Molecular Dynamics Simulations of the Mononuclear Zinc β-lactamase from *Bacillus cereus*

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Supporting Information

- Bond and Angle Parameters for the **ZNOH** Model.

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BOND
ZN-NB    103.00      2.08 ! NB: Atom type for the Nε2 atom in His86 and His149
ZN-NH    103.00      2.08 ! NH=NB: Atom type for the Nδ1 atom in His88
ZN-OW    180.00      1.86 ! OW: Atom type for the zinc-bound hydroxide

ANGLE
ZN-NB-CV     20.00    138.00 !
ZN-NB-CR     20.00    115.50 !
ZN-NH-CR     20.00    115.50 !
ZN-NH-CC     20.00    124.50 !
ZN-NH-CW     20.00    129.50 !
ZN-OW-HW     29.00    122.00 !
OW-ZN-NB     30.00    102.00 !
OW-ZN-NH     30.00    124.00 !
NB-ZN-NB     20.00    109.50 !
NB-ZN-NH     20.00    109.50 !
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- Bond and Angle Parameters for the **$ZNOH_2$** Model

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BOND
ZN-NB    121.00      2.02 !
ZN-NH    121.00      2.02 !
ZN-OW     80.00      2.12 !

ANGLE
ZN-NB-CV     20.00    125.00 !
ZN-NB-CR     20.00    129.00 !
ZN-NH-CR     20.00    123.00 !
ZN-NH-CC     20.00    123.00 !
ZN-OW-HW     18.00    125.00 !
OW-ZN-NB     30.00    106.00 !
OW-ZN-NH     30.00    104.00 !
NB-ZN-NB     20.00    110.00 !
NB-ZN-NH     20.00    114.00 !
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- **HF/6-31G* RESP Atomic Charges**

ZnOH				$ZnOH_2$			
CB	HID	86	0.109	CB	HID	86	0.168
HB2	HID	86	0.018	HB2	HID	86	0.016
HB3	HID	86	0.018	HB3	HID	86	0.016
CG	HID	86	0.076	CG	HID	86	0.096
ND1	HID	86	-0.260	ND1	HID	86	-0.216
HD1	HID	86	0.347	HD1	HID	86	0.351
CE1	HID	86	0.022	CE1	HID	86	0.023
HE1	HID	86	0.195	HE1	HID	86	0.200
NE2	HID	86	-0.140	NE2	HID	86	-0.195
CD2	HID	86	-0.304	CD2	HID	86	-0.317
HD2	HID	86	0.210	HD2	HID	86	0.208
CB	HIE	88	0.021	CB	HIE	88	0.045
HB2	HIE	88	0.035	HB2	HIE	88	0.038
HB3	HIE	88	0.035	HB3	HIE	88	0.038
CG	HIE	88	0.124	CG	HIE	88	0.087
ND1	HIE	88	-0.323	ND1	HIE	88	-0.247
CE1	HIE	88	0.010	CE1	HIE	88	-0.032
HE1	HIE	88	0.183	HE1	HIE	88	0.209
NE2	HIE	88	-0.157	NE2	HIE	88	-0.151
HE2	HIE	88	0.342	HE2	HIE	88	0.367
CD2	HIE	88	-0.284	CD2	HIE	88	-0.243
HD2	HIE	88	0.238	HD2	HIE	88	0.258
CB	HID	149	0.153	CB	HID	149	0.210
HB2	HID	149	0.002	HB2	HID	149	0.004
HB3	HID	149	0.002	HB3	HID	149	0.004
CG	HID	149	0.051	CG	HID	149	0.057
ND1	HID	149	-0.249	ND1	HID	149	-0.191
HD1	HID	149	0.335	HD1	HID	149	0.350
CE1	HID	149	0.104	CE1	HID	149	-0.027
HE1	HID	149	0.174	HE1	HID	149	0.211
NE2	HID	149	-0.259	NE2	HID	149	-0.137
CD2	HID	149	-0.274	CD2	HID	149	-0.365
HD2	HID	149	0.205	HD2	HID	149	0.241
Zn1	ZNW		0.849	Zn1	ZNW		0.816
OZn	ZNW		-0.990	HZ2	WZN		0.516
HZn	ZNW		0.384	HZ1	WZN		0.516
				OZn	WZN		-0.920

Table S3. Summary of the RMS Deviations and RMS Fluctuations.

	ZnOH	$ZnOH_2$
	RMSD (Å)	
total	1.77 ± 0.06	1.89 ± 0.06
backbone	1.33 ± 0.07	1.44 ± 0.08
N-domain	1.82 ± 0.10	1.91 ± 0.09
C-domain	1.58 ± 0.08	1.76 ± 0.09
	Rad_{gyr} (Å) [a]	
protein average	16.47 ± 0.15	16.41 ± 0.15
	RMSF (Å)	
total	0.92 ± 0.07	0.94 ± 0.08
backbone	0.68 ± 0.07	0.70 ± 0.08
N-domain total	0.94 ± 0.09	0.94 ± 0.09
C-domain total	0.81 ± 0.07	0.87 ± 0.09
$\alpha_1\alpha_2$	0.85 ± 0.09	0.80 ± 0.11
$\beta_1\beta_2\beta_3$	0.83 ± 0.14	0.74 ± 0.13
$\beta_4\beta_5\beta_6\beta_7$	0.64 ± 0.08	0.65 ± 0.06
α_3	0.65 ± 0.12	0.67 ± 0.13
$\beta_8\beta_9\beta_{10}\beta_{11}\beta_{12}$	0.66 ± 0.09	0.72 ± 0.09
$\alpha_4\alpha_5$	0.73 ± 0.08	0.67 ± 0.08

[a] The radius of gyration of the protein from X-ray is 16.2 Å

Table S4. Summary of RMSF values of selected residues in the active site.

	RMSF (Å)			RMSF (Å)	
Residue	**ZnOH**	**$ZnOH_2$**	**Residue**	**ZnOH**	**$ZnOH_2$**
His86	0.13	0.14	Arg91	0.18	0.18
His88	0.14	0.21	Asp56	0.22	0.21
His149	0.15	0.15	Phe34	0.28	0.54
Asp90	0.16	0.36	Trp59	0.17	0.17
His210	0.15	0.23	Val39	0.25	0.56
Cys168	0.11	0.18	Asn180	0.28	0.38
Lys171	0.34	0.40	Gly179	0.14	0.19

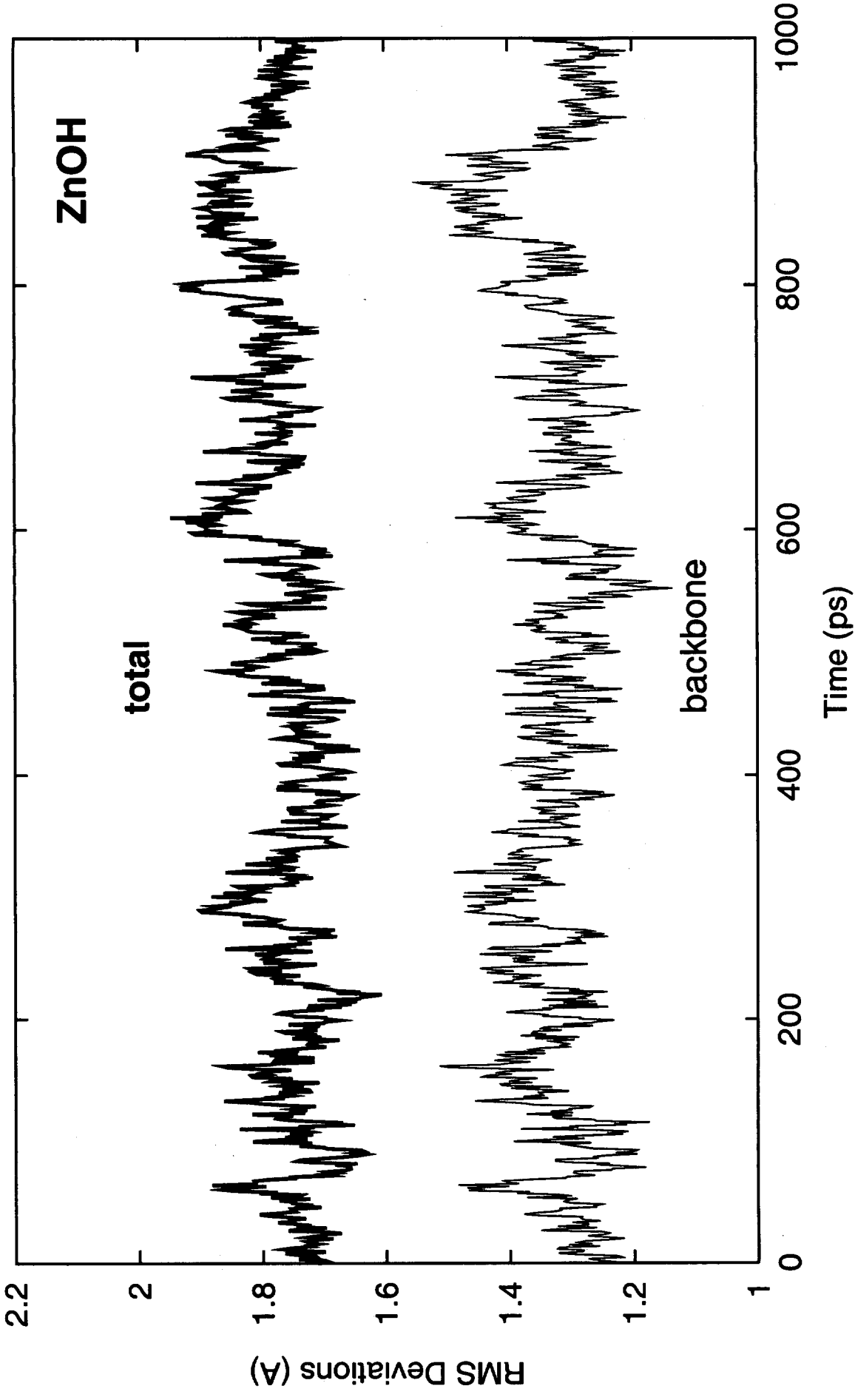

Figure S5.

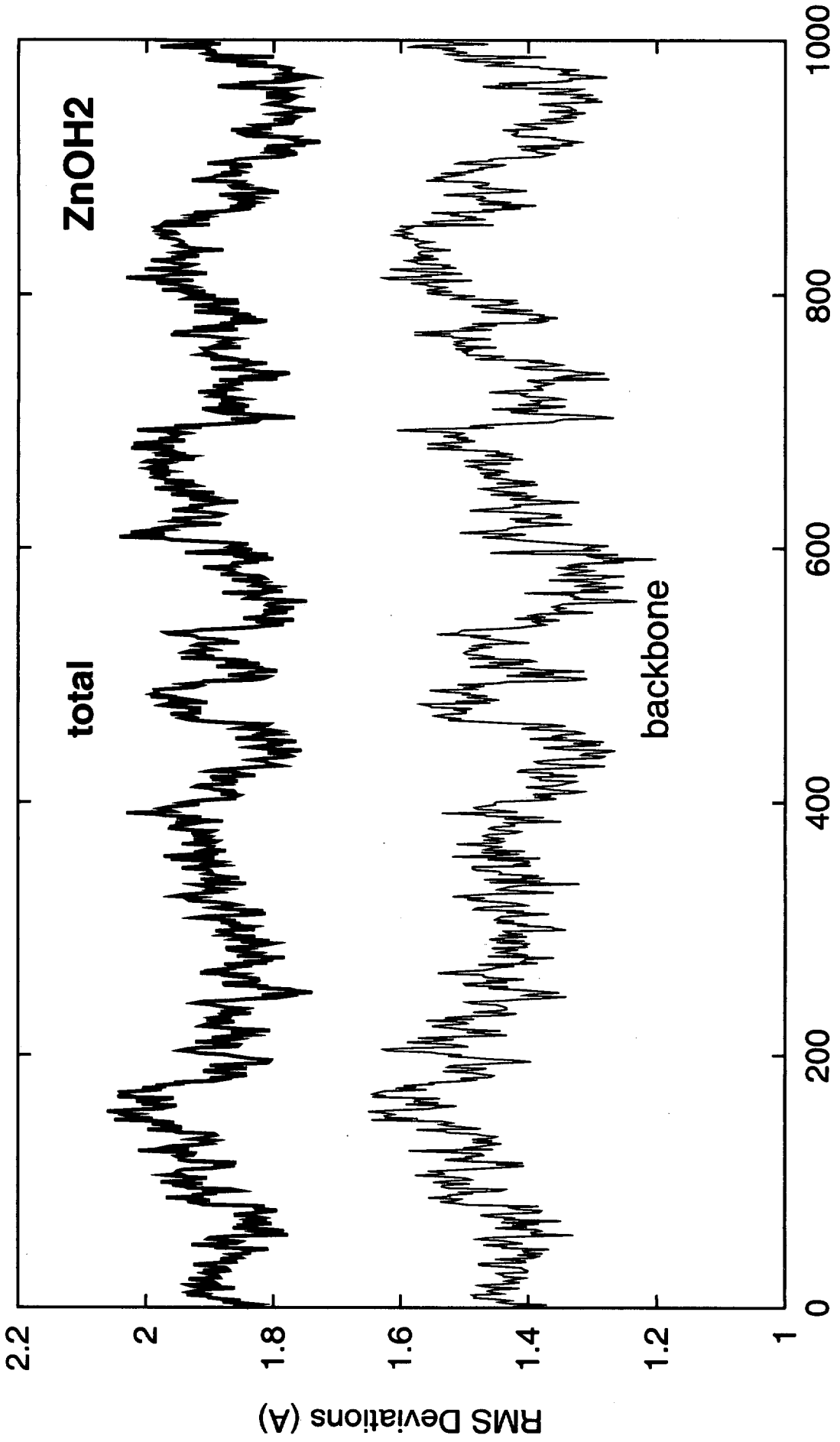

Figure S6.