

Table S4. Interactions in AgPGRPLC3-MTP/TCT model structures*Hydrogen bonds*

PGRPLC3 atoms		Atoms of MTP		PGRPLC3 atoms		Atoms of TCT	
H57	Nε2	AMU	O7	H34	Nε2	GlcNAc	O7
T35	O		N2	S152	N		O7
Y70	Oη		O10	E151	N		O3
R63	Nε/Nη2	L-Ala	O (W74) ¹	T35	O	MurNAc	N2
H92	O	D-isoGln	N	H57	Nε2		O7
H144	Nε2		N2	R63	Nε/Nη2		O7 (W74) ¹
N97	Nδ2		Oε1	Y70	Oη		O10
N97	Nδ2	Lys	O	R63	Nη2	L-Ala	O (W74) ¹
G90	O		O (W22) ¹	H92	O	D-Glu	N
				H144	Nε2		Oε2
				N97	Nδ2		Oδ
				R84	Nη1	Meso-DAP	Oζ1
					Nη2		Oζ2
				S66	N		Oζ2
				N97	Nδ2	D-Ala	O
				G95	N		O

Hydrophobic contacts

PGRPLC3 residues		Atoms of MTP		PGRPLC3 residues		Atoms of TCT	
T35		AMU	C8	A36		GlcNAc	C8
S152			C11	H34			C8
F150		D-isoGln	C	E151			C8
K94			Cβ				C7
A91			Cδ	F150			C4
A91		Lys	Cα				C5
F65			Cγ				C6
			Cδ	S152		MurNAc	C11
				H57		L-Ala	Cβ
				F150		D-Glu	Cε
				H92			Cβ
				A91			Cγ
							Cδ
				F65		Meso-DAP	Cβ
							Cδ
				A91			Cα
							Cβ
				S66			Cζ
				K94		D-Ala	Cα
							C

¹Structural water molecules observed in *DmPGRP-LCx-TCT-LCa* structure