

## REFERENCES

## 12.1 (cont.)

- Hendrickson, W. A., Horton, J. R. & LeMaster, D. M. (1990). Selenomethionyl proteins produced for analysis by multiwavelength anomalous diffraction (MAD): a vehicle for direct determination of three-dimensional structure. *EMBO J.* **9**, 1665–1672.
- Islam, S. A., Carvin, D., Sternberg, M. J. E. & Blundell, T. L. (1998). HAD, a data bank of heavy-atom binding sites in protein crystals: a resource for use in multiple isomorphous replacement and anomalous scattering. *Acta Cryst.* **D54**, 1199–1206.
- Labahn, J., Scharer, O. D., Long, A., Ezaz-Nikpay, K., Verdine, O. L. & Ellenberger, T. E. (1996). Structural basis for the excision repair of alkylation-damaged DNA. *Cell*, **86**, 321–329.
- Leahy, D. J., Erickson, H. P., Aukhil, I., Joshi, P. & Hendrickson, W. A. (1994). Crystallization of a fragment of human fibronectin: introduction of methionine by site-directed mutagenesis to allow phasing via selenomethionine. *Proteins Struct. Funct. Genet.* **19**, 48–54.
- Lipka, J. J., Lippard, S. J. & Wall, J. S. (1976). Visualisation of polymercurimethane-labelled fd bacteriophage in the scanning transmission electron microscope. *Science*, **206**, 1419–1421.
- Lipscomb, W. N., Reeke, G. N., Hartsuck, J. A., Quijcho, F. A. & Bethge, P. H. (1970). The structure of carboxypeptidase. VIII. Atomic interpretation at 0.2 nm resolution, a new study of the complex of glycyl-L-tyrosine with CPA, and mechanistic deductions. *Philos. Trans. R. Soc. London Ser. B*, **257**, 177–214.
- Lustbader, J. W., Wu, H., Birken, S., Pollak, S., Kolks-Gawinowicz, M. A., Pound, A. M., Austen, D., Hendrickson, W. A. & Canfield, R. E. (1995). The expression, characterization and crystallization of wild-type and selenomethionyl human chorionic gonadotrophin. *Endocrinology*, **136**, 640–650.
- Miller, J. H. (1972). Cysteine auxotrophic strains, in which proteins can be synthesised with the seleno derivative. In *Experiments in molecular genetics*. Cold Spring Harbour Laboratory Press.
- Muller, S., Senn, H., Gsell, B., Vetter, W., Baron, C. & Bock, A. (1994). The formation of diselenide bridges in proteins by incorporation of selenocysteine residues: biosynthesis and characterization of (Se)2-thioredoxin. *Biochemistry*, **33**, 3404–3412.
- O'Halloran, T. V., Lippard, S. J., Richmond, T. J. & Klug, A. (1987). Multiple heavy-atom reagents for macromolecular X-ray structure determination application to the nucleosome core particle. *J. Mol. Biol.* **194**, 705–712.
- Petsko, G. A., Phillips, D. C., Williams, R. J. P. & Wilson, I. A. (1978). On the protein crystal chemistry of chloroplatinite ions: general principles and interactions with triose phosphate isomerase. *J. Mol. Biol.* **120**, 345–359.
- Ringe, D., Petsko, G. A., Yamakura, F., Suzuki, K. & Ohmori, D. (1983). Structure of iron superoxide dismutase from *Pseudomonas ovalis* at 2.9 Å resolution. *Proc. Natl Acad. Sci. USA*, **80**, 3879–3883.
- Sasaki, K., Dockerill, S., Adamiak, D. A., Tickle, I. J. & Blundell, T. L. (1975). X-ray analysis of glucagon and its relationship to receptor binding. *Nature (London)*, **257**, 751–757.
- Schiltz, M. (1997). Xenon & krypton at LURE. <http://www.lure.u-psud.fr/sections/Xenon/XENONENG.HTM>.
- Schoenborn, B. P., Watson, H. C. & Kendrew, J. C. (1965). Binding of xenon to sperm whale myoglobin. *Nature (London)*, **207**, 28–30.
- Sigler, P. B. & Blow, D. M. (1965). A means of promoting heavy atom binding in protein crystals. *J. Mol. Biol.* **14**, 640–644.
- Sigler, P. B., Blow, D. M., Matthews, B. W. & Henderson, R. (1968). Structure of crystalline alpha-chymotrypsin II. A preliminary report including a hypothesis for the activation mechanism. *J. Mol. Biol.* **35**, 143–164.
- Sperling, R., Burstein, Y. & Steinberg, I. Z. (1969). Selective reduction and mercuration of cysteine IV–V in bovine pancreatic ribonuclease. *Biochemistry*, **8**, 3810–3820.
- Sperling, R. & Steinberg, I. Z. (1974). Simultaneous reduction and mercuration of disulphide bond A6–A11 of insulin by monovalent mercury. *Biochemistry*, **13**, 2007–2013.
- Thygesen, J., Weinstein, S., Franceschi, F. & Yonath, A. (1996). The suitability of metal clusters for phasing in macromolecular crystallography of large macromolecular assemblies. *Structure*, **4**, 513–518.
- Tsernoglou, D. & Petsko, G.-A. (1976). The crystal structure of a post-synaptic neurotoxin from sea snake at 2.2 Å resolution. *FEBS Lett.* **68**, 1–4.
- Wood, S. P., Tickle, I. J., Treharne, A. M., Pitts, J. E., Mascarenhas, Y., Li, J. Y., Husain, J., Cooper, S., Blundell, T. L., Hruby, V. J., Buku, A., Fischman, A. J. & Wyssbrod, H. R. (1986). Crystal structure analysis of deamino-oxytocin: conformational flexibility and receptor binding. *Science*, **232**, 633–636.
- Yonath, A., Saper, M. A., Makowski, I., Mussig, J., Piefke, J., Bartunik, H. D., Bartels, K. S. & Wittmann, H. G. (1986). Characterization of single crystals of the large ribosomal particles from *Bacillus stearothermophilus*. *J. Mol. Biol.* **187**, 633–636.

## 12.2

- Adman, E. T., Stenkamp, R. E., Sieker, L. C. & Jensen, L. H. (1978). A crystallographic model for azurin at 3.0 Å resolution. *J. Mol. Biol.* **123**, 35–47.
- Argos, P. & Rossmann, M. G. (1976). A method to determine heavy-atom positions for virus structures. *Acta Cryst.* **B32**, 2975–2983.
- Arnold, E., Vriend, G., Luo, M., Griffith, J. P., Kamer, G., Erickson, J. W., Johnson, J. E. & Rossmann, M. G. (1987). The structure determination of a common cold virus, human rhinovirus 14. *Acta Cryst.* **A43**, 346–361.
- Badger, J. & Athay, R. (1998). Automated and graphical methods for locating heavy-atom sites for isomorphous replacement and multiwavelength anomalous diffraction phase determination. *J. Appl. Cryst.* **31**, 270–274.
- Blow, D. M. & Crick, F. H. C. (1959). The treatment of errors in the isomorphous replacement method. *Acta Cryst.* **12**, 794–802.
- Budisa, N., Karnbrock, W., Steinbacher, S., Humm, A., Prade, L., Neufeind, T., Moroder, L. & Huber, R. (1997). Bioincorporation of telluromethionine into proteins: a promising new approach for X-ray structure analysis of proteins. *J. Mol. Biol.* **270**, 616–623.
- Buerger, M. J. (1959). *Vector space*. New York: Wiley.
- Chang, G. & Lewis, M. (1994). Using genetic algorithms for solving heavy-atom sites. *Acta Cryst.* **D50**, 667–674.
- Crick, F. H. C. & Magdoff, B. S. (1956). The theory of the method of isomorphous replacement for protein crystals. I. *Acta Cryst.* **9**, 901–908.
- Dumas, P. (1994a). The heavy-atom problem: a statistical analysis. I. A priori determination of best scaling, level of substitution, lack of isomorphism and phasing power. *Acta Cryst.* **A50**, 526–537.
- Dumas, P. (1994b). The heavy-atom problem: a statistical analysis. II. Consequences of the a priori knowledge of the noise and heavy-atom powers and use of a correlation function for heavy-atom-site determination. *Acta Cryst.* **A50**, 537–546; erratum, **A50**, 793.
- Green, D. W., Ingram, V. M. & Perutz, M. F. (1954). The structure of haemoglobin IV. Sign determination by the isomorphous replacement method. *Proc. R. Soc. London Ser. A*, **225**, 287–307.
- Harker, D. (1956). The determination of the phases of the structure factors of non-centrosymmetric crystals by the method of double isomorphous replacement. *Acta Cryst.* **9**, 1–9.
- Hendrickson, W. A., Horton, J. R. & LeMaster, D. M. (1990). Selenomethionyl proteins produced for analysis by multiwavelength anomalous diffraction (MAD): a vehicle for direct determination of three-dimensional structure. *EMBO J.* **9**, 1665–1672.
- Löwe, J., Stock, D., Jap, B., Zwickl, P., Baumeister, W. & Huber, R. (1995). Crystal structure of the 20S proteasome from the archaeon *T. acidophilum* at 3.4 Å resolution. *Science*, **268**, 533–539.
- McRee, D. E. (1998). *Practical protein crystallography*. San Diego: Academic Press.

## 12. ISOMORPHOUS REPLACEMENT

### 12.2 (cont.)

- Messerschmidt, A., Rossi, A., Ladenstein, R., Huber, R., Bolognesi, M., Gatti, G., Marchesini, A., Petruzzelli, R. & Finazzi-Agro, A. (1989). X-ray crystal structure of the blue oxidase ascorbate oxidase from zucchini. Analysis of the polypeptide fold and a model of the copper sites and ligands. *J. Mol. Biol.* **206**, 513–529.
- Nar, H., Huber, R., Meining, W., Schmid, C., Weinkauff, S. & Bacher, A. (1995). Atomic structure of GTP cyclohydrolase I. *Structure*, **3**, 459–466.
- Nar, H., Messerschmidt, A., Huber, R., van de Kamp, M. & Canters, G. W. (1991). X-ray crystal structure of the two site-specific mutants His35Gln and His235Leu of azurin from *Pseudomonas aeruginosa*. *J. Mol. Biol.* **218**, 427–447.
- Patterson, A. L. (1934). A Fourier series method for the determination of the components of interatomic distances in crystals. *Phys. Rev.* **46**, 372–376.
- Perutz, M. F. (1956). Isomorphous replacement and phase determination in non-centrosymmetric space groups. *Acta Cryst.* **9**, 867–873.
- Richardson, J. W. & Jacobson, R. A. (1987). In *Patterson and Pattersons*, edited by J. P. Glusker, B. K. Patterson & M. Rossi. Oxford University Press.
- Rogers, D. (1965). In *Computing methods in crystallography*, edited by J. S. Rollett, pp.133–148. Oxford University Press.
- Romao, M. J., Turk, D., Gomis-Ruth, F. X., Huber, R., Schumacher, G., Mollering, H. & Russmann, L. (1992). Crystal structure analysis, refinement and enzymatic reaction mechanism of N-carbamoylsarcosine amidohydrolase from *Arthrobacter sp.* at 2.0 Å resolution. *J. Mol. Biol.* **226**, 1111–1130.
- Rossmann, M. G. (1960). The accurate determination of the position and shape of heavy-atom replacement groups in proteins. *Acta Cryst.* **13**, 221–226.
- Rossmann, M. G. (1972). Editor. *The molecular replacement method*. New York: Gordon and Breach.
- Rossmann, M. G., Arnold, E. & Vriend, G. (1986). Comparison of vector search and feedback methods for finding heavy-atom sites in isomorphous derivatives. *Acta Cryst.* **A42**, 325–334.
- Sheldrick, G. M. (1990). Phase annealing in SHELX-90: direct methods for larger structures. *Acta Cryst.* **A46**, 467–473.
- Sheldrick, G. M., Dauter, Z., Wilson, K. S., Hope, H. & Sieker, L. C. (1993). The application of direct methods and Patterson interpretation to high-resolution native protein data. *Acta Cryst.* **D49**, 18–23.
- Steigemann, W. (1991). Recent advances in the PROTEIN program system for the X-ray structure analysis of biological macromolecules. In *Crystallographic computing 5: from chemistry to biology*, edited by D. Moras, A. D. Podjarny & J. C. Thierry, pp. 115–125. Oxford University Press.
- Stubbs, M. T., Nar, H., Löwe, J., Huber, R., Ladenstein, R., Spangfort, M. D. & Svensson, L. A. (1996). Locating a local symmetry axis from Patterson map cross vectors: application to crystal data from GroEL, GTP cyclohydrolase I and the proteosome. *Acta Cryst.* **D52**, 447–452.
- Stubbs, M. T., Summers, L., Mayr, I., Schneider, M., Bode, W., Huber, R., Ries, A. & Kühn, K. (1990). Crystals of the NC1 domain of type IV collagen. *J. Mol. Biol.* **211**, 683–684.
- Terwilliger, T. C. & Berendzen, J. (1999). Automated MAD and MIR structure solution. *Acta Cryst.* **D55**, 849–861.
- Terwilliger, T. C. & Eisenberg, D. (1983). Unbiased three-dimensional refinement of heavy-atom parameters by correlation of origin-removed Patterson functions. *Acta Cryst.* **A39**, 813–817.
- Terwilliger, T. C. & Eisenberg, D. (1987). Isomorphous replacement: effects of errors on the phase probability distribution. *Acta Cryst.* **A43**, 6–13.
- Terwilliger, T. C., Kim, S.-H. & Eisenberg, D. (1987). Generalized method of determining heavy-atom positions using the difference Patterson function. *Acta Cryst.* **A43**, 1–5.
- Tong, L. & Rossmann, M. G. (1993). Patterson-map interpretation with noncrystallographic symmetry. *J. Appl. Cryst.* **26**, 15–21.
- Vagin, A. & Teplyakov, A. (1998). A translation-function approach for heavy-atom location in macromolecular crystallography. *Acta Cryst.* **D54**, 400–402.
- Wilson, A. J. C. (1949). The probability distribution of X-ray intensities. *Acta Cryst.* **2**, 318–321.