

The original values of the 6 physical structural properties (DNA) taken from Goni et al. (2007)

| Physicochemical properties | AA | AC | AG | AT | CA | CC | CG | CT | GA | GC | GG | GT | TA | TC | TG | TT |
|----------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Rise (DNA) | 7.65 | 8.93 | 7.08 | 9.07 | 6.38 | 8.04 | 6.23 | 7.08 | 8.56 | 9.53 | 8.04 | 8.93 | 6.23 | 8.56 | 6.38 | 7.65 |
| Roll (DNA) | 2.26 | 3.03 | 2.03 | 3.83 | 1.78 | 1.65 | 2 | 2.03 | 1.93 | 2.61 | 1.65 | 3.03 | 1.2 | 1.93 | 1.78 | 2.26 |
| Shift (DNA) | 1.69 | 1.32 | 1.46 | 1.03 | 1.07 | 1.43 | 1.08 | 1.46 | 1.32 | 1.2 | 1.43 | 1.32 | 0.72 | 1.32 | 1.07 | 1.69 |
| Slide (DNA) | 0.026 | 0.036 | 0.031 | 0.033 | 0.016 | 0.026 | 0.014 | 0.031 | 0.025 | 0.025 | 0.026 | 0.036 | 0.017 | 0.025 | 0.016 | 0.026 |
| Tilt (DNA) | 0.02 | 0.023 | 0.019 | 0.022 | 0.017 | 0.019 | 0.016 | 0.019 | 0.02 | 0.026 | 0.019 | 0.023 | 0.016 | 0.02 | 0.017 | 0.02 |
| Twist (DNA) | 0.038 | 0.038 | 0.037 | 0.036 | 0.025 | 0.042 | 0.026 | 0.037 | 0.038 | 0.036 | 0.042 | 0.038 | 0.018 | 0.038 | 0.025 | 0.038 |

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|----------------------------|-------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|-------|-------|-------|-------|
| Rise (DNA) | -0.11 | 1.04 | -0.62 | 1.17 | -1.25 | 0.24 | -1.39 | -0.62 | 0.71 | 1.59 | 0.24 | 1.04 | -1.39 | 0.71 | -1.25 | -0.11 |
| Roll (DNA) | 0.11 | 1.29 | -0.24 | 2.51 | -0.62 | -0.82 | -0.29 | -0.24 | -0.39 | 0.65 | -0.82 | 1.29 | -1.51 | -0.39 | -0.62 | 0.11 |
| Shift (DNA) | 1.59 | 0.13 | 0.68 | -1.02 | -0.86 | 0.56 | -0.82 | 0.68 | 0.13 | -0.35 | 0.56 | 0.13 | -2.24 | 0.13 | -0.86 | 1.59 |
| Slide (DNA) | 0.06 | 1.5 | 0.78 | 1.07 | -1.38 | 0.06 | -1.66 | 0.78 | -0.08 | -0.08 | 0.06 | 1.5 | -1.23 | -0.08 | -1.38 | 0.06 |
| Tilt (DNA) | 0.09 | 1.19 | -0.28 | 0.83 | -1.01 | -0.28 | -1.38 | -0.28 | 0.09 | 2.3 | -0.28 | 1.19 | -1.38 | 0.09 | -1.01 | 0.09 |
| Twist (DNA) | 0.5 | 0.5 | 0.36 | 0.22 | -1.36 | 1.08 | -1.22 | 0.36 | 0.5 | 0.22 | 1.08 | 0.5 | -2.37 | 0.5 | -1.36 | 0.5 |