M. & Crothers, D. M. (1984). The locus of sequence-directed and protein-induced DNA bending. *Nature (London)*, **308**, 509–513.
- Yang, W. & Steitz, T. A. (1995). Crystal structure of the site-specific recombinase gamma delta resolvase complexed with a 34 bp cleavage site. *Cell*, **82**, 193–207.
- Brooks, C. L. & Karplus, M. (1989). Solvent effects on protein motion and protein effects on solvent motion. Dynamics of the active site region of lysozyme. *J. Mol. Biol.* **208**, 159–181.
- Bryant, R. G. (1996). The dynamics of water–protein interactions. *Annu. Rev. Biophys. Biomol. Struct.* **25**, 29–53.
- Chervenak, M. C. & Toone, E. J. (1994). A direct measure of the contribution of solvent reorganization to the enthalpy of ligand binding. *J. Am. Chem. Soc.* **116**, 10533–10539.
- Clackson, T. & Wells, J. T. (1995). A hot spot of binding energy in a hormone–receptor interface. *Science*, **267**, 383–386.
- Clark, K. L., Halay, E. D., Lai, E. & Burley, S. K. (1993). Co-crystal structure of the HNF-3/fork head DNA-recognition motif resembles histone H5. *Nature (London)*, **364**, 412–420.
- Clore, G. M., Bax, A., Omichinski, J. G. & Gronenborn, A. M. (1994). Localization of bound water in the solution structure of a complex of the erythroid transcription factor GATA-1 with DNA. *Curr. Biol.* **2**, 89–94.
- Condon, P. & Royer, W. (1994). Crystal structure of oxygenated Scapharca dimeric hemoglobin at 1.7 Å resolution. *J. Biol. Chem.* **269**, 25259–25267.
- Deisenhofer, J. & Steigemann, W. (1975). Crystallographic refinement of the structure of bovine pancreatic trypsin inhibitor at 1.5 Å resolution. *Acta Cryst.* **B31**, 238–250.
- Edsall, J. T. & McKenzie, H. A. (1978). Water and proteins. I. The significance and structure of water; its interaction with electrolytes and non-electrolytes. *Adv. Biophys.* **10**, 137–207.
- Edsall, J. T. & McKenzie, H. A. (1983). Water and proteins. II. The location and dynamics of water in protein systems and its relation to their stability and properties. *Adv. Biophys.* **16**, 53–183.
- Gunsteren, W. F. van, Luque, F. J., Timms, D. & Torda, A. E. (1994). Molecular mechanics in biology: from structure to function, taking account of solvation. *Annu. Rev. Biophys. Biomol. Struct.* **23**, 847–863.
- Hayward, S., Kitao, A., Hirata, F. & Go, N. (1993). Effect of solvent on collective motions in globular protein. *J. Mol. Biol.* **234**, 1207–1217.
- Hendrickson, W. A. & Teeter, M. M. (1981). Structure of the hydrophobic protein crambin determined directly from the anomalous scattering of sulphur. *Nature (London)*, **290**, 107–113.
- Hendsch, Z. S., Jonsson, T., Sauer, R. T. & Tidor, B. (1996). Protein stabilization by removal of unsatisfied polar groups: computational approaches and experimental tests. *Biochemistry*, **35**, 7621–7625.
- Hendsch, Z. S. & Tidor, B. (1994). Do salt bridges stabilize proteins? A continuum electrostatic analysis. *Protein Sci.* **3**, 211–226.
- Herron, J. N., Terry, A. H., Johnston, S., He, S.-M., Guddat, L. W., Voss, E. W. & Edmundson, A. B. (1994). High resolution structures of the 4-4-20 Fab–fluorescein complex in two solvent systems: effects of solvent on structure and antigen-binding affinity. *Biophys. J.* **67**, 2167–2175.
- Holdgate, G., Tunnicliffe, A., Ward, W. H. J., Weston, S. A., Rosenbrock, G., Barth, P. T., Taylor, I. W. F., Pauptit, R. A. & Timms, D. (1997). The entropic penalty of ordered water accounts for weaker binding of the antibiotic Novobiocin to a resistant mutant of DNA gyrase: a thermodynamic and crystallographic study. *Biochemistry*, **36**, 9663–9673.
- Hubbard, S. J., Gross, K.-H. & Argos, P. (1994). Intramolecular cavities in globular proteins. *Protein Eng.* **7**, 613–626.
- Jiang, J.-S. & Brünger, A. (1994). Protein hydration observed by X-ray diffraction. Solvation properties of penicillopepsin and neuraminidase crystal structures. *J. Mol. Biol.* **243**, 100–115.
- Karplus, P. A. & Faerman, C. (1994). Ordered water in macromolecular structure. *Curr. Opin. Struct. Biol.* **4**, 770–776.
- Kauzmann, W. (1959). Some factors in the interpretation of protein denaturation. *Adv. Protein Chem.* **14**, 1–63.
- Kendrew, J. C. (1963). Myoglobin and the structure of proteins. *Science*, **139**, 1259–1266.
- Komives, E. A., Loughheed, J. C., Liu, K., Sugio, S., Zhang, Z., Petsko, G. A. & Ringe, D. (1995). The structural basis for pseudoreversion of the E165D lesion by the secondary S96P

23.4

- Allen, K. N., Bellamacina, C. R., Ding, X., Jeffery, C. J., Mattos, C., Petsko, G. A. & Ringe, D. (1996). An experimental approach to mapping the binding surfaces of crystalline proteins. *J. Phys. Chem.* **100**, 2605–2611.
- Badger, J. (1993). Multiple hydration layers in cubic insulin crystals. *Biophys. J.* **65**, 1656–1659.
- Baker, E. N. & Hubbard, R. E. (1984). Hydrogen bonding in globular proteins. *Prog. Biophys. Mol. Biol.* **44**, 97–179.
- Beglov, D. & Roux, B. (1997). An integral equation to describe the solvation of polar molecules in liquid water. *J. Phys. Chem.* **101**, 7821–7826.
- Bellamacina, C., Mattos, C., Griffith, D., Ivanov, D., Stanton, M., Petsko, G. A. & Ringe, D. (1999). Unpublished results.
- Berman, H. M., Westbrook, J., Feng, Z., Gilliland, G., Bhat, T. N., Weissig, H., Shindyalov, I. N. & Bourne, P. E. (2000). The Protein Data Bank. *Nucleic Acids Res.* **28**, 235–242.
- Bhat, T. N., Bentley, G. A., Boulot, G., Greene, M. I., Tello, D., Dall'Acqua, W., Souchon, H., Schwarz, F. P., Maiuzza, R. A. & Poljak, R. J. (1994). Bound water molecules and conformational stabilization help mediate an antigen–antibody association. *Proc. Natl Acad. Sci. USA*, **91**, 1089–1093.
- Blake, C. C. F., Pulford, W. C. A. & Artymiuk, P. J. (1983). X-ray studies of water in crystals of lysozyme. *J. Mol. Biol.* **167**, 693–723.