

**Table S2. Interactions in AgPGRPLC1-MTP/TCT model structures***Hydrogen bonds*

PGRPLC1 atoms		Atoms of MTP		PGRPLC1 atoms		Atoms of TCT	
H57	Nε2	AMU	O7	H34	Nε2	GlcNAc	O7
T149	Oγ1		O4 (W5) <sup>1</sup>	T149	Oγ1		O5 (W5) <sup>1</sup>
T35	O		N2	Y56	Oη		O6 (anh)
Y68	Oη	L-Ala	O10	I150	N		O3
H90	O	D-isoGln	N	T35	O	MurNAc	N2
K92	N		O	H57	Nε2		O7
N95	Nδ2		Oε1	Y68	Oη		O10
N95	Nδ2	Lys	O	H90	O	D-Glu	N
G88	O		O (W22) <sup>1</sup>	K147	Nζ		Oε1
				K92	N		Oε1
				N95	Nδ2		Oδ
				R82	Nη1	Meso-DAP	Oζ1
					Nη2		Oζ2
				G64	N		Oζ2
				G88	O	D-Ala	N (W22) <sup>1</sup>
				N93	N		O

*Hydrophobic contacts*

PGRPLC1 residues		Atoms of MTP		PGRPLC1 residues		Atoms of TCT	
T35		AMU	C8	A36		GlcNAc	C8
S151			C11	I150			C8
K147		D-isoGln	C				C7
K92			Cβ	H34			C8
A89		Lys	Cα	S151		MurNAc	C11
			Cδ	H57		L-Ala	Cβ
Y63			Cβ	K147		D-Glu	Cε
			Cγ	H90			Cβ
			Cδ	A89			Cδ
			Cε	Y63		Meso-DAP	Cβ
							Cδ
				A89			Cβ
							Cα
				K92		D-Ala	Cα
							C

<sup>1</sup>Structural water molecules observed in *DmPGRP-LCx-TCT-LCa* structure