BIOCHEMISTRY
including biophysical chemistry & molecular biology

Supporting information for *Biochemistry*, **1995**, 34(42), 13858 – 13870, DOI: 10.1021/bi00042a018

# ZHOU
# 13858-13870

Table S1: $^{15}N$ and $^{1}H$ Resonance Assignments for $CheA_{1-134}$ at pH 6.3 and 30 °C[a]

| residue | amide N | amide H | αH | others |
|---|---|---|---|---|
| M1 | | | | |
| S2 | | | | |
| M3 | 122.9 | 8.46 | 4.53 | 2.75, 2.59, 2.00 |
| D4 | 123.3 | 8.55 | 4.69 | 2.73, 2.60 |
| | 122.9 | 8.46 | 4.69 | 2.73, 2.60 |
| I5 | 122.2 | 8.16 | 4.23 | 1.93, 0.94, 1.25 |
| | 122.1 | 8.22 | 4.23 | 1.93, 0.94, 1.25 |
| S6 | 122.1 | 8.28 | 4.42 | Hβ(3.85) |
| D7 | 122.9 | 8.26 | 4.54 | Hβ(2.55,2.60) |
| F8 | 120.3 | 7.97 | 4.52 | Hβ(3.09), Hδ(7.21), Hε(7.35) |
| Y9 | 119.4 | 7.72 | 3.71 | Hβ(2.82, 2.58), Hδ(6.79), Hε(6.85) |
| Q10 | 118.6 | 7.94 | 3.97 | 2.23, 2.14, Hγ(2.47), Nε2(115.4), Hε2(6.92, 7.89) |
| T11 | 113.1 | 7.91 | 4.28 | Hβ(4.13), Hγ(1.31) |
| F12 | 122.6 | 7.53 | 4.51 | Hβ(3.23, 2.56), Hδ(7.09), Hε(7.22) |
| F13 | 119.1 | 8.31 | 4.02 | Hβ(3.30), Hδ(7.17), Hε(7.25) |
| D14 | 118.5 | 8.29 | 4.39 | Hβ(2.79) |
| E15 | 122.4 | 8.06 | 4.06 | Hβ(2.06), Hγ(2.43, 2.19) |
| A16 | 122.9 | 9.21 | 3.82 | Hβ(0.93) |
| D17 | 118.9 | 8.32 | 4.44 | Hβ(2.90, 2.59) |
| E18 | 121.1 | 7.44 | 4.13 | 2.22, 2.47 |
| L19 | 122.5 | 8.69 | 4.21 | 1.99,1.32, 0.96 |
| L20 | 121.5 | 8.92 | 4.11 | 2.08, 0.93 |
| A21 | 123.0 | 7.61 | 4.26 | Hβ(1.52) |
| D22 | 121.4 | 8.33 | 4.41 | Hβ(2.84) |
| M23 | 121.1 | 8.94 | 3.95 | 2.65, 2.39, 2.27, Hγ(2.89) |
| E24 | 119.3 | 8.21 | 3.78 | 2.35, 2.17, 1.93 |
| Q25 | 116.0 | 7.92 | 3.91 | 2.40, 2.09, Nε2(113.2), Hε2(6.78, 7.47) |
| H26 | 114.8 | 7.86 | 4.41 | Hβ(3.06) |
| L27 | 121.1 | 8.57 | 3.96 | Hβ(2.30, 1.86), Hγ(1.28), Hδ(0.78, 1.09) |
| L28 | 115.8 | 7.92 | 4.15 | 1.89, 1.50, Hβ(0.92) |
| V29 | 109.6 | 7.07 | 4.53 | Hβ(2.42), Hγ(0.97) |
| L30 | 125.5 | 7.20 | 4.19 | 1.78, 1.57, Hδ(0.95, 0.82) |
| Q31 | 126.6 | 8.89 | 4.79 | Hβ(2.04, 2.15), Hγ(2.45) |
| P32 | | | | |
| E33 | 114.5 | 8.81 | 4.22 | Hβ(2.00), Hγ(2.30, 2.08) |
| A34 | 121.8 | 7.43 | 4.63 | Hβ(1.23) |
| P35 | | | | |
| D36 | 125.8 | 8.20 | 4.59 | Hβ(2.71) |
| A37 | 130.8 | 8.99 | 3.96 | Hβ(1.51) |
| E38 | 118.0 | 8.39 | 4.26 | 2.35, 2.15 |
| Q39 | 121.2 | 8.14 | 3.98 | 2.22, 2.14, Hγ(2.52), Nε2(112.2), Hε2(6.96, 7.73) |
| L40 | 118.0 | 8.00 | 4.02 | 1.86,1.36, 1.67, 0.82 |
| N41 | 118.4 | 8.58 | 4.43 | Hβ(2.98, 2.78), Nδ2(112.5), Hδ2(6.91, 7.59) |
| A42 | 123.4 | 7.89 | 4.03 | Hβ(1.05) |
| I43 | 120.8 | 7.85 | 3.59 | 2.01, 1.85, 0.89, 0.81 |
| F44 | 120.2 | 8.45 | 3.88 | Hβ(3.29, 2.87*), Hδ(7.05), Hε(6.81) |
| R45 | 119.1 | 8.85 | 3.79 | 1.97, 1.86, 1.62, 0.94, Hβ(3.25) |
| A46 | 122.3 | 7.57 | 4.20 | Hβ(1.58) |
| A47 | 120.1 | 7.96 | 3.73 | Hβ(1.23) |
| H48 | 116.9 | 8.92 | 4.26 | Hβ(2.99, 2.40) |
| S49 | 117.4 | 8.36 | 4.24 | Hβ(3.92) |
| I50 | 124.6 | 8.18 | 3.84 | 1.96, 1.42, 1.39, 1.05, 0.81 |
| K51 | 121.6 | 8.55 | 3.69 | 1.81, 1.04 |
| G52 | 105.6 | 7.82 | 3.85, 3.63 | |
| G53 | 110.8 | 7.93 | 3.63, 3.60 | |
| A54 | 123.3 | 8.89 | 3.78 | Hβ(1.56) |
| G55 | 103.7 | 8.06 | 3.82, 3.64 | |
| T56 | 120.6 | 7.60 | 3.56 | Hγ(0.37) |
| F57 | 116.5 | 6.90 | 4.24 | Hβ(2.31, 1.19), Hδ(6.60), Hε(6.86) |
| G58 | 107.3 | 7.21 | 3.94, 3.78 | |
| F59 | 122.4 | 8.14 | 4.86 | Hβ(3.76, 2.74), Hδ(6.53), Hε(6.94) |
| S60 | 119.8 | 8.05 | 4.08 | Hβ(3.94) |
| V61 | 122.2 | 7.91 | 3.36 | Hβ(1.75), Hγ(0.54, 0.17) |
| L62 | 122.5 | 6.78 | 4.95 | 1.97, 1.77, 1.57, 1.30*, 1.19* |
| Q63 | 122.8 | 8.65 | 3.67 | 2.33, 1.65, Nε2(110.2), Hε2(6.79, 7.17) |
| E64 | 119.0 | 8.39 | 4.41 | Hβ(2.19), Hγ(2.49, 2.26) |
| T65 | 117.1 | 8.17 | 3.92 | Hβ(4.44), Hγ(1.23) |
| T66 | 113.2 | 8.21 | 3.85 | Hβ(4.05), Hγ(1.34) |
| H67 | 122.8 | 8.63 | 4.31 | Hβ(3.25) |
| L68 | 118.4 | 7.91 | 3.94 | 2.09, 1.38, 1.03, 0.82 |
| M69 | 119.5 | 7.81 | 4.00 | 2.18, 2.05 |
| E70 | 121.4 | 9.40 | 3.76 | Hβ(2.05), Hγ(2.24, 2.35) |

| | | | | |
|---|---|---|---|---|
| N71 | 117.8 | 8.05 | 4.57 | $H^{\beta}$(2.84), $N^{\varepsilon 2}$(109.9), $H^{\varepsilon 2}$(6.39, 7.52) |
| L72 | 120.1 | 7.30 | 4.20 | 2.15, 1.58, 1.98, $H^{\delta 1}$(1.13), $H^{\delta 2}$(0.89) |
| L73 | 120.1 | 8.58 | 3.96 | 2.21, 1.38, $H^{\delta 1}$(0.40), $H^{\delta 2}$(0.66*) |
| D74 | 120.5 | 8.84 | 4.29 | $H^{\beta}$(2.87) |
| E75 | 117.7 | 7.67 | 3.97 | 2.57, 2.36 |
| A76 | 121.7 | 8.41 | 4.52 | $H^{\beta}$(1.58) |
| R77 | 120.8 | 8.88 | 4.08 | 2.03, 1.66, $H^{\delta}$(3.20) |
| R78 | 117.7 | 7.65 | 4.33 | 2.03, 1.72, 1.58, $H^{\delta}$(3.10) |
| G79 | 107.9 | 7.83 | 4.19, 3.91 | |
| E80 | 118.5 | 8.02 | 4.29 | 2.21, 1.84 |
| M81 | 117.2 | 7.00 | 4.55 | 1.92, 1.63, 2.37, 2.26 |
| Q82 | 126.2 | 8.66 | 4.37 | $H^{\beta}$(2.09, 1.93), $H^{\gamma}$(2.40), $N^{\varepsilon 2}$(113.8), $H^{\varepsilon 2}$(6.82, 7.62) |
| L83 | 122.5 | 8.91 | 4.33 | 2.07, 1.87, 2.38, $H^{\delta 1}$(1.11), $H^{\delta 2}$(0.85) |
| N84 | 112.6 | 6.72 | 4.58 | $H^{\beta}$(3.21, 3.04), $N^{\delta 2}$(113.8), $H^{\delta 2}$(7.01, 7.48) |
| T85 | 114.8 | 8.78 | 3.85 | $H^{\beta}$(4.12), $H^{\gamma}$(1.23) |
| D86 | 122.5 | 7.96 | 4.43 | $H^{\beta}$(2.74, 2.57) |
| I87 | 122.9 | 8.37 | 3.39 | 2.01, 1.78*, 1.35, 0.82, 0.23 |
| I88 | 120.2 | 7.78 | 3.54 | 2.00, 1.14, 1.07, 0.77 |
| N89 | 118.7 | 8.45 | 4.63 | $H^{\beta}$(3.02, 2.89), $N^{\delta 2}$(112.1), $H^{\delta 2}$(6.81, 7.74) |
| L90 | 124.9 | 7.97 | 4.44 | 1.84, 1.61, 0.86, 0.78 |
| F91 | 123.6 | 8.86 | 3.73 | $H^{\beta}$(3.12, 2.26), $H^{\delta}$(7.00), $H^{\varepsilon}$(7.05) |
| L92 | 123.3 | 8.74 | 4.07 | 2.13, 1.71, 0.99 |
| E93 | 122.0 | 8.46 | 4.18 | 2.34, 2.15, $H^{\gamma}$(2.55) |
| T94 | 118.1 | 8.67 | 3.82 | $H^{\beta}$(4.32), 1.24 |
| K95 | 124.3 | 8.35 | 4.07 | 1.88, 2.18, 1.23 |
| D96 | 121.4 | 8.00 | 4.53 | $H^{\beta}$(2.99, 2.76) |
| I97 | 124.2 | 8.37 | 3.90 | 2.02, 1.02, 1.23, 0.70 |
| M98 | 122.6 | 9.20 | 4.09 | 2.39 |
| Q99 | 119.4 | 8.39 | 4.42 | 2.50, 2.26, $N^{\varepsilon 2}$(115.8), $H^{\varepsilon 2}$(7.19, 7.45) |
| E100 | 119.9 | 7.84 | 4.07 | 2 53, 2.27, 2.12 |
| Q101 | 122.3 | 8.62 | 3.69 | 2.71, $N^{\varepsilon 2}$(102.4), $H^{\varepsilon 2}$(6.24, 6.82) |
| L102 | 119.9 | 8.60 | 4.00 | 2.00, 1.60, 0.95 |
| D103 | 118.5 | 8.61 | 4.10 | $H^{\beta}$(2.69, 2.50) |
| A104 | 124.8 | 7.71 | 3.98 | $H^{\beta}$(0.98) |
| Y105 | 119.4 | 7.85 | 4.37 | $H^{\beta}$(2.65, 2.61), $H^{\delta}$(6.96), $H^{\varepsilon}$(6.71) |
| K106 | 121.1 | 8.40 | 3.36 | 1.54 |
| Q107 | 116.2 | 7.27 | 4.48 | 2.35, 1.84, $N^{\varepsilon 2}$(110.1), $H^{\varepsilon 2}$(6.72, 7.21) |
| S108 | 113.5 | 8.17 | 4.18 | |
| Q109 | 118.4 | 8.17 | 4.55 | 2.29, 2.00, 1.64, $N^{\varepsilon 2}$(112.2), $H^{\varepsilon 2}$(6.77, 7.31) |
| E110 | 120.9 | 8.29 | 4.52 | 2.36, 1.98, 1.84 |
| P111 | | | | |
| D112 | 122.5 | 8.87 | 4.40 | $H^{\beta}$(2.71) |
| A113 | 133.0 | 8.84 | 4.21 | $H^{\beta}$(1.55) |
| A114 | 121.9 | 8.33 | 4.25 | $H^{\beta}$(1.50) |
| S115 | 116.5 | 8.39 | 4.42 | $H^{\beta}$(3.98) |
| F116 | 122.7 | 7.30 | 4.49 | $H^{\beta}$(3.19), $H^{\delta}$(7.26), $H^{\varepsilon}$(7.37), $H^{\zeta}$(7.32) |
| D117 | 121.1 | 8.42 | 4.09 | $H^{\beta}$(2.76, 2.68) |
| Y118 | 119.1 | 8.03 | 4.21 | $H^{\beta}$(3.31, 3.12), $H^{\delta}$(7.10), $H^{\varepsilon}$(6.77) |
| I119 | 122.7 | 8.40 | 3.85 | 1.96*, 1.30, 0.89*, 1.02* |
| C120 | 121.1 | 8.14 | 4.00 | $H^{\beta}$(2.66, 2.22) |
| Q121 | 118.6 | 7.67 | 3.97 | 2.08, 2.31, 2.48 |
| A122 | 122.9 | 7.73 | 3.99 | $H^{\beta}$(1.20) |
| L123 | 118.4 | 8.53 | 4.05 | 1.95, 1.26, 0.89, 0.99* |
| R124 | 120.2 | 8.41 | 4.00 | 1.91, 1.59, 1.81, 3.16 |
| Q125 | 119.2 | 8.09 | 4.01 | 2.19, 2.07, 2.41 |
| L126 | 119.3 | 7.49 | 4.16 | 1.72, 1.63, 0.86 |
| A127 | 120.7 | 7.52 | 4.10 | $H^{\beta}$(1.48) |
| L128 | 119.5 | 7.79 | 4.16 | 1.79, 1.61, 0.86* |
| E129 | 120.4 | 8.15 | 4.13 | $H^{\beta}$(2.07, 2.12), $H^{\gamma}$(2.26, 2.41) |
| A130 | 123.4 | 8.15 | 4.29 | $H^{\beta}$(1.43) |
| K131 | 118.6 | 7.82 | 4.36 | 2.99, 1.94, 1.83, 1.67, 1.50 |
| G132 | 109.5 | 8.13 | 3.95, 4.05 | |
| E133 | 121.3 | 8.27 | 4.41 | 2.25, 2.10, 1.89, |
| T134 | 120.9 | 7.81 | 4.18 | $H^{\gamma}$(1.13) |

[a] $^{1}H$ chemical shifts are relatavie to DSS. $^{15}N$ chemical shifts are relative to $^{15}NH_3$. Chemical shift values indicated by asterisks (*) were obtained from a 3D $^{15}N$-edited NOESY.

Table S2

| residue | $T_1$ (sec) | $T_2$ (sec) | NOE | $\tau_m$ (ns) | $S^2$ | $\tau_e$ (ps) | error (%) |
|---|---|---|---|---|---|---|---|
| 4 | 0.7857 | 0.2498 | | 5.51 | | | |
| 4 | 0.0451 | 0.0229 | | | | | |
| 5 | 0.6543 | 0.2844 | | 4.19 | | | |
| 5 | 0.0306 | 0.0302 | | | | | |
| 6 | 1.8723 | 0.4323 | -3.966 | 6.94 | 0.163 | 0.8264E+02 | |
| 6 | 0.2493 | 0.0686 | | | | | 33.55 |
| 7 | 0.5533 | 0.1678 | 0.467 | 5.71 | 0.518 | 0.1930E+04 | |
| 7 | 0.0219 | 0.0104 | | | | | 33.63 |
| 9 | 0.5428 | 0.1180 | 0.736 | 7.23 | 0.808 | 0.4536E+02 | |
| 9 | 0.0207 | 0.0052 | | | | | 11.14 |
| 11 | 0.5256 | 0.1098 | 0.765 | 7.42 | 0.853 | 0.4146E+02 | |
| 11 | 0.0197 | 0.0044 | | | | | 8.86 |
| 12 | 0.5563 | 0.1057 | 0.738 | 7.89 | 0.843 | 0.3437E+02 | |
| 12 | 0.0221 | 0.0043 | | | | | 2.15 |
| 14 | 0.5324 | 0.0980 | 0.806 | 8.06 | 0.904 | 0.8086E-07 | |
| 14 | 0.0201 | 0.0035 | | | | | 0.86 |
| 15 | 0.5343 | 0.1053 | 0.789 | 7.71 | 0.866 | 0.2183E+02 | |
| 15 | 0.0203 | 0.0041 | | | | | 5.29 |
| 16 | 0.5467 | 0.0978 | 0.747 | 8.20 | 0.888 | 0.3136E+02 | |
| 16 | 0.0213 | 0.0035 | | | | | 1.84 |
| 17 | 0.5366 | 0.0861 | 0.870 | 8.77 | 0.963 | 0.4249E-05 | |
| 17 | 0.0205 | 0.0027 | | | | | 9.97 |
| 18 | 0.5248 | 0.0989 | 0.802 | 7.93 | 0.904 | 0.9125E+01 | |
| 18 | 0.0197 | 0.0036 | | | | | 2.45 |
| 19 | 0.5090 | 0.0988 | 0.799 | 7.79 | 0.918 | 0.2364E+02 | |
| 19 | 0.0183 | 0.0037 | | | | | 4.34 |
| 20 | 0.5808 | 0.0898 | 0.800 | 8.98 | 0.912 | 0.3988E-05 | |
| 20 | 0.0245 | 0.0030 | | | | | 11.48 |
| 21 | 0.5574 | 0.0942 | 0.872 | 8.50 | 0.900 | 0.3153E-05 | |
| 21 | 0.0219 | 0.0033 | | | | | 6.82 |
| 22 | 0.5386 | 0.0961 | 0.854 | 8.21 | 0.905 | 0.7826E-05 | |
| 22 | 0.0206 | 0.0034 | | | | | 3.41 |
| 23 | 0.5548 | 0.0965 | 0.808 | 8.35 | 0.892 | 0.2879E-07 | |
| 23 | 0.0219 | 0.0035 | | | | | 3.21 |
| 24 | 0.5764 | 0.0927 | 0.864 | 8.76 | 0.895 | 0.2320E-05 | |
| 24 | 0.0238 | 0.0032 | | | | | 9.70 |
| 25 | 0.5505 | 0.0937 | 0.766 | 8.46 | 0.909 | 0.1094E+02 | |
| 25 | 0.0217 | 0.0032 | | | | | 4.95 |
| 26 | 0.5459 | 0.0960 | 0.841 | 8.29 | 0.901 | 0.9753E-05 | |
| 26 | 0.0213 | 0.0034 | | | | | 3.47 |
| 27 | 0.5749 | 0.0865 | 0.801 | 9.12 | 0.937 | 0.9384E-06 | |
| 27 | 0.0238 | 0.0027 | | | | | 13.33 |
| 28 | 0.5414 | 0.0903 | 0.740 | 8.57 | 0.933 | 0.3754E+02 | |
| 28 | 0.0208 | 0.0031 | | | | | 6.62 |
| 29 | 0.5660 | 0.1099 | 0.737 | 7.78 | 0.819 | 0.3233E+02 | |
| 29 | 0.0231 | 0.0045 | | | | | 3.58 |
| 30 | 0.5701 | 0.1179 | 0.833 | 7.47 | 0.798 | 0.5461E+01 | |
| 30 | 0.0236 | 0.0054 | | | | | 9.10 |
| 31 | 0.5143 | 0.1229 | 0.685 | 6.79 | 0.743 | 0.1630E+04 | |
| 31 | 0.0187 | 0.0055 | | | | | 18.93 |
| 33 | 0.5434 | 0.1246 | 0.635 | 6.98 | 0.776 | 0.7575E+02 | |
| 33 | 0.0209 | 0.0058 | | | | | 13.21 |
| 34 | 0.6290 | 0.1295 | 0.632 | 7.50 | 0.705 | 0.4294E+02 | |
| 34 | 0.0282 | 0.0062 | | | | | 6.04 |
| 36 | 0.6052 | 0.1442 | 0.598 | 6.80 | 0.681 | 0.5535E+02 | |
| 36 | 0.0262 | 0.0079 | | | | | 15.22 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 37 | 0.5198 | 0.0925 | 0.800 | 8.23 | 0.941 | 0.7490E-04 | |
| 37 | 0.0191 | 0.0034 | | | | | 1.51 |
| 38 | 0.5353 | 0.1098 | 0.727 | 7.51 | 0.841 | 0.5155E+02 | |
| 38 | 0.0201 | 0.0045 | | | | | 7.13 |
| 39 | 0.5670 | 0.1066 | 0.788 | 7.95 | 0.837 | 0.1047E+02 | |
| 39 | 0.0231 | 0.0042 | | | | | 2.09 |
| 40 | 0.5294 | 0.1002 | 0.671 | 7.91 | 0.880 | 0.9292E+02 | |
| 40 | 0.0199 | 0.0038 | | | | | 0.93 |
| 42 | 0.5123 | 0.0976 | 0.764 | 7.88 | 0.917 | 0.4914E+02 | |
| 42 | 0.0186 | 0.0036 | | | | | 2.65 |
| 43 | 0.5346 | 0.1004 | 0.789 | 7.95 | 0.888 | 0.1540E+02 | |
| 43 | 0.0206 | 0.0038 | | | | | 2.00 |
| 44 | 0.5262 | 0.1008 | 0.710 | 7.85 | 0.884 | 0.7109E+02 | |
| 44 | 0.0195 | 0.0038 | | | | | 2.29 |
| 45 | 0.4983 | 0.0991 | 0.829 | 7.67 | 0.930 | 0.5507E+01 | |
| 45 | 0.0179 | 0.0036 | | | | | 6.40 |
| 46 | 0.5148 | 0.0983 | 0.773 | 7.87 | 0.912 | 0.3856E+02 | |
| 46 | 0.0186 | 0.0035 | | | | | 2.91 |
| 47 | 0.5376 | 0.1065 | 0.760 | 7.69 | 0.856 | 0.3490E+02 | |
| 47 | 0.0207 | 0.0041 | | | | | 5.20 |
| 48 | 0.5222 | 0.0972 | 0.774 | 8.00 | 0.912 | 0.2952E+02 | |
| 48 | 0.0196 | 0.0035 | | | | | 1.19 |
| 49 | 0.5064 | 0.0963 | 0.718 | 7.89 | 0.923 | 0.1052E+03 | |
| 49 | 0.0186 | 0.0034 | | | | | 1.89 |
| 50 | 0.5325 | 0.0904 | 0.884 | 8.48 | 0.940 | 0.2005E-06 | |
| 50 | 0.0200 | 0.0029 | | | | | 7.01 |
| 51 | 0.4992 | 0.0960 | 0.766 | 7.83 | 0.936 | 0.6842E+02 | |
| 51 | 0.0180 | 0.0034 | | | | | 3.30 |
| 52 | 0.5164 | 0.1025 | 0.806 | 7.68 | 0.896 | 0.1858E+02 | |
| 52 | 0.0193 | 0.0039 | | | | | 5.99 |
| 53 | 0.4945 | 0.1018 | 0.782 | 7.50 | 0.915 | 0.5833E+02 | |
| 53 | 0.0174 | 0.0038 | | | | | 8.12 |
| 54 | 0.5045 | 0.0963 | 0.837 | 7.87 | 0.936 | 0.1010E-04 | |
| 54 | 0.0185 | 0.0035 | | | | | 3.87 |
| 55 | 0.5063 | 0.1176 | 0.709 | 6.92 | 0.770 | 0.1640E+04 | |
| 55 | 0.0183 | 0.0051 | | | | | 16.27 |
| 56 | 0.5389 | 0.1075 | 0.800 | 7.65 | 0.855 | 0.1670E+02 | |
| 56 | 0.0210 | 0.0042 | | | | | 6.20 |
| 57 | 0.5477 | 0.1021 | 0.836 | 7.99 | 0.872 | 0.1549E-08 | |
| 57 | 0.0215 | 0.0039 | | | | | 2.60 |
| 58 | 0.5882 | 0.1093 | 0.897 | 8.01 | 0.812 | 0.6075E-06 | |
| 58 | 0.0249 | 0.0044 | | | | | 5.39 |
| 59 | 0.5212 | 0.1210 | 0.912 | 6.92 | 0.838 | 0.5144E-03 | |
| 59 | 0.0196 | 0.0054 | | | | | 17.79 |
| 60 | 0.5439 | 0.0998 | 0.776 | 8.07 | 0.883 | 0.1713E+02 | |
| 60 | 0.0215 | 0.0037 | | | | | 0.28 |
| 61 | 0.5099 | 0.0960 | 0.744 | 7.94 | 0.925 | 0.7217E+02 | |
| 61 | 0.0184 | 0.0034 | | | | | 1.58 |
| 62 | 0.5449 | 0.0998 | 0.766 | 8.08 | 0.881 | 0.2254E+02 | |
| 62 | 0.0211 | 0.0037 | | | | | 0.00 |
| 63 | 0.5128 | 0.0940 | 0.861 | 8.08 | 0.938 | 0.3300E-05 | |
| 63 | 0.0188 | 0.0033 | | | | | 3.44 |
| 64 | 0.5045 | 0.0952 | 0.767 | 7.93 | 0.936 | 0.5704E+02 | |
| 64 | 0.0184 | 0.0034 | | | | | 2.07 |
| 65 | 0.5716 | 0.0921 | 0.865 | 8.75 | 0.902 | 0.1167E-05 | |
| 65 | 0.0242 | 0.0032 | | | | | 9.57 |
| 66 | 0.4936 | 0.0917 | 0.835 | 8.01 | 0.969 | 0.5575E-05 | |
| 66 | 0.0172 | 0.0032 | | | | | 2.40 |
| 67 | 0.4937 | 0.1030 | 0.770 | 7.43 | 0.910 | 0.6953E+02 | |
| 67 | 0.0170 | 0.0039 | | | | | 8.82 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 70 | 0.5162 | 0.0963 | 0.806 | 7.99 | 0.925 | 0.4073E+01 | |
| 70 | 0.0189 | 0.0035 | | | | | 1.76 |
| 71 | 0.4789 | 0.0953 | 0.759 | 7.66 | 0.914 | 0.1818E+04 | |
| 71 | 0.0163 | 0.0034 | | | | | 2.57 |
| 72 | 0.5381 | 0.0979 | 0.795 | 8.12 | 0.898 | 0.4733E+01 | |
| 72 | 0.0209 | 0.0035 | | | | | 0.06 |
| 73 | 0.5185 | 0.0958 | 0.767 | 8.04 | 0.921 | 0.3862E+02 | |
| 73 | 0.0191 | 0.0034 | | | | | 0.60 |
| 74 | 0.4771 | 0.1041 | 0.830 | 7.21 | 0.849 | 0.2357E+04 | |
| 74 | 0.0164 | 0.0040 | | | | | 10.26 |
| 76 | 0.5305 | 0.0995 | 0.749 | 7.96 | 0.891 | 0.4241E+02 | |
| 76 | 0.0201 | 0.0037 | | | | | 1.41 |
| 77 | 0.5384 | 0.1060 | 0.825 | 7.72 | 0.865 | 0.3058E+01 | |
| 77 | 0.0207 | 0.0043 | | | | | 5.68 |
| 79 | 0.5441 | 0.1083 | 0.755 | 7.66 | 0.843 | 0.3441E+02 | |
| 79 | 0.0214 | 0.0044 | | | | | 5.50 |
| 80 | 0.5849 | 0.1015 | 0.738 | 8.36 | 0.844 | 0.2073E+02 | |
| 80 | 0.0245 | 0.0038 | | | | | 4.00 |
| 81 | 0.5842 | 0.1203 | 0.711 | 7.49 | 0.767 | 0.3662E+02 | |
| 81 | 0.0246 | 0.0053 | | | | | 7.17 |
| 82 | 0.6096 | 0.1320 | 0.717 | 7.25 | 0.719 | 0.3100E+02 | |
| 82 | 0.0264 | 0.0064 | | | | | 10.59 |
| 83 | 0.5813 | 0.1404 | 0.683 | 6.73 | 0.715 | 0.4700E+02 | |
| 83 | 0.0241 | 0.0073 | | | | | 17.29 |
| 84 | 0.6163 | 0.1131 | 0.773 | 8.07 | 0.779 | 0.8793E+01 | |
| 84 | 0.0270 | 0.0046 | | | | | 0.24 |
| 85 | 0.6576 | 0.1017 | 0.859 | 8.98 | 0.804 | 0.1032E-04 | |
| 85 | 0.0317 | 0.0038 | | | | | 12.24 |
| 86 | 0.6169 | 0.0959 | 0.814 | 8.95 | 0.855 | 0.8504E-06 | |
| 86 | 0.0277 | 0.0034 | | | | | 11.17 |
| 87 | 0.5336 | 0.0995 | 0.764 | 7.99 | 0.891 | 0.3053E+02 | |
| 87 | 0.0202 | 0.0037 | | | | | 1.17 |
| 89 | 0.5811 | 0.0941 | 0.751 | 8.73 | 0.887 | 0.8347E+01 | |
| 89 | 0.0243 | 0.0033 | | | | | 8.50 |
| 90 | 0.5164 | 0.0907 | 0.800 | 8.30 | 0.954 | 0.5295E-05 | |
| 90 | 0.0190 | 0.0031 | | | | | 2.47 |
| 91 | 0.5195 | 0.0945 | 0.833 | 8.12 | 0.930 | 0.1225E-04 | |
| 91 | 0.0194 | 0.0033 | | | | | 1.89 |
| 92 | 0.5452 | 0.0932 | 0.842 | 8.44 | 0.915 | 0.5744E-05 | |
| 92 | 0.0209 | 0.0033 | | | | | 5.12 |
| 93 | 0.5437 | 0.0900 | 0.828 | 8.61 | 0.935 | 0.5553E-07 | |
| 93 | 0.0213 | 0.0030 | | | | | 7.01 |
| 94 | 0.5287 | 0.0979 | 0.773 | 8.03 | 0.903 | 0.2601E+02 | |
| 94 | 0.0196 | 0.0036 | | | | | 0.83 |
| 95 | 0.5423 | 0.0917 | 0.788 | 8.50 | 0.927 | 0.5593E-04 | |
| 95 | 0.0212 | 0.0031 | | | | | 5.15 |
| 96 | 0.5943 | 0.0965 | 0.809 | 8.71 | 0.865 | 0.2166E-05 | |
| 96 | 0.0251 | 0.0035 | | | | | 8.11 |
| 97 | 0.5415 | 0.0944 | 0.803 | 8.34 | 0.913 | 0.1732E-04 | |
| 97 | 0.0208 | 0.0033 | | | | | 3.03 |
| 98 | 0.5491 | 0.0961 | 0.836 | 8.32 | 0.897 | 0.1085E-04 | |
| 98 | 0.0219 | 0.0035 | | | | | 3.53 |
| 99 | 0.5385 | 0.0917 | 0.761 | 8.46 | 0.929 | 0.2017E+02 | |
| 99 | 0.0207 | 0.0031 | | | | | 4.99 |
| 100 | 0.5810 | 0.0972 | 0.761 | 8.56 | 0.870 | 0.7229E+01 | |
| 100 | 0.0246 | 0.0046 | | | | | 6.22 |
| 101 | 0.5282 | 0.0958 | 0.793 | 8.13 | 0.916 | 0.6707E+01 | |
| 101 | 0.0202 | 0.0034 | | | | | 0.26 |
| 102 | 0.5344 | 0.0923 | 0.868 | 8.39 | 0.928 | 0.1571E-05 | |
| 102 | 0.0204 | 0.0032 | | | | | 5.52 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 104 | 0.5531 | 0.0969 | 0.799 | 8.31 | 0.892 | 0.6100E-04 | |
| 104 | 0.0217 | 0.0035 | | | | | 2.62 |
| 105 | 0.5672 | 0.0944 | 0.852 | 8.58 | 0.893 | 0.3993E-05 | |
| 105 | 0.0226 | 0.0033 | | | | | 7.17 |
| 107 | 0.5885 | 0.1034 | 0.735 | 8.30 | 0.832 | 0.2206E+02 | |
| 107 | 0.0247 | 0.0039 | | | | | 3.23 |
| 108 | 0.5017 | 0.1049 | 0.812 | 7.42 | 0.899 | 0.2997E+02 | |
| 108 | 0.0180 | 0.0040 | | | | | 9.58 |
| 109 | 0.5439 | 0.1184 | 0.830 | 7.22 | 0.817 | 0.1436E+02 | |
| 109 | 0.0210 | 0.0053 | | | | | 12.51 |
| 110 | 0.5669 | 0.1315 | 0.664 | 6.92 | 0.743 | 0.5558E+02 | |
| 110 | 0.0228 | 0.0063 | | | | | 14.41 |
| 112 | 0.5298 | 0.1175 | 0.734 | 7.14 | 0.820 | 0.5331E+02 | |
| 112 | 0.0201 | 0.0051 | | | | | 12.40 |
| 113 | 0.5459 | 0.1040 | 0.817 | 7.88 | 0.866 | 0.1037E+01 | |
| 113 | 0.0213 | 0.0041 | | | | | 3.37 |
| 114 | 0.5646 | 0.1046 | 0.730 | 8.02 | 0.841 | 0.3358E+02 | |
| 114 | 0.0229 | 0.0041 | | | | | 0.29 |
| 115 | 0.5671 | 0.0976 | 0.831 | 8.40 | 0.877 | 0.1266E-05 | |
| 115 | 0.0230 | 0.0036 | | | | | 4.42 |
| 116 | 0.5367 | 0.0997 | 0.804 | 8.01 | 0.891 | 0.3674E+01 | |
| 116 | 0.0209 | 0.0037 | | | | | 1.48 |
| 118 | 0.5547 | 0.0988 | 0.772 | 8.22 | 0.880 | 0.1296E+02 | |
| 118 | 0.0215 | 0.0036 | | | | | 1.78 |
| 119 | 0.5409 | 0.0931 | 0.800 | 8.41 | 0.921 | 0.4763E-04 | |
| 119 | 0.0211 | 0.0032 | | | | | 3.92 |
| 120 | 0.5143 | 0.1038 | 0.898 | 7.59 | 0.894 | 0.1785E-04 | |
| 120 | 0.0189 | 0.0040 | | | | | 8.82 |
| 121 | 0.5234 | 0.0985 | 0.830 | 7.94 | 0.908 | 0.1359E-04 | |
| 121 | 0.0196 | 0.0036 | | | | | 2.85 |
| 122 | 0.5538 | 0.0950 | 0.828 | 8.42 | 0.900 | 0.7511E-05 | |
| 122 | 0.0216 | 0.0033 | | | | | 4.58 |
| 123 | 0.5486 | 0.0967 | 0.808 | 8.28 | 0.896 | 0.8766E-06 | |
| 123 | 0.0217 | 0.0034 | | | | | 2.30 |
| 124 | 0.5253 | 0.1095 | 0.741 | 7.44 | 0.852 | 0.5260E+02 | |
| 124 | 0.0198 | 0.0045 | | | | | 8.36 |
| 125 | 0.5305 | 0.1050 | 0.844 | 7.69 | 0.876 | 0.4197E-03 | |
| 125 | 0.0202 | 0.0041 | | | | | 6.32 |
| 126 | 0.5544 | 0.0975 | 0.793 | 8.29 | 0.888 | 0.4897E-03 | |
| 126 | 0.0217 | 0.0035 | | | | | 2.37 |
| 127 | 0.5447 | 0.1070 | 0.726 | 7.73 | 0.845 | 0.4589E+02 | |
| 127 | 0.0214 | 0.0043 | | | | | 4.20 |
| 129 | 0.5349 | 0.1315 | 0.541 | 6.65 | 0.692 | 0.1476E+04 | |
| 129 | 0.0203 | 0.0064 | | | | | 20.81 |
| 130 | 0.5613 | 0.1447 | 0.384 | 6.43 | 0.683 | 0.1165E+03 | |
| 130 | 0.0227 | 0.0078 | | | | | 17.08 |
| 131 | 0.6228 | 0.2077 | 0.130 | 5.30 | 0.423 | 0.1727E+01 | |
| 131 | 0.0273 | 0.0159 | | | | | 59.9 |
| 132 | 0.6296 | 0.2361 | -1.292 | 4.80 | 0.289 | 0.4224E+03 | |
| 132 | 0.0284 | 0.0204 | | | | | 6.46 |
| 133 | 0.7454 | 0.3310 | -5.162 | 4.10 | 0.182 | 0.3423E+03 | |
| 133 | 0.0399 | 0.0402 | | | | | 32.35 |
| 134 | 1.0003 | 0.5532 | -14.305 | 3.18 | 0.097 | 0.2144E+03 | |
| 134 | 0.0717 | 0.1199 | | | | | 41.15 |

For each residue, the bottom row of numbers give the standard deviations of the T1 and T2 values, and the total relative deviation of theoretical values from experimental values in the fitting of order parameter and effective correlation time of internal motion.