

Table S2: Distance between active site CA atoms. The residues were identified using a structure of TpMan in complex with β -D-glucose (PDB id: 3PZI), where the distances between ligand and residue are lower than 5 Å.

Pairs	Distances between CA atoms (Å)			Distance between CB atoms (Å)		
	pH 8	pH 6	pH 4	pH 8	pH 6	pH 4
TRP:134-GLU:198	7.8	7.3	8.4	6.6	6.3	7.5
TRP:134-ARG:200	9.3	9.9	9.8	9.3	9.6	9.8
TRP:134-GLU:235	12.6	13	13.7	11.4	12	12.5
TRP:134-TRP:253	18.3	19	18.9	17.1	18	18.1
TRP:134-TYR:280	15.7	16.3	16.3	13	13.8	13.7
TRP:134-HIS:283	14.8	14.4	15.4	12.2	11.9	12.8
TRP:134-TRP:284	15.7	15.5	17	14.9	14.8	16.2
GLU:198-ARG:200	6.4	6.4	6.1	6.8	6.8	6.4
GLU:198-GLU:235	5.3	6	5.7	5.2	6	5.4
GLU:198-TRP:253	14.8	15.4	15.3	14.2	15	15.1
GLU:198-TYR:280	12	12.6	12.5	9.9	10.7	10.3
GLU:198-HIS:283	13.5	13.1	14	11.1	10.8	11.4
GLU:198-TRP:284	13.3	13.1	14.3	11.8	11.8	12.7
ARG:200-GLU:235	8.7	8.6	9	7.8	7.5	7.6
ARG:200-TRP:253	12.3	12.8	13.1	10.8	11.8	11.9
ARG:200-TYR:280	15.5	16	16	13.7	14.3	13.9
ARG:200-HIS:283	15.6	15.4	15.9	13.6	13.5	13.3
ARG:200-TRP:284	14.3	14.2	15.4	12.7	12.7	13.3
GLU:235-TRP:253	12.3	12.8	13.2	11.2	11.7	12.6
GLU:235-TYR:280	9.3	10	10.1	8.2	9.3	9.1
GLU:235-HIS:283	12.4	12.7	13.1	10.5	11.1	11
GLU:235-TRP:284	11.3	11.5	12.4	8.9	9.3	10.1
TRP:253-TYR:280	13.2	13.3	13.6	12.9	13	13.7
TRP:253-HIS:283	12.2	12.2	11.6	12.2	12.2	11.5
TRP:253-TRP:284	8.7	8.8	8.6	7.9	7.9	8.2
TYR:280-HIS:283	5.6	6	5.7	4.4	4.7	4.6
TYR:280-TRP:284	6.2	6.3	6.5	5.5	5.4	6.3
HIS:283-TRP:284	3.7	3.5	3.6	5.5	5.3	5.2
Sum of distances	320.8	326.1	335.2	289.3	297.2	304.2
Average	11.5	11.6	12	10.3	10.6	10.9
Standard deviation	3.7	3.8	3.9	3.2	3.3	3.4