

Investigation on the Inter-Molecular Electrostatic Interactions Stabilizing the Structure of the PD-1/PD-L1 Axis: An In Silico Study

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Supplementary materials

No.	PDB ID	Structure Title
1	1NPU	Crystal structure of the extracellular domain of murine PD-1
2	2M2D	Human programmed cell death 1 receptor
3	3BIK	Crystal Structure of the PD-1/PD-L1 Complex
4	3BP5	Crystal structure of the mouse PD-1 and PD-L2 complex
5	3BP6	Crystal structure of the mouse PD-1 Mutant and PD-L2 complex
6	3RNK	Crystal structure of the complex between mouse PD-1 mutant and PD-L2 IgV domain
7	3RNQ	Crystal structure of the complex between the extracellular domains of mouse PD-1 mutant and PD-L2
8	3RRQ	Crystal structure of the extracellular domain of human PD-1
9	3SBW	Crystal structure of the complex between the extracellular domains of mouse PD-1 mutant and human PD-L1
10	4ZQK	Structure of the complex of human programmed death-1 (PD-1) and its ligand PD-L1.
11	5B8C	High resolution structure of the human PD-1 in complex with pembrolizumab Fv
12	5GGR	PD-1 in complex with nivolumab Fab
13	5GGS	PD-1 in complex with pembrolizumab Fab
14	5IUS	Crystal structure of human PD-L1 in complex with high affinity PD-1 mutant
15	5JXE	Human PD-1 ectodomain complexed with Pembrolizumab Fab
16	5WT9	Complex structure of PD-1 and nivolumab-Fab
17	6HIG	hPD-1/NBO1a Fab complex
18	6J14	Complex structure of GY-14 and PD-1
19	6J15	Complex structure of GY-5 Fab and PD-1
20	6JBT	Complex structure of toripalimab-Fab and PD-1
21	6JJP	Crystal structure of Fab of a PD-1 monoclonal antibody MW11-h317 in complex with PD-1
22	6K0Y	Study of the interactions of a novel monoclonal antibody, mAb059c, with the hPD-1 receptor
23	6UMT	High-affinity human PD-1 PD-L2 complex
24	6UMU	Human apo PD-1 triple mutant
25	6UMV	Human apo PD-1 double mutant

Table 1: PD-1-related experimental structures as of December 24, 2019 in the Protein Data Bank with a **Text Search** for: pd1 and **Molecule** : Programmed cell death protein 1. In this table, each shaded gray row represents an experimentally determined structure of the PD-1/PD-L1 complex.

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Table 2: PD-1-related experimental structures as of December 24, 2019 in the Protein Data Bank with a **Text Search** for: pd1 and **Molecule** : Programmed cell death protein 1. In this table, each shaded gray row represents an experimentally determined structure of the PD-1/PD-L2 complex.

No.	PDB ID	Structure Title
1	3BIK	Crystal Structure of the PD-1/PD-L1 Complex
2	3BIS	Crystal Structure of the PD-L1
3	3FN3	Dimeric Structure of PD-L1
4	3SBW	Crystal structure of the complex between the extracellular domains of mouse PD-1 mutant and human PD-L1
5	4Z18	Crystal structure of human PD-L1
6	4ZQK	Structure of the complex of human programmed death-1 (PD-1) and its ligand PD-L1.
7	5C3T	PD-1 binding domain from human PD-L1
8	5GGT	PD-L1 in complex with BMS-936559 Fab
9	5GRJ	Crystal structure of human PD-L1 with monoclonal antibody avelumab
10	5IUS	Crystal structure of human PD-L1 in complex with high affinity PD-1 mutant
11	5J89	Structure of human Programmed cell death 1 ligand 1 (PD-L1) with low molecular mass inhibitor
12	5J8O	Structure of human Programmed cell death 1 ligand 1 (PD-L1) with low molecular mass inhibitor
13	5JDR	Structure of PD-L1
14	5JDS	Crystal structure of PD-L1 complexed with a nanobody at 1.7 Angstrom resolution
15	5N2D	Structure of PD-L1/small-molecule inhibitor complex
16	5N2F	Structure of PD-L1/small-molecule inhibitor complex
17	5NIU	Structure of human Programmed cell death 1 ligand 1 (PD-L1) with low molecular mass inhibitor
18	5O45	Structure of human PD-L1 in complex with inhibitor
19	5O4Y	Structure of human PD-L1 in complex with inhibitor
20	5X8L	PD-L1 in complex with atezolizumab
21	5X8M	PD-L1 in complex with durvalumab
22	5XJ4	Complex structure of durvalumab-scFv/PD-L1
23	5XXY	Crystal structure of PD-L1 complexed with atezolizumab fab at 2.9A
24	6NM7	PD-L1 IgV domain bound to fragment
25	6NM8	IgV-V76T BMS compound 105
26	6NNV	PD-L1 IgV domain complex with macro-cyclic peptide
27	6NOJ	PD-L1 IgV domain V76T with fragment
28	6NOS	PD-L1 IgV domain V76T with fragment
29	6NP9	PD-L1 IgV domain V76T with fragment
30	6R3K	Structure of human Programmed cell death 1 ligand 1 (PD-L1) with low molecular mass inhibitor
31	6RPG	Structure of human Programmed cell death 1 ligand 1 (PD-L1) with inhibitor

Table 3: PD-L1-related experimental structures as of December 24, 2019 in the Protein Data Bank with a **Text Search** for: pdl1 and **Molecule** : Programmed cell death 1 ligand 1. In this table, each shaded gray row represents an experimentally determined structure of the PD-1/PD-L1 complex.

PD-1	Uniform resource locators (URLs)
Gene	https://www.ncbi.nlm.nih.gov/gene/5133
Uniprot	https://www.uniprot.org/uniprot/Q15116
Protein	https://www.ncbi.nlm.nih.gov/protein/AJS10360.1
BioMuta	https://hive.biochemistry.gwu.edu/biomuta/proteinview/Q15116
PD-L1	Uniform resource locators (URLs)
Gene	https://www.ncbi.nlm.nih.gov/gene/29126
Uniprot	https://www.uniprot.org/uniprot/Q9NZQ7
Protein	https://www.ncbi.nlm.nih.gov/protein/AAP13470.1
BioMuta	https://hive.biochemistry.gwu.edu/biomuta/proteinview/Q9NZQ7

Table 4: Online resources for gene sequences, protein sequences, structural and functional information of the two immune checkpoints.