Table II: Ligand-CRT docking characteristics

Ligand[a]	Docking energy (kcal/mol)	Interacting residues			
		CRT[b]	Ligand[c]	Distance (Å)	Chemical bond[d]
SE (^{70}QKRAA^{74})	-207	Asp209	R72	3.5	ES
		Asp209	R72	3.5	ES
		Glu223	K71	3.2	ES
HS(4-4)c Trp (DKCLA)	-109	Glu257	K	2.1	HB
		Glu257	K	2.6	ES
HS(3-4)c Trp (DKCLA)	-21.9	Asp209	A	1.8	HB
		Glu223	D	2.1	HB
		Gly256	D	2.1	HB

a, Core amino acid sequences are shown in parentheses; b, CRT residues are shown in a three-letter format. Numbers correspond to the location of the amino acid residue in the CRT sequence; c, ligand residues are shown in a single-letter format. Numbers correspond to the location of the amino acid residue in the DRβ chain sequence; d, ES, electrostatic; HB, hydrogen bond.