Table S1. Temperature coefficients (Δδ/ΔT) of H^N involved in Hydrogen Bond restraints. Here are only reported the temperature coefficients of H^N involved in a hydrogen bond (Backbone amide H^N as well as side chain H^N). It is usually considered that amide H^N's exhibiting a temperature coefficient lower than 5.10^{-3} ppb/K (in absolute value) are engaged in a hydrogen bond.

H^N group	Temp. coeff. (10^3ppm/K)	H^N group	Temp. coeff. (10^3ppm/K)
H^N_7 (O_{60})	-4.85	H^N_{62} (O_7)	-0.41
H^N_9 (O_{62})	0.07	H^N_{63} (O_{32})	-2.69
H^N_{16} (O_{12})	-3.93	H^N_{64} (O_9)	-3.86
H^N_{17} (O_{13})	-3.15	H^N_{65} (O_{34})	-2.68
H^N_{18} (O_{14})	-2.57	H^N_{68} (O_{65})	-0.26
H^N_{21} (O_{17})	5.06	H^N_{72} (O_{68})	-2.27
H^N_{22} (O_{18})	2.09	H^N_{73} (O_{69})	-2.69
H^N_{23} (O_{19})	1.82	H^N_{74} (O_{70})	-3.62
H^N_{25} (O_{21})	-0.67	H^N_{75} (O_{71})	-1.66
H^N_{28} (O_{57})	-4.00	H^N_{76} (O_{72})	-3.42
H^N_{29} (O_{86})	-3.13	H^N_{77} (O_{73})	-3.28
H^N_{30} (O_{59})	-2.81	H^N_{82} (O_{33})	-4.16
H^N_{31} (O_{84})	-2.88	H^N_{83} (O_{95})	-3.39
H^N_{32} (O_{61})	-2.14	H^N_{84} (O_{31})	-2.19
H^N_{33} (O_{82})	-3.88	H^N_{85} (O_{93})	-3.42
H^N_{34} (O_{63})	-2.38	H^N_{86} (O_{29})	-3.73
H^N_{42} (O_{38})	-1.48	H^N_{88} (O_{27})	3.55
H^N_{43} (O_{39})	-3.04	H^N_{93} (O_{85})	-1.99
H^N_{44} (O_{40})	-3.69	H^N_{95} (O_{83})	-2.13
H^N_{45} (O_{41})	-1.92	H^N_{97} (O_{81})	-4.41
H^N_{47} (O_{43})	-1.59	H^N_{105} (O_{101})	-1.18
H^N_{48} (O_{44})	-2.35	H^N_{106} (O_{102})	-4.01
H^N_{49} (O_{45})	-3.60	H^N_{107} (O_{103})	-2.66
H^N_{50} (O_{46})	-3.72	H^N_{108} (O_{104})	-1.51
H^N_{51} (O_{47})	-2.37	H^N_{109} (O_{105})	-1.50
H^N_{52} (O_{48})	-2.57	H^N_{110} (O_{106})	-1.26
H^N_{53} (O_{49})	-0.72	H^N_{111} (O_{107})	-1.07
H^N_{54} (O_{50})	-3.93	H^N_{112} (O_{108})	-3.66
H^N_{55} (O_{51})	-3.14		
H^N_{59} (O_{28})	-1.69	$H^{N\xi 1}_{37}$ ($O\delta_{66}$)	0.01
H^N_{60} (O_5)	-2.51	H^N_{41} ($S\gamma_{38}$)	-1.79
H^N_{61} (O_{30})	-3.27		

Table S2. Statistical data about the active site Ala_{35}-Lys_{42}.

Residue	Backbone rmsd (Å)	Heavy rmsd (Å)	ϕ (degrees)	ψ (degrees)	χ^1 (degrees.)
Ala_{35}	0.33	0.37	-82 ± 7.5	144 ± 10	
Ser_{36}	0.51	0.65	-52 ± 6	-43 ± 5	-168 ± 12
Trp_{37}	0.54	0.70	-67 ± 6	78 ± 10	56 ± 6
Cys_{38}	0.39	0.39	-165.5 ± 5.5	89.5 ± 7	-179 ± 7
Pro_{39}	0.39	0.46	-52.8 ± 5	89.5 ± 7	
Pro_{40}	0.39	0.45	-47.7 ± 5	-43 ± 4	
Cys_{41}	0.28	0.37	-66 ± 6	-25 ± 6	-51 ± 10
Lys_{42}	0.34	0.74	-55 ± 6	-48 ± 8	-156 ± 22
S^{γ}_{38} S^{γ}_{41} distance: 3.6 ± 0.4 Å					