TABLE 2.4. Groups of Hydrogen Atoms in the Common Amino Acid Residues with Similar Random Coil $^1$H Chemical Shifts*

<table>
<thead>
<tr>
<th>Code</th>
<th>$\delta$(ppm)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH$_3$</td>
<td>0.9-1.4</td>
<td></td>
</tr>
<tr>
<td>$\beta$(a)</td>
<td>1.6-2.3</td>
<td>$\beta$H of V,I,L,E,Q,M,P,R,K</td>
</tr>
<tr>
<td>$\beta$(b)</td>
<td>2.7-3.3</td>
<td>$\beta$H of C,D,N,F,Y,H,W</td>
</tr>
<tr>
<td>$\cdot\cdot\cdot$</td>
<td>1.2-3.3</td>
<td>Other Aliphatic CH</td>
</tr>
<tr>
<td>$\alpha,\beta$(S,T)</td>
<td>3.9-4.8</td>
<td>All $\alpha$H, $\beta$H of S and T</td>
</tr>
<tr>
<td>Ring</td>
<td>6.5-7.7</td>
<td>Aromatic CH of F,Y,W; 4H of H</td>
</tr>
<tr>
<td>2H(H)</td>
<td>7.7-8.6</td>
<td>2H of H in the pH range 1-11</td>
</tr>
<tr>
<td>NH(sc)*</td>
<td>6.6-7.6</td>
<td>Side Chain NH of N,Q,K,R</td>
</tr>
<tr>
<td>NH(bb)*</td>
<td>8.1-8.8</td>
<td>Backbone NH</td>
</tr>
<tr>
<td>NH(W)*</td>
<td>10.2</td>
<td>Indole NH of W</td>
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</tbody>
</table>

* In model peptides the labile protons (identified by *) are only observed in H2O solution. The singlet resonance of $\epsilon$CH$_3$ in Met is at 2.13 ppm (Table 2.3).
<table>
<thead>
<tr>
<th>Residue</th>
<th>NH</th>
<th>αH</th>
<th>βH</th>
<th>Others</th>
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<tr>
<td>Gly</td>
<td>8.39</td>
<td>3.97</td>
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<tr>
<td>Ala</td>
<td>8.25</td>
<td>4.35</td>
<td>1.39</td>
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<tr>
<td>Val</td>
<td>8.44</td>
<td>4.18</td>
<td>2.13</td>
<td>γCH$_3$ 0.97, 0.94</td>
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<tr>
<td>Ile</td>
<td>8.19</td>
<td>4.23</td>
<td>1.90</td>
<td>γCH$_2$ 1.48, 1.19</td>
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<td></td>
<td></td>
<td>γCH$_3$ 0.95</td>
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<td></td>
<td>δCH$_3$ 0.89</td>
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<tr>
<td>Leu</td>
<td>8.42</td>
<td>4.38</td>
<td>1.65, 1.65</td>
<td>γH 1.64</td>
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<tr>
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<td>δCH$_3$ 0.94, 0.90</td>
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<td>γCH$_2$ 2.03, 2.03</td>
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<td>δCH$_2$ 3.68, 3.65</td>
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<tr>
<td>Pro b</td>
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<td>Thr</td>
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<td>2.84, 2.75</td>
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<td>Glu</td>
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<td>2.09, 1.97</td>
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<tr>
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<td>δCH$_2$ 3.32, 3.32</td>
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<tr>
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</table>

a Data for the nonterminal residues X in tetrapeptides GGXX, pH 7.0, 35°C [from Bundi and Wüthrich (1979a), except that more precise data were obtained for Leu, Pro, Lys, Arg, Met, and Phe using new measurements at 500 MHz].

b Data for trans-Pro.