

BIOCHEMISTRY

including biophysical chemistry & molecular biology

Supporting information for *Biochemistry*, 1994, 33(10), 3055 – 3062, DOI: [10.1021/bi00176a039](https://doi.org/10.1021/bi00176a039)

GEIER
STANGER
3055-3062

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>.

Supplementary Material. Listings of the intermolecular ligand-DNA and ligand-ligand restraints used to derive the molecular model of the 1:1:1 2-ImN:Dst:DNA complex with d(GCCTAACAAGG):d(CCTTGTTAGGC) and achieved distances.^a

2-ImN	DNA	Dst	restraints in Å	achieved distance in Å
	A8 C2H	C(19)H ^b	2.5-3.7	3.71
	A8 C2H	NH-4	1.8-3.7	1.98
	A8 C1'H	NH-4	2.5-3.7	3.71
	A8 C1'H	H3-3	2.5-3.7	3.14
H4-1	G16 C1'H		2.5-3.7	2.53
H4-1	G16 NH ₂ H22 ^c		2.5-4.2	4.25
H4-1	G16 NH ₂ H21		1.8-3.7	2.66
	G16 NH ₂ H22	H3-3	2.5-3.7	2.58
	G16 NH ₂ H21	H3-3	2.5-3.7	2.48
	G16 NH ₂ H22	NH-3	2.5-3.7	2.51
	G16 NH ₂ H21	NH-3	2.5-3.7	3.15
NH-2	G16 NH ₂ H22		3.7-4.2	3.69
NH-2	G16 NH ₂ H21		2.5-4.2	2.84
	C7 C1'H	NH-3	2.5-3.7	2.68
	C7 C1'H	H3-2	2.5-3.7	2.65
NH-2	T17 C1'H		2.5-3.7	2.68
NH-3	A6 C2H		3.7-4.2	3.68
	A6 C2H	NH-2	2.5-3.7	2.72
	A6 C2H	H3-2	2.5-3.7	2.45
	A6 C1'H	NH-2	2.5-3.7	2.56
H3-2	A6 C2H		2.5-3.7	2.52
H3-2	T18 C1'H		2.5-3.7	3.10
NH-3	T18 C1'H		2.5-3.7	2.49
H3-3	A5 C2H		1.8-2.5	2.50
	A5 C2H	NH-1	2.5-3.7	2.69
	A5 C1'H	NH-1	2.5-3.7	2.50
	A5 C1'H	HF	2.5-3.7	2.76
H3-3	A19 C1'H		2.5-3.7	2.96
NH-4	A19 C1'H		2.5-3.7	2.80
NH-4	A19 C2H		2.5-3.7	2.52
C(19)H ^b	A19 C2H		2.5-4.7	2.48
C(19)H ^b	Ligand-Ligand	HF	2.5-4.7	3.15

^a Derived from H₂O NOESY data acquired at 100 msec mixing time.

^b C(19)H protons not stereospecifically assigned. Restraints defined to C(19)H pseudo atoms.

^c Restraints defined to individual NH₂ protons based on initial models derived by defining restraints to NH₂ pseudo atom.