

**Table S3. Interactions in AgPGRPLC2-MTP/TCT model structures***Hydrogen bonds*

PGRPLC2 atoms		Atoms of MTP		PGRPLC2 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	V150	N		O3
Y68	Oη		O10	T35	O	MurNAc	N2
K61	Nζ	L-Ala	O (W74) <sup>1</sup>	H57	Nε2		O7
T90	O	D-isoGln	N	K61	Nζ		O7 (W74) <sup>1</sup>
D147	Oδ2		N2	Y68	Oη		O10
N95	Nδ2		Oε1	K61		L-Ala	O (W74) <sup>1</sup>
N95	Nδ2	Lys	O	T90	O	D-Glu	N
G88	O		O (W22) <sup>1</sup>	D147	Oδ2		Oε2 (W190) <sup>1</sup>
				N95	Nδ2		Oδ
				R82	Nη1	Meso-DAP	Oζ1
					Nη2		Oζ2
				D64	N		Oζ2
				N95	Nδ2	D-Ala	O
				G93	N		O

*Hydrophobic contacts*

PGRPLC2 residues		Atoms of MTP		PGRPLC2 residues		Atoms of TCT	
T35		AMU	C8	A36		GlcNAc	C8
H57		L-Ala	Cβ	H34			C8
Y63		D-isoGln	Cγ	V150			C7
P92			Cβ	H57		L-Ala	Cβ
			C	Y68			Cβ
Y63	Lys		Cα	T90			Cβ
			Cγ	P92		D-Glu	Cε
			Cε				Cβ
A89			Cα				Cγ
				Y63			Cγ
				A89			Cδ
				Y63		Meso-DAP	Cβ
				A89			Cα
				P92		D-Ala	C

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