

Table 3. Hydrogen bonding distances between the glycone moieties of dhurrin and DIMBOAGlc and the amino acid side chains in the glycone-binding site of Glu1 E191D

Glucose position	Amino acid	Hydrogen bonding distance	
		Dhurrin	DIMBOAGlc*
O6	E464 OE2	2.6 Å	2.6- 2.7 Å
O6	W457 NE1	2.9 Å	2.6- 3.2 Å
O4	Q38 OE1	4.4 Å	3.3 Å
O4	W465 NE1	-	4.2 Å
O4	W457 NE1	2.4 Å	-
H2O	Q38 OE1	2.7 Å	-
H2O	W465 NE1	2.9 Å	-
O3	H142 NE2	3.6 Å	3.0 Å
O3	N190 ND2	3.8 Å	3.2 Å
O2	E406 OE2	3.1 Å	2.3- 3.1 Å
O2	D191 OD2	2.6 Å	2.7- 3.7 Å
C1	E406 OE2	4.3 Å	3.6-3.8 Å

*The indicated range corresponds to the two possible conformers, 4C_1 chair- and the 1S_3 skew-boat.