Variation of different local and global parameters for the four datasets

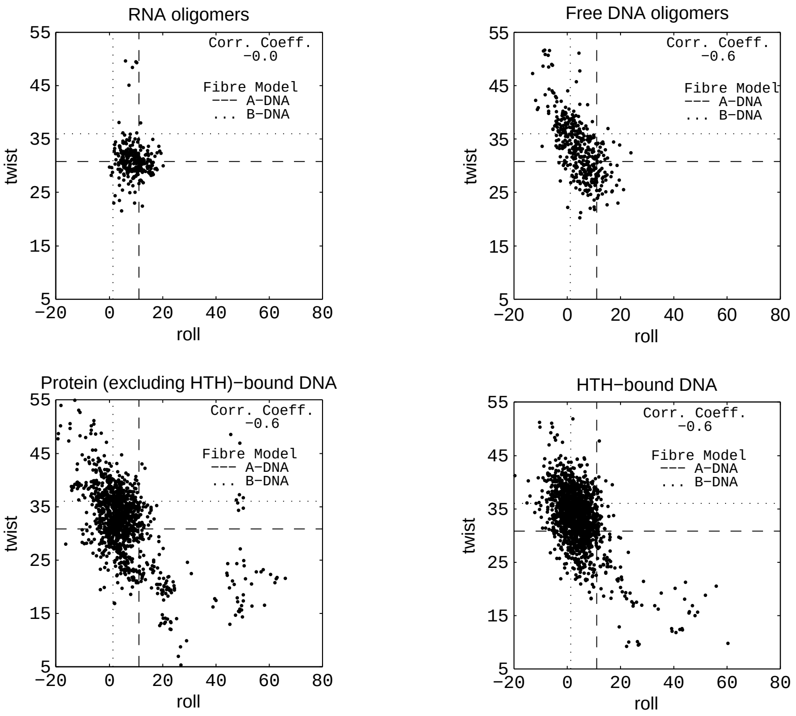

Figure 1: Twist versus Roll for the RNA, free DNA oligomers, protein (excluding HTH)-bound DNA and HTH-bound DNA datasets. Dashed and dotted lines have been drawn to highlight the values for the A and B-DNA fibre models.

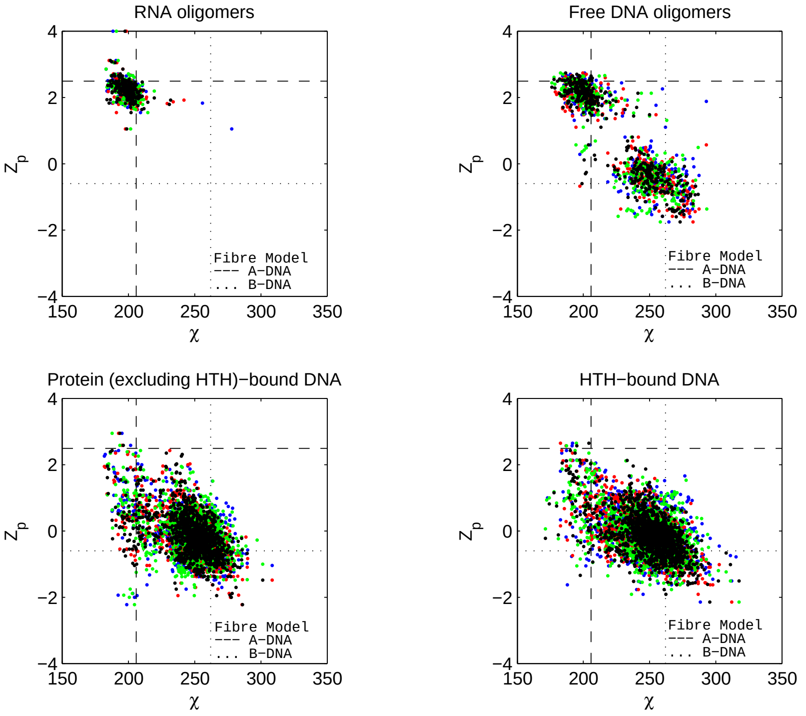

Figure 2: Z_p versus backbone torsion angle χ for the four datasets. The four nucleotides constituting a basepaired dinucleotide step corresponding to a particular Z_p value have been colour coded as follows: *5'-end Strand 1 - blue; 3'-end Strand 1 - Red; 5'-end Strand 2 - Green; 3'-end Strand 2 - Black.*

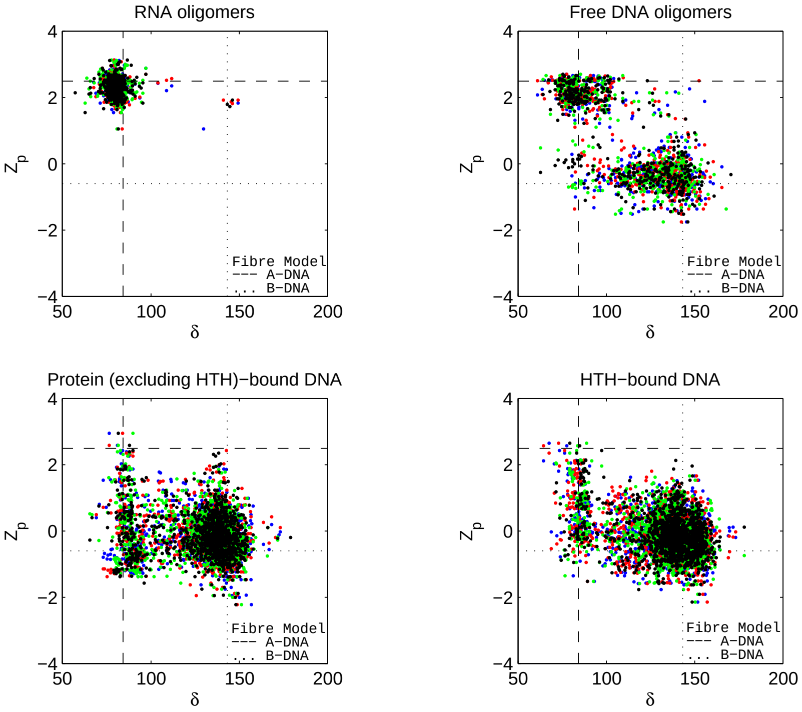

Figure 3: Z_p versus backbone torsion angle δ for the four datasets. The four nucleotides constituting a basepaired dinucleotide step corresponding to a particular Z_p value have been colour coded as follows: *5'-end Strand 1 - blue; 3'-end Strand 1 - Red; 5'-end Strand 2 - Green; 3'-end Strand 2 - Black.*

Table 1: Mean and standard deviation values (in parentheses) for global helical basepair orientation parameters and groove widths. The linear global helical axis has been fitted to the backbone C_1' atoms. For the complex and HTH datasets, structures which are curved or whose geometry of curvature could not be assigned are excluded, since a linear global helical axis cannot be fitted to such structures.

	Fibre-model		RNA	Free		Complex	HTH
	A-DNA	B-DNA		A-like	B-like	Excl. TEH†	Excl. TC ‡
				($Z_p > 1.3$ Å)	($Z_p \leq 0.8$ Å)		
Inclination (°)	19.3	2.0	15.4 (4.8)	16.5 (5.1)	2.0 (3.5)	6.4 (6.2)	5.9 (6.5)
Helical twist (°)	32.7	36.0	32.7 (6.1)	32.1 (3.7)	35.9 (6.0)	34.1 (4.6)	34.0 (4.8)
X-displacement (Å)	-4.5	0.6	-4.3 (1.2)	-4.3 (0.9)	0.1 (0.8)	-1.1 (1.1)	-0.9 (1.3)
Helical rise (Å)	2.6	3.4	2.7 (0.3)	2.7 (0.3)	3.3 (0.1)	3.2 (0.1)	3.2 (0.2)
Smallest P-P distance (Å) (across minor groove)	17.0	11.7	15.7 (0.6)	15.8 (0.6)	11.1 (1.5)	12.4 (1.7)	12.5 (1.8)
Smallest P-P distance (Å) (across major groove)	8.2	17.2	11.1 (2.0)	11.6 (2.7)	17.1 (0.9)	17.3 (1.7)	17.1 (1.3)

†TEH - TBP, Endonuclease and Hyperthermophile chromosomal protein SAC7D containing structures (excluded)

‡TC - TBP and CAP containing structures (excluded)