Supplementary Material

Two high-resolution crystal structures of potato 1,3-β-glucanase reveal subdomain flexibility with implications for substrate binding

Agnieszka Wojtkowiak^a, Kamil Witek^b, Jacek Hennig^b and Mariusz Jaskolski^{a,c,*}

^aDepartment of Crystallography, Faculty of Chemistry, A. Mickiewicz University, Poznan, Poland; ^bInstitute of Biochemistry and Biophysics, Polish Academy of Sciences, Warsaw and ^cCenter for Biocrystallographic Research, Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, Poland

Correspondence e-mail: mariuszj@amu.edu.pl

Table S1

Analysis of surface area $[Å^2]$ buried on packing interactions.

	HD	HD with His-tag omitted	HD with His-tag & Q223B-D227B omitted	LD	LD with His-tag omitted
Total solvent-accessible area with generated symmetry-related atoms $[Å^2]$	19390	19480	19810	20110	20360
Total solvent-accessible area without considering symmetry- related atoms [Å ²]	27460	27200	27510	26460	25950
Total area difference owing to presence of symmetry-related atoms $[Å^2]$	-8060	-7710	-7690	-6350	-5590
Chain A area difference [Å ²] / % of total contact surface	-3930/48.8	-3800/49.3	-3800/49.4	-3600/56.7	-3210/57.4
Chain B area difference $[Å^2] / \%$ of total contact surface	-4130/51.2	-3910/50.7	-3890/50.6	-2750/43.3	-2380/42.6