Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Material

A quantum biochemistry investigation of the protein-protein interactions for the description of allosteric modulation on biomass-degrading chimera

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Table S1: Amino-acids numbering of xylanase domain with the corresponding secondary structure for Xyl_{bound} and Xyl_{free} system

Secondary Structure	Amino acids numbering	
	Xyl_{bound}	Xyl_{free}
B2	276 to 282	276 to 282
A2	286 to 291	286 to 292
A3	297 to 302	296 to 302
B3	307 to 313	306 to 313
A5	322 to 331	321 to 330
B5	334 to 344	333 to 344
B6	348 to 356	348 to 353
B9	364 to 371	364 to 371
B8	374 to 386	374 to 382
B7	394 to 404	397 to 402
A6	411 to 415	413 to 416
H1	417 to 427	417 to 427
B4	434 to 445	434 to 447
A4	449 to 455	450 to 454

Table S2: Amino-acids numbering of XBP domain with the corresponding secondary structure for Xyl_{bound} and Xyl_{free} system

Secondary Structure	Amino acids numbering	
	Xyl_{bound}	Xyl_{free}
B1	03 to 09	03 to 09
H1	15 to 31	19 to 31
B2	33 to 39	33 to 39
H2	44 to 57	44 to 57
B3	61 to 64	61 to 64
H3	72 to 82	72 to 82
B4	85 to 89	85 to 89
B5	100 to 102	100 to 102
H4	106 to 117	106 to 120
B6	126 to 129	125 to 129
H5	136 to 148	136 to 149
B7	159 to 164	159 to 161
H6	171 to 181	171 to 184
B8	189 to 194	191 to 194
H7	197 to 206	197 to 210
B9	212 to 221	217 to 221
H8	225 to 230	225 to 233
B10	238 to 240	238 to 240
H9	244 to 259	244 to 258
H10	465 to 470	463 to 469

Table S3: Interdomain interaction pair energies that present Δ_{IE} < -2.0 kcal/mol for Xyl_{bound} and Xyl_{free} system

Interaction pairs	Interaction Energy (kcal/mol)		Δ_{IE} (kcal/mol)
	Xyl_{bound}	Xyl_{free}	
$A272_{Xyl}$-$D105_{XBP}$	-6.65	-0.96	-5.69
$S273_{Xyl}$-$D105_{XBP}$	-5.55	-0.09	-5.46
$S273_{Xyl}$-$E107_{XBP}$	-8.57	0.08	-8.64
$T274_{Xyl}$-$K108_{XBP}$	-3.36	-0.55	-2.80
$S293_{Xyl}$-$K108_{XBP}$	-4.43	-0.14	-4.29
$S293_{Xyl}$-$E111_{XBP}$	-11.12	-8.26	-2.86
$G294_{Xyl}$-$K108_{XBP}$	-3.18	-0.10	-3.08
$N296_{Xyl}$-$K115_{XBP}$	-7.31	-0.11	-7.20
$N296_{Xyl}$-$D119_{XBP}$	-3.95	-0.51	-3.45
$S298_{Xyl}$-$D119_{XBP}$	-5.59	-0.65	-4.94
$G316_{Xyl}$-$N271_{XBP}$	-3.39	-0.11	-3.27
$S317_{Xyl}$-$F104_{XBP}$	-2.31	-0.03	-2.28
$D372_{Xyl}$-$D465_{XBP}$	-4.50	1.13	-5.63
$D372_{Xyl}$-$D470_{XBP}$	-2.16	0.66	-2.82
$G373_{Xyl}$-$D465_{XBP}$	-2.64	-0.62	-2.03
$R403_{Xyl}$-$D465_{XBP}$	-6.93	-1.11	-5.82
$N412_{Xyl}$-$N461_{XBP}$	-14.42	-8.14	-6.28
$N412_{Xyl}$-$N462_{XBP}$	-4.27	-1.75	-2.52
$T414_{Xyl}$-$K464_{XBP}$	-3.28	-0.04	-3.24
$T416_{Xyl}$-$T466_{XBP}$	-5.73	-0.16	-5.56
$N419_{Xyl}$-$D470_{XBP}$	-2.49	-0.10	-2.39
$N434_{Xyl}$-$D267_{XBP}$	-9.56	-0.11	-9.45
$W456_{Xyl}$-$I120_{XBP}$	-3.09	-0.29	-2.79
$W456_{Xyl}$-$N459_{XBP}$	-2.75	-0.10	-2.65

Table S4: Interdomain interaction pair energies that present Δ_{IE} > 2.0 kcal/mol for Xyl_{bound} and Xyl_{free} system

Interaction pairs	Interaction Energy (kcal/mol)		Δ_{IE} (kcal/mol)
	Xyl_{bound}	Xyl_{free}	
$A272_{Xyl}$-$F104_{XBP}$	0.81	-2.03	2.84
$A272_{Xyl}$-$K108_{XBP}$	0.02	-2.00	2.02
$S273_{Xyl}$-$E111_{XBP}$	-0.17	-5.54	5.37
$S273_{Xyl}$-$N271_{XBP}$	-0.28	-6.86	6.57
$T274_{Xyl}$-$E111_{XBP}$	0.07	-2.25	2.32
$T274_{Xyl}$-$N271_{XBP}$	-0.03	-6.61	6.59
$S293_{Xyl}$-$D119_{XBP}$	0.03	-3.76	3.79
$T314_{Xyl}$-$N271_{XBP}$	-0.05	-3.10	3.04
$T315_{Xyl}$-$D267_{XBP}$	-0.16	-4.35	4.19
$G316_{Xyl}$-$D267_{XBP}$	-0.16	-5.03	4.87
$F319_{Xyl}$-$L246_{XBP}$	-0.25	-2.73	2.48
$F319_{Xyl}$-$N249_{XBP}$	-0.07	-2.28	2.21
$R320_{Xyl}$-$N271_{XBP}$	-0.33	-2.97	2.64
$T321_{Xyl}$-$Y241_{XBP}$	-0.33	-4.37	4.04
$N323_{Xyl}$-$Y241_{XBP}$	-2.70	-5.87	3.18
$N323_{Xyl}$-$D457_{XBP}$	-0.46	-4.17	3.72
$N323_{Xyl}$-$V458_{XBP}$	0.14	-2.41	2.55
$Y324_{Xyl}$-$D457_{XBP}$	-0.13	-2.66	2.53
$N325_{Xyl}$-$D457_{XBP}$	-0.29	-2.86	2.57
$S411_{Xyl}$-$N461_{XBP}$	-0.09	-3.62	3.54
$N412_{Xyl}$-$D457_{XBP}$	-0.14	-5.60	5.46
$N412_{Xyl}$-$N459_{XBP}$	-0.10	-6.61	6.51
$N412_{Xyl}$-$K460_{XBP}$	-0.11	-3.55	3.44
$N412_{Xyl}$-$D465_{XBP}$	-1.34	-4.46	3.12
$A413_{Xyl}$-$D465_{XBP}$	-0.39	-5.16	4.77
$T414_{Xyl}$-$N462_{XBP}$	-0.12	-4.24	4.12
$T414_{Xyl}$-$D465_{XBP}$	-2.74	-4.91	2.17
$T414_{Xyl}$-$T466_{XBP}$	-1.47	-4.18	2.71
$T414_{Xyl}$-$K469_{XBP}$	0.00	-5.69	5.69
$N452_{Xyl}$-$D119_{XBP}$	-4.25	-6.71	2.46
$W456_{Xyl}$-$A116_{XBP}$	-0.53	-4.64	4.11
$W456_{Xyl}$-$D119_{XBP}$	-0.23	-2.30	2.07
$W456_{Xyl}$-$V240_{XBP}$	-0.40	-4.33	3.93

Table S5: Interdomain interaction pair energies that present values higher than 2.0 kcal/mol or lower -2.0 kcal/mol and are exclusive of Xyl_{bound} or Xyl_{free} system

Interaction pairs	Interaction Energy (kcal/mol)	
	Xyl_{bound}	Xyl_{free}
$A272_{Xyl}$-$Y241_{XBP}$		-4.79
$V290_{Xyl}$-$D119_{XBP}$		-3.45
$G316_{Xyl}$-$E253_{XBP}$		-4.77
$S317_{Xyl}$-$E253_{XBP}$		-2.40
$F319_{Xyl}$-$T245_{XBP}$		-3.98
$R320_{Xyl}$-$Y241_{XBP}$		-2.01
$T321_{Xyl}$-$D470_{XBP}$		-3.92
$D372_{Xyl}$-$K469_{XBP}$		-10.94
$S418_{Xyl}$-$D470_{XBP}$		-2.41
$N419_{Xyl}$-$K469_{XBP}$		2.16
$G295_{Xyl}$-$D105_{XBP}$	-5.26	
$W313_{Xyl}$-$D105_{XBP}$	-7.24	
$S317_{Xyl}$-$S103_{XBP}$	-3.00	
$S317_{Xyl}$-$N271_{XBP}$	-4.17	
$F319_{Xyl}$-$F100_{XBP}$	-2.89	
$F319_{Xyl}$-$I102_{XBP}$	-3.88	
$R320_{Xyl}$-$D105_{XBP}$	-6.46	
$T321_{Xyl}$-$F104_{XBP}$	-3.79	
$N325_{Xyl}$-$I120_{XBP}$	-2.86	
$V328_{Xyl}$-$D119_{XBP}$	-6.40	
$R407_{Xyl}$-$K464_{XBP}$	-2.15	
$G410_{Xyl}$-$N461_{XBP}$	-3.36	
$N412_{Xyl}$-$K464_{XBP}$	-8.46	
$N419_{Xyl}$-$L246_{XBP}$	-2.11	
$N419_{Xyl}$-$N249_{XBP}$	-5.47	
$N422_{Xyl}$-$K27_{XBP}$	-4.87	
$N422_{Xyl}$-$E253_{XBP}$	-9.82	
$K425_{Xyl}$-$E253_{XBP}$	-3.98	
$K425_{Xyl}$-$E257_{XBP}$	-8.63	
$N430_{Xyl}$-$Q262_{XBP}$	-4.06	
$S433_{Xyl}$-$Q262_{XBP}$	-3.58	
$S433_{Xyl}$-$E263_{XBP}$	-2.73	
$S433_{Xyl}$-$P264_{XBP}$	-10.96	

$S433_{Xyl}$-$K265_{XBP}$	-3.26
$N434_{Xyl}$-$P264_{XBP}$	-2.49
$N434_{Xyl}$-$K265_{XBP}$	-10.46
$N434_{Xyl}$-$A266_{XBP}$	-3.02
$W435_{Xyl}$-$K265_{XBP}$	-3.52
$W435_{Xyl}$-$A266_{XBP}$	-3.66

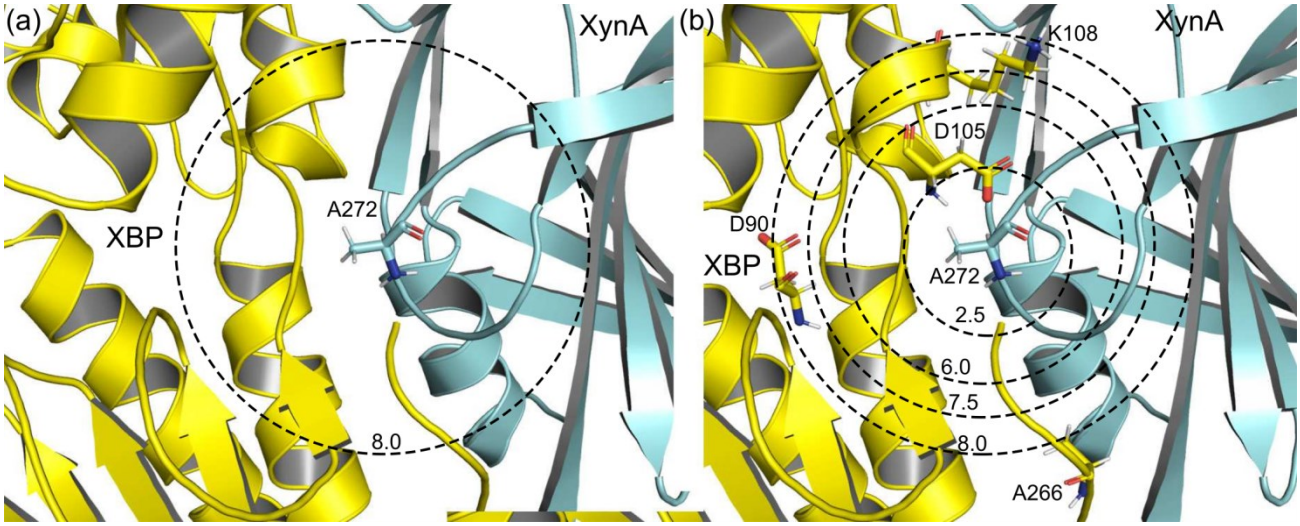

Fig. S1 - (a) Schematic view depicting the 8.0 Å radius around A272 Xyl residue and (b) the selection of some XBP amino acids within the r = 2.5, 6.0, 7.5 and 8.0 Å.

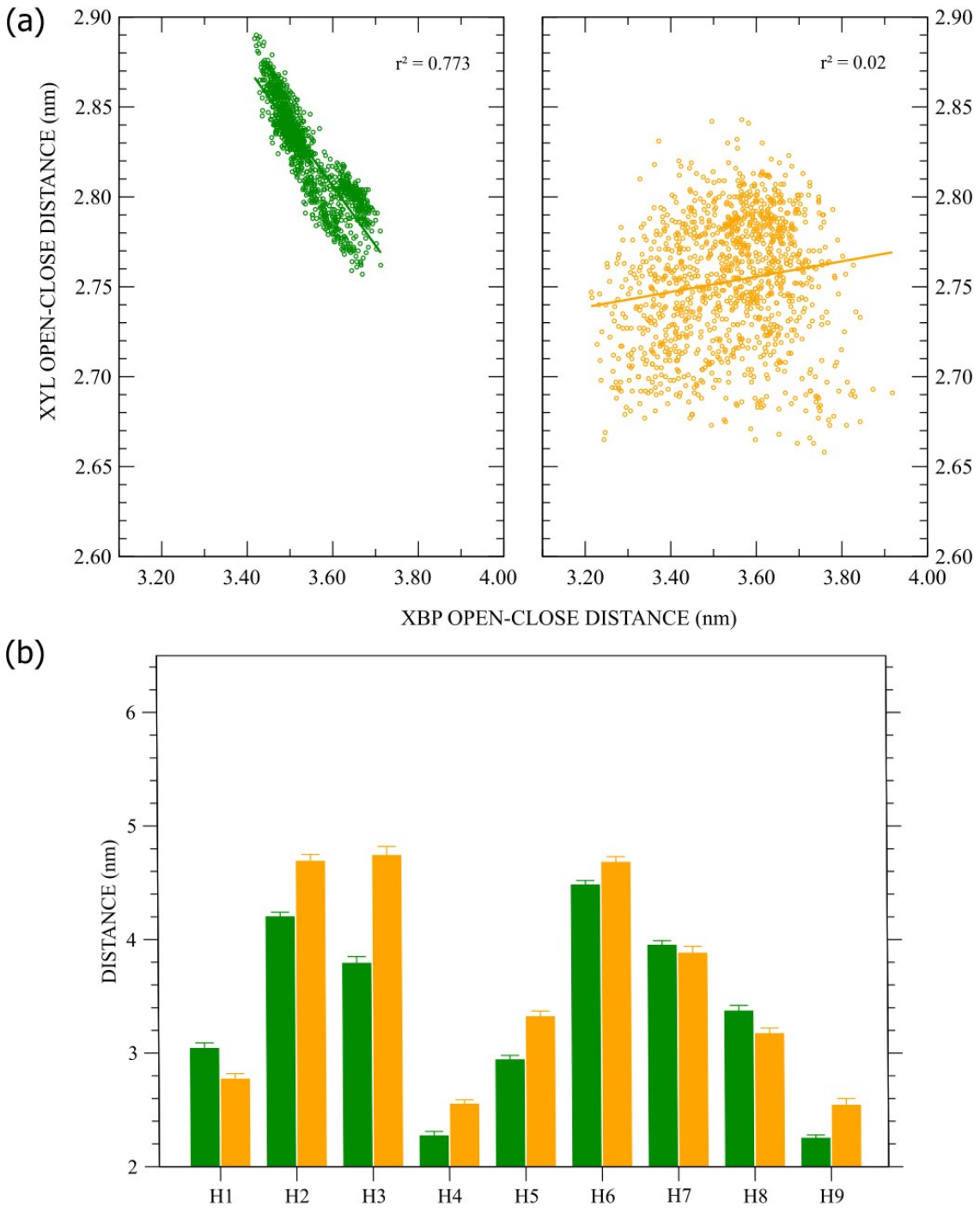

Fig. S2 - (a) Linear regression between the open-close distances, calculated from essential dynamics filtered trajectories according to the Methodology, for XBP and xylanase. Xyl_{free} (right) and Xyl_{bound} (left) states. The p-values for the linear regression models were < 0.0001. (b) Distances between the center of mass of XBP α-helixes (H1 to H9) and xylanase domain for Xyl_{free} (orange bars) and Xyl_{bound} (green bars).

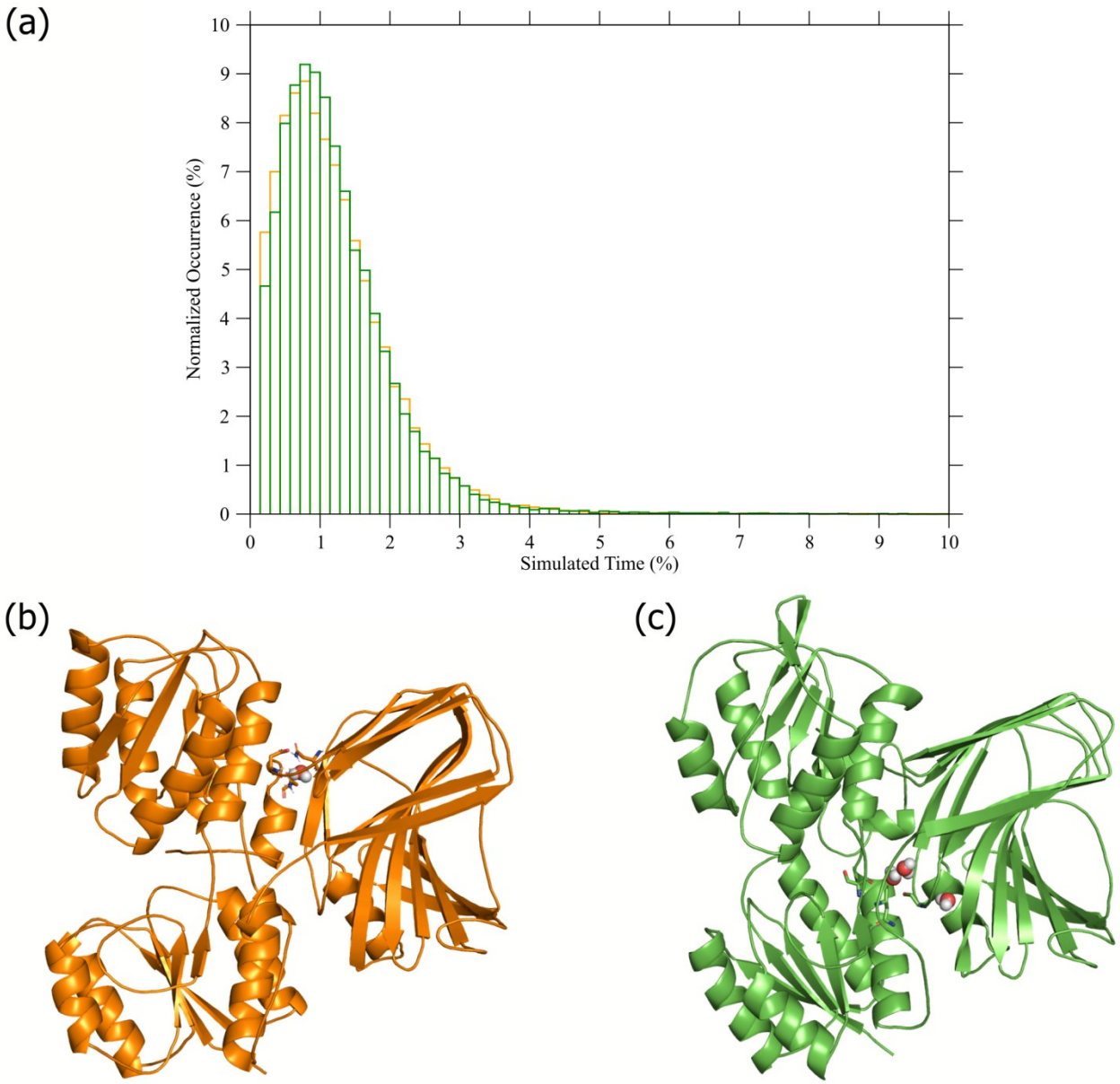

Fig. S3 - (a) Histogram of water molecules frequency into the interfacial region over simulated time with a bin size of 100 ps. (b) Schematic view depicting the interfacial waters molecules for (b) Xyl_{free} (orange) and (c) Xyl_{bound} (green) states.

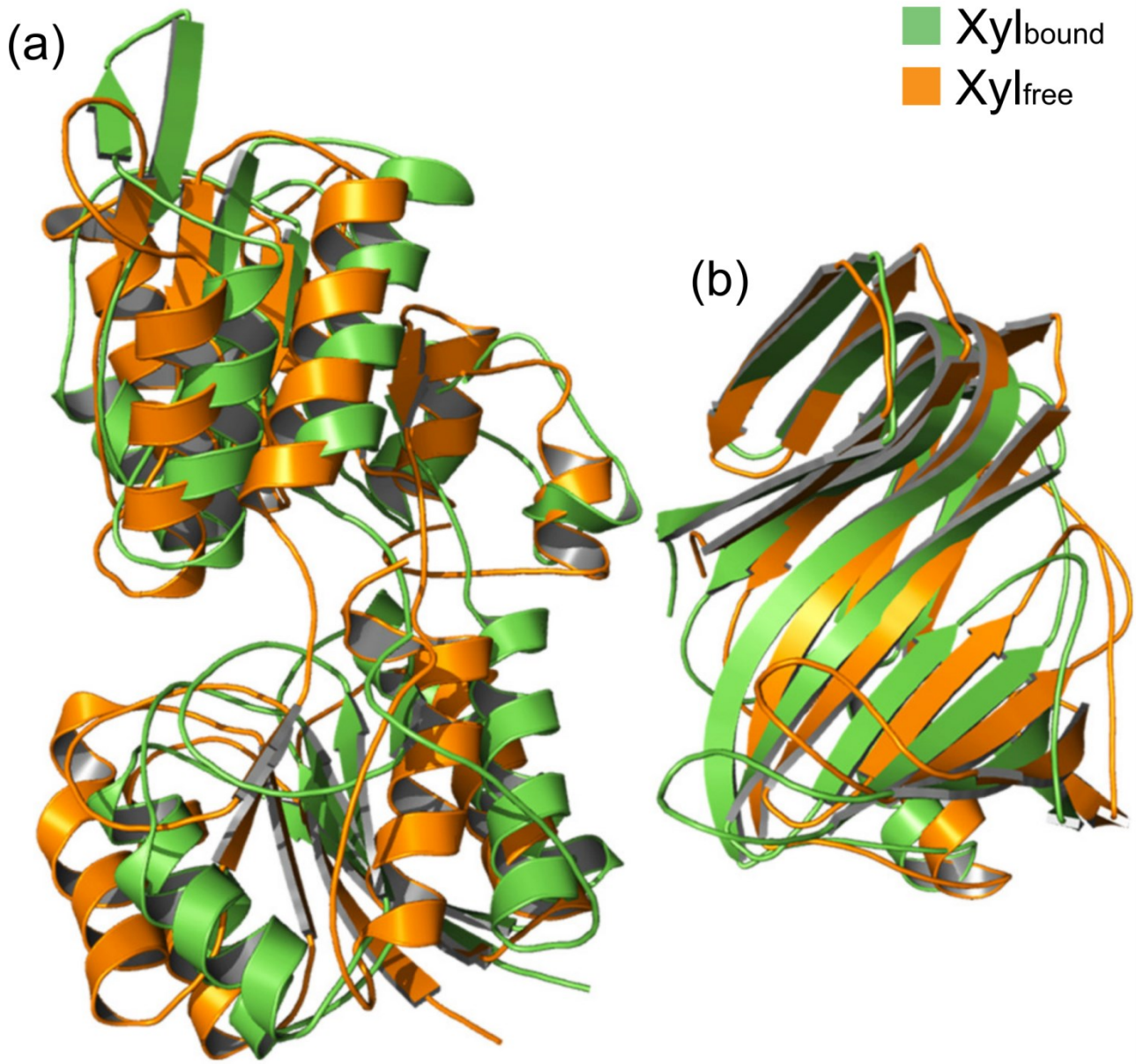

Fig. S4 - Supperposing structure of two domains, a) XBP and b) xylanase on the Xyl-XBP chimera for Xyl_{bound} (green) and Xyl_{Free} (orange) states.

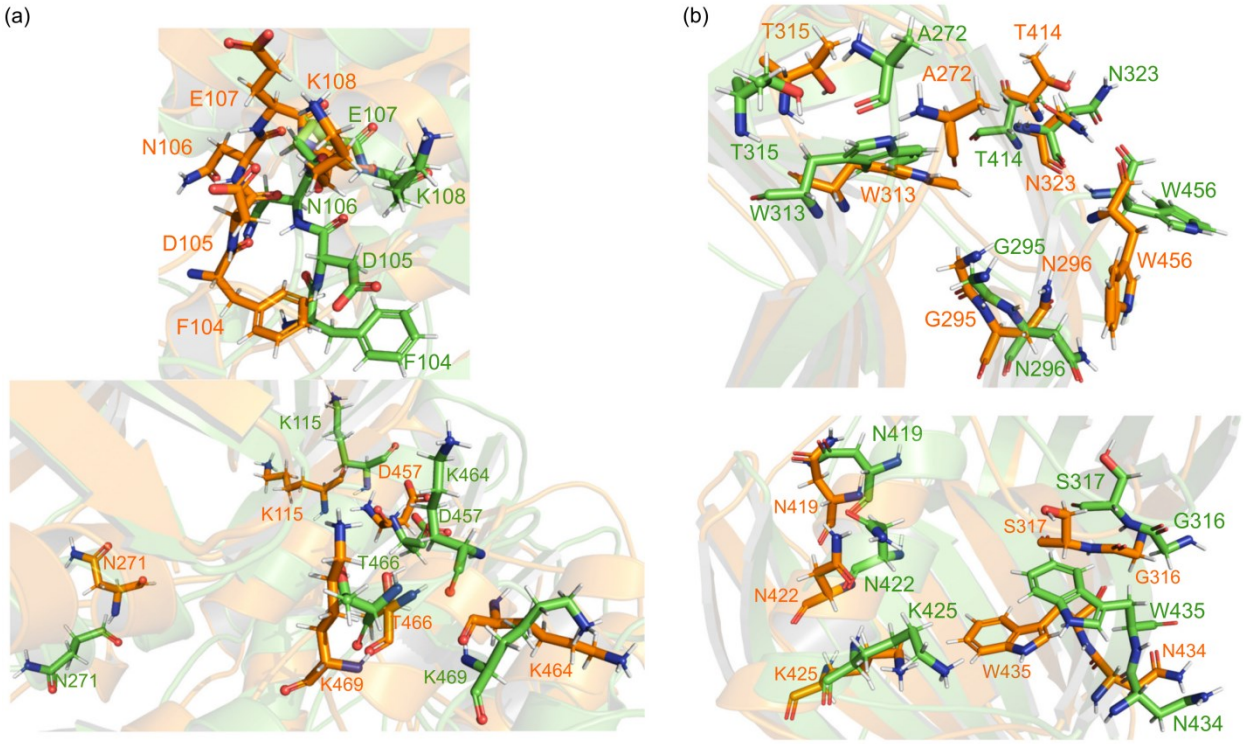

Fig. S5 - Supperposing structure of the amino acids forming the chimera interface in Xyl_{bound} (green) and Xyl_{Free} (orange) showing their difference in the position.