

**TABLE 1.2 A summary of the the main types of electrostatic interactions found in proteins.**

Van der Waals interactions are also described here because of their electrostatic nature.  $q$  is the full charge (in electron charges),  $\mu$  is the dipole moment (in Debye),  $r_{ij}$  is the distance between the charges (in Å), and  $\epsilon_r$  is the relative dielectric constant of the medium. The  $\theta$  angles in the second and third equations are defined in Figure 1.15b. To obtain the energy in kcal/mol, the following pre-factors should be used: **332** for the first equation, **69.1** for the second equation, and **14.4** for the third equation.

| Interaction                     | Example                    | Potential energy  | Distance dependence                            | Typical distance (Å)  | Typical strength in vacuum <sup>*a</sup> (kcal/mol) |
|---------------------------------|----------------------------|---|--|-----------------------|---|
| Charge-charge (ionic)           | Salt bridge                | $U = \frac{q_i q_j}{\epsilon_r r_{ij}}$   | $1/r$  | < 4 (salt bridge)     | ~80   |
| Charge-fixed dipole             | Hydrogen bond              | $U = \frac{q_i \mu_j (\cos \theta)}{\epsilon_r r_{ij}^2}$   | $1/r^2$  | 2.8–3.0 <sup>*b</sup> | 0–7 <sup>*c</sup>                                   |
| Fixed dipole – fixed dipole     | Hydrogen bond              | $U = \frac{\mu_i \mu_j (2 \cos \theta_i \cos \theta_j - \sin \theta_i \sin \theta_j)}{\epsilon_r r_{ij}^3}$ | $1/r^3$  |                       |   |
| Induced dipole – induced dipole | Van-der Waals interactions | $U = \frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^6}$  | $1/r^6$ (attractive)<br>$1/r^{12}$ (repulsive) | 3.5 <sup>*d</sup>     | 0.1–0.5 <sup>*e</sup>                               |

<sup>\*a</sup>In proteins, the strength of these interactions is difficult to determine, and different values have been suggested by different studies (e.g., <sup>[136]</sup>; see Chapter 4 for details).

<sup>\*b</sup><sup>[133]</sup>. In the case of hydrogen bonds, if the bond is described as donor-hydrogen-acceptor (D–H···A), the reported values correspond to the D···A distance. The corresponding H···A distance is typically 2 Å <sup>[134]</sup>.

<sup>\*c</sup><sup>[166–168]</sup>.

<sup>\*d</sup><sup>[169]</sup>.

<sup>\*e</sup><sup>[167,170]</sup>.