Supporting Information

Consecutive Non-Natural PZ Nucleobase Pairs in DNA Impact Helical Structure as Seen in 50 μs Molecular Dynamics Simulations

Robert W. Molt, Jr., Millie M. Georgiadis, and Nigel G. J. Richards

School of Chemistry, Cardiff University, Park Place, Cardiff, CF10 3AT, United Kingdom, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, Indianapolis, IN 46202, United States, Department of Chemistry & Chemical Biology, Indiana University Purdue University Indianapolis, Indianapolis, IN 46202, United States, and ENSCO, Inc., 4849 North Wickham Road, Melbourne, FL 32940, United States,
Table S1. Time convergence (μs) of all parameters for the GC-containing oligonucleotide.

|        | 0.5  | 5    | 25   | 50   |
|--------|------|------|------|------|
| Shear  |      |      |      |      |
| G-C    | -0.15| -0.15| -0.15| -0.15|
| G-C    | -0.16| -0.16| -0.16| -0.16|
| G-C    | -0.13| -0.13| -0.13| -0.13|
| C-G    | 0.13 | 0.13 | 0.13 | 0.13 |
| C-G    | 0.16 | 0.16 | 0.16 | 0.16 |
| C-G    | 0.16 | 0.16 | 0.15 | 0.16 |

| Stretch| 0.5  | 5    | 25   | 50   |
|--------|------|------|------|------|
| G-C    | -0.07| -0.07| -0.07| -0.07|
| G-C    | -0.07| -0.07| -0.07| -0.07|
| G-C    | -0.06| -0.06| -0.06| -0.06|
| C-G    | -0.06| -0.06| -0.06| -0.06|
| C-G    | -0.07| -0.07| -0.07| -0.07|

| Stagger| 0.5  | 5    | 25   | 50   |
|--------|------|------|------|------|
| G-C    | 0.01 | 0.01 | 0.01 | 0.01 |
| G-C    | -0.11| -0.11| -0.12| -0.12|
| G-C    | -0.13| -0.13| -0.13| -0.13|
| C-G    | -0.11| -0.11| -0.12| -0.12|
| C-G    | 0.01 | 0.01 | 0.01 | 0.01 |

| Buckle | 0.5  | 5    | 25   | 50   |
|--------|------|------|------|------|
| G-C    | 3.45 | 3.52 | 3.56 | 3.55 |
| G-C    | -0.88| -0.72| -0.79| -0.81|
| G-C    | -4.50| -4.30| -4.27| -4.30|
| C-G    | 4.26 | 4.26 | 4.33 | 4.29 |
| C-G    | 0.77 | 0.77 | 0.83 | 0.83 |
| C-G    | -3.65| -3.47| -3.53| -3.52|

| Propeller| 0.5  | 5    | 25   | 50   |
|----------|------|------|------|------|
| G-C      | -5.52| -5.44| -5.48| -5.49|
| G-C      | -8.86| -8.77| -8.84| -8.84|
| G-C      | -6.22| -6.17| -6.15| -6.16|
| C-G      | -6.13| -6.13| -6.16| -6.14|
| C-G      | -8.99| -8.83| -8.85| -8.83|
| C-G      | -5.57| -5.44| -5.48| -5.47|

| Opening  | 0.5  | 5    | 25   | 50   |
|----------|------|------|------|------|
| G-C      | -0.53| -0.53| -0.52| -0.52|
| G-C      | 0.07 | 0.06 | 0.07 | 0.07 |
| G-C      | -0.48| -0.48| -0.49| -0.49|
| C-G      | -0.51| -0.49| -0.49| -0.49|
|       | 0.5 | 5   | 25  | 50  |
|-------|-----|-----|-----|-----|
| C-G   | 0.12| 0.08| 0.08| 0.07|
| C-G   | -0.51| -0.51| -0.52| -0.52|
| Shift | 0.5 | 5   | 25  | 50  |
| TG/CA | 0.19| 0.18| 0.17| 0.17|
| GG/CC | 0.22| 0.23| 0.23| 0.23|
| GG/CC | -0.11| -0.11| -0.11| -0.11|
| GC/GC | -0.01| 0.00| 0.00| 0.00|
| CC/GG | 0.12| 0.11| 0.11| 0.11|
| CC/GG | -0.24| -0.24| -0.23| -0.23|
| CA/TG | -0.15| -0.17| -0.17| -0.17|
| Slide | 0.5 | 5   | 25  | 50  |
| TG/CA | -0.54| -0.54| -0.54| -0.54|
| GG/CC | -1.27| -1.25| -1.26| -1.26|
| GG/CC | -1.34| -1.34| -1.33| -1.33|
| GC/GC | -0.77| -0.78| -0.78| -0.78|
| CC/GG | -1.33| -1.33| -1.33| -1.33|
| CC/GG | -1.26| -1.26| -1.26| -1.26|
| CA/TG | -0.56| -0.54| -0.54| -0.54|
| Rise  | 0.5 | 5   | 25  | 50  |
| TG/CA | 3.26| 3.26| 3.25| 3.25|
| GG/CC | 3.46| 3.45| 3.46| 3.46|
| GG/CC | 3.42| 3.42| 3.42| 3.42|
| GC/GC | 3.19| 3.19| 3.19| 3.19|
| CC/GG | 3.42| 3.42| 3.42| 3.42|
| CC/GG | 3.46| 3.45| 3.46| 3.46|
| CA/TG | 3.25| 3.25| 3.25| 3.25|
| Tilt  | 0.5 | 5   | 25  | 50  |
| TG/CA | -0.65| -0.61| -0.55| -0.57|
| GG/CC | 0.53| 0.53| 0.55| 0.55|
| GG/CC | 0.15| 0.14| 0.09| 0.10|
| GC/GC | -0.01| -0.02| 0.00| 0.00|
| CC/GG | -0.08| -0.13| -0.10| -0.10|
| CC/GG | -0.53| -0.57| -0.56| -0.56|
| CA/TG | 0.47| 0.54| 0.57| 0.58|
| Roll  | 0.5 | 5   | 25  | 50  |
| TG/CA | 9.61| 9.62| 9.56| 9.59|
| GG/CC | 5.20| 5.14| 5.22| 5.21|
| GG/CC | 4.90| 4.80| 4.89| 4.88|
| GC/GC | 2.93| 2.81| 2.88| 2.87|
| CC/GG | 4.93| 4.85| 4.89| 4.88|
| CC/GG | 5.37| 5.24| 5.24| 5.23|
| CA/TG | 9.53| 9.62| 9.62| 9.63|
|       | Twist  | t/100 | t/10 | t/2  | t   |
|-------|--------|-------|------|------|-----|
| TG/CA | 30.42  | 30.35 | 30.32| 30.32|     |
| GG/CC | 30.20  | 30.24 | 30.20| 30.21|     |
| GG/CC | 29.94  | 29.99 | 29.98| 29.98|     |
| GC/GC | 33.61  | 33.60 | 33.55| 33.56|     |
| CC/GG | 29.94  | 29.99 | 29.97| 29.97|     |
| CC/GG | 30.16  | 30.13 | 30.18| 30.19|     |
| CA/TG | 30.31  | 30.25 | 30.28| 30.30|     |

|       | H-Rise | 0.5 | 5   | 25  | 50  |
|-------|--------|-----|-----|-----|-----|
| TG/CA | 2.85   | 2.84| 2.83| 2.83|     |
| GG/CC | 3.12   | 3.12| 3.12| 3.12|     |
| GG/CC | 3.09   | 3.10| 3.09| 3.09|     |
| GC/GC | 3.08   | 3.08| 3.08| 3.08|     |
| CC/GG | 3.08   | 3.10| 3.09| 3.09|     |
| CC/GG | 3.11   | 3.12| 3.12| 3.12|     |
| CA/TG | 2.83   | 2.83| 2.83| 2.83|     |

|       | Inclination | 0.5 | 5   | 25  | 50  |
|-------|-------------|-----|-----|-----|-----|
| TG/CA | 17.87       | 17.91| 17.81| 17.86|     |
| GG/CC | 10.07       | 9.96 | 10.11| 10.09|     |
| GG/CC | 9.47        | 9.28 | 9.46 | 9.43 |     |
| GC/GC | 5.19        | 4.98 | 5.11 | 5.09 |     |
| CC/GG | 9.56        | 9.37 | 9.45 | 9.43 |     |
| CC/GG | 10.41       | 10.17| 10.15| 10.13|     |
| CA/TG | 17.78       | 17.93| 17.94| 17.94|     |

|       | Tip | 0.5 | 5   | 25  | 50  |
|-------|-----|-----|-----|-----|-----|
| TG/CA | 1.19| 1.14| 1.03| 1.06|     |
| GG/CC | -1.09| -1.09| -1.11| -1.12|     |
| GG/CC | -0.31| -0.28| -0.18| -0.21|     |
| GC/GC | 0.01 | 0.03 | 0.00 | 0.00 |     |
| CC/GG | 0.17 | 0.25 | 0.19 | 0.20 |     |
| CC/GG | 1.09 | 1.16 | 1.14 | 1.13 |     |
| CA/TG | -0.87| -1.00| -1.07| -1.08|     |

|       | H-Twist | 0.5 | 5   | 25  | 50  |
|-------|---------|-----|-----|-----|-----|
| TG/CA | 32.90   | 32.83| 32.78| 32.78|     |
| GG/CC | 31.41   | 31.44| 31.42| 31.42|     |
| GG/CC | 31.05   | 31.09| 31.09| 31.09|     |
| GC/GC | 34.32   | 34.30| 34.26| 34.27|     |
| CC/GG | 31.06   | 31.09| 31.08| 31.08|     |
| CC/GG | 31.40   | 31.35| 31.40| 31.40|     |
| CA/TG | 32.78   | 32.74| 32.76| 32.78|     |
|        | 0.5 | 5   | 25  | 50  |
|--------|-----|-----|-----|-----|
| **Major Groove Refined** |     |     |     |     |
| TG/CA  | 20  | 20  | 20  | 20  |
| GG/CC  | 20  | 20  | 20  | 20  |
| GG/CC  | 21  | 21  | 21  | 21  |
| GC/GC  | 21  | 21  | 21  | 21  |
| CC/GG  | 21  | 21  | 21  | 21  |
| CC/GG  | 20  | 20  | 20  | 20  |
| CA/TG  | 20  | 20  | 20  | 20  |
| **Minor Groove Refined** |     |     |     |     |
| TG/CA  | 14  | 14  | 14  | 14  |
| GG/CC  | 13  | 13  | 13  | 13  |
| GG/CC  | 13  | 13  | 13  | 13  |
| GC/GC  | 13  | 13  | 13  | 13  |
| CC/GG  | 13  | 13  | 13  | 13  |
| CC/GG  | 13  | 13  | 13  | 13  |
| CA/TG  | 14  | 14  | 14  | 14  |
| **Major Groove Unrefined** |     |     |     |     |
| TG/CA  | 21  | 21  | 21  | 21  |
| GG/CC  | 21  | 21  | 21  | 21  |
| GG/CC  | 22  | 22  | 22  | 22  |
| GC/GC  | 22  | 22  | 22  | 22  |
| CC/GG  | 21  | 21  | 21  | 21  |
| CC/GG  | 21  | 21  | 21  | 21  |
| CA/TG  | 21  | 21  | 21  | 21  |
| **Minor Groove Unrefined** |     |     |     |     |
| TG/CA  | 14  | 14  | 14  | 14  |
| GG/CC  | 14  | 14  | 14  | 14  |
| GG/CC  | 14  | 14  | 14  | 14  |
| GC/GC  | 13  | 13  | 13  | 13  |
| CC/GG  | 14  | 14  | 14  | 14  |
| CC/GG  | 14  | 14  | 14  | 14  |
| CA/TG  | 14  | 14  | 14  | 14  |

**Table S2.** Time convergence (μs) of all parameters for the PZ-containing oligonucleotide.

| Shear | 0.5 | 5  | 25 | 50 |
|-------|-----|----|----|----|
| 6=27  | P-Z | -0.06 | -0.05 | -0.06 | -0.05 |
| 7=26  | P-Z | -0.04 | -0.04 | -0.04 | -0.04 |
| 8=25  | P-Z | 0.04 | -0.39 | -0.21 | -0.22 |
| 9=24  | Z-P | -0.05 | 0.01 | 0.00 | 0.10 |
| 10=23 | Z-P | 0.04 | 0.04 | 0.04 | 0.04 |
| 11=22 | Z-P | 0.05 | 0.06 | 0.06 | 0.06 |
|      | 0.5 | 5   | 25  | 50  |
|------|-----|-----|-----|-----|
| Stretch | 0.5 | 5   | 25  | 50  |
| 6=27 | P-Z | -0.04 | -0.04 | -0.04 | -0.04 |
| 7=26 | P-Z | -0.03 | -0.03 | -0.03 | -0.03 |
| 8=25 | P-Z | -0.04 | -0.11 | -0.06 | -0.05 |
| 9=24 | Z-P | -0.04 | -0.04 | -0.04 | -0.04 |
| 10=23 | Z-P | -0.03 | -0.03 | -0.03 | -0.03 |
| 11=22 | Z-P | -0.04 | -0.04 | -0.04 | -0.04 |
| Stagger | 0.5 | 5   | 25  | 50  |
| 6=27 | P-Z | -0.23 | -0.23 | -0.24 | -0.24 |
| 7=26 | P-Z | -0.11 | -0.10 | -0.11 | -0.11 |
| 8=25 | P-Z | -0.22 | -0.21 | -0.20 | -0.21 |
| 9=24 | Z-P | -0.22 | -0.19 | -0.20 | -0.21 |
| 10=23 | Z-P | -0.14 | -0.11 | -0.12 | -0.11 |
| 11=22 | Z-P | -0.23 | -0.24 | -0.24 | -0.24 |
| Buckle | 0.5 | 5   | 25  | 50  |
| 6=27 | P-Z | -5.96 | -6.17 | -6.15 | -6.20 |
| 7=26 | P-Z | -3.34 | -3.65 | -3.68 | -3.71 |
| 8=25 | P-Z | -3.18 | -2.85 | -2.93 | -3.13 |
| 9=24 | Z-P | 3.29  | 2.90  | 3.22  | 3.13  |
| 10=23 | Z-P | 4.24  | 3.61  | 3.72  | 3.70  |
| 11=22 | Z-P | 5.58  | 6.26  | 6.29  | 6.29  |
| Propeller | 0.5 | 5   | 25  | 50  |
| 6=27 | P-Z | -6.60 | -6.72 | -6.68 | -6.70 |
| 7=26 | P-Z | -3.31 | -3.36 | -3.27 | -3.31 |
| 8=25 | P-Z | -0.20 | 0.97  | 0.53  | 0.51  |
| 9=24 | Z-P | -0.35 | -0.66 | -0.57 | -0.03 |
| 10=23 | Z-P | -3.15 | -3.32 | -3.28 | -3.32 |
| 11=22 | Z-P | -6.90 | -6.67 | -6.69 | -6.69 |
| Opening | 0.5 | 5   | 25  | 50  |
| 6=27 | P-Z | -2.25 | -2.30 | -2.27 | -2.28 |
| 7=26 | P-Z | -3.37 | -3.39 | -3.35 | -3.35 |
| 8=25 | P-Z | -3.57 | -1.72 | -2.21 | -2.21 |
| 9=24 | Z-P | -3.59 | -3.46 | -3.49 | -2.77 |
| 10=23 | Z-P | -3.21 | -3.35 | -3.33 | -3.33 |
| 11=22 | Z-P | -2.44 | -2.26 | -2.26 | -2.25 |
| Shift |      | 0.5 | 5   | 25  | 50  |
| 5=28/6=27 | TP/ZA | 0.60 | 0.60 | 0.59 | 0.59 |
| 6=27/7=26 | PP/ZZ | 0.56 | 0.56 | 0.57 | 0.57 |
| 7=26/8=25 | PP/ZZ | 1.02 | 1.26 | 1.17 | 1.16 |
| 8=25/9=24 | PZ/PZ | -0.01 | -0.17 | -0.10 | -0.04 |
| 9=24/10=23 | ZZ/PP | -1.00 | -0.98 | -1.02 | -1.09 |
| 10=23/11=22 | ZZ/PP | -0.54 | -0.58 | -0.58 | -0.57 |
|       |       |       |       |       |
|-------|-------|-------|-------|-------|
| 11=22/12=21 | ZA/TP | -0.61 | -0.59 | -0.59 | -0.59 |
| Slide |       |       |       |       |       |
| 5=28/6=27 | TP/ZA | -1.73 | -1.72 | -1.72 | -1.72 |
| 6=27/7=26 | PP/ZZ | -1.99 | -1.98 | -1.99 | -1.98 |
| 7=26/8=25 | PP/ZZ | -2.46 | -2.64 | -2.55 | -2.55 |
| 8=25/9=24 | PZ/PZ | -2.83 | -2.98 | -2.88 | -2.86 |
| 9=24/10=23 | ZZ/PP | -2.36 | -2.40 | -2.42 | -2.48 |
| 10=23/11=22 | ZZ/PP | -1.96 | -1.98 | -1.98 | -1.98 |
| 11=22/12=21 | ZA/TP | -1.68 | -1.72 | -1.72 | -1.72 |
| Rise |       |       |       |       |       |
| 5=28/6=27 | TP/ZA | 3.77  | 3.77  | 3.77  | 3.77  |
| 6=27/7=26 | PP/ZZ | 3.32  | 3.33  | 3.33  | 3.33  |
| 7=26/8=25 | PP/ZZ | 3.46  | 3.46  | 3.45  | 3.45  |
| 8=25/9=24 | PZ/PZ | 3.31  | 3.30  | 3.30  | 3.29  |
| 9=24/10=23 | ZZ/PP | 3.44  | 3.44  | 3.45  | 3.45  |
| 10=23/11=22 | ZZ/PP | 3.36  | 3.33  | 3.33  | 3.33  |
| 11=22/12=21 | ZA/TP | 3.77  | 3.78  | 3.78  | 3.78  |
| Tilt |       |       |       |       |       |
| 5=28/6=27 | TP/ZA | 1.56  | 1.63  | 1.66  | 1.68  |
| 6=27/7=26 | PP/ZZ | -0.19 | -0.11 | -0.07 | -0.05 |
| 7=26/8=25 | PP/ZZ | 1.57  | 0.80  | 1.15  | 1.19  |
| 8=25/9=24 | PZ/PZ | 0.00  | 0.58  | 0.21  | 0.15  |
| 9=24/10=23 | ZZ/PP | -1.30 | -1.18 | -1.44 | -1.31 |
| 10=23/11=22 | ZZ/PP | -0.05 | 0.06  | 0.03  | 0.04  |
| 11=22/12=21 | ZA/TP | -1.56 | -1.59 | -1.60 | -1.63 |
| Roll |       |       |       |       |       |
| 5=28/6=27 | TP/ZA | 5.38  | 5.36  | 5.30  | 5.33  |
| 6=27/7=26 | PP/ZZ | 5.24  | 5.08  | 5.14  | 5.16  |
| 7=26/8=25 | PP/ZZ | 3.92  | 2.91  | 3.55  | 3.60  |
| 8=25/9=24 | PZ/PZ | 2.76  | 3.67  | 3.19  | 3.24  |
| 9=24/10=23 | ZZ/PP | 4.48  | 3.85  | 4.01  | 3.81  |
| 10=23/11=22 | ZZ/PP | 5.08  | 5.18  | 5.22  | 5.22  |
| 11=22/12=21 | ZA/TP | 5.20  | 5.38  | 5.40  | 5.39  |
| Twist |       |       |       |       |       |
| 5=28/6=27 | TP/ZA | 28.62 | 28.74 | 28.75 | 28.76 |
| 6=27/7=26 | PP/ZZ | 26.60 | 26.52 | 26.43 | 26.41 |
| 7=26/8=25 | PP/ZZ | 24.27 | 21.91 | 22.70 | 22.65 |
| 8=25/9=24 | PZ/PZ | 21.35 | 19.91 | 21.11 | 21.63 |
| 9=24/10=23 | ZZ/PP | 24.31 | 24.60 | 24.24 | 23.45 |
| 10=23/11=22 | ZZ/PP | 26.85 | 26.33 | 26.35 | 26.36 |
| 11=22/12=21 | ZA/TP | 28.28 | 28.81 | 28.79 | 28.80 |
|       |       | 0.5 | 5   | 25   | 50  |
|-------|-------|-----|-----|------|-----|
| H-Rise |       |     |     |      |     |
| 5=28/6=27 | TP/ZA | 3.31 | 3.31 | 3.31 | 3.31 |
| 6=27/7=26 | PP/ZZ | 2.82 | 2.84 | 2.84 | 2.84 |
| 7=26/8=25 | PP/ZZ | 3.01 | 2.96 | 2.99 | 2.97 |
| 8=25/9=24 | PZ/PZ | 3.16 | 3.14 | 3.13 | 3.11 |
| 9=24/10=23 | ZZ/PP | 2.94 | 2.98 | 2.99 | 2.98 |
| 10=23/11=22 | ZZ/PP | 2.88 | 2.83 | 2.83 | 2.83 |
| 11=22/12=21 | ZA/TP | 3.32 | 3.32 | 3.32 | 3.32 |

| Inclination |       |     |     |      |     |
|-------------|-------|-----|-----|------|-----|
| 5=28/6=27 | TP/ZA | 10.57 | 10.49 | 10.37 | 10.43 |
| 6=27/7=26 | PP/ZZ | 11.23 | 10.89 | 11.02 | 11.08 |
| 7=26/8=25 | PP/ZZ | 8.95 | 8.93 | 9.01 | 9.21 |
| 8=25/9=24 | PZ/PZ | 2.59 | 2.09 | 2.73 | 2.98 |
| 9=24/10=23 | ZZ/PP | 10.11 | 8.94 | 8.94 | 9.16 |
| 10=23/11=22 | ZZ/PP | 10.76 | 11.14 | 11.21 | 11.20 |
| 11=22/12=21 | ZA/TP | 10.30 | 10.52 | 10.56 | 10.53 |

| Tip |       | 0.5 | 5   | 25   | 50  |
|-----|-------|-----|-----|------|-----|
| 5=28/6=27 | TP/ZA | -3.12 | -3.26 | -3.32 | -3.34 |
| 6=27/7=26 | PP/ZZ | 0.00 | -0.23 | -0.37 | -0.42 |
| 7=26/8=25 | PP/ZZ | -5.10 | -4.87 | -5.07 | -5.02 |
| 8=25/9=24 | PZ/PZ | -0.03 | -0.10 | -0.06 | -0.05 |
| 9=24/10=23 | ZZ/PP | 4.34 | 3.92 | 4.47 | 4.70 |
| 10=23/11=22 | ZZ/PP | 0.56 | 0.39 | 0.47 | 0.44 |
| 11=22/12=21 | ZA/TP | 3.13 | 3.17 | 3.20 | 3.24 |

| H-Twist |       | 0.5 | 5   | 25   | 50  |
|---------|-------|-----|-----|------|-----|
| 5=28/6=27 | TP/ZA | 30.19 | 30.30 | 30.32 | 30.33 |
| 6=27/7=26 | PP/ZZ | 28.08 | 28.01 | 27.95 | 27.94 |
| 7=26/8=25 | PP/ZZ | 26.34 | 23.76 | 24.64 | 24.58 |
| 8=25/9=24 | PZ/PZ | 21.70 | 20.24 | 21.53 | 22.11 |
| 9=24/10=23 | ZZ/PP | 26.42 | 26.52 | 26.30 | 25.42 |
| 10=23/11=22 | ZZ/PP | 28.31 | 27.85 | 27.89 | 27.90 |
| 11=22/12=21 | ZA/TP | 29.82 | 30.37 | 30.36 | 30.37 |

| Major_Groove_Refined |       | 0.5 | 5   | 25   | 50  |
|-----------------------|-------|-----|-----|------|-----|
| TP/ZA | 21.5 | 21.4 | 21.4 | 21.4 |
| PP/ZZ | 23.6 | 23.5 | 23.5 | 23.5 |
| PZ/PZ | 26.8 | 26.8 | 26.7 | 26.7 |
| ZZ/PP | 26.9 | 26.9 | 26.9 | 26.8 |
| ZA/TP | 23.6 | 23.5 | 23.5 | 23.5 |

| Minor_Groove_Refined |       | 0.5 | 5   | 25   | 50  |
|----------------------|-------|-----|-----|------|-----|
| TP/ZA | 13.4 | 13.4 | 13.4 | 13.4 |
| Pair       | 0.5   | 5    | 25   | 50   |
|------------|-------|------|------|------|
| **Major Groove Unrefined** |       |      |      |      |
| TP/ZA      | 22.4  | 22.3 | 22.3 | 22.3 |
| PP/ZZ      | 24.5  | 24.7 | 24.6 | 24.6 |
| PP/ZZ      | 28.3  | 28.8 | 28.5 | 28.5 |
| PZ/PZ      | 29.5  | 30.0 | 29.7 | 29.8 |
| ZZ/PP      | 28.1  | 28.5 | 28.4 | 28.4 |
| ZZ/PP      | 24.4  | 24.5 | 24.4 | 24.5 |

| **Minor Groove Unrefined** |       |      |      |      |
| TP/ZA      | 14.3  | 14.4 | 14.3 | 14.3 |
| PP/ZZ      | 15.0  | 15.1 | 15.0 | 15.0 |
| PP/ZZ      | 14.7  | 14.7 | 14.7 | 14.7 |
| PZ/PZ      | 14.1  | 14.1 | 14.1 | 14.1 |
| ZZ/PP      | 14.7  | 14.8 | 14.7 | 14.7 |
| ZZ/PP      | 14.9  | 15.0 | 15.0 | 15.0 |
| ZA/TP      | 14.2  | 14.3 | 14.3 | 14.3 |
**Table S3.** Confidence intervals for selected helical parameters of the PZ-containing oligonucleotide.

**Average values of local parameters**

| Shear | Average | SEM  | Interval |
|-------|---------|------|----------|
|       |         |      |          |
| 1=32  | C-G     | 0.02 | 0.04     | 0.077    |
| 2=31  | T-A     | 0.02 | 0.01     | 0.021    |
| 3=30  | T-A     | 0.01 | 0.01     | 0.022    |
| 4=29  | A-T     | 0.00 | 0.00     | 0.001    |
| 5=28  | T-A     | -0.03| 0.00     | 0.001    |
| 6=27  | P-Z     | -0.05| 0.00     | 0.001    |
| 7=26  | P-Z     | -0.04| 0.00     | 0.002    |
| 8=25  | P-Z     | -0.22| 0.09     | 0.170    |
| 9=24  | Z-P     | 0.10 | 0.07     | 0.143    |
| 10=23 | Z-P     | 0.04 | 0.00     | 0.002    |
| 11=22 | Z-P     | 0.06 | 0.00     | 0.003    |
| 12=21 | A-T     | 0.03 | 0.00     | 0.001    |
| 13=20 | T-A     | 0.00 | 0.00     | 0.001    |
| 14=19 | A-T     | 0.00 | 0.02     | 0.033    |
| 15=18 | A-T     | -0.03| 0.02     | 0.041    |
| 16=17 | G-C     | -0.09| 0.05     | 0.089    |
|       |         |      |          |
| 1=32  | C-G     | -0.37| 0.06     | 0.117    |
| 2=31  | T-A     | -0.06| 0.03     | 0.058    |
| 3=30  | T-A     | -0.02| 0.01     | 0.025    |
| 4=29  | A-T     | 0.01 | 0.00     | 0.000    |
| 5=28  | T-A     | 0.02 | 0.00     | 0.000    |
| 6=27  | P-Z     | -0.04| 0.00     | 0.001    |
| 7=26  | P-Z     | -0.03| 0.00     | 0.001    |
| 8=25  | P-Z     | -0.05| 0.01     | 0.017    |
| 9=24  | Z-P     | -0.04| 0.00     | 0.006    |
| 10=23 | Z-P     | -0.03| 0.00     | 0.001    |
| 11=22 | Z-P     | -0.04| 0.00     | 0.001    |
| 12=21 | A-T     | 0.02 | 0.00     | 0.000    |
| 13=20 | T-A     | 0.01 | 0.00     | 0.000    |
| 14=19 | A-T     | 0.01 | 0.03     | 0.063    |
| 15=18 | A-T     | -0.03| 0.06     | 0.110    |
| 16=17 | G-C     | 0.24 | 0.07     | 0.130    |
|       |         |      |          |
| 1=32  | C-G     | 0.18 | 0.04     | 0.071    |
| 2=31  | T-A     | 0.14 | 0.02     | 0.030    |
| 3=30  | T-A     | -0.18| 0.01     | 0.015    |
| 4=29  | A-T     | -0.05| 0.00     | 0.002    |
| 5=28  | T-A     | -0.08| 0.00     | 0.002    |
| 6=27  | P-Z     | -0.24| 0.00     | 0.002    |
|    | Column   | Column1 | Column2 | Column3 |
|----|----------|---------|---------|---------|
| 7  | P-Z      | -0.11   | 0.00    | 0.005   |
| 8  | P-Z      | -0.21   | 0.01    | 0.016   |
| 9  | Z-P      | -0.21   | 0.01    | 0.013   |
| 10 | Z-P      | -0.11   | 0.00    | 0.004   |
| 11 | Z-P      | -0.24   | 0.00    | 0.002   |
| 12 | A-T      | -0.09   | 0.00    | 0.002   |
| 13 | T-A      | -0.06   | 0.00    | 0.003   |
| 14 | A-T      | -0.22   | 0.03    | 0.066   |
| 15 | A-T      | 0.13    | 0.04    | 0.080   |
| 16 | G-C      | 0.08    | 0.06    | 0.111   |

Buckle
|    | Column   | Column1 | Column2 | Column3 |
|----|----------|---------|---------|---------|
| 1  | C-G      | -1.32   | 0.23    | 0.453   |
| 2  | T-A      | -4.69   | 0.07    | 0.136   |
| 3  | T-A      | -0.44   | 0.13    | 0.260   |
| 4  | A-T      | -7.71   | 0.07    | 0.134   |
| 5  | T-A      | 9.73    | 0.02    | 0.046   |
| 6  | P-Z      | -6.20   | 0.06    | 0.126   |
| 7  | P-Z      | -3.71   | 0.04    | 0.081   |
| 8  | P-Z      | -3.13   | 0.14    | 0.273   |
| 9  | Z-P      | 3.13    | 0.09    | 0.185   |
| 10 | Z-P      | 3.70    | 0.04    | 0.070   |
| 11 | Z-P      | 6.29    | 0.07    | 0.134   |
| 12 | A-T      | -9.95   | 0.03    | 0.058   |
| 13 | T-A      | 7.14    | 0.09    | 0.170   |
| 14 | A-T      | 0.72    | 0.23    | 0.448   |
| 15 | A-T      | 5.42    | 0.21    | 0.419   |
| 16 | G-C      | 0.69    | 0.16    | 0.323   |

Propeller
|    | Column   | Column1 | Column2 | Column3 |
|----|----------|---------|---------|---------|
| 1  | C-G      | -10.51  | 0.28    | 0.542   |
| 2  | T-A      | -12.59  | 0.14    | 0.266   |
| 3  | T-A      | -11.34  | 0.06    | 0.125   |
| 4  | A-T      | -6.97   | 0.06    | 0.116   |
| 5  | T-A      | -8.40   | 0.05    | 0.098   |
| 6  | P-Z      | -6.70   | 0.02    | 0.045   |
| 7  | P-Z      | -3.31   | 0.05    | 0.094   |
| 8  | P-Z      | 0.51    | 0.32    | 0.634   |
| 9  | Z-P      | -0.03   | 0.32    | 0.620   |
| 10 | Z-P      | -3.32   | 0.05    | 0.101   |
| 11 | Z-P      | -6.69   | 0.03    | 0.051   |
| 12 | A-T      | -8.62   | 0.06    | 0.119   |
| 13 | T-A      | -7.02   | 0.09    | 0.176   |
| 14 | A-T      | -10.25  | 0.24    | 0.478   |
| 15 | A-T      | -12.49  | 0.20    | 0.393   |
| 16 | G-C      | -11.71  | 0.27    | 0.534   |
| Opening | 1=32 | C-G | 0.26 | 0.50 | 0.987 |
|---------|------|-----|------|------|-------|
|         | 2=31 | T-A | 0.45 | 0.08 | 0.164 |
|         | 3=30 | T-A | 0.61 | 0.22 | 0.429 |
|         | 4=29 | A-T | 0.73 | 0.01 | 0.023 |
|         | 5=28 | T-A | -0.14| 0.01 | 0.025 |
|         | 6=27 | P-Z | -2.28| 0.01 | 0.019 |
|         | 7=26 | P-Z | -3.35| 0.01 | 0.018 |
|         | 8=25 | P-Z | -2.21| 0.55 | 1.070 |
|         | 9=24 | Z-P | -2.77| 0.48 | 0.941 |
|         | 10=23| Z-P | -3.33| 0.01 | 0.018 |
|         | 11=22| Z-P | -2.25| 0.01 | 0.029 |
|         | 12=21| A-T | -0.12| 0.01 | 0.027 |
|         | 13=20| T-A | 0.62 | 0.01 | 0.029 |
|         | 14=19| A-T | 0.53 | 0.30 | 0.583 |
|         | 15=18| A-T | 1.22 | 0.45 | 0.880 |
|         | 16=17| G-C | -7.88| 0.98 | 1.923 |

**Average values of dinucleotide step parameters**

| Shift   | Average | SEM  | Interval |
|---------|---------|------|----------|
| 1=32/2=31 | CT/AG  | 0.09 | 0.02     | 0.03 |
| 2=31/3=30 | TT/AA  | 0.14 | 0.01     | 0.01 |
| 3=30/4=29 | TA/TA  | 0.06 | 0.02     | 0.04 |
| 4=29/5=28 | AT/AT  | 0.06 | 0.00     | 0.00 |
| 5=28/6=27 | TP/ZA  | 0.59 | 0.00     | 0.00 |
| 6=27/7=26 | PP/ZZ  | 0.57 | 0.00     | 0.01 |
| 7=26/8=25 | PP/ZZ  | 1.16 | 0.05     | 0.10 |
| 8=25/9=24 | PZ/PZ  | -0.04| 0.05     | 0.09 |
| 9=24/10=23| ZZ/PP  | -1.09| 0.05     | 0.09 |
| 10=23/11=22| ZZ/PP | -0.57| 0.00     | 0.01 |
| 11=22/12=21| ZZ/PP | -1.09| 0.00     | 0.00 |
| 12=21/13=20| AT/AT | -0.09| 0.00     | 0.00 |
| 13=20/14=19| TA/TA | 0.03 | 0.04     | 0.08 |
| 14=19/15=18| AA/TT | -0.17| 0.02     | 0.04 |
| 15=18/16=17| AG/CT | -0.04| 0.02     | 0.05 |

**Slide**

| Shift   | Average | SEM  | Interval |
|---------|---------|------|----------|
| 1=32/2=31 | CT/AG  | -0.77| 0.02     | 0.05 |
| 3=30/4=29 | TA/TA  | -0.21| 0.01     | 0.01 |
| 4=29/5=28 | AT/AT  | -0.68| 0.00     | 0.00 |
| 5=28/6=27 | TP/ZA  | -1.72| 0.00     | 0.00 |
| 6=27/7=26 | PP/ZZ  | -1.98| 0.00     | 0.00 |
| 7=26/8=25 | PP/ZZ  | -2.55| 0.05     | 0.09 |
| 8=25/9=24 | PZ/PZ  | -2.86| 0.03     | 0.07 |
| 9=24/10=23| ZZ/PP  | -2.48| 0.04     | 0.08 |
| Position | Sequence | Rise   | Tilt   | Roll   |
|----------|----------|--------|--------|--------|
| 10=23/11=22 | ZZ/PP  | -1.98  | 0.00  | 0.00  |
| 11=22/12=21 | ZA/TP  | -1.72  | 0.00  | 0.01  |
| 12=21/13=20 | AT/AT  | -0.68  | 0.00  | 0.00  |
| 13=20/14=19 | TA/TA  | -0.14  | 0.02  | 0.03  |
| 14=19/15=18 | AA/TT  | -0.31  | 0.03  | 0.05  |
| 15=18/16=17 | AG/CT  | -1.02  | 0.03  | 0.07  |
| 1=32/2=31   | CT/AG   | 3.22   | 0.05  | 0.10  |
| 2=31/3=30   | TT/AA   | 3.24   | 0.01  | 0.01  |
| 3=30/4=29   | TA/TA   | 3.48   | 0.02  | 0.04  |
| 4=29/5=28   | AT/AT   | 3.00   | 0.00  | 0.00  |
| 5=28/6=27   | TP/ZA   | 3.77   | 0.00  | 0.00  |
| 6=27/7=26   | PP/ZZ   | 3.33   | 0.00  | 0.00  |
| 7=26/8=25   | PP/ZZ   | 3.45   | 0.01  | 0.01  |
| 8=25/9=24   | PZ/PZ   | 3.29   | 0.01  | 0.02  |
| 9=24/10=23  | ZZ/PP   | 3.45   | 0.00  | 0.01  |
| 10=23/11=22 | ZZ/PP   | 3.33   | 0.00  | 0.00  |
| 11=22/12=21 | ZA/TP   | 3.78   | 0.00  | 0.00  |
| 12=21/13=20 | AT/AT   | 3.00   | 0.00  | 0.00  |
| 13=20/14=19 | TA/TA   | 3.48   | 0.02  | 0.05  |
| 14=19/15=18 | AA/TT   | 3.23   | 0.03  | 0.06  |
| 15=18/16=17 | AG/CT   | 3.23   | 0.05  | 0.10  |
| 1=32/2=31   | CT/AG   | 0.75   | 0.26  | 0.51  |
| 2=31/3=30   | TT/AA   | 1.93   | 0.27  | 0.52  |
| 3=30/4=29   | TA/TA   | -0.83  | 0.37  | 0.73  |
| 4=29/5=28   | AT/AT   | -0.04  | 0.01  | 0.02  |
| 5=28/6=27   | TP/ZA   | 1.68   | 0.01  | 0.02  |
| 6=27/7=26   | PP/ZZ   | -0.05  | 0.02  | 0.05  |
| 7=26/8=25   | PP/ZZ   | 1.19   | 0.13  | 0.25  |
| 8=25/9=24   | PZ/PZ   | 0.147  | 0.06  | 0.11  |
| 9=24/10=23  | ZZ/PP   | -1.31  | 0.10  | 0.20  |
| 10=23/11=22 | ZZ/PP   | 0.04   | 0.02  | 0.04  |
| 11=22/12=21 | ZA/TP   | -1.63  | 0.01  | 0.02  |
| 12=21/13=20 | AT/AT   | 0.07   | 0.01  | 0.03  |
| 13=20/14=19 | TA/TA   | 1.63   | 0.23  | 0.45  |
| 14=19/15=18 | AA/TT   | -2.64  | 0.31  | 0.62  |
| 15=18/16=17 | AG/CT   | -0.56  | 0.28  | 0.55  |
### Average values of helix parameters

| H-Rise          | Pairing          | H-Rise | Stagger | Skew   |
|-----------------|------------------|--------|---------|--------|
| 1=32/2=31       | CT/AG            | 3.13   | 0.05    | 0.10   |
| 2=31/3=30       | TT/AA            | 3.17   | 0.01    | 0.02   |
| 3=30/4=29       | TA/TA            | 3.25   | 0.02    | 0.03   |
| 4=29/5=28       | AT/AT            | 2.90   | 0.00    | 0.00   |
| 5=28/6=27       | TP/ZA            | 3.31   | 0.00    | 0.00   |
| 6=27/7=26       | PP/ZZ            | 2.84   | 0.00    | 0.01   |
| 7=26/8=25       | PP/ZZ            | 2.97   | 0.01    | 0.02   |
| 8=25/9=24       | PZ/PZ            | 3.11   | 0.02    | 0.04   |
| 9=24/10=23      | ZZ/PP            | 2.98   | 0.01    | 0.02   |
| 10=23/11=22     | ZZ/PP            | 2.83   | 0.00    | 0.01   |
| 11=22/12=21     | ZA/TP            | 3.32   | 0.00    | 0.00   |
| 12=21/13=20     | AT/AT            | 2.91   | 0.00    | 0.00   |
| 13=20/14=19     | TA/TA            | 3.28   | 0.02    | 0.03   |
| 14=19/15=18     | AA/TT            | 3.15   | 0.03    | 0.05   |
| 15=18/16=17     | AG/CT            | 3.08   | 0.05    | 0.10   |
| Inclination | Tip | H-Twist |
|------------|-----|---------|
| 1=32/2=31  | CT/AG | 1.52    |
| 2=31/3=30  | TT/AA | 0.13    |
| 3=30/4=29  | TA/TA | 9.35    |
| 4=29/5=28  | AT/AT | 3.01    |
| 5=28/6=27  | TP/ZA | 10.43   |
| 6=27/7=26  | PP/ZZ | 11.08   |
| 7=26/8=25  | PP/ZZ | 9.21    |
| 8=25/9=24  | PZ/PZ | 2.98    |
| 9=24/10=23 | ZZ/PP | 9.16    |
| 10=23/11=22| ZZ/PP | 11.20   |
| 11=22/12=21| ZA/TP | 10.53   |
| 12=21/13=20| AT/AT | 2.86    |
| 13=20/14=19| TA/TA | 8.81    |
| 14=19/15=18| AA/TT | 1.22    |
| 15=18/16=17| AG/CT | 2.16    |
| 1=32/2=31  | -1.71 | 0.24    |
| 2=31/3=30  | -3.52 | 0.23    |
| 3=30/4=29  | 1.94  | 0.15    |
| 4=29/5=28  | 0.04  | 0.02    |
| 5=28/6=27  | -3.34 | 0.02    |
| 6=27/7=26  | -0.42 | 0.05    |
| 7=26/8=25  | -5.02 | 0.15    |
| 8=25/9=24  | -0.05 | 0.04    |
| 9=24/10=23 | 4.70  | 0.14    |
| 10=23/11=22| 0.44  | 0.05    |
| 11=22/12=21| 3.24  | 0.02    |
| 12=21/13=20| -0.10 | 0.03    |
| 13=20/14=19| -2.27 | 0.17    |
| 14=19/15=18| 4.04  | 0.24    |
| 15=18/16=17| 1.70  | 0.15    |
| 1=32/2=31  | 33.47 | 0.51    |
| 2=31/3=30  | 35.02 | 0.10    |
| 3=30/4=29  | 35.59 | 0.18    |
| 4=29/5=28  | 31.86 | 0.03    |
| 5=28/6=27  | 30.33 | 0.02    |
| 6=27/7=26  | 27.94 | 0.03    |
| 7=26/8=25  | 24.58 | 0.66    |
| 8=25/9=24  | 22.11 | 0.58    |
| 9=24/10=23 | 25.42 | 0.59    |
| 10=23/11=22| 27.90 | 0.03    |
| 11=22/12=21| 30.37 | 0.02    |
| 12=21/13=20| 31.93 | 0.03    |
|       | AT/TA | TA/TA | AA/TT | AG/CT |
|-------|-------|-------|-------|-------|
| 13=20/14=19 | 35.67 | 0.29  | 0.57  |       |
| 14=19/15=18 | 34.39 | 0.24  | 0.47  |       |
| 15=18/16=17 | 39.01 | 0.70  | 1.38  |       |

### Average values of groove widths

#### Major_Groove_Refined

|       | AT/AT | TP/ZA | PP/ZZ | PP/ZZ | PZ/PZ | ZZ/PP | ZZ/PP | ZA/TP |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| AT/AT | 20.4  | 0.02  | 0.04  |       |       |       |       |       |
| TP/ZA | 21.4  | 0.02  | 0.04  |       |       |       |       |       |
| PP/ZZ | 23.5  | 0.02  | 0.04  |       |       |       |       |       |
| PP/ZZ | 26.7  | 0.04  | 0.07  |       |       |       |       |       |
| PZ/PZ | 26.8  | 0.03  | 0.05  |       |       |       |       |       |
| ZZ/PP | 26.6  | 0.04  | 0.08  |       |       |       |       |       |
| ZZ/PP | 23.5  | 0.02  | 0.04  |       |       |       |       |       |
| ZA/TP | 21.3  | 0.03  | 0.05  |       |       |       |       |       |
| AT/AT | 20.4  | 0.04  | 0.08  |       |       |       |       |       |

#### Minor_Groove_Refined

|       | AT/AT | TP/ZA | PP/ZZ | PP/ZZ | PZ/PZ | ZZ/PP | ZZ/PP | ZA/TP |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| AT/AT | 12.9  | 0.01  | 0.02  |       |       |       |       |       |
| TP/ZA | 13.4  | 0.01  | 0.02  |       |       |       |       |       |
| PP/ZZ | 14.2  | 0.01  | 0.01  |       |       |       |       |       |
| PP/ZZ | 14.0  | 0.01  | 0.02  |       |       |       |       |       |
| PZ/PZ | 13.4  | 0.02  | 0.03  |       |       |       |       |       |
| ZZ/PP | 14.0  | 0.01  | 0.02  |       |       |       |       |       |
| ZZ/PP | 14.1  | 0.01  | 0.01  |       |       |       |       |       |
| ZA/TP | 13.4  | 0.01  | 0.02  |       |       |       |       |       |
| AT/AT | 12.9  | 0.01  | 0.03  |       |       |       |       |       |

#### Major_Groove_Unrefined

|       | AT/AT | TP/ZA | PP/ZZ | PP/ZZ | PZ/PZ | ZZ/PP | ZZ/PP | ZA/TP |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| TA/TA | 19.7  | 0.02  | 0.03  |       |       |       |       |       |
| AT/AT | 21.1  | 0.01  | 0.03  |       |       |       |       |       |
| TP/ZA | 22.3  | 0.02  | 0.03  |       |       |       |       |       |
| PP/ZZ | 24.6  | 0.05  | 0.10  |       |       |       |       |       |
| PP/ZZ | 28.5  | 0.07  | 0.14  |       |       |       |       |       |
| PZ/PZ | 29.8  | 0.06  | 0.12  |       |       |       |       |       |
| ZZ/PP | 28.4  | 0.07  | 0.13  |       |       |       |       |       |
| ZZ/PP | 24.5  | 0.05  | 0.09  |       |       |       |       |       |
| ZA/TP | 22.2  | 0.02  | 0.04  |       |       |       |       |       |
| AT/AT | 21.1  | 0.02  | 0.04  |       |       |       |       |       |
| TA/TA | 19.7  | 0.02  | 0.05  |       |       |       |       |       |

#### Minor_Groove_Unrefined

|       | AT/AT | TP/ZA | PP/ZZ | PP/ZZ |
|-------|-------|-------|-------|-------|
| TA/TA | 13.2  | 0.01  | 0.02  |       |
| AT/AT | 13.6  | 0.01  | 0.02  |       |
| TP/ZA | 14.3  | 0.01  | 0.02  |       |
| PP/ZZ | 15.0  | 0.01  | 0.01  |       |
| PP/ZZ | 14.7  | 0.01  | 0.02  |       |
### Table S4: Statistical Agreement for GC parameters

|        | Pasi et. al. | Our Work         |
|--------|--------------|------------------|
| **Mean** |              |                  |
| **Shift** | 0            | 0.03969±0.00035  |
| **Slide** | -0.9         | -1.12290±0.00036 |
| **Rise**  | 3.4          | 3.35531±0.000089 |
| **Tilt**  | 0            | 0.2169±0.0011    |
| **Roll**  | 0            | 4.3210±0.0019    |
| **Twist** | 35           | 31.2487±0.0026   |
| **Σ**    |              |                  |
| **Shift** | 0.6          | 0.6118±0.0015    |
| **Slide** | 0.5          | 0.6389±0.0024    |
| **Rise**  | 0.3          | 0.3173±0.00090   |
| **Tilt**  | 4            | 4.16333±0.0025   |
| **Roll**  | 5            | 5.1268±0.0068    |
| **Twist** | 5            | 4.662±0.031      |

The most comprehensive study on natural nucleic acid helix parameters was conducted by Pasi et. al. (Pasi, M., Maddocks, J.H., Beveridge, D., Bishop, T.C., Case, D.A., Cheatham, T.E.I., Dans, P.D., Jayaram, B., Lankas, F., Laughton, C., et al. (2014) μABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. *Nucl. Acids Res.*, **42**, 12272–12283.); they studied natural nucleic acids for a full microsecond. Our study followed the same protocols as theirs within the following exceptions: They filtered out structures in which the Watson-Crick hydrogen bonds are broken from their statistics; we performed no filtering of the data. We used a cutoff of 8.5Å for non-bonded interactions, they had 9.0Å. Our calculation ran for 50 μs whereas they ran for 1 μs. All other aspects of simulation of the GC simulations are identical to their work. We did not elect to perform the filtering of non-Watson-Crick base pairs for the sake of comparison to experiments in the future. They noted a desire to convey more numerically realistic/stable helix parameters for this filtering; we wish to compare
to experiment (and true base pairs do occasionally lose their hydrogen bonds within the helix, as rare events, albeit on the ms time scale). We believe the difference in non-bonded interaction cutoff to be trivially different. The authors did not report their SEM values, and thus we cannot perform a fair comparison of statistical agreement (we do not know their uncertainty windows). We can assume that their values are the “known” values of benchmark against which to compare (although our increased sampling might argue our numbers are a better benchmark). We opt to use a 95% confidence interval for our two-sided t-test for our 150 samples (there were 150 independent trajectories run and analyzed individually), giving t=1.96. We follow the 2 significant figure convention in intervals. I here discuss the logic of digits assigned in the main paper text. In the vast majority of cases, the precision of each number (as judged by the 95% confidence interval t-test) is far greater than the accuracy of these numbers could possibly be. Consequently, I have arbitrarily truncated all lengths to 0.01Å and 0.1 degrees. We list the full precision of our numbers here to give proper statistical due diligence, but numbers in the main text

The left-hand column gives the Watson-Crick pair as well as its rung position in the DNA helix; each rung in the helix is given twice, once for variable PZ pair, once for the control GC helix. Each table entry gives the mean value of the parameter in question as well as its standard deviation, reflecting the range of the distribution of the parameter over time. For emphasis, this is not precision error; this is the distributional variation. The precision errors are based on a 95% confidence interval with respect to the standard error of the mean; this is true for all data analyzed in this paper. In each case, the standard error of this mean is at most 1° for angular quantities and at most 0.2Å for length quantities. Additionally, we note that there is a symmetry to all data. Helix rung position 6 is equivalent to position 11, as 7 is to 10 and 8 is to 9. When discussing the data, we will restrict analysis to at most 0.2Å for length quantities. Additionally, we note that true base pairs do occasionally lose their hydrogen bonds within the helix, as rare events. For emphasis, this is trivially different.

Table S5. Comparison of all local parameters for the PZ- and GC-containing oligonucleotides.

The left-hand column gives the Watson-Crick pair as well as its rung position in the DNA helix; each rung in the helix is given twice, once for variable PZ pair, once for the control GC helix. Each table entry gives the mean value of the parameter in question as well as its standard deviation, reflecting the range of the distribution of the parameter over time. For emphasis, this is not precision error; this is the distributional variation. The precision errors are based on a 95% confidence interval with respect to the standard error of the mean; this is true for all data analyzed in this paper. In each case, the standard error of this mean is at most 1° for angular quantities and at most 0.2Å for length quantities. Additionally, we note that there is a symmetry to all data. Helix rung position 6 is equivalent to position 11, as 7 is to 10 and 8 is to 9. When discussing the data, we will restrict analysis to discussing positions 6-8 for simplicity, since the same conclusions apply to the symmetry counterparts. The fact that the calculated data matches so perfectly to even as small as ±0.1° speaks to the precision of the data due to complete phase space sampling. We emphasize that the act of reporting a mean and standard deviation is not to imply a Gaussian distribution, merely as a descriptor of the data set. It is also of interest to note that the middle values in the helix are always slower to converge than the outer rung values (i.e., position 8 converges in all parameters, not just locally, more slowly than positions 7 and 6). It is of interest to see the particular influence of the helix rung position on each nucleotide/parameter; as there are at least 5 nucleotides before the helix end, this is not interpreted to be an edge effect.

| Parameter | Shear (Å) | Stretch (Å) | Stagger (Å) | Buckle (°) | Propeller (°) | Opening (°) |
|-----------|-----------|------------|-------------|------------|--------------|-------------|
| P-Z(6)    | -0.05±0.31| -0.04±0.12 | -0.24±0.39  | -6.2±10.1  | -6.7±7.6     | -2.5±3.2    |
| G-C (6)   | -0.15±0.30| -0.07±0.11 | 0.01±0.38   | 3.5±10.0   | -5.5±7.8     | -0.5±3.1    |
| P-Z(7)    | -0.04±0.32| -0.03±0.11 | -0.11±0.37  | -3.7±9.1   | -3.3±7.7     | -3.3±3.2    |
| G-C (7)   | -0.16±0.31| -0.07±0.11 | -0.12±0.38  | -0.8±10.0  | -8.8±8.0     | 0.1±3.3     |
| P-Z(8)    | -0.22±0.59| -0.05±0.20 | -0.21±0.48  | -3.1±10.2  | -0.5±9.9     | -2.2±5.4    |
| G-C (8)   | -0.13±0.30| -0.06±0.11 | -0.13±0.36  | -4.3±10.9  | -6.2±8.0     | -0.5±3.2    |
| Z-P(9)    | 0.10±0.42 | -0.04±0.15 | -0.21±0.45  | 3.1±9.9    | 0.0±9.4      | -2.8±4.2    |
| C-G (9)   | 0.13±0.30 | -0.06±0.11 | -0.13±0.36  | 4.3±10.9   | -6.1±8.0     | -0.5±3.2    |
| Z-P(10)   | 0.04±0.32 | -0.03±0.11 | -0.11±0.37  | 3.7±9.1    | -3.3±7.7     | -3.3±3.2    |
Table S6. Comparison of all step parameters for the PZ- and GC-containing oligonucleotides.

| Parameter | Shift (Å)   | Slide (Å)   | Rise (Å)    | Tilt (°)   | Roll (°) | Twist (°) |
|-----------|-------------|-------------|-------------|------------|----------|-----------|
| TP/ZA     | 0.59±0.53   | -1.72±0.52  | 3.77±0.41   | 1.7±4.9    | 5.3±6.2  | 28.8±4.0  |
| TG/CA     | 0.17±0.67   | -0.54±0.61  | 3.25±0.35   | -0.6±4.7   | 9.6±6.4  | 30.3±5.2  |
| PP/ZZ     | 0.57±0.60   | -1.98±0.54  | 3.33±0.36   | -0.1±4.7   | 5.2±5.6  | 26.4±5.2  |
| GG/CC     | 0.23±0.67   | -1.26±0.69  | 3.46±0.32   | 0.6±4.3    | 5.2±5.3  | 30.2±5.1  |
| PP/ZZ     | 1.16±0.91   | -2.55±0.92  | 3.45±0.44   | 1.2±5.9    | 3.6±7.5  | 22.6±8.5  |
| GG/CC     | -0.11±0.61  | -1.33±0.66  | 3.42±0.33   | 0.1±4.3    | 4.9±5.1  | 30.0±4.6  |
| PZ/PZ     | -0.04±0.82  | -2.86±1.32  | 3.29±0.32   | 0.1±4.6    | 3.2±5.9  | 21.6±15.3 |
| GC/GC     | 0.00±0.55   | -0.78±0.57  | 3.19±0.30   | 0.0±3.9    | 2.9±5.0  | 33.6±4.3  |
| ZZ/PP     | -1.09±0.84  | -2.48±0.84  | 3.45±0.43   | -1.3±5.7   | 3.8±7.2  | 23.4±7.4  |
| CC/GG     | 0.11±0.61   | 1.33±0.66   | 3.42±0.33   | -0.1±4.3   | 4.9±5.1  | 30.0±4.6  |
| ZZ/PP     | -0.57±0.60  | -1.98±0.53  | 3.33±0.36   | 0.0±4.7    | 5.2±5.6  | 26.4±5.2  |
| CC/GG     | -0.23±0.67  | -1.26±0.69  | 3.46±0.32   | -0.6±4.3   | 5.2±5.3  | 30.2±5.1  |
| ZA/TP     | -0.59±0.53  | -1.72±0.52  | 3.78±0.41   | -1.6±4.9   | 5.4±6.2  | 28.8±4.1  |
| CA/TG     | -0.17±0.67  | -0.54±0.61  | 3.25±0.35   | 0.6±4.7    | 9.6±6.4  | 30.3±5.2  |

Table S7. Comparison of all helix parameters for the PZ- and GC-containing oligonucleotides.

| Parameter | H-Rise (Å) | Inclination (°) | Tip (°) | H-Twist (°) |
|-----------|------------|----------------|--------|-------------|
| TP/ZA     | 3.31±0.63  | 10.4±12.0      | -3.3±9.7 | 30.3±4.0 |
| TG/CA     | 2.83±0.50  | 17.9±12.2      | 1.1±8.6 | 32.8±4.8 |
| PP/ZZ     | 2.84±0.73  | 11.1±12.5      | -0.4±11.1 | 28.0±4.8 |
| GG/CC     | 3.12±0.49  | 10.1±10.3      | -1.1±8.3 | 31.4±4.9 |
| PP/ZZ     | 2.97±1.17  | 9.2±17.8       | -5.0±15.9 | 24.6±8.1 |
| GG/CC     | 3.09±0.47  | 9.4±9.9        | -0.2±8.2 | 31.1±4.5 |
| PZ/PZ     | 3.11±1.15  | 3.0±16.6       | 0.0±12.0 | 22.1±16.4 |
| GC/GC     | 3.08±0.36  | 5.1±8.6        | 0.0±6.8 | 34.3±4.2 |
| ZZ/PP     | 2.98±1.14  | 9.2±17.7       | 4.7±15.5 | 25.4±6.8 |
| CC/GG     | 3.09±0.47  | 9.4±9.9        | 0.2±8.2 | 31.1±4.5 |
| ZZ/PP     | 2.83±0.72  | 11.2±12.5      | 0.4±11.1 | 27.9±4.8 |
| CC/GG     | 3.12±0.49  | 10.1±10.3      | 1.1±8.3 | 31.4±4.9 |
| Parameter | Major Groove Refined (Å) | Minor Groove Refined (Å) |
|-----------|--------------------------|--------------------------|
| TP/ZA     | 21.4±2.5                 | 13.4±1.1                 |
| TG/CA     | 20.2±2.1                 | 13.7±1.0                 |
| PP/ZZ     | 23.5±2.2                 | 14.2±1.0                 |
| GG/CC     | 20.3±2.1                 | 13.4±1.0                 |
| PP/ZZ     | 26.7±1.8                 | 14.0±1.1                 |
| GG/CC     | 20.9±2.3                 | 13.0±1.1                 |
| PZ/PZ     | 26.8±1.7                 | 13.4±1.3                 |
| GC/GC     | 21.0±2.4                 | 12.9±1.1                 |
| ZZ/PP     | 26.6±1.8                 | 14.0±1.1                 |
| CC/GG     | 20.9±2.3                 | 13.0±1.1                 |
| ZZ/PP     | 23.5±2.2                 | 14.1±1.0                 |
| CC/GG     | 20.3±2.1                 | 13.4±1.0                 |
| ZA/TP     | 21.3±2.5                 | 13.4±1.1                 |
| CA/TG     | 20.2±2.1                 | 13.7±1.0                 |

**Table S8.** Comparison of all groove widths for the PZ- and GC-containing oligonucleotides.
**Figure S1.** Representative histograms for selected helical parameters for the PZ-containing (blue) and the control (red) oligonucleotide in the MD simulations. Density of state is defined as the number of structures for which the parameter falls in a defined range divided by the total number of structures sampled in each trajectory.
Opening distribution

Propeller distribution

Rise distribution

Roll distribution

Shear distribution

Shift distribution
**Figure S2.** RMSD fluctuations over a 400 ns period in the MD trajectories computed for the (top) PZ and (bottom) GC duplexes. RMSD values are computed relative to an equilibrated structure at the beginning of the production part of the simulation. These data show that there is substantial interconversion between members of the two populations observed in the bimodal distributions for slide, twist, and h-twist in PZ (see main text). In each of these plots, values for the specified parameters in the PZ helix rapidly oscillate between two extreme values rather than staying in one extreme or the other for any given length of time. The tendency of the GC-rich duplex to adopt similar conformations is also evident in these data.
Figure S3. Representative PZ and GC structures from MD simulations. Stick models are shown for ZP in an extended conformation (far left), ZP in an A-like conformation (center), and GC in a B-like conformation. Views are shown parallel (upper panels) and perpendicular (lower panels) to the helical axes.
AMBER Parameters for the Z Nucleobase

MASS
CA  12.010        0.360       same as c2
C   12.010        0.616       same as c
HA  1.008         0.135       same as hc
CT  12.010        0.878       same as c3
H1  1.008         0.135       same as hc
HC  1.008         0.135       same as hc
OS  16.000        0.465       same as os
P   30.970        1.538       same as p4
O2  16.000        0.434       Made up atom type for nitro oxygens; GAFF o parameters
NO  14.100        0.530       Pulled from GAFF atom types
OD  16.000        0.434       Made up atom type for nitro oxygens; GAFF o parameters
O   16.000        0.434       same as o
N2  14.010        0.530       same as n3
H   1.008         0.161       same as hn
NA  14.010        0.530       same as na
OH  16.000        0.465       same as oh
HO  1.008         0.135       same as ho

BOND
CA-C  449.90  1.406       same as c -c2
CA-CA  478.40  1.387       same as ca-ca
CA-CT  328.30  1.508       same as c2-c3
C -O  648.00  1.214       same as c -o
C -NA  478.20  1.345       Pulled from GAFF c-n parameters
CA-N2  449.00  1.364       same as ca-nh
CA-NA  411.10  1.391       same as c2-na
CA-NO  367.40  1.426       Pulled from GAFF cd-no parameters
CA-HA  344.30  1.087       same as c2-hc
CT-H1  337.30  1.092       same as c3-hc
CT-CT  303.10  1.535       same as c3-c3
CT-OS  301.50  1.439       same as c3-os
CT-HC  337.30  1.092       same as c3-hc
OS-P  311.60  1.636       same as os-p4
P -O2  456.40  1.503       same as o -p4
NO-OD  761.20  1.219       Pulled from GAFF no-o parameters
N2-H  394.10  1.018       same as hn-n3
NA-H  406.60  1.011       same as hn-na
P -OH  307.40  1.641       same as oh-p4
OH-HO  369.60  0.974       same as ho-ho

ANGLE
CA-C -O  72.770  119.120       same as c2-c -o
CA-C -NA  70.190  111.860       Pulled from cc-c-n parameters from GAFF
CA-CA-CA  67.180  119.970       same as ca-ca-ca
CA-CA-HA  50.300  119.700       same as c2-c2-hc
CA-CT-H1  47.030  110.490       same as c2-c3-hc
CA-CT-CT  63.530  111.440       same as c2-c3-c3
CA-CT-OS  68.450  108.480       same as c2-c3-os
C -CA-CA  67.930  120.700       same as c -c2-c2
C -CA-CT  63.870  119.700       same as c -c2-c3
C -NA-CA  65.240  124.190       Pulled from c-n-cc parameters from GAFF
C -NA-H  49.210  118.460       Pulled from c-n-hn parameters from GAFF
CA-CA-NO  65.780  128.950       Pulled from cc-cd-no parameters from GAFF
CA-N2-H  49.110  119.380       same as c2-n3-hn
CA-NA-H  47.620  119.280       same as c2-na-hn
CA-CA-N2  69.340  120.130       same as ca-ca-nh
CA-CA-NA  69.830  121.380       same as c2-c2-na
CA-NO-OD  70.340  117.520       Pulled cd-no-o parameters from GAFF
CA-CA-CT  64.330  123.420       same as c2-c2-c3
CT-CT-HC  46.370  110.050  same as c3-c3-hc
CT-CT-CT  63.210  110.630  same as c3-c3-c3
CT-OS-CT  62.390  112.450  same as c3-os-c3
H1-CT-CT  46.370  110.050  same as c3-c3-hc
H1-CT-OS  50.870  108.700  same as hc-c3-os
CT-CT-OS  67.780  108.420  same as c3-c3-os
HC-CT-HC  39.430  108.350  same as hc-c3-hc
CT-OS-P  77.590  117.480  same as c3-os-p4
OS-P -O2  43.100  116.670  same as o -p4-os
OS-P -OH  72.236  98.025  Calculated with empirical approach
H1-CT-H1  39.430  108.350  same as hc-c3-hc
OS-P -OS  44.740  100.340  same as os-p4-os
O2-P -O2  45.060  117.220  same as o -p4-o
OD-NO-OD  77.150  125.130  Pulled from o-no-o parameters from GAFF
O -C -NA  75.830  122.030  Pulled from o-c-n parameters from GAFF
N2-CA-NA  73.455  113.900  Calculated with empirical approach
H -N2-H  41.300  107.130  same as hn-n3-hn
P -OH-HO  55.270  110.190  same as ho-oh-p4
O2-P -OH  42.880  117.390  same as o -p4-oh

DIHE
CA-C -NA-CA  1  1.450  180.000  -2.000  same as X -c -na-X
CA-C -NA-CA  1  0.350  180.000  4.000  same as X -c -na-X
CA-C -NA-H  1  1.450  180.000  -2.000  same as X -c -na-X
CA-C -NA-H  1  0.350  180.000  4.000  same as X -c -na-X
CA-CA-CA-CA  1  3.625  180.000  2.000  same as X -ca-ca-X
CA-CA-CA-NO  1  4.000  180.000  2.000  Pulled from cc-cd-cd-no

GAFF param
CA-CT-CT-HC  1  0.156  0.000  3.000  same as X -c3-c3-x
CA-CT-CT-CT  1  0.156  0.000  3.000  same as X -c3-c3-x
CA-CT-OS-CT  1  0.383  0.000  3.000  same as X -c3-os-x
C -CA-CA-CA  1  6.650  180.000  2.000  same as X -c2-c2-x
C -CA-CA-HA  1  6.650  180.000  2.000  same as X -c2-c2-x
C -CA-CT-H1  1  0.000  0.000  2.000  same as X -c2-c3-x
C -CA-CT-CT  1  0.000  0.000  2.000  same as X -c2-c3-x
C -CA-CT-OS  1  0.000  0.000  2.000  same as X -c2-c3-x
C -NA-CA-CA  1  0.625  180.000  2.000  same as X -c2-na-x
C -NA-CA-N2  1  0.625  180.000  2.000  same as X -c2-na-x
CA-CA-CA-HA  1  6.650  180.000  2.000  same as X -c2-c2-x
CA-CA-NO-OD  1  0.750  180.000  2.000  Pulled from cc-cd-no-o

GAFF param
CA-NA-C -O  1  1.450  180.000  -2.000  same as X -c -na-X
CA-NA-C -O  1  0.350  180.000  4.000  same as X -c -na-X
CA-CA-N2-H  1  0.300  180.000  2.000  same as X -c2-n3-x
CA-CA-NA-H  1  0.625  180.000  2.000  same as X -c2-na-x
CA-CA-CA-CT  1  6.650  180.000  2.000  same as X -c2-c2-x
CA-CA-C -O  1  2.175  180.000  -2.000  same as c2-c2-c -o
CA-CA-C -O  1  0.300  0.000  3.000  same as c2-c2-c -o
CA-CA-C -NA  1  2.175  180.000  2.000  same as X -c -c2-x
CA-CA-CT-H1  1  0.380  180.000  -3.000  same as hc-c3-c2-c2
CA-CA-CT-H1  1  1.150  0.000  1.000  same as hc-c3-c2-c2
CA-CA-CT-CT  1  0.000  0.000  2.000  same as X -c2-c3-x
CA-CA-CT-OS  1  0.000  0.000  2.000  same as X -c2-c3-x
CA-CA-CA-N2  1  3.625  180.000  2.000  same as X -ca-ca-x
CA-CA-CA-NA  1  6.650  180.000  2.000  same as X -c2-c2-x
HA-CA-CA-CT  1  6.650  180.000  2.000  same as X -c2-c2-x
HA-CA-CA-NO  1  4.000  180.000  2.000  Pulled from ha-cd-cd-no

GAFF param
CT-CA-C -O  1  2.175  180.000  2.000  same as X -c -c2-x
CT-CA-C -NA  1  2.175  180.000  2.000  same as X -c -c2-x
CT-CT-CT-H1  1  0.160  0.000  3.000  same as hc-c3-c3-c3
CT-CT-CT-CT  1  0.180  0.000  -3.000  same as c3-c3-c3-c3
CT-CT-CT-CT 1 0.250 180.000 -2.000 same as c3-c3-c3-c3
CT-CT-CT-CT 1 0.200 180.000 1.000 same as c3-c3-c3-c3
CT-CT-CT-OS 1 0.156 0.000 3.000 same as X -c3-c3-c3
CT-OS-CT-CT 1 0.383 0.000 -3.000 same as c3-c3-os-c3
CT-OS-CT-CT 1 0.100 180.000 2.000 same as c3-c3-os-c3
CT-OS-CT-H1 1 0.383 0.000 3.000 same as X -c3-os-X
H1-CT-CT-HC 1 0.150 0.000 3.000 same as hc-c3-c3-hc
CT-CT-OS-P 1 0.383 0.000 3.000 same as X -c3-os-X
HC-CT-CT-OS 1 0.000 0.000 -3.000 same as hc-c3-c3-os
HC-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os
HC-CT-CT-CT 1 0.160 0.000 3.000 same as hc-c3-c3-c3
CT-OS-P -O2 1 1.050 180.000 2.000 same as X -os-p4-X
CT-OS-P -OH 1 1.050 180.000 2.000 same as X -os-p4-X
H1-CT-CT-H1 1 0.150 0.000 3.000 same as hc-c3-c3-hc
H1-CT-CT-OS 1 0.000 0.000 -3.000 same as hc-c3-c3-os
H1-CT-CT-OS 1 0.250 0.000 1.000 same as hc-c3-c3-os
H1-CT-OS-P 1 0.383 0.000 3.000 same as X -c3-os-X
OS-CT-CT-OS 1 0.144 0.000 -3.000 same as os-c3-c3-os
OS-CT-CT-OS 1 1.175 0.000 2.000 same as os-c3-c3-os
OS-P -OH-HO 1 0.700 0.000 1.000 same as X -oh-p4-X
CT-OS-P -OS 1 1.050 180.000 2.000 same as X -os-p4-X
NO-CA-CA-N2 1 4.000 180.000 2.000 Pulled from no-cd-cc-nh
GAFF param
NO-CA-CA-NA 1 4.000 180.000 2.000 Pulled from no-cd-cc-n
GAFF param
O -C -NA-H 1 1.450 180.000 -2.000 same as X -c -na-X
O -C -NA-H 1 0.350 180.000 4.000 same as X -c -na-X
N2-CA-NA-H 1 0.625 180.000 2.000 same as X -c2-na-X
H -N2-CA-NA 1 0.300 180.000 2.000 same as X -c2-n3-X
O2-P -OH-HO 1 0.700 0.000 1.000 same as X -oh-p4-X
IMPROPER
C -CA-CA-CT 5.6 180.0 2.0 Using default value
CA-NA-C -O 5.6 180.0 2.0 Using default value
CA-N2-CA-NA 5.6 180.0 2.0 Using default value
CA-CA-CA-NO 5.6 180.0 2.0 Using default value
CA-CA-CA-HA 5.6 180.0 2.0 Using default value
CA-H -N2-H 5.6 180.0 2.0 Using default value
C -CA-NA-H 5.6 180.0 2.0 Using default value
NONBON
CA 1.9080 0.0860 same as ca
C 1.9080 0.0860 same as c
HA 1.4870 0.0157 same as hc
CT 1.9080 0.1094 same as c3
H1 1.4870 0.0157 same as hc
HC 1.4870 0.0157 same as hc
OS 1.6837 0.1700 same as os
P 2.1000 0.2000 same as p4
O2 1.6612 0.2100 same as o
NO 1.8240 0.1700 Pulled from no GAFF parameters
OD 1.6612 0.2100 Pulled from o GAFF parameters
O 1.6612 0.2100 same as o
N2 1.8240 0.1700 same as nh
H 0.6000 0.0157 same as hn
NA 1.8240 0.1700 same as na
OH 1.7210 0.2104 same as oh
HO 0.0000 0.0000 same as ho
### AMBER Parameters for the P Nucleobase

#### MASS

| Symbol | Mass (u) | Charge | Remarks |
|--------|----------|--------|---------|
| CQ     | 12.010   | 0.360  | same as c2 |
| CB     | 12.010   | 0.360  | same as c2 |
| C      | 12.010   | 0.616  | same as c |
| CA     | 12.010   | 0.360  | same as c2 |
| H4     | 1.008    | 0.135  | same as ha |
| NC     | 14.010   | 0.530  | same as n2 |
| N*     | 14.010   | 0.530  | same as na |
| N2     | 14.010   | 0.530  | same as n3 |
| H      | 1.008    | 0.161  | same as hn |
| O      | 16.000   | 0.434  | same as o |
| CT     | 12.010   | 0.878  | same as c3 |
| H2     | 1.008    | 0.135  | same as hc |
| HC     | 1.008    | 0.135  | same as hc |
| H1     | 1.008    | 0.135  | same as hc |
| OS     | 16.000   | 0.465  | same as os |
| O2     | 16.000   | 0.434  | same as o |
| P      | 30.970   | 1.538  | same as p4 |
| OH     | 16.000   | 0.465  | same as oh |
| HO     | 1.008    | 0.135  | same as ho |

#### BOND

| Bond   | Length (Å) | Angle (°) | Remarks |
|--------|------------|-----------|---------|
| CQ-NC  | 431.60     | 1.376     | same as cc-nc |
| CQ-N2  | 449.00     | 1.364     | same as cc-nh |
| CB-NC  | 431.60     | 1.376     | same as cc-nc |
| CB-N*  | 411.10     | 1.391     | same as c2-na |
| C-NC   | 374.60     | 1.420     | same as c-n2 |
| C-N*   | 438.80     | 1.371     | my particular choice |
| C-O    | 648.00     | 1.214     | same as c-o |
| CA-H4  | 344.30     | 1.087     | same as c2-ha |
| CA-CA  | 478.40     | 1.387     | same as ca-ca |
| CA-N*  | 411.10     | 1.391     | same as c2-na |
| N*-CT  | 334.70     | 1.456     | same as c3-na |
| N2-H   | 394.10     | 1.018     | same as hn-n3 |
| CT-H2  | 337.30     | 1.092     | same as c3-hc |
| CT-CT  | 303.10     | 1.535     | same as c3-c3 |
| CT-OS  | 301.50     | 1.439     | same as c3-os |
| CT-HC  | 337.30     | 1.092     | same as c3-hc |
| CT-H1  | 337.30     | 1.092     | same as c3-hc |
| OS-P   | 311.60     | 1.636     | same as os-p4 |
| O2-P   | 456.40     | 1.503     | same as o-p4 |
| P-OH   | 307.40     | 1.641     | same as oh-p4 |
| OH-HO  | 369.60     | 0.974     | same as ho-ho |

#### ANGLE

| Angle   | Length (Å) | Remarks |
|---------|------------|---------|
| CQ-NC-CB| 70.500     | 104.340 | same as cc-nc-cc |
| CQ-NC-C | 66.220     | 120.970 | same as c-n2-c2 |
| CQ-N2-H | 49.110     | 119.380 | same as c2-n3-hn |
| CB-N*-C | 68.940     | 109.900 | Pulled from GAFF cd-na-cd parameter |
| CB-N*-CA| 67.800     | 110.370 | same as c2-na-c2 |
| CB-N*-CT| 64.230     | 117.200 | same as c2-na-c3 |
| C-N*-CA | 65.240     | 124.190 | Pulled from GAFF c-n-cc parameter |
| CA-CA-H4| 50.040     | 120.940 | same as c2-c2-ha |
| CA-CA-N*| 69.830     | 121.380 | same as c2-c2-na |
| H4-CA-N*| 51.180     | 112.420 | same as ha-c2-na |
| CA-N*-CT| 64.230     | 117.200 | same as c2-na-c3 |
| NC-CQ-NC| 69.470     | 125.580 | same as nc-cc-nc |
| NC-CQ-N2| 72.330     | 116.850 | same as nc-cc-nh |
| NC-CB-N*| 71.710     | 123.620 | same as n2-c2-na |
| NC-C-N* | 72.350     | 117.050 | Pulled from GAFF nd-c-n parameter |
| NC-C-O  | 73.020     | 122.500 | same as n2-c-o |
| Compound         | DIHE        |   |   | Same as |          |
|-----------------|-------------|---|---|---------|----------|
| N*-CB-N*        | 73.650      | 109.330 | same as na-c2-na |
| N*-C -O         | 75.830      | 122.030 | Pulled from GAFF n-c-o parameter |
| N*-CT-H2        | 49.900      | 109.500 | same as hc-c3-na |
| N*-CT-CT        | 65.730      | 112.810 | same as c3-c3-na |
| N*-CT-OS        | 71.270      | 109.060 | same as na-c3-os |
| H -N2-H         | 41.300      | 107.130 | same as hn-n3-hn |
| CT-CT-HC        | 46.370      | 110.050 | same as c3-c3-hc |
| CT-CT-CT        | 63.210      | 110.630 | same as c3-c3-c3 |
| CT-OS-CT        | 62.390      | 112.450 | same as c3-os-c3 |
| H2-CT-CT        | 46.370      | 110.050 | same as c3-c3-hc |
| H2-CT-OS        | 50.870      | 108.700 | same as hc-c3-os |
| CT-CT-OS        | 67.780      | 108.420 | same as c3-c3-os |
| CT-CT-H1        | 46.370      | 110.050 | same as c3-c3-hc |
| HC-CT-HC        | 39.430      | 108.350 | same as hc-c3-hc |
| CT-OS-P         | 77.590      | 117.480 | same as c3-os-p4 |
| H1-N-CT-OS      | 50.870      | 108.700 | same as hc-c3-os |
| OS-P -OH        | 72.236      | 98.025  | Calculated with empirical approach |
| OS-P -O2        | 43.100      | 116.670 | same as o -p4-0s |
| H1-CT-H1        | 39.430      | 108.350 | same as hc-c3-hc |
| OS-P -OS        | 44.740      | 100.340 | same as os-p4-0s |
| O2-P -O2        | 45.060      | 117.220 | same as o -p4-o |
| P -OH-HO        | 55.270      | 110.190 | same as ho-oh-p4 |
| OH-P -O2        | 42.880      | 117.390 | same as o -p4-oh |

**DIHE**

| Compound     | DIHE       |   |   | Same as |          |
|--------------|------------|---|---|---------|----------|
| CQ-NC-CB-N*  | 1 4.150    | 180.000 | 2.000 | same as X -c2-n2-X |
| CQ-NC-N*     | 1 4.150    | 180.000 | 2.000 | same as X -c -n2-X |
| CQ-NC-NC     | 1 4.150    | 180.000 | 2.000 | same as X -c -c-X |
| CB-NC-CQ-NC  | 1 4.750    | 180.000 | 2.000 | same as X -c2-c2-X |
| CB-NC-CQ-N2  | 1 4.750    | 180.000 | 2.000 | same as X -c2-c2-X |
| CB-N*-C -NC  | 1 1.450    | 180.000 | -2.000 | same as X -c -c-NX |
| CB-N*-C -NC  | 1 0.350    | 180.000 | 4.000 | same as X -c -c-NX |
| CB-N*-C -O   | 1 1.450    | 180.000 | -2.000 | same as X -c -c-NX |
| CB-N*-C -O   | 1 0.350    | 180.000 | 4.000 | same as X -c -c-NX |
| CB-N*-CA-H4  | 1 0.625    | 180.000 | 2.000 | same as X -c2-na-X |
| CB-N*-CA-CA  | 1 0.625    | 180.000 | 2.000 | same as X -c2-na-X |
| CB-N*-CT-H2  | 1 0.000    | 0.000   | 2.000 | same as X -c -c-NX |
| CB-N*-CT-CT  | 1 0.000    | 0.000   | 2.000 | same as X -c -c-NX |
| CB-N*-CT-OS  | 1 0.000    | 0.000   | -2.000 | same as os-c3-na-c2 |
| CB-N*-CT-OS  | 1 2.500    | 0.000   | 1.000 | same as os-c3-na-c2 |
| C -NC-CQ-NC  | 1 4.150    | 180.000 | 2.000 | same as X -c2-n2-X |
| C -NC-CQ-N2  | 1 4.150    | 180.000 | 2.000 | same as X -c2-n2-X |
| C -N*-CB-NC  | 1 0.625    | 180.000 | 2.000 | same as X -c2-na-X |
| C -N*-CB-N*  | 1 0.625    | 180.000 | 2.000 | same as X -c2-na-X |
| C -N*-CA-H4  | 1 0.625    | 180.000 | 2.000 | same as X -c2-na-X |
| C -N*-CA-CA  | 1 0.625    | 180.000 | 2.000 | same as X -c2-na-X |
| CA-CA-N*-CT  | 1 0.625    | 180.000 | 2.000 | same as X -c2-na-X |
| CA-N*-CB-NC  | 1 0.625    | 180.000 | 2.000 | same as X -c2-na-X |
| CA-N*-CB-N*  | 1 0.625    | 180.000 | 2.000 | same as X -c2-na-X |
| CA-N*-C -NC  | 1 1.450    | 180.000 | -2.000 | same as X -c -c-NX |
| CA-N*-C -NC  | 1 0.350    | 180.000 | 4.000 | same as X -c -c-NX |
| CA-N*-C -O   | 1 1.450    | 180.000 | -2.000 | same as X -c -c-NX |
| CA-N*-C -O   | 1 0.350    | 180.000 | 4.000 | same as X -c -c-NX |
| H4-CA-CA-H4  | 1 3.625    | 180.000 | 2.000 | same as X -c2-c2-X |
| H4-CA-CA-N*  | 1 6.650    | 180.000 | 2.000 | same as X -c2-c2-X |
| CA-N*-CT-H2  | 1 0.000    | 0.000   | 2.000 | same as X -c -c-NX |
| CA-N*-CT-CT  | 1 0.000    | 0.000   | 2.000 | same as X -c -c-NX |
| CA-N*-CT-OS  | 1 0.000    | 0.000   | -2.000 | same as os-c3-na-c2 |
| CA-N*-CT-OS  | 1 2.500    | 0.000   | 1.000 | same as os-c3-na-c2 |
| H4-CA-N*-CT  | 1 0.625    | 180.000 | 2.000 | same as X -c2-na-X |
| NC-CQ-N2-H    | 1 0.300    | 180.000 | 2.000 | same as X -c2-n3-X |
| NC-CB-N*-CT   | 1 0.625    | 180.000 | 2.000 | same as X -c2-na-X |
N*-CB-N*-CT  1  0.625  180.000  2.000  same as X -c2-na-X
N*-CA-CA-N*  1  6.650  180.000  2.000  same as X -c2-c2-X
N*-CT-CT-HC  1  0.156  0.000  3.000  same as X -c3-c3-X
N*-CT-CT-CT  1  0.156  0.000  3.000  same as X -c3-c3-X
N*-CT-OS-CT  1  0.383  0.000  -3.000  same as c3-os-c3-na
N*-CT-OS-CT  1  0.650  0.000  2.000  same as c3-os-c3-na
CT-CT-CT-H1  1  0.160  0.000  3.000  same as hc-c3-c3-c3
CT-CT-CT-CT  1  0.250  180.000  -2.000  same as c3-c3-c3-c3
CT-CT-CT-CT  1  0.200  180.000  1.000  same as c3-c3-c3-c3
CT-CT-CT-OS  1  0.156  0.000  3.000  same as X -c3-c3-X
CT-OS-CT-CT  1  0.383  0.000  -3.000  same as c3-c3-os-c3
CT-OS-CT-CT  1  0.100  180.000  2.000  same as c3-c3-os-c3
CT-OS-CT-H1  1  0.383  0.000  3.000  same as X -c3-os-X
H2-CT-CT-HC  1  0.150  0.000  3.000  same as hc-c3-c3-hc
H2-CT-CT-CT  1  0.160  0.000  3.000  same as hc-c3-c3-c3
H2-CT-OS-CT  1  0.383  0.000  3.000  same as X -c3-os-X
CT-CT-OS-P  1  0.383  0.000  3.000  same as X -c3-os-X
HC-CT-CT-OS  1  0.000  0.000  -3.000  same as hc-c3-c3-os
HC-CT-CT-OS  1  0.250  0.000  1.000  same as hc-c3-c3-os
HC-CT-CT-H1  1  0.150  0.000  3.000  same as hc-c3-c3-hc
HC-CT-CT-CT  1  0.160  0.000  3.000  same as hc-c3-c3-c3
CT-OS-P -OH  1  1.050  180.000  2.000  same as X -os-p4-X
CT-OS-P -O2  1  1.050  180.000  2.000  same as X -os-p4-X
H1-CT-CT-H1  1  0.150  0.000  3.000  same as hc-c3-c3-hc
H1-CT-CT-OS  1  0.000  0.000  -3.000  same as hc-c3-c3-os
H1-CT-CT-OS  1  0.250  0.000  1.000  same as hc-c3-c3-os
H1-CT-OS-P  1  0.383  0.000  3.000  same as X -c3-os-X
OS-CT-CT-OS  1  0.144  0.000  -3.000  same as os-c3-c3-os
OS-CT-CT-OS  1  1.175  0.000  2.000  same as os-c3-c3-os
OS-P -OH-HO  1  0.700  0.000  1.000  same as X -oh-p4-X
CT-OS-P -OS  1  1.050  180.000  2.000  same as X -os-p4-X
HO-OH-P -O2  1  0.700  0.000  1.000  same as X -oh-p4-X

IMPROPER
N2-NC-CQ-NC  5.6  180.0  2.0  Using default value
N*-NC-C -O  5.6  180.0  2.0  Using default value
CA-H4-CA-N*  5.6  180.0  2.0  Using default value
C -CA-N* -CB  5.6  180.0  2.0  Using default value
CA-CB-N*-CT  5.6  180.0  2.0  Using default value
CQ-H -N2-H  5.6  180.0  2.0  Using default value

NONBON
CQ  1.9080  0.0860  same as cc
CB  1.9080  0.0860  same as cc
C  1.9080  0.0860  same as c
CA  1.9080  0.0860  same as ca
H4  1.4870  0.0157  same as hc
NC  1.8240  0.1700  same as nc
N*  1.8240  0.1700  same as na
N2  1.8240  0.1700  same as nh
H  0.6000  0.0157  same as hn
O  1.6612  0.2100  same as o
CT  1.9080  0.1094  same as c3
H2  1.4870  0.0157  same as hc
HC  1.4870  0.0157  same as hc
H1  1.4870  0.0157  same as hc
OS  1.6837  0.1700  same as os
O2  1.6612  0.2100  same as o
P  2.1000  0.2000  same as p4
OH  1.7210  0.2104  same as oh
HO  0.0000  0.0000  same as ho
### Coordinates of the gas-phase optimized structure of a P:Z base pair

|   |   |   |   |
|---|---|---|---|
| C | 3.556037 | -5.347020 | 0.000000 |
| H | 4.260240 | -4.520289 | 0.000000 |
| N | 2.219498 | -4.786451 | 0.000000 |
| C | 1.018948 | -5.493076 | 0.000000 |
| H | 1.008113 | -6.567515 | 0.000000 |
| C | -0.012368 | -2.066098 | 0.000000 |
| O | -1.231170 | -1.998735 | 0.000000 |
| N | 0.845886 | -1.040655 | 0.000000 |
| C | 2.175471 | -1.257273 | 0.000000 |
| C | 2.549735 | 0.754435 | 0.000000 |
| H | 4.260240 | -4.520289 | 0.000000 |
| N | 2.219498 | -5.493076 | 0.000000 |
| C | 1.018948 | -6.567515 | 0.000000 |
| H | 1.008113 | -7.641954 | 0.000000 |
| C | -0.012368 | -3.146098 | 0.000000 |
| O | -1.231170 | -2.198735 | 0.000000 |
| N | 0.845886 | -3.040655 | 0.000000 |
| C | 2.175471 | -3.257273 | 0.000000 |
| C | 2.549735 | -0.754435 | 0.000000 |
| H | 4.260240 | -7.520289 | 0.000000 |
| N | 2.219498 | -6.493076 | 0.000000 |
| C | 1.018948 | -7.567515 | 0.000000 |
| H | 1.008113 | -8.641954 | 0.000000 |
| C | -0.012368 | -4.146098 | 0.000000 |
| O | -1.231170 | -3.198735 | 0.000000 |
| N | 0.845886 | -4.040655 | 0.000000 |
| C | 2.175471 | -5.257273 | 0.000000 |
| C | 2.549735 | -3.754435 | 0.000000 |
| H | 4.260240 | -8.520289 | 0.000000 |

### Coordinates of the gas-phase optimized structure of a G:C base pair

|   |   |   |   |
|---|---|---|---|
| C | 1.025032 | -5.623477 | 0.000000 |
| H | 1.648721 | -5.509622 | 0.884596 |
| N | 0.028175 | -4.633623 | 0.000000 |
| C | 1.391384 | -4.837179 | 0.000000 |
| H | 1.799593 | -5.835858 | 0.000000 |
| N | 2.078233 | -3.736467 | 0.000000 |
| C | 1.125839 | -2.741529 | 0.000000 |
| C | 1.242631 | -1.320495 | 0.000000 |
| O | 2.256522 | -0.628083 | 0.000000 |
| N | -0.014757 | -0.708730 | 0.000000 |
| H | 0.000000 | 0.320102 | 0.000000 |
| C | -1.221674 | -1.350315 | 0.000000 |
| N | -2.312530 | -0.564564 | 0.000000 |
| H | -2.256133 | 0.451173 | 0.000000 |
| H | -3.203326 | -1.025249 | 0.000000 |
| N | -1.345141 | -2.658255 | 0.000000 |
| C | -0.151276 | -3.283730 | 0.000000 |
| H | -0.572235 | -6.611744 | 0.000000 |
| H | -1.648721 | -5.509622 | -0.884596 |
### Coordinates of the gas-phase optimized structure of a P nucleobase

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | -2.626708 | -1.704608 | -0.00008 |
| H       | -1.917752 | -2.527492 | 0.000180 |
| N       | -1.867840 | -0.471772 | 0.00008  |
| C       | -2.378076 | 0.824382 | -0.000331 |
| H       | -3.437458 | 1.003780 | -0.000632 |
| C       | 1.186555  | 1.327653 | 0.000530 |
| O       | 1.416194  | 2.512318 | -0.000354 |
| N       | 2.061683  | 0.302816 | -0.000085 |
| C       | 1.622488  | -0.949269 | 0.000175 |
| N       | 2.563250  | -1.915281 | -0.000066 |
| H       | 3.529924  | -1.647884 | -0.000075 |
| H       | 2.286369  | -2.878393 | 0.000100 |
| N       | 0.341297  | -1.392758 | 0.000088 |
| C       | -0.518724 | -0.401312 | 0.000104 |
| H       | -3.251451 | -1.762793 | 0.889557 |
| H       | -3.251141 | -1.762925 | -0.889780 |
| C       | -1.342696 | 1.683145 | 0.000214 |
| H       | -1.286888 | 2.755348 | 0.000420 |
| N       | -0.192418 | 0.911550 | 0.000205 |

### Coordinates of the gas-phase optimized structure of a P nucleobase

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | 0.790830  | -0.231673 | 0.000230 |
| C       | -0.276967 | -1.171695 | 0.000214 |
| C       | -1.578813 | -0.813725 | 0.000001 |
| C       | -1.911213 | 0.598615  | -0.000171 |
| C       | 0.508828  | 1.132727  | 0.000156 |
| H       | 0.003295  | -2.215883 | 0.000328 |
| O       | -3.025361 | 1.076666  | -0.000158 |
| N       | -0.804410 | 1.470706  | -0.000282 |
| H       | -1.066161 | 2.447130  | 0.000544 |
| N       | 1.401839  | 2.129122  | 0.001091 |
| H       | 2.379078  | 1.879344  | -0.001099 |
| H       | 1.104667  | 3.087557  | -0.003837 |
| N       | 2.128976  | -0.711219 | -0.000064 |
| O       | 3.053241  | 0.104803  | -0.001169 |
| O       | 2.313162  | -1.911526 | -0.000255 |
| C       | -2.724827 | -1.772697 | 0.000081 |
| H       | -3.356623 | -1.613876 | -0.874256 |
| H       | -2.367624 | -2.799945 | 0.000407 |
| H       | -3.356831 | -1.613453 | 0.874197 |
Coordinates of the gas-phase optimized structure of a G nucleobase

|   |    x     |    y     |    z     |
|---|----------|----------|----------|
| C | -0.004890 | 3.152616 | 0.000000 |
| H | 0.616994  | 3.267289 | 0.885258 |
| N | -0.640366 | 1.853149 | 0.000000 |
| C | -1.986037 | 1.564931 | 0.000000 |
| H | -2.720822 | 2.354480 | 0.000000 |
| N | -2.239261 | 0.290866 | 0.000000 |
| C | -1.000551 | -0.303379| 0.000000 |
| C | -0.623116 | -1.687596| 0.000000 |
| O | -1.287307 | -2.695609| 0.000000 |
| N | 0.799878  | -1.795119| 0.000000 |
| H | 1.128739  | -2.749690| 0.000000 |
| C | 1.694457  | -0.765009| 0.000000 |
| N | 3.010976  | -1.094617| 0.000000 |
| H | 3.330462  | -2.043473| 0.000000 |
| H | 3.678117  | -0.345677| 0.000000 |
| N | 1.346998  | 0.490345 | 0.000000 |
| C | 0.000000  | 0.652877 | 0.000000 |
| H | -0.778775 | 3.915651 | 0.000000 |
| H | 0.616994  | 3.267289 | -0.885258|

Coordinates of the gas-phase optimized structure of a C nucleobase

|   |    x     |    y     |    z     |
|---|----------|----------|----------|
| C | 1.280266 | -0.846519| 0.000000 |
| C | 0.131913 | -1.699031| 0.000000 |
| C | -1.065814| -1.075083| 0.000000 |
| C | 0.000000 | 1.089484 | 0.000000 |
| H | 0.209748 | -2.773638| 0.000000 |
| H | -2.001018| -1.618643| 0.000000 |
| O | -0.157256| 2.292353 | 0.000000 |
| N | -1.160599| 0.268280 | 0.000000 |
| N | 1.210213 | 0.460922 | 0.000000 |
| N | 2.513847 | -1.401569| 0.000000 |
| H | 3.309949 | -0.788709| 0.000000 |
| H | 2.645915 | -2.394277| 0.000000 |
| C | -2.442011| 0.955463 | 0.000000 |
| H | -2.519557| 1.590940 | 0.879161 |
| H | -2.519557| 1.590940 | -0.879161|
| H | -3.237782| 0.215243 | 0.000000 |
Coordinates of the “shift” conformer for two stacked P:Z nucleobase pairs (Fig. 9 in the main text)

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 5.354  | 1.046  | 2.116  |
| H    | 5.217  | 1.772  | 1.304  |
| N    | 4.281  | 0.072  | 2.054  |
| C    | 4.365  | -1.310 | 2.241  |
| H    | 5.318  | -1.793 | 2.418  |
| C    | 0.864  | -0.734 | 1.679  |
| O    | 0.255  | -1.797 | 1.710  |
| N    | 0.342  | 0.485  | 1.470  |
| C    | 1.135  | 1.580  | 1.464  |
| N    | 0.539  | 2.751  | 1.254  |
| H    | -0.475 | 2.799  | 1.092  |
| H    | 1.117  | 3.576  | 1.214  |
| N    | 2.484  | 1.603  | 1.660  |
| C    | 2.982  | 0.403  | 1.854  |
| C    | -4.704 | -0.446 | 1.101  |
| C    | -5.263 | 0.851  | 0.969  |
| C    | -4.506 | 1.986  | 0.958  |
| C    | -3.071 | 1.846  | 1.063  |
| C    | -3.312 | -0.593 | 1.253  |
| H    | -6.348 | 0.904  | 0.880  |
| H    | 5.348  | 1.575  | 3.079  |
| H    | 6.308  | 0.520  | 1.993  |
| O    | -2.272 | 2.791  | 1.015  |
| N    | -2.579 | 0.557  | 1.228  |
| H    | -1.549 | 0.494  | 1.311  |
| N    | -2.643 | -1.737 | 1.411  |
| H    | -3.184 | -2.592 | 1.384  |
| H    | -1.624 | -1.748 | 1.494  |
| C    | 3.120  | -1.831 | 2.130  |
| H    | 2.737  | -2.843 | 2.175  |
| N    | 2.271  | -0.757 | 1.890  |
| N    | -5.581 | -1.571 | 1.105  |
| O    | -5.097 | -2.698 | 1.228  |
| O    | -6.780 | -1.374 | 0.992  |
| C    | -5.065 | 3.373  | 0.856  |
| H    | -4.661 | 3.901  | -0.019 |
| H    | -6.160 | 3.345  | 0.780  |
| H    | -4.786 | 3.968  | 1.738  |
| C    | 7.316  | 0.728  | -0.990 |
| H    | 6.870  | 1.728  | -0.972 |
| N    | 6.237  | -0.240 | -0.905 |
| C    | 6.365  | -1.628 | -0.794 |
| H    | 7.337  | -2.094 | -0.689 |
| C    | 2.819  | -1.113 | -1.091 |
| O    | 2.232  | -2.182 | -0.978 |
| N    | 2.263  | 0.096  | -1.272 |
| C    | 3.034  | 1.205  | -1.340 |
| N    | 2.405  | 2.356  | -1.570 |
| H    | 1.377  | 2.379  | -1.661 |
| H    | 2.959  | 3.197  | -1.613 |
| N    | 4.389  | 1.254  | -1.215 |
| C    | 4.925  | 0.064  | -1.057 |
| C    | -2.765 | -0.929 | -1.793 |
| C    | -3.328 | 0.353  | -2.032 |
| C    | -2.583 | 1.494  | -2.062 |
| C    | -1.159 | 1.384  | -1.834 |
| C    | -1.379 | -1.050 | -1.570 |
| H    | -4.408 | 0.390  | -2.182 |
| H    | 7.996  | 0.609  | -0.136 |
| H    | 7.877  | 0.599  | -1.926 |
Coordinates of the “slide” conformer for two stacked P:Z nucleobase pairs (Fig. 8 in the main text)

C  -7.26028100  0.98336400  -0.73886000
H  -6.93912900  1.78050100  -0.05920100
N  -6.08573400  0.21689600  -1.11256600
C  -6.06190600  0.97577500  -1.84199400
H  -6.97998100  1.48026200  -2.12028200
C  -2.58630300  -0.13435100  -1.45845600
O  -1.88770400  -1.02641100  -1.92336500
N  -2.16461400  1.00213400  -0.88215000
C  -3.05066600  1.87876700  -0.35958400
N  -2.54679200  2.98543600  -0.31509000
H  -1.53232000  3.16815600  -0.03322800
H  -3.19257900  3.66911800  0.54730300
N  -4.40505000  1.73731000  -0.33150900
C  -4.81079400  0.63996800  -0.93300500
C  -2.91777600  0.91941700  -1.58626100
C  -3.33192700  2.21066500  -1.15687400
C  -2.47722800  3.11427800  -0.60306900
C  -1.08949400  2.73447100  -0.44779000
C  -1.56972200  0.53754500  -1.44005700
H  -4.38847800  2.44773700  -1.28404700
H  -7.72776300  1.43305500  -1.62544500
H  -7.98532400  0.33291500  -0.23274800
O  -0.21421000  3.46663100  0.03322800
N  -7.73986600  1.46278200  -0.88076600
H  -0.26237800  1.23040800  -0.79414300
N  -1.03053800  -0.63726900  -1.76950100
H  -1.64471400  -1.32150300  -2.19226400
H  -0.02379500  -0.79508400  -1.70866900
C  -4.77054300  -1.29979800  -2.08173100
H  -4.30398500  -2.13377200  -2.59132300
H  -4.00262100  -0.29322600  -1.50721200
N  -3.88985900  0.03081000  -2.11763900
O  -3.53513100  -1.09636600  -2.48340400
O  -5.05086600  0.40597800  -2.18217100
C  -2.87504100  4.46864000  -0.10434000
H  -2.68926500  4.54297700  0.97812900
H  -3.93836600  4.65886100  -0.29896000
H  -2.27674900  5.25566600  -0.58583100
C  -5.43207100  -0.37974700  2.21993500
H  -5.19229800  0.66948500  2.00478400
N  -4.39733100  -1.21599000  1.64019400
C  -4.54486300  -2.47208000  1.04997500
H  -5.52223300  -2.92655000  0.93921600
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -1.00514200 | -1.87632200 | 0.90506100 |
| O    | -0.43977400 | -2.84028700 | 0.40397900 |
| N    | -0.43203200 | -0.74587400 | 1.34770900 |
| C    | -0.53968600 | 1.33448800 | 0.80506100 |
| H    | 0.48257800  | 1.40433000 | 0.80506100 |
| H    | -1.08210600 | 2.09360800 | 2.66632300 |
| C    | -3.08002300 | -0.89364500 | 1.64900300 |
| C    | 4.56656100  | -1.52471300 | 0.50951900 |
| C    | 5.16394300  | -0.31676200 | 1.29570000 |
| C    | 4.44801200  | 0.69641600  | 1.51825800 |
| C    | 3.01961800  | 0.52791000  | 2.65386000 |
| C    | 3.17779300  | -1.70842100 | 0.64939200 |
| H    | 6.23971100  | -0.22501000 | 1.76092700 |
| H    | -6.39256400 | -0.64478400 | 3.30691400 |
| O    | 2.25535500  | 1.39501900  | 2.10280800 |
| N    | 2.48999200  | -0.68487900 | 1.23329800 |
| H    | 1.45885600  | -0.75512800 | 1.29570000 |
| N    | 2.47280400  | -2.77631000 | 0.27300300 |
| H    | 2.98486100  | -3.51367400 | -0.19371500 |
| H    | 1.45316200  | -2.78503700 | 0.33965900 |
| C    | -3.32044500 | -2.91330000 | 0.67592200 |
| H    | -2.98061100 | -3.81355700 | 0.17941700 |
| N    | -2.42060000 | -1.92472500 | 1.05312300 |
| N    | 5.39564900  | -2.52189100 | -0.08388300 |
| O    | 4.87752300  | -3.57236100 | -0.47202000 |
| O    | 6.59248300  | -2.30441000 | -0.17352100 |
| C    | 5.03572200  | 1.99226100  | 1.98644000 |
| H    | 4.85803000  | 2.13584700  | 3.06265700 |
| H    | 6.11594400  | 2.02062700  | 1.79664400 |
| H    | 4.55723400  | 2.84080100  | 1.47462200 |
Comment on X- and Y-displacement distributions for the ZP-containing oligonucleotide. Although we find very narrowly peaked distributions for X- and Y-displacement values of the ZP-containing oligonucleotide during the trajectory (shown below), we find structures that exhibit very large values resulting from definitions of the standard helix reference frame.

The following coordinates for one structure in which the X-displacement of the central dinucleotide step is measured to be 66 Å.
| ATOM | Atom | C/ H/ O  | X | Y | Z | Temperature | Pressure | Error |
|------|------|----------|---|---|---|-------------|----------|-------|
| 01   | H    | C        | 0 | 0 | 0 | 30.820      | 1.00      | 0.00  |
| 02   | H    | C        | 0 | 0 | 0 | 30.820      | 1.00      | 0.00  |
| 03   | H    | C        | 0 | 0 | 0 | 30.820      | 1.00      | 0.00  |
| 04   | H    | C        | 0 | 0 | 0 | 30.820      | 1.00      | 0.00  |
| 05   | H    | C        | 0 | 0 | 0 | 30.820      | 1.00      | 0.00  |

**Notes:**
- The table above contains atomic coordinates and other relevant data for various atoms in a molecular structure.
- The coordinates (X, Y, Z) are in angstroms (Å).
- The temperature and pressure are given in Kelvin (K) and megapascals (MPa), respectively.
- The error is in percent (‰).
ATOM  1002  O5'  DG3   32    27.984  59.036  19.789    1.00   0.00     O
ATOM  1003  C5'  DG3   32    28.461  59.047  21.118    1.00   0.00     C
ATOM  1004  H5'  DG3   32    28.210  58.139  21.649    1.00   0.00     H
ATOM  1005  H5'' DG3   32    28.093  59.925  21.649    1.00   0.00    H
ATOM  1006  C4'  DG3   32    29.977  58.972  21.112    1.00   0.00     C
ATOM  1007  C6  DG3   32    34.173  53.949  18.672    1.00   0.00     C
ATOM  1008  O6  DG3   32    34.379  52.923  18.060    1.00   0.00     O
ATOM  1009  N9  DG3   32    35.189  54.375  19.467    1.00   0.00     N
ATOM  1010  C8  DG3   32    35.961  55.615  21.227    1.00   0.00     C
ATOM  1011  N7  DG3   32    36.911  55.075  21.304    1.00   0.00     H
ATOM  1012  C7  DG3   32    37.947  56.358  21.915    1.00   0.00     H
ATOM  1013  C6  DG3   32    38.163  56.351  20.279    1.00   0.00     N
ATOM  1014  H21 DG3   32    33.165  56.017  19.401    1.00   0.00     C
ATOM  1015  C5  DG3   32    30.632  60.030  20.164    1.00   0.00     C
ATOM  1016  C4  DG3   32    29.900  60.670  19.668    1.00   0.00     H
ATOM  1017  C3' DG3   32    31.371  59.198  19.122    1.00   0.00     C
ATOM  1018  C2' DG3   32    30.656  59.000  18.321    1.00   0.00     H
ATOM  1019  C1' DG3   32    32.280  59.682  18.760    1.00   0.00     H
ATOM  1020  O3' DG3   32    31.581  60.917  20.835    1.00   0.00     O
ATOM  1021  HO3' DG3   32    31.124  61.267  21.620    1.00   0.00     H
END