Table 18.3.2.3
Bond lengths (Å) and angles (°) of peptide backbone fragments

EH denotes parameters from Engh & Huber (1991). Bold values mark important updates for angles involving proline (with cis and trans distinction) and branched CB atoms (isoleucine, valine, threonine). The number of fragments used for the statistics is given. The standard deviation of each value is given in parentheses following the value and is on the scale of the least significant digit of the value.

18.3.2.6. Non-bonded interactions

Like the potential parameterization of torsion-angle statistics with the CSD, parameterization of non-bonded interactions, typically into terms representing packing (an empirical mix of London dispersion forces and solvent effects), electrostatics and hydrogen bonding, is probably more strongly influenced by protein environment than are bond and angle terms. Specific chemical questions are likely to be best addressed with fragment structure databases, however, for improved parameterization or structure-quality evaluation. Possible examples include hydrogen bonds, salt bridges (see, e.g., the discussion on charge delocalization of Glu and Asp above) etc. These are particularly relevant for structures generally atypical among proteins, such as at enzyme reactive sites.

18.3.2.7. Effects of hydrogen atoms in parameterization

While many CSD fragments include hydrogen-atom positions, their accuracy is necessarily the most limited. Evaluation of CSD statistics without hydrogens and the subsequent addition of parameters to refine hydrogens adds an additional artifactual coupling between parameters involving non-hydrogen atoms as well. This artifactual coupling might theoretically be of some concern, but is a second-order effect and presumably introduces effects smaller than the artifactual coupling between non-hydrogen parameters, for example.

18.3.2.8. Special geometries: cofactors, ligands, metals etc.

Most crystallographers will experience neither the need nor desire to derive their own parameterization for general protein structure refinement; many, however, need new parameters for ligands or other entities that are not amino-acid residues. The desire to derive their own parameterization for general protein environment than are bond and angle terms. Specific chemical questions are likely to be best addressed with fragment structure databases, however, for improved parameterization or structure-quality evaluation. Possible examples include hydrogen bonds, salt bridges (see, e.g., the discussion on charge delocalization of Glu and Asp above) etc. These are particularly relevant for structures generally atypical among proteins, such as at enzyme reactive sites.