

**Table 4. Contribution of single amino acids in the FMO trimer of *P. aestuarii* to calculated site energies of BChl *a***

| <i>m</i> | Axial ligand     |                                      | Hydrogen bond donor to<br>3-acetyl group |                                      | Hydrogen bond donor to<br>13 <sup>1</sup> -keto group |                                      |
|----------|------------------|--------------------------------------|--|--------------------------------------|---|--------------------------------------|
|          | Group            | $\Delta\Delta G_{\text{back}}^{(m)}$ | Group                                    | $\Delta\Delta G_{\text{back}}^{(m)}$ | Group   | $\Delta\Delta G_{\text{back}}^{(m)}$ |
| 1        | His-110          | 30                                   | H <sub>2</sub> O                         | -117                                 | –   | –                                    |
| 2        | H <sub>2</sub> O | 75                                   | Ser-72                                   | -86                                  | Ile-137 (B)<br>Tyr-138 (B)                            | -48<br>-41                           |
| 3        | His-298          | 88                                   | Tyr-15                                   | -131                                 | Ala-40 (B)  | -35                                  |
| 4        | His-290          | 38                                   | –  | –                                    | Tyr-345   | -49                                  |
| 5        | Leu-242 (B)      | 117                                  | –  | –                                    | –   | –                                    |
| 6        | His-145          | 66                                   | Trp-184                                  | -48                                  | Arg-95 <sup>a</sup>                                   | -96                                  |
| 7        | His-297          | 21                                   | –  | –                                    | –   | –                                    |

Energy shifts are given in wavenumber units (cm<sup>-1</sup>, i.e., energy/*hc*). Only shifts of magnitude  $\geq 20$  cm<sup>-1</sup> are considered. (B) Effects of backbone partial charges are included.

<sup>a</sup> Positively charged.