Table S1. E111-DIII interface

16007 DIII – E111 scFv			Western Pacific-74 DIII – E111 Fab	
Van der Waals contacts[a]				
DIII	**E111 scFv**		**E111 Fab**	
Val300	AsnL53			
Met301	AsnL53		AsnL53 LeuL50	
Lys334	AsnL30D		AsnL30D	
Pro336	TrpH99		TrpH99	
Phe337	TyrL30B		TyrL30B	
Ser338	HisL30A ProH98		PheL32 HisL30A ProH98	
Thr339 or Ser339	HisL30A TyrL30B		HisL30A TyrL30B	
Gln340	TrpH95 PheH97 ProH98		PheH97 ProH98	
Glu342	ValH56			
Lys343	TrpH33 ArgH50 ValH56 AspH57 LysH58		TrpH33 ArgH50 AspH57	
Gly344	ArgH50 TrpH95		ArgH50 TrpH95	
Ala345 or Val345	AspL94 ArgH50		AspL94 ArgH50 LysH58	
Thr346	HisL30A AsnL91 AsnL92		HisL30A AsnL91 AsnL92	
Gln347	HisL30A		HisL30A	
Gly349	TyrL30B		TyrL30B	
Arg350	TryL30B		TyrL30B	
Leu351	TyrL30B		TyrL30B	
Pro372	TyrL30B		TyrL30B	
Val379	PheH97		PheH97	
Ala382	PheH96 PheH97 TrpH99		PheH96 PheH97 TrpH99	
Gly383	PheH96 PheH97		PheH96 PheH97	

Glu384	AsnH31 TrpH32		AsnH31 TrpH32	
E111/DIII putative hydrogen bonds[b]				
DIII	**E111 scFv**	**Distance (Å)**	**E111 Fab**	**Distance (Å)**
Thr/Ser339 (OG1)	TyrL30B (OH)	2.96	TyrL30B (OH)	2.71
Ser339 (O)			HisL30A (NE2)	2.95
Lys343(O)	ArgH50 (NE)	2.93	ArgH50 (NE)	3.29
Lys343(O)	ArgH50 (NH1)	2.90	ArgH50 (NH1)	3.20
Lys343(NZ)	AsnH57 (O)	3.00	AsnH57 (O)	3.32
Thr346 (OG1)	AsnL91 (O)	2.77	AsnL91 (O)	2.81
Gly383 (N)	PheH97 (O)	2.59	PheH97 (O)	2.84
E111/DIII water mediated hydrogen bonds[b,c]				
DIII	**E111**			
Ile335 (O)	AsnL53 (OD1)			
Phe337 (O)	AsnL30D (OD1) HisL30A (O)			
Asp341 (OD2)	LysH58 (NZ)			
Lys343 (NZ)	AsnH57 (O) AsnH57 (OD1)			
Gly344 (O)	TyrL96 (OH)			
Thr346 (O)	AspL92 (O)			
Thr346 (OG1/N)	AspL91 (O) AsnL92 (O) AsnL94 (OD1)			
Asn348 (OD1)	HisL30A (ND1) AsnL92 (OD1)			
Asn348 (OD1)	AsnL92 (O)			
Gly349 (O)	TyrL30B (N)			

[a]Van der Waals contacts have interatomic distance ≤ 4.0 Å

[b]Putative H-bonds defined by HBPlus (McDonald IK)

[c]Water molecules were not placed in the E111 Fab-West Pac-74 DIII structure.