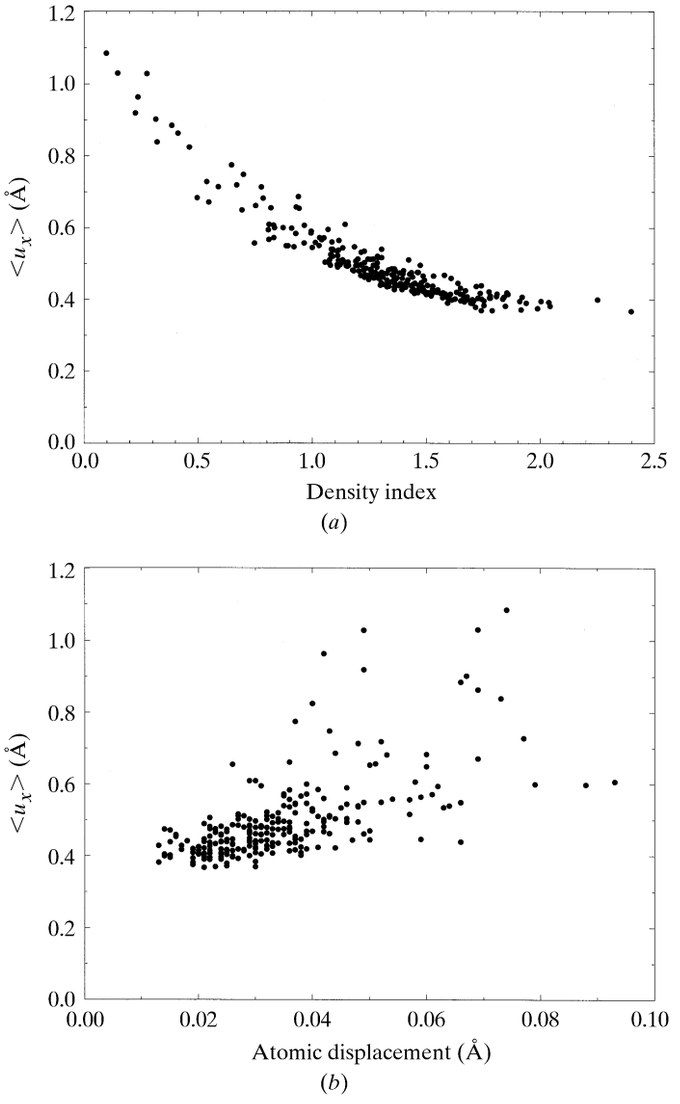

Fig. 21.2.3.5. Pairwise correlations between the various local quality indicators computed by *SFCHECK*. (*a*) Correlation between the average residue *B* factor and the density index, and (*b*) between the *B* factor and the atomic displacement. The values displayed were computed for residues in the crystal structure of carboxypeptidase (1YME). The meaning of the parameters displayed is given in Table 21.2.3.3.

resolution (Longhi *et al.*, 1997; EU 3-D Validation Network, 1998). The EU 3-D Validation Network study showed that in the atomic resolution structures, most of the geometrical validation parameters are more tightly clustered about their mean value than in structures determined at lower resolution, including tighter clustering in the core regions of the Ramachandran plot, tighter clustering of the atomic volumes and smaller s.u.'s in the distributions of the χ_1, χ_2 dihedral angles. In contrast, the ω torsion angle about the peptide bond exhibits a wider distribution, with a mean of 179.0 (56)° compared to 179.6 (47)° previously computed in protein structures determined at various resolution levels (Morris *et al.*, 1992).

Recently, atomic resolution structures have also been used to derive atomic s.u values for proteins. Remarkably, the estimated coordinate errors for concanavalin A at 0.94 Å (Deacon *et al.*, 1997) were found to be equivalent to those of small-molecule crystal structures, despite the large size of the protein (237 residues).

Atomic resolution structures of proteins and other macromolecules thus promise to represent a valuable source of accurate information on geometric and conformational parameters of these molecules. But the analysis and validation of such structures also brings about additional complications, such as, for example, the problem of dealing with equilibria between multiple conformations, which atomic resolution data tend to resolve with much higher detail and accuracy. Handling these equilibria will require an adaptation of the current validation procedures.

21.2.5. Concluding remarks

The coming years will see an ever-increasing number of crystal structures of proteins and nucleic acids determined at high resolution and a substantial growth in the number of atomic resolution structures. This will most certainly help in obtaining better data on the geometric and stereochemical parameters of these macromolecules and thus improve the target values for both refinement and structure validation. It should also make it possible to derive better criteria for evaluating the agreement of the model with the electron density and to improve upon and generalize comprehensive and systematic approaches, such as that implemented in the software *SFCHECK*.

references