

## APPENDIX

Table IV.6.A1. Inter-residue contact potentials  $e_{AB}$  for  $R_C = 6.5 \text{ \AA}$  {Miyazawa & Jernigan 1996 ID: 174}

|   | A    | C    | D     | E     | F     | G    | H    | I     | K     | L     | M     | N     | P     | Q     | R     | S     | T     | V     | W     | Y     |       |
|---|------|------|-------|-------|-------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| A |      |      | 0.51  | 0.26  | 0.30  | 0.17 | 0.18 | 0.47  | 0.05  | 0.11  | 0.13  | 0.15  | 0.36  | 0.20  | 0.24  | 0.30  | 0.18  | 0.10  | 0.08  | 0.07  | 0.09  |
| C | 0.51 |      |       | 0.91  | 0.91  | 0.54 | 0.68 | 0.65  | 0.49  | 0.83  | 0.57  | 0.46  | 0.97  | 0.53  | 0.64  | 0.93  | 0.69  | 0.67  | 0.52  | 0.30  | 0.64  |
| D | 0.26 | 0.91 |       |       | 0.05  | 0.75 | 0.13 | -0.19 | 0.71  | -1.01 | 0.89  | 0.77  | -0.24 | 0.14  | -0.09 | -0.91 | -0.19 | -0.14 | 0.89  | 0.30  | -0.07 |
| E | 0.30 | 0.91 | 0.05  |       |       | 0.52 | 0.36 | -0.16 | 0.46  | -1.28 | 0.55  | 0.30  | -0.21 | 0.07  | -0.19 | -1.04 | -0.19 | -0.22 | 0.55  | 0.00  | -0.25 |
| F | 0.17 | 0.54 | 0.75  | 0.52  |       |      | 0.62 | 0.39  | 0.06  | 0.33  | 0.03  | -0.20 | 0.72  | 0.25  | 0.30  | 0.42  | 0.44  | 0.41  | 0.10  | 0.00  | 0.05  |
| G | 0.18 | 0.68 | 0.13  | 0.36  | 0.62  |      |      | 0.50  | 0.62  | 0.03  | 0.65  | 0.46  | 0.22  | 0.13  | 0.24  | 0.18  | 0.14  | 0.10  | 0.51  | 0.24  | 0.20  |
| H | 0.47 | 0.65 | -0.19 | -0.16 | 0.39  | 0.50 |      |       | 0.66  | 0.23  | 0.67  | 0.28  | 0.29  | 0.15  | 0.31  | 0.14  | 0.26  | 0.16  | 0.70  | 0.08  | 0.09  |
| I | 0.05 | 0.49 | 0.71  | 0.46  | 0.06  | 0.62 | 0.66 |       |       | 0.32  | -0.08 | -0.01 | 0.87  | 0.39  | 0.37  | 0.41  | 0.59  | 0.30  | -0.01 | 0.02  | 0.11  |
| K | 0.11 | 0.83 | -1.01 | -1.28 | 0.33  | 0.03 | 0.23 | 0.32  |       |       | 0.37  | 0.31  | -0.30 | -0.04 | -0.46 | 0.24  | -0.15 | -0.19 | 0.33  | -0.10 | -0.46 |
| L | 0.13 | 0.57 | 0.89  | 0.55  | 0.03  | 0.65 | 0.67 | -0.08 | 0.37  |       |       | 0.01  | 0.79  | 0.35  | 0.42  | 0.43  | 0.60  | 0.40  | -0.04 | 0.08  | 0.10  |
| M | 0.15 | 0.46 | 0.77  | 0.30  | -0.20 | 0.46 | 0.28 | -0.01 | 0.31  | 0.01  |       |       | 0.62  | 0.16  | 0.20  | 0.38  | 0.53  | 0.28  | 0.18  | -0.29 | -0.10 |
| N | 0.36 | 0.97 | -0.24 | -0.21 | 0.72  | 0.22 | 0.29 | 0.87  | -0.30 | 0.79  | 0.62  |       |       | 0.18  | -0.10 | -0.02 | 0.10  | 0.02  | 0.77  | 0.30  | 0.17  |
| P | 0.20 | 0.53 | 0.14  | 0.07  | 0.25  | 0.13 | 0.15 | 0.39  | -0.04 | 0.35  | 0.16  | 0.18  |       |       | -0.08 | -0.05 | 0.14  | 0.04  | 0.31  | -0.33 | -0.23 |
| Q | 0.24 | 0.64 | -0.09 | -0.19 | 0.30  | 0.24 | 0.31 | 0.37  | -0.46 | 0.42  | 0.20  | -0.10 | -0.08 |       |       | -0.26 | 0.11  | -0.08 | 0.46  | 0.19  | -0.12 |
| R | 0.30 | 0.93 | -0.91 | -1.04 | 0.42  | 0.18 | 0.14 | 0.41  | 0.24  | 0.43  | 0.38  | -0.02 | -0.05 | -0.26 |       |       | -0.01 | -0.07 | 0.47  | -0.11 | -0.30 |
| S | 0.18 | 0.69 | -0.19 | -0.19 | 0.44  | 0.14 | 0.26 | 0.59  | -0.15 | 0.60  | 0.53  | 0.10  | 0.14  | 0.11  | -0.01 |       |       | -0.06 | 0.55  | 0.38  | 0.14  |
| T | 0.10 | 0.67 | -0.14 | -0.22 | 0.41  | 0.10 | 0.16 | 0.30  | -0.19 | 0.40  | 0.28  | 0.02  | 0.04  | -0.08 | -0.07 | -0.06 |       |       | 0.36  | 0.37  | 0.13  |
| V | 0.08 | 0.52 | 0.89  | 0.55  | 0.10  | 0.51 | 0.70 | -0.01 | 0.33  | -0.04 | 0.18  | 0.77  | 0.31  | 0.46  | 0.47  | 0.55  | 0.36  |       |       | 0.11  | 0.23  |
| W | 0.07 | 0.30 | 0.30  | 0.00  | 0.00  | 0.24 | 0.08 | 0.02  | -0.10 | 0.08  | -0.29 | 0.30  | -0.33 | 0.19  | -0.11 | 0.38  | 0.37  | 0.11  |       |       | -0.04 |
| Y | 0.09 | 0.64 | -0.07 | -0.25 | 0.05  | 0.20 | 0.09 | 0.11  | -0.46 | 0.10  | -0.10 | 0.17  | -0.23 | -0.12 | -0.30 | 0.14  | 0.13  | 0.23  | -0.04 |       |       |