Supporting Information for

Computational Analysis of the SARS-CoV-2 RBD–ACE2 Binding Process Based on MD and the 3D-RISM Theory

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Table S1. List of the ten most frequently formed hydrogen bonds at windows = 50 and 89. The details are same as for Table 1 in the main text. 0MB618 denotes the β-L-mannose at the terminal of glycan connected to ACE2/ASN90.

Acceptor residue	Atom	Donor residue	Atom	Fraction
Window = 50				
RBD		ACE2		
THR415	O	0MB618	H4O	0.18
ASN501	OD1	LYS353	HZ2	0.18
ASN501	OD1	LYS353	HZ3	0.18
ASN501	OD1	LYS353	HZ1	0.17
ASN487	OD1	GLN24	HE22	0.12
ASN487	OD1	SER19	HG	0.11
THR500	OG1	LYS353	HZ2	0.11
GLN409	NE2	0MB618	H4O	0.11
THR415	O	0MB618	H3O	0.1
THR500	OG1	LYS353	HZ1	0.09
ACE2		RBD		
0MB618	O6	ARG408	HH11	0.12
0MB618	O3	GLN409	HE21	0.1
0MB618	O3	VAL417	H	0.1
GLN24	OE1	TYR489	HH	0.07

0MB618	O4	ARG408	HH11	0.07
ASP38	OD1	GLN498	HE22	0.07
THR20	O	ASN487	HD21	0.07
0MB618	O3	THR415	HG1	0.06
0MB618	O4	ARG408	HH21	0.05
0MB618	O6	ARG408	HH21	0.05
Window = 89				
RBD		ACE2		
ASN487	OD1	TYR83	HH	0.58
ALA475	O	SER19	HG	0.54
THR415	O	0MB618	H3O	0.32
THR446	O	GLN42	HE21	0.29
TYR449	OH	GLN42	HE22	0.25
GLN498	OE1	LYS353	HZ2	0.24
GLN498	OE1	LYS353	HZ3	0.21
GLN498	OE1	LYS353	HZ1	0.18
THR415	O	0MB618	H4O	0.13
GLN493	OE1	LYS31	HZ3	0.13
ACE2		RBD		
LYS353	O	GLY502	H	0.81
TYR41	OH	THR500	HG1	0.69
ASP38	OD2	TYR449	HH	0.51
GLU329	OE2	ARG439	HH11	0.43
GLU329	OE2	ARG439	HH21	0.36
GLU329	OE1	ARG439	HH11	0.34
GLU37	OE1	TYR505	HH	0.33

GLU35	OE1	GLN493	HE21	0.31
GLU329	OE1	ARG439	HH21	0.26
GLU35	OE2	GLN493	HE21	0.18

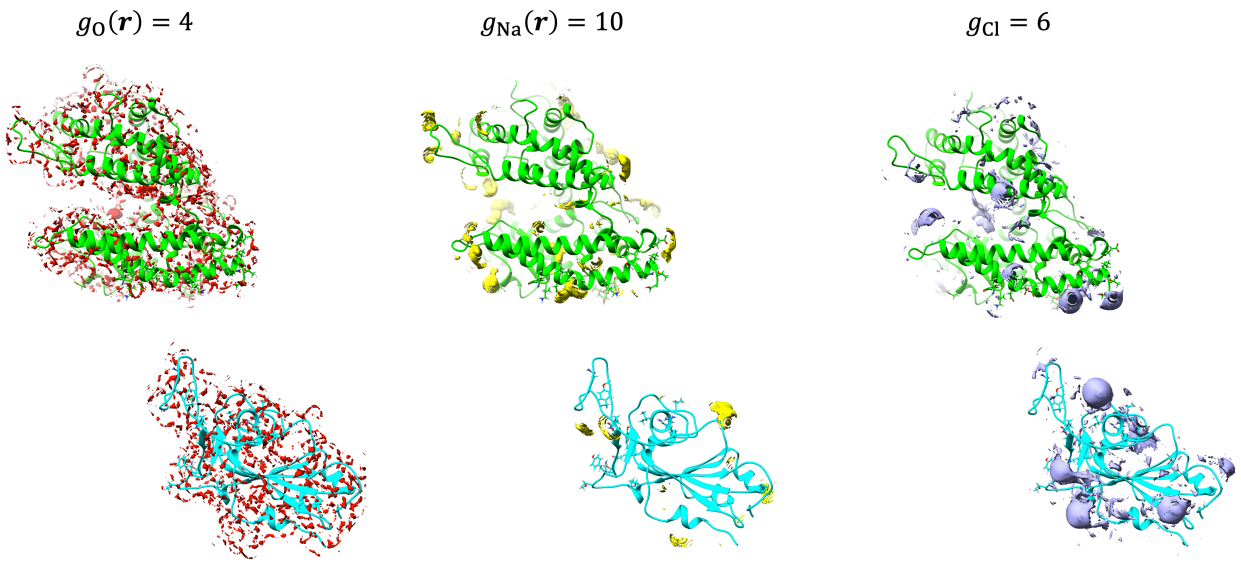

Figure S1. The iso-value surfaces of 3D-DFs of water oxygen, sodium ion, and chloride ion at window = 1 depicted in red-, yellow- and purple-colored surfaces, respectively. The iso-values of each 3D-DF are indicated in each panel.

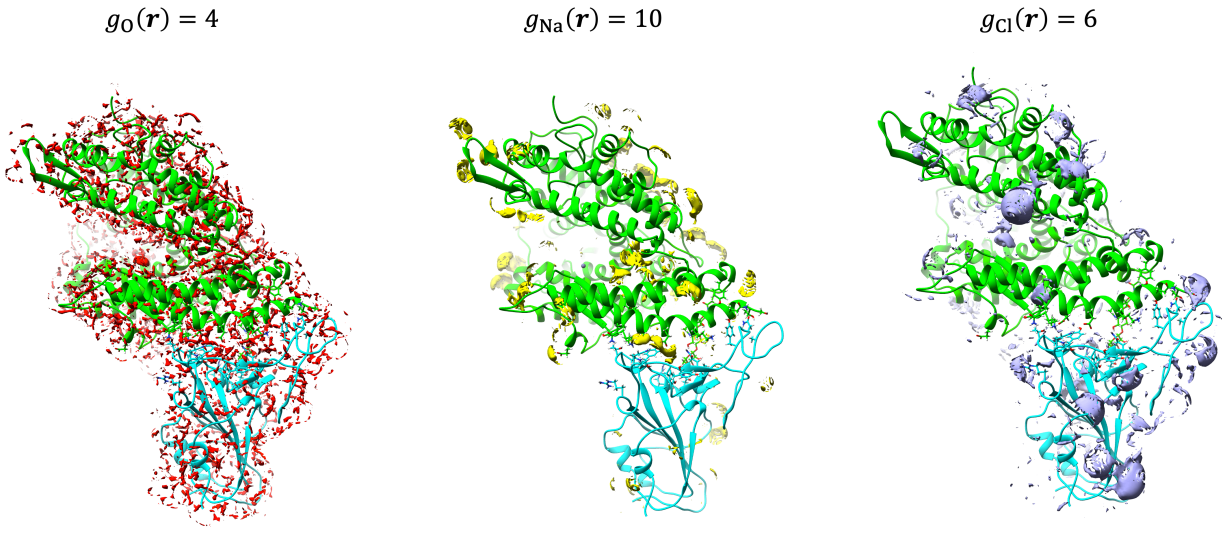

Figure S2. The iso-value surfaces of 3D-DFs of water oxygen, sodium ion, and chloride ion at window = 50 depicted in red-, yellow- and purple-colored surfaces, respectively. The iso-values of each 3D-DF are indicated in each panel.

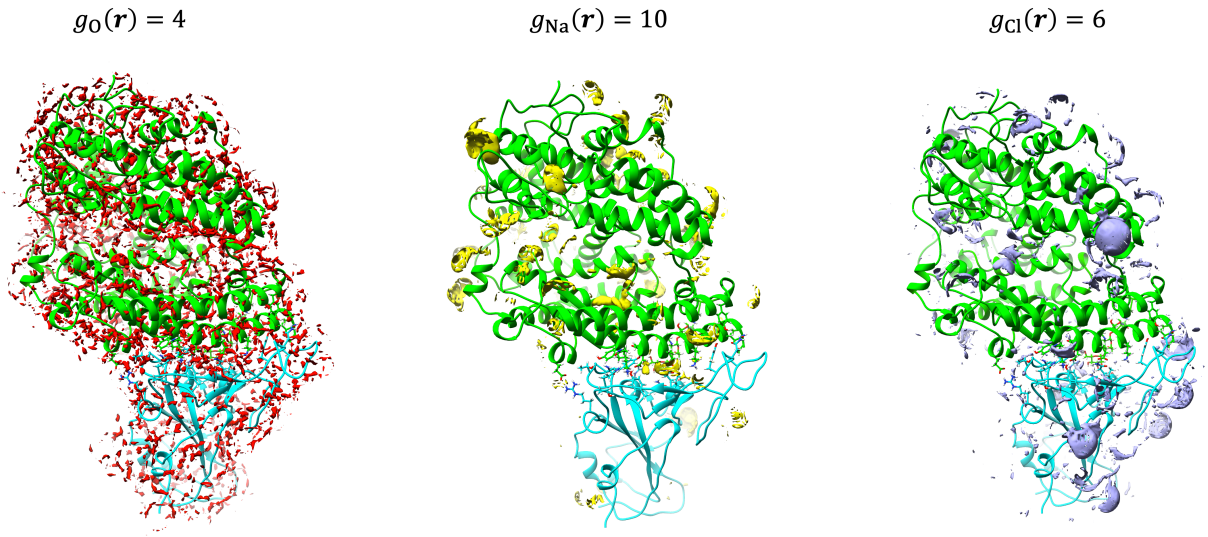

Figure S3. The iso-value surfaces of 3D-DFs of water oxygen, sodium ion, and chloride ion at window = 89 depicted in red-, yellow- and purple-colored surfaces, respectively. The iso-values of each 3D-DF are indicated in each panel.