PDB	Acceptor (A)	Donor (D)	Hydrogen (H)	D-A (Å)	H-A (Å)	$\angle ADH(°)$
5O4Y	O, D_PHE_1	NH2, E_ARG_125	HH21, E_ARG_125	2.98	2.14	12.47

Table 1: The hydrogen bond formed between Arg125 of PD-1 and Phe1 of its inhibitor (PDB ID: 5O4Y). In this table, the residue naming scheme is **Chain ID_residue name_residue number**, $\angle ADH$ represents the angle formed by acceptor (A), donor (D) and hydrogen (H) ($\angle ADH$).

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
3BIK	A_ARG_125	NH2	B_GLU_136	OE1	3.033
3BIK	A_ARG_125	NH2	B_GLU_136	OE2	3.001
3SBW	C_ARG_125	NH1	B_GLU_136	OE1	3.198
3SBW	C_ARG_125	NH1	B_GLU_136	OE2	2.810
5IUS	C_ARG_125	NH1	A_GLU_70	OE1	3.144
5IUS	C_ARG_125	NH1	A_GLU_70	OE2	2.870
5IUS	C_ARG_125	NH2	A_GLU_70	OE2	2.861
5IUS	D_ARG_125	NH2	B_GLU_70	OE1	3.305
5IUS	D_ARG_125	NH2	B_GLU_70	OE2	3.337
5J89	C_ARG_125	NH1	D_ASP_61	OD1	3.128
5J89	A_ARG_125	NH1	B_ASP_61	OD2	3.707
5J8O	B_ARG_125	NH1	A_ASP_61	OD2	3.401
5N2D	A_ARG_125	NH1	B_ASP_61	OD2	3.726
5N2D	B_ARG_125	NH2	A_GLU_58	OE1	3.996
5N2D	B_ARG_125	NH2	A_ASP_61	OD2	3.034
5N2D	C_ARG_125	NH1	D_ASP_61	OD2	3.979
5N2F	B_ARG_125	NH2	A_ASP_61	OD1	3.490
5NIU	A_ARG_125	NH2	B_ASP_61	OD1	3.287
5NIU	B_ARG_125	NH2	A_ASP_61	OD1	3.247
5NIU	C_ARG_125	NH2	D_ASP_61	OD1	3.661
5NIX	B_ARG_125	NH1	A_ASP_61	OD2	3.957
5NIX	C_ARG_125	NH1	D_ASP_61	OD1	3.476
5NIX	C_ARG_125	NH2	D_ASP_61	OD1	1.493
5NIX	C_ARG_125	NH2	D_ASP_61	OD2	3.393
5X8L	A_ARG_125	NH1	F_ASP_31	OD1	3.967
5X8L	A_ARG_125	NH2	F_ASP_31	OD1	2.989
5X8L	B_ARG_125	NH2	G_ASP_31	OD1	2.787
5X8L	B_ARG_125	NH2	G_ASP_31	OD2	3.932
5X8L	C_ARG_125	NH2	H_ASP_31	OD1	2.813
5X8L	C_ARG_125	NH2	H_ASP_31	OD2	3.969
5X8L	D_ARG_125	NH1	S_ASP_31	OD1	3.645
5X8L	D_ARG_125	NH2	S_ASP_31	OD1	3.477
5X8L	E_ARG_125	NH2	J_ASP_31	OD1	3.207
5XXY	A_ARG_125	NH2	H_ASP_31	OD1	3.134

Table 2: Arg125-linked salt bridging networks within the experimentally determined PD-1/PD-L1 structures. In this table, the residue naming scheme is **Chain ID_residue name_residue number**.