

Table 4: HB type and count per trajectory recorded during  $R^*(4,8)$  events. The three most important HBs in each trajectory are marked in bold.

Hydrogen Bonds	Trajectory				
	[RC]	[P1]	[P2]	[DU]	[RCS]
Glu-22(O $_{\epsilon}$ )–Lys-28(H $_{\zeta}$ )	<b>1,833</b>	1,595	0	0	<b>4,740</b>
Asp-23(O $_{\delta}$ )–Lys-28(H $_{\zeta}$ )	<b>1,590</b>	3,311	72	<b>253</b>	<b>5,106</b>
<b>SB</b>	33.3%	14.1%	1.0%	9.9%	68.7%
Glu-22(O $_{\epsilon}$ )–Glu-22(H)	348	0	330	0	0
Glu-22(O $_{\epsilon}$ )–Asp-23(H)	164	0	0	0	0
Glu-22(O $_{\epsilon}$ )–Ser-26(H)	854	0	0	0	0
Glu-22(O $_{\epsilon}$ )–Ser-26(H $_{\gamma}$ )	522	0	0	0	0
Gln-22(O $_{\epsilon}$ )–Lys-28(H $_{\zeta}$ )	0	0	0	51	0
Asp-23(O $_{\delta}$ )–Gln-22(H $_{\epsilon}$ )	0	0	0	164	0
Asp-23(O $_{\delta}$ )–Val-24(H)	191	0	403	105	221
Asp-23(O $_{\delta}$ )–Ser-26(H $_{\gamma}$ )	0	0	<b>600</b>	0	0
Asp-23(O $_{\delta}$ )–Ser-26(H)	0	0	274	0	0
Asp-23(O $_{\delta}$ )–Gly-29(H)	0	0	0	0	257
<b>Charged-SD</b>	20.2%	0.0%	22.5%	12.5%	3.3%
Ala-21(O)–Gly-25(H)	0	0	227	0	0
Ala-21(O)–Ser-26(H)	0	2,078	0	0	0
Glu-22(O)–Asn-27(H)	0	2,977	0	0	0
Glu-22(O)–Gly-29(H)	0	0	0	0	447
Asp-23(O)–Asn-27(H)	0	412	209	0	0
Asp-23(O)–Lys-28(H)	36	<b>8,252</b>	182	245	0
Val-24(O)–Lys-28(H)	0	0	460	0	0
Val-24(O)–Gly-29(H)	57	0	<b>1,713</b>	0	0
Asn-27(O)–Val-24(H)	0	0	0	0	<b>1,335</b>
Asn-27(O)–Gly-25(H)	164	0	419	108	862
Lys-28(O)–Val-24(H)	0	0	0	43	118
Lys-28(O)–Gly-25(H)	<b>4,430</b>	<b>8,098</b>	0	<b>796</b>	548
Gly-29(O)–Ser-26(H)	0	0	0	97	96
<b>Backbone HBs</b>	45.6%	62.9%	45.0%	50.2%	23.8%
Glu-22(O)–Asn-27(H $_{\delta}$ )	0	2,265	0	0	0
Asp-23(O)–Asn-27(H $_{\delta}$ )	0	0	355	0	0
Gly-25(O)–Gln-22(H $_{\epsilon}$ )	0	0	0	32	0
Asn-27(O $_{\delta}$ )–Asp-23(H)	0	0	599	0	0
<b>SD-Backbone</b>	0%	6.5%	13.4%	1.2%	0.0%
Val-24(O)–Ala-21(H $_{\tau}$ )	83	<b>4,633</b>	212	<b>385</b>	169
Gly-25(O)–Ala-21(H $_{\tau}$ )	0	0	301	0	0
Asn-27(O)–Ala-21(H $_{\tau}$ )	0	0	131	0	0
Ala-30(O $_{\tau}$ )–Ala-21(H $_{\tau}$ )	0	204	0	0	203
Ala-30(O $_{\tau}$ )–Ser-26(H $_{\gamma}$ )	0	0	0	202	28
Ala-30(O $_{\tau}$ )–Lys-28(H $_{\zeta}$ )	0	869	<b>645</b>	85	192
<b>N- C-terminal HBs</b>	0.8%	16.4%	18.1%	26.2%	4.1%