Peptide atoms		Antibody atoms		Distances (Å)	Type of interaction	CDR loop	Peptide (φ,ψ) angles[§] (degrees)	Peptide B factor[£] ($Å^2$) Mainchain/sidechain
Q1	OE1	Ser26	O	2.36	HB	L1	N.A.	47.9±2.2/53.0±2.6
	OE1	His28	N	3.38	HB	L1		
	NE2	Ser29	OG	2.48	HB	L1		
	CB	Gln27	O	2.98	VDW	L1		
	NE2	Thr30	CG2	2.91	VDW	L1		
Q2	O	Thr30	OG	2.87/2.51	sHB	L1	-89±19,148±7	41.4±2.5/43.8±2.5
	N	Gln27	O	3.10	HB	L1		
	OE1	Gln27	NE2	2.64	HB	L1		
	NE2	Asp96	OD1	3.31	HB	L3		
	NE2	Asp96	OD2	3.13/2.69	sHB	L3		
	NE2	Asp96	OD1	3.38/2.74	sHB	L3		
	OE1	His28	NE2	3.45	VDW	L1		
	CG	Tyr31	OH	3.28	VDW	L1		
	NE2	Ile98	CD1	3.86	VDW	L3		
Q3	O	Asp96	OD2	2.68/2.69	sHB	L3	-101±7,122±5	34.4±2.9/42.9±2.6
Q4	N	Thr30	OG	2.85/2.87	sHB	L1	-66±3,135±4	27.7±3.3/24.3±3.9
	CA	Tyr31	CZ	3.42	VDW	L1		
	NE2	Gly95	O	2.95	HB	L3		
	NE2	Thr32	O	2.89	HB	L1		
	OE1	Thr32	N	2.78	HB	L1		
	NE2	Glu34	OE2	3.34/2.81	sHB	L1		
	NE2	Gly95	N	3.34/2.94	sHB	L3		
	OE1	Thr32	CB	3.39	VDW	L1		
Q5	N	Asp98	OD2	2.95	HB	L3	-102±3,135±4	26.5±3.6/31.7±2.9
	O	Thr97	N	2.86	HB	L3		
	O	Thr97	OG2	2.92	HB	L3		
	O	Trp104	NE1	2.80/3.15	sHB	H3		
	CB	Thr97	C	3.76	VDW	L3		
Q6	N	Asp98	OD2	3.16	HB	L3	-131±6,166±6	26.3±4.8/28.9±2.2
	O	Thr97	OG1	3.02/2.97	sHB	L3		
	OE1	Thr32	OG1	3.26/2.68	sHB	L1		
	NE2	Glu49	OE1	2.85/2.65	sHB	L2		
	NE2	Glu34	OE2	3.22/2.61	sHB	L1		
	NE2	Glu49	OE2	3.22/3.02	sHB	L2		
	NE2	Tyr102	CB	3.57	VDW	H3		
Q7	O	Gly101	O	3.44	HB	H3	-143±5,142±9	27.4±5.1/38.8±3.0
	N	Trp104	NE1	2.84/3.24	sHB	H3		
	N	Tyr102	O	2.84/2.93	sHB	H3		
	C	Tyr102	CD2	3.16	VDW	H3		
	OE1	Tyr33	OH	2.57	HB	H1		
	NE2	Thr99	CB	2.66	VDW	H3		
Q8	O	Tyr33	OH	2.78/2.99	sHB	H1	-72±7,132±2	27.9±5.6/38.6±2.6
	O	Tyr33	CE2	3.67	VDW	H1		
	OE1	Gly101	O	3.23	HB	H3		
	NE2	Tyr102	CE1	3.56	VDW	H3		
Q9	N	Gly101	O	2.72	HB	H3	-76±3,-26±9	28.5±7.3/23.2±5.8
	O	Tyr33	N	3.44	HB	H1		
	O	Tyr32	CD2	3.62	VDW	H1		
	OE1	Tyr35	OH	2.54	HB	H1		
	OE1	Tyr33	O	2.88/2.68	sHB	H1		
	OE1	Gly99	N	2.88/2.73	sHB	H3		
	NE2	Tyr35	OH	2.97/2.57	sHB	H1		
	CB	Gly99	CA	3.74	VDW	H3		
	CG	Gly101	O	3.30	VDW	H3		
	CG	Val103	O	3.26	VDW	H3		
Q10	N	Arg100	N	3.36/2.81	sHB	H3	-106±9,136±9	35.7±7.4/42.0±5.3
	NE2	Tyr32	OH	3.08	HB	H1		
	NE2	Asp31	OD2	2.72/2.78	sHB	H1		
	CB	Tyr32	CE2	3.58	VDW	H1		
G11	N	Asp31	O	2.88	HB	H1	N.A.	44.6±5.2/N.A.

[§]Peptide φ,ψ angles are the average of angles for the six peptides in two different crystal forms of the complex.

[£]Peptide B-factors are the average for the mainchain and sidechain atoms of the four peptides in the 1.68 Å resolution $P2_1$ structure.

HB, hydrogen bond; sHB, solvent-mediated hydrogen bond; VDW, van der Waals interaction.

Supplementary Table 1. Interactions between $GQ_{10}G$ and the MW1 Fv. Peptide mainchain and sidechain atoms are highlighted in green and red, respectively. Average mainchain φ, ϕ angles for secondary structures are -75°, +150° (polyproline II helix), -135°, +135° (β-strand) and -57°, -47° (α-helix). Peptide residue Q9 exhibits the dihedral angles of a α-helix, but is classified as random coil because it does not make mainchain hydrogen bonds with other peptide residues.