Supporting Information for

Interaction of serum proteins with SARS-CoV-2 RBD

Yue-wen Yin[1], Yan-jing Sheng[1], Min Wang[1], Yu-qiang Ma[2,*], Hong-ming Ding[1,*]

[1] Center for Soft Condensed Matter Physics and Interdisciplinary Research, School of Physical Science and Technology, Soochow University, Suzhou 215006, China.

[2] National Laboratory of Solid State Microstructures and Department of Physics, Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, China.
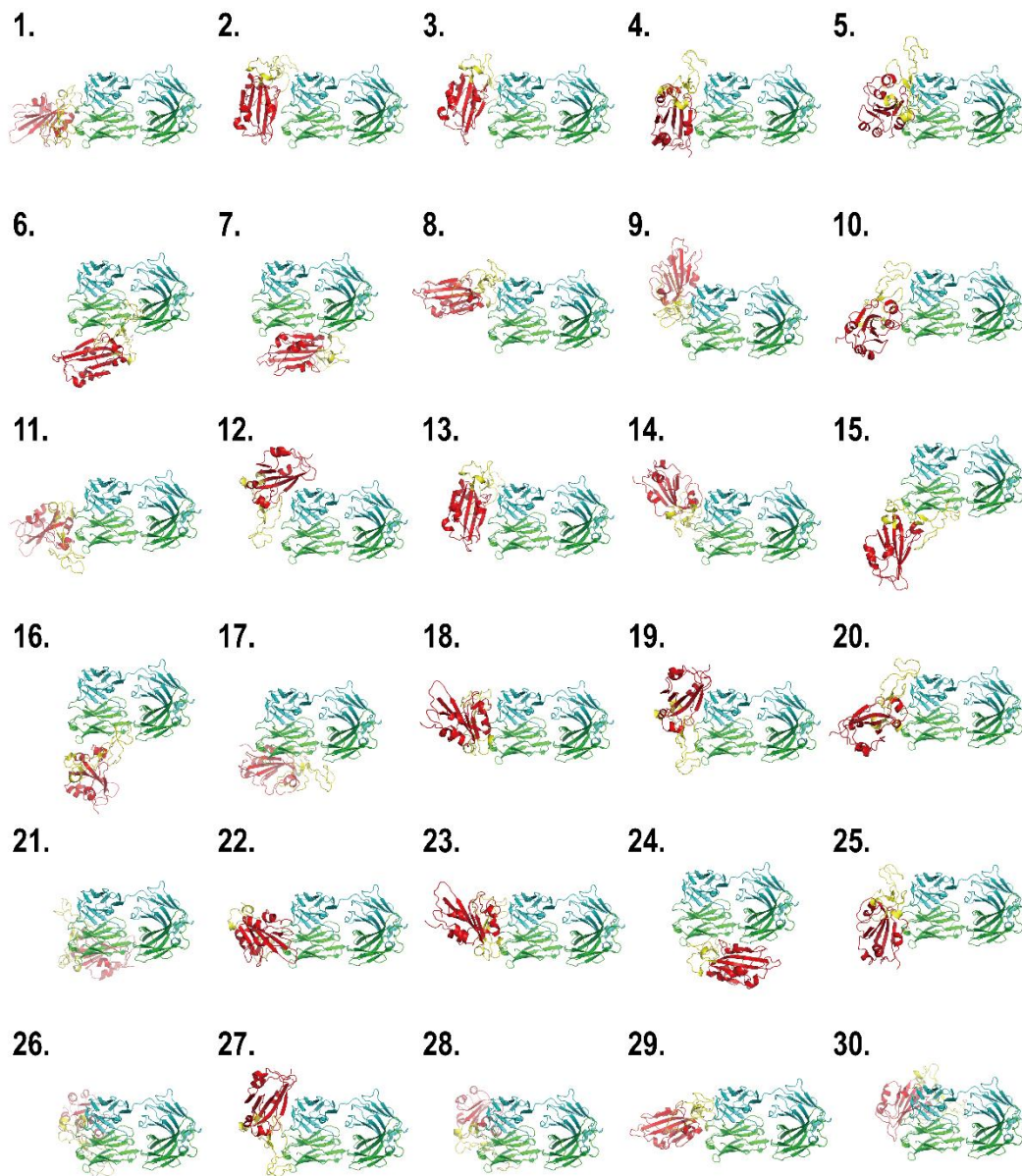
*Email: myqiang@nju.edu.cn, dinghm@suda.edu.cn

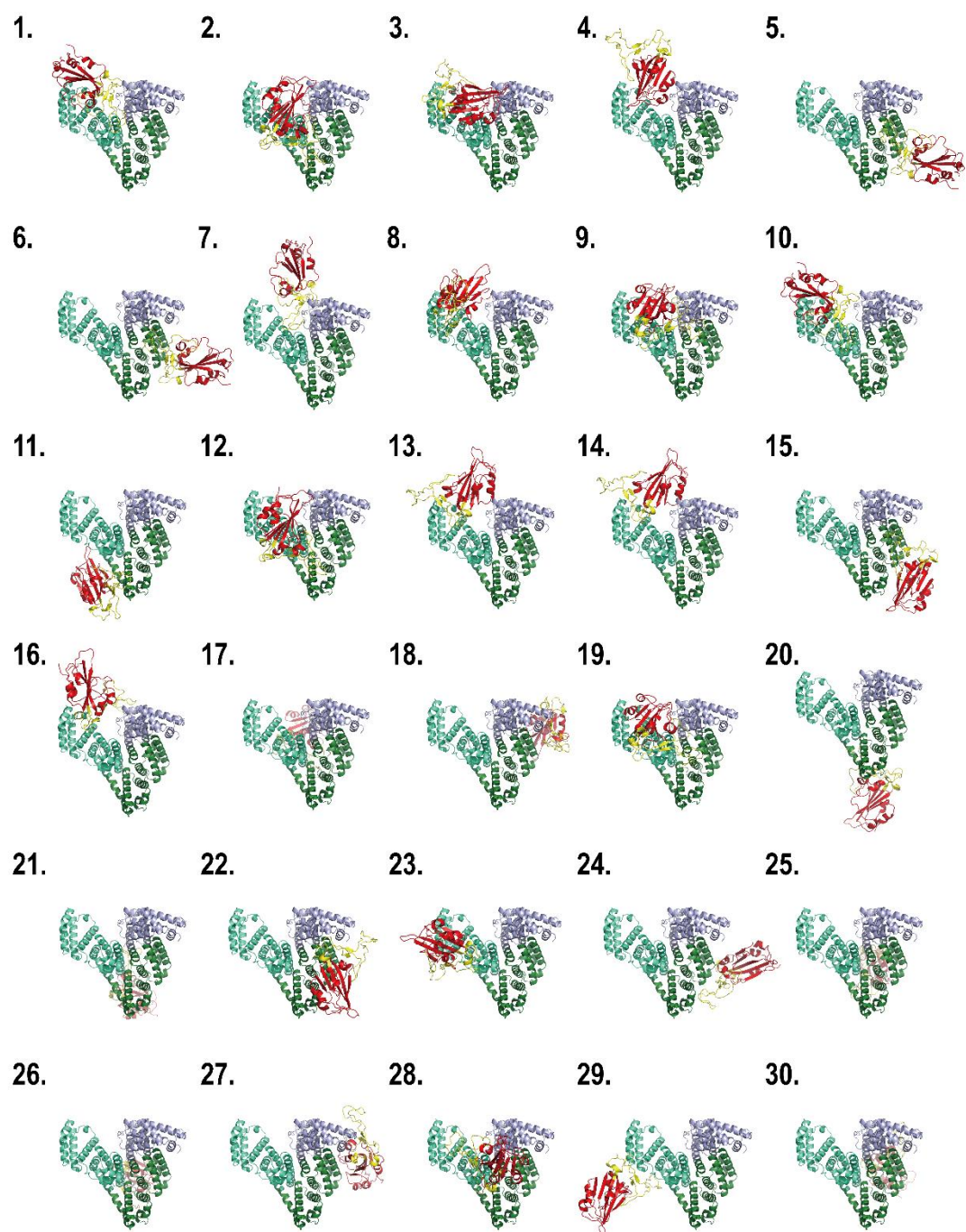**Figure S1.** Snapshots of the top 30 conformations of the IgM-RBD complexes in the docking.

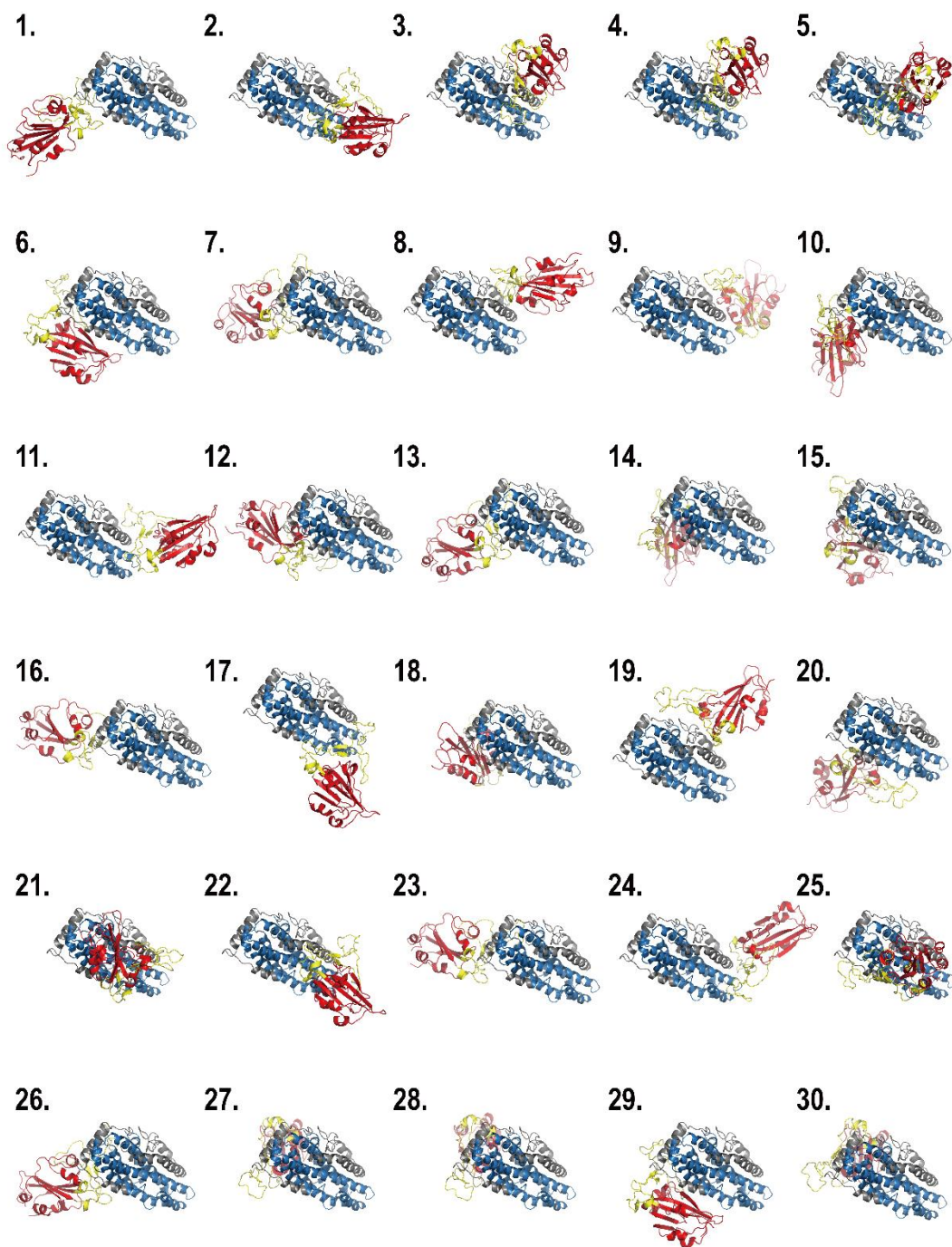**Figure S2.** Snapshots of the top 30 conformations of the HSA-RBD complexes in the docking.

Figure S3. Snapshots of the top 30 conformations of the ApoE-RBD complexes in the docking.
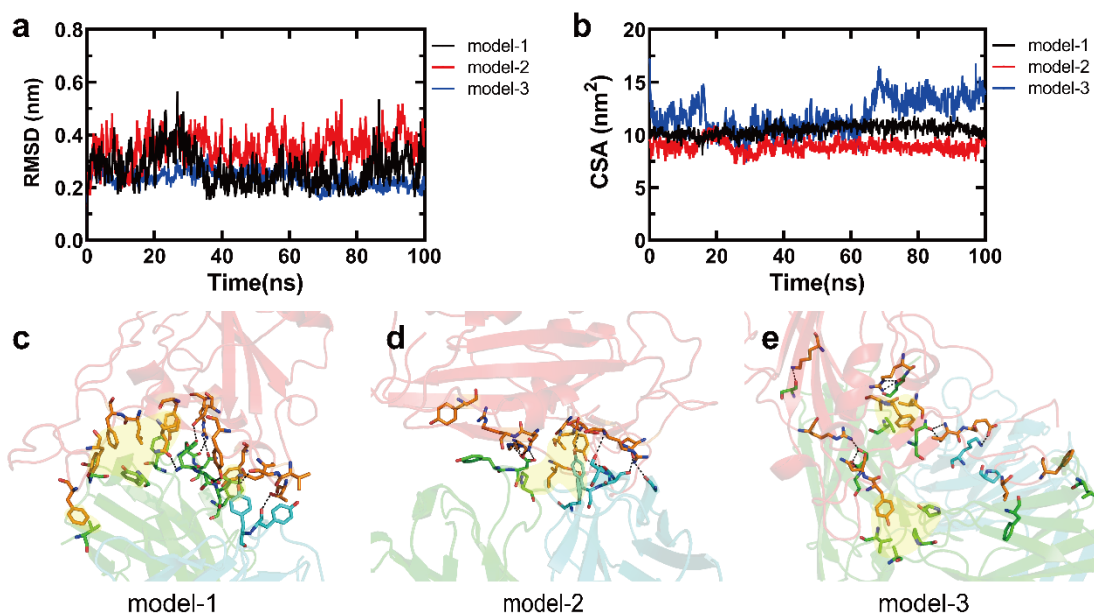
Figure S4. (a) The root mean square deviation (RMSD) of the backbone atoms in the three models of IgM and RBD as a function of time. (b) The contact surface areas (CSA) between the IgM and RBD in the three models as a function of time. Structural depiction of key interfacial interactions between the IgM and the RBD of SARS-CoV-2 in the three models (c-e), where the hydrogen bonds are highlighted with dashed lines, and the hydrophobic contacts are shaded in yellow.
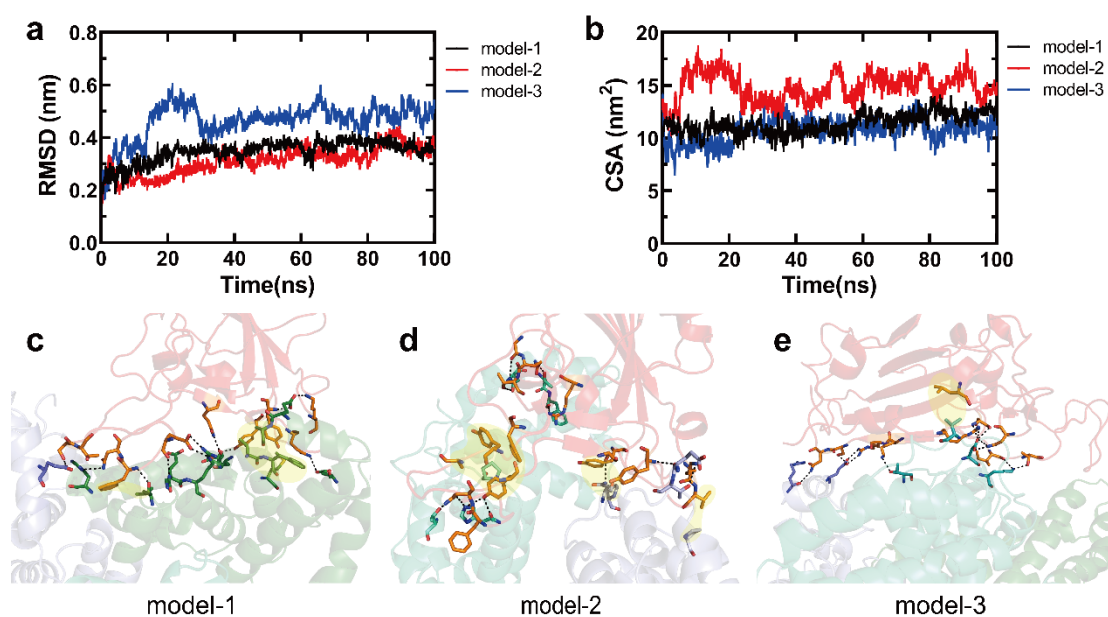
Figure S5. (a) The RMSD of the backbone atoms in the three models of HSA and

RBD as a function of time. (b) The CSA between the HSA and RBD in the three models as a function of time. Structural depiction of key interfacial interactions between the HSA and the RBD of SARS-CoV-2 in the three models (c-e), where the hydrogen bonds are highlighted with dashed lines, and the hydrophobic contacts are shaded in yellow.

Figure S6. (a) The RMSD of the backbone atoms in the three models of ApoE and RBD as a function of time. (b) The CSA between the ApoE and RBD in the three models as a function of time. Structural depiction of key interfacial interactions between the ApoE and the RBD of SARS-CoV-2 in the three models (c-e), where the hydrogen bonds are highlighted with dashed lines, and the hydrophobic contacts are shaded in yellow.
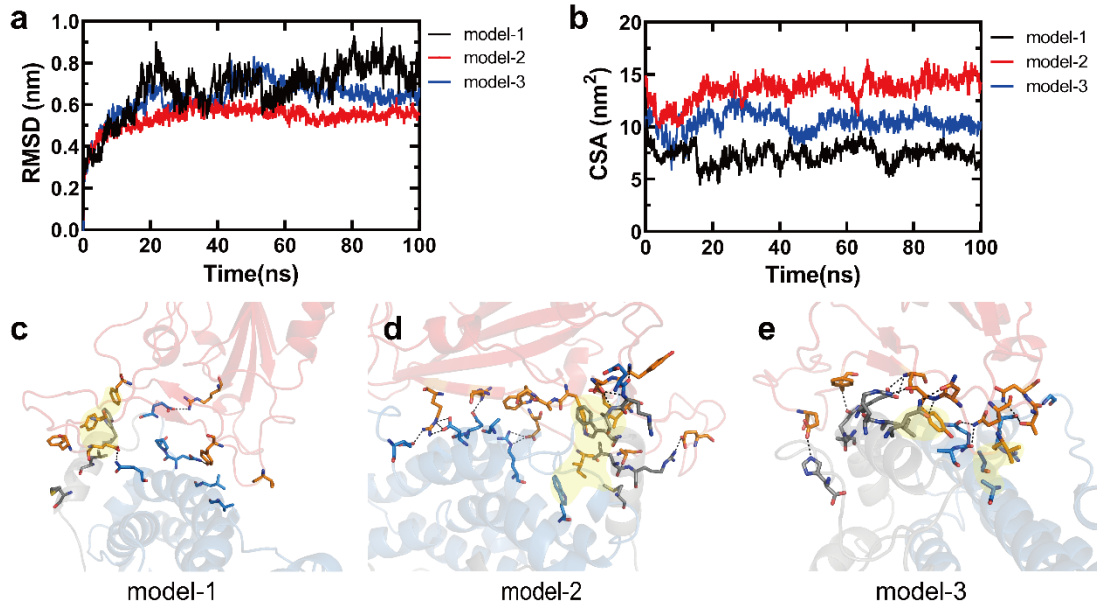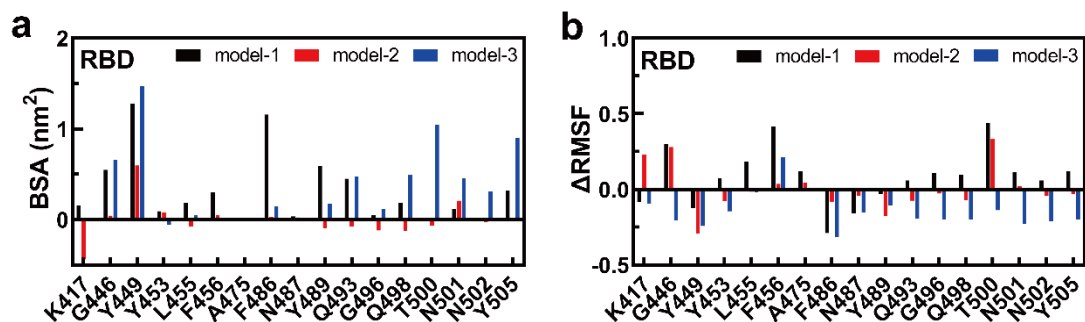

Figure S7. The BSA (a) and ΔRMSF (b) of the epitope site of RBD in the three models.

Table S1. The binding energy (BE) in the unit of kcal/mol and the root mean square deviation (RMSD) in the unit of Å for the Top 30 conformations in IgM/RBD system.

Conf.	1	2	3	4	5	6	7	8	9	10
BE[1]	-30.98	-30.18	-30.14	-28.75	-28.30	-27.20	-26.69	-26.32	-25.18	-24.81
RMSD[2]	0.00	18.86	18.14	19.33	22.79	27.36	32.86	12.94	20.32	19.42
Note[3]	model-1	model-2				model-3				
Conf.	11	12	13	14	15	16	17	18	19	20
BE	-22.21	-21.30	-20.54	-20.03	-19.10	-14.57	-11.20	-10.96	-9.69	-8.41
RMSD	5.34	24.72	19.38	18.52	25.14	27.73	21.54	24.27	22.66	23.66
Conf.	21	22	23	24	25	26	27	28	29	30
BE	-7.71	-7.00	-6.80	-6.14	-4.67	-3.53	-1.18	-0.02	1.36	3.61
RMSD	24.81	19.63	22.42	36.01	18.43	19.25	21.63	18.70	7.16	20.52

[1]The BE was calculated by the MM/PBSA method, which could be different from that after 100-ns molecular dynamics simulations.

[2]The RMSD was calculated by using the backbone atoms of the proteins, where the first conformation was taken as the reference. The binding models were clustered with an RMSD cutoff of 5 Å, i.e., the two conformations with the RMSD difference smaller than 5 Å were treated as one conformation.

[3]The model-1, model-2, and model-3 were corresponding to the models used in the main text.

Table S2. The binding energy (BE) in the unit of kcal/mol and the root mean square deviation (RMSD) in the unit of Å for the Top 30 conformations in HSA/RBD system.

Conf.	1	2	3	4	5	6	7	8	9	10
BE	-45.85	-39.68	-39.53	-39.12	-38.49	-38.28	-36.54	-35.74	-33.83	-28.42
RMSD	0.00	16.36	16.89	15.67	40.80	41.14	13.54	13.08	14.16	3.25
Note	model-2	model-3			model-1					
Conf.	11	12	13	14	15	16	17	18	19	20
BE	-26.09	-23.09	-18.86	-18.61	-16.92	-14.24	-14.03	-13.70	-10.94	-9.38
RMSD	30.21	17.24	15.60	17.35	38.92	12.75	32.22	36.36	14.66	44.80
Conf.	21	22	23	24	25	26	27	28	29	30
BE	-9.04	-8.73	-5.65	-5.31	-4.72	-3.43	2.01	2.07	5.06	7.76
RMSD	41.56	34.00	18.10	41.86	38.45	37.95	39.41	22.59	27.02	38.95

Table S3. The binding energy (BE) in the unit of kcal/mol and the root mean square deviation (RMSD) in the unit of Å for the Top 30 conformations in ApoE/RBD system.

Conf.	1	2	3	4	5	6	7	8	9	10
BE	-33.13	-32.59	-31.08	-30.01	-29.74	-27.22	-26.59	-26.38	-25.57	-22.83
RMSD	0.00	48.91	46.79	47.24	45.14	19.62	19.21	54.48	56.57	21.68
Note	model-1	model-3				model-2				
Conf.	11	12	13	14	15	16	17	18	19	20
BE	-21.94	-19.12	-17.72	-17.44	-15.76	-15.23	-13.24	-13.08	-13.02	-12.79
RMSD	57.08	19.37	14.39	28.81	26.47	19.76	40.27	24.03	51.66	25.86
Conf.	21	22	23	24	25	26	27	28	29	30
BE	-11.28	-8.88	-8.51	-7.99	-4.83	-4.04	-1.12	0.36	1.35	7.77
RMSD	35.66	44.93	19.84	58.18	36.52	13.61	33.40	32.86	20.43	34.72