

Studies of base pair sequence effects on DNA solvation based on all-atom molecular dynamics simulations

SURJIT B DIXIT, MIHALY MEZEI and DAVID L BEVERIDGE

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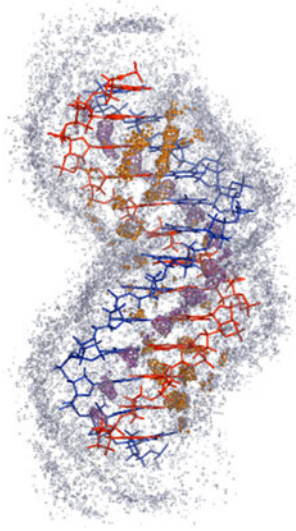
Supplementary material

Supplementary table 1. List of PDB IDs

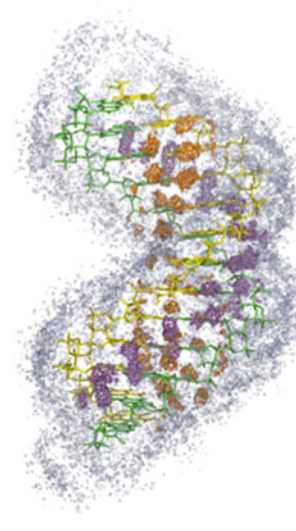
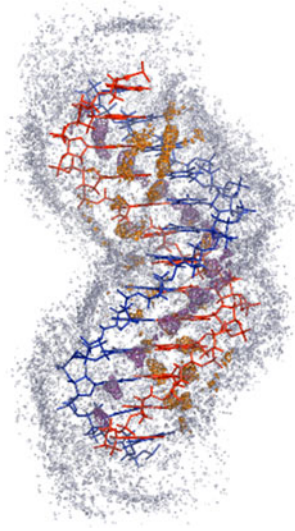
PDB ID	Resolution (Å)	Sequence
119d.pdb1	2.25	CGTAGATCTACG
126d.pdb1	2.00	CATGGCCATG
158d.pdb1	1.90	CCAAGCTTGG
167d.pdb1	2.30	CCATTAATGG
194d.pdb1	2.30	CGCGTTAACGCG
196d.pdb1	1.70	CTCTCGAGAG
1bd1.pdb1	1.60	CCAGGCCTGG
1bdn.pdb1	2.60	CGCAAAAATGCG
1bna.pdb1	1.90	CGCGAATTCGCG
1cgc.pdb1	2.20	CCGGCGCCGG
1d23.pdb1	1.50	CGATCGATCG
1d28.pdb1	2.70	CGTGAATTCACG
1d29.pdb1	2.50	CGTGAATTCACG
1d49.pdb1	1.50	CGATTAATCG
1d56.pdb1	1.70	CGATATATCG
1d57.pdb1	2.00	CGATATATCG
1d65.pdb1	2.20	CGCAAAATTTGCG
1d89.pdb1	2.30	CGCGAAAAAACG
1d8g.pdb1	0.74	CCAGTACTGG
1d98.pdb1	2.50	CGCAAAAAAGCG
1dc0.pdb1	1.30	CATGGGCCCATG
1dev.pdb1	2.50	CCGCTAGCGG
1dn9.pdb1	2.20	CGCATATATGCG
1en3.pdb1	0.99	CCAACGTTGG
1en8.pdb1	0.99	CCAACGTTGG
1en9.pdb1	0.99	CCAGCGCTGG
1ene.pdb1	0.99	CCAGCGCTGG
1f6c.pdb1	2.70	GGCGCC

Supplementary table 1. (continued)

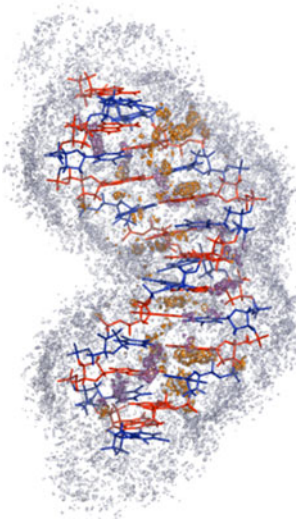
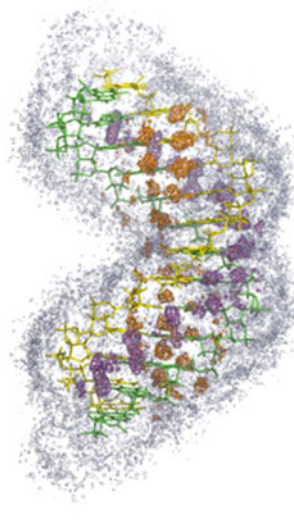
1fq2.pdb1	1.20	CGCGAATTCGCG
1jgr.pdb1	1.20	CGCGAATTCGCG
1qc1.pdb1	2.50	CCGCCGGCGG
206d.pdb1	2.50	CGGTGG
250d.pdb1	2.47	CGCTAGCG
251d.pdb1	1.90	CTCGAG
252d.pdb1	2.30	CGCAATTGCG
287d.pdb1	2.20	CGCGATATCGCG
2bna.pdb1	2.70	CGCGAATTCGCG
307d.pdb1	1.85	CAAAGAAAAG
330d.pdb1	2.70	ACCGCCGGCGCC
355d.pdb1	1.40	CGCGAATTCGCG
423d.pdb1	1.60	ACCGACGTCGGT
424d.pdb1	2.70	ACCGACGTCGGT
425d.pdb1	2.80	ACCGGTACCGGT
426d.pdb1	3.00	CGCGAATTCGCG
428d.pdb1	1.75	CGCGAATTCGCG
477d.pdb1	1.70	GGCGAATTCGCG
5dnb.pdb1	1.40	CCAACGTTGG
7bna.pdb1	1.90	CGCGAATTCGCG
9bna.pdb1	1.90	CGCGAATTCGCG



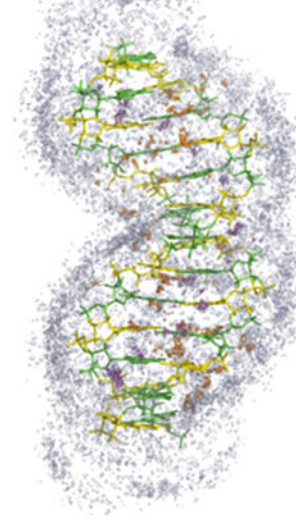
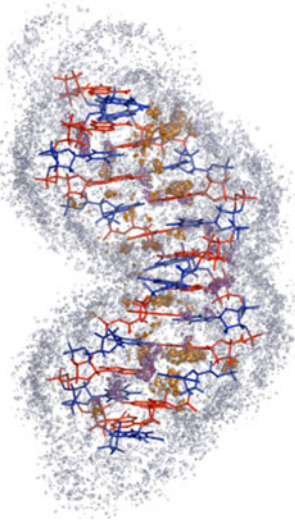
Poly A



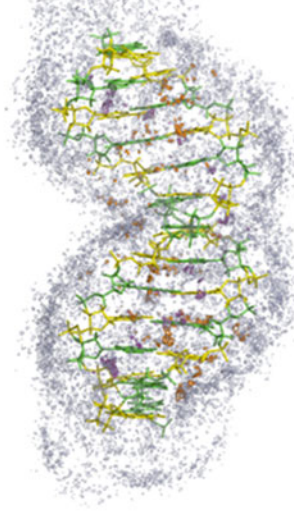
Poly (G)



Poly (ApT)



Poly (GpC)



Supplementary figure 1. Stereo images of hydration density maps around the poly A, poly G, poly (ApT) and poly (GpC) sequences.