

Table 2. Interactions between Munc18c and Stx4₁₋₁₉

The Stx4 N-peptide forms 13 hydrogen bonds (<3.4 Å) and 140 atom:atom van der Waals contacts (<4 Å) with Munc18c. The atoms involved in the hydrogen bonds are listed in the first section of the table, and the residues (rather than atoms) involved in van der Waals interactions are listed in the second section. Stx4 intramolecular hydrogen bonds are shown in the third section of the table. For hydrogen bonds, residues conserved in the Stx or SM protein are shown in bold, and, where they are not conserved, the aligned residue is shown in parentheses for Stx1a, Sed5p, Munc18-1 (M18-1), and Sly1p.

Hydrogen bonds		
Stx4	Munc18c	Distance, Å
Arg2:O (Stx1a:Lys2; Sed5p:Lys4)	Glu135:N (Sly1p:Asp158)	2.6
Arg2:NE	Asn137:OD1 (Sly1p:Tyr160)	3.4
Arg2:NH2	Ile136:O	2.6
Asp3:N	Glu223:OE1 (M18-1:Asp216)	2.8
Asp3:OD2	Arg132:NH2 (M18-1:Thr129; Sly1p:Gln155)	2.5
Asp3:OD2	Lys134:NZ (M18-1:Thr131; Sly1p:Tyr157)	2.8
Arg4:N	Cys133:O (M18-1:Leu130; Sly1p:Val156)	2.8
Arg4:NH1	Cys114:O (Slyp:Leu132)	2.8
Arg4:NH1	Glu135:OE1	2.9
Thr5:N	Cys133:O	3.1
Thr5:OG1	Cys133:N	3.1
Arg9:NH1 (Sed5p:Gln11)	Ile130:O (Sly1p:Ile153)	3.3
Arg9:NH1	Ile130:O	2.7
Van der Waals contacts		
Met1	Phe113, Glu135 , Ile221, Glu223	
Arg2	Glu135 , Ile136 , Asn137 , Tyr218 , Asp222 , Glu223, Lys224	
Asp3	Arg132, Cys133, Lys134, Glu223,	
Arg4	Cys114 , Phe119 , Cys133, Glu135	

Thr5	Arg131, Arg132, Cys133
Glu7	Phe119
Leu8	Phe119 , Ile122, Cys126, Ile130
Arg9	Lys128 , Ile130 , Arg131
Asp12	Phe119 , Asn120
Asp16	Asn120

Intramolecular hydrogen bonds		Distance, Å
Asp3:OD1	Thr5:N	3.3
Asp3:OD1	Thr5:OG1	2.9
Asp3:OD2	Thr5:OG1	3.5
Arg4:O	Glu7:N	3.3
Arg4:O	Leu8:N	3.2
Glu7:OE1	Arg4:NE	2.9
Glu7:OE1	Arg4:NH2	3.1
