Supplementary Online Material for

The Structure of the *Staphylococcus aureus* Sortase-Substrate Complex Reveals how the Universally Conserved LPXTG Sorting Signal is Recognized

Nuttee Suree, Chu Kong Liew, Valerie A. Villareal, William Thieu, Evgeny A. Fadeev, Jeremy J. Clemens, Michael E. Jung, and Robert T. Clubb

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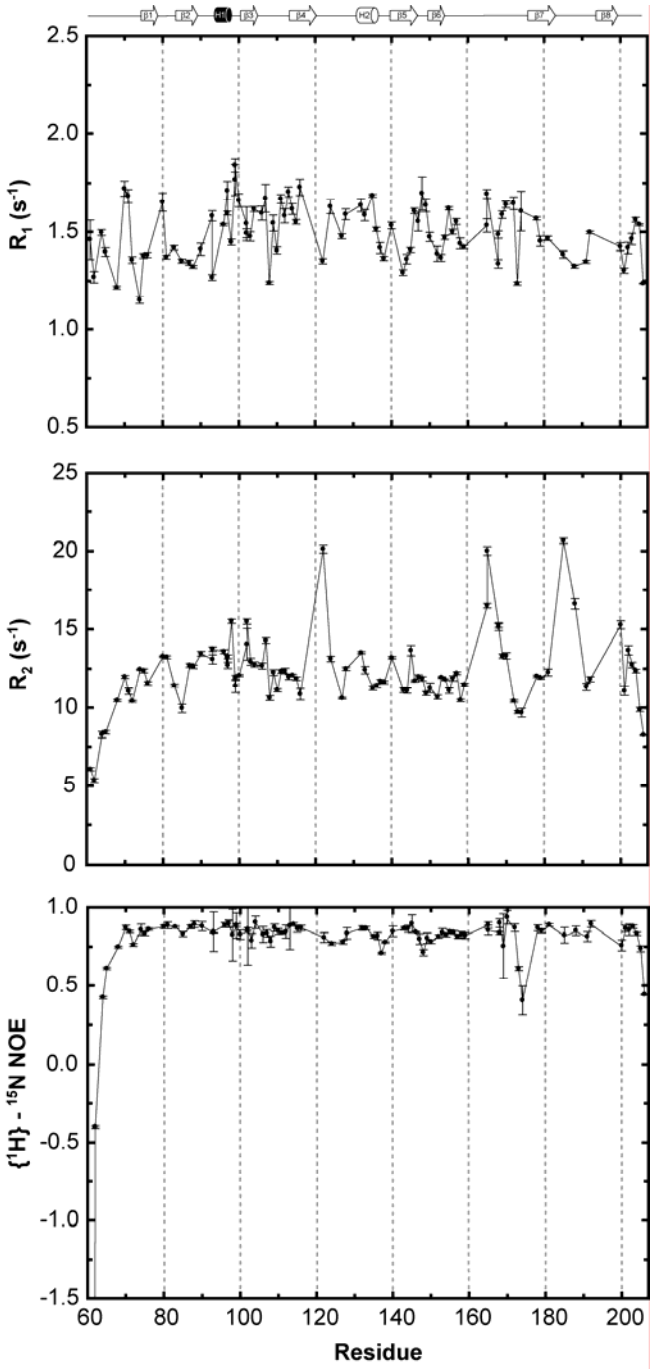

Fig. S1: Backbone amide ^{15}N spin relaxation data. The connecting lines represent only the trends of the data and are not necessarily representing residues with no data available (due to low signal or overlapped resonance).

Table S1: Model-free parameters for the SrtA-LPAT* complex

Residue		Model	S^2	S^2_f	τ_e (ps)	R_{ex} (s^{-1})
A61		1	0.496 (± 0.009)			
K62		5	0.350 (± 0.011)	0.849 (± 0.015)	570 (± 17)	
Q64		5	0.628 (± 0.019)	0.898 (± 0.011)	923 (± 47)	
I65		5	0.652 (± 0.011)	0.825 (± 0.008)	1217 (± 66)	
D68		4	0.760 (± 0.005)		15 (± 1)	
S70		1	0.981 (± 0.007)			
K71		1	0.928 (± 0.013)			
V72		1	0.831 (± 0.004)			
G74	β1	3	0.740 (± 0.011)			3.3 (± 0.2)
Y75	β1	3	0.884 (± 0.008)			1.4 (± 0.2)
I76	β1	1	0.912 (± 0.006)			
D80		1	1.000 (± 0.002)			
I83	β2	1	0.916 (± 0.005)			
E85	β2	1	0.869 (± 0.006)			
G90		1	1.000 (± 0.006)			
T93	H1	1	1.000 (± 0.008)			
Q96	H1	1	1.000 (± 0.002)			
L97	H1	1	1.000 (± 0.008)			
N98	H1	3	0.961 (± 0.010)			3.2 (± 0.2)
G100		1	0.930 (± 0.004)			
F103	β3	3	0.936 (± 0.015)			1.5 (± 0.3)
A104	β3	1	1.000 (± 0.004)			
E106		1	1.000 (± 0.008)			
N107		3	1.000 (± 0.026)			2.1 (± 0.4)
E108		3	0.807 (± 0.005)			0.5 (± 0.2)
S109		1	0.997 (± 0.008)			
L110		1	0.904 (± 0.006)			
D111		1	1.000 (± 0.004)			
D112		1	1.000 (± 0.007)			
Q113	β4	1	0.997 (± 0.007)			
N114	β4	1	0.936 (± 0.005)			
I115	β4	1	0.980 (± 0.006)			
S116	β4	1	1.000 (± 0.011)			
F122		3	0.867 (± 0.009)			9.4 (± 0.3)
D124		1	1.000 (± 0.007)			
N127		1	0.876 (± 0.004)			
Y128		1	1.000 (± 0.005)			
L133	H2	1	1.000 (± 0.009)			
A136	H2	1	0.951 (± 0.005)			
K138		1	0.907 (± 0.005)			
S140	β5	3	0.981 (± 0.011)			1.1 (± 0.2)
Y143	β5	1	0.856 (± 0.007)			
F144	β5	1	0.888 (± 0.011)			
K145	β5	3	0.904 (± 0.008)			2.5 (± 0.3)
V146	β5	1	0.970 (± 0.005)			
G147		1	0.974 (± 0.009)			
N148		1	0.925 (± 0.011)			
E149	β6	1	0.898 (± 0.010)			

Residue		**Model**	S^2	S^2_f	τ_e (ps)	R_{ex} (s^{-1})
T150	β6	2	0.926 (± 0.013)		31 (± 12)	
K152	β6	1	0.848 (± 0.009)			
Y153	β6	3	0.877 (± 0.010)			1.1 (± 0.1)
K154	β6	1	0.935 (± 0.004)			
T156		1	0.962 (± 0.007)			
S157		1	0.989 (± 0.006)			
I158		1	0.851 (± 0.006)			
R159		1	0.922 (± 0.005)			
V168		3	0.866 (± 0.014)			4.4 (± 0.2)
L169		1	1.000 (± 0.005)			
D170		1	1.000 (± 0.005)			
Q172		1	0.839 (± 0.006)			
K173		5	0.750 (± 0.008)	0.826 (± 0.008)	471 (± 97)	
G174		2	0.780 (± 0.023)		400 (± 101)	
Q178	β7	1	0.990 (± 0.004)			
L179	β7	1	0.947 (± 0.005)			
L181	β7	1	0.940 (± 0.007)			
D185		3	0.880 (± 0.011)			9.9 (± 0.2)
N188		3	0.851 (± 0.005)			6.1 (± 0.3)
T191		1	0.893 (± 0.005)			
G192		1	0.952 (± 0.004)			
F200	β8	3	0.915 (± 0.013)			3.9 (± 0.3)
V201	β8	1	0.835 (± 0.008)			
A202		3	0.924 (± 0.019)			2.1 (± 0.4)
T203		1	0.997 (± 0.007)			
E204		1	1.000 (± 0.004)			
V205		5	0.752 (± 0.013)	0.894 (± 0.009)	2106 (± 565)	
K206		5	0.595 (± 0.004)	0.795 (± 0.002)	848 (± 12)	

Note: For model 5: $S^2=S^2_f.S^2_s$. and $\tau_e = \tau_s$. For models 1 to 4 $\tau_e = \tau_f$.