materials

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Supplementary Materials

Characterization of Structural and Energetic Differences between Conformations of the SARS-CoV-2 Spike Protein

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Table S1. Number of intrachain (AA, BB, CC) and interchain (AB, AC, BC) contacts, and respective residues, from the differential contact map (dCM > 0.9) analysis using high-frequency contacts. Amino acids are classified as Polar (Q, N, T, S), Hydrophobic (A, V, I, L, M, F, Y, W), Charged (R, K, D, E) and Other (H, C, U, G, P). Stabilizing/Destabilizing contacts and residues are shown in Figures 2 and 3. The relative stability of spike protein with one and two open RBD are compared to the closed conformation and compared between themselves.

Chains	Contacts											Residues				
	TOTAL	P-P	P-H	P-C	P-O	H-H	H-C	O-H	C-C	O-C	O-O	TOTAL	P	H	C	O
1up2down stabilized compared to 3down																
AA	3	0	1	0	1	1	0	0	0	0	0	6	2	3	0	1
BB	24	2	3	0	1	4	5	3	2	4	0	32	7	9	11	5
CC	11	1	0	0	4	3	1	2	0	0	0	14	4	5	1	4
AB	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
AC	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BC	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1up2down destabilized compared to 3down																
AA	9	1	1	0	0	2	1	2	1	1	0	17	3	7	4	3
BB	26	1	5	0	1	3	3	9	2	0	2	37	7	15	6	9
CC	3	0	0	0	0	0	1	2	0	0	0	6	0	3	1	2
AB	10	0	0	3	0	0	3	3	0	1	0	15	2	5	5	3
AC	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BC	16	1	5	4	0	2	2	1	0	1	0	19	6	8	4	1
2up1down stabilized compared to 3down																
AA	9	0	1	0	1	4	0	2	0	1	0	18	2	11	1	4
BB	32	3	3	1	3	6	3	5	3	5	0	47	11	15	12	9
CC	13	1	1	1	3	4	0	3	0	0	0	17	6	6	1	4
AB	19	0	2	2	0	7	1	5	1	1	0	21	3	10	3	5

AC	2	1	0	0	0	1	0	0	0	0	0	4	2	2	0	0
BC	1	0	0	0	0	0	0	0	0	1	0	2	0	0	1	1
2up1down destabilized compared to 3down																
AA	18	0	6	3	0	6	3	0	0	0	0	29	8	17	4	0
BB	61	4	10	3	4	7	8	20	1	0	4	75	19	31	9	16
CC	10	0	1	1	1	2	4	1	0	0	0	16	3	7	4	2
AB	20	0	3	4	0	0	4	4	1	3	1	26	5	8	6	7
AC	4	0	0	2	0	0	2	0	0	0	0	6	1	2	3	0
BC	24	1	6	7	1	3	3	1	1	1	0	21	7	7	5	2
2up1down stabilized compared to 1up2down																
AA	6	0	1	0	0	3	1	0	0	1	0	12	1	8	2	1
BB	3	0	0	0	2	0	0	0	0	1	0	6	2	0	1	3
CC	2	0	0	0	0	0	0	2	0	0	0	4	0	2	0	2
AB	20	0	2	3	0	7	1	5	1	1	0	21	3	10	3	5
AC	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BC	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2up1down destabilized compared to 1up2down																
AA	15	0	4	1	1	5	3	1	0	0	0	22	3	14	3	2
BB	18	0	1	0	1	3	4	7	0	0	2	22	2	11	3	6
CC	2	0	1	0	0	0	1	0	0	0	0	4	1	2	1	0
AB	2	0	0	0	0	0	0	1	0	1	0	4	0	1	1	2
AC	10	0	1	2	0	1	3	2	0	1	0	11	1	4	4	2
BC	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table S2. List of 10 high-frequency contacts involved in detachment of the RBD in chain B from S2 domain in chain A mediated by hinge domain. Value of the dCM analysis is given in the last column.

Residue 1 RBD	**Residue2 S2**	**dCM (freq >0.9)**
S383(B)	R983(A)	1
V382(B)	R983(A)	1
S383(B)	D985(A)	1
K386(B)	S982(A)	0.97
G381(B)	R983(A)	0.96
Y396(B)	P230(A)	0.94
K386(B)	L984(A)	0.94
G381(B)	L984(A)	0.91
K386(B)	R983(A)	0.91
V382(B)	L984(A)	0.9