Table 2. Refinement statistics for Glu1E191D, mutant -DIMBOAGlc, -DIMBOA, and -dhurrin complexes

	Glu1E191D	*Glu1E191D in complex with DIMBOAglc*	*Glu1E191D in complex with DIMBOA*	*Glu1E191D in complex with dhurrin*
Resolution range (Å)	20- 2.2	30- 2.1	30- 2.1	30- 2.0
sigma-cutoff	0.01	0.1	0.1	0.05
R factor (%) (no. of refl.)	20.73 (51715)	22.77 (58739)	21.84 (58462)	19.55 (69029)
R_{free} factor (%) (5% of refl.)	24.38 (2592)	26.70 (2964)	26.60 (2962)	23.47 (3513)
No. of non-H protein atoms	7934	7918	7918	7950
No. of hetero-atoms	18	52	30	44
No. of solvent atoms	386	326	437	606
rms deviation from ideal geometry				
Bond lengths (Å)	0.007	0.006	0.007	0.006
Bond angles (°)	1.30	1.3	1.4	1.4
dihedrals (°)	22.5	22.3	22.3	22.5
impropers (°)	0.8	0.8	0.8	0.9
Average B factor ($Å^2$) (all atoms)	21.3	44.4	38.4	26.1
Luzzati coor. error (Å)	0.26	0.32	0.30	0.23
Ramachandran outliers	1	0	0	0
Residues in most favorable regions (%)	87.7	86.3	86.0	86.9