Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The origin of specificity and insight into recognition between aminoacyl carrier protein and its protein partner

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Supporting Information

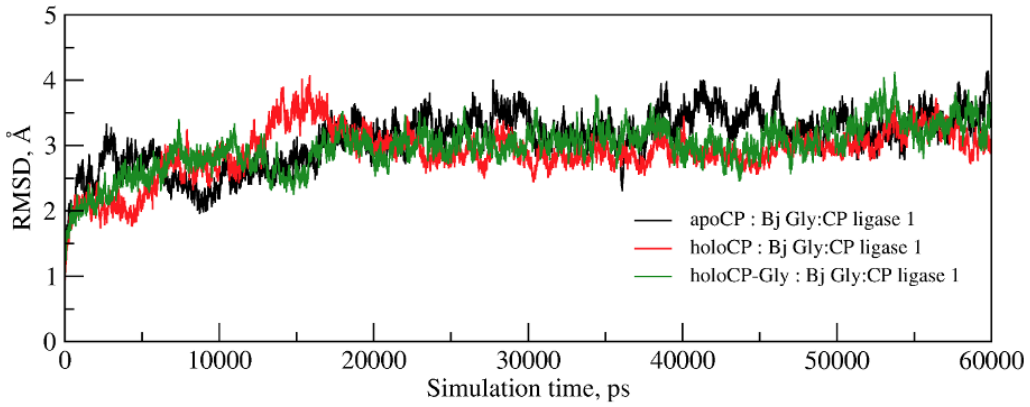

Figure S1. The time evolution of RMSD values obtained for the simulated complexes during the 60 ns of MD simulations.

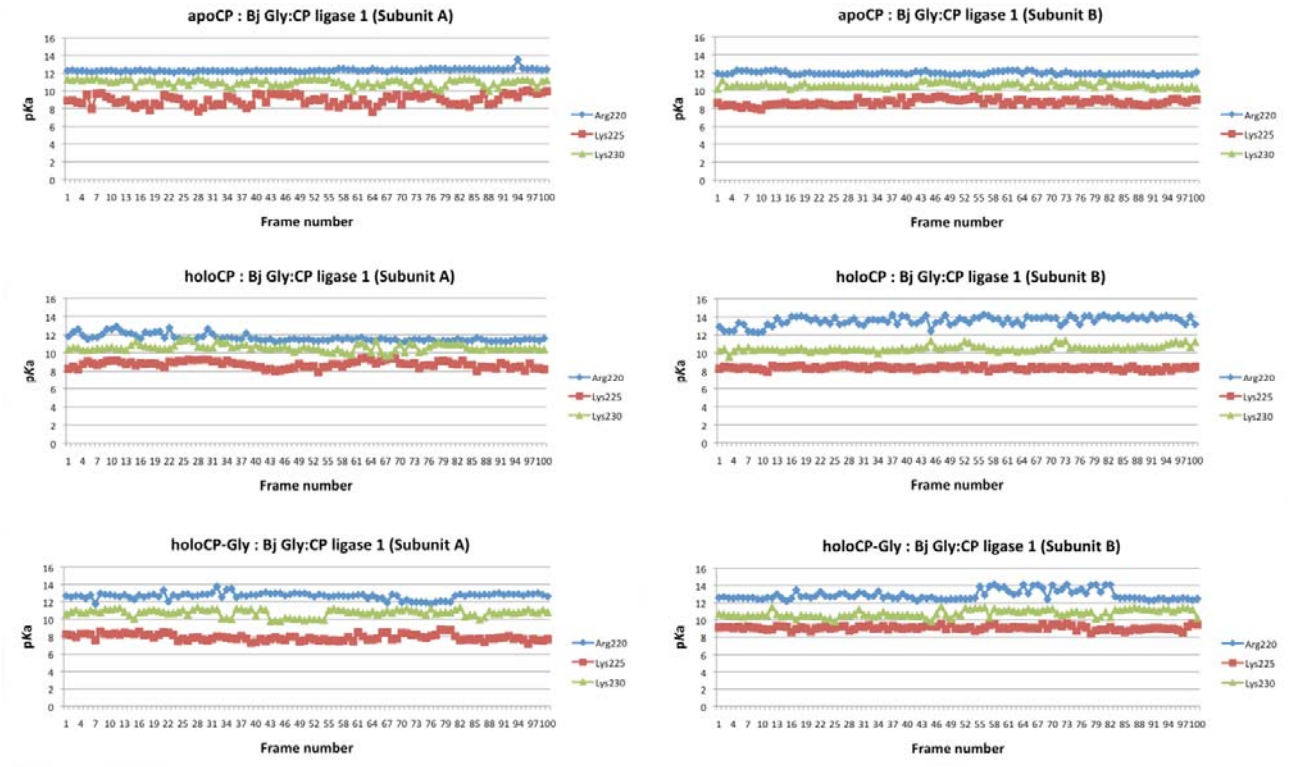

Figure S2. PROPKA pK_a values obtained on snapshot structures sampled at 0.05 ns intervals from the last 5 ns of MD trajectories corresponding to all three complexes.

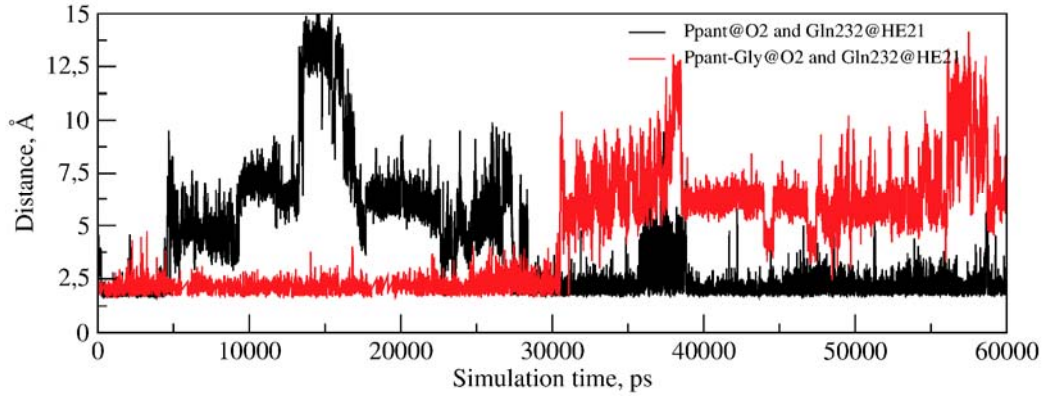

Figure S3. Distance between phosphate oxygens of **Ppant** (black) and **Ppant–Gly** (red) and side-chain of Gln232 within the active site of the ligase.

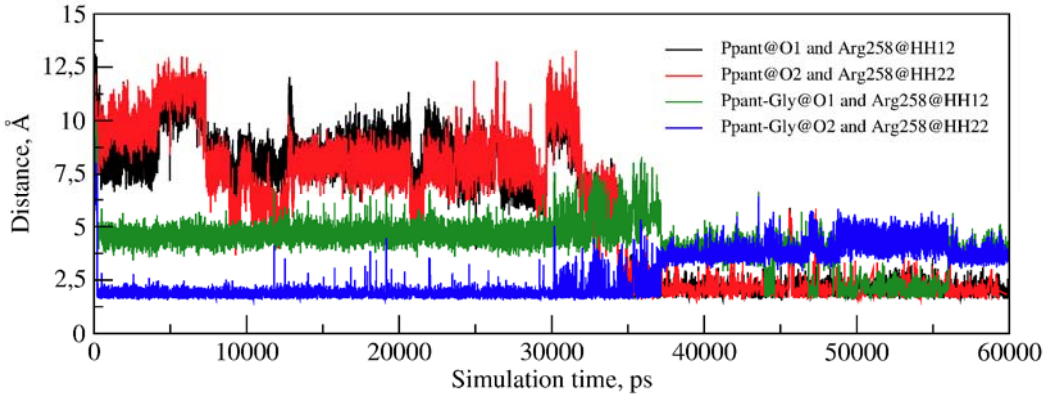

Figure S4. Distance between phosphate oxygens of **Ppant** (black and red) and **Ppant–Gly** (green and blue) and side-chain of Arg258 within the active site of the ligase.

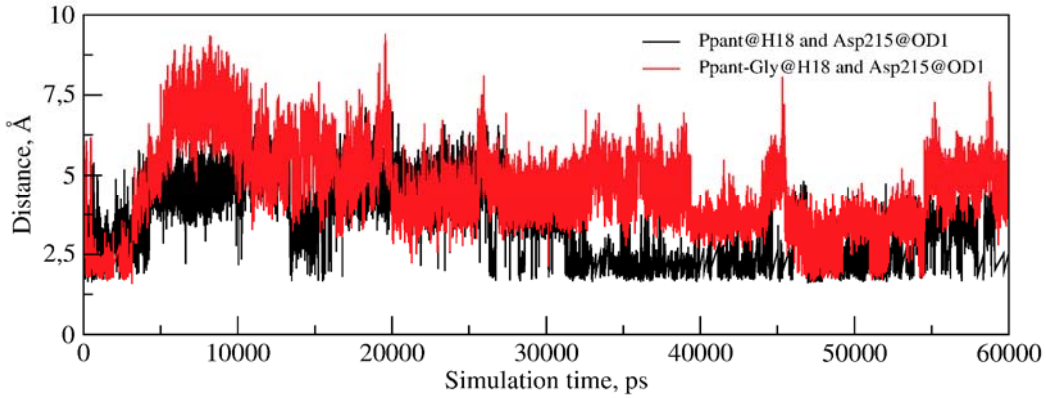

Figure S5. Distance between hydrogen (H18) of **Ppant** (black) and **Ppant–Gly** (red) and side-chain of Asp215 within the active site of the ligase.

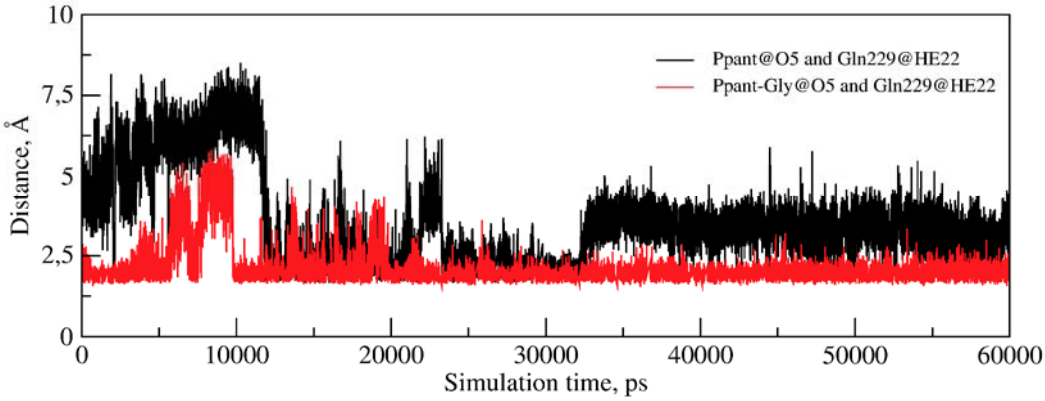

Figure S6. Distance between oxygen (O5) of **Ppant** (black) and **Ppant–Gly** (red) and side-chain of Gln229 within the active site of the ligase.

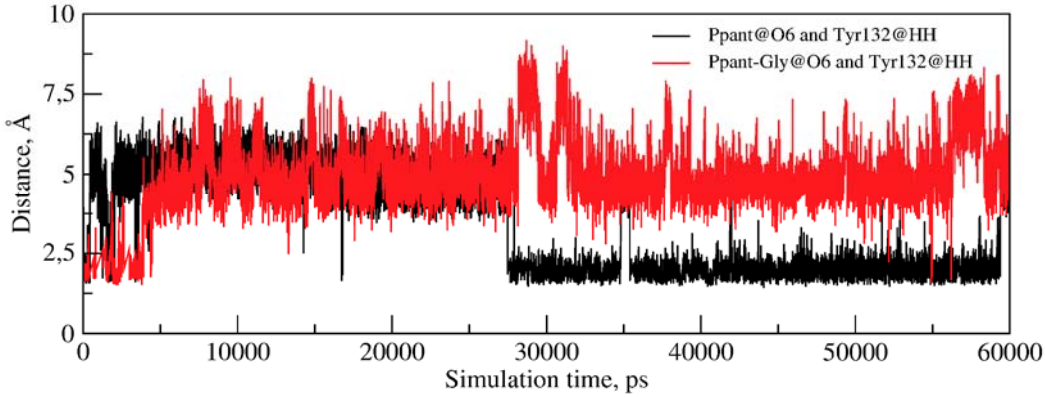

Figure S7. Distance between oxygen (O6) of **Ppant** (black) and **Ppant–Gly** (red) and side-chain of Tyr132 within the active site of the ligase.

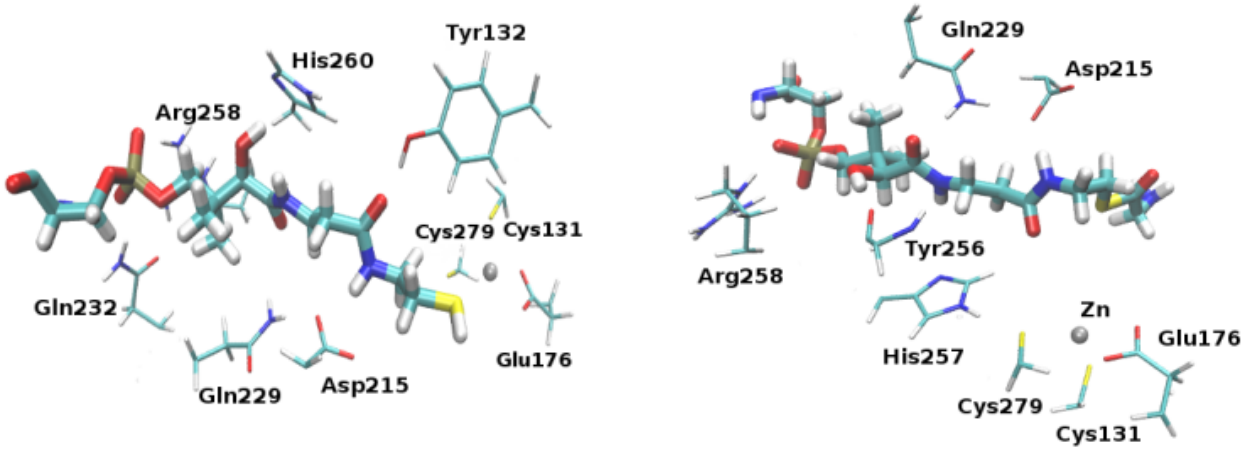

Figure S8. Orientation of the model **Ppant** (left) and **Ppant–Gly** (right) prosthetic groups within the ligase active site.

Table S1. Alanine scanning results obtained for complexes formed between holoCP and subunit A of Bj Gly:CP ligase 1 and holoCP and subunit B of Bj Gly:CP ligase 1. Binding free energy is a sum of energy components of Van der Waals (VDW), electrostatic interactions (EEL), and polar (EPB) and non-polar (ENPOLAR) terms of solvatation free energies. All values are in kcal/mol.[a]

System (subunit A)	VDW	EEL	EGB	ESURF	ΔH_{gas}	ΔH_{solv}	ΔH_{bind}	$\Delta\Delta H_{bind}$
wild–type complex	–104.5	–364.4	412.3	–12.4	–468.9	399.9	**–69.0**	
(R220A) complex	–100.5	–163.8	220.9	–11.4	–264.3	209.5	**–54.8**	**14.2**
(V221A) complex	–103.0	–364.6	411.5	–12.3	–467.6	399.2	**–68.4**	**0.6**
(Q223A) complex	-101.0	-370.4	416.8	-12.0	-471.4	404.7	**-66.8**	**2.2**
(M224A) complex	–96.7	–362.5	409.4	–11.7	–459.2	397.8	**–61.5**	**7.5**
(K225A) complex	–100.1	–250.8	295.9	–11.9	–350.9	283.9	**–66.9**	**2.1**
(V227A) complex	–102.3	–363.8	410.9	–12.2	–466.3	398.6	**–67.6**	**1.4**
(S228A) complex	–103.4	–362.9	411.9	–12.3	–466.3	399.6	**–66.7**	**2.3**
(Q229A) complex	–102.5	-365.7	414.0	-12.2	-468.3	401.7	**-66.6**	**2.4**
(K230A) complex	–103.7	–238.7	285.0	–12.4	–342.4	272.6	**–69.8**	**–0.8**
(Q231A) complex	–99.6	–353.9	398.8	–11.8	–453.5	387.0	**–66.5**	**2.5**
(Q232A) complex	–99.3	–361.6	407.4	–11.9	–460.9	395.4	**–65.5**	**3.5**

System (Subunit B)	VDW	EEL	EGB	ESURF	ΔH_{gas}	ΔH_{solv}	ΔH_{bind}	$\Delta\Delta H_{bind}$
wild–type complex	-107.2	-378.5	420.1	-12.9	-485.7	407.2	**-78.5**	
(R220A) complex	-107.4	-170.3	221.8	-12.4	-277.7	209.4	**-68.3**	**10.2**
(V221A) complex	-106.0	-378.5	419.5	-12.7	-484.5	406.8	**-77.7**	**0.8**
(Q223A) complex	-106.1	-380.4	420.9	-12.7	-486.5	408.1	**-78.4**	**0.1**
(M224A) complex	-100.4	-376.3	416.5	-12.3	-476.7	404.3	**-72.4**	**6.0**
(K225A) complex	-104.2	-274.0	313.1	-12.5	-378.3	300.6	**-77.7**	**0.8**
(V227A) complex	-104.1	-378.0	418.1	-12.5	-482.1	405.5	**-76.6**	**1.9**
(S228A) complex	-106.8	-375.2	418.5	-12.8	-481.9	405.7	**-76.3**	**2.2**
(Q229A) complex	-105.8	-377.5	417.5	-12.5	-483.3	405.0	**-78.3**	**0.2**
(K230A) complex	-106.1	-161.1	214.1	-12.4	-267.2	201.7	**-65.5**	**12.9**
(Q231A) complex	-103.6	-369.9	419.2	-12.8	-473.6	406.9	**-66.7**	**11.8**
(Q232A) complex	-100.6	-367.1	407.8	-12.2	-467.7	395.6	**-72.1**	**6.4**

[a] VDW = van der Waals contribution from MM; EEL = electrostatic energy as calculated by the MM force field; EGB = the electrostatic contribution to the solvation free energy calculated by GB; ESURF = nonpolar contribution to the solvation free energy calculated by an empirical model