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Supporting information for article:

Structures of the *N*-acetyltransferase domain of *Xylella fastidiosa* *N*-acetyl-L-glutamate synthase/kinase with and without His tag bound with *N*-acetyl-L-glutamate

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Supplemental Materials

Table S1. Average temperature factor (Å^2) for the main-chain, the side-chain, whole protein and NAG for the different subunits of xfNAT structure

Subunit	Main chain	Side chain	Protein	NAG
A	12.4	17.6	15.2	13.4
B	22.1	27.2	24.7	18.4
C	13.4	17.7	15.5	14.2
D	19.3	23.8	21.7	16.3
E	15.2	20.3	17.8	14.6
F	20.0	25.6	23.2	18.9
G	15.4	20.5	18.1	15.4
H	26.8	31.2	29.1	22.5

Table S2. Interactions between *N*-acetyl-L-glutamate and protein atoms for the subunit B of xfNAT-ht structure

Arginine	Protein	Distance (Å)
N2	Arg385 O	3.30
	Asp354 O	3.23
O7	Phe356 N	2.95
OXT	Lys355 NZ	2.77
O	Asp354 O	3.07
OE1	Asn390 ND	2.92
	Arg387 N	3.07
	Arg317 NH2	
OE2	Arg317 NE	
	Arg317 NH1	
	Arg317 NH2	
	Arg387 NE	

Figure S1. Stereo diagrams of the superimposition of eight subunits in xfNAT. A: Superimposition of eight subunits in xfNAT in ribbons. B: superimposition of NAG molecules in eight subunits in sticks. Two major conformations were observed. Subunits A, B, C, D, E, F, G and H are colored in red, green, blue, yellow, magentas, cyan, orange, light-pink, respectively.

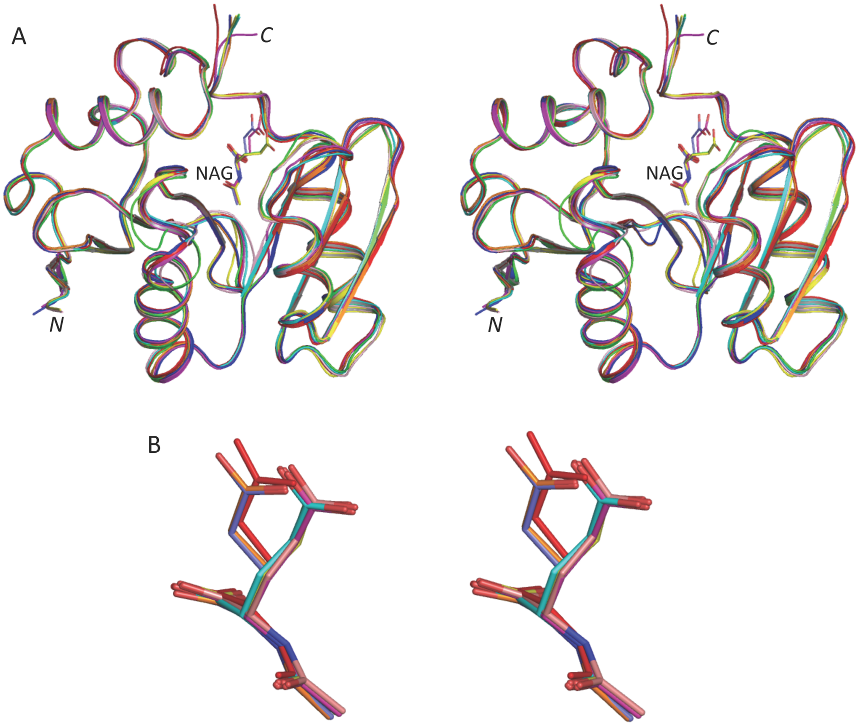

Figure S2. Cartoon drawing to illustrate the calculations of the possible dimer orientation differences in different dimers.

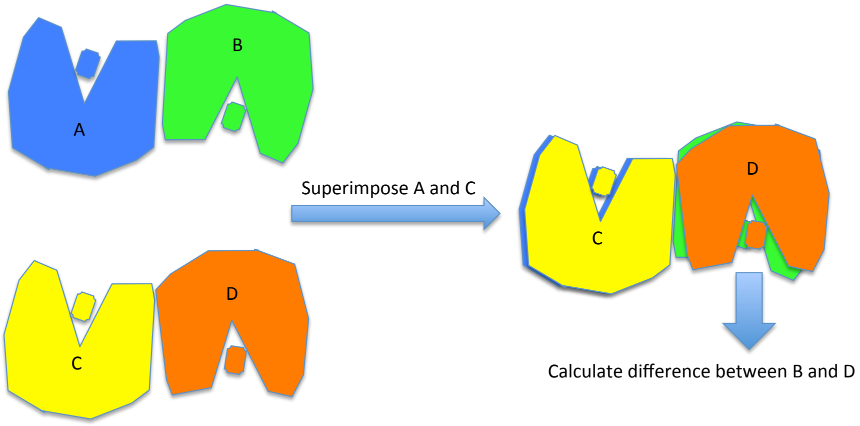

Figure S3. NAG binding site. E: NAG binding site for subunit E for xfNAT. F: NAG binding site for subunit F for xfNAT. G: NAG binding site for subunit G for xfNAT. H: NAG binding site for subunit H for xfNAT. The conformation of NAG in subunit G is close to those in subunits A and C, representing the first NAG binding conformation. The conformations of NAG in subunits E, F and G are close to those in subunits B and D, representing the second NAG binding conformation. Bound NAG is shown in sky-blue sticks. Side-chains involved in hydrogen bonding interactions with NAG are shown in sky-blue sticks. Electron density map ($2F_o$-F_c) around bound NAG (contoured at 1.0 σ) is shown as a blue cage. Potential hydrogen bonding interactions are shown in red dashed lines.