

21. STRUCTURE VALIDATION

References

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- Aalten, D. M. F. van, Bywater, R., Findlay, J. B. C., Hendlich, M., Hooft, R. W. W. & Vriend, G. (1996). *PRODRG, a program for generating molecular topologies and unique molecular descriptors from coordinates of small molecules*. *J. Comput. Aided Mol. Des.* **10**, 255–262.
- Abagyan, R. A. & Totrov, M. M. (1997). *Contact area difference (CAD): a robust measure to evaluate accuracy of protein models*. *J. Mol. Biol.* **268**, 678–685.
- Abola, E. E., Bairoch, A., Barker, W. C., Beck, S., Benson, D. A., Berman, H., Cantor, C., Doubet, S., Hubbard, T. J. P., Jones, T. A., Kleywegt, G. J., Kolaskar, A. S., van Kuik, A., Lesk, A. M., Mewes, H. W., Neuhaus, D., Pfeiffer, F., Ten Eyck, L. F., Simpson, R. J., Stoesser, G., Sussman, J. L., Tateno, Y., Tsugita, A., Ulrich, E. L. & Vliegthart, J. F. G. (2000). *Quality control in databanks for molecular biology*. *BioEssays*, **22**, 1024–1034.
- Adams, P. D., Pannu, N. S., Read, R. J. & Brünger, A. T. (1997). *Cross-validated maximum likelihood enhances crystallographic simulated annealing refinement*. *Proc. Natl Acad. Sci. USA*, **94**, 5018–5023.
- Akker, F. van den & Hol, W. G. J. (1999). *Difference density quality (DDQ): a method to assess the global and local correctness of macromolecular crystal structures*. *Acta Cryst.* **D55**, 206–218.
- 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.* **B35**, 2331–2339.
- Allen, F. H. & Johnson, O. (1991). *Automated conformational analysis from crystallographic data. 4. Statistical descriptors for a distribution of torsion angles*. *Acta Cryst.* **B47**, 62–67.
- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *Tables of bond lengths determined by X-ray and neutron diffraction. Part 1. Bond lengths in organic compounds*. *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.
- Ammon, H. L., Weber, I. T., Wlodawer, A., Harrison, R. W., Gilliland, G. L., Murphy, K. C., Sjölin, L. & Roberts, J. (1988). *Preliminary crystal structure of Acinetobacter glutaminasificans glutaminase-asparaginase*. *J. Biol. Chem.* **263**, 150–156.
- Bacchi, A., Lamzin, V. S. & Wilson, K. S. (1996). *A self-validation technique for protein structure refinement: the extended Hamilton test*. *Acta Cryst.* **D52**, 641–646.
- Balasubramanian, R. (1977). *New type of representation for mapping chain-folding in protein molecules*. *Nature (London)*, **266**, 856–857.
- Bernstein, F. C., Koetzle, T. F., Williams, G. J. B., Meyer, E. F. Jr, 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.
- Bhat, T. N. (1988). *Calculation of an OMIT map*. *J. Appl. Cryst.* **21**, 279–281.
- Bhat, T. N. & Cohen, G. H. (1984). *OMITMAP: an electron density map suitable for the examination of errors in a macromolecular model*. *J. Appl. Cryst.* **17**, 244–248.
- Borgstahl, G. E. O., Williams, D. R. & Getzoff, E. D. (1995). *1.4 Å structure of photoactive yellow protein, a cytosolic photoreceptor: unusual fold, active site, and chromophore*. *Biochemistry*, **34**, 6278–6287.
- Bott, R. & Sarma, R. (1976). *Crystal structure of turkey egg-white lysozyme: results of the molecular replacement method at 5 Å resolution*. *J. Mol. Biol.* **106**, 1037–1046.
- Bowie, J. U., Lüthy, R. & Eisenberg, D. (1991). *A method to identify protein sequences that fold into a known three-dimensional structure*. *Science*, **253**, 164–170.
- Brändén, C.-I. & Jones, T. A. (1990). *Between objectivity and subjectivity*. *Nature (London)*, **343**, 687–689.
- Bricogne, G. & Irwin, J. (1996). *Maximum-likelihood refinement of incomplete models with BUSTER + TNT*. In *Proceedings of the CCP4 study weekend. Macromolecular refinement*, edited by E. Dodson, M. Moore, A. Ralph & S. Bailey, pp. 85–92. Warrington: Daresbury Laboratory.
- Brünger, A. T. (1992a). *Free R value: a novel statistical quantity for assessing the accuracy of crystal structures*. *Nature (London)*, **355**, 472–475.
- Brünger, A. T. (1992b). *X-PLOR. A system for crystallography and NMR*. Yale University, New Haven, Connecticut, USA.
- Brünger, A. T. (1993). *Assessment of phase accuracy by cross validation: the free R value*. *Methods and applications*. *Acta Cryst.* **D49**, 24–36.
- Brünger, A. T. (1997). *The free R value: a more objective statistic for crystallography*. *Methods Enzymol.* **277**, 366–396.
- Carson, M., Buckner, T. W., Yang, Z., Narayana, S. V. L. & Bugg, C. E. (1994). *Error detection in crystallographic models*. *Acta Cryst.* **D50**, 900–909.
- Carugo, O. & Bordo, D. (1999). *How many water molecules can be detected by protein crystallography?* *Acta Cryst.* **D55**, 479–483.
- Chapman, M. S. (1995). *Restrained real-space macromolecular atomic refinement using a new resolution-dependent electron-density function*. *Acta Cryst.* **A51**, 69–80.
- Colovos, C. & Yeates, T. O. (1993). *Verification of protein structures: patterns of nonbonded atomic interactions*. *Protein Sci.* **2**, 1511–1519.
- Cruickshank, D. W. J. (1949). *The accuracy of electron-density maps in X-ray analysis with special reference to dibenzyl*. *Acta Cryst.* **2**, 65–82.
- Cruickshank, D. W. J. (1950). *The convergence of the least-squares or Fourier refinement methods*. *Acta Cryst.* **3**, 10–13.
- Cruickshank, D. W. J. (1999). *Remarks about protein structure precision*. *Acta Cryst.* **D55**, 583–601.
- Diederichs, K. & Karplus, P. A. (1997). *Improved R-factors for diffraction data analysis in macromolecular crystallography*. *Nature Struct. Biol.* **4**, 269–275.
- Dodson, E., Kleywegt, G. J. & Wilson, K. S. (1996). *Report of a workshop on the use of statistical validators in protein X-ray crystallography*. *Acta Cryst.* **D52**, 228–234.
- Drenth, J. (1994). *Principles of protein X-ray crystallography*. New York: Springer-Verlag.
- Engh, R. A. & Huber, R. (1991). *Accurate bond and angle parameters for X-ray protein structure refinement*. *Acta Cryst.* **A47**, 392–400.
- EU 3-D Validation Network (1998). *Who checks the checkers? Four validation tools applied to eight atomic resolution structures*. *J. Mol. Biol.* **276**, 417–436.
- Flocco, M. M. & Mowbray, S. L. (1995). *C α -based torsion angles: a simple tool to analyze protein conformational changes*. *Protein Sci.* **4**, 2118–2122.
- Greaves, R. B., Vagin, A. A. & Dodson, E. J. (1999). *Automated production of small-molecule dictionaries for use in crystallographic refinements*. *Acta Cryst.* **D55**, 1335–1339.
- Gunasekaran, K., Ramakrishnan, C. & Balaram, P. (1996). *Disallowed Ramachandran conformations of amino acid residues in protein structures*. *J. Mol. Biol.* **264**, 191–198.
- Hamilton, W. C. (1965). *Significance tests on the crystallographic R factor*. *Acta Cryst.* **18**, 502–510.
- Hendrickson, W. A. (1985). *Stereochemically restrained refinement of macromolecular structures*. *Methods Enzymol.* **115**, 252–270.
- Hendrickson, W. A. & Konnert, J. H. (1980). *Incorporation of stereochemical information into crystallographic refinement*. In *Computing in crystallography*, edited by R. Diamond, S. Ramaseshan & K. Venkatesan, pp. 13.01–13.25. Bangalore: Indian Academy of Science.
- Herzberg, O. & Moulton, J. (1991). *Analysis of the steric strain in the polypeptide backbone of protein molecules*. *Proteins Struct. Funct. Genet.* **11**, 223–229.
- Hodel, A., Kim, S.-H. & Brünger, A. T. (1992). *Model bias in macromolecular crystal structures*. *Acta Cryst.* **A48**, 851–858.

REFERENCES

21.1 (cont.)

- Hoier, H., Schlömann, M., Hammer, A., Glusker, J. P., Carrell, H. L., Goldman, A., Stezowski, J. J. & Heinemann, U. (1994). Crystal structure of chloromuconate cycloisomerase from *Alcaligenes eutrophus* JMP134 (pJP4) at 3 Å resolution. *Acta Cryst.* **D50**, 75–84.
- Hooft, R. W. W., Sander, C. & Vriend, G. (1994). Reconstruction of symmetry-related molecules from Protein Data Bank (PDB) files. *J. Appl. Cryst.* **27**, 1006–1009.
- Hooft, R. W. W., Sander, C. & Vriend, G. (1996a). Verification of protein structures: side-chain planarity. *J. Appl. Cryst.* **29**, 714–716.
- Hooft, R. W. W., Sander, C. & Vriend, G. (1996b). Positioning hydrogen atoms by optimizing hydrogen-bond networks in protein structures. *Proteins Struct. Funct. Genet.* **26**, 363–376.
- Hooft, R. W. W., Sander, C. & Vriend, G. (1997). Objectively judging the quality of a protein structure from a Ramachandran plot. *Comput. Appl. Biosci.* **13**, 425–430.
- Hooft, R. W. W., Vriend, G., Sander, C. & Abola, E. E. (1996). Errors in protein structures. *Nature (London)*, **381**, 272.
- IUPAC-IUB Commission on Biochemical Nomenclature (1970). Abbreviations and symbols for the description of the conformation of polypeptide chains. *J. Mol. Biol.* **52**, 1–17.
- James, M. N. G. & Sielecki, A. R. (1983). Structure and refinement of penicillopepsin at 1.8 Å resolution. *J. Mol. Biol.* **163**, 299–361.
- Janin, J. (1990). Errors in three dimensions. *Biochimie*, **72**, 705–709.
- Janin, J., Wodak, S., Levitt, M. & Maigret, B. (1978). Conformation of amino acid side-chains in proteins. *J. Mol. Biol.* **125**, 357–386.
- Jones, T. A. & Kjeldgaard, M. (1994). Making the first trace with *O*. In *Proceedings of the CCP4 study weekend. From first map to final model*, edited by S. Bailey, R. Hubbard & D. A. Waller, pp. 1–13. Warrington: Daresbury Laboratory.
- Jones, T. A. & Kjeldgaard, M. (1997). Electron density map interpretation. *Methods Enzymol.* **277**, 173–208.
- Jones, T. A., Kleywegt, G. J. & Brünger, A. T. (1996). Storing diffraction data. *Nature (London)*, **381**, 18–19.
- Jones, T. A. & Thirup, S. (1986). Using known substructures in protein model building and crystallography. *EMBO J.* **5**, 819–822.
- 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.* **A47**, 110–119.
- Karplus, P. A. (1996). Experimentally observed conformation-dependent geometry and hidden strain in proteins. *Protein Sci.* **5**, 1406–1420.
- Keller, P. A., Henrick, K., McNeil, P., Moodie, S. & Barton, G. J. (1998). Deposition of macromolecular structures. *Acta Cryst.* **D54**, 1105–1108.
- Kelly, J. A., Dideberg, O., Charlier, P., Wery, J. P., Libert, M., Moews, P. C., Knox, J. R., Duez, C., Fraipoint, C., Joris, B., Dusart, J., Frère, J. M. & Ghuysen, J. M. (1986). On the origin of bacterial resistance to penicillin: comparison of a β -lactamase and a penicillin target. *Science*, **231**, 1429–1431.
- Kelly, J. A. & Kuzin, A. P. (1995). The refined crystallographic structure of a DD-peptidase penicillin-target enzyme at 1.6 Å resolution. *J. Mol. Biol.* **254**, 223–236.
- Kleywegt, G. J. (1996). Use of non-crystallographic symmetry in protein structure refinement. *Acta Cryst.* **D52**, 842–857.
- Kleywegt, G. J. (1997). Validation of protein models from C α coordinates alone. *J. Mol. Biol.* **273**, 371–376.
- Kleywegt, G. J. (1999). Experimental assessment of differences between related protein crystal structures. *Acta Cryst.* **D55**, 1878–1884.
- Kleywegt, G. J., Bergfors, T., Senn, H., Le Motte, P., Gsell, B., Shudo, K. & Jones, T. A. (1994). Crystal structures of cellular retinoic acid binding proteins I and II in complex with all-trans-retinoic acid and a synthetic retinoid. *Structure*, **2**, 1241–1258.
- Kleywegt, G. J. & Brünger, A. T. (1996). Checking your imagination: applications of the free R value. *Structure*, **4**, 897–904.
- Kleywegt, G. J., Hoier, H. & Jones, T. A. (1996). A re-evaluation of the crystal structure of chloromuconate cycloisomerase. *Acta Cryst.* **D52**, 858–863.
- Kleywegt, G. J. & Jones, T. A. (1995a). Braille for pugilists. In *Proceedings of the CCP4 study weekend. Making the most of your model*, edited by W. N. Hunter, J. M. Thornton & S. Bailey, pp. 11–24. Warrington: Daresbury Laboratory.
- Kleywegt, G. J. & Jones, T. A. (1995b). Where freedom is given, liberties are taken. *Structure*, **3**, 535–540.
- Kleywegt, G. J. & Jones, T. A. (1996a). Efficient rebuilding of protein structures. *Acta Cryst.* **D52**, 829–832.
- Kleywegt, G. J. & Jones, T. A. (1996b). Phi/Psi-chology: Ramachandran revisited. *Structure*, **4**, 1395–1400.
- Kleywegt, G. J. & Jones, T. A. (1997). Model-building and refinement practice. *Methods Enzymol.* **277**, 208–230.
- Kleywegt, G. J. & Jones, T. A. (1998). Databases in protein crystallography. *Acta Cryst.* **D54**, 1119–1131.
- Kleywegt, G. J. & Read, R. J. (1997). Not your average density. *Structure*, **5**, 1557–1569.
- Kleywegt, G. J., Zou, J. Y., Divne, C., Davies, G. J., Sinning, I., Ståhlberg, J., Reinikainen, T., Srisodsuk, M., Teeri, T. T. & Jones, T. A. (1997). The crystal structure of the catalytic core domain of endoglucanase I from *Trichoderma reesei* at 3.6 Å resolution, and a comparison with related enzymes. *J. Mol. Biol.* **272**, 383–397.
- Korn, A. P. & Rose, D. R. (1994). Torsion angle differences as a means of pinpointing local polypeptide chain trajectory changes for identical proteins in different conformational states. *Protein Eng.* **7**, 961–967.
- Kuriyan, J. & Weiss, W. I. (1991). Rigid protein motion as a model for crystallographic temperature factors. *Proc. Natl Acad. Sci. USA*, **88**, 2773–2777.
- Laskowski, R. A., MacArthur, M. W., Moss, D. S. & Thornton, J. M. (1993). PROCHECK: a program to check the stereochemical quality of protein structures. *J. Appl. Cryst.* **26**, 283–291.
- Laskowski, R. A., MacArthur, M. W. & Thornton, J. M. (1994). Evaluation of protein coordinate data sets. In *Proceedings of the CCP4 study weekend. From first map to final model*, edited by S. Bailey, R. Hubbard & D. A. Waller, pp. 149–159. Warrington: Daresbury Laboratory.
- Laskowski, R. A., MacArthur, M. W. & Thornton, J. M. (1998). Validation of protein models derived from experiment. *Curr. Opin. Struct. Biol.* **8**, 631–639.
- Laskowski, R. A., Moss, D. S. & Thornton, J. M. (1993). Main-chain bond lengths and bond angles in protein structures. *J. Mol. Biol.* **231**, 1049–1067.
- Lubkowski, J., Wlodawer, A., Housset, D., Weber, I. T., Ammon, H. L., Murphy, K. C. & Swain, A. L. (1994). Refined crystal structure of *Acinetobacter glutaminasificans* glutaminase-asparaginase. *Acta Cryst.* **D50**, 826–832.
- Lüthy, R., Bowie, J. U. & Eisenberg, D. (1992). Assessment of protein models with three-dimensional profiles. *Nature (London)*, **356**, 83–85.
- Luzzati, V. (1952). Traitement statistique des erreurs dans la détermination des structures cristallines. *Acta Cryst.* **5**, 802–810.
- MacArthur, M. W., Laskowski, R. A. & Thornton, J. M. (1994). Knowledge-based validation of protein structure coordinates derived by X-ray crystallography and NMR spectroscopy. *Curr. Opin. Struct. Biol.* **4**, 731–737.
- MacArthur, M. W. & Thornton, J. M. (1996). Deviations from planarity of the peptide bond in peptides and proteins. *J. Mol. Biol.* **264**, 1180–1195.
- MacArthur, M. W. & Thornton, J. M. (1999). Protein side-chain conformation: a systematic variation of χ_1 mean values with resolution – a consequence of multiple rotameric states? *Acta Cryst.* **D55**, 994–1004.
- McDonald, I. K. & Thornton, J. M. (1995). The application of hydrogen bonding analysis in X-ray crystallography to help orientate asparagine, glutamine and histidine side chains. *Protein Eng.* **8**, 217–224.
- McRee, D. E., Tainer, J. A., Meyer, T. E., van Beeumen, J., Cusanovich, M. A. & Getzoff, E. D. (1989). Crystallographic

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21.1 (cont.)

- structure of a photoreceptor protein at 2.4 Å resolution. *Proc. Natl Acad. Sci. USA*, **86**, 6533–6537.
- Maiorov, V. & Abagyan, R. (1998). Energy strain in three-dimensional protein structures. *Fold. Des.* **3**, 259–269.
- Marsh, R. E. (1995). Some thoughts on choosing the correct space group. *Acta Cryst.* **B51**, 897–907.
- Marsh, R. E. (1997). The perils of Cc revisited. *Acta Cryst.* **B53**, 317–322.
- Melo, F. & Feytmans, E. (1998). Assessing protein structures with a non-local atomic interaction energy. *J. Mol. Biol.* **277**, 1141–1152.
- Merritt, E. A. (1999). Expanding the model: anisotropic displacement parameters in protein structure refinement. *Acta Cryst.* **D55**, 1109–1117.
- Merritt, E. A., Kuhn, P., Sarfaty, S., Erbe, J. L., Holmes, R. K. & Hol, W. G. J. (1998). The 1.25 Å resolution refinement of the cholera toxin B-pentamer: evidence of peptide backbone strain at the receptor-binding site. *J. Mol. Biol.* **282**, 1043–1059.
- Morris, A. L., MacArthur, M. W., Hutchinson, E. G. & Thornton, J. M. (1992). Stereochemical quality of protein structure coordinates. *Proteins Struct. Funct. Genet.* **12**, 345–364.
- Murshudov, G. N., Vagin, A. A. & Dodson, E. J. (1997). Refinement of macromolecular structures by the maximum-likelihood method. *Acta Cryst.* **D53**, 240–255.
- Nayal, M. & Di Cera, E. (1996). Valence screening of water in protein crystals reveals potential Na⁺ binding sites. *J. Mol. Biol.* **256**, 228–234.
- Noble, M. E. M., Zeelen, J. P., Wierenga, R. K., Mainfroid, V., Goraj, K., Gohimont, A. C. & Martial, J. A. (1993). Structure of triosephosphate isomerase from *Escherichia coli* determined at 2.6 Å resolution. *Acta Cryst.* **D49**, 403–417.
- Nunn, R. S., Artymiuk, P. J., Baker, P. J., Rice, D. W. & Hunter, C. N. (1995). Retraction – Purification and crystallization of the light harvesting LH1 complex from *Rhodobacter sphaeroides*. *J. Mol. Biol.* **252**, 153.
- Oldfield, T. J. & Hubbard, R. E. (1994). Analysis of C α geometry in protein structures. *Proteins Struct. Funct. Genet.* **18**, 324–337.
- Pannu, N. S., Murshudov, G. N., Dodson, E. J. & Read, R. J. (1998). Incorporation of prior phase information strengthens maximum-likelihood structure refinement. *Acta Cryst.* **D54**, 1285–1294.
- Pannu, N. S. & Read, R. J. (1996). Improved structure refinement through maximum likelihood. *Acta Cryst.* **A52**, 659–668.
- Parkinson, G., Vojtechovsky, J., Clowney, L., Brünger, A. T. & Berman, H. M. (1996). New parameters for the refinement of nucleic acid-containing structures. *Acta Cryst.* **D52**, 57–64.
- Ponder, J. W. & Richards, F. M. (1987). Tertiary templates for proteins. Use of packing criteria in the enumeration of allowed sequences for different structural classes. *J. Mol. Biol.* **193**, 775–791.
- Pontius, J., Richelle, J. & Wodak, S. J. (1996). Deviations from standard atomic volumes as a quality measure for protein crystal structures. *J. Mol. Biol.* **264**, 121–136.
- Priestle, J. P. (1994). Stereochemical dictionaries for protein structure refinement and model building. *Structure*, **2**, 911–913.
- Ramachandran, G. N. & Mitra, A. K. (1976). An explanation for the rare occurrence of cis peptide units in proteins and polypeptides. *J. Mol. Biol.* **107**, 85–92.
- Ramachandran, G. N. & Srinivasan, R. (1961). An apparent paradox in crystal structure analysis. *Nature (London)*, **190**, 159–161.
- Ramakrishnan, C. & Ramachandran, G. N. (1965). Stereochemical criteria for polypeptide and protein chain conformations. II. Allowed conformations for a pair of peptide units. *Biophys. J.* **5**, 909–933.
- Read, R. J. (1986). Improved Fourier coefficients for maps using phases from partial structures with errors. *Acta Cryst.* **A42**, 140–149.
- Read, R. J. (1990). Structure-factor probabilities for related structures. *Acta Cryst.* **A46**, 900–912.
- Read, R. J. (1994). Model bias and phase combination. In *Proceedings of the CCP4 study weekend. From first map to final model*, edited by S. Bailey, R. Hubbard & D. A. Waller, pp. 31–40. Warrington: Daresbury Laboratory.
- Read, R. J. (1997). Model phases: probabilities and bias. *Methods Enzymol.* **277**, 110–128.
- Schomaker, V. & Trueblood, K. N. (1968). On the rigid-body motion of molecules in crystals. *Acta Cryst.* **B24**, 63–76.
- Schultze, P. & Feigon, R. (1997). Chirality errors in nucleic acid structures. *Nature (London)*, **387**, 668.
- Sevcik, J., Dauter, Z., Lamzin, V. S. & Wilson, K. S. (1996). Ribonuclease from *Streptomyces aureofaciens* at atomic resolution. *Acta Cryst.* **D52**, 327–344.
- Sheldrick, G. M. (1996). Least-squares refinement of macromolecules: estimated standard deviations, NCS restraints and factors affecting convergence. In *Proceedings of the CCP4 study weekend. Macromolecular refinement*, edited by E. Dodson, M. Moore, A. Ralph & S. Bailey, pp. 47–58. Warrington: Daresbury Laboratory.
- Sinning, I., Kleywegt, G. J., Cowan, S. W., Reinemer, P., Dirr, H. W., Huber, R., Gilliland, G. L., Armstrong, R. N., Ji, X., Board, P. G., Olin, B., Mannervik, B. & Jones, T. A. (1993). Structure determination and refinement of human alpha class glutathione transferase A1-1, and a comparison with the mu and pi class enzymes. *J. Mol. Biol.* **232**, 192–212.
- Sippl, M. J. (1993). Recognition of errors in three-dimensional structures of proteins. *Proteins Struct. Funct. Genet.* **17**, 355–362.
- Stewart, D. E., Sarkar, A. & Wampler, J. E. (1990). Occurrence and role of cis peptide bonds in protein structures. *J. Mol. Biol.* **214**, 253–260.
- Swindells, M. B., MacArthur, M. W. & Thornton, J. M. (1995). Intrinsic φ , ψ propensities of amino acids, derived from the coil regions of known structures. *Nature Struct. Biol.* **2**, 596–603.
- Taylor, R. & Kennard, O. (1986). Accuracy of crystal structure error estimates. *Acta Cryst.* **B42**, 112–120.
- Ten Eyck, L. F. (1996). Full matrix least squares. In *Proceedings of the CCP4 study weekend. Macromolecular refinement*, edited by E. Dodson, M. Moore, A. Ralph & S. Bailey, pp. 37–45. Warrington: Daresbury Laboratory.
- Tickle, I. J., Laskowski, R. A. & Moss, D. S. (1998). R_{free} and the R_{free} ratio. I. Derivation of expected values of cross-validation residuals used in macromolecular least-squares refinement. *Acta Cryst.* **D54**, 547–557.
- Vaguine, A. A., Richelle, J. & Wodak, S. J. (1999). SFCHECK: a unified set of procedures for evaluating the quality of macromolecular structure-factor data and their agreement with the atomic model. *Acta Cryst.* **D55**, 191–205.
- 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.
- Vriend, G. (1990). WHAT IF: a molecular modeling and drug design program. *J. Mol. Graphics*, **8**, 52–56.
- Vriend, G. & Sander, C. (1993). Quality control of protein models: directional atomic contact analysis. *J. Appl. Cryst.* **26**, 47–60.
- Walther, D. & Cohen, F. E. (1999). Conformational attractors on the Ramachandran map. *Acta Cryst.* **D55**, 506–517.
- Watkin, D. (1996). Pseudo symmetry. In *Proceedings of the CCP4 study weekend. Macromolecular refinement*, edited by E. Dodson, M. Moore, A. Ralph & S. Bailey, pp. 171–184. Warrington: Daresbury Laboratory.
- Weaver, L. H., Tronrud, D. E., Nicholson, H. & Matthews, B. W. (1990). Some uses of the Ramachandran (φ , ψ) diagram in the structural analysis of lysozymes. *Curr. Sci.* **59**, 833–837.
- Weiss, M. S. & Hilgenfeld, R. (1997). On the use of the merging R factor as a quality indicator for X-ray data. *J. Appl. Cryst.* **30**, 203–205.
- Wilson, A. J. C. (1949). The probability distribution of X-ray intensities. *Acta Cryst.* **2**, 318–321.
- Zou, J. Y. & Mowbray, S. L. (1994). An evaluation of the use of databases in protein structure refinement. *Acta Cryst.* **D50**, 237–249.

21.2

- Abagyan, R. A. & Totrov, M. M. (1997). Contact area difference (CAD): a robust measure to evaluate accuracy of protein models. *J. Mol. Biol.* **268**, 678–685.