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Supporting Information Table 1: Final energies obtained for the three minimized average structures†

	shift restraints			shift +NOE restraints			NOE restraints			initial structures[b]		
	P	B	A	P	B	A	P	B	A	P	B	A
E_{total}[a]	-2423	-2373	-2426	-2110	-2102	-2079	-2518	-2476	-2298	-2563	-2588	-2489
E_{bond}	75	73	75	85	81	97	67	71	81	69	66	66
E_{angl}	230	241	240	340	346	353	230	217	302	201	191	244
E_{dihe}	173	158	171	199	172	188	154	162	169	136	166	183
E_{impr}	1.71	1.40	1.53	2.18	1.76	2.19	2.57	1.43	2.45	1.12	1.44	3.03
E_{vdw}	-56	-14	-39	26	30	25	-96	-88	-41	-116	-139	-70
E_{shift}	35	45	29	54	63	44	-	-	-	-	-	-
E_{NOE}	-	-	-	42	48	74	29	33	57	-	-	-

† In kcal/mol, final f_{pc} = 5 kcal/mol.ppm^2; scale(NOE)= 50 kcal/mol.Å^2.

[a] Total energy is composed of bond, angle, dihedral, improper, van der Waals and electrostatic, as well as pseudocontact shift and NOE energies where indicated. Bond, angle, dihedral, van der Waals and improper energies are also listed.

b Initial structures (see text); minimized with no experimental restraints

Supporting Information Table 2: RMSD of average structures against families of structures for different models†

		shift restraints			shift +NOE restraints			NOE restraints		
		P	B	A	P	B	A	P	B	A
shift	P	0.29	0.67	1.03	0.80	1.14	1.11	2.20	1.77	1.99
restraints	B	0.68	0.31	1.13	0.94	1.24	1.28	2.20	1.80	1.86
	A	1.06	1.15	0.22	1.20	1.33	0.96	2.33	1.83	1.93
shift + NOE	P	0.78	0.91	1.20	0.38	1.05	0.94	2.10	1.69	1.83
restraints	B	1.14	1.24	1.31	1.02	0.37	1.02	2.14	1.69	2.01
	A	1.14	1.31	0.97	0.95	1.05	0.31	2.19	1.69	1.78
NOE	P	2.18	2.20	2.31	2.10	2.16	2.17	0.46	2.24	2.10
restraints	B	1.65	1.58	1.64	1.49	1.67	1.52	2.47	1.53	1.71
	A	1.98	1.88	1.91	1.82	2.00	1.74	2.07	1.71	0.48
initial	P	1.65	1.67	1.71	1.60	1.70	1.58	2.06	1.65	1.59
structures	B	1.93	2.10	1.92	1.74	1.61	1.54	2.63	1.90	2.32
	A	2.59	2.50	2.54	2.42	2.74	2.55	3.02	2.15	2.47

†In Å, minimized average structure vertically, families of structures (20 for P, B; 10 for A) horizontally; excluding hydrogens and DNA terminal base pairs; see text for definition of P,B and A. See footnote of Suppporting Information Table 1 for details on refinement force constants and initial structures.

Supporting Information Table 3: Structural statistics of the minimized averaged structures and of initial structures†

	shift restraints			shift +NOE restraints			NOE restraints			initial structures		
	P	B	A	P	B	A	P	B	A	P	B	A
rmsd bond [a]	0.017	0.016	0.017	0.018	0.017	0.019	0.016	0.016	0.016	0.016	0.016	0.016
rmsd angle [b]	2.89	2.96	2.97	3.75	3.72	3.74	3.04	2.84	3.57	2.73	3.12	2.68
rmsd impr [c]	4.22	3.81	3.97	4.16	3.43	3.74	4.11	3.32	3.52	2.38	5.29	3.38
rmsd NOE [d]	0.328	0.331	0.355	0.031	0.035	0.043	0.027	0.029	0.038	0.231	0.378	0.292
# NOE [e]	53	54	58	0	0	0	0	0	0	55	87	68
rmsd shift [f]	0.30	0.32	0.30	0.34	0.35	0.43	5.38	7.33	11.08	7.06	57.52	29.94
# shift [g]	28	37	30	38	42	29	230	190	262	197	272	275

†See footnote of Supporting Information Table 1 for details on refinement force constants and initial structures.

[a]r.m.s.d. of bond lengths from ideal geometry (Å)

[b]r.m.s.d. of bond angles from ideal geometry (deg)

[c]r.m.s.d. of improper angles from ideal geometry (deg)

[d]r.m.s.d. of NOE violations from experimental distance restraints (Å)

[e]no. NOE violations > 0.3Å

[f]r.m.s.d. of pseudocontact shifts from experimental pseudocontact shifts (ppm)

[g]no. of shift violations exceeding tol (experimental error) + gradient error (see text)