

13. MOLECULAR REPLACEMENT

13.3 (cont.)

- Colman, P. M., Fehlhammer, H. & Bartels, K. (1976). *Patterson search methods in protein structure determination: β -trypsin and immunoglobulin fragments*. In *Crystallographic computing techniques*, edited by F. R. Ahmed, K. Huml & B. Sedlacek, pp. 248–258. Copenhagen: Munksgaard.
- Crowther, R. A. & Blow, D. M. (1967). *A method of positioning a known molecule in an unknown crystal structure*. *Acta Cryst.* **23**, 544–548.
- Driessen, H. P. C., Bax, B., Slingsby, C., Lindley, P. F., Mahadevan, D., Moss, D. S. & Tickle, I. J. (1991). *Structure of oligomeric β B2-crystallin: an application of the T_2 translation function to an asymmetric unit containing two dimers*. *Acta Cryst.* **B47**, 987–997.
- Fujinaga, M. & Read, R. J. (1987). *Experiences with a new translation-function program*. *J. Appl. Cryst.* **20**, 517–521.
- Harada, Y., Lifchitz, A., Berthou, J. & Jolles, P. (1981). *A translation function combining packing and diffraction information: an application to lysozyme (high-temperature form)*. *Acta Cryst.* **A37**, 398–406.
- Hendrickson, W. A. & Ward, K. B. (1976). *A packing function for delimiting the allowable locations of crystallized macromolecules*. *Acta Cryst.* **A32**, 778–780.
- Hirshfeld, F. L. (1968). *Symmetry in the generation of trial structures*. *Acta Cryst.* **A24**, 301–311.
- Navaza, J. (1994). *AMoRe: an automated package for molecular replacement*. *Acta Cryst.* **A50**, 157–163.
- Navaza, J. & Vernoslova, E. (1995). *On the fast translation functions for molecular replacement*. *Acta Cryst.* **A51**, 445–449.
- Nixon, P. E. & North, A. C. T. (1976). *Crystallographic relationship between human and hen-egg lysozymes. I. Methods for the establishment of molecular orientational and positional parameters*. *Acta Cryst.* **A32**, 320–325.
- Rabinovich, D. & Shakked, Z. (1984). *A new approach to structure determination of large molecules by multi-dimensional search methods*. *Acta Cryst.* **A40**, 195–200.
- Rae, A. D. (1977). *The use of structure factors to find the origin of an oriented molecular fragment*. *Acta Cryst.* **A33**, 423–425.
- Read, R. J. & Schierbeek, A. J. (1988). *A phased translation function*. *J. Appl. Cryst.* **21**, 490–495.
- Rossmann, M. G. (1972). Editor. *The molecular replacement method*. New York: Gordon & Breach.
- Rossmann, M. G. (1990). *The molecular replacement method*. *Acta Cryst.* **A46**, 73–82.
- Rossmann, M. G. & Blow, D. M. (1962). *The detection of sub-units within the crystallographic asymmetric unit*. *Acta Cryst.* **15**, 24–31.
- Tickle, I. J. (1985). *Review of space group general translation functions that make use of known structure information and can be expanded as Fourier series*. In *Proceedings of the Daresbury study weekend. Molecular replacement*, edited by P. A. Machin, pp. 22–26. Warrington: Daresbury Laboratory.
- Tollin, P. (1966). *On the determination of molecular location*. *Acta Cryst.* **21**, 613–614.
- Tollin, P. & Rossmann, M. G. (1966). *A description of various rotation function programs*. *Acta Cryst.* **21**, 872–876.
- Tong, L. (1993). *Replace, a suite of computer programs for molecular-replacement calculations*. *J. Appl. Cryst.* **26**, 748–751.
- Tong, L. (1996a). *Combined molecular replacement*. *Acta Cryst.* **A52**, 782–784.
- Tong, L. (1996b). *The locked translation function and other applications of a Patterson correlation function*. *Acta Cryst.* **A52**, 476–479.
- Tong, L. & Rossmann, M. G. (1990). *The locked rotation function*. *Acta Cryst.* **A46**, 783–792.
- Tong, L. & Rossmann, M. G. (1997). *Rotation function calculations with GLRF program*. *Methods Enzymol.* **276**, 594–611.
- Urzhumtsev, A. & Podjarny, A. (1995). *On the solution of the molecular-replacement problem at very low resolution: application to large complexes*. *Acta Cryst.* **D51**, 888–895.

- Wu, H., Kwong, P. D. & Hendrickson, W. A. (1997). *Dimeric association and segmental variability in the structure of human CD4*. *Nature (London)*, **387**, 527–530.

13.4

- Abad-Zapatero, C., Abdel-Meguid, S. S., Johnson, J. E., Leslie, A. G. W., Rayment, I., Rossmann, M. G., Suck, D. & Tsukihara, T. (1980). *Structure of southern bean mosaic virus at 2.8 Å resolution*. *Nature (London)*, **286**, 33–39.
- Argos, P., Ford, G. C. & Rossmann, M. G. (1975). *An application of the molecular replacement technique in direct space to a known protein structure*. *Acta Cryst.* **A31**, 499–506.
- Argos, P. & Rossmann, M. G. (1980). *Molecular replacement method*. In *Theory and practice of direct methods in crystallography*, edited by M. F. C. Ladd & R. A. Palmer, pp. 361–417. New York: Plenum.
- Arnold, E. & Rossmann, M. G. (1986). *Effect of errors, redundancy, and solvent content in the molecular replacement procedure for the structure determination of biological macromolecules*. *Proc. Natl Acad. Sci. USA*, **83**, 5489–5493.
- Arnold, E. & Rossmann, M. G. (1988). *The use of molecular-replacement phases for the refinement of the human rhinovirus 14 structure*. *Acta Cryst.* **A44**, 270–282.
- 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.
- Bjorkman, P. J., Saper, M. A., Samraoui, B., Bennett, W. S., Strominger, J. L. & Wiley, D. C. (1987). *Structure of the human class I histocompatibility antigen, HLA-A2*. *Nature (London)*, **329**, 506–512.
- Bloomer, A. C., Champness, J. N., Bricogne, G., Staden, R. & Klug, A. (1978). *Protein disk of tobacco mosaic virus at 2.8 Å resolution showing the interactions within and between subunits*. *Nature (London)*, **276**, 362–368.
- Bolin, J. T., Smith, J. L. & Muchmore, S. W. (1993). *Considerations in phase refinement and extension: experiments with a rapid and automatic procedure*. American Crystallographic Association Annual Meeting, May 23–28, Albuquerque, New Mexico, Vol. 21, p. 51.
- Bragg, L. & Perutz, M. F. (1952). *The structure of haemoglobin*. *Proc. R. Soc. London Ser. A*, **213**, 425–435.
- Bricogne, G. (1974). *Geometric sources of redundancy in intensity data and their use for phase determination*. *Acta Cryst.* **A30**, 395–405.
- Bricogne, G. (1976). *Methods and programs for direct-space exploitation of geometric redundancies*. *Acta Cryst.* **A32**, 832–847.
- Buehner, M., Ford, G. C., Moras, D., Olsen, K. W. & Rossmann, M. G. (1974). *Structure determination of crystalline lobster D-glyceraldehyde-3-phosphate dehydrogenase*. *J. Mol. Biol.* **82**, 563–585.
- Champness, J. N., Bloomer, A. C., Bricogne, G., Butler, P. J. G. & Klug, A. (1976). *The structure of the protein disk of tobacco mosaic virus at 5 Å resolution*. *Nature (London)*, **259**, 20–24.
- Chapman, M. S., Tsao, J. & Rossmann, M. G. (1992). *Ab initio phase determination for spherical viruses: parameter determination for spherical-shell models*. *Acta Cryst.* **A48**, 301–312.
- Cornea-Hasegan, M. A., Zhang, Z., Lynch, R. E., Marinescu, D. C., Hadfield, A., Muckelbauer, J. K., Munshi, S., Tong, L. & Rossmann, M. G. (1995). *Phase refinement and extension by means of non-crystallographic symmetry averaging using parallel computers*. *Acta Cryst.* **D51**, 749–759.
- Cowtan, K. D. & Main, P. (1993). *Improvement of macromolecular electron-density maps by the simultaneous application of real and reciprocal space constraints*. *Acta Cryst.* **D49**, 148–157.
- Crowther, R. A. (1969). *The use of non-crystallographic symmetry for phase determination*. *Acta Cryst.* **B25**, 2571–2580.
- Das, K., Ding, J., Hsiou, Y., Clark, A. D. Jr, Moereels, H., Koymans, L., Andries, K., Pauwels, R., Janssen, P. A. J., Boyer, P. L., Clark,

REFERENCES

13.4 (cont.)

- P., Smith, R. H. Jr, Kroeger Smith, M. B., Michejda, C. J., Hughes, S. H. & Arnold, E. (1996). *Crystal structure of 8-Cl and 9-Cl TIBO complexed with wild-type HIV-1 RT and 8-Cl TIBO complexed with the Tyr181Cys HIV-1 RT drug-resistant mutant*. *J. Mol. Biol.* **264**, 1085–1100.
- Ding, J., Das, K., Tantillo, C., Zhang, W., Clark, A. D. Jr, Jessen, S., Lu, X., Hsiou, Y., Jacobo-Molina, A., Andries, K., Pauwels, R., Moereels, H., Koymans, L., Janssen, P. A. J., Smith, R. H. Jr, Kroeger Koepke, M., Michejda, C. J., Hughes, S. H. & Arnold, E. (1995). *Structure of HIV-1 reverse transcriptase in a complex with the non-nucleoside inhibitor α -APA R 95845 at 2.8 Å resolution*. *Structure*, **3**, 365–379.
- Dodson, E. J., Gover, S. & Wolf, W. (1992). Editors. *Proceedings of the CCP4 study weekend. Molecular replacement*. Warrington: Daresbury Laboratory.
- Dokland, T., McKenna, R., Sherman, D. M., Bowman, B. R., Bean, W. F. & Rossmann, M. G. (1998). *Structure determination of the φ X174 closed procapsid*. *Acta Cryst. D* **54**, 878–890.
- Esnouf, R., Ren, J., Ross, C., Jones, Y., Stammers, D. & Stuart, D. (1995). *Mechanism of inhibition of HIV-1 reverse transcriptase by non-nucleoside inhibitors*. *Nature Struct. Biol.* **2**, 303–308.
- Fletterick, R. J. & Steitz, T. A. (1976). *The combination of independent phase information obtained from separate protein structure determinations of yeast hexokinase*. *Acta Cryst. A* **32**, 125–132.
- Furey, W. & Swaminathan, S. (1990). *PHASES: a program package for the processing and analysis of diffraction data from macromolecules*. Am. Crystallogr. Assoc. Meeting Abstracts, **18**, PA33, p. 73.
- Furey, W. & Swaminathan, S. (1997). *PHASES-95: a program package for the processing and analysis of diffraction data from macromolecules*. *Methods Enzymol.* **277**, 590–620.
- Gaykema, W. P. J., Hol, W. G. J., Vereijken, J. M., Soeter, N. M., Bak, H. J. & Beintema, J. J. (1984). *3.2 Å structure of the copper-containing, oxygen-carrying protein Panulirus interruptus haemocyanin*. *Nature (London)*, **309**, 23–29.
- Harrison, S. C., Olson, A. J., Schutt, C. E., Winkler, F. K. & Bricogne, G. (1978). *Tomato bushy stunt virus at 2.9 Å resolution*. *Nature (London)*, **276**, 368–373.
- Hogle, J. M., Chow, M. & Filman, D. J. (1985). *Three-dimensional structure of poliovirus at 2.9 Å resolution*. *Science*, **229**, 1358–1365.
- Johnson, J. E. (1978). *Appendix II. Averaging of electron density maps*. *Acta Cryst. B* **34**, 576–577.
- Johnson, J. E., Akimoto, T., Suck, D., Rayment, I. & Rossmann, M. G. (1976). *The structure of southern bean mosaic virus at 22.5 Å resolution*. *Virology*, **75**, 394–400.
- Johnson, J. E., Argos, P. & Rossmann, M. G. (1975). *Rotation function studies of southern bean mosaic virus at 22 Å resolution*. *Acta Cryst. B* **31**, 2577–2583.
- Jones, T. A. (1992). *a, yaap, asap, @#*? A set of averaging programs*. In *Proceedings of the CCP4 study weekend. Molecular replacement*, edited by E. Dodson, S. Gover & W. Wolf, pp. 91–105. Warrington: Daresbury Laboratory.
- Jones, T. A., Zou, J.-Y., Cowan, S. W. & Kjeldgaard, M. (1991). *Improved methods for building protein models in electron density maps and the location of errors in these models*. *Acta Cryst. A* **47**, 110–119.
- Kleywegt, G. J. & Jones, T. A. (1994). *Halloween, masks and bones*. In *From first map to final model*, edited by S. Bailey, R. Hubbard & D. Waller, pp. 59–66. Warrington: Daresbury Laboratory.
- Kleywegt, G. J. & Jones, T. A. (1996). *xdlMAPMAN and xdlDATA-MAN – programs for reformatting, analysis and manipulation of biomacromolecular electron-density maps and reflection data sets*. *Acta Cryst. D* **52**, 826–828.
- Lin, Z., Konno, M., Abad-Zapatero, C., Wierenga, R., Murthy, M. R. N., Ray, W. J. Jr & Rossmann, M. G. (1986). *The structure of rabbit muscle phosphoglucomutase at intermediate resolution*. *J. Biol. Chem.* **261**, 264–274.
- Luo, M., Vriend, G., Kamer, G. & Rossmann, M. G. (1989). *Structure determination of Mengo virus*. *Acta Cryst. B* **45**, 85–92.
- McKenna, R., Xia, D., Willingmann, P., Ilag, L. L., Krishnaswamy, S., Rossmann, M. G., Olson, N. H., Baker, T. S. & Incardona, N. L. (1992). *Atomic structure of single-stranded DNA bacteriophage φ X174 and its functional implications*. *Nature (London)*, **355**, 137–143.
- McKenna, R., Xia, D., Willingmann, P., Ilag, L. L. & Rossmann, M. G. (1992). *Structure determination of the bacteriophage φ X174*. *Acta Cryst. B* **48**, 499–511.
- Main, P. (1967). *Phase determination using non-crystallographic symmetry*. *Acta Cryst.* **23**, 50–54.
- Matthews, B. W., Sigler, P. B., Henderson, R. & Blow, D. M. (1967). *Three-dimensional structure of tosyl- α -chymotrypsin*. *Nature (London)*, **214**, 652–656.
- Muckelbauer, J. K., Kremer, M., Minor, I., Tong, L., Zlotnick, A., Johnson, J. E. & Rossmann, M. G. (1995). *Structure determination of coxsackievirus B3 to 3.5 Å resolution*. *Acta Cryst. D* **51**, 871–887.
- Muirhead, H., Cox, J. M., Mazzarella, L. & Perutz, M. F. (1967). *Structure and function of haemoglobin. III. A three-dimensional Fourier synthesis of human deoxyhaemoglobin at 5.5 Å resolution*. *J. Mol. Biol.* **28**, 117–156.
- Nordman, C. E. (1980). *Procedures for detection and idealization of non-crystallographic symmetry with application to phase refinement of the satellite tobacco necrosis virus structure*. *Acta Cryst. A* **36**, 747–754.
- Perutz, M. F. (1946). *Trans. Faraday Soc.* **42B**, 187.
- Rayment, I. (1983). *Molecular replacement method at low resolution: optimum strategy and intrinsic limitations as determined by calculations on icosahedral virus models*. *Acta Cryst. A* **39**, 102–116.
- Ren, J., Esnouf, R., Garman, E., Somers, D., Ross, C., Kirby, I., Keeling, J., Darby, G., Jones, Y., Stuart, D. & Stammers, D. (1995). *High resolution structures of HIV-1 RT from four RT-inhibitor complexes*. *Nature Struct. Biol.* **2**, 293–302.
- Rossmann, M. G. (1972). Editor. *The molecular replacement method*. New York: Gordon & Breach.
- Rossmann, M. G. (1990). *The molecular replacement method*. *Acta Cryst. A* **46**, 73–82.
- Rossmann, M. G. & Arnold, E. (2001). *Patterson and molecular-replacement techniques*. In *International tables for crystallography*, Vol. B. *Reciprocal space*, edited by U. Shmueli, pp. 235–263. Dordrecht: Kluwer Academic Publishers.
- Rossmann, M. G., Arnold, E., Erickson, J. W., Frankenberger, E. A., Griffith, J. P., Hecht, H. J., Johnson, J. E., Kamer, G., Luo, M., Mosser, A. G., Rueckert, R. R., Sherry, B. & Vriend, G. (1985). *Structure of a human common cold virus and functional relationship to other picornaviruses*. *Nature (London)*, **317**, 145–153.
- Rossmann, M. G. & Blow, D. M. (1962). *The detection of sub-units within the crystallographic asymmetric unit*. *Acta Cryst.* **15**, 24–31.
- Rossmann, M. G. & Blow, D. M. (1963). *Determination of phases by the conditions of non-crystallographic symmetry*. *Acta Cryst.* **16**, 39–45.
- Rossmann, M. G., Blow, D. M., Harding, M. M. & Collier, E. (1964). *The relative positions of independent molecules within the same asymmetric unit*. *Acta Cryst.* **17**, 338–342.
- Rossmann, M. G., McKenna, R., Tong, L., Xia, D., Dai, J.-B., Wu, H., Choi, H.-K. & Lynch, R. E. (1992). *Molecular replacement real-space averaging*. *J. Appl. Cryst.* **25**, 166–180.
- Schuller, D. J. (1996). *MAGICSSQUASH: more versatile non-crystallographic averaging with multiple constraints*. *Acta Cryst. D* **52**, 425–434.
- Sim, G. A. (1959). *The distribution of phase angles for structures containing heavy atoms. II. A modification of the normal heavy-atom method for non-centrosymmetrical structures*. *Acta Cryst.* **12**, 813–815.

13. MOLECULAR REPLACEMENT

13.4 (cont.)

- Tong, L., Qian, C., Davidson, W., Massariol, M.-J., Bonneau, P. R., Cordingley, M. G. & Lagacé, L. (1997). *Experiences from the structure determination of human cytomegalovirus protease*. *Acta Cryst. D***53**, 682–690.
- Tong, L. & Rossmann, M. G. (1995). *Reciprocal-space molecular-replacement averaging*. *Acta Cryst. D***51**, 347–353.
- Tsao, J., Chapman, M. S. & Rossmann, M. G. (1992). *Ab initio phase determination for viruses with high symmetry: a feasibility study*. *Acta Cryst. A***48**, 293–301.
- Tsao, J., Chapman, M. S., Wu, H., Agbandje, M., Keller, W. & Rossmann, M. G. (1992). *Structure determination of monoclinic canine parvovirus*. *Acta Cryst. B***48**, 75–88.
- Valegård, K., Liljas, L., Fridborg, K. & Unge, T. (1990). *The three-dimensional structure of the bacterial virus MS2*. *Nature (London)*, **345**, 36–41.
- Varghese, J. N., Laver, W. G. & Colman, P. M. (1983). *Structure of the influenza virus glycoprotein antigen neuraminidase at 2.9 Å resolution*. *Nature (London)*, **303**, 35–40.
- Vellieux, F. M. D. A. P., Hunt, J. F., Roy, S. & Read, R. J. (1995). *DEMON/ANGEL: a suite of programs to carry out density modification*. *J. Appl. Cryst.* **28**, 347–351.
- Wang, J., Yan, Y., Garrett, T. P. J., Liu, J., Rodgers, D. W., Garlick, R. L., Tarr, G. E., Husain, Y., Reinherz, E. L. & Harrison, S. C. (1990). *Atomic structure of a fragment of human CD4 containing two immunoglobulin-like domains*. *Nature (London)*, **348**, 411–418.
- Wilson, I. A., Skehel, J. J. & Wiley, D. C. (1981). *Structure of the haemagglutinin membrane glycoprotein of influenza virus at 3 Å resolution*. *Nature (London)*, **289**, 366–373.
- Zhang, K. Y. J. (1993). *SQUASH – combining constraints for macromolecular phase refinement and extension*. *Acta Cryst. D***49**, 213–222.