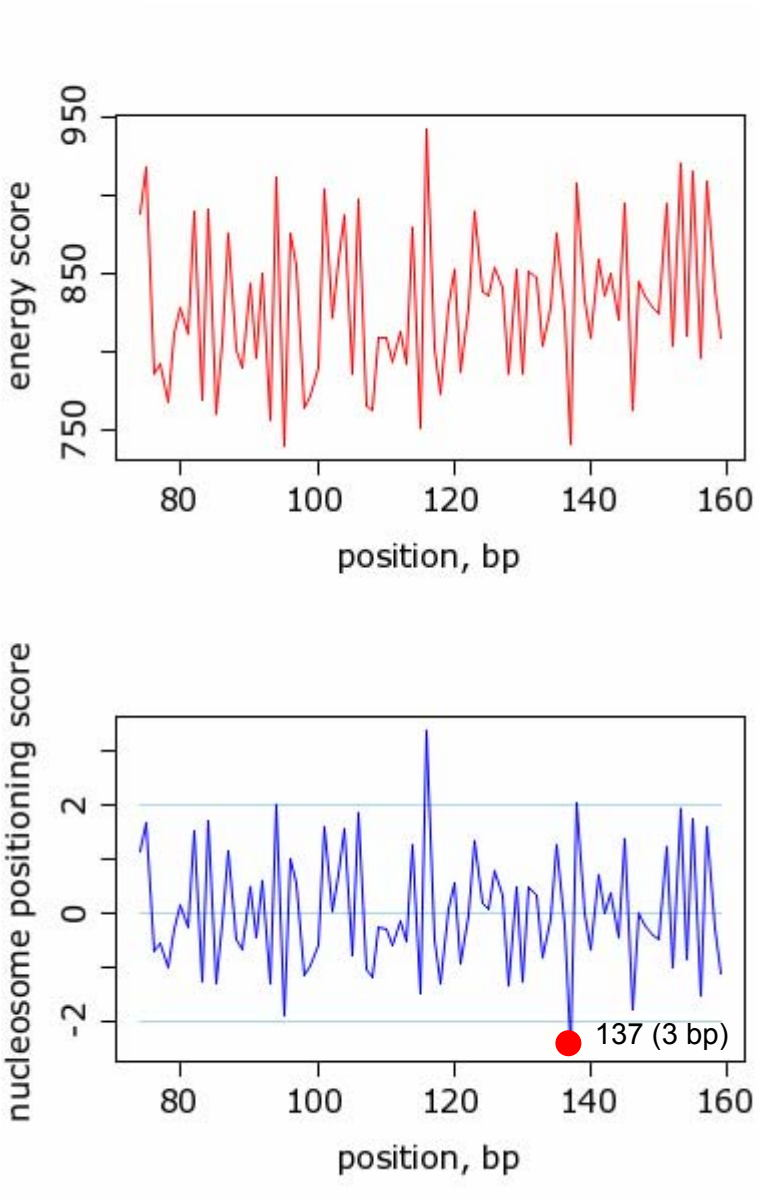
SUPPLEMENTARY MATERIAL

Table 1. Comparison of experimental and theoretical nucleosomal arrangements on selected sequences*

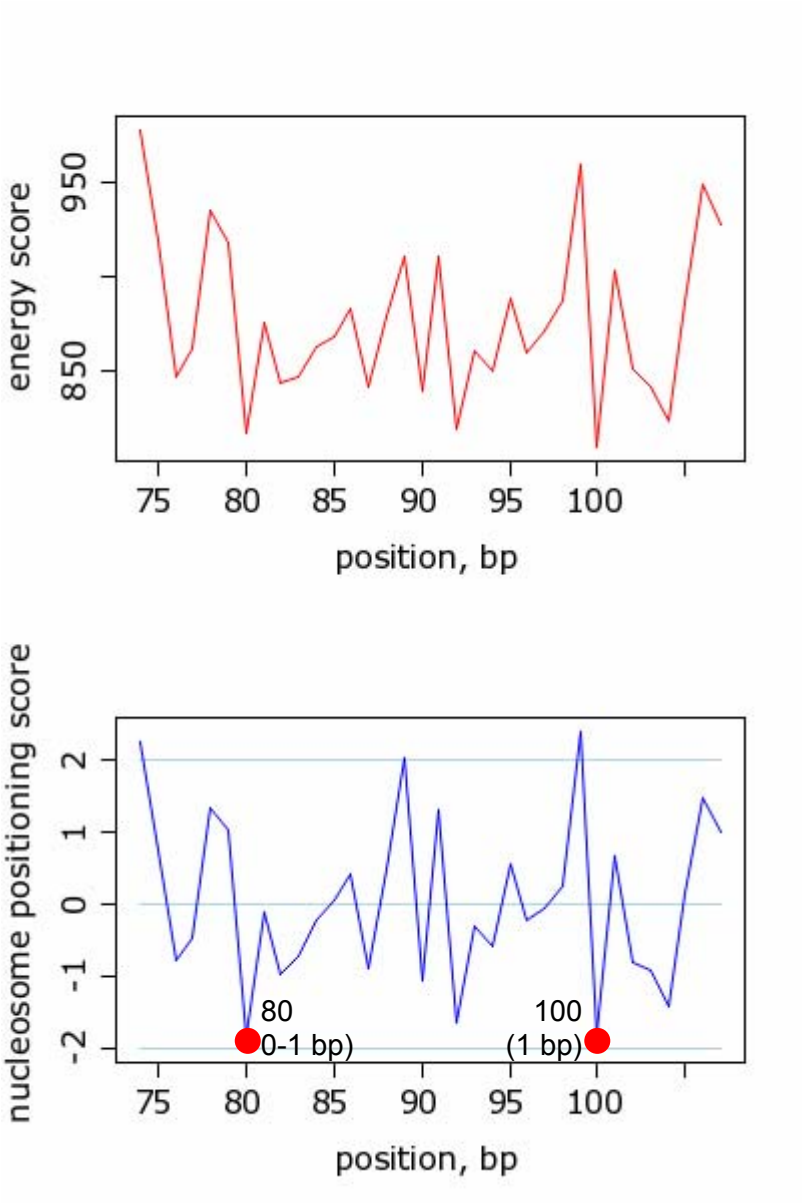
	Sequence	experimental method	Reference	number of experiment-ally mapped nucleosomes	number of predicted nucleosomes (3 bp/4 bp accuracy)	number of false predic-tions
1	High-affinity '601' synthetic sequence	site-directed hydroxyl-radical cleavage of the sugar-phosphate backbone by modified histone residues in the vicinity of the nucleosomal dyad	[1]	1	1/1	0
2	*L. variegatus* 5S rRNA gene	Same	[2]	2	2/2	0
3	183-bp pGUB plasmid positioning sequence	Photochemical cross-linking and subsequent cleavage, by heat and alkali treatment, of DNA photoadducts formed with specifically tailored amino-acid groups	[5]	2	2/2	1
4	fragment of chicken β^A-globin promoter	enzymatic (combined MNase and DNase I) digestion	[6]	1	1/1	0
5	*X. borealis* 5S rRNA gene (somatic)	site-directed hydroxyl-radical cleavage of the sugar-phosphate backbone by modified histone residues in the vicinity of the nucleosomal dyad	[3]	6	2/4	0
6	*X. borealis* 5S rRNA gene (oocyte)	Same	[3]	6	3/4	1
7	Mouse mammary tumor virus 3'LTR sequence	Same	[4]	2	0/1	6
	Total			**20**	**11 (55%) / 15 (75%)**	**8**

*Sequences available in the literature for which nucleosome locations were experimentally determined *in vitro* with base-pair resolution. We note that using the nucleosome positioning data with the resolution lower than 5 bp may be misleading, because a 5-bp shift of the nucleosome on a positioning sequence would result in completely opposite rotational setting. Predictions are based on the calculations of nucleosome positioning-scores performed with the template that comprises central 129 bp of the DNA structure from the best-resolved nucleosome core particle structure (NCP147) [7]. The 147-bp window was used to calculate nucleosome positioning score. Threshold of $P \leq -2$ was used to call predicted nucleosome locations (the nucleosome positioning score does not reach –2 at any position on the sea urchin 5S rRNA gene sequence; experimental nucleosome locations on this sequence correspond to the two strongest minima in the positioning score profile ($P = -1.8$ for both positions); therefore they were taken as correctly predicted). The sequences are available at: http://compbio.med.harvard.edu/tolstorukov/nuseq/hi-res.positioning.seq.txt

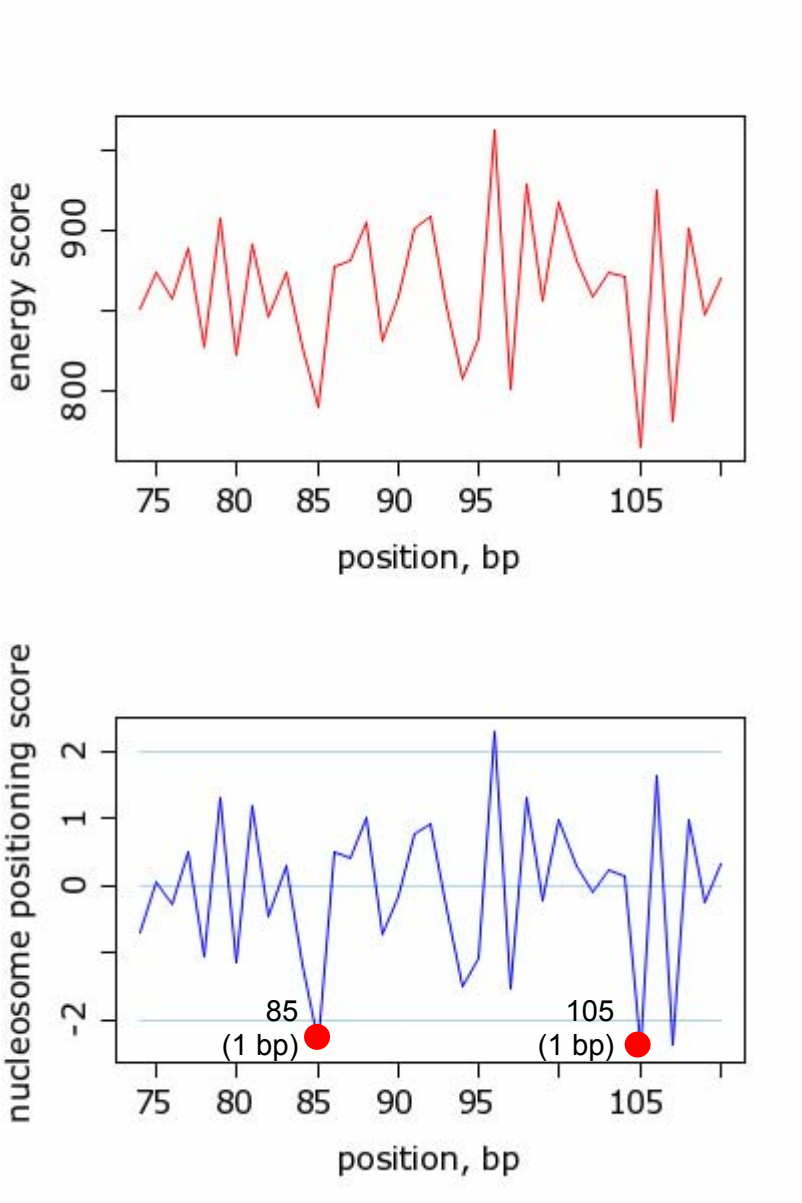
Examples of the nucleosome deformation energy and positioning score profiles
(predicted positions are indicated with red cycles, the accuracy of predictions is shown in parentheses)



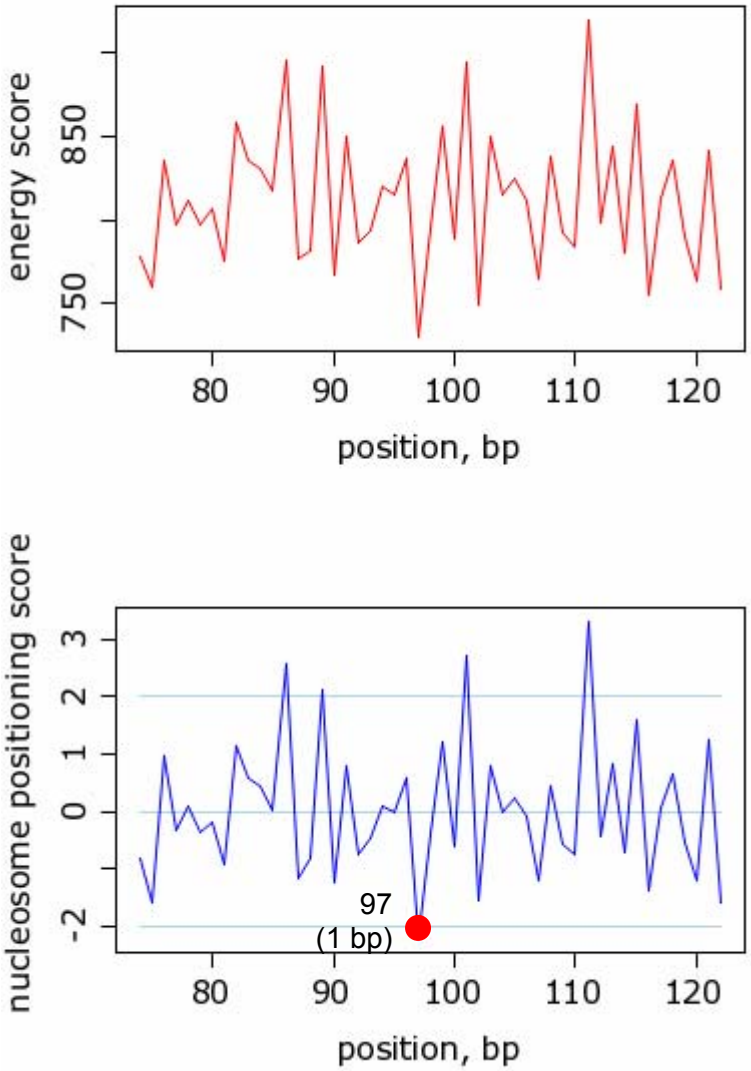
The high-affinity sequence '601'. The experimentally determined dyad position is at base pair 134 (J. Widom, personal communication).



Sea urchin 5S rDNA (clone ASYM180). The experimentally determined dyad positions are at base pairs 81 and 99 on the sequence (corresponding positions relative to the transcription start site are base pairs –11/–12 and +8; note that there is no position “0” in these coordinates).



The 183-bp sequence from the pGUB plasmid. The experimentally determined dyad positions are at base pairs 84 and 104.



The 195-bp fragment from the sequence of the chicken β-globin[A] gene. The experimentally determined nucleosome location (nucleosome 5A) is reported at position 95.5 on the sequence fragment (corresponding position relative to the transcription start site is –281.5).

References

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