

Table 4. Hydrogen bond interactions in the PGRP-I β C–GMPP and PGRP-I α C–MPP complexes

Atoms of GMPP or MPP		Atoms of PGRP-I β C		Atoms of PGRP-I α C	
NAG	O4	R353	N η 1		
	O5	<i>T354*</i>	<i>Oγ1</i>		
	O7	T354	<i>Oγ1</i>		
	NAM	N2	T241	O	T209
	O1				T209
	O3	<i>T354*</i>	<i>Oγ1</i>		
	O4	<i>T354*</i>	<i>Oγ1</i>		
	O7			H231	N ε 2
	O10	Y263	O η		
	O10	Y274	O η	Y242	O η
ALA1	O			R235	N η 2
	O	<i>R353*</i>	<i>O</i>		
GDG	O ε 1	D301	O δ 1	N269	N δ 2
	N	S296	O	H264	O
	O	S296	O	Y266	O
	O2	<i>R353*</i>	O		
LYS	N ζ	<i>K268*</i>	O	N236	O
ALA4	O			G267	N
	O			N269	N82
	O			<i>N269*</i>	N
ALA5	OXT	Q293	N ε 2		
	OXT	D302	N		
	OXT	<i>G262*</i>	O		

Alanines at GMPP or MPP positions 1, 4, and 5 are designated ALA1, ALA4, and ALA5. NAG, *N*-acetylglucosidic acid (in GMPP only); NAM, *N*-acetylmuramic acid; GDG, γ -D-glutamate (in GMPP) or γ -D-glutamine (in MPP). O2 is the carboxyl O atom of GDG.

*Water-mediated hydrogen bonds are in italics.