Intrinsic contribution of the 2’-hydroxyl to RNA conformational heterogeneity

Elizabeth J. Denning and Alexander D. MacKerell Jr.*
Department of Pharmaceutical Sciences, University of Maryland, 20 Penn Street, Baltimore, MD 21201

Supporting Information

Figure S1: Reference structure (Front and side view) for the 3D water probability distribution calculations. This template structure was used to align the individual nucleotides in the crystal structures using the ribose atoms for reference: C1', C2', C3', C4', and O4' atoms. The template structure was built within the CHARMM program and minimized using steepest decent while constraining the nucleotide geometry to an ideal RNA A-form commonly found in duplex RNA (see Table S1).

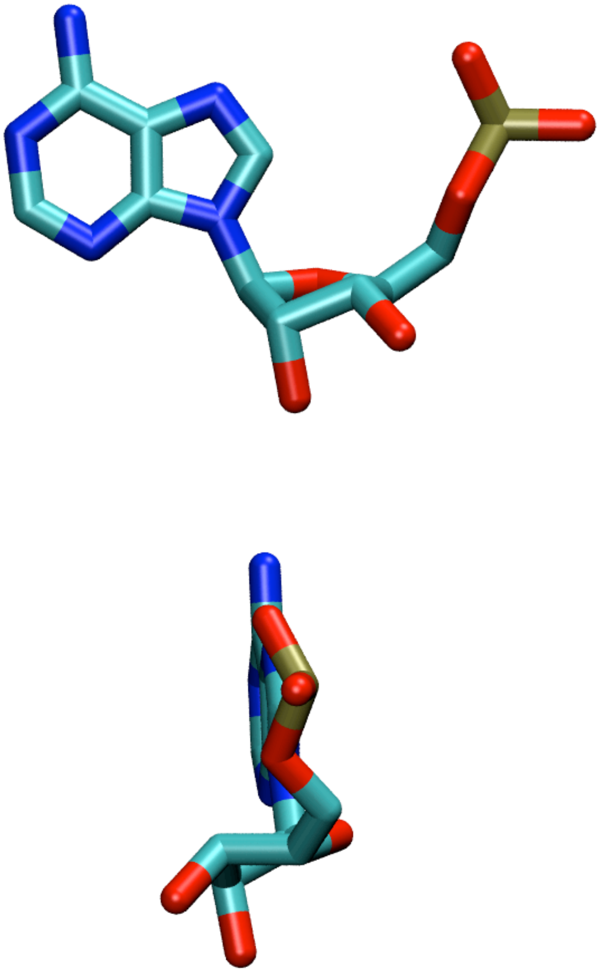

Figure S2: The initial starting geometry for the QM calculations using the NUSU model compound, containing the phosphodiester backbone and a uracil base, and a single water molecule. The water was placed at a distance of 2.77 Å between the water H and the O2' oxygen near the additional water distribution site found for non-canonical structures (see Figure 4, in main text). The QM calculations were performed at the MP2/6-31+G(d) level using the Gaussian03 package. **(A)** Side view **(B)** Bottom view.

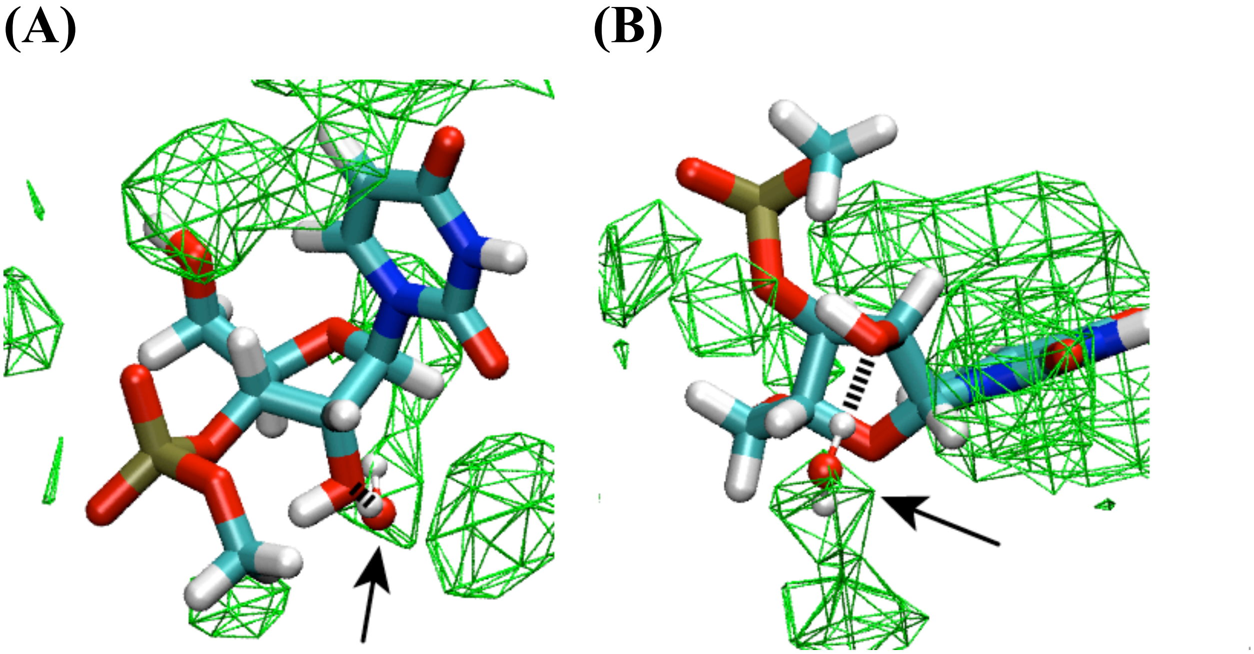

Table S1. The constraints used for the QM calculations.

Target Dihedral	A DNA	B_I DNA	B_{II} DNA	A-RNA
α (O3′-P-O5′-C5′)	291	298	298	291
β (P-O5′-C5′-C4′)	175	168	168	174
γ (O5′-C5′-C4′-C3′)	57	51	51	57
ε (C4′-C3′-O3′-P)	205	195.7	267.2	211
ζ (C3′-O3′-P-O5′)	287	270.3	159.2	287
Sugar constraints:				
C2′ endo (south, B-form)	C3′-C4′-O4′-C1′ = 0			
C3′ endo (north, A-form)	C4′-O4′-C1′-C2′ = 0			

Table S2. List of DNA structures used for the survey data.

PDB ID	Type	Ref.	PDB ID	Type	Ref.
137D	A-form	Ramakrishnan *et al* [1]	477D	B-form	Minasov *et al* [2]
1ZEX	A-form	Hays *et al* [3]	158D	B-form	Grzeskowiak *et al* [4]
1ZEY	A-form	Hays *et al* [3]	194D	B-form	Balendiran *et al* [5]
1ZF1	A-form	Hays *et al* [3]	1CGC	B-form	Heinemann *et al* [6]
1ZF6	A-form	Hays *et al* [3]	1D29	B-form	Larsen *et al* [7]
1ZF8	A-form	Hays *et al* [3]	1D57	B-form	Yuan *et al* [8]
1ZF9	A-form	Hays *et al* [3]	1D65	B-form	Edwards *et al* [9]
1ZFA	A-form	Hays *et al* [3]	1D8G	B-form	Kielkopf *et al* [10]
2PKV	A-form	Girard *et al* [11]	1DCV	B-form	Eichman *et al* [12]
2PL4	A-form	Girard *et al* [11]	1DN9	B-form	Yoon *et al* [13]
2PL8	A-form	Girard *et al* [11]	1EN3	B-form	Chiu *et al* [14]
2PLB	A-form	Girard *et al* [11]	1EN9	B-form	Chiu *et al* [14]
440D	A-form	Gao *et al* [15]	1HQ7	B-form	Locasale *et al* [16]
1D78 + 1D79	A-form	Thota *et al* [17]	1IH1	B-form	Vargason *et al* [18]
368D	A-form	Fernandez *et al* [19]	1QC1	B-form	Timsit *et al* [20]
369D	A-form	Fernandez *et al* [19]	1S23	B-form	Valls *et al* [21]
370D	A-form	Fernandez *et al* [19]	1WQY	B-form	Arai *et al* [22]
371D	A-form	Fernandez *et al* [19]	1ZEW	B-form	Hays *et al* [3]
414D	A-form	Savitha *et al* [23]	1ZF5	B-form	Hays *et al* [3]
116D	A-form	Bingman *et al* [24]	1ZFC	B-form	Hays *et al* [3]
126D	A-form	Goodsell *et al* [25]	1ZFE	B-form	Hays *et al* [3]
138D	A-form	Ramakrishnan *et al* [1]	1ZFF	B-form	Hays *et al* [3]
160D	A-form	Ramakrishnan *et al* [26]	1ZFM	B-form	Hays *et al* [3]
1DNZ	A-form	Robinson *et al* [27]	251D	B-form	Wahl *et al* [28]
1G00	A-form	Urpi *et al* [29]	3DNB	B-form	Prive *et al* [30]
257D	A-form	Mooers *et al* [31]	3GGB	B-form	Maehigashi *et al* [32]
260D	A-form	Ban *et al* [33]	3GGI	B-form	Maehigashi *et al* [32]
287D	A-form	Shatzky-Schwartz *et al* [34]	3GGK	B-form	Maehigashi *et al* [32]
28DN	A-form	Courseille *et al* [35]	5DNB	B-form	Prive *et al* [30]
401D	A-form	Finley *et al* [36]	436D	B-form	Tereshko *et al* [37]
441D	A-form	Gao *et al* [15]	460D	B-form	Tereshko *et al* [38]
9DNA	A-form	Heinemann *et al* [39]	461D	B-form	Tereshko *et al* [38]
196D	B-form	Goodsell *et al* [40]	1BNA	B-form	Drew *et al* [41]
1D49	B-form	Quintana *et al* [42]	1D23	B-form	Grzeskowiak *et al* [43]
1D56	B-form	Yuan *et al* [8]	1JGR	B-form	Howerton *et al* [44]
1FQ2	B-form	Sines *et al* [45]	431D	B-form	Vlieghe *et al* [46]
1ZF0	B-form	Hays *et al* [3]	476D	B-form	Minasov *et al* [2]
1ZF7	B-form	Hays *et al* [3]	355D	B-form	Shui *et al* [47]
1ZFB	B-form	Hays *et al* [3]			
1ZFG	B-form	Hays *et al* [3]			

Table S3. List of RNA structures used for the survey data.

PDB ID	Type	Ref.
157D	Canonical	Leonard *et al* [48]
1DQH	Canonical with Bulge	Xiong *et al* [49]
1EHZ	tRNA	Shi *et al* [50]
1F27	Pseudoknot	Nix *et al* [51]
1L2X	Pseudoknot	Egli *et al* [52]
1MME	Ribozyme	Scott *et al* [53]
1MSY	Tetraloop	Correll *et al* [54]
1Q9A	Hairpin	Correll *et al* [55]
1RNA	Canonical	Dock-Bregeon *et al* [56]
1SA9	Canonical	Jang *et al* [57]
1SDR	Canonical	Schindelin *et al* [58]
1XPE	Kissing complex	Ennifar *et al* [59]
1Y26	Riboswitch	Serganov *et al* [60]
1ZCI	Kissing complex	Ennifar *et al* [59]
1ZEV	Canonical	Mooers *et al* [61]
259D	Canonical	Egli *et al* [62]
280D	Canonical	Lietzke *et al* [63]
2FD0	Kissing complex	Ennifar *et al* [64]
2V6W	tRNA acceptor	Forster *et al* [65]
353D	Canonical	Betzel *et al* [66]
397D	Canonical with Bulge	Ippolito *et al* [67]
3DW5	Hairpin	Olieric *et al* [68]
3DW7	Hairpin	Olieric *et al* [68]
3FAR	Canonical	Ennifar *et al* [69]
3L0U	tRNA	Byrne *et al* [70]
402D	Canonical	Jang *et al* [71]
405D	Canonical	Pan *et al* [72]
433D	Canonical	Trikha *et al* [73]
434D	Canonical	Mueller *et al* [74]
435D	Canonical	Mueller *et al* [74]
437D	Pseudoknot	Su *et al* [75]
438D	Canonical	Shi *et al* [76]
472D	Canonical	Deng *et al* [77]
480D	Canonical	Correll *et al* [78]
483D	Canonical	Correll *et al* [78]

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