Supporting Information for

Computational Design of Stapled Peptide Inhibitor against SARS-CoV-2 Receptor Binding Domain

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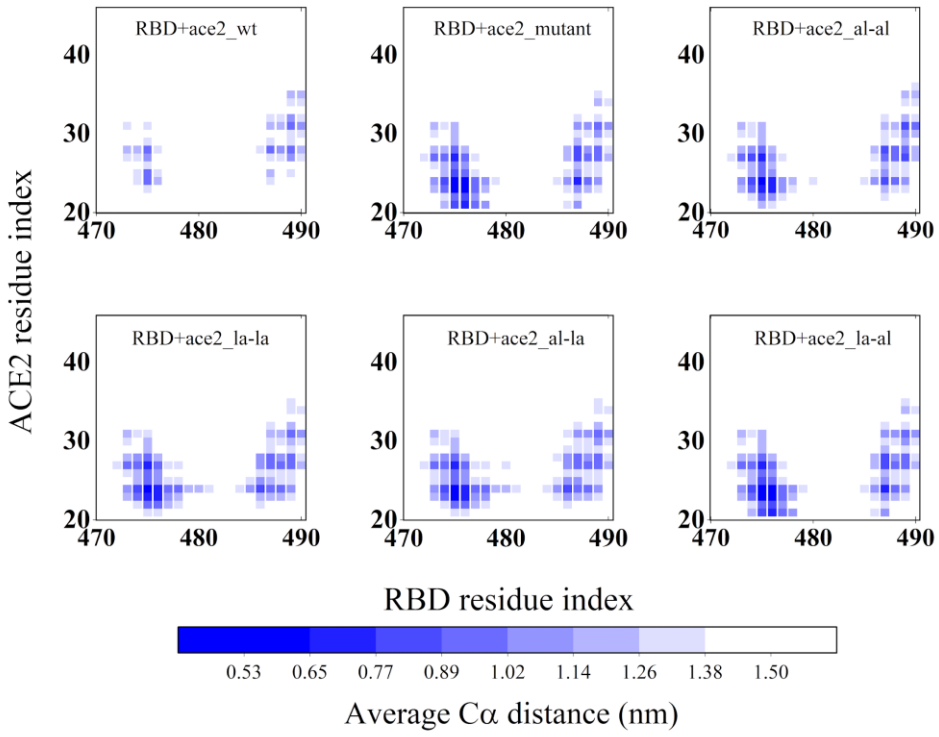

Figure S1: The contact maps between ACE2-peptide and RBD for different peptides bound to RBD. The average distance between the alpha carbons of the amino acids of ACE2-peptides and the loop region of RBD (470 to 490) are plotted using a blue-to-white color scale. The blue colored sections represent smaller distances between the residues and hence higher contact whereas residue pairs appearing in white colored sections are at a larger distance therefore forming weaker contacts.

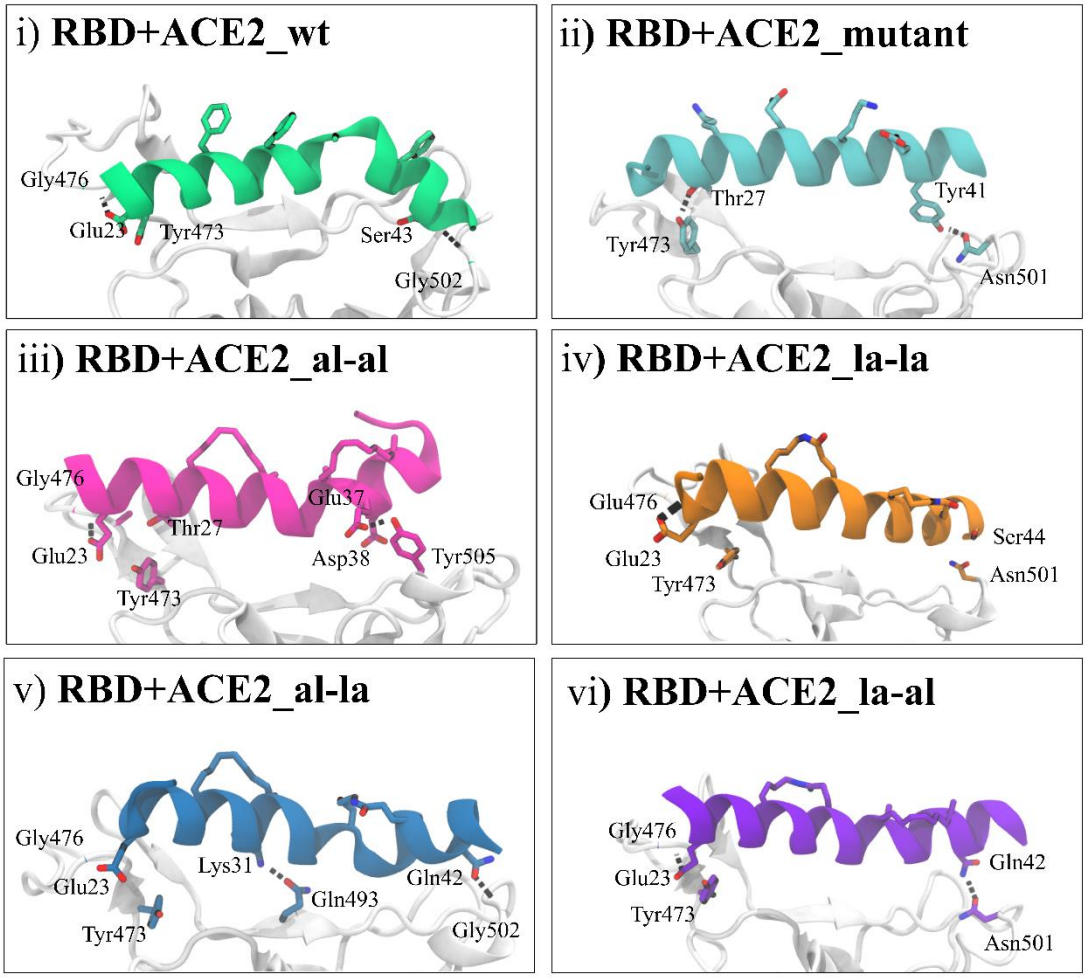

Figure S2: The hydrogen bonds between residues (in stick) of RBD (white ribbon) and ACE2-peptides (colored ribbon) are shown for different systems. The hydrogen bonds are shown as black dots.

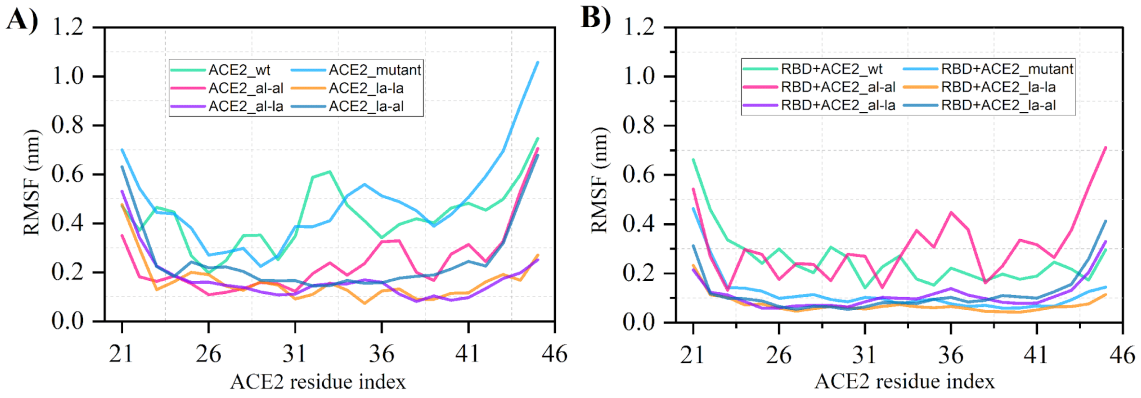

Figure S3: The root mean square fluctuation (RMSF) of ACE2 residues for (A) the free peptides and (B) in their complexes with RBD.

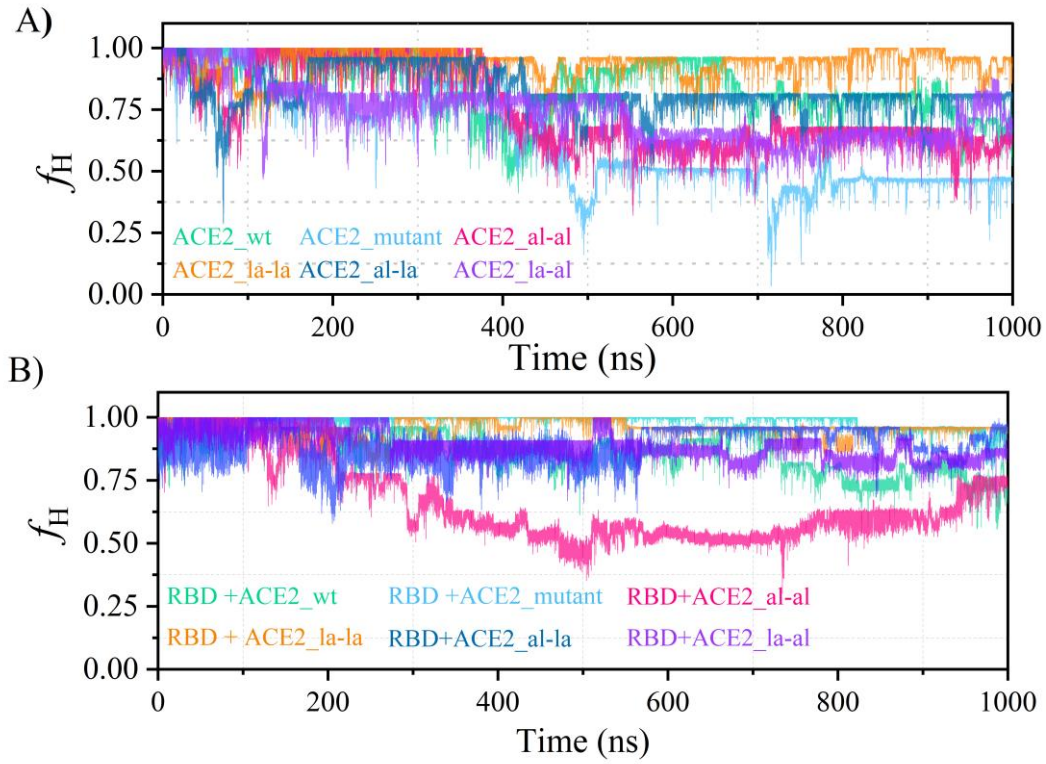

Figure S4: The helical fraction of ACE2-peptides in (A) the free states and (B) in their complexes with RBD.

Table S1: Binding energy components of **RBD** in three different simulations. All energy values and standard errors are in kcal/mol.

Energy Components	Simulation1	Simulation2	Simulation3	Average
E_{Elec}	-3,806.58 ± 303.18	-3,786.82 ± 305.88	-3,769.62 ± 305.12	-3,787.67 ± 15.10
E_{vdw}	-545.85 ± 22.73	-552.59 ± 23.41	-550.72 ± 21.78	-549.72 ± 2.84
$E_{Internal}$	4,073.15 ± 40.60	4,071.75 ± 40.72	4,071.54 ± 40.77	4,072.15 ± 0.71
$E_{Solv(polar)}$	-2,217.49 ± 297.56	-2,232.67 ± 301.20	-2,238.67 ± 299.70	-2,229.61 ± 8.91
$E_{Solv(non-polar)}$	65.42 ± 0.95	64.70 ± 1.07	65.56 ± 0.83	65.22 ± 0.38
$E_{Elec+Solv(polar)}$	-6,024.07 ± 24.03	-6,019.49 ± 23.83	-6,008.29 ± 23.67	-6,017.28 ± 6.63
H	-2,431.34 ± 39.73	-2,435.62 ± 41.07	-2,421.92 ± 39.83	-2,429.63 ± 5.72
$-TS$	-863.35	-899.67	-866.62	-876.55 ± 16.40

Table S2: Binding energy components of **RBD+ACE2_wt** in three different simulations. All energy values and standard errors are in kcal/mol.

Energy Components	Simulation1	Simulation2	Simulation3	Average
E_{Elec}	-4,467.63 ± 350.29	-4,310.30 ± 366.47	-4,351.86 ± 359.34	-4,376.60 ± 66.57
E_{vdw}	-611.79 ± 23.20	-601.10 ± 25.18	-612.42 ± 24.92	-608.44 ± 5.19
$E_{Internal}$	4,662.87 ± 43.67	4,660.95 ± 43.91	4,664.46 ± 44.18	4,662.76 ± 1.44
$E_{Solv(polar)}$	-2,619.31 ± 343.62	-2,770.17 ± 359.26	-2,729.11± 352.70	-2,706.20 ± 63.68
$E_{Solv(non-polar)}$	76.18 ± 0.93	76.65 ± 1.12	76.24 ±1.09	76.35 ± 0.21
$E_{Elec+Solv(polar)}$	-7,086.94 ± 26.98	-7,080.47 ± 25.71	-7,080.97 ± 26.89	-7,082.79 ± 2.94
H	-2,959.67 ± 43.25	-2,943.98 ± 43.77	-2,952.69 ± 44.12	-2,952.11 ± 6.42
$-TS$	-997.11	-1,015.73	-996.89	-1,003.24 ± 8.83

Table S3: Binding energy components of **RBD+ACE2_mutant** in three different simulations. All energy values and standard errors are in kcal/mol.

Energy Components	simulation1	simulation2	simulation3	Average
E_{Elec}	-4,431.40 ± 354.15	-4,478.70 ± 356.51	-4,389.58 ± 350.60	-4,433.23 ± 36.41
E_{vdw}	-648.31 ± 22.87	-660.23 ± 23.69	-630.71 ± 23.67	-646.41 ± 12.13
$E_{Internal}$	4,631.40 ± 43.72	4,644.78 ± 43.70	4,633.05 ± 43.35	4,636.41 ± 5.96
$E_{Solv(polar)}$	-2,933.45 ± 346.48	-2,907.71 ± 350.49	-2,987.06 ± 344.68	-2,942.74 ± 33.05
$E_{Solv(non-polar)}$	75.59 ± 0.92	74.64 ± 0.94	76.83 ± 0.97	75.69 ± 0.90
$E_{Elec+Solv(polar)}$	-7,364.85 ± 26.76	-7,386.41 ± 26.08	-7,376.64 ± 25.81	-7,375.97 ± 8.81
H	-3,306.17 ±43.01	-3,327.21 ± 43.68	-3,297.47 ± 43.07	-3,310.28 ± 12.48
$-TS$	-998.82	-996.54	-992.02	-995.79 ± 2.83

Table S4: Binding energy components of **RBD+ACE2_al-al** in three different simulations. All energy values and standard errors are in kcal/mol.

Energy Components	simulation1	simulation2	simulation3	Average
E_{Elec}	-4,172.79 ± 361.79	-4,370.40 ±350.80	-4,376.29 ± 339.51	-4,306.49 ± 94.57
E_{Vdw}	-640.65 ± 24.65	-646.11 ± 24.12	-645.03 ± 24.16	-643.93 ± 2.36
$E_{Internal}$	4,684.43 ± 44.05	4,683.97 ± 43.46	4,677.10 ± 43.76	4,681.83 ± 3.35
$E_{Solv(polar)}$	-2,854.44 ± 357.25	-2,677.61 ± 343.69	-2,658.79 ± 333.78	-2,730.28 ± 88.13
$E_{Solv(non-polar)}$	75.64 ± 0.99	74.50 ± 0.95	75.62 ± 1.00	75.25 ± 0.53
$E_{Elec+Solv(polar)}$	-7,027.23 ± 24.84	-7,048.01 ± 27.23	-7,035.08 ± 25.47	-7,036.77 ± 8.57
H	-2,907.82 ± 43.32	-2,935.65 ± 43.44	-2,927.39 ± 43.01	-2,923.62 ± 11.67
$-TS$	-990.80	-1004.49	-1,023.49	-1006.26 ± 13.40

Table S5: Binding energy components of **RBD+ACE2_la-la** in three different simulations. All energy values and standard errors are in kcal/mol.

Energy Components	simulation1	simulation2	simulation3	Average
E_{Elec}	-4,346.24 ± 352.11	-4,552.89 ± 356.37	-4,402.40 ± 364.36	-4,433.84 ± 87.25
E_{Vdw}	-648.59 ± 23.37	-653.64 ± 23.66	-651.61 ± 26.67	-651.28 ± 2.07
$E_{Internal}$	4,645.75 ± 43.85	4,644.80 ± 43.80	4,647.02 ± 43.56	4,645.86 ± 0.91
$E_{Solv(polar)}$	-2,850.91 ± 345.80	-2,645.43 ± 350.09	-2,787.74 ± 359.31	-2,761.36 ± 85.94
$E_{Solv(non-polar)}$	75.25 ± 0.95	74.17 ± 0.94	75.00 ± 1.26	74.81 ± 0.46
$E_{Elec+Solv(polar)}$	-7,197.15 ± 25.69	-7,198.32 ± 26.35	-7,190.14 ± 27.12	-7,195.20 ± 3.61
H	-3,124.74 ± 43.29	-3,132.98 ± 42.86	-3,119.73 ± 44.81	-3,125.82 ± 5.46
$-TS$	-997.12	-994.47	-966.15	-985.91 ± 14.02

Table S6: Binding energy components of **RBD+ACE2_al-la** in three different simulations. All energy values and standard errors are in kcal/mol.

Energy Components	simulation1	simulation2	simulation3	Average
E_{Elec}	-4,260.50 ± 366.82	-4,207.51 ± 342.74	-4,513.91 ± 344.28	-4,327.31 ± 133.71
E_{Vdw}	-623.80 ± 23.49	-630.04 ± 27.03	-647.49 ± 23.48	-633.78 ± 10.02
$E_{Internal}$	4,662.14 ± 43.59	4,661.76 ± 43.82	4,669.79 ± 43.50	4,664.56 ± 3.70
$E_{Solv(polar)}$	-2,854.24 ± 357.84	-2,913.86 ± 336.54	-2,613.68 ± 338.53	-2,793.93 ± 129.76
$E_{Solv(non-polar)}$	76.81 ± 0.99	76.47 ± 1.27	74.42 ± 0.88	75.90 ± 1.05
$E_{Elec+Solv(polar)}$	-7,114.74 ± 27.57	-7,121.37 ± 26.01	-7,127.59 ± 25.41	-7,121.23 ±5.25
H	-2,999.60 ± 43.08	-3,013.19 ± 45.16	-3,030.86 ± 43.24	-3,014.55 ± 12.80
$-TS$	-1,021.55	-999.96	-985.45	-1002.32 ± 14.83

Table S7: Binding energy components of **RBD+ACE2_la-al** in three different simulations. All energy values and standard errors are in kcal/mol.

Energy Components	simulation1	simulation2	simulation3	Average
E_{Elec}	-4,437.03 ± 358.56	-4,469.12 ± 349.38	-4,406.19 ± 345.09	-4,437.45 ± 25.69
E_{Vdw}	-638.32 ± 23.82	-661.21 ± 23.28	-638.74 ± 23.56	-646.09 ± 10.70
$E_{Internal}$	4,674.81 ± 43.81	4,661.90 ± 43.33	4,665.56 ± 43.33	4,667.42 ± 5.43
$E_{Solv(polar)}$	-2,703.36 ± 352.53	-2,635.71 ± 343.79	-2,710.20 ± 338.79	-2,683.09 ± 33.62
$E_{Solv(non-polar)}$	75.22 ± 0.98	74.37 ± 0.95	76.06 ± 0.93	75.22 ± 0.69
$E_{Elec+Solv(polar)}$	-7,140.39 ± 25.74	-7,104.83 ± 25.97	-7,116.39 ± 26.21	-7,120.54 ± 14.81
H	-3,028.67 ± 42.80	-3,029.77 ± 42.38	-3,013.51 ± 42.66	-3,023.98 ± 7.42
$-TS$	-987.53	-995.00	-1012.40	-998.31 ± 10.42

Table S8: Binding energy components of **ACE2_wt** in three different simulations. All energy values and standard errors are in kcal/mol.

Energy Components	simulation1	simulation2	simulation3	Average
E_{Elec}	-315.53 ± 80.10	-314.60 ± 77.77	-317.50 ± 71.42	-315.87 ± 1.21
E_{Vdw}	-24.96 ± 7.83	-33.37 ± 8.22	-25.61 ± 7.88	-27.98 ± 3.82
$E_{Internal}$	571.44 ± 15.43	572.09 ± 15.57	569.00 ± 15.35	570.85 ± 1.33
$E_{Solv(polar)}$	-726.47 ± 75.40	-717.26 ± 74.69	-721.94 ± 67.30	-721.89 ± 3.76
$E_{Solv(non-polar)}$	12.92 ± 0.26	12.37 ± 0.32	12.88 ± 0.25	12.73 ± 0.25
$E_{Elec+Solv(polar)}$	-1,042.49 ± 9.85	-1,031.86 ± 9.04	-1,039.44 ± 9.39	-1,037.77 ± 4.31
H	-482.60 ± 16.03	-480.76 ± 15.52	-483.17 ± 15.69	-482.17 ± 1.03
$-TS$	-153.24	-182.84	-109.92	-148.66 ± 29.94

Table S9: Binding energy components of **ACE2_mutant** in three different simulations. All energy values and standard errors are in kcal/mol.

Energy Components	simulation1	simulation2	simulation3	Average
E_{Elec}	-382.76 ± 98.19	-371.78 ± 83.70	-363.53 ± 85.82	-372.69 ± 7.88
E_{Vdw}	-54.18 ± 8.70	-62.76 ± 7.99	-59.06 ± 7.62	-58.67 ± 3.51
$E_{Internal}$	565.78 ± 15.39	565.64 ± 15.38	564.31 ± 15.44	565.24 ± 0.66
$E_{Solv(polar)}$	-966.73 ± 92.84	-975.32 ± 79.22	-985.33 ± 81.45	-975.79 ± 7.60
$E_{Solv(non-polar)}$	12.95 ± 0.32	12.43 ± 0.24	12.85 ± 0.25	12.75 ± 0.23
$E_{Elec+Solv(polar)}$	-1,349.49 ± 10.82	-1,347.10 ± 9.97	-1,348.86 ± 9.88	-1,348.48 ± 1.01
H	-824.93 ± 15.99	-831.80 ± 15.34	-830.75 ± 15.63	-829.16 ± 3.02
$-TS$	-192.04	-121.83	-127.36	-147.08 ± 31.87

Table S10: Binding energy components of **ACE2_al-al** in three different simulations. All energy values and standard errors are in kcal/mol.

Energy Components	simulation1	simulation2	simulation3	Average
E_{Elec}	-265.04 ± 78.85	-196.40 ± 75.69	-211.41 ± 81.72	-224.28 ± 29.46
E_{Vdw}	-52.56 ± 7.82	-46.86 ± 7.50	-46.27 ± 8.41	-48.56 ± 2.83
$E_{Internal}$	611.87 ± 15.57	606.26 ± 15.62	612.00 ± 16.00	610.04 ± 2.67
$E_{Solv(polar)}$	-757.67 ± 75.32	-811.12 ± 73.63	-797.71 ± 77.87	-788.83 ± 22.70
$E_{Solv(non-polar)}$	12.50 ± 0.23	13.07 ± 0.25	13.18 ± 0.36	12.92 ± 0.30
$E_{Elec+Solv(polar)}$	-1,022.71 ± 9.10	-1,007.52 ± 8.10	-1,009.12 ± 9.93	-1,013.11 ±6.81
H	-450.90 ± 15.61	-435.04 ± 15.29	-430.21 ± 16.39	-438.71 ± 8.84
$-TS$	-136.71	-162.04	-160.62	-153.12 ± 11.62

Table S11: Binding energy components of **ACE2_la-la** in three different simulations. All energy values and standard errors are in kcal/mol.

Energy Components	simulation1	simulation2	simulation3	Average
E_{Elec}	-382.44 ± 91.05	-390.62 ± 79.84	-308.06 ± 82.47	-360.37 ± 37.14
E_{Vdw}	-54.17 ± 8.02	-56.00 ± 8.03	-52.22 ± 8.78	-54.13 ± 1.54
$E_{Internal}$	576.95 ± 15.40	573.03 ± 15.13	572.87 ± 15.62	574.28 ± 1.89
$E_{Solv(polar)}$	-789.86 ± 84.46	-781.11 ± 75.74	-840.49 ± 79.38	-803.82 ± 26.18
$E_{Solv(non-polar)}$	12.70 ± 0.38	12.64 ± 0.32	13.16 ± 0.39	12.83 ± 0.23
$E_{Elec+Solv(polar)}$	-1,172.30 ±11.38	-1,171.73 ± 9.45	-1,148.55± 11.04	-1,164.19 ± 11.06
H	-636.81 ± 17.37	-642.06 ± 15.49	-614.75 ± 16.71	-631.21 ± 11.83
$-TS$	-112.07	-132.04	-141.22	-128.45 ± 12.17

Table S12: Binding energy components of **ACE2_al-la** in three different simulations. All energy values and standard errors are in kcal/mol.

Energy Components	simulation1	simulation2	simulation3	Average
E_{Elec}	-334.16 ± 77.69	-324.17 ± 76.83	-313.02 ± 81.20	-323.78 ± 8.64
E_{Vdw}	-51.03 ± 8.37	-54.93 ± 7.70	-54.73 ± 7.86	-53.56 ± 1.79
$E_{Internal}$	590.81 ± 15.64	596.29 ± 15.56	596.86 ± 15.52	594.65 ± 2.73
$E_{Solv(polar)}$	-759.35 ± 73.03	-776.76 ± 72.79	-785.37 ± 77.89	-773.83 ± 10.82
$E_{Solv(non-polar)}$	12.70 ± 0.41	12.46 ± 0.23	12.54 ± 0.25	12.56 ± 0.10
$E_{Elec+Solv(polar)}$	-1,093.52 ± 10.33	-1,100.94 ± 9.40	-1,098.39 ± 8.96	-1,097.61 ± 3.08
H	-541.05 ± 16.77	-547.12 ± 15.69	-543.73 ± 15.55	-543.96 ± 2.48
$-TS$	-131.94	-106.62	-163.70	-134.09 ± 23.35

Table S13: Binding energy components of **ACE2_la-al** in three different simulations. All energy values and standard errors are in kcal/mol.

Energy Components	simulation1	simulation2	simulation3	Average
E_{Elec}	-301.52 ± 87.00	-284.33 ± 80.32	-315.94 ± 86.53	-300.60 ± 12.92
E_{Vdw}	-53.86 ± 8.81	-58.88 ± 7.96	-52.07 ± 7.94	-54.93 ± 2.88
$E_{Internal}$	592.38 ± 15.46	594.04 ± 15.60	590.27 ± 15.55	592.23 ± 1.54
$E_{Solv(polar)}$	-788.75 ± 83.41	-806.76 ± 77.03	-774.45 ± 80.75	-789.99 ± 13.22
$E_{Solv(non-polar)}$	12.75 ± 0.37	12.37 ± 0.25	12.81 ± 0.33	12.64 ± 0.19
$E_{Elec+Solv(polar)}$	-1,090.27 ± 9.96	-1,091.09± 9.19	-1,090.39 ± 10.57	-1,090.58 ± 0.36
H	-538.99 ± 17.27	-543.55 ± 15.78	-539.38 ± 16.40	-540.64 ± 2.06
$-TS$	-140.61	-159.87	-160.02	-153.50 ±9.11

Table S14: Binding free energy of **RBD-ACE2_wt** binding. All energy values and standard errors are in kcal/mol.

Energy Components	RBD+ACE2_wt	RBD	ACE2_wt	ΔE
E_{Elec}	-4,376.60 ± 66.57	-3,787.67 ± 15.10	-315.87 ± 1.21	-273.05
E_{Vdw}	-608.44 ± 5.19	-549.72 ± 2.84	-27.98 ± 3.82	-30.74
$E_{Internal}$	4,662.76 ± 1.44	4,072.15 ± 0.71	570.85 ± 1.33	19.77
$E_{Solv(polar)}$	-2,706.20 ± 63.68	-2,229.61 ± 8.91	-721.89 ± 3.76	245.30
$E_{Solv(non-polar)}$	76.35 ± 0.21	65.22 ± 0.38	12.73 ± 0.25	-1.60
$E_{Elec+Solv(polar)}$	-7,082.79 ± 2.94	-6,017.28 ±6.63	-1,037.77 ± 4.31	-27.44
H	-2,952.11 ± 6.42	-2,429.63 ± 5.72	-482.17 ± 1.03	-40.31
$-TS$	-1,003.24 ± 8.83	-876.55 ± 16.40	-148.66 ± 29.94	21.97
G				-18.34

Table S15: Binding free energy of **RBD-ACE2_mutant** binding. All energy values and standard errors are in kcal/mol.

Energy Components	RBD+ACE2_mutant	RBD	ACE2_mutant	ΔE
E_{Elec}	-4,433.23 ± 36.41	-3,787.67 ± 15.10	-372.69 ± 7.88	-272.86
E_{Vdw}	-646.41 ± 12.13	-549.72 ± 2.84	-58.67 ± 3.51	-38.03
$E_{Internal}$	4,636.41 ± 5.96	4,072.15 ± 0.71	565.24 ± 0.66	-0.98
$E_{Solv(polar)}$	-2,942.74 ± 33.05	-2,229.61 ± 8.91	-975.79 ± 7.60	262.66
$E_{Solv(non-polar)}$	75.69 ± 0.90	65.22 ± 0.38	12.75 ± 0.23	-2.28
$E_{Elec+Solv(polar)}$	-7,375.97 ± 8.81	-6,017.28 ± 6.63	-1,348.48±1.01	-10.20
H	-3,310.28 ± 12.48	-2,429.63 ± 5.72	-829.16 ± 3.02	-51.50
$-TS$	-995.79 ± 2.83	-876.55 ± 16.40	-147.08 ± 31.87	27.83
G				-23.67

Table S16: Binding free energy of **RBD-ACE2_al-al** binding. All energy values and standard errors are in kcal/mol.

Energy Components	RBD+ACE2_al-al	RBD	ACE2_al-al	ΔE
E_{Elec}	-4,306.49 ± 94.57	-3,787.67 ± 15.10	-224.28 ± 29.46	-294.54
E_{Vdw}	-643.93 ± 2.36	-549.72 ± 2.84	-48.56 ± 2.83	-45.65
$E_{Internal}$	4,681.83 ± 3.35	4,072.15 ± 0.71	610.04 ± 2.67	-0.36
$E_{Solv(polar)}$	-2,730.28 ± 88.13	-2,229.61 ± 8.91	-788.83 ± 22.70	288.16
$E_{Solv(non-polar)}$	75.25 ± 0.53	65.22 ± 0.38	12.92 ± 0.30	-2.89
$E_{Elec+Solv(polar)}$	-7,036.77 ± 8.57	-6,017.28 ± 6.63	-1,013.11± 6.81	-6.38
H	-2,923.62 ± 11.67	-2,429.63 ± 5.72	-438.71 ± 8.84	-55.28
$-TS$	-1006.26± 13.40	-876.55 ± 16.40	-153.12 ± 11.62	23.41
G				-31.87

Table S17: Binding free energy of **RBD-ACE2_la-la** binding. All energy values and standard errors are in kcal/mol.

Energy Components	RBD+ACE2_la-la	RBD	ACE2_la-la	ΔE
E_{Elec}	-4,433.84 ± 87.25	-3,787.67 ± 15.10	-360.37 ± 37.14	-285.80
E_{Vdw}	-651.28 ± 2.07	-549.72 ± 2.84	-54.13 ± 1.54	-47.43
$E_{Internal}$	4,645.86 ± 0.91	4,072.15 ± 0.71	574.28 ± 1.89	-0.57
$E_{Solv(polar)}$	-2,761.36 ± 85.94	-2,229.61 ± 8.91	-803.82 ± 26.18	272.07
$E_{Solv(non-polar)}$	74.81 ± 0.46	65.22 ± 0.38	12.83 ± 0.23	-3.25
$E_{Elec+Solv(polar)}$	-7,195.20 ± 3.61	-6,017.28 ± 6.63	-1,164.19 ±11.06	-13.73
H	-3,125.82 ± 5.46	-2,429.63 ± 5.72	-631.21 ± 11.83	-64.98
$-TS$	-985.91 ± 14.02	-876.55 ± 16.40	-128.45 ± 12.17	19.08
G				-45.90

Table S18: Binding free energy of **RBD-ACE2_al-la** binding. All energy values and standard errors are in kcal/mol.

Energy Components	RBD+ACE2_al-la	RBD	ACE2_al-la	ΔE
E_{Elec}	-4,327.31 ± 133.71	-3,787.67 ± 15.10	-323.78 ± 8.64	-215.85
E_{Vdw}	-633.78 ± 10.02	-549.72 ± 2.84	-53.56 ± 1.79	-30.50
$E_{Internal}$	4,664.56 ± 3.70	4,072.15 ± 0.71	594.65 ± 2.73	-2.23
$E_{Solv(polar)}$	-2,793.93 ± 129.76	-2,229.61 ± 8.91	-773.83 ± 10.82	209.51
$E_{Solv(non-polar)}$	75.90 ± 1.05	65.22 ± 0.38	12.56 ± 0.10	-1.89
$E_{Elec+Solv(polar)}$	-7,121.23 ±5.25	-6,017.28 ± 6.63	-1,097.61 ± 3.08	-6.34
H	-3,014.55 ± 12.80	-2,429.63 ± 5.72	-543.96 ± 2.48	-40.96
$-TS$	-1002.32 ± 14.83	-876.55 ± 16.40	-134.09 ± 23.35	8.31
G				-32.65

Table S19: Binding free energy of **RBD-ACE2_la-al** binding. All energy values and standard errors are in kcal/mol.

Energy Components	RBD+ACE2_la-al	RBD	ACE2_la-al	ΔE
E_{Elec}	-4,437.45 ± 25.69	-3,787.67 ± 15.10	-300.60 ± 12.92	-349.18
E_{Vdw}	-646.09 ± 10.70	-549.72 ± 2.84	-54.93 ± 2.88	-41.44
$E_{Internal}$	4,667.42 ± 5.43	4,072.15 ± 0.71	592.23 ± 1.54	3.05
$E_{Solv(polar)}$	-2,683.09 ± 33.62	-2,229.61 ± 8.91	-789.99 ± 13.22	336.51
$E_{Solv(non-polar)}$	75.22 ± 0.69	65.22 ± 0.38	12.64 ± 0.19	-2.65
$E_{Elec+Solv(polar)}$	-7,120.54 ± 14.81	-6,017.28 ± 6.63	-1,090.58 ± 0.36	-12.67
H	-3,023.98 ± 7.42	-2,429.63 ± 5.72	-540.64 ± 2.06	-53.72
$-TS$	-998.31 ± 10.42	-876.55 ± 16.40	-153.50 ± 9.11	31.74
G				-21.98