Table 2. Dimer interactions

Interface*	Hydrogen bonds	Hydrogen bond distance, Å <4 Å		
		12Y-2 A	12Y-2 B	12Y-1
D-D_s strands	Main-chain H-bonds:			
	Val59(N)–Val59(O)$_s$	2.88	2.93	3.15
	Val59(O)–Val59(N)$_s$	2.88	2.93	3.15
	Side-chain H-bonds:			
	Lys61(Nζ)–Glu57(Oε1)$_s$	2.65		3.16
	Water mediated H-bonds:			
	W(20)/W(37)–Lys61(N)	3.37	3.12	
	W(20)/W(37)–Gly62(N)	3.09	2.64	
	W(20)/W(37)–Glu57(O)$_s$	2.73	2.88	
	W(20)/W(37)–Glu57(N)$_s$	2.75	2.92	
	W(1)/W(11)–Glu57(Oε1)$_s$	2.96	2.66	
	W(1)/W(11)–Lys61(N)	2.81	3.00	
	W(1)/W(11)–Val59(O)	2.81	3.13	
	W(81)–Thr58(Oγ1)			3.01
	W(81)–Asn60(Oδ1))$_s$			3.13
CDR3-CDR3$_s$	Main-chain H-bonds:			
	Asn95(N)–Arg101(O)$_s$	3.25	3.05	
	Arg101(N)–Asn95(O)$_s$	3.25	3.05	
	Ser97(N)–Leu99(O)$_s$	2.90	3.11	
	Ser97(O)–Leu99(N)$_s$	3.09	2.74	
	Side-chain H-bonds:			
	Asn95(Oδ1)–Arg101(Nε)$_s$	2.72		
	Tyr94(O)–Arg101(Nε)$_s$		2.69	
	Tyr94(Oη)–Arg101(Nη1)$_s$		3.36	
CDR1-CDR1$_s$	Side-chain H-bonds:			
	Lys 32(O)–Asp33(Oδ1)$_s$	2.42	3.25	
	Lys 32(O –Lys61(Nζ)$_s$		2.84	

*Subscript “s” is for a twofold symmetry-related molecule.