Table S1. Statistical analysis of the energy minimized family of conformers and of the mean structure of apoNTKII from *Listeria monocytogenes*.

	REM[a]	<REM>[a]
RMS violations per meaningful distance constraint (Å) [b]	(20 structures)	(mean)
Intraresidue (238)	0.0168 ± 0.0025	0.0183
Sequential (314)	0.0212 ± 0.0019	0.0186
Medium range[c] (266)	0.0975 ± 0.0021	0.0082
Long range (451)	0.0189 ± 0.0014	0.0190
Total (1269)	0.0177 ± 0.0009	0.0170
RMS violations per meaningful dihedral angle constraints (deg)[b]		
ϕ (45)	0.5865 ± 0.4500	0.00
ψ (37)	0.00	0.00
χ_1 (44)	0.3074 ± 0.2500	0.00
Average number of violations per structure		
Intraresidue	6.45 ± 1.50	7
Sequential	6.30 ± 1.10	5
Medium range[c]	3.95 ± 1.24	4
Long range	12.45 ± 1.68	11
Total	29.15 ± 2.60	27
ϕ	1.06 ± 0.86	0
ψ	0.00	0
χ_1	0.66 ± 0.41	0
Average no. of NOE violations larger than 0.3 Å	0.0 ± 0.0	0.00
Average NOE target function (Å^2)	0.43 ± 0.04	0.40
Average angle target function (rad^2)	0.05 ± 0.01	0.04
RMSD to the mean structure (Å) (BB)[d] **(HA)**	0.42 ± 0.09 Å 1.17 ± 0.07	
Structural analysis[e]		
% of residues in most favorable regions	78.6	84.1
% of residues in allowed regions	15.6	11.1
% of residues in generously allowed regions	4.9	3.2
% of residues in disallowed regions	1.0	0.0
H-bond energy (kJ mol^{-1})	2.86 ± 0.12	2.84
Overall G-factor	-0.22± 0.02	-0.22

[a]REM indicates the energy minimized family of 20 structures, <REM> is the energy minimized average structure of the ensemble.
[b]The number of meaningful constraints for each class is reported in parenthesis.
[c]Medium range distance constraints are those between residues (i,i+2), (i,i+3), (i,i+4) and (i,i+5).
[d]The RMSD to the mean structure is reported considering residues (4-68).
[e]Resulted from the Ramachandran plot analysis. In the PROCHECK statistics, the average hydrogen-bond energy within 2.5-4.0 kJ mol^{-1} and overall G-factor over -0.5 is expected to be a good-quality structure.

Table S2. Acquisition parameters for NMR experiments performed on apo and CdNTKII from *Listeria monocytogenes*.

Experiments[a]	Dimension of acquired data (nucleus)			Spectral width (ppm)			n[b]
	t_1	t_2	t_3	F_1	F_2	F_3	
[^{1}H-^{1}H]-NOESY[c]	1024(^{1}H)	2048(^{1}H)		15	15		64
[^{1}H-^{1}H]-TOCSY[d]	1024(^{1}H)	2048(^{1}H)		15	15		64
^{1}H-^{15}N-HSQC[c]	512(^{15}N)	1024(^{1}H)		40	15		8
$^2J_{NH}$-^{1}H-^{15}N-HSQC[e]	256(^{15}N)	2048(^{1}H)		180	25		64
^{15}N-edited [^{1}H-^{1}H]-NOESY[c]	272(^{1}H)	40(^{15}N)	1024(^{1}H)	15	40	15	16
HNHA[c]	128(^{1}H)	40(^{15}N)	1024(^{1}H)	15	40	15	16
HNHB[f]	128(^{1}H)	40(^{15}N)	1024(^{1}H)	15	40	15	32
^{15}N R_1[g]	256(^{15}N)	2048(^{1}H)		40	15		8
^{15}N R_2[g]	256(^{15}N)	2048(^{1}H)		40	15		8
^{1}H–^{15}N NOEs[g]	256(^{15}N)	2048(^{1}H)		40	15		48

[a]All 3D and 2D spectra were collected at 298 K, processed using the standard Bruker software (XWINNMR) and analyzed through the XEASY program. [b]Number of acquired scans. [c]Data acquired on the 700 MHz spectrometer. 2D NOESY and 3D NOESY-^{15}N HSQC maps were acquired with a mixing time of 100 ms and a recycle time of 1.5 s. [d]2D TOCSY spectra were recorded on the 600 MHz spectrometer with a spin-lock time of 90 ms and a recycle time of 1.5 s. [e]To identify the tautomeric state of His 62, a ^{1}H-^{15}N HSQC experiment was performed for measuring $^2J_{NH}$ coupling constants within the His ring. In this experiment, the INEPT delay was set to 22 ms. [f]Data acquired on a 500 MHz spectrometer equipped with a triple resonance cryoprobe. [g] In all experiments the water signal was suppressed with 'water flipback' scheme. A recycle delay of 3 s was used for R_1 and R_2 relaxation experiments, while of 5 s for ^{1}H–^{15}N NOE experiments. A refocusing delay of 450 μs were used in the R_2 measurements.

Fig. S1. ^{15}N relaxation parameters R_1, R_2 and heteronuclear NOE versus residue number of apoNTKII (A) and CdNTKII (B) collected at 600 MHz.

Fig. S2. Spectral density functions $J(\omega_N)$, $J(\omega_H)$ and $J(0)$ versus the residue number as obtained from ^{15}N relaxation data of apoNTKII (A) and CdNTKII (B).

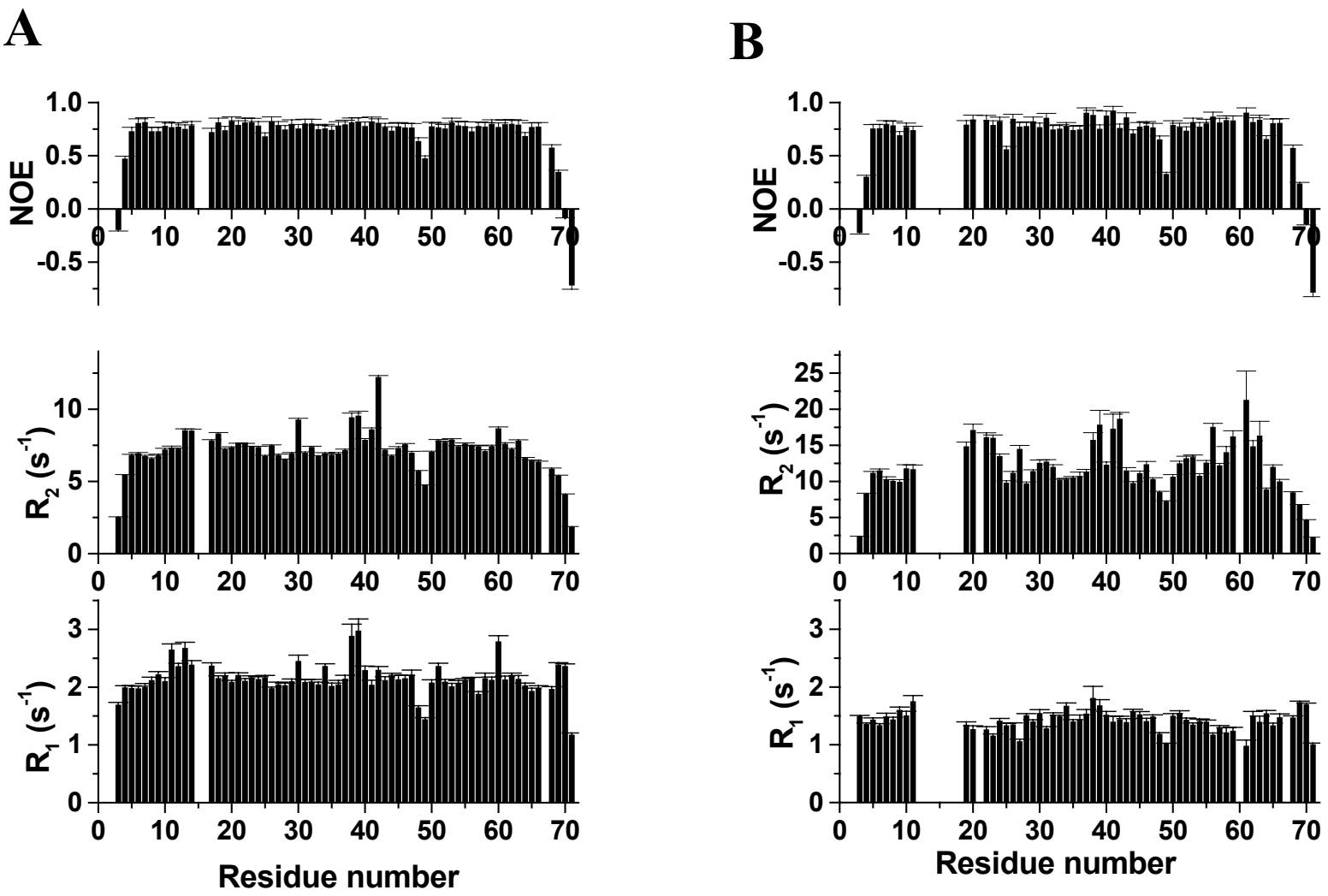

Fig. S1

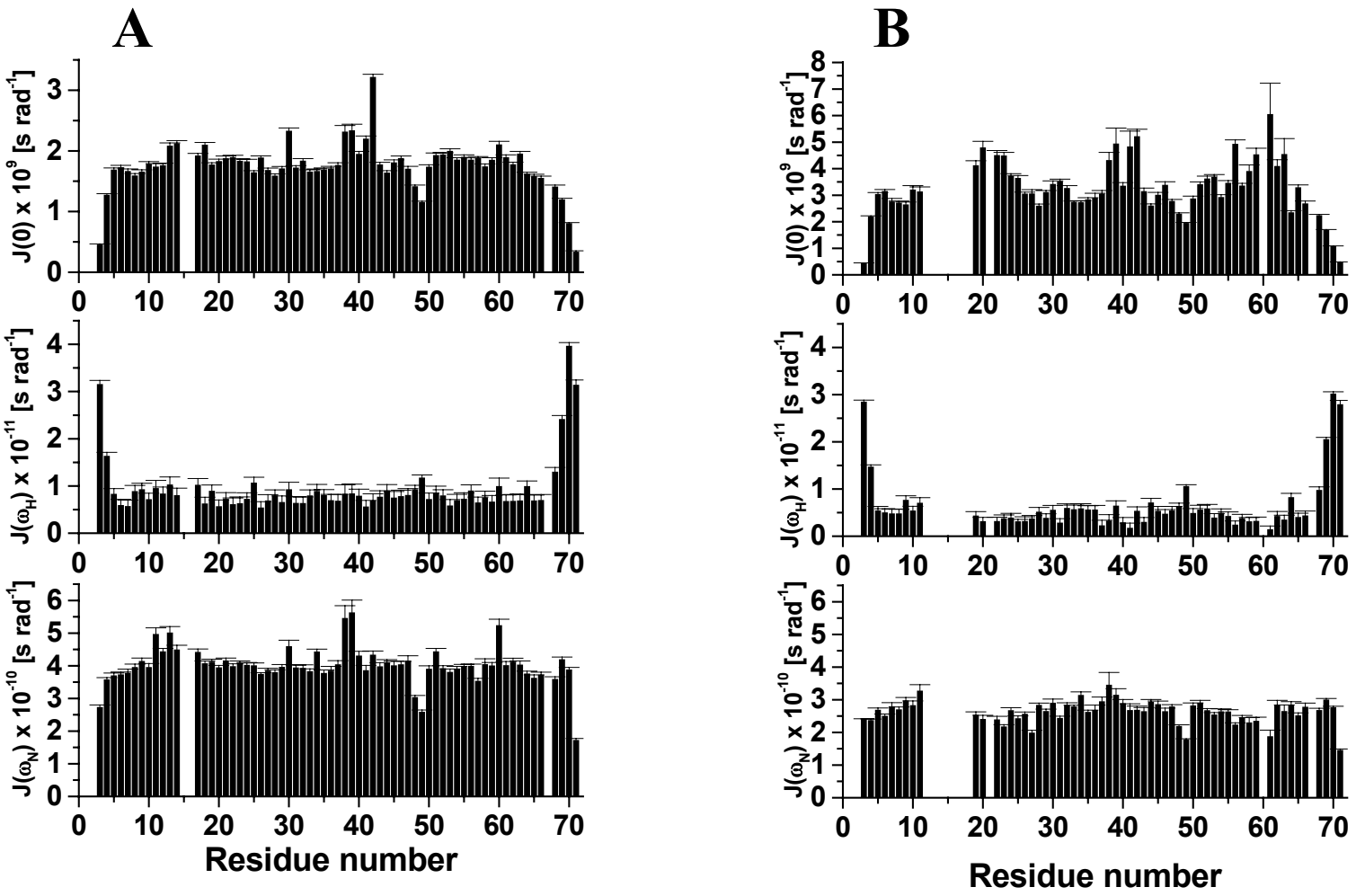
A
B
J(0) x 10^9 [s rad^-1]
J(ω_H) x 10^-11 [s rad^-1]
J(ω_N) x 10^-10 [s rad^-1]
Residue number

Fig. S2