STRUCTURAL BIOLOGY

Volume 75 (2019)

Supporting information for article:

Relationship between the induced-fit loop and the activity of *Klebsiella pneumoniae* pullulanase

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Table S1 Sugar puckering parameters and torsion angles. The table shows Cremer-Pople parameters and torsion angles for maltotriose molecules bound to the active site. Cremer-Pople parameters were calculated using a Web-site calculator (http://enzyme13.bt.a.u-tokyo.ac.jp/CP/). The torsion angles were calculated using the program COOT (Emsley and Cowtan, 2004). Torsion angles were defined as O5 – C1 – O4' – C4' (Φ) and C1 – O4' – C4' – C5' (ψ) between glucose molecules on the side of the non-reducing end (including the C1 atom) and glucose molecules on the side of the reducing end (including the O4 atom; dash number).

		+2	+1	0	-1	-2	-3
PulA G680	Φ (°)	210.268	270.745	117.646	172.924	242.811	257.772
	Θ (°)	7.062	7.061	0.886	16.390	5.607	1.060
	Q	0.569	0.594	0.584	0.607	0.583	0.566
	conformation	$^4C_1$	$^4C_1$	$^4C_1$	$^4C_1$	$^4C_1$	$^4C_1$
	Φ (°)		102.77	101.30		85.61	99.52
	Ψ (°)		-132.30	-131.48		-155.75	-141.17
PulA G680L	Φ (°)	248.041	289.720	45.549	123.135	259.581	269.902
	Θ (°)	5.995	6.464	5.629	11.731	3.402	1.296
	Q	0.575	0.608	0.584	0.590	0.607	0.578
	conformation	$^4C_1$	$^4C_1$	$^4C_1$	$^4C_1$	$^4C_1$	$^4C_1$
	Φ (°)		103.71	102.16		87.69	98.65
	Ψ (°)		-138.91	-132.36		-152.22	-142.19

Table S2 Dihedral angles of residues 706-710. Dihedral angle parameters were calculated using a Web-site calculator (http://cib.cf.ocha.ac.jp/bitool/DIHED/). Dihedral angles were defined as C^{n-1}-N^n-$C\alpha^n$-C^n (Φ) and N^n-$C\alpha^n$-C^n-N^{n+1} (Ψ).

		Glu706		Gly707		Trp708		Asp709		Ser710	
		Φ	Ψ	Φ	Ψ	Φ	Ψ	Φ	Ψ	Φ	Ψ
PulA G680	ligand-free_chain_A	-81.1	100.2	-95.9	38.0	-65.8	149.6	-56.2	174.7	-107.4	-1.6
	ligand-free_chain_B	-80.0	101.0	-98.8	38.5	-71.2	159.4	-60.5	132.1	-106.5	-3.8
	G3	-80.1	103.7	-98.0	36.5	-68.4	156.4	-57.5	133.6	-111.5	-0.8
PulA-L680	ligand-free_chain_A	-82.3	105.7	-109.8	46.3	-68.3	170.3	-74.8	121.5	-108.7	170.4
	ligand-free_chain_B_Alt_A	-88.1	111.1	-82.3	42.2	113.2	159.2	-2.0	130.6	-162.2	172.6
	ligand-free_chain_B_Alt_B	-158.9	106.3	138.9	-27.0	57.5	160.0	-85.5	67.7	-116.1	44.8
	G3	-82.0	101.0	-107.1	47.5	-66.2	169.4	-72.8	124.8	-116.0	165.0
KPP	ligand-free	-145.4	168.0	169.1	-88.9	71.2	9.8	-124.7	-0.7	-65.1	133.8
	G3	-79.1	109.4	-105.9	48.6	-76.8	-165.7	-97.3	118.1	-91.8	-5.6