PDB	Acceptor (A)	Donor (D)	Hydrogen (H)	D-A (Å)	H-A (Å)	$\angle ADH(°)$
5O45	OD2, A_ASP_122	N, A_VAL_21	H, A_VAL_21	2.94	2.10	10.32
5O45	O, A_ASP_122	N, A_ILE_116	H, A_ILE_116	2.98	2.13	6.64
5O45	OD1, A_ASP_122	N, A_TYR_123	H, A_TYR_123	2.93	2.22	29.46
5O4Y	O, B_ASP_122	N, B_ILE_116	H, B_ILE_116	3.00	2.16	11.79
5O4Y	OD1, C_ASP_122	N, C_TYR_123	H, C_TYR_123	2.73	2.01	27.76
5O4Y	O, E_ASP_122	N, E_ILE_116	H, E_ILE_116	2.99	2.19	18.05
5O4Y	O, E_ILE_116	N, E_ASP_122	H, E_ASP_122	2.97	2.20	22.39
5O4Y	OD1, E_ASP_122	N, E_TYR_123	H, E_TYR_123	2.81	2.07	25.74
5XXY	OD2, A_ASP_122	OG1, A_THR_20	HG1, A_THR_20	2.93	2.22	28.25
5XXY	OD2, A_ASP_122	N, A_VAL_21	H, A_VAL_21	2.79	1.95	10.31
5XXY	OD1, A_ASP_122	N, A_TYR_123	H, A_TYR_123	2.80	2.08	28.06

Table 1: The Asp22-linked hydrogen bonding (including both side chain and main chain) network formed within the experimentally determined PD-1/PD-L1 structures. 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	Acceptor (A)	Donor (D)	Hydrogen (H)	D-A (Å)	H-A (Å)	$\angle ADH(°)$
5XXY	OD2, A_ASP_122	OG1, A_THR_20	HG1, A_THR_20	2.93	2.22	28.25

Table 2: The Asp22-linked hydrogen bonding (including only side chain) network formed within the experimentally determined PD-1/PD-L1 structures. 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_LYS_124	NZ	A_ASP_122	OD1	3.019
3BIK	A_LYS_124	NZ	A_ASP_122	OD2	3.912
3BIS	A_LYS_124	NZ	A_ASP_122	OD1	3.773
3BIS	B_LYS_124	NZ	B_ASP_122	OD1	3.846
3FN3	B_LYS_124	NZ	B_ASP_122	OD1	3.034
3SBW	C_LYS_124	NZ	C_ASP_122	OD2	3.377
4Z18	B_LYS_124	NZ	B_ASP_122	OD1	3.214
4ZQK	A_LYS_124	NZ	A_ASP_122	OD2	3.631
5C3T	A_LYS_124	NZ	A_ASP_122	OD1	3.985
5C3T	A_LYS_124	NZ	A_ASP_122	OD2	3.140
5GGR	L_LYS_126	NZ	L_ASP_122	OD1	3.367
5GGT	A_LYS_124	NZ	A_ASP_122	OD2	3.321
5GRJ	A_LYS_124	NZ	A_ASP_122	OD1	3.729
5GRJ	A_LYS_124	NZ	A_ASP_122	OD2	3.641
5IUS	A_HIS_68	NE2	C_ASP_122	OD1	2.880
5IUS	B_HIS_68	NE2	D_ASP_122	OD1	2.672
5IUS	B_HIS_68	NE2	D_ASP_122	OD2	3.787
5IUS	C_LYS_124	NZ	C_ASP_122	OD2	2.898
5IUS	D_LYS_124	NZ	D_ASP_122	OD2	3.022
5J89	C_LYS_124	NZ	C_ASP_122	OD2	3.308
5J89	A_LYS_124	NZ	A_ASP_122	OD2	3.320
5J89	D_LYS_124	NZ	D_ASP_122	OD2	3.158
5J8O	A_LYS_124	NZ	A_ASP_122	OD2	3.299
5J8O	B_LYS_124	NZ	B_ASP_122	OD2	2.851
5JDR	A_LYS_124	NZ	A_ASP_122	OD1	3.201
5JDR	A_LYS_124	NZ	A_ASP_122	OD2	3.566
5JDS	A_LYS_124	NZ	A_ASP_122	OD1	3.048
5N2D	A_LYS_124	NZ	A_ASP_122	OD1	3.814
5N2D	B_LYS_124	NZ	B_ASP_122	OD2	3.206
5N2D	C_LYS_124	NZ	C_ASP_122	OD2	3.423
5N2D	D_LYS_124	NZ	D_ASP_122	OD2	2.935
5N2F	A_LYS_124	NZ	A_ASP_122	OD2	3.363
5N2F	B_LYS_124	NZ	B_ASP_122	OD2	3.084
5NIU	A_LYS_124	NZ	A_ASP_122	OD2	3.492
5NIU	B_LYS_124	NZ	B_ASP_122	OD2	3.475
5NIU	C_LYS_124	NZ	C_ASP_122	OD2	3.481
5NIU	D_LYS_124	NZ	D_ASP_122	OD2	3.508
5NIX	A_LYS_124	NZ	A_ASP_122	OD1	3.930
5NIX	A_LYS_124	NZ	A_ASP_122	OD2	3.158
5NIX	B_LYS_124	NZ	B_ASP_122	OD1	3.633
5NIX	B_LYS_124	NZ	B_ASP_122	OD2	3.267
5NIX	C_LYS_124	NZ	C_ASP_122	OD1	3.855

5NIX	C_LYS_124	NZ	C_ASP_122	OD2	3.349
5NIX	D_LYS_124	NZ	D_ASP_122	OD2	3.416
5O45	A_LYS_124	NZ	A_ASP_122	OD2	3.319
5O4Y	B_LYS_124	NZ	B_ASP_122	OD2	3.125
5O4Y	C_LYS_124	NZ	C_ASP_122	OD1	3.781
5O4Y	C_LYS_124	NZ	C_ASP_122	OD2	2.940
5O4Y	E_LYS_124	NZ	E_ASP_122	OD2	3.678
5WT9	H_LYS_214	NZ	L_ASP_122	OD1	3.763
5WT9	H_LYS_214	NZ	L_ASP_122	OD2	3.182
5X8L	A_LYS_124	NZ	A_ASP_122	OD2	3.334
5X8L	B_LYS_124	NZ	B_ASP_122	OD1	3.752
5X8L	B_LYS_124	NZ	B_ASP_122	OD2	3.564
5X8L	C_LYS_124	NZ	C_ASP_122	OD2	3.819
5X8L	D_LYS_124	NZ	D_ASP_122	OD2	3.701
5X8L	E_LYS_124	NZ	E_ASP_122	OD2	3.645
5X8M	A_LYS_124	NZ	A_ASP_122	OD2	3.674
5XJ4	A_LYS_124	NZ	A_ASP_122	OD2	3.456
5XXY	A_LYS_124	NZ	A_ASP_122	OD2	3.664

Table 3: Asp122-linked salt bridging network within the experimentally determined PD-1/PD-L1 structures. In this table, the residue naming scheme is **Chain ID_residue name_residue number**.