

27. Vitagliano, L., Berisio, R., Mastrangelo, A., Mazzarella, L. & Zagari, A. Preferred proline puckerings in *cis* and *trans* peptide groups: implications for collagen stability. *Protein Sci.* **10**, 2627–2632 (2001).
28. Zydowsky, L.D. *et al.* Active site mutants of human cyclophilin A separate peptidyl-prolyl isomerase activity from cyclosporin A binding and calcineurin inhibition. *Protein Sci.* **1**, 1092–1099 (1992).
29. Stein, R.L. Mechanism of enzymatic and nonenzymatic prolyl *cis-trans* isomerization. *Adv. Protein Chem.* **44**, 1–24 (1993).
30. Fischer, S., Michnick, S. & Karplus, M. A mechanism for rotamase catalysis by the FK506 binding protein (FKBP). *Biochemistry* **32**, 13830–13837 (1993).
31. Hur, S. & Bruice, T.C. The mechanism of *cis-trans* isomerization of prolyl peptides by cyclophilin. *J. Am. Chem. Soc.* **124**, 7303–7313 (2002).
32. Otwinowski, Z. & Minor, W. Processing of X-ray diffraction data collected in oscillation mode. *Methods Enzymol.* **276**, 307–326 (1997).
33. Leslie, A.G.W. *Joint CCP4 and ESF-EACMB Newsletter on Protein Crystallography* Vol. 26 (Daresbury Laboratory, Warrington, 1992).
34. Collaborative Computational Project, Number 4. CCP4 Suite: programs for protein crystallography. *Acta Crystallogr. D* **50**, 760–763 (1994).
35. Brünger, A.T. *X-PLOR Version 3.843: A System for X-ray Crystallography and NMR* (Yale University, New Haven, Connecticut, 1996).
36. Jones, T.A., Zou, J.-Y., Cowan, S.W. & Kjeldgaard, M. Improved methods for building protein models in electron density maps and location of errors in these models. *Acta Crystallogr. A* **47**, 110–119 (1991).
37. Lamzin, V.S. & Wilson, K.S. Automated building of solvent structure combined with standard restrained refinement. *Methods Enzymol.* **277**, 269–305 (1997).
38. Murshudov, G.N., Vagin, A.A. & Dodson, E.J. Refinement of macromolecular structures by the maximum-likelihood method. *Acta Crystallogr. D* **53**, 240–255 (1997).
39. Murshudov, G.N., Vagin, A.A., Lebedev, A., Wilson, K.S. & Dodson, E.J. Efficient anisotropic refinement of macromolecular structures using FFT. *Acta Crystallogr. D* **55**, 247–255 (1999).
40. Kraulis, P.J. Molscript: a program to produce both detailed and schematic plots of protein structures. *J. Appl. Crystallogr.* **24**, 946–950 (1991).
41. Merritt, E.A. & Bacon, D.J. Raster3D: photorealistic molecular graphics. *Methods Enzymol.* **277**, 505–524 (1997).
42. Laskowski, R.A., MacArthur, M.W., Moss, D.S. & Thornton, J.M. PROCHECK: a program to check the stereochemical quality of protein structures. *J. Appl. Crystallogr.* **26**, 283–291 (1993).
43. Morris, A.L., MacArthur, M.W., Hutchinson, E.G. & Thornton, J.M. Stereochemical quality of protein structure coordinates. *Proteins* **12**, 345–364 (1992).