

Table S1. Coordination shell of the Mg²⁺ ion in the different SPP-ligand complexes. As described in the text, Mg²⁺ ions occupy two positions in the complex with sucrose + PO₄, and the residues involved in the coordination shells in each position are shown separately, ^a catalytic position, ^b non-catalytic position.

FORM 1			FORM 2											
Empty			Empty			Glc			Suc & PO ₄			Suc		
Residue	Atom	Distance (Å)	Residue	Atom	Distance (Å)	Residue	Atom	Distance (Å)	Residue	Atom	Distance (Å)	Residue	Atom	Distance (Å)
Asp9	OD2	2.2	Asp9	OD2	2.7	Asp9	OD2	2.5	Asp11 ^a	O	2.6	Asp9	OD2	2.9
Asp11	O	2.2	Asp186	OD1	2.6	Asp186	OD1	2.6	Asp186 ^a	OD1	2.5	Asp186	OD1	2.8
Asp186	OD1	2.3	Ser187	OG	2.7	Ser187	OG	2.7	PO ₄ ^a	O2	2.6	Ser187	OG	2.6
H ₂ O 40	O	2.3	Asn189	OD1	2.7	Asn189	OD1	2.4	H ₂ O 219 ^a	O	2.5	Asn189	OD1	2.5
H ₂ O 67	O	2.3	Asp190	OD2	2.7	Asp190	OD2	2.6	Asp9 ^b	OD2	2.2	Asp190	OD2	2.5
H ₂ O73	O	2.5				H ₂ O 212	O	2.9	Asp186 ^b	OD1	2.5	H ₂ O 91	O	2.7
									Ser187 ^b	OG	2.6			
									Asn189 ^b	OD1	2.5			
									Asp190 ^b	OD2	2.6			
									H ₂ O 219 ^b	O	2.7			