Table S1 Hydrogen bonds between BoNT/A-RBD and SV2C-LD in four mutate systems

R1294A		
BONT/A-RBD	SV2C-LD	Occupancy
M1144-N	C560-O	93.4%
S1142-O	F562-N	91.7%
S1142-N	F562-O	74.9%
M1144-O	C560-N	72.0%
T1146-OG1	F557-N	43.3%
A1294-N	S561-OG	33.9%
T1145-OG1	N559-N	23.3%
T1146-OG1	E556-OE1	19.1%
T1145-OG1	N559-OD1	15.5%
T1146-N	F557-O	15.0%
T1146-OG1	E556-OE2	13.2%
N954-ND2	F557-O	13.1%
G1292-O	N559-ND2	11.7%

F563A		
BONT/A-RBD	SV2C-LD	Occupancy
M1144-N	C560-O	94.4%
S1142-O	F562-N	92.1%
T1146-N	F557-O	85.3%
M1144-O	C560-N	78.2%
Y1149-OH	N559-OD1	70.5%
T1146-OG1	F557-N	68.6%
T1145-OG1	N559-N	66.2%
S1142-N	F562-O	48.2%
R1294-NH1	D539-OD1	46.4%
R1294-NE	D539-OD1	36.4%
R1294-NE	D539-OD2	35.8%
E1293-OE2	S561-OG	28.7%
K1187-NZ	E523-OE1	28.3%
R1294-NH1	D539-OD2	28.0%
K1187-NZ	D543-OD1	22.9%
R1156-NH1	S561-OG	22.7%
R1156-NH2	F542-O	19.1%
T1146-OG1	E556-OE1	17.1%
T1146-OG1	E556-OE2	17.1%
K1187-NZ	D543-OD2	16.7%
G1292-O	N559-ND2	14.8%
K1137-NZ	N565-OT1	14.0%
K1137-NZ	N565-OT2	13.7%
K1187-NZ	E523-OE2	13.6%

R1156E		
BONT/A-RBD	SV2C-LD	Occupancy
M1144-N	C560-O	91.4%
M1144-O	C560-N	89.4%
T1146-N	F557-O	84.4%
T1146-OG1	F557-N	62.5%
T1145-OG1	N559-N	59.6%
E1156-OE2	H564-NE2	42.1%
S1142-O	F562-N	36.9%
T1146-OG1	E556-OE1	28.3%
T1146-OG1	E556-OE2	24.3%
E1156-OE1	H564-NE2	24.2%
K1137-NZ	N565-OT2	21.2%
K1137-NZ	N565-OT1	18.2%
R1294-NH2	T521-OG1	15.4%
Y952-O	K558-NZ	13.2%
F953-O	K558-NZ	12.9%
N1147-ND2	E556-OE2	12.7%
R1294-NH1	D539-OD2	12.0%
R1294-NH2	D539-OD2	11.7%

TT1145/6AA		
BONT/A-RBD	SV2C-LD	Occupancy
S1142-O	F562-N	91.9%
Y1122-OH	N565-OT1	88.9%
R1156-NH2	N565-OT2	87.0%
R1156-NE	N565-OT1	86.6%
M1144-N	C560-O	81.0%
S1142-N	F562-O	79.1%
R1294-NH1	D539-OD1	54.8%
R1294-NH2	D539-OD2	54.1%
R1156-NH2	D543-OD1	50.9%
R1156-NH1	D543-OD2	48.8%
R1156-NH2	D543-OD2	45.8%
R1156-NH1	D543-OD1	44.7%
R1294-NH2	D539-OD1	41.4%
R1294-NH1	D539-OD2	40.5%
R1156-NH2	N565-OT1	14.2%