

Table 3. Interactions between PD-1 and PD-L1 in the complex

Hydrogen bonds and salt bridges					
PD-1 contact atom	PD-1 residue location	PD-L1 contact atom	PD-L1 residue location	Distance, Å	*** < 3.3 Å * > 3.3 Å
N 66 Nδ2	C strand	A 121 O	G strand	3.5	*
N 68 Nδ2	C strand	Y 123 OH	G strand	2.8	***
S 73 Oγ	CC' loop	D 26 Oδ2	A strand	3.1	***
N 74 Oδ1	CC' loop	R 125 NH1	G strand	3.2	***
Q 75 Oε1	CC' loop	R 125 N	G strand	2.8	***
Q 75 Nε2	CC' loop	R 125 O	G strand	2.7	***
Q 75 Nε2	CC' loop	D 26 Oδ1	A strand	3.0	***
T 76 Oγ1	C' strand	Y 123 O	G strand	3.0	***
T 76 O	C' strand	K 124 Nζ	G strand	3.0	***
K 78 Nζ	C' strand	A 121 O	G strand	3.2	***
K 78 Nζ	C' strand	F 19 O	N-terminus	2.9	***
P 130 O	FG loop	Q 66 Nε2	C' strand	3.5	*
A 132 N	FG loop	Q 66 Oε1	C' strand	3.2	***
E 136 Oε1	G strand	Y 123 OH	G strand	2.6	***
E 136 Oε1	G strand	R 125 NH2	G strand	3.0	***
E 136 Oε2	G strand	R 113 Ne	F strand	3.3	*
E 136 Oε2	G strand	R 113 NH2	F strand	3.2	***
E 136 Oε2	G strand	R 125 NH2	G strand	3.0	***
Water-mediated hydrogen bonds					
I 134 O	G strand	Y 56 OH	C strand	3.0 / 3.0	*** / ***
I 134 N	G strand	Y 56 OH	C strand	3.0	***