**Structure of the HIV-1 frameshift site RNA bound to a small molecule
inhibitor of viral replication**

Supplemental Information

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Table S1. Structural statistics. The best 50 docking solutions were selected for refinement in implicit solvent with HADDOCK. Structures chosen for refinement in AMBER had no angle violations $> 5^\circ$ and no distance constraint violations $> 0.5 \text{ \AA}$. The 10 lowest energy structures with no angle violations $> 5^\circ$ and no distance constraint violations $> 0.5 \text{ \AA}$ after AMBER refinement were accepted and analyzed.

Figure S1. Effect of DB213 on RNA stability in 100 mM KCl. All samples contained 2 μM RNA.. First derivative plots of UV-monitored (270 nm) thermal denaturation in the presence of 0 μM DB213 (black circles) or 100 μM DB213 (red circles) are shown. Data fitting results are indicated by black and red lines for 0 μM DB213 and 100 μM DB213, respectively. (a) At 0 μM DB213, the transition melting temperature for the lower helix (Tm_l) is $71.9 \pm 0.3^\circ\text{C}$, while at 100 μM DB213 it is $75.5 \pm 0.3^\circ\text{C}$. Transition melting temperatures for the upper stem-loop could not be determined, as they are greater than 97°C at both 0 μM DB213 and 100 μM DB213. (b) UV-monitored thermal denaturations performed as in (a), with the addition of 6 M urea, which shifts the upper melting transition into an observable range. At 0 μM DB213, the transition melting temperatures for the lower helix (Tm_l) and upper stem-loop (Tm_u) are $61.7 \pm 0.3^\circ\text{C}$ and $86.6 \pm 0.3^\circ\text{C}$, respectively, while at 100 μM DB213 these temperatures are $63.1 \pm 0.3^\circ\text{C}$ and $87.7 \pm 0.3^\circ\text{C}$.

Figure S2. HIV-1_{NMR} RNA and DB213 NMR reference spectra. (a) DB213-only reference experiment, with resonance assignments indicated and numbered as in Figures 1b and 2. (b) RNA-only reference experiment, with resonance assignments indicated and numbered as in Figure 1a. (c) Combined DB213 and RNA (1:1 molar ratio) experiment. Resonance assignments for the RNA are indicated and numbered as in Figure 1a. Peaks indicated by asterisks are indicative of amino groups on DB213 that are hydrogen-bonded to the HIV-1 RNA. (d) Spectrum in (b) zoomed in to the region containing imino

and amino resonances. (e) Spectrum in (c) zoomed in to the region containing imino and amino resonances

Figure S3. Change in the magnitude of combined chemical shift changes (in ppm) for indicated ^1H - ^{13}C correlations plotted vs. RNA sequence as indicated and numbered in Figure 1a.

Figure S4. Change in HIV-1_{NMR} bulge conformation upon DB213 binding. Top panel, free conformation. Bottom panel, bound conformation. Interphosphate distances across the bulge are indicated.

Figure S5. Pulse sequence for carbon-decoupled ^1H - ^{13}C TROSY-HSQC experiments. The experiment for acquiring decoupled ^1H - ^{13}C TROSY spectra is based on the gradient-selected ^1H - ^{13}C TROSY pulse program (1). Narrow and wide bars indicate non-selective 90° and 180° pulses, respectively. Three shaped pulses are used on ^{13}C : (a) an ISNOB3 inversion pulse (2), (b) a HYPERBOLIC-SECANT inversion pulse (3) and (c) a REBURP refocusing pulse (4). All three pulses are given on-resonance. The ISNOB3 and REBURP pulses have narrower bandwidth covering only the ^{13}C nuclei that are being observed (see below), while the HYPERBOLIC-SECANT pulse is a 1ms long pulse with a 200ppm bandwidth. The ^{13}C carrier frequency and the ^{13}C shaped pulses have been optimized for recording a spectrum that either contains C^6H^6 , C^8H^8 and C^2H^2 peaks, or $\text{C}^{1'}\text{H}^{1'}$, C^5H^5 and $\text{C}^{4'}\text{H}^{4'}$ peaks. For obtaining the former spectrum, the ^{13}C offset is set at 146ppm with a bandwidth of about 23 ppm for the (a) and (c) ^{13}C shaped pulses, while the $\text{C}^5/\text{C}^{1'}/\text{C}^{4'}$ spectrum is collected by setting the ^{13}C offset at 97 ppm, with a bandwidth of 30 ppm. The carrier frequency for ^1H is set on resonance with water at 4.77 ppm; Delay durations: $\delta = 1/(2J_{CH})$, where $J_{CH} = 190$ Hz (an average of ribose and aromatic J_{CH} couplings); Δ_1 = duration of G_3 and 0.2s for recovery; Δ_2 = duration of G_6 and 0.2s for recovery. Phase

cycling: $\phi_1 = y, -y$, $\phi_2 = y$, $\phi_3 = x$, $\phi_{\text{rec}} = x, -x$. To accomplish quadrature detection for the ^{13}C indirect dimension the Rance-Kay method where a second FID is collected for each increment by changing the phases $\phi_2 = -y$, $\phi_3 = -x$ and inverting the sign of the G_6 gradient. Adjacent FIDs are then added and subtracted during processing to obtain the real and imaginary components (5). For States-TPPI acquisition, the ϕ_1 and ϕ_{rec} phases are also incremented by 180° every other ^{13}C increment. Gradients are WURST-shaped z -axis gradients with a length of 0.5 ms, except for G_2 and G_6 that are 1 and 2ms long, respectively. Gradient strengths (G/cm): G_1 : 5, G_2 : 17, G_4 : 6, G_5 : 7. G_3 and G_6 are the gradients for coherence selection with $G_6 = \gamma_{\text{C}} / \gamma_{\text{H}} \bullet G_3$, where γ_{C} and γ_{H} are the gyromagnetic ratios for ^{13}C and ^1H respectively. A total of 2048 points were acquired in the direct dimension and 256 points in the indirect dimension with sweep widths of 11000 Hz and 5100 Hz ($\text{C}^2/\text{C}^6/\text{C}^8$), or 6000 Hz and 3800 Hz ($\text{C}^5/\text{C}^{1'}/\text{C}^{4'}$), respectively. A similar experiment was used for collection of dipolar couplings at natural abundance ^{13}C , with the following modifications: pulse (b) was removed, pulse (c) was replaced with a non-selective 180° pulse, the ^{15}N channel was removed, the second $t_1/2$ time was removed and the first $t_1/2$ time changed to t_1 , and a second set of FIDs was acquired for each increment to collect the bottom-right and bottom-left TROSY components by changing the initial phase of ϕ_3 to $-x$. Corresponding Varian pulse programs and NMRpipe data processing macros are available at <http://www.nmrfam.wisc.edu>.

Figure S6. Residual dipolar coupling validation. The forty-two experimentally observed RDCs are plotted against RDCs that have been back-calculated from the lowest energy structure of the DB213:HIV-1_{NMR} complex. The overall agreement between observed and back-calculated RDCs is very good, as indicated by the Cornilescu Q-value of less than 0.25, and the r^2 value of greater than 0.95.

Text: DB213 parameter files

Table S1.

	RNA	Ligand
NMR constraints		
Intramolecular distance restraints		
Total NOE	786	26
Intra-residue	321	26
Inter-residue	465	n/a
Sequential ($ i - j = 1$)	369	n/a
Non-sequential ($ i - j > 1$)	96	n/a
Hydrogen bonds	96	0
Based on A-form geometry	85	n/a
Intermolecular distance restraints	42	
Dihedral angle restraints		
Nucleic acid	324	n/a
Sugar-Base glycosidic (χ)	45	n/a
Sugar pucker (ν_1, ν_2)	78	n/a
Backbone ($\alpha, \beta, \gamma, \delta, \epsilon, \zeta$)	202	n/a
Based on A-form geometry	202	n/a
Residual dipolar couplings	42	n/a
Structure statistics		
Number of structures		
Initially docked with HADDOCK	500	
Refined with HADDOCK	50	
Refined with AMBER	26	
Accepted after refinement	10	
Violations (mean and s.d.)		
Distance constraints (Å)	0.0514 ± 0.0001	
Dihedral angle constraints (°)	0.497 ± 0.091	n/a
Residual dipolar couplings (Hz)	4.26 ± 0.14	n/a
Number of dihedral angle violations ($> 5^\circ$)	0	n/a
Number of distance constraint violations (> 0.5 Å)	0	0
Deviations from idealized geometry		
Bond lengths (Å)	0.00441 ± 0.00031	
Bond angles (°)	0.886 ± 0.021	
Impropers (°)	0.842 ± 0.032	
r.m.s. deviation to mean structure (Å)		
RNA		
All heavy atoms	0.97	n/a
Upper stem-loop (residues 17-40)	0.39	n/a
Lower helix (residues 8-14,46-52)	0.30	n/a
Bulge (residues 15, 16, 41-45)	0.78	n/a
Ligand		
All heavy atoms	n/a	0.89
Complex		
All heavy atoms	0.97	
Ligand & RNA upper stem-loop (residues 17-40, 53)	0.39	
Ligand & RNA upper stem-loop, bulge (residues 15-45, 53)	0.66	
Ligand & RNA in frameshift position (residues 13-47, 53)	0.79	

Figure S1.

FigureS2.

Figure S3.

Figure S4.

Figure S6.

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!DB213 parameter file
!
!/var/tmp/xdict_5343.par
!Created by XPLO2D V. 050802/3.3.2 at Thu Mar 25 19:23:17 2010
!Auto-generated by XPLO2D from file /var/tmp/xdict_5343.pdb
!Parameters for residue type DB
!
!modified by RJM

set echo=off message=off end

checkversion 1.2

evaluate ($kbond = 1000)
evaluate ($kangle = 500)
evaluate ($kimpr = 750)
evaluate ($kdihe = 750)

!Define bonding
BOND HX1 CX2 $kbond 1.087
BOND CX2 CX3 $kbond 1.398
BOND CX2 CX9 $kbond 1.401
BOND CX3 CX4 $kbond 1.401
BOND CX3 HX60 $kbond 1.086
BOND CX4 CX5 $kbond 1.400
BOND CX4 CX35 $kbond 1.405
BOND CX5 HX6 $kbond 1.086
BOND CX5 CX7 $kbond 1.399
BOND CX7 HX8 $kbond 1.086
BOND CX7 CX9 $kbond 1.401
BOND CX9 CX10 $kbond 1.405
BOND CX10 NX11 $kbond 1.372
BOND CX10 NX14 $kbond 1.384
BOND NX11 HX12 $kbond 1.032
BOND NX11 HX13 $kbond 1.028
BOND NX14 HX15 $kbond 1.011
BOND NX14 CX16 $kbond 1.621
BOND CX16 HX17 $kbond 1.104
BOND CX16 HX18 $kbond 1.104
BOND CX16 CX19 $kbond 1.559
BOND CX19 HX20 $kbond 1.101
BOND CX19 HX21 $kbond 1.102
BOND CX19 CX22 $kbond 1.563
BOND CX22 HX23 $kbond 1.105
BOND CX22 HX24 $kbond 1.104
BOND CX22 NX25 $kbond 1.501
BOND NX25 CX26 $kbond 1.499
BOND NX25 HX30 $kbond 1.094
BOND NX25 CX31 $kbond 1.497
BOND CX26 HX27 $kbond 1.104
BOND CX26 HX28 $kbond 1.104
BOND CX26 HX29 $kbond 1.104
BOND CX31 HX32 $kbond 1.103
BOND CX31 HX33 $kbond 1.104
BOND CX31 HX34 $kbond 1.102
BOND CX35 NX36 $kbond 1.371
BOND CX35 NX39 $kbond 1.384
BOND NX36 HX37 $kbond 1.032
BOND NX36 HX38 $kbond 1.028
BOND NX39 HX40 $kbond 1.011
BOND NX39 CX41 $kbond 1.633
BOND CX41 HX42 $kbond 1.103
BOND CX41 HX43 $kbond 1.104

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BOND CX41 CX44 $kbond 1.558
BOND CX44 HX45 $kbond 1.102
BOND CX44 HX46 $kbond 1.101
BOND CX44 CX47 $kbond 1.563
BOND CX47 HX48 $kbond 1.105
BOND CX47 HX49 $kbond 1.105
BOND CX47 NX50 $kbond 1.501
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!Define angles

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ANGLE HX1 CX2 CX9 $kangle 120.30
ANGLE CX3 CX2 CX9 $kangle 121.08
ANGLE CX2 CX3 CX4 $kangle 120.73
ANGLE CX2 CX3 HX60 $kangle 118.48
ANGLE CX4 CX3 HX60 $kangle 120.78
ANGLE CX3 CX4 CX5 $kangle 118.23
ANGLE CX3 CX4 CX35 $kangle 121.44
ANGLE CX5 CX4 CX35 $kangle 120.33
ANGLE CX4 CX5 HX6 $kangle 120.38
ANGLE CX4 CX5 CX7 $kangle 121.00
ANGLE HX6 CX5 CX7 $kangle 118.61
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ANGLE CX5 CX7 CX9 $kangle 120.77
ANGLE HX8 CX7 CX9 $kangle 120.77
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ANGLE CX2 CX9 CX10 $kangle 120.36
ANGLE CX7 CX9 CX10 $kangle 121.47
ANGLE CX9 CX10 NX11 $kangle 118.92
ANGLE CX9 CX10 NX14 $kangle 120.50
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ANGLE CX22 NX25 CX26 $kangle 109.91

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DIHEdral	CX2	CX3	CX4	CX35	\$kdihe	0	180.00	!	Value =	-179.35
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DIHEdral	HX23	CX22	NX25	CX26	\$kdihe	0	-60.00	!	Value =	-56.08
DIHEdral	HX23	CX22	NX25	HX30	\$kdihe	0	60.00	!	Value =	61.55
DIHEdral	HX23	CX22	NX25	CX31	\$kdihe	0	180.00	!	Value =	-178.36
DIHEdral	HX24	CX22	NX25	CX26	\$kdihe	0	60.00	!	Value =	61.07
DIHEdral	HX24	CX22	NX25	HX30	\$kdihe	0	180.00	!	Value =	178.70
DIHEdral	HX24	CX22	NX25	CX31	\$kdihe	0	-60.00	!	Value =	-61.21
DIHEdral	CX22	NX25	CX26	HX27	\$kdihe	0	180.00	!	Value =	176.67
DIHEdral	CX22	NX25	CX26	HX28	\$kdihe	0	60.00	!	Value =	57.22
DIHEdral	CX22	NX25	CX26	HX29	\$kdihe	0	-60.00	!	Value =	-63.13

DIHEdral	HX30	NX25	CX26	HX27	\$kdihe	0	60.00	!	Value =	58.39
DIHEdral	HX30	NX25	CX26	HX28	\$kdihe	0	-60.00	!	Value =	-61.06
DIHEdral	HX30	NX25	CX26	HX29	\$kdihe	0	180.00	!	Value =	178.59
DIHEdral	CX31	NX25	CX26	HX27	\$kdihe	0	-60.00	!	Value =	-58.81
DIHEdral	CX31	NX25	CX26	HX28	\$kdihe	0	180.00	!	Value =	-178.25
DIHEdral	CX31	NX25	CX26	HX29	\$kdihe	0	60.00	!	Value =	61.40
DIHEdral	CX22	NX25	CX31	HX32	\$kdihe	0	60.00	!	Value =	54.19
DIHEdral	CX22	NX25	CX31	HX33	\$kdihe	0	180.00	!	Value =	174.21
DIHEdral	CX22	NX25	CX31	HX34	\$kdihe	0	-60.00	!	Value =	-66.86
DIHEdral	CX26	NX25	CX31	HX32	\$kdihe	0	-60.00	!	Value =	-68.49
DIHEdral	CX26	NX25	CX31	HX33	\$kdihe	0	60.00	!	Value =	51.53
DIHEdral	CX26	NX25	CX31	HX34	\$kdihe	0	180.00	!	Value =	170.46
DIHEdral	HX30	NX25	CX31	HX32	\$kdihe	0	180.00	!	Value =	174.61
DIHEdral	HX30	NX25	CX31	HX33	\$kdihe	0	-60.00	!	Value =	-65.37
DIHEdral	HX30	NX25	CX31	HX34	\$kdihe	0	60.00	!	Value =	53.56
DIHEdral	CX4	CX35	NX39	HX40	\$kdihe	0	0.00	!	Value =	2.72
DIHEdral	CX4	CX35	NX39	CX41	\$kdihe	0	180.00	!	Value =	-178.63
DIHEdral	NX36	CX35	NX39	HX40	\$kdihe	0	180.00	!	Value =	-177.23
DIHEdral	NX36	CX35	NX39	CX41	\$kdihe	0	0.00	!	Value =	1.42
DIHEdral	CX35	NX39	CX41	HX42	\$kdihe	0	60.00	!	Value =	52.21
DIHEdral	CX35	NX39	CX41	HX43	\$kdihe	0	-60.00	!	Value =	-66.11
DIHEdral	CX35	NX39	CX41	CX44	\$kdihe	0	180.00	!	Value =	172.76
DIHEdral	HX40	NX39	CX41	HX42	\$kdihe	0	-120.00	!	Value =	-129.14
DIHEdral	HX40	NX39	CX41	HX43	\$kdihe	0	120.00	!	Value =	112.55
DIHEdral	HX40	NX39	CX41	CX44	\$kdihe	0	0.00	!	Value =	-8.59
DIHEdral	NX39	CX41	CX44	HX45	\$kdihe	0	60.00	!	Value =	60.27
DIHEdral	NX39	CX41	CX44	HX46	\$kdihe	0	-60.00	!	Value =	-56.65
DIHEdral	NX39	CX41	CX44	CX47	\$kdihe	0	180.00	!	Value =	-178.28
DIHEdral	HX42	CX41	CX44	HX45	\$kdihe	0	180.00	!	Value =	-179.09
DIHEdral	HX42	CX41	CX44	HX46	\$kdihe	0	60.00	!	Value =	63.99
DIHEdral	HX42	CX41	CX44	CX47	\$kdihe	0	-60.00	!	Value =	-57.64
DIHEdral	HX43	CX41	CX44	HX45	\$kdihe	0	-60.00	!	Value =	-60.53
DIHEdral	HX43	CX41	CX44	HX46	\$kdihe	0	180.00	!	Value =	-177.45
DIHEdral	HX43	CX41	CX44	CX47	\$kdihe	0	60.00	!	Value =	60.92
DIHEdral	CX41	CX44	CX47	HX48	\$kdihe	0	60.00	!	Value =	63.79
DIHEdral	CX41	CX44	CX47	HX49	\$kdihe	0	-60.00	!	Value =	-51.04
DIHEdral	CX41	CX44	CX47	NX50	\$kdihe	0	180.00	!	Value =	-172.61
DIHEdral	HX45	CX44	CX47	HX48	\$kdihe	0	180.00	!	Value =	-175.19
DIHEdral	HX45	CX44	CX47	HX49	\$kdihe	0	60.00	!	Value =	69.98
DIHEdral	HX45	CX44	CX47	NX50	\$kdihe	0	-60.00	!	Value =	-51.59
DIHEdral	HX46	CX44	CX47	HX48	\$kdihe	0	-60.00	!	Value =	-56.19
DIHEdral	HX46	CX44	CX47	HX49	\$kdihe	0	180.00	!	Value =	-171.02
DIHEdral	HX46	CX44	CX47	NX50	\$kdihe	0	60.00	!	Value =	67.42
DIHEdral	CX44	CX47	NX50	CX51	\$kdihe	0	-60.00	!	Value =	-61.33
DIHEdral	CX44	CX47	NX50	CX55	\$kdihe	0	180.00	!	Value =	176.37
DIHEdral	CX44	CX47	NX50	HX59	\$kdihe	0	60.00	!	Value =	58.74
DIHEdral	HX48	CX47	NX50	CX51	\$kdihe	0	60.00	!	Value =	61.18
DIHEdral	HX48	CX47	NX50	CX55	\$kdihe	0	-60.00	!	Value =	-61.12
DIHEdral	HX48	CX47	NX50	HX59	\$kdihe	0	180.00	!	Value =	-178.75
DIHEdral	HX49	CX47	NX50	CX51	\$kdihe	0	180.00	!	Value =	178.36
DIHEdral	HX49	CX47	NX50	CX55	\$kdihe	0	60.00	!	Value =	56.06
DIHEdral	HX49	CX47	NX50	HX59	\$kdihe	0	-60.00	!	Value =	-61.57
DIHEdral	CX47	NX50	CX51	HX52	\$kdihe	0	180.00	!	Value =	-174.17
DIHEdral	CX47	NX50	CX51	HX53	\$kdihe	0	60.00	!	Value =	66.80
DIHEdral	CX47	NX50	CX51	HX54	\$kdihe	0	-60.00	!	Value =	-54.22
DIHEdral	CX55	NX50	CX51	HX52	\$kdihe	0	-60.00	!	Value =	-51.47
DIHEdral	CX55	NX50	CX51	HX53	\$kdihe	0	180.00	!	Value =	-170.50
DIHEdral	CX55	NX50	CX51	HX54	\$kdihe	0	60.00	!	Value =	68.49
DIHEdral	HX59	NX50	CX51	HX52	\$kdihe	0	60.00	!	Value =	65.38
DIHEdral	HX59	NX50	CX51	HX53	\$kdihe	0	-60.00	!	Value =	-53.65
DIHEdral	HX59	NX50	CX51	HX54	\$kdihe	0	180.00	!	Value =	-174.67
DIHEdral	CX47	NX50	CX55	HX56	\$kdihe	0	-60.00	!	Value =	-57.26
DIHEdral	CX47	NX50	CX55	HX57	\$kdihe	0	180.00	!	Value =	-176.61
DIHEdral	CX47	NX50	CX55	HX58	\$kdihe	0	60.00	!	Value =	63.20

DIHEdral	CX51	NX50	CX55	HX56	\$kdihe	0	180.00	!	Value =	178.16
DIHEdral	CX51	NX50	CX55	HX57	\$kdihe	0	60.00	!	Value =	58.80
DIHEdral	CX51	NX50	CX55	HX58	\$kdihe	0	-60.00	!	Value =	-61.39
DIHEdral	HX59	NX50	CX55	HX56	\$kdihe	0	60.00	!	Value =	61.05
DIHEdral	HX59	NX50	CX55	HX57	\$kdihe	0	-60.00	!	Value =	-58.31
DIHEdral	HX59	NX50	CX55	HX58	\$kdihe	0	180.00	!	Value =	-178.50

!Define planar/chiral atoms/bonds

IMPRoper	CX2	HX1	CX3	CX9	\$kimpr	0	0.000	!	Value =	0.525
IMPRoper	CX3	CX2	CX4	HX60	\$kimpr	0	0.000	!	Value =	-0.554
IMPRoper	CX4	CX3	CX5	CX35	\$kimpr	0	0.000	!	Value =	-0.078
IMPRoper	CX5	CX4	HX6	CX7	\$kimpr	0	0.000	!	Value =	-0.545
IMPRoper	CX7	CX5	HX8	CX9	\$kimpr	0	0.000	!	Value =	-0.661
IMPRoper	CX9	CX2	CX7	CX10	\$kimpr	0	0.000	!	Value =	-0.059
IMPRoper	CX10	CX9	NX11	NX14	\$kimpr	0	0.000	!	Value =	-0.034
IMPRoper	NX11	CX10	HX12	HX13	\$kimpr	0	0.000	!	Value =	-0.047
IMPRoper	NX14	CX10	HX15	CX16	\$kimpr	0	0.000	!	Value =	0.816
IMPRoper	CX16	NX14	HX17	HX18	\$kimpr	0	35.000	!	Value =	33.964
IMPRoper	CX19	CX16	HX20	HX21	\$kimpr	0	35.000	!	Value =	34.683
IMPRoper	CX22	CX19	HX23	HX24	\$kimpr	0	35.000	!	Value =	35.844
IMPRoper	NX25	CX22	CX26	HX30	\$kimpr	0	-35.000	!	Value =	-32.218
IMPRoper	CX26	NX25	HX27	HX28	\$kimpr	0	35.000	!	Value =	33.478
IMPRoper	CX31	NX25	HX32	HX33	\$kimpr	0	-35.000	!	Value =	-33.186
IMPRoper	CX35	CX4	NX36	NX39	\$kimpr	0	0.000	!	Value =	0.030
IMPRoper	NX36	CX35	HX37	HX38	\$kimpr	0	0.000	!	Value =	0.015
IMPRoper	NX39	CX35	HX40	CX41	\$kimpr	0	0.000	!	Value =	-0.822
IMPRoper	CX41	NX39	HX42	HX43	\$kimpr	0	35.000	!	Value =	34.047
IMPRoper	CX44	CX41	HX45	HX46	\$kimpr	0	35.000	!	Value =	35.330
IMPRoper	CX47	CX44	HX48	HX49	\$kimpr	0	35.000	!	Value =	36.462
IMPRoper	NX50	CX47	CX51	CX55	\$kimpr	0	35.000	!	Value =	34.452
IMPRoper	CX51	NX50	HX52	HX53	\$kimpr	0	35.000	!	Value =	33.569
IMPRoper	CX55	NX50	HX56	HX57	\$kimpr	0	35.000	!	Value =	33.588

!Define nonbonded values

NONBonded	HX1	0.0498	1.4254	0.0498	1.4254
NONBonded	CX2	0.1200	3.7418	0.1000	3.3854
NONBonded	CX3	0.1200	3.7418	0.1000	3.3854
NONBonded	CX4	0.1200	3.7418	0.1000	3.3854
NONBonded	CX5	0.1200	3.7418	0.1000	3.3854
NONBonded	HX6	0.0498	1.4254	0.0498	1.4254
NONBonded	CX7	0.1200	3.7418	0.1000	3.3854
NONBonded	HX8	0.0498	1.4254	0.0498	1.4254
NONBonded	CX9	0.1200	3.7418	0.1000	3.3854
NONBonded	CX10	0.1200	3.7418	0.1000	3.3854
NONBonded	NX11	0.2384	2.8509	0.2384	2.8509
NONBonded	HX12	0.0498	1.4254	0.0498	1.4254
NONBonded	HX13	0.0498	1.4254	0.0498	1.4254
NONBonded	NX14	0.2384	2.8509	0.2384	2.8509
NONBonded	HX15	0.0498	1.4254	0.0498	1.4254
NONBonded	CX16	0.1200	3.7418	0.1000	3.3854
NONBonded	HX17	0.0498	1.4254	0.0498	1.4254
NONBonded	HX18	0.0498	1.4254	0.0498	1.4254
NONBonded	CX19	0.1200	3.7418	0.1000	3.3854
NONBonded	HX20	0.0498	1.4254	0.0498	1.4254
NONBonded	HX21	0.0498	1.4254	0.0498	1.4254
NONBonded	CX22	0.1200	3.7418	0.1000	3.3854
NONBonded	HX23	0.0498	1.4254	0.0498	1.4254
NONBonded	HX24	0.0498	1.4254	0.0498	1.4254
NONBonded	NX25	0.2384	2.8509	0.2384	2.8509
NONBonded	CX26	0.1200	3.7418	0.1000	3.3854
NONBonded	HX27	0.0498	1.4254	0.0498	1.4254
NONBonded	HX28	0.0498	1.4254	0.0498	1.4254
NONBonded	HX29	0.0498	1.4254	0.0498	1.4254
NONBonded	HX30	0.0498	1.4254	0.0498	1.4254

NONBonded	CX31	0.1200	3.7418	0.1000	3.3854
NONBonded	HX32	0.0498	1.4254	0.0498	1.4254
NONBonded	HX33	0.0498	1.4254	0.0498	1.4254
NONBonded	HX34	0.0498	1.4254	0.0498	1.4254
NONBonded	CX35	0.1200	3.7418	0.1000	3.3854
NONBonded	NX36	0.2384	2.8509	0.2384	2.8509
NONBonded	HX37	0.0498	1.4254	0.0498	1.4254
NONBonded	HX38	0.0498	1.4254	0.0498	1.4254
NONBonded	NX39	0.2384	2.8509	0.2384	2.8509
NONBonded	HX40	0.0498	1.4254	0.0498	1.4254
NONBonded	CX41	0.1200	3.7418	0.1000	3.3854
NONBonded	HX42	0.0498	1.4254	0.0498	1.4254
NONBonded	HX43	0.0498	1.4254	0.0498	1.4254
NONBonded	CX44	0.1200	3.7418	0.1000	3.3854
NONBonded	HX45	0.0498	1.4254	0.0498	1.4254
NONBonded	HX46	0.0498	1.4254	0.0498	1.4254
NONBonded	CX47	0.1200	3.7418	0.1000	3.3854
NONBonded	HX48	0.0498	1.4254	0.0498	1.4254
NONBonded	HX49	0.0498	1.4254	0.0498	1.4254
NONBonded	NX50	0.2384	2.8509	0.2384	2.8509
NONBonded	CX51	0.1200	3.7418	0.1000	3.3854
NONBonded	HX52	0.0498	1.4254	0.0498	1.4254
NONBonded	HX53	0.0498	1.4254	0.0498	1.4254
NONBonded	HX54	0.0498	1.4254	0.0498	1.4254
NONBonded	CX55	0.1200	3.7418	0.1000	3.3854
NONBonded	HX56	0.0498	1.4254	0.0498	1.4254
NONBonded	HX57	0.0498	1.4254	0.0498	1.4254
NONBonded	HX58	0.0498	1.4254	0.0498	1.4254
NONBonded	HX59	0.0498	1.4254	0.0498	1.4254
NONBonded	HX60	0.0498	1.4254	0.0498	1.4254

!Special solute-solute hydrogen bonding potential parameters

!From dna-rna parameter file, not currently in use

!AEXP=4

!REXP=6

!HAEX=4

!AAEX=2

set echo=on message=on end

!DB213 topology file

!

!/var/tmp/xdict_5343.top

!Created by XPLO2D V. 050802/3.3.2 Thu Mar 25 19:23:17 2010 for A. Nonymous

!Auto-generated by XPLO2D from file /var/tmp/xdict_5343.pdb

!You *MUST* check/edit MASSes and CHARGes !!!

!Check DONORs and ACCEptors

!Verify IMPROpers yourself

!DIHEdrals which are not flat are commented out

!

!modified by RJM

!charges from CHARMM

set echo=false end

MASS	HX1	1.00800
MASS	CX2	12.01100
MASS	CX3	12.01100
MASS	CX4	12.01100
MASS	CX5	12.01100
MASS	HX6	1.00800
MASS	CX7	12.01100
MASS	HX8	1.00800
MASS	CX9	12.01100
MASS	CX10	12.01100

```

MASS NX11    14.00700
MASS HX12     1.00800
MASS HX13     1.00800
MASS NX14    14.00700
MASS HX15     1.00800
MASS CX16    12.01100
MASS HX17     1.00800
MASS HX18     1.00800
MASS CX19    12.01100
MASS HX20     1.00800
MASS HX21     1.00800
MASS CX22    12.01100
MASS HX23     1.00800
MASS HX24     1.00800
MASS NX25    14.00700
MASS CX26    12.01100
MASS HX27     1.00800
MASS HX28     1.00800
MASS HX29     1.00800
MASS HX30     1.00800
MASS CX31    12.01100
MASS HX32     1.00800
MASS HX33     1.00800
MASS HX34     1.00800
MASS CX35    12.01100
MASS NX36    14.00700
MASS HX37     1.00800
MASS HX38     1.00800
MASS NX39    14.00700
MASS HX40     1.00800
MASS CX41    12.01100
MASS HX42     1.00800
MASS HX43     1.00800
MASS CX44    12.01100
MASS HX45     1.00800
MASS HX46     1.00800
MASS CX47    12.01100
MASS HX48     1.00800
MASS HX49     1.00800
MASS NX50    14.00700
MASS CX51    12.01100
MASS HX52     1.00800
MASS HX53     1.00800
MASS HX54     1.00800
MASS CX55    12.01100
MASS HX56     1.00800
MASS HX57     1.00800
MASS HX58     1.00800
MASS HX59     1.00800
MASS HX60     1.00800

```

```
autogenerate angles=true end
```

```
RESIdue DB
```

```

{ Note: electrostatics should normally not be used in }
{ crystallographic refinement since it can produce }
{ artefacts. For this reason, all charges are set to }
{ zero by default. Edit them if necessary }

```

```
GROUP
```

```

ATOM H5 TYPE HX1 CHARge 0.1150 END
ATOM C5 TYPE CX2 CHARge -0.1150 END
ATOM C6 TYPE CX3 CHARge -0.1150 END
ATOM C1 TYPE CX4 CHARge 0.1200 END

```

```

ATOM  C2      TYPE CX5      CHARGE -0.1150  END
ATOM  H2      TYPE HX6      CHARGE  0.1150  END
ATOM  C3      TYPE CX7      CHARGE  0.1150  END
ATOM  H3      TYPE HX8      CHARGE  0.1150  END
ATOM  C4      TYPE CX9      CHARGE  0.1200  END
ATOM  C14     TYPE CX10     CHARGE  0.6400  END
ATOM  N114    TYPE NX11     CHARGE -0.8000  END
ATOM  H114    TYPE HX12     CHARGE  0.4600  END
ATOM  H124    TYPE HX13     CHARGE  0.4600  END
ATOM  N24     TYPE NX14     CHARGE -0.7000  END
ATOM  H214    TYPE HX15     CHARGE  0.4400  END
ATOM  C34     TYPE CX16     CHARGE  0.2000  END
ATOM  H314    TYPE HX17     CHARGE  0.0900  END
ATOM  H324    TYPE HX18     CHARGE  0.0900  END
ATOM  C44     TYPE CX19     CHARGE -0.1800  END
ATOM  H414    TYPE HX20     CHARGE  0.0900  END
ATOM  H424    TYPE HX21     CHARGE  0.0900  END
ATOM  C54     TYPE CX22     CHARGE -0.1000  END
ATOM  H514    TYPE HX23     CHARGE  0.2500  END
ATOM  H524    TYPE HX24     CHARGE  0.2500  END
ATOM  N64     TYPE NX25     CHARGE -0.6000  END
ATOM  C74     TYPE CX26     CHARGE -0.3500  END
ATOM  H714    TYPE HX27     CHARGE  0.2500  END
ATOM  H724    TYPE HX28     CHARGE  0.2500  END
ATOM  H734    TYPE HX29     CHARGE  0.2500  END
ATOM  H614    TYPE HX30     CHARGE  0.4500  END
ATOM  C84     TYPE CX31     CHARGE -0.3500  END
ATOM  H814    TYPE HX32     CHARGE  0.2500  END
ATOM  H824    TYPE HX33     CHARGE  0.2500  END
ATOM  H834    TYPE HX34     CHARGE  0.2500  END
ATOM  C11     TYPE CX35     CHARGE  0.6400  END
ATOM  N111    TYPE NX36     CHARGE -0.8000  END
ATOM  H111    TYPE HX37     CHARGE  0.4600  END
ATOM  H121    TYPE HX38     CHARGE  0.4600  END
ATOM  N21     TYPE NX39     CHARGE -0.7000  END
ATOM  H211    TYPE HX40     CHARGE  0.4400  END
ATOM  C31     TYPE CX41     CHARGE  0.2000  END
ATOM  H311    TYPE HX42     CHARGE  0.0900  END
ATOM  H321    TYPE HX43     CHARGE  0.0900  END
ATOM  C41     TYPE CX44     CHARGE -0.1800  END
ATOM  H411    TYPE HX45     CHARGE  0.0900  END
ATOM  H421    TYPE HX46     CHARGE  0.0900  END
ATOM  C51     TYPE CX47     CHARGE -0.1000  END
ATOM  H511    TYPE HX48     CHARGE  0.2500  END
ATOM  H521    TYPE HX49     CHARGE  0.2500  END
ATOM  N61     TYPE NX50     CHARGE -0.6000  END
ATOM  C71     TYPE CX51     CHARGE -0.3500  END
ATOM  H711    TYPE HX52     CHARGE  0.2500  END
ATOM  H721    TYPE HX53     CHARGE  0.2500  END
ATOM  H731    TYPE HX54     CHARGE  0.2500  END
ATOM  C81     TYPE CX55     CHARGE -0.3500  END
ATOM  H811    TYPE HX56     CHARGE  0.2500  END
ATOM  H821    TYPE HX57     CHARGE  0.2500  END
ATOM  H831    TYPE HX58     CHARGE  0.2500  END
ATOM  H611    TYPE HX59     CHARGE  0.4000  END
ATOM  H6      TYPE HX60     CHARGE  0.1150  END

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BOND  H5      C5      BOND  C5      C6      BOND  C5      C4      BOND  C6      C1
BOND  C6      H6      BOND  C1      C2      BOND  C1      C11     BOND  C2      H2
BOND  C2      C3      BOND  C3      H3      BOND  C3      C4      BOND  C4      C14
BOND  C14    N114     BOND  C14    N24     BOND  N114  H114     BOND  N114  H124
BOND  N24    H214     BOND  N24    C34     BOND  C34   H314     BOND  C34   H324
BOND  C34    C44     BOND  C44   H414     BOND  C44   H424     BOND  C44   C54
BOND  C54    H514     BOND  C54   H524     BOND  C54   N64     BOND  N64   C74

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DIHEdral H321 C31 C41 H421 ! flat ? (180 degrees = trans) 182.55
DIHEdral C31 C41 C51 N61 ! flat ? (180 degrees = trans) 187.39
DIHEdral H411 C41 C51 H511 ! flat ? (180 degrees = trans) 184.80
DIHEdral H421 C41 C51 H521 ! flat ? (180 degrees = trans) 188.98
DIHEdral C41 C51 N61 C81 ! flat ? (180 degrees = trans) 176.37
DIHEdral H511 C51 N61 H611 ! flat ? (180 degrees = trans) 181.25
DIHEdral H521 C51 N61 C71 ! flat ? (180 degrees = trans) 178.36
DIHEdral C51 N61 C71 H711 ! flat ? (180 degrees = trans) 185.83
DIHEdral C81 N61 C71 H721 ! flat ? (180 degrees = trans) 189.50
DIHEdral H611 N61 C71 H731 ! flat ? (180 degrees = trans) 185.33
DIHEdral C51 N61 C81 H821 ! flat ? (180 degrees = trans) 183.39
DIHEdral C71 N61 C81 H811 ! flat ? (180 degrees = trans) 178.16
DIHEdral H611 N61 C81 H831 ! flat ? (180 degrees = trans) 181.50

IMPRoper C5 H5 C6 C4 ! chirality or flatness improper 0.53
IMPRoper C6 C5 C1 H6 ! chirality or flatness improper -0.55
IMPRoper C1 C6 C2 C11 ! chirality or flatness improper -0.08
IMPRoper C2 C1 H2 C3 ! chirality or flatness improper -0.55
IMPRoper C3 C2 H3 C4 ! chirality or flatness improper -0.66
IMPRoper C4 C5 C3 C14 ! chirality or flatness improper -0.06
IMPRoper C14 C4 N114 N24 ! chirality or flatness improper -0.03
IMPRoper N114 C14 H114 H124 ! chirality or flatness improper -0.05
IMPRoper N24 C14 H214 C34 ! chirality or flatness improper 0.82
IMPRoper C34 N24 H314 H324 ! chirality or flatness improper 33.96
IMPRoper C44 C34 H414 H424 ! chirality or flatness improper 34.68
IMPRoper C54 C44 H514 H524 ! chirality or flatness improper 35.84
IMPRoper N64 C54 C74 H614 ! chirality or flatness improper -32.22
IMPRoper C74 N64 H714 H724 ! chirality or flatness improper 33.48
IMPRoper C84 N64 H814 H824 ! chirality or flatness improper -33.19
IMPRoper C11 C1 N111 N21 ! chirality or flatness improper 0.03
IMPRoper N111 C11 H111 H121 ! chirality or flatness improper 0.01
IMPRoper N21 C11 H211 C31 ! chirality or flatness improper -0.82
IMPRoper C31 N21 H311 H321 ! chirality or flatness improper 34.05
IMPRoper C41 C31 H411 H421 ! chirality or flatness improper 35.33
IMPRoper C51 C41 H511 H521 ! chirality or flatness improper 36.46
IMPRoper N61 C51 C71 C81 ! chirality or flatness improper 34.45
IMPRoper C71 N61 H711 H721 ! chirality or flatness improper 33.57
IMPRoper C81 N61 H811 H821 ! chirality or flatness improper 33.59

{ Note: edit any DONOrs and ACCEptors if necessary }

END { RESIdue DB }

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Supplemental References

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4. Geen, H.F., R. (1991) Band-selective radiofrequency pulses. *J Magn. Reson.*, **93**, 93-141.
5. Kay, L., Keifer, P. and Saarinen, T. (1992) Pure absorption gradient enhanced heteronuclear single quantum correlation spectroscopy with improved sensitivity. *Journal of the American Chemical Society*, **114**, 10663-10665.