



b)

Homology model	Homology model							Volumen	Surf. Area
	P03126	A1:a	A1:b	A1:c	A2:a	A2:b	A3:a		
Homology model P03126	0	3.49	3.22	4.21	2.92	1.82	1.35	1,222.6 Å ³	271.3 Å ²
A1:a	3.66	0	0.76	1.08	1.23	2.33	4.03	799.6 Å ³	244.8 Å ²
A1:b	3.65	1.31	0	1.45	0.89	2.08	3.81	862.0 Å ³	277.3 Å ²
A1:c	4.27	1.47	1.49	0	1.92	3.11	4.75	671.0 Å ³	238.7 Å ²
A2:a	3.42	1.2	1.42	2	0	1.79	3.5	904.8 Å ³	297.3 Å ²
A2:b	2.42	2.56	2.61	3.32	2.21	0	2.36	1,073.3 Å ³	308.4 Å ²
A3:a	1.51	4.38	4.46	5.02	4.13	3.05	0	1,204.4 Å ³	305.3 Å ²

RMSD (Å)

Figure S8: Representative conformations of E6 protein. a) Superimposed structures of the six conformations selected from apo-E6 trajectories. b) RMSD values of each conformer pair, the homology model P03126 is also included. Squares represent the RMSD value of the whole backbone. Circles correspond to the RMSD values of the pocket residues.