Table S1: Frequencies of hydrophobic contacts and hydrogen bonds in the simulations of ThEG3-pt* and CfCBM-pt. Only frequencies above 8% are shown.

ThEG3-pt*	**Hydrophobic Contacts / %**				
	Trp23	Ile131	Tyr112	Phe203	Val58
	100	100	99	98	94
	Tyr61	Ile128	Tyr7	Phe102	Trp121
	94	72	67	42	19
	Hydrogen Bonds / %				
	Gly129	Glu201	Asn21	Asn152	
	41	36	26	17	
CfCBM-pt	**Hydrophobic Contacts / %**				
	Tyr19	Val17	Val48	Tyr43	Tyr85
	100	100	98	100	98
	Hydrogen Bonds / %				
	Gln124	Asn81	Ala18	Arg75	
	37	33	34	29	

Hydrophobic contact:
It was considered that the hydrophobic contacts exist if the distances between carbon atoms in the lateral chains of hydrophobic residues (Val, Leu, Met, Ile, Pro, Trp , Phe and Tyr) and atoms in glycosidic rings "backbone" are smaller than 5 Å.

Hydrogen bonding:
The adopted criteria to consider a hydrogen bond were *D-A* distance less than 3 Å, *D-H-A* angle less than 20^{o}, being *D*, the donor and *A*, the acceptor of proton.