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

Supporting Information

Recognition of PDL1/L2 by Different Induce-fit Mechanisms of PD1: A Comparative Study of Molecular Dynamics Simulations

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Table S1. PD1, PDL1 crystal structure data statistics

System	PDB code	Resolution
PD1	2M2D	--
	3RRQ	2.10
	4ZQK	2.45
	5B8C	2.15
	5GGR	3.30
	5GGS	2.00
	5IUS	2.89
	5JXE	2.90
	5WT9	2.40
	6HIG	2.20
	6JBT	2.47
PDL1	3BIK	2.65
	3BIS	2.64
	3FN3	2.70
	3SBW	2.28
	4Z18	1.95
	4ZQK	2.45
	5C3T	1.80
	5GGT	2.80
	5GRJ	3.21
	5IUS	2.89
	5J89	2.20
	5J8O	2.30
	5JDR	2.70
	5JDS	1.70
	5N3D	2.35
	5N2F	1.70
	5MIU	2.10
	5O45	0.99
	5O4Y	2.30
	5X8L	3.10
	5X8M	2.66
	5XJ4	2.30
	5XXY	2.90
	6MNM7	2.43
	6NM8	2.79
	6NNV	1.92
	6NOJ	2.33
	6NOS	2.70
	6NP9	1.27

	6R3K	2.20

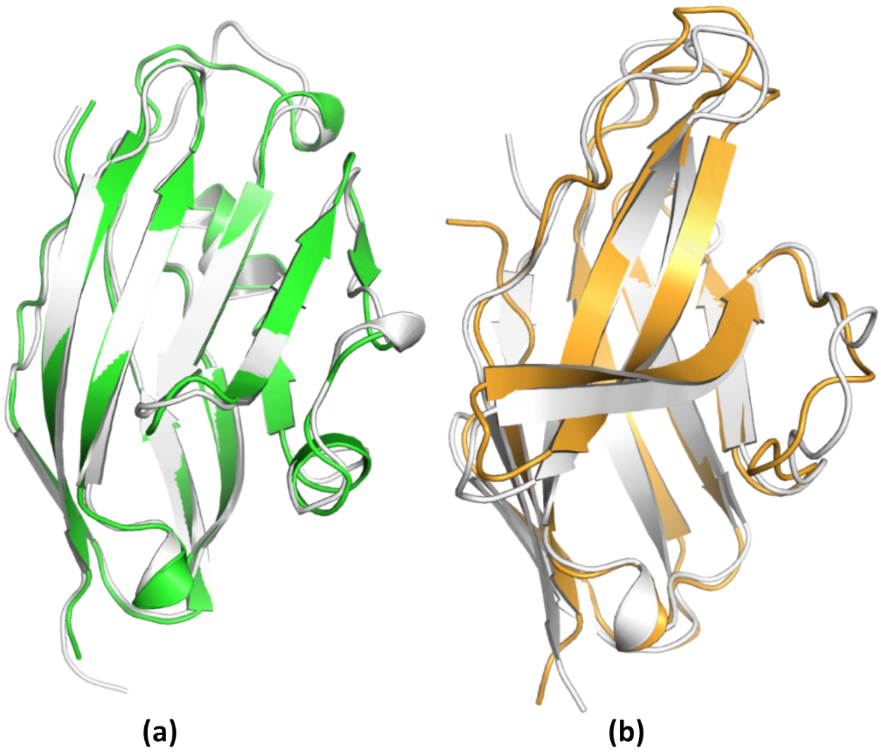
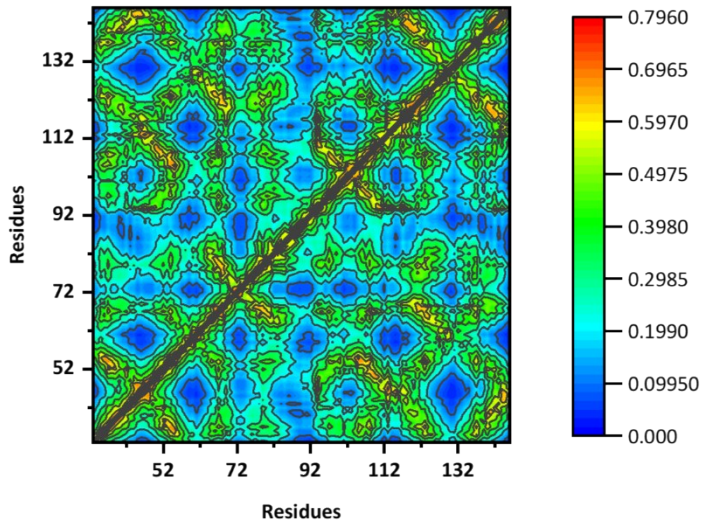
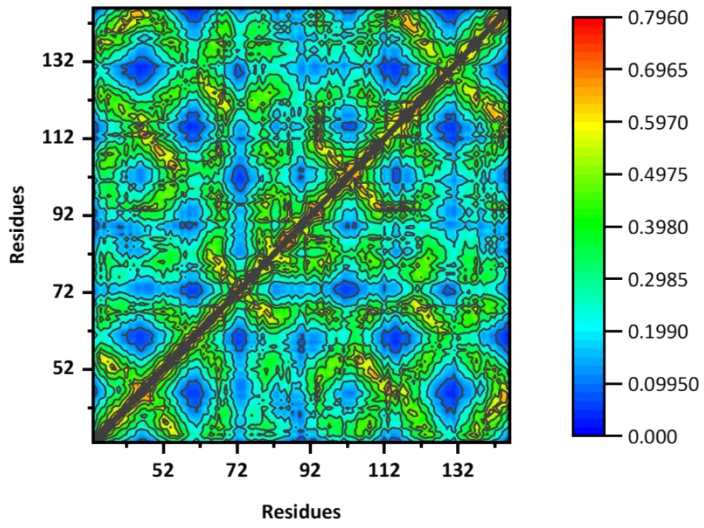


Figure S1. Schematic diagram of protein secondary structure superposition. (a) PDL1 monomer (gray) and PDL1 in PD1/PDL1 complex (green). (b) PD1 monomer (gray) and PD1 in PD1/PDL2 complex (orange).



(a)



(b)

Figure S2. Correlation analysis of PD1 residues in PD1/Ligand complex (a) PD1/PDL1 (b) PD1/PDL2

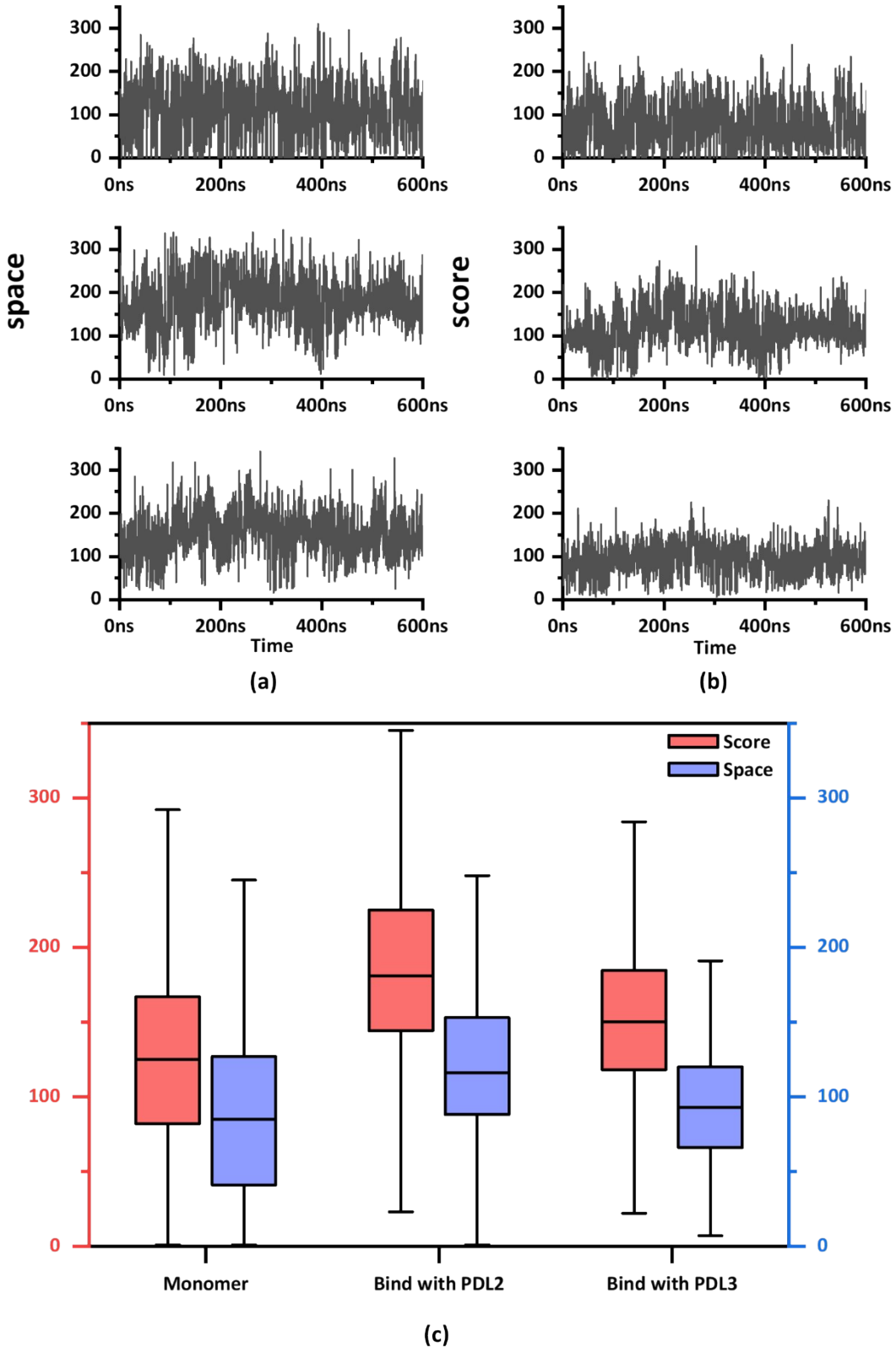


Figure S3. (a) Schematic diagram of pocket volume change. (b) Schematic diagram of pocket scoring changes. From top to bottom, the models are PD1 monomer, PD1 combined with PDL1 and PD1 combined with PDL2. (c) Box plot of the distributions of pocket volume and pocket scoring.

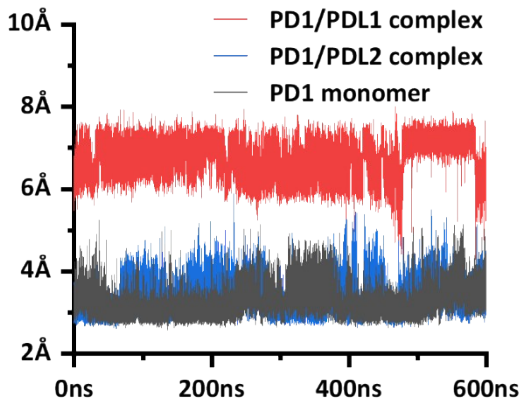


Figure S4. Distance time curve of D92-O (O atom at D92) and F95-N (N atom at F95).

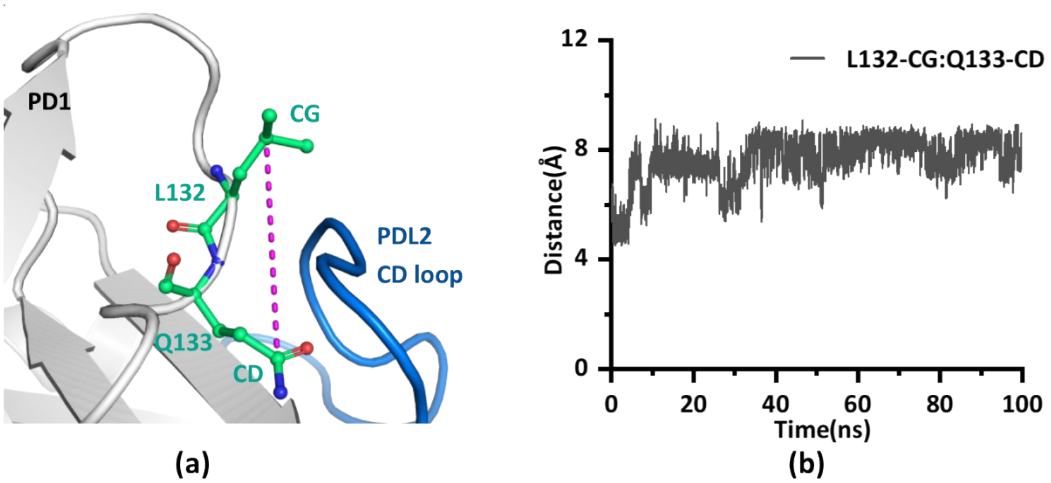


Figure S5. (a) Diagram of distance between L132-CG and Q133-CD. (b) Distance time curve of L132-CG and Q133-CD.