Supplementary Material

Structural changes of Zn(II)bleomycin complexes when bound to DNA hairpins containing the 5'-GT-3' and 5'-GC-3' binding sites studied through NMR spectroscopy

Shelby E. Follett, Sally A. Murray, Azure D. Ingersoll, Teresa M. Reilly, Teresa E. Lehmann*

Supplementary Table S1. Chemical shifts for the bleomycin residues for each of the free Zn(II)BLMs under study with a 1:1 molar ratio for Zn²⁺:BLM.

Residue	Zn(II)BLM-A2 (ppm)	Zn(II)PEP (ppm)	Zn(II)BLM-B2 (ppm)	Zn(II)BLM-A5 (ppm)
Val C ^a H	1.65	1.65	1.66	1.64
Val C ^β H	3.12	3.12	3.13	3.13
Val C ^y H	3.33	3.34	3.33	3.33
Val C ^a CH ₃	0.70	0.70	0.69	0.69
Val C ^γ CH ₃	0.64	0.65	0.65	0.65
Val NH	7.26	7.26	7.29	7.26
Thr C ^a H	3.81	3.82	3.80	3.81
Thr C ^β H	3.73	3.73	3.72	3.72
Thr CH ₃	0.73	0.74	0.73	0.73
Thr NH	7.68	7.68	7.67	7.68
Bit C ^α H ₂	2.91	2.91	2.91	2.91
Bit $C^{\beta}H_2$	3.27	3.28	3.25	3.27
Bit NH	8.07	8.07	8.06	8.07
Ala CαH	3.45	3.44	3.44	3.45
Ala C ^β H _{2a}	2.18	2.17	2.17	2.18
Ala $C^{\beta}H_{2b}$	3.08	3.07	3.07	3.07
Ala NH	7.26	7.26	7.29	7.26
Ala NH _{2a}	6.64	6.63	6.64	6.63
Ala NH _{2b}	7.06	7.06	7.06	7.06
Ala CONH _{2a}	6.82	6.81	6.81	6.83
Ala CONH _{2b}	7.60	7.59	7.60	7.60
Pyr CαH2a	2.59	2.58	2.58	2.59
Pyr C ^a H _{2b}	2.95	2.95	2.96	2.96
Pyr C ^β H	4.21	4.20	4.20	4.22
Pyr CH ₃	2.09	2.09	2.09	2.09
Pyr NH2	6.73	6.72	6.72	6.72
Pyr CONH2a	7.18	7.18	7.18	7.18
Pyr CONH _{2b}	7.60	7.59	7.60	7.60
Hist C2H	7.72	7.72	7.72	7.72
Hist C4H	7.02	7.02	7.01	7.02
Hist C ^a H	5.02	5.02	5.02	5.01
Hist C ^β H	5.14	5.13	5.13	5.14
Mann C1H	4.60	4.59	4.60	4.60
Mann C2H	3.80	3.80	3.79	3.80
Mann C3H	3.74	3.73	3.74	3.74
Mann C4H	3.42	3.41	3.41	3.42
Mann C5H	3.41	3.37	3.41	3.42
Mann C6H	3.68	3.66	3.68	3.67
Mann C6H'	3.51	3.50	3.51	3.51
Mann NH _{2a}	5.62	5.62	5.62	5.62
Mann NH _{2b}	6.27	6.27	6.27	6.27

Residue	Zn(II)BLM-A ₂ (ppm)	Zn(II)PEP	Zn(II)BLM-B ₂ (ppm)	Zn(II)BLM-A5 (ppm)
		(ppm)		
Gul C1H	5.02	5.01	5.01	5.01
Gul C2H	3.77	3.77	3.77	3.77
Mann NH _{2b}	6.27	6.27	6.27	6.27
Gul C1H	5.02	5.01	5.01	5.01
Gul C2H	3.77	3.77	3.77	3.77
Gul C3H	3.75	3.74	3.74	3.75
Gul C4H	3.43	3.43	3.42	3.42
Gul C5H	3.56	3.55	3.55	3.56
Gul C6H	3.43	3.42	3.42	3.43
Gul C6H'	3.33	3.33	3.32	3.33
$^{a}A_{2} C^{\alpha}H_{2}$	3.05			
$A_2 C^{\beta} H_2$	1.85			
$A_2 C^{\gamma} H_2$	3.31			
A ₂ NH	8.66			
PEP $C^{\alpha}H_2$		3.09		
$PEP C^{\beta}H_{2a}$		1.58		
PEP C ^β H _{2b}		1.67		
$PEP C^{\gamma}H_{2a}$		2.51		
PEP $C^{\gamma}H_{2b}$		2.61		
PEP C ⁸ H		4.06		
PEP CH ₃		1.32		
PEP NH (2)		8.45		
$B_2 C^{\alpha} H_{2a}$			3.13	
$B_2 C^{\alpha} H_{2b}$			3.32	
$B_2 C^{\beta} H_{2a}$			1.05	
$B_2 C^{\beta} H_{2b}$			1.36	
$B_2 C^{\gamma} H_{2a}$			0.55	
$B_2 C^{\gamma} H_{2b}$			1.01	
$B_2 C^{\delta} H_{2a}$			<i>b</i> _	
$B_2 C^{\delta} H_{2b}$			2.89	
B2 NH (1)			8.51	
B2 NH (2)				
A5 $C^{\alpha}H_2$				3.22
$A_5 C^{\beta} H_2$				1.71
$A_5 C^{\gamma} H_2$				2.80
$A_5 C^{\delta}H_2$				2.69
A5 $C^{\epsilon}H_2$				1.43
$A_5 C^{\zeta}H_2$				1.44
$A_5 C^{\eta}H_2$				2.75
A5 NH2 (1)				8.64
$A_5 \text{ NH}_2(2)$				-

Supplementary Table S1 (Cont.)

^{*a*}Unassignable. ^{*b*}Red labels indicate tail protons for each Zn(II)BLM.



Figure S1. Base and sugar sections of the NOESY spectra for both free Zn(II)BLM-A₂ and Zn(II)BLM-A₂ (red) bound to each of the DNA strands under study (black). Spectra were acquired at 5 °C in H₂O. OL:Zn(II)BLM in 1:1 molar ratio. Corresponding assignments for the bleomycin cross peaks are located in Supplementary Tables S2 and S3.

F2 (ppm)	F1 (ppm)	Assignment	OL ₁ + Zn(II)BLM-A ₂	OL ₂ + Zn(II)BLM-A ₂
7.26	5.02	Ala NH - Gul C1H ^a	*c	*
7.26	4.56	Ala NH - Mann C1H	*	*
3.74	2.93	Thr $C^{\beta}H$ - Bit $C^{\alpha}H_{2b}$		*
7.68	1.65	Thr NH - Val CαH		*
7.67	3.12	Thr NH - Val C ^β H	*	*
7.68	3.33	Thr NH - Val C ^y H	*	*
7.68	0.70	Thr NH - Val C ^a CH ₃	*	*
8.07	3.81	Bit NH - Thr C ^a H		*
8.07	3.72	Bit NH - Thr C ^β H	*	*
8.07	0.73	Bit NH - Thr CH ₃	*	*
8.07	7.74	Bit NH - Thr NH	*	*
3.31	2.90	A2 C γ H2 - Bit C α H2	*	*
3.44	2.58	Ala C ^a H - Pyr C ^a H _{2a}	*	
3.45	2.93	Ala C ^a H - Pyr C ^a H _{2b}		*
3.10	2.58	Ala C ^β H _{2b} - Pyr C ^α H _{2a}		
7.06	2.93	Ala NH _{2b} - Bit C ^a H _{2b}		
7.06	3.56	Ala NH _{2b} - Gul C5H	*	
7.06	4.20	Ala NH2b - Pyr CβH		*
2.94	2.17	Pyr C ^α H _{2b} - Ala C ^β H _{2a}		
2.58	2.18	Pyr C ^a H _{2a} - Ala C ^β H _{2a}		
4.22	2.17	Pyr C ^β H - Ala C ^β H _{2a}		
4.22	3.08	Pyr C ^β H - Ala C ^β H _{2b}		*
4.20	3.45	Pyr C ^β H - Ala C ^α H		
4.19	3.74	Pyr C ^β H - Mann C5H	*	*
4.22	3.80	Pyr C ^β H - Mann C2H	*	*
7.73	1.64	Hist C2H - Val C ^a H	*	*
7.72	4.22	Hist C2H - Pyr C ^β H	*	*
7.72	2.92	Hist C2H - Bit C ^{\alpha} H ₂	*	*
7.72	3.08	Hist C2H - Ala C ^β H _{2b}	*	*
7.72	0.68	Hist C2H - Val C ^a CH ₃	*	*
7.02	0.69	Hist C4H - Val C ^a CH ₃		*
7.02	0.64	Hist C4H - Val C ^Y CH ₃	*	
7.02	1.64	Hist C4H - Val C ^a H		*
7.01	3.11	Hist C4H - Val C ^β H	*	*
7.02	3.33	Hist C4H - Gul C6H'		*
7.02	3.44	Hist C4H - Gul C6H	*	*
7.02	3.56	Hist C4H - Gul C5H		*
7.01	5.01	Hist C4H - Gul C1H	*	
3.80	2.93	Mann C2H - Bit C ^a H _{2b}		*
3.41	5.02	Mann C4H - Gul C1H	*	*
3.51	5.02	Mann C6H' - Gul C1H		*
5.62	2.09	Mann NH _{2a} - Pyr CH ₃	*	*
6.28	2.09	Mann NH _{2b} - Pyr CH ₃	*	
5.02	4.56	Gul C1H - Mann C1H		
3.76	3.06	Thr $C^{\beta}H - Ala C^{\beta}H_{2b}b$	$+^d$	
7.54	0.66	Thr NH – Val CYCH ₃	+	
8.08	0.66	Bit NH – Val C ^Y CH ₃	+	
5.12	4.57	Hist C ^p H – Mann C1H	+	

Supplementary Table S2. Inter-residue intramolecular NOEs for free Zn(II)BLM-A2 and Zn(II)BLM-A2 bound to both OLs. Spectra were acquired at 5 °C in H2O. OL:Zn(II)BLM in 1:1 molar ratio. Missing NOE (*) and new NOE (+) connections upon DNA binding correspond to Figures 3, 4, 5, and S1.

F2 (ppm)	F1 (ppm)	Assignment	$OL_1 + Zn(II)BLM-A_2$	$OL_2 + Zn(II)BLM-A_2$
7.74	0.75	Hist C2H – Thr CH3	+	
7.75	3.75	Hist C2H – Thr C $^{\beta}$ H	+	
3.19	2.61	Val C ^β H – Pyr C ^α H _{2a}		+
7.37	3.07	Val NH – Ala C ^β H _{2b}		+
7.36	1.75	Val NH – $A_2 C^{\beta} H$		+
3.76	3.17	Thr $C^{\beta}H$ – Val $C^{\beta}H$		+
7.69	3.10	Thr NH – Ala C ^β H _{2b}		+
3.45	1.79	Ala $C^{\alpha}H - A_2 C^{\beta}H_2$		+
3.10	4.20	Ala C ^β H _{2b} – Pyr C ^β H		+
2.60	1.78	Pyr $C^{\alpha}H_{2a}$ – A ₂ $C^{\beta}H_{2}$		+
2.60	3.05	Pyr C $^{\alpha}$ H _{2a} – A ₂ C $^{\alpha}$ H ₂		+
2.96	3.46	$Pvr C^{\alpha}H_{2b} - Ala C^{\alpha}H$		+

Supplementary Table S2 (Cont.)

^{*a*}Blue colored labels indicate that the inter-residue NOE was detected for the free Zn(II)BLM-A₂. ^{*b*}Pink colored labels indicated that the NOE is only detected when the specified OL is bound. ^{*c*}Asterisks (*) indicate that the specific NOE is missing upon complexation with the specified OL, ^{*d*}Plus (+) indicates that the specific NOE connection is found upon complexation with the specified OL. The color coding of the NOE assignments corresponds to the color coding for Figures 3, 4, and 5.

F2 (ppm)	F1 (ppm)	Assignment	$OL_1 + Zn(II)BLM-A_2$	OL ₂ + Zn(II)BLM-A ₂
1.65	0.64	Val C ^a H - Val C ^y CH ₃ ^a	* c	*
1.65	0.69	Val C ^a H - Val C ^a CH ₃		
3.12	0.64	Val C ^β H - Val C ^γ CH ₃		
3.12	0.69	Val C ^β H - Val C ^α CH ₃	*	*
3.12	1.65	Val C ^β H - Val C ^α H		*
3.33	1.65	Val C ^γ H - Val C ^α H	*	
3.32	0.65	Val CYH - Val CYCH3		
3.33	3.12	Val C ^γ H - Val C ^β H	*	*
7.26	1.65	Val NH - Val C ^a H	*	*
7.25	3.33	Val NH - Val C ^y H	*	*
7.26	3.12	Val NH - Val C ^β H		*
7.27	0.71	Val NH -Val C ^a CH ₃	*	*
7.26	0.64	Val NH -Val CYCH3		*
3.81	0.73	Thr C ^a H - Thr CH ₃		
3.71	0.73	Thr C ^β H - Thr CH ₃		
3.87	3.74	Thr $C^{\alpha}H$ -Thr $C^{\beta}H$	*	*
7.68	3.72	Thr NH - Thr C ^β H	*	*
7.67	3.81	Thr NH - Thr C ^a H		*
3.22	2.92	Bit $C^{\beta}H_{2b}$ - Bit $C^{\alpha}H_{2b}$	*	*
3.24	2.91	Bit $C^{\beta}H_{2a}$ - Bit $C^{\alpha}H_{2a}$		
8.07	3.30	Bit NH - Bit $C^{\beta}H_{2b}$	*	*
8.08	3.25	Bit NH - Bit $C^{\beta}H_{2a}$		
8.07	2.90	Bit NH - Bit C ^α H ₂		*
3.05	1.85	$A_2 C^{\alpha}H_2$ - $A_2 C^{\beta}H_2$		
3.29	1.85	$A_2 C^{\gamma}H_2$ - $A_2 C^{\beta}H_2$		
8.66	3.29	$A_2 NH - A_2 C^{\gamma}H_2$		
3.45	2.18	Ala C ^α H - Ala C ^β H _{2a}		
3.45	3.08	Ala C ^α H - Ala C ^β H _{2b}		
3.08	2.18	Ala $C^{\beta}H_{2b}$ - Ala $C^{\beta}H_{2a}$		
7.06	3.08	Ala NH _{2b} - Ala C ^β H _{2b}		*
7.60	6.82	Ala CONH _{2b} - Ala CONH _{2a}		
7.06	6.64	Ala NH2b - Ala NH2a		
7.06	3.45	Ala NH _{2b} - Ala C ^α H		*
2.96	2.58	Pyr C ^a H _{2b} - Pyr C ^a H _{2a}		
4.23	2.59	Pyr C ^β H - Pyr C ^α H _{2a}		
4.20	2.93	Pyr C ^β H - Pyr C ^α H _{2b}		
6.72	2.10	Pyr NH ₂ - Pyr CH ₃		
7.60	7.18	Pyr CONH2b - Pyr CONH2a		
5.14	5.02	Hist C ^β H - Hist C ^α H		
7.72	7.02	Hist C ² H - Hist C4H		
3.80	3.74	Mann C2H - Mann C3H	*	*
3.80	3.44	Mann C2H - Mann C4H	*	
3.77	4.60	Mann C2H - Mann C1H		*
3.75	4.60	Mann C3H - Mann C1H	*	*
3.41	4.56	Mann C4H - Mann C1H		
3.41	3.73	Mann C5H - Mann C3H	*	*
3.68	3.42	Mann C6H - Mann C4H	*	*
3.52	3.42	Mann C6H' - Mann C4H	*	*

Supplementary Table S3. Intra-residue intramolecular NOEs for free Zn(II)BLM-A2 and Zn(II)BLM-A2 bound to both OLs. Spectra were acquired at 5 °C in H2O. OL:Zn(II)BLM in 1:1 molar ratio. Missing NOE (*) and new NOE (+) connections upon DNA binding correspond to Figure S1.

Supprimentary Table 55 (Cont.)				
F2 (ppm)	F1 (ppm)	Assignment	$OL_1 + Zn(II)BLM-A_2$	$OL_2 + Zn(II)BLM-A_2$
3.68	3.51	Mann C6H - Mann C6H'	*	*
6.27	5.62	Mann NH2b - Mann NH2a		
5.02	3.42	Gul C1H - Gul C4H		
5.02	3.77	Gul C1H - Gul C2H		
5.01	3.56	Gul C1H - Gul C5H		
3.77	3.43	Gul C2H - Gul C4H	*	*
3.75	5.01	Gul C3H - Gul C1H	*	*
3.74	3.44	Gul C3H - Gul C4H	*	*
3.75	3.56	Gul C3H - Gul C5H	*	*
3.44	3.56	Gul C4H - Gul C5H	*	*
3.42	3.55	Gul C6H - Gul C5H	*	*
3.55	3.33	Gul C5H - Gul C6H'	*	*
3.55	3.43	Gul C5H - Gul C6H	*	*
3.42	3.33	Gul C6H - Gul C6H'	*	*
8.57	3.25	$A_2 NH - A_2 C^{\beta}H_2^{b}$	$+^d$	
7.60	2.57	Pyr CONH2b – Pyr C¤H2a	+	
7.60	2.97	Pyr CONH _{2b} – Pyr C ^a H _{2b}	+	

Supplementary Table S3 (Cont.)

^{*a*}Blue colored labels indicate that the inter-residue NOE was detected for the free Zn(II)BLM-A₂. ^{*b*}Pink colored labels indicated that the NOE is only detected when the specified OL is bound. ^{*c*}Asterisks (*) indicate that the specific NOE is missing upon complexation with the specified OL, ^{*d*}Plus (+) indicates that the specific NOE connection is found upon complexation with the specified OL.



Figure S2. Base and sugar sections of the NOESY spectra for both free Zn(II)PEP (red) and Zn(II)PEP bound to each of the OLs under study (black). Spectra were acquired at 5 °C in H₂O. OL:Zn(II)BLM in 1:1 molar ratio. Corresponding assignments for the bleomycin cross peaks are located in Supplementary Tables S4 and S5.

F2 (ppm)	F1 (ppm)	Assignment	OL ₁ + Zn(II)PEP	$OL_2 + Zn(II)PEP$
3.13	4.57	Val C ^β H - Mann C1H ^a	$*_{\mathcal{C}}$	*
3.33	5.01	Val C ^y H - Gul C1H	*	*
0.64	4.56	Val C ^Y CH3 - Mann C1H	*	*
7.27	2.09	Ala NH - Pyr CH ₃	*	*
7.26	4.56	Ala NH - Mann C1H		*
7.25	5.02	Ala NH - Gul C1H/Hist CªH		*
7.26	3.42	Ala NH - Gul C6H		*
3.83	3.33	Thr C ^a H - Gul C6H'	*	*
3.73	2.09	Thr C ^β H - Pyr CH ₃	*	*
3.73	2.93	Thr $C^{\beta}H$ - Bit $C^{\alpha}H_{2b}$	*	*
7.68	0.65	Thr NH - Val C ^Y CH ₃		*
7.68	0.69	Thr NH - Val C ^a CH ₃	*	*
7.68	1.65	Thr NH - Val C¤H		*
7.68	3.13	Thr NH - Val C ^β H	*	*
7.68	3.34	Thr NH - Val CYH	*	*
8.07	0.74	Bit NH - Thr CH3		*
8.07	3.73	Bit NH - Thr C ^β H	*	
8.07	3.82	Bit NH - Thr C ^a H		*
8.07	7.67	Bit NH - Thr NH	*	*
2.59	2.17	PEP $C^{\gamma}H_{2b}$ - Ala $C^{\beta}H_{2a}$	*	*
2.55	2.17	PEP C γ H _{2a} - Ala C β H _{2a}	*	*
3.44	2.58	Ala C ^a H - Pyr C ^a H _{2a}		*
3.45	2.93	Ala C ^a H -Bit C ^a H _{2b}		*
3.08	2.58	Ala $C^{\beta}H_{2b}$ - Pyr $C^{\alpha}H_{2a}$		*
3.05	2.95	Ala $C^{\beta}H_{2b}$ - Pyr $C^{\alpha}H_{2b}$	*	*
3.06	1.67	Ala C ^β H _{2b} - PEP C ^β H _{2b}	*	*
7.06	2.93	Ala NH _{2b} - Bit C ^α H _{2b}		*
7.06	3.55	Ala NH _{2b} - Gul C5H		*
7.06	4.20	Ala NH _{2b} - Pyr C ^β H		*
6.81	2.57	Ala CONH2a - Pyr C¤H2a	*	*
2.57	2.17	Pyr C ^a H _{2b} - Ala C ^β H _{2a}	*	*
4.20	2.17	Pyr C ^β H - Ala C ^β H _{2a}		
4.20	3.07	Pyr C ^β H - Ala C ^β H _{2b}		
4.19	3.44	Pyr C ^β H - Ala C ^α H		*
4.21	3.79	Pyr C ^β H - Mann C2H	*	*
4.19	3.73	Pyr C ^β H - Mann C5H	*	*
6.72	5.60	Pyr NH2 - Mann NH2a	*	*
7.18	6.67	Pyr CONH2a - Ala NH2a	*	*
7.72	1.65	Hist C2H - Val CªH		*
7.72	0.69	Hist C2H - Val C ^a CH ₃		*
7.72	2.17	Hist C2H - Ala C ^β H _{2a}	*	*
7.72	2.92	Hist C2H - Bit C ^a H _{2b}	*	*
7.72	3.08	Hist C2H - Ala C ^β H _{2b}	*	*
7.72	3.44	Hist C2H - Ala C ^a H	*	*
7.72	4.20	Hist C2H - Pyr C ^β H	*	*
7.72	7.26	Hist C2H - Val NH	*	*
7.02	0.65	Hist C4H - Val C ^Y CH ₃	*	
7.02	0.69	Hist C4H - Val C ^a CH ₃		*

Supplementary Table S4. Inter-residue intramolecular NOEs for free Zn(II)PEP and Zn(II)PEP bound to both OLs. Spectra were acquired at 5 °C in H₂O. OL:Zn(II)BLM in 1:1 molar ratio. Missing NOE (*) and new NOE (+) connections upon DNA binding correspond to Figures 3, 4, 5, and S2.

F2 (ppm)	F1 (ppm)	Assignment	OL1 + Zn(II)PEP	OL ₂ + Zn(II)PEP
7.02	1.65	Hist C4H - Val C ^a H		*
7.01	3.11	Hist C4H - PEP C ^a H ₂	*	*
7.02	3.32	Hist C4H - Gul C6H'		*
7.01	3.42	Hist C4H - Gul C6H		
7.02	3.56	Hist C4H - Gul C5H		
7.02	4.56	Hist C4H - Mann C1H	*	*
7.01	5.01	Hist C4H - Gul C1H		*
5.14	4.56	Hist C ^β H - Mann C1H	*	*
3.80	2.93	Mann C2H - Bit C ^a H _{2b}	*	*
3.41	5.01	Mann C4H - Gul C1H		
3.41	2.09	Mann C ⁴ H/Gul C6H - Pyr CH ³	*	*
3.65	5.01	Mann C6H - Gul C1H	*	*
3.50	5.01	Mann C6H' - Gul C1H	*	*
5.62	2.09	Mann NH _{2a} - Pyr CH ₃	*	*
6.27	2.09	Mann NH _{2b} - Pyr CH ₃		
5.01	4.56	Gul C1H - Mann C1H		*
3.75	4.60	Gul C3H - Mann C1H	*	*
3.55	4.57	Gul C5H - Mann C1H	*	*
6.77	1.48	Pyr NH ₂ – Val C $^{\alpha}$ H b	$+^d$	
7.75	5.63	Hist C2H – Mann NH _{2a}	+	
7.73	0.75	Hist C2H – Thr CH ₃	+	
7.04	3.78	Hist C4H – Thr C $^{\beta}$ H		+
7.03	4.03	Hist C4H – PEP C ^₅ H		+

Supplementary Table S4 (Cont.)

^{*a*}Blue colored labels indicate that the inter-residue NOE was detected for the free Zn(II)PEP. ^{*b*}Pink colored labels indicated that the NOE is only detected when the specified OL is bound. ^{*c*}Asterisks (*) indicate that the specific NOE is missing upon complexation with the specified OL, ^{*d*}Plus (+) indicates that the specific NOE connection is found upon complexation with the specified OL. The color coding of the NOE assignments corresponds to the color coding for Figures 3, 4, and 5.

F2 (ppm)	F1 (ppm)	Assignment	OL1 + Zn(II)PEP	OL ₂ + Zn(II)PEP
1.65	0.64	Val C ^a H - Val C ^y CH3 ^a		
1.65	0.70	Val C ^a H - Val C ^a CH ₃	$*_{C}$	*
3.12	0.65	Val C ^β H - Val C ^γ CH ₃		
3.12	0.69	Val C ^β H - Val C ^α CH ₃	*	*
3.12	1.65	Val C ^β H - Val C ^α H		*
3.33	0.64	Val CYH - Val CYCH3		
3.33	0.70	Val C ^Y H - Val C ^a CH ₃	*	*
3.33	1.65	Val C ^γ H - Val C ^α H		
3.33	3.12	Val $C^{\gamma}H$ - Val $C^{\beta}H$		*
7.25	0.64	Val NH -Val CYCH3		*
7.25	0.70	Val NH -Val C ^a CH ₃	*	*
7.25	1.65	Val NH - Val CªH	*	*
7.27	3.12	Val NH - Val C ^β H		*
7.26	3.34	Val NH - Val C ^y H	*	*
3.82	0.74	Thr C ^a H - Thr CH ₃		*
3.82	3.73	Thr $C^{\alpha}H$ - Thr $C^{\beta}H$	*	*
3.72	0.74	Thr C ^β H - Thr CH ₃		
7.68	3.72	Thr NH - Thr C ^β H	*	*
7.67	3.82	Thr NH - Thr CαH		*
3.25	2.92	Bit $C^{\beta}H_{2a}$ - Bit $C^{\alpha}H_{2b}$		
3.30	2.93	Bit $C^{\beta}H_{2b}$ - Bit $C^{\alpha}H_{2b}$	*	*
3.31	3.25	Bit $C^{\beta}H_{2b}$ -Bit $C^{\beta}H_{2a}$	*	*
8.07	2.90	Bit NH - Bit C ^a H ₂		*
8.07	3.25	Bit NH - Bit C ^β H _{2a}		*
8.08	3.31	Bit NH - Bit $C^{\beta}H_{2b}$	*	*
3.09	1.58	$PEP C^{\alpha}H_2 - PEP C^{\beta}H_{2a}$		
3.09	1.67	$PEP C^{\alpha}H_2 - PEP C^{\beta}H_{2b}$	*	*
1.67	1.58	$PEP C^{\beta}H_{2b} - PEP C^{\beta}H_{2a}$	*	*
2.62	1.58	$PEP C^{\gamma}H_{2b} - PEP C^{\beta}H_{2a}$	*	
2.51	1.58	$PEP C^{\gamma}H_{2a} - PEP C^{\beta}H_{2a}$		
2.62	1.67	$PEP C^{\gamma}H_{2b} - PEP C^{\beta}H_{2b}$		*
2.51	1.68	$PEP C^{\gamma}H_{2a} - PEP C^{\beta}H_{2b}$	*	*
2.61	2.51	$PEP C^{\gamma}H_{2b} - PEP C^{\gamma}H_{2a}$		*
4.06	1.32	PEP C ^o H - PEP CH ₃		
8.45	3.11	$PEP NH(2) - PEP C^{\alpha}H_2$		*
3.44	2.17	Ala $C^{\alpha}H$ - Ala $C^{\beta}H_{2a}$		
3.44	3.07	Ala $C^{\alpha}H$ - Ala $C^{\beta}H_{2b}$		
3.07	2.17	Ala C ^β H _{2b} - Ala C ^β H _{2a}		
7.06	3.07	Ala NH2b - Ala C ^β H2b		*
7.06	3.44	Ala NH _{2b} - Ala C $^{\alpha}$ H	*	*
7.06	6.63	Ala NH2b - Ala NH2a		
7.59	6.81	Ala CONH _{2b} - Ala		
		CONH _{2a}		
7.59	7.18	Pyr CONH _{2b} - Pyr		
	2	CONH _{2a}		¥.
7.59	2.57	$Pyr CONH_{2b} - Pyr C^{\alpha}H_{2a}$		r v.
7.59	2.95	$Pyr CONH_{2b} - Pyr C^{\alpha}H_{2b}$		r
2.95	2.58	PVr C ^a H2b - PVr C ^a H2a		

Supplementary Table S5. Intra-residue intramolecular NOEs for free Zn(II)PEP and Zn(II)PEP bound to both OLs. Spectra were acquired at 5 °C in H₂O. OL:Zn(II)BLM in 1:1 molar ratio. Missing NOE (*) and new NOE (+) connections upon DNA binding correspond to Figure S2.

F2 (ppm)	F1 (ppm)	Assignment	$OL_1 + Zn(II)PEP$	OL ₂ + Zn(II)PEP
4.22	2.57	Pyr C ^β H - Pyr C ^α H _{2a}		
4.20	2.94	Pyr C ^β H - Pyr C ^α H _{2b}		
6.72	2.09	Pyr NH ₂ - Pyr CH ₃		
7.72	7.02	Hist C2H - Hist C4H		
7.02	5.13	Hist C4H - Hist C ^β H	*	*
5.14	5.02	Hist $C^{\beta}H$ - Hist $C^{\alpha}H$		
3.80	3.73	Mann C2H - Mann C3H	*	*
3.80	3.43	Mann C2H - Mann C4H	*	
3.80	4.60	Mann C2H - Mann C1H	*	*
3.73	3.41	Mann C3H - Mann C4H	*	*
3.41	4.56	Mann C4H - Mann C1H	*	*
3.65	4.58	Mann C6H - Mann C1H	*	*
3.67	3.50	Mann C6H - Mann C6H'	*	
3.67	3.42	Mann C6H - Mann C4H	*	*
3.51	3.42	Mann C6H' - Mann C4H	*	*
3.50	4.56	Mann C6H' - Mann C1H	*	*
6.27	5.62	Mann NH2b - Mann NH2a		
5.01	3.77	Gul C1H - Gul C2H		
5.02	3.56	Gul C1H - Gul C5H		*
3.77	3.56	Gul C2H - Gul C5H	*	*
3.77	3.33	Gul C2H - Gul C6H'	*	*
3.77	3.43	Gul C2H - Gul C4H	*	*
3.74	3.32	Gul C3H - Gul C6H'	*	*
3.74	3.43	Gul C3H - Gul C4H	*	*
3.75	3.56	Gul C3H - Gul C5H	*	*
3.75	5.01	Gul C3H - Gul C1H	*	*
3.55	3.42	Gul C5H - Gul C6H	*	
3.55	3.33	Gul C5H - Gul C6H'	*	*
3.42	3.33	Gul C6H - Gul C6H'	*	*
7.49	0.78	Thr NH – Thr CH_{3}^{b}	$+^d$	
4.05	1.65	$PEP C^{\delta}H - PEP C^{\beta}H_{2b}$	+	

Supplementary Table S5 (Cont.)

^{*a*}Blue colored labels indicate that the inter-residue NOE was detected for the free Zn(II)PEP. ^{*b*}Pink colored labels indicated that the NOE is only detected when the specified OL is bound. ^{*c*}Asterisks (*) indicate that the specific NOE is missing upon complexation with the specified OL, ^{*d*}Plus (+) indicates that the specific NOE connection is found upon complexation with the specified OL.



Figure S3. Base and sugar sections of the NOESY spectra for both free Zn(II)BLM-B₂ (red) and Zn(II)BLM-B₂ bound to each of the OLs under study (black). Spectra were acquired at 5 °C in H₂O. OL:Zn(II)BLM in 1:1 molar ratio. Corresponding assignments for the bleomycin cross peaks are located in Supplementary Tables S6 and S7.

F2 (ppm)	F1 (ppm)	Assignment	$OL_1 + Zn(II)BLM-B_2$
3.79	2.93	Thr $C^{\alpha}H$ - Bit $C^{\alpha}H_{2b}a$	*c
3.73	2.93	Thr $C^{\beta}H$ - Bit $C^{\alpha}H_{2b}$	*
7.67	0.69	Thr NH - Val C ^a CH ₃	*
7.67	1.66	Thr NH - Val CαH	
7.67	3.33	Thr NH - Val C ^Y H	*
7.67	3.13	Thr NH - Val C ^β H	*
8.06	0.73	Bit NH - Thr CH ₃	
8.06	3.72	Bit NH - Thr C ^β H	*
8.06	3.81	Bit NH - Thr C ^a H	
8.05	7.68	Bit NH - Thr NH	*
3.44	2.93	Ala C ^α H - Pyr C ^α H _{2b}	
3.06	2.58	Ala C ^β H _{2b} - Pyr C ^α H _{2a}	
7.06	4.21	Ala NH ₂ _b - Pyr C ^β H	
7.06	3.55	Ala NH _{2b} - Gul C5H	
7.06	2.93	Ala NH _{2b} - Bit C ^α H _{2b}	
7.29	5.01	Ala NH - Gul C1H/Hist CαH	*
7.29	4.56	Ala NH - Mann C1H	*
6.63	3.55	Ala NH _{2a} - Gul C5H	*
2.95	2.17	Pyr C ^α H _{2b} - Ala C ^β H _{2a}	
4.21	3.79	Pyr C ^β H - Mann C2H	*
4.20	3.44	Pyr C ^β H - Ala C ^α H	
4.19	3.07	Pyr C ^β H - Ala C ^β H _{2b}	*
4.21	2.17	Pyr C ^β H - Ala C ^β H _{2a}	
7.71	4.21	Hist C2H - Pyr C ^β H	*
7.01	3.33	Hist C4H - Gul C6H'	*
7.01	3.42	Hist C4H - Gul C6H	*
7.01	3.56	Hist C4H - Gul C5H	*
7.01	0.69	Hist C4H - Val C ^a CH ₃	
7.01	1.66	Hist C4H - Val C ^α H	*
3.41	5.01	Mann C4H - Gul C1H	
6.27	2.09	Mann NH _{2b} - Pyr CH ₃	*
7.50	0.66	Thr NH – Val C γ CH $_3^b$	$+^d$
8.11	0.75	Hist C2H – Thr CH ₃	+

Supplementary Table S6. Inter-residue intramolecular NOEs for free Zn(II)BLM-B2 and Zn(II)BLM-B2 bound to OL1. Spectra were acquired at 5 °C in H2O. OL:Zn(II)BLM in 1:1 molar ratio. Missing NOE (*) and new NOE (+) connections upon DNA binding correspond to Figures 3, 4, and S3.

^{*a*}Blue colored labels indicate that the inter-residue NOE was detected for the free Zn(II)BLM-B₂. ^{*b*}Pink colored labels indicated that the NOE is only detected when the OL₁ is bound. ^{*c*}Asterisks (*) indicate that the specific NOE is missing upon complexation with OL₁, ^{*d*}Plus (+) indicates that the specific NOE connection is found upon complexation with OL₁. The color coding of the NOE assignments corresponds to the color coding for Figures 3 and 4.

F2 (ppm)	F1 (ppm)	Assignment	$OL_1 + Zn(II)BLM-B_2$
1.66	0.64	Val C ^{\alpha} H - Val C ^{\alpha} CH3 ^a	· · · · · · · · · · · · · · · · · · ·
3.13	0.65	Val C ^β H - Val C ^γ CH ₃	
3.13	0.69	Val C ^β H - Val C ^α CH ₃	*c
3.13	1.66	Val C ^β H - Val C ^α H	
3.33	1.66	Val CYH - Val CaH	
3.32	0.64	Val CYH - Val CYCH3	
3.32	3.13	$Val C^{\gamma}H$ - $Val C^{\beta}H$	*
7.29	0.64	Val NH -Val CYCH3	
7.29	1.66	Val NH - Val CªH	*
7.29	3.33	Val NH - Val C ^y H	
7.29	3.13	Val NH - Val C ^β H	
3.81	0.74	Thr C ^a H - Thr CH ₃	
3.72	3.80	Thr C ^α H -Thr C ^β H	*
3.71	0.73	Thr C ^β H - Thr CH ₃	
7.67	3.81	Thr NH - Thr CαH	
7.67	3.72	Thr NH - Thr $C^{\beta}H$	*
3.24	2.90	Bit $C^{\beta}H_{2a}$ - Bit $C^{\alpha}H_2$	
8.06	2.88	Bit NH - Bit C ^{\alpha} H _{2a}	
8.06	3.26	Bit NH - Bit C ^β H _{2b}	
3.12	1.36	$B_2 C^{\alpha} H_{2a}$ - $B_2 C^{\beta} H_{2b}$	
1.37	1.05	$B_2 C^{\beta} H_{2b}$ - $B_2 C^{\beta} H_{2a}$	
1.01	0.55	$B_2 C^{\gamma} H_{2b}$ - $B_2 C^{\gamma} H_{2a}$	
2.89	1.34	$B_2 C^{\delta}H_{2b}$ - $B_2 C^{\beta}H_{2b}$	
8.51	1.36	B2 NH - B2 $C^{\beta}H_{2b}$	
8.51	3.12	B2 NH - B2 $C^{\alpha}H_{2a}$	
3.44	2.17	Ala C ^α H - Ala C ^β H _{2a}	
3.45	3.07	Ala C ^α H - Ala C ^β H _{2b}	
3.07	2.17	Ala $C^{\beta}H_{2b}$ - Ala $C^{\beta}H_{2a}$	
6.64	3.44	Ala NH2a - Ala C ^α H	
7.06	6.64	Ala NH _{2b} - Ala NH _{2a}	
7.60	6.81	Ala CONH2b - Ala CONH2a	
7.60	2.95	Pyr CONH _{2b} - Pyr C ^a H _{2b}	
7.60	2.58	Pyr CONH _{2b} - Pyr C ^a H _{2a}	*
7.06	3.44	Ala NH2b - Ala CªH	*
7.06	3.07	Ala NH _{2b} - Ala C ^β H _{2b}	*
2.93	2.58	Pyr C $^{\alpha}H_{2b}$ - Pyr C $^{\alpha}H_{2a}$	
4.21	2.95	$Pyr C^{\beta}H$ - $Pyr C^{\alpha}H_{2b}$	
4.21	2.58	$Pyr C^{\beta}H$ - $Pyr C^{\alpha}H_{2a}$	
6.72	2.09	Pyr NH ₂ - Pyr CH ₃	
7.59	7.18	Pyr CONH2b - Pyr CONH2a	
5.13	5.02	Hist $C^{\beta}H$ - Hist $C^{\alpha}H$	*
3.79	4.60	Mann C2H - Mann C1H	
3.78	3.43	Mann C2H - Mann C4H	*
3.41	4.56	Mann C4H - Mann C1H	
3.41	3.68	Mann C5H - Mann C6H	*
3.67	3.51	Mann C6H - Mann C6H'	*
3.51	3.68	Mann C6H' - Mann C6H	*
3.51	3.42	Mann C6H' - Mann C4H	*

Supplementary Table S7. Intra-residue intramolecular NOEs for free Zn(II)BLM-B2 and Zn(II)BLM-B2 bound to OL1. Spectra were acquired at 5 °C in H2O. OL:Zn(II)BLM in 1:1 molar ratio. Missing NOE (*) and new NOE (+) connections upon DNA binding correspond to Figure S3.

Supplementally Tuble 57 (Conti)					
F2 (ppm)	F1 (ppm)	Assignment	$OL_1 + Zn(II)BLM-B_2$		
6.27	5.62	Mann NH _{2b} - Mann NH _{2a}			
5.01	3.77	Gul C1H - Gul C2H			
3.73	3.41	Gul C3H - Gul C4H	*		
3.43	3.55	Gul C4H - Gul C5H	*		
3.42	3.33	Gul C4H - Gul C6H'	*		
3.56	5.01	Gul C5H - Gul C1H			
3.55	3.42	Gul C5H - Gul C6H	*		
3.54	3.33	Gul C5H - Gul C6H'	*		
3.55	3.75	Gul C5H - Gul C3H	*		
3.40	3.73	Gul C6H - Gul C3H	*		
3.32	3.42	Gul C6H' - Gul C6H	*		
7.74	7.07	Hist C2H – Hist C4H ^b	$+^d$		
5.02	3 41	Gul C1H – Gul C4H	+		

Supplementary Table S7 (Cont.)

^{*a*}Blue colored labels indicate that the inter-residue NOE was detected for the free Zn(II)BLM-B₂. ^{*b*}Pink colored labels indicated that the NOE is only detected when OL₁ is bound. ^{*c*}Asterisks (*) indicate that the specific NOE is missing upon complexation with OL₁, ^{*d*}Plus (+) indicates that the specific NOE connection is found upon complexation with OL₁.



Figure S4. Base and sugar sections of the NOESY spectra for both free Zn(II)BLM-A₅ (red) and Zn(II)BLM-A₅ bound to each of the DNA strands under study (black). Spectra were acquired at 5 °C in H₂O. OL:Zn(II)BLM in 1:1 molar ratio. Corresponding assignments for the bleomycin cross peaks are located in Supplementary Tables S8 and S9.

F2 (ppm)	F1 (ppm)	Assignment	OL ₁ + Zn(II)BLM-A ₅
7.68	0.69	Thr NH - Val $C^{\alpha}CH_{3}^{a}$	*c
7.68	1.64	Thr NH - Val CαH	
7.68	3.13	Thr NH - Val C ^β H	*
7.68	3.33	Thr NH - Val C ^y H	*
8.07	3.81	Bit NH - Thr C ^a H	
8.07	3.72	Bit NH - Thr C ^β H	*
8.07	0.73	Bit NH - Thr CH ₃	
8.07	7.68	Bit NH - Thr NH	*
3.45	2.93	Ala $C^{\alpha}H$ - Pyr $C^{\alpha}H_{2b}$	
3.07	2.59	Ala C ^β H _{2b} - Pyr C ^α H _{2a}	
7.26	4.56	Ala NH - Mann C1H	*
7.26	5.02	Ala NH - Gul C1H/Hist C¤H	*
7.06	4.20	Ala NH₂ь - Pyr C ^β H	*
7.06	3.56	Ala NH _{2b} - Gul C5H	*
7.06	2.93	Ala NH _{2b} - Bit C ^α H ₂	*
6.63	3.56	Ala NH _{2a} - Gul C5H	
6.63	4.20	Ala NH₂a - Pyr C ^β H	
2.58	2.17	Pyr CαH2a - Ala CβH2a	*
2.97	2.17	Pyr C ^α H _{2b} - Ala C ^β H _{2a}	
4.23	3.79	Pyr C ^β H - Mann C2H	*
4.19	3.45	Pyr C ^β H - Ala C ^α H	
4.23	3.07	$Pyr C^{\beta}H$ - Ala $C^{\beta}H_{2b}$	
4.23	2.17	Pyr C ^β H - Ala C ^β H _{2a}	
7.73	4.23	Hist C2H - Pyr C ^β H	*
7.72	3.12	Hist C2H - Val C ^β H	*
7.72	2.92	Hist C2H - Bit C ^a H ₂	*
7.73	1.65	Hist C2H - Val C ^a H	*
7.73	0.69	Hist C2H - Val C ^a CH ₃	*
7.72	6.63	Hist C2H - Ala NH _{2a}	*
7.01	4.56	Hist C4H - Mann C1H	*
7.01	3.56	Hist C4H - Gul C5H	
7.01	3.42	Hist C4H - Gul C6H	*
7.01	3.33	Hist C4H - Gul C6H'/Val C ^y H	
7.01	3.12	Hist C4H - Val C ^β H	*
7.01	0.68	Hist C4H - Val C ^a CH ₃	*
7.01	1.64	Hist C4H - Val C ^a H	*
3.80	2.93	Mann C2H - Pyr C ^a H _{2b}	
3.75	2.93	Mann C3H - Pyr C ^a H _{2b}	
6.27	2.09	Mann NH _{2b} - Pyr CH ₃	*
3.85	0.67	Thr $C^{\alpha}H - Val C^{\gamma}CH_{3}^{b}$	+ ^d
7.41	1.32	Thr NH – Val CYCH3	+
7.76	0.78	Hist C2H – Thr CH ₃	+
7.05	0.63	Hist C4H – Val C ^Y CH ₃	+
8.42	7.75	A5 NH (1) – Hist C2H	+
3.06	1.69	Ala $C^{\beta}H_{2b} - A_5 C^{\beta}H_2$	+

Supplementary Table S8. Inter-residue intramolecular NOEs for free Zn(II)BLM-A5 and Zn(II)BLM-A5 bound to OL1. Spectra were acquired at 5 °C in H2O. OL:Zn(II)BLM in 1:1 molar ratio. Missing NOE (*) and new NOE (+) connections upon DNA binding correspond to Figures 3, 4, and S4.

^{*a*}Blue colored labels indicate that the inter-residue NOE was detected for the free Zn(II)BLM-A₅. ^{*b*}Pink colored labels indicated that the NOE is only detected when OL₁ is bound. ^{*c*}Asterisks (*) indicate that the specific NOE is missing

upon complexation with OL₁, ^{*d*}Plus (+) indicates that the specific NOE connection is found upon complexation with OL₁. The color coding of the NOE assignments corresponds to the color coding for Figures 3 and 4.

F2 (ppm)	F1 (ppm)	Assignment	$OL_1 + Zn(II)BLM-A_5$
1.64	0.64	Val C ^a H - Val C ^y CH ₃ ^a	
1.64	0.69	Val C ^a H - Val C ^a CH ₃	
3.13	0.65	Val C ^β H - Val C ^γ CH ₃	
3.13	0.68	Val C ^β H - Val C ^α CH ₃	*c
3.13	1.64	Val C ^β H - Val C ^α H	
3.33	0.65	Val CYH - Val CYCH3	
3.32	3.13	Val C ^y H - Val C ^β H	*
3.33	1.64	Val C ^y H - Val C ^a H	
7.26	0.64	Val NH -Val C ^Y CH ₃	*
7.26	1.64	Val NH - Val C ^a H	*
7.26	3.13	Val NH - Val C ^β H	
7.26	3.33	Val NH - Val C ^y H	
3.72	0.73	Thr C ^β H - Thr CH ₃	
3.81	0.73	Thr C ^α H - Thr CH ₃	
3.87	3.74	Thr $C^{\alpha}H$ -Thr $C^{\beta}H$	*
7.68	3.72	Thr NH - Thr $C^{\beta}H$	*
7.68	3.81	Thr NH - Thr CαH	*
3.26	2.91	Bit $C^{\beta}H_2$ - Bit $C^{\alpha}H_2$	
3.29	3.24	Bit $C^{\beta}H_{2b}$ - Bit $C^{\beta}H_{2a}$	*
8.07	3.30	Bit NH - Bit C ^β H _{2b}	*
8.07	3.24	Bit NH - Bit C ^β H _{2a}	
8.07	2.89	Bit NH - Bit $C^{\alpha}H_2$	
3.22	1.71	A5 $C^{\alpha}H_2$ - A5 $C^{\beta}H_2$	
2.80	1.71	$A_5 C^{\gamma}H_2$ - $A_5 C^{\beta}H_2$	
2.68	1.43	$A_5 C^{\delta}H_2 - A_5 C^{\varepsilon}H_2$	
2.75	1.44	A ₅ C ^{η} H ₂ - A ₅ C ^{ζ} H ₂	
8.64	1.71	A5 NH (1) - A5 $C^{\beta}H_2$	*
8.64	3.22	A ₅ NH(1) - A ₅ C^{α} H ₂	
3.45	2.18	Ala C $^{\alpha}$ H - Ala C $^{\beta}$ H _{2a}	
3.45	3.08	Ala $C^{\alpha}H$ - Ala $C^{\beta}H_{2b}$	
3.07	2.17	Ala $C^{\beta}H_{2b}$ - Ala $C^{\beta}H_{2a}$	
7.60	6.82	Ala CONH2b - Ala CONH2a	
7.06	6.63	Ala NH2b - Ala NH2a	
7.26	3.42	Ala NH - Ala CªH	*
7.06	3.45	Ala NH _{2b} - Ala C^{α} H	
7.06	3.08	Ala NH2b - Ala C^{β} H2b	*
6.63	3.45	Ala NH _{2a} - Ala C $^{\alpha}$ H	
7.06	2.18	Ala NH _{2b} - Ala C^{β} H _{2a}	*
7.06	6.84	Ala NH2b - Ala CONH2a	*
2.97	2.59	$Pyr C^{\alpha}H_{2b} - Pyr C^{\alpha}H_{2a}$	
4.19	2.93	$Pyr C^{p}H - Pyr C^{\alpha}H_{2b}$	
4.23	2.59	Pyr C ^p H - Pyr C ^a H _{2a}	
7.60	7.18	Processing Constraints of the Co	
7.60	2.96	$Pyr CONH_{2b} - Pyr C^{\alpha}H_{2b}$	
7.60	2.59	Pyr CONH _{2b} - Pyr C ^α H _{2a}	
6.72	2.09	Pyr NH2 - Pyr CH3	

Supplementary Table S9. Intra-residue intramolecular NOEs for free Zn(II)BLM-A5 and Zn(II)BLM-A5 bound to OL1. Spectra were acquired at 5 °C in H2O. OL:Zn(II)BLM in 1:1 molar ratio. Missing NOE (*) and new NOE (+) connections upon DNA binding correspond to Figure S4.

F2 (ppm)	F1 (ppm)	Assignment	OL ₁ + Zn(II)BLM-A ₅
5.14	5.01	Hist C ^β H - Hist C ^α H	
7.72	7.02	Hist C2H - Hist C4H	*
7.01	5.01	Hist C4H - Hist C ^a H	
3.77	4.60	Mann C2H - Mann C1H	*
3.80	3.73	Mann C2H - Mann C3H	*
3.80	3.43	Mann C2H - Mann C4H	*
3.41	4.56	Mann C4H - Mann C1H	*
3.67	3.42	Mann C6H - Mann C4H	*
3.67	3.51	Mann C6H - Mann C6H'	*
3.51	3.41	Mann C6H' - Mann C4H	*
3.49	3.42	Mann C6H' - Mann C5H	*
6.27	5.62	Mann NH2b - Mann NH2a	
5.01	3.77	Gul C1H - Gul C2H	
5.01	3.42	Gul C1H - Gul C4H	
3.77	3.43	Gul C2H - Gul C4H	*
3.74	3.43	Gul C3H - Gul C4H	*
3.75	3.56	Gul C3H - Gul C5H	*
3.56	5.01	Gul C5H - Gul C1H	
3.55	3.43	Gul C5H - Gul C6H	*
3.55	3.33	Gul C5H - Gul C6H'	*
7.18	0.67	Val NH -Val C ^a CH ₃ ^b	+d

Supplementary Table S9 (Cont.)

^{*a*}Blue colored labels indicate that the inter-residue NOE was detected for the free Zn(II)BLM-A₅. ^{*b*}Pink colored labels indicated that the NOE is only detected when OL₁ is bound. ^{*c*}Asterisks (*) indicate that the specific NOE is missing upon complexation with OL₁, ^{*d*}Plus (+) indicates that the specific NOE connection is found upon complexation with OL₁.