

Table 4. Murine PD-1 mutations and binding data from Zhang *et al.* (1) reconciled with the PD-1/PD-L1 complex structure

mPD-1 residue (numbering from this work)	Residue number in ref. 1	Human equivalent	Mutation from ref. 1	Location from crystal structures [ref. 1 and this work]	Is any atom within 4 Å of PD-L1?	Binding BIAcore, %	Side chain located in interface or solvent	mPD-1 residue (numbering from this work)
D 62	29	S	A	BC loop	no	115	solvent	D 62
D 62	29	S	S	BC loop	no	125	solvent	D 62
M 64*	31	V	A	C strand	yes	67	interface	M 64*
N 66*	33	same	A	C strand	yes	52	interface	N 66*
N 68*	35	Y	none	C strand	yes	not done	interface	N 68*
S 73*	40	same	none	CC' loop	yes	not done	interface	S 73*
N 74*	41	same	none	CC' loop	yes	not done	interface	N 74*
Q 75*	42	same	none	CC' loop	yes	not done	interface	Q 75*
T 76*	43	same	none	C' strand	yes	not done	interface	T 76*
K 78*	45	same	A	C' strand	yes	2	interface	K 78*
N 84	51	E	A	C'C" loop	no	101	solvent	N 84
L 86	53	R	A	C" strand	no	102	solvent	L 86
Q 88	55	same	S	C" strand	no	88	solvent	Q 88
V 90*	57	G	A	C"D loop	yes	87	interface	V 90*
H 107	74	same	S	E strand	no	96	solvent	H 107
R 114	81	same	S	EF loop	no	89	solvent	R 114
L 122*	89	same	none	F strand	yes	not done	interface	L 122*
G 124*	91	same	none	F strand	yes	not done	interface	G 124*
I 126*	93	same	A	F strand	yes	0	interface	I 126*
L 128*	95	same	A	F strand/FG loop	yes	3	interface	L 128*
H 129	96	A	A	FG loop	no	60	solvent	H 129
P 130*	97	same	A	FG loop	yes	83	interface	P 130*
K 131*	98	same	A	FG loop	yes	42	interface	K 131*
A 132*	99	same	L	FG loop	yes	121	interface	A 132*
I 134*	101	same	A	G strand	yes	4	interface	I 134*
E 136*	103	same	A	G strand	yes	9	interface	E 136*
D 62/ A 132	99/ 29	same/ S	L/ A	FG loop/ BC loop	yes/ no	135	solvent/ interface	D 62/ A 132

*Denotes a residue in the interface of the PD-1/PD-L1 complex.

Binding by wildtype mPD-1 was 100% in Zhang *et al.* (1).

1. Zhang X, *et al.* (2004) Structural and functional analysis of the costimulatory receptor programmed death-1. *Immunity* 20:337–347.