Supplemental material for

Multi-LZerD: Multiple protein docking for asymmetric complexes

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Table SI. The number of decoys in the final population with a correctly predicted subcomplex.

| A. Bound cases						
PDB ID [a]	Number of Subunits in the correctly predicted sub-complexes [b]					
	6	5	4	3	2	0
2AZE (3)	-	-	-	1	29	0
1A0R (3)	-	-	-	1	121	0
1VCB (3)	-	-	-	1	40	112
1K6N (3)	-	-	-	1	198	0
1B9X (3)	-	-	-	1	198	0
6RLX (4)	-	-	0	1	131	68
1QGW (4)	-	-	1	0	198	0
1LOG (4)	-	-	1	0	111	0
1NNU (4)	-	-	1	1	138	0
1RHM (4)	-	-	1	1	82	0
1I3O (6)	5	190	4	0	0	0

The analysis was performed on the bound multiple docking prediction results shown in Table 2.

a) The number of chains in the complex is shown in parentheses.

b) In each decoy structure, the maximum number of subunits which are assembled within a global RMSD of 4.0 Å is counted.

B. Unbound Cases

| PDB ID [a]	Number of Subunits in the correctly predicted sub-complexes [b]					
	6	5	4	3	2	0
1A0Rbg (3)	-	-	-	0	19	180
1A0Rb (3)	-	-	-	1	168	30
1A0Rg (3)	-	-	-	1	141	57
1VCBabc (3)	-	-	-	1	180	18
1QGWabcd (3)		-	1	7	191	0
1NNUabcd (4)	-	-	1	3	195	0
1NNUab (4)	-	-	1	1	193	4
1NNUcd (4)	-	-	1	3	111	84
1LOGabcd (4)	-	-	1	1	197	0
1RHMabcd (4)	-	-	1	0	39	159

The analysis was performed on the unbound multiple docking prediction results shown in Table 3.

Figure S1. RMSD and physics-based scores in final GA generation.
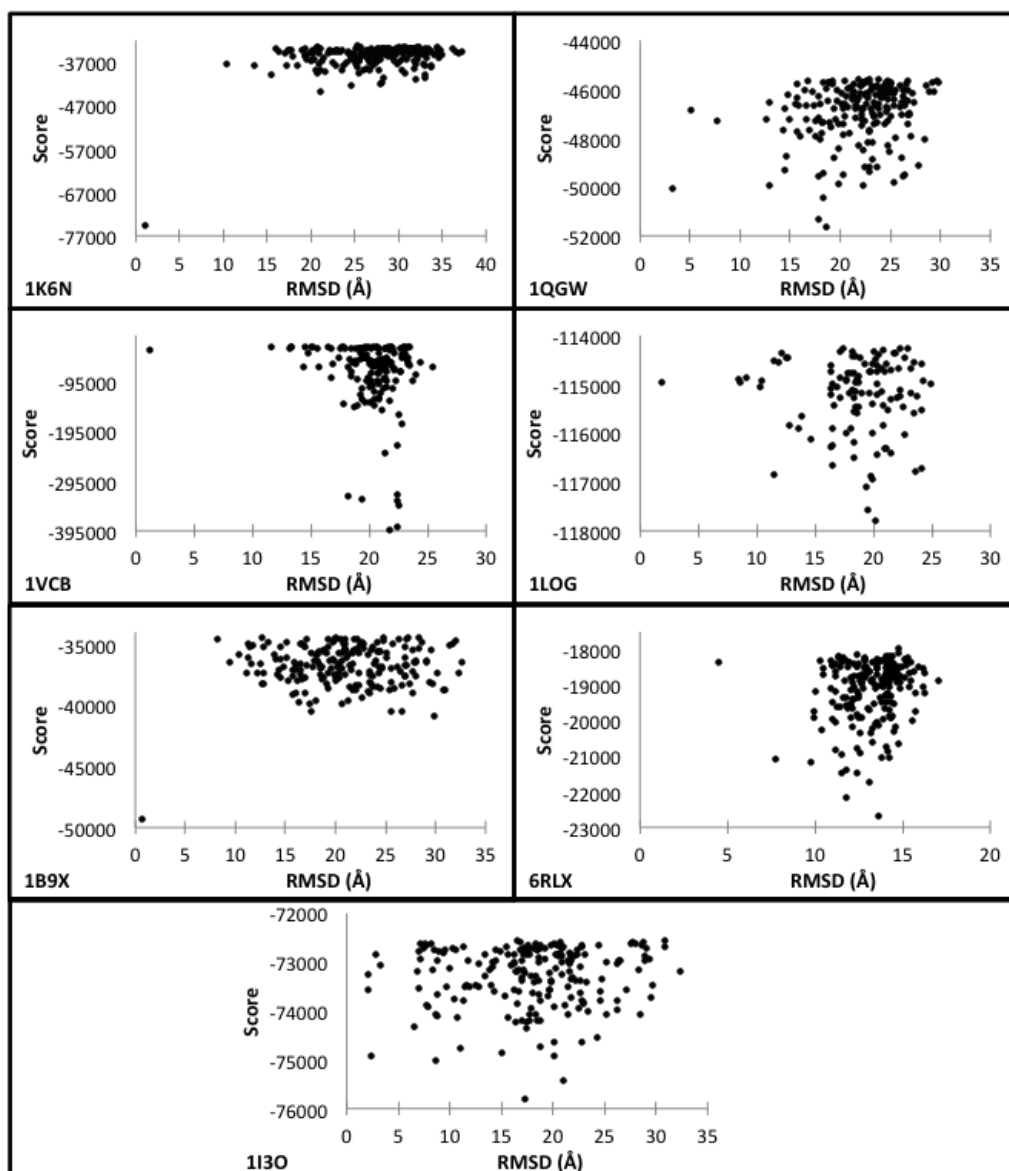
Plots for the other four protein complexes in the dataset (Table 1) are shown as Figure 3 in the main text.

Figure S2. The evolution of the fitness score and the RMSD.
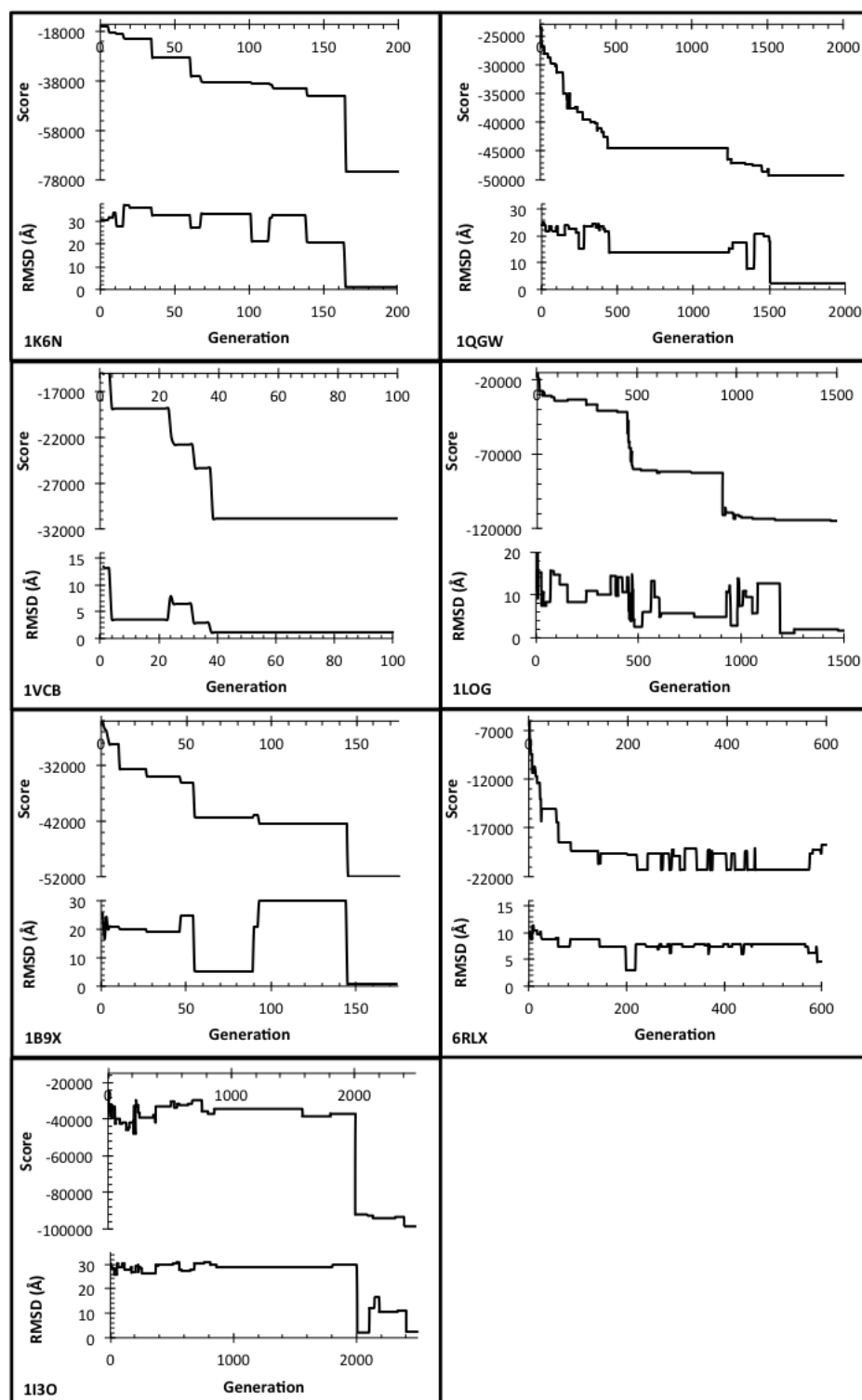
Plots for the other four protein complexes in the dataset (Table 1) are shown as Figure 4 in the main text.