

Table S2. HADDOCK output for modeling the E2~Ub-E2 complex.

	Haddock score	# structures	RMSD (Å)	Evdw (kcal mol⁻¹)	Eelec (kcal mol⁻¹)	Edesov (kcal mol⁻¹)	EAIR (kcal mol⁻¹)	buried surface area (Å²)
Cluster 2	-123.2 ± 10.1	22	17.6 ± 1.6	-19.2 ± 3.5	-246.6 ± 50.9	17.1±5.8	9.4 ±8.84	1065.9 ±62.3
Cluster 3	-122.1 ± 12.7	16	8.8 ± 6.4	-25.8 ± 4.9	-252.2 ± 40.3	17.1± 7.0	35.5± 26.41	1079.4± 173.0
Cluster 1	-121.7± 23.9	22	8.3± 5.3	-25.3± 3.0	-204.6± 68.9	16.7± 3.6	34.2± 1.53	1041.4± 201.6
Cluster 4	-118.9± 14.0	15	12.8± 3.9	-22.4± 2.0	-223.8± 74.3	12.8± 10.5	19.5± 14.38	962.3± 134.6
Cluster 5	-108.1± 8.6	14	10.6± 2.3	-22.2± 6.9	-161.3± 35.7	13.0± 6.1	25.6± 11.19	889.8± 48.9
Cluster 10	-105.2±9.6	10	14.2± 3.3	-19.8± 4.8	-183.4± 86.1	8.7± 6.9	19.2± 15.59	902.9± 104.3
Cluster 7	-104.9± 11.8	13	14.2± 3.1	-22.8± 0.9	-185.8± 80.4	12.8± 10.3	13.5± 14.62	954.1± 177.0
Cluster 8	-103.2± 8.0	11	12.9± 2.1	-19.7± 2.1	-137.8± 33.4	5.9± 1.6	20.9± 15.03	840.2± 73.3
Cluster 6	-98.3± 9.5	14	11.9± 2.7	-18.6± 2.3	-165.4± 59.8	10.4± 6.3	18.4± 15.61	793.8± 49.3
Cluster 12	-98.0± 11.7	7	13.3± 2.3	-20.5± 1.2	-147.0± 43.8	7.3± 2.6	11.8± 11.18	862.7± 83.5