3.3.4.2.5. Cartesian coordinates

Importing Cartesian coordinates can allow the display of incommensurate and quasicrystal structures if the refinement software has this as an output option. Using Cartesian coordinates can sometimes be more convenient for the slight modification of structures for the display of distortions or individual molecules. A structure defined as triclinic with space group *P*1 and a cubic cell with edges of unit length would also work for importing a structure or molecule originally defined in a Cartesian frame of reference.

3.3.4.2.6. Comparing or overlaying crystal structures

The graphical comparison of crystallographic structures can be useful and time-saving for comparison of polymorphs or a chemically similar series of small-molecule structures. One program that can perform this function is *CrystMol*, where multiple molecular structures can be compared using a point and click menu or *via* the *CrystMol* scripting system. RMS differences are also listed. Superposition of structures is discussed in Section 3.3.1.2.2.

3.3.4.2.7. Extended structures and topology analysis

Currently, the only available program that rigorously analyses extended structures (involving overlapping or interpenetrating molecules) is *OLEX*. For graphical viewing of extended structures *OLEX* displays particular fragments in a single colour. *GRETEP* also has this display functionality, making it useful for viewing extended structures.

3.3.4.2.8. Magnetic crystal structure display

The software listed in Tables 3.3.4.1 and 3.3.4.2 includes programs that can display graphics representing magnetic vectors without necessarily having the ability to understand magnetic symmetry. Programs that can display magnetic structures include *ATOMS*, *CrystalMaker*, *Diamond*, *DrawXTL*, *FpStudio*, *VENUS* and *Xtal-3D*.

3.3.4.2.9. Incommensurate crystal structures

PRJMS and *FpStudio* are currently the only programs that can plot modulated structures in three-dimensional space; *FpStudio* is currently restricted to incommensurate magnetic structures. However, importing Cartesian coordinates can be used to display incommensurate structures when incommensurate refinement software can output coordinates in this format. *BALSAC* provides a good example of software which by default uses Cartesian coordinates, from which plots of incommensurate and quasicrystal structures can be generated.

References

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.

Abi-Ezzi, S. S. & Bunshaft, A. J. (1986). *An implementer's view of PHIGS. IEEE Comput. Graphics Appl.* Vol. 6, Part 2.

Aharonov, Y., Farach, H. A. & Poole, C. P. (1977). *Non-linear vector product to describe rotations. Am. J. Phys.* **45**, 451–454.

Allen, F. H., Bellard, S., Brice, M. D., Cartwright, B. A., Doubleday, A., Higgs, H., Hummelink, T., Hummelink-Peters, B. G., Kennard, O., Motherwell, W. D. S., Rodgers, J. R. & Watson, D. G. (1979). *The Cambridge Crystallographic Data Centre: computer-based search, retrieval, analysis and display of information. Acta Cryst.* B**35**, 2331–2339.

Allinger, N. L. (1976). *Calculation of molecular structure and energy by force field methods. Adv. Phys. Org. Chem.* **13**, 1–82.

Altona, C. & Sundaralingam, M. (1972). *Conformational analysis of the sugar ring in nucleosides and nucleotides. A new description using the concept of pseudorotation. J. Am. Chem. Soc.* **94**, 8205–8212.

American National Standards Institute, American National Standard for Information Processing Systems – Computer Graphics – Graphical Kernel System (GKS) Functional Description (1985). ISO 7942, ISO Central Secretariat, Geneva, Switzerland.

American National Standards Institute, American National Standard for Information Processing Systems – Computer Graphics – Programmer's Hierarchical Graphics System (PHIGS) Functional Description, Archive File Format, Clear-Text Encoding of Archive File (1988). ANSI X3.144–1988. ANSI, New York, USA.

Anderson, S. (1984). *Graphical representation of molecules and substructure-search queries in MACCS. J. Mol. Graphics*, **2**, 83–90.

Arnold, D. B. & Bono, P. R. (1988). *CGM and CGI: Metafile and Interface Standards for Computer Graphics.* Berlin: Springer-Verlag.

Atwood, J. L. & Barbour, L. J. (2003). *Molecular graphics: from science to art. Cryst. Growth Des.* **3**, 3.

Barbour, L. J. (2001). *X-Seed – A software tool for supramolecular crystallography. J. Supramol. Chem.* **1**, 189.

Barry, C. D. & North, A. C. T. (1971). *The use of a computer-controlled display system in the study of molecular conformations. Cold Spring Harbour Symp. Quant. Biol.* **36**, 577–584.

Bash, P. A., Pattabiraman, N., Huang, C., Ferrin, T. E. & Langridge, R. (1983). *Van der Waals surfaces in molecular modelling: implementation with real-time computer graphics. Science*, **222**, 1325–1327.

Beddell, C. J. (1970). *An X-ray Crystallographic Study of the Activity of Lysozyme.* DPhil thesis, University of Oxford, England.

Bennett, D. W. (2004). *MolXtl: molecular graphics for small-molecule crystallography. J. Appl. Cryst.* **37**, 1038.

Bernstein, F. C., Koetzle, T. F., Williams, G. J. B., Meyer, E. F., Brice, M. D., Rodgers, J. R., Kennard, O., Shimanouchi, T. & Tasumi, M. (1977). *The Protein Data Bank: a computer-based archival file for macromolecular structures. J. Mol. Biol.* **112**, 535–542.

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.

Boyd, D. B. & Lipkowitz, K. B. (1982). *Molecular mechanics, the method and its underlying philosophy. J. Chem. Educ.* **59**, 269–274.

Brandenburg, N. P., Dempsey, S., Dijkstra, B. W., Lijk, L. J. & Hol, W. G. J. (1981). *An interactive graphics system for comparing and model building of macromolecules. J. Appl. Cryst.* **14**, 274–279.

Brooks, B. R., Brucolleri, R. E., Olafson, B. D., States, D. J., Swaminathan, S. & Karplus, M. (1983). *CHARMM: a program for macromolecular energy, minimization, and dynamics calculations. J. Comput. Chem.* **4**, 187–217.

Brown, M. D. (1985). *Understanding PHIGS.* Template, Megatek Corp., San Diego, California, USA.

Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *New software for searching the Cambridge Structural Database and visualizing crystal structures. Acta Cryst.* B**58**, 389–397.

Burkert, U. & Allinger, N. L. (1982). *Molecular Mechanics. ACS Monogr.* No. 177.

Burnett, M. N. & Johnson, C. K. (1996). *ORTEP-III: Oak Ridge thermal ellipsoid plot program for crystal structure illustrations*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.

Cambillau, C. & Horjales, E. (1987). *TOM: a FRODO subpackage for protein-ligand fitting with interactive energy minimization. J. Mol. Graphics*, **5**, 174–177.

Cambillau, C., Horjales, E. & Jones, T. A. (1984). *TOM, a display program for fitting ligands into protein receptors and performing interactive energy minimization. J. Mol. Graphics*, **2**, 53–54.

Cambridge Structural Database (1994). Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, England.

Chapon, L. C. & Rodriguez-Carvajal, J. (2005). *FpStudio*. Rutherford Appleton Laboratory, UK, and Laboratoire Léon Brillouin, Saclay, France.

Cockcroft, J. K. & Stephenson, R. (2005). *EPSRC-funded Collaborative Computational Project Number 14 for Single Crystal and Powder Diffraction (CCP14)*, http://www.ccp14.ac.uk/.

Cockrell, P. R. (1983). *A new general purpose method for large volume production of contour charts. Comput. Graphics Forum*, **2**, 35–47.

Cohen, N. C. (1971). *GEMO: a computer program for the calculation of the preferred conformations of organic molecules. Tetrahedron*, **27**, 789–797.

Cohen, N. C., Colin, P. & Lemoine, G. (1981). *Script: interactive molecular geometrical treatments on the basis of computer-drawn chemical formula. Tetrahedron*, **37**, 1711–1721.

Collins, D. M., Cotton, F. A., Hazen, E. E., Meyer, E. F. & Morimoto, C. N. (1975). *Protein crystal structures: quicker, cheaper approaches. Science*, **190**, 1047–1053.

Connolly, M. L. (1983*a*). *Solvent-accessible surfaces of proteins and nucleic acids. Science*, **221**, 709–713.

Connolly, M. L. (1983*b*). *Analytical molecular surface calculation. J. Appl. Cryst.* **16**, 548–558.

Dam, A. van (1988). *PHIGS+ functional description, revision 3.0. Comput. Graphics*, **22**, 125–218.

Dayringer, H. E., Tramontano, A., Sprang, S. R. & Fletterick, R. J. (1986). *Interactive program for visualization and modelling of proteins, nucleic acids and small molecules. J. Mol. Graphics*, **4**, 82–87.

Diamond, R. (1966). *A mathematical model-building procedure for proteins. Acta Cryst.* **21**, 253–266.

Diamond, R. (1971). *A real-space refinement procedure for proteins. Acta Cryst.* A**27**, 436–452.

Diamond, R. (1976*a*). *On the comparison of conformations using linear and quadratic transformations. Acta Cryst.* A**32**, 1–10.

Diamond, R. (1976*b*). *Model building techniques for macromolecules.* In *Crystallographic Computing Techniques*, edited by F. R. Ahmed, K. Huml & B. Sedlacek, pp. 336–343. Copenhagen: Munksgaard.

Diamond, R. (1980*a*). *Some problems in macromolecular map interpretation.* In *Computing in Crystallography*, edited by R. Diamond, S. Ramaseshan & K. Venkatesan, pp. 21.01–21.19. Bangalore: Indian Academy of Sciences for the International Union of Crystallography.

Diamond, R. (1980*b*). *Inter-active graphics.* In *Computing in Crystallography*, edited by R. Diamond, S. Ramaseshan & K. Venkatesan, pp. 27.01–27.16. Bangalore: Indian Academy of Sciences for the International Union of Crystallography.

Diamond, R. (1981*a*). *BILDER: a computer graphics program for biopolymers and its application to the interpretation of the structure of tobacco mosaic virus protein discs at 2.8 Å resolution.* In *Biomolecular Structure, Conformation, Function and Evolution*, Vol. 1, edited by R. Srinivasan, pp. 567–588. Oxford: Pergamon Press.

Diamond, R. (1981*b*). *A review of the principles and properties of the method of least squares.* In *Structural Aspects of Biomolecules*, edited by R. Srinivasan & V. Pattabhi, pp. 81–122. Delhi: Macmillan India Ltd.

Diamond, R. (1982*a*). *Two contouring algorithms.* In *Computational Crystallography*, edited by D. Sayre, pp. 266–272. Oxford University Press.

Diamond, R. (1982*b*). *BILDER: an interactive graphics program for biopolymers.* In *Computational Crystallography*, edited by D. Sayre, pp. 318–325. Oxford University Press.

Diamond, R. (1984*a*). *Applications of computer graphics in molecular biology. Comput. Graphics Forum*, **3**, 3–11.

Diamond, R. (1984*b*). *Least squares and related optimisation techniques.* In *Methods and Applications in Crystallographic Computing*, edited by S. R. Hall & T. Ashida, pp. 174–192. Oxford University Press.

Diamond, R. (1988). *A note on the rotational superposition problem. Acta Cryst.* A**44**, 211–216.

Diamond, R. (1989). *A comparison of three recently published methods for superimposing vector sets by pure rotation. Acta Cryst.* A**45**, 657.

Diamond, R. (1990*a*). *On the factorisation of rotations with special reference to diffractometry. Proc. R. Soc. London Ser. A*, **428**, 451–472.

Diamond, R. (1990*b*). *Chirality in rotational superposition. Acta Cryst.* A**46**, 423.

Diamond, R. (1992). *On the multiple simultaneous superposition of molecular structures by rigid body transformations. Protein Sci.* **1**, 1279–1287.

Diamond, R. (1995). *Coordinate based cluster analysis. Acta Cryst.* D**51**, 127–135.

Diamond, R., Wynn, A., Thomsen, K. & Turner, J. (1982). *Three-dimensional perception for one-eyed guys, or, the use of dynamic parallax.* In *Computational Crystallography*, edited by D. Sayre, pp. 286–293. Oxford University Press.

Dodson, E. J., Isaacs, N. W. & Rollett, J. S. (1976). *A method for fitting satisfactory models to sets of atomic positions in protein structure refinements. Acta Cryst.* A**32**, 311–315.

Dodson, G. G., Eliopoulos, E. E., Isaacs, N. W., McCall, M. J., Niall, H. D. & North, A. C. T. (1982). *Rat relaxin: insulin-like fold predicts a likely receptor binding region. Int. J. Biol. Macromol.* **4**, 399–405.

Dolomanov, O. V., Blake, A. J., Champness, N. R. & Schröder, M. (2003). *OLEX: new software for visualization and analysis of extended crystal structures. J. Appl. Cryst.* **36**, 1283–1284.

Downs, R. T. & Hall-Wallace, M. (2003). *The American Mineralogist Crystal Structure Database. Am. Mineral.* **88**, 247–250.

Dowty, E. (2005). *Cryscon*. Shape Software, 521 Hidden Valley Road, Kingsport, TN 37663, USA. http://www.shapesoftware.com/.

Enderle, G., Kansy, K. & Pfaff, G. (1984). *Computer Graphics Programming, GKS – the Graphics Standard.* Berlin: Springer-Verlag.

Evans, P. R., Farrants, G. W. & Hudson, P. J. (1981). *Phosphofructokinase: structure and control. Philos. Trans. R. Soc. London Ser. B*, **293**, 53–62.

Farrugia, L. J. (1997). *ORTEP-3 for Windows – a version of ORTEP-III with a Graphical User Interface (GUI). J. Appl. Cryst.* **30**, 565.

Feldmann, R. J. (1976). *The design of computing systems for molecular modeling. Annu. Rev. Biophys. Bioeng.* **5**, 477–510.

Feldmann, R. J. (1983). *Directions in macromolecular structure representation and display.* In *Computer Applications in Chemistry*, edited by S. R. Heller & R. Potenzone Jr, pp. 9–18. Amsterdam: Elsevier.

Feldmann, R. J., Bing, D. H., Furie, B. C. & Furie, B. (1978). *Interactive computer surface graphics approach to the study of the active site of bovine trypsin. Proc. Natl Acad. Sci. Biochemistry*, **75**, 5409–5412.

Ferrin, T. E., Huang, C., Jarvis, L. & Langridge, R. (1984). *Molecular inter-active display and simulation: MIDAS. J. Mol. Graphics*, **2**, 55.

Finger, L. W., Kroeker, M. & Toby, B. H. (2007). *DRAWxtl, an open-source computer program to produce crystal structure drawings. J. Appl. Cryst.* **40**, 188–192.

Fischer, R. X. (1985). *STRUPLO84, a Fortran plot program for crystal structure illustrations in polyhedral representation. J. Appl. Cryst.* **18**, 258–262.

Foley, J. D., van Dam, A., Feiner, S. K. & Hughes, J. F. (1990). *Computer Graphics Principles and Practice*, 2nd ed. New York: Addison Wesley.

Ford, L. O., Johnson, L. N., Machin, P. A., Phillips, D. C. & Tjian, R. (1974). *Crystal structure of a lysozyme-tetrasaccharide lactone complex. J. Mol. Biol.* **88**, 349–371.

Gallo, L., Huang, C. & Ferrin, T. (1983). *UCSF MIDAS, molecular interactive display and simulation, users' guide.* Computer Graphics Laboratory, School of Pharmacy, University of California, San Francisco, USA.

Gill, P. E., Murray, W. & Wright, M. H. (1981). *Practical Optimization.* Orlando: Academic Press.

Gilliland, G. L. & Quiocho, F. A. (1981). *Structure of the* L*-arabinose-binding protein from Escherichia coli at 2.4 Å resolution. J. Mol. Biol.* **146**, 341–362.

Girling, R. L., Houston, T. E., Schmidt, W. C. Jr & Amma, E. L. (1980). *Macromolecular structure refinement by restrained least-squares and interactive graphics as applied to sickling deer type III hemoglobin. Acta Cryst.* A**36**, 43–50.

Gossling, T. H. (1967). *Two methods of presentation of electron-density maps using a small-store computer. Acta Cryst.* **22**, 465–468.

Greer, J. (1974). *Three-dimensional pattern recognition: an approach to automated interpretation of electron density maps of proteins. J. Mol. Biol.* **82**, 279–302.

Harris, M. R., Geddes, A. J. & North, A. C. T. (1985). *A liquid crystal stereo-viewer for molecular graphics. J. Mol. Graphics*, **3**, 121–122.

Hass, B. S., Willoughby, T. V., Morimoto, C. N., Cullen, D. L. & Meyer, E. F. (1975). *The solution of the structure of spirodienone by visual packing analysis. Acta Cryst.* B**31**, 1225–1229.

Heap, B. R. & Pink, M. G. (1969). *Three contouring algorithms*, DNAM Rep. 81. National Physical Laboratory, Teddington, England.

Hermans, J. (1985). *Rationalization of molecular models.* In *Methods in Enzymology*, Vol. 115, *Diffraction Methods for Biological Molecules*, Part B, edited by H. W. Wyckoff, C. H. W. Hirs & S. N. Timasheff, pp. 171–189. Orlando: Academic Press.

Hermans, J. & McQueen, J. E. (1974). *Computer manipulation of (macro) molecules with the method of local change. Acta Cryst.* A**30**, 730–739.

Hewat, A. (2002). *Databases linked to electronic publications. Acta Cryst.* A**58** (Suppl.), C216.

Hogle, J., Rao, S. T., Mallikarjunan, M., Beddell, C., McMullan, R. K. & Sundaralingam, M. (1981). *Studies of monoclinic hen egg white lysozyme. Structure solution at 4 Å resolution and molecular-packing*

comparisons with tetragonal and triclinic lysozymes. Acta Cryst. B**37**, 591–597.

Hopgood, F. R. A., Duce, D. A., Gallop, J. R. & Sutcliffe, D. C. (1986). *Introduction to the Graphical Kernel System*, 2nd ed. London: Academic Press.

Hubbard, R. E. (1983). *Colour molecular graphics on a microcomputer. J. Mol. Graphics*, **1**, 13–16, C3–C4.

Hubbard, R. E. (1985). *The representation of protein structure.* In *Computer Aided Molecular Design*, pp. 99–106. Proceedings of a two-day conference, London, October 1984. London: Oyez Scientific.

Hummel, W., Hauser, J. & Bürgi, H.-B. (1990). *PEANUT: computer graphics program to represent atomic displacement parameters. J. Mol. Graphics*, **8**, 214–220.

Hummel, W., Raselli, A. & Bürgi, H.-B. (1990). *Analysis of atomic displacement parameters and molecular motion in crystals. Acta Cryst.* B**46**, 683–692.

International Standards Organisation, International Standard Information Processing Systems – Computer Graphics – Graphical Kernel System for Three Dimensions (GKS-3D), Functional Description (1988). ISO Document No. 8805:1988(E). American National Standards Institute, New York, USA.

International Tables for Crystallography (2001). Vol. F. *Crystallography of Biological Macromolecules*, edited by M. G. Rossmann & E. Arnold. Dordrecht: Kluwer Academic Publishers.

International Tables for Crystallography (2005). Vol. A. *Space-Group Symmetry*, edited by Th. Hahn. Heidelberg: Springer.

International Tables for Crystallography (2005). Vol. G. *Definition and Exchange of Crystallographic Data*, edited by S. R. Hall & B. McMahon. Heidelberg: Springer.

IUPAC–IUB Commission on Biochemical Nomenclature (1970). *Abbreviations and symbols for the description of the conformation of polypeptide chains. J. Biol. Chem.* **245**, 6489–6497.

Izumi, F. (2004). *Beyond the ability of Rietveld analysis: MEM-based pattern fitting. Solid State Ionics*, **172**, 1–6.

Izumi, F. & Dilanian, R. A. (2002). *Structure refinement based on the maximum-entropy method from powder diffraction data.* In *Recent Research Developments in Physics*, Vol. 3, Part II, pp. 699–726. Trivandrum: Transworld Research Network.

Johnson, C. K. (1970). *Drawing crystal structures by computer.* In *Crystallographic Computing*, edited by F. R. Ahmed, pp. 227–230. Copenhagen: Munksgaard.

Johnson, C. K. (1976). *ORTEP-II. A Fortran thermal-ellipsoid plot program for crystal structure illustrations.* Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Johnson, C. K. (1980). *Computer-generated illustrations.* In *Computing in Crystallography*, edited by R. Diamond, S. Ramaseshan & K. Venkatesan, pp. 26.01–26.10. Bangalore: Indian Academy of Sciences for the International Union of Crystallography.

Jones, T. A. (1978). *A graphics model building and refinement system for macromolecules. J. Appl. Cryst.* **11**, 268–272.

Jones, T. A. (1982). *FRODO: a graphics fitting program for macromolecules.* In *Computational Crystallography*, edited by D. Sayre, pp. 303–317. Oxford University Press.

Jones, T. A. (1985). *Interactive computer graphics: FRODO.* In *Methods in Enzymology*, Vol. 115, *Diffraction Methods for Biological Molecules*, Part B, edited by H. W. Wyckoff, C. H. W. Hirs & S. N. Timasheff, pp. 157–171. Orlando: Academic Press.

Jones, T. A. & Liljas, L. (1984). *Crystallographic refinement of macromolecules having non-crystallographic symmetry. Acta Cryst.* A**40**, 50–57.

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.

Kabsch, W. (1976). *A solution for the best rotation to relate two sets of vectors. Acta Cryst.* A**32**, 922–923.

Kabsch, W. (1978). *A discussion of the solution for the best rotation to relate two sets of vectors. Acta Cryst.* A**34**, 827–828.

Katz, L. & Levinthal, C. (1972). *Interactive computer graphics and representation of complex biological structures. Annu. Rev. Biophys. Bioeng.* **1**, 465–504.

Kearsley, S. K. (1989). *On the orthogonal transformation used for structural comparisons. Acta Cryst.* A**45**, 208–210.

Kearsley, S. K. (1990). *An algorithm for the simultaneous superposition of a structural series. J. Comput. Chem.* **11**, 1187–1192.

Keller, E. (1999). *SCHAKAL 99, a computer program for the graphic representation of molecular and solid-state structure models*. University of Freiburg, Germany.

Kraus, W. & Nolze, G. (1996). *POWDER CELL – a program for the representation and manipulation of crystal structures and calculation of the resulting X-ray powder patterns. J. Appl. Cryst.* **29**, 301–303.

Langridge, R., Ferrin, T. E., Kuntz, I. D. & Connolly, M. L. (1981). *Real-time color graphics in studies of molecular interactions. Science*, **211**, 661–666.

Le Bail, A. (1996). *VRML as a tool for exploring complex structures. Acta Cryst.* A**52** (Suppl.), C78.

Lederer, F., Glatigny, A., Bethge, P. H., Bellamy, H. D. & Mathews, F. S. (1981). *Improvement of the 2.5 Å resolution model of cytochrome b_{562} by re-determining the primary structure and using molecular graphics. J. Mol. Biol.* **148**, 427–448.

Lesk, A. M. (1991). *Protein Architecture: A Practical Approach.* Oxford: IRL Press.

Lesk, A. M. & Hardman, K. D. (1982). *Computer-generated schematic diagrams of protein structures. Science*, **216**, 539–540.

Lesk, A. M. & Hardman, K. D. (1985). *Computer-generated pictures of proteins.* In *Methods in Enzymology*, Vol. 115, *Diffraction Methods for Biological Molecules*, Part B, edited by H. W. Wyckoff, C. H. W. Hirs & S. N. Timasheff, pp. 381–390. Orlando: Academic Press.

Levinthal, C. (1966). *Molecular model-building by computer. Sci. Am.* **214**, 42–52.

Levitt, M. (1971). PhD Dissertation, ch. 2. University of Cambridge, England.

Levitt, M. (1974). *Energy refinement of hen egg-white lysozyme. J. Mol. Biol.* **82**, 393–420.

Levitt, M. & Lifson, S. (1969). *Refinement of protein conformations using a macromolecular energy minimization procedure. J. Mol. Biol.* **46**, 269–279.

Levitt, M. & Warshel, A. (1975). *Computer simulation of protein folding. Nature (London)*, **253**, 694–698.

Lieth, C. W. van der, Carter, R. E., Dolata, D. P. & Liljefors, T. (1984). *RINGS – a general program to build ring systems. J. Mol. Graphics*, **2**, 117–123.

Liljefors, T. (1983). *MOLBUILD – an interactive computer graphics interface to molecular mechanics. J. Mol. Graphics*, **1**, 111–117.

Luenberger, D. G. (1984). *Linear and Nonlinear Programming.* Reading: Addison Wesley.

McArdle, P. (1994). *ORTEX2.1 – a 1677-atom version of ORTEP with automatic cell outline and cell packing for use on a PC. J. Appl. Cryst.* **27**, 438–439.

McArdle, P., Gilligan, K., Cunningham, D., Dark, R. & Mahon, M. (2004). *A method for the prediction of the crystal structure of ionic organic compounds? The crystal structures of o-toluidinium chloride and bromide and polymorphism of bicifadine hydrochloride. CrystEngComm*, **6**, 303.

Mackay, A. L. (1984). *Quaternion transformation of molecular orientation. Acta Cryst.* A**40**, 165–166.

McLachlan, A. D. (1972). *A mathematical procedure for superimposing atomic coordinates of proteins. Acta Cryst.* A**28**, 656–657.

McLachlan, A. D. (1979). *Gene duplications in the structural evolution of chymotrypsin. Appendix: Least squares fitting of two structures. J. Mol. Biol.* **128**, 49–79.

McLachlan, A. D. (1982). *Rapid comparison of protein structures. Acta Cryst.* A**38**, 871–873.

Max, N. L. (1984). *Computer representation of molecular surfaces. J. Mol. Graphics*, **2**, 8–13, C2–C4.

Meyer, E. F. (1970). *Three-dimensional graphical models of molecules and a time-slicing computer. J. Appl. Cryst.* **3**, 392–395.

Meyer, E. F. (1971). *Interactive computer display for the three dimensional study of macromolecular structures. Nature (London)*, **232**, 255–257.

Meyer, E. F. (1974). *Storage and retrieval of macromolecular structural data. Biopolymers*, **13**, 419–422.

Miller, J. R., Abdel-Meguid, S. S., Rossmann, M. G. & Anderson, D. C. (1981). *A computer graphics system for the building of macromolecular models into electron density maps. J. Appl. Cryst.* **14**, 94–100.

Morffew, A. J. (1983). *Bibliography for molecular graphics. J. Mol. Graphics*, **1**, 17–23.

Morffew, A. J. (1984). *Bibliography for molecular graphics, 1983/84. J. Mol. Graphics*, **2**, 124–128.

Morimoto, C. N. & Meyer, E. F. (1976). *Information retrieval, computer graphics, and remote computing.* In *Crystallographic Computing Techniques*, edited by F. R. Ahmed, K. Huml & B. Sedlacek, pp. 488–496. Copenhagen: Munksgaard.

Motherwell, W. D. S. (1978). *Pluto – a program for displaying molecular and crystal structures.* Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, England.

Newman, W. M. & Sproull, R. F. (1973). *Principles of Inter-active Computer Graphics.* New York: McGraw-Hill.

North, A. C. T. (1982). *Use of interactive computer graphics in studying molecular structures and interactions. Chem. Ind.* pp. 221–225.

North, A. C. T., Denson, A. K., Evans, A. C., Ford, L. O. & Willoughby, T. V. (1981). *The use of an interactive computer graphics system in the study of protein conformations.* In *Biomolecular Structure, Conformation, Function and Evolution*, Vol. 1, edited by R. Srinivasan, pp. 59–72. Oxford: Pergamon Press.

O'Donnell, T. J. & Olson, A. J. (1981). *GRAMPS – a graphics language interpreter for real-time, interactive, three-dimensional picture editing and animation. Comput. Graphics*, **15**, 133–142.

Olson, A. J. (1982). *GRAMPS: a high level graphics interpreter for expanding graphics utilization.* In *Computational Crystallography*, edited by D. Sayre, pp. 326–336. Oxford University Press.

Opdenbosch, N. van, Cramer, R. III & Giarrusso, F. F. (1985). *Sybyl, the integrated molecular modelling system. J. Mol. Graphics*, **3**, 110–111.

Ozawa, T. C. & Kang, S. J. (2004). *Balls&Sticks: easy-to-use structure visualization and animation program. J. Appl. Cryst.* **37**, 679.

Pearl, L. H. & Honegger, A. (1983). *Generation of molecular surfaces for graphic display. J. Mol. Graphics*, **1**, 9–12, C2.

Phillips, S. E. V. (1980). *Structure and refinement of oxymyoglobin at 1.6 Å resolution. J. Mol. Biol.* **142**, 531–554.

Phong, B. T. (1975). *Illumination for computer generated images. Commun. ACM*, **18**, 311–317.

Porter, T. K. (1978). *Spherical shading. Comput. Graphics*, **12**, 282–285.

Potenzone, R., Cavicchi, E., Weintraub, H. J. R. & Hopfinger, A. J. (1977). *Molecular mechanics and the CAMSEQ processor. Comput. Chem.* **1**, 187–194.

Potterton, E. A., Geddes, A. J. & North, A. C. T. (1983). *Attempts to design inhibitors of dihydrofolate reductase using interactive computer graphics with real time energy calculations.* In *Chemistry and Biology of Pteridines*, edited by J. A. Blair, pp. 299–303. Berlin, New York: Walter de Gruyter.

Purisima, E. O. & Scheraga, H. A. (1986). *An approach to the multiple-minima problem by relaxing dimensionality. Proc. Natl Acad. Sci. USA*, **83**, 2782–2786.

Richardson, J. S. (1977). *β-Sheet topology and the relatedness of proteins. Nature (London)*, **268**, 495–500.

Richardson, J. S. (1981). *The anatomy and taxonomy of protein structure. Adv. Protein Chem.* **34**, 167–339.

Richardson, J. S. (1985). *Schematic drawings of protein structures.* In *Methods in Enzymology*, Vol. 115, *Diffraction Methods for Biological Molecules*, Part B, edited by H. W. Wyckoff, C. H. W. Hirs & S. N. Timasheff, pp. 359–380. Orlando: Academic Press.

Shapiro, A., Botha, J. D., Pastore, A. & Lesk, A. M. (1992). *A method for multiple superposition of structures. Acta Cryst.* A**48**, 11–14.

Siegrist, T. (1997). *Crystallographica – a software toolkit for crystallography. J. Appl. Cryst.* **30**, 418–419.

Soyer, A. (1993). *LMCTEP: software for crystal structure representation. J. Appl. Cryst.* **26**, 495.

Spek, A. L. (1998). *PLATON. A multipurpose crystallographic tool*. University of Utrecht, Utrecht, The Netherlands.

Spek, A. L. (2003). *Single-crystal structure validation with the program PLATON. J. Appl. Cryst.* **36**, 7–13.

Sundaram, K. & Radhakrishnan, R. (1979). *A computer program for topographic analysis of biomolecular systems. Comput. Programs Biomed.* **10**, 34–42.

Sutcliffe, D. C. (1980). *Contouring over rectangular and skewed rectangular grids – an introduction.* In *Mathematical Methods in Computer Graphics and Design*, edited by K. W. Brodie, pp. 39–62. London: Academic Press.

Sutherland, I. E., Sproull, R. F. & Schumacker, R. A. (1974). *A characterization of ten hidden surface algorithms. Comput. Surv.* **6**, 1–55.

Swanson, S. M., Wesolowski, T., Geller, M. & Meyer, E. F. (1989). *Animation: a useful tool for protein molecular dynamicists, applied to hydrogen bonds in the active site of elastase. J. Mol. Graphics*, **7**, 240–242, 223–224.

Takenaka, A. & Sasada, Y. (1980). *Computer manipulation of crystal and molecular models. J. Crystallogr. Soc. Jpn*, **22**, 214–225.

Thomas, D. J. (1993). *Toward more reliable printed stereo. J. Mol. Graphics*, **11**, 15–22.

Tsernoglou, D., Petsko, G. A., McQueen, J. E. & Hermans, J. (1977). *Molecular graphics: application to the structure determination of a snake venom neurotoxin. Science*, **197**, 1378–1381.

Vedani, A. & Meyer, E. F. (1984). *Structure–activity relationships of sulfonamide drugs and human carbonic anhydrase C: modelling of inhibitor molecules into receptor site of the enzyme with an interactive computer graphics display. J. Pharm. Sci.* **73**, 352–358.

Walsh, G. R. (1975). *Methods of Optimization.* London: John Wiley.

Warme, P. K., Go, N. & Scheraga, H. A. (1972). *Refinement of X-ray data of proteins. 1. Adjustment of atomic coordinates to conform to a specified geometry. J. Comput. Phys.* **9**, 303–317.

Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.

Williams, T. V. (1982). Thesis. University of North Carolina at Chapel Hill, NC, USA.

Willoughby, T. V., Morimoto, C. N., Sparks, R. A. & Meyer, E. F. (1974). *Mini-computer control of a stereo graphics display. J. Appl. Cryst.* **7**, 430–434.

Wipke, W. T. (1974). *Computer assisted three-dimensional synthetic analysis.* In *Computer Representation and Manipulation of Chemical Information*, edited by W. T. Wipke, S. R. Heller, R. J. Feldmann & E. Hyde, pp. 147–174. New York: John Wiley.

Wipke, W. T., Braun, H., Smith, G., Choplin, F. & Sieber, W. (1977). *SECS – simulation and evaluation of chemical synthesis: strategy and planning. ACS Symp. Ser.* **61**, 97–125.

Wipke, W. T. & Dyott, T. M. (1974). *Simulation and evaluation of chemical synthesis. Computer representation and manipulation of stereochemistry. J. Am. Chem. Soc.* **96**, 4825–4834.

Yamamoto, A. (1982). *Structure factor of modulated crystal structures. Acta Cryst.* A**38**, 87–92.