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Impact of Mutations in the SARS-CoV-2 Spike RBD Region of BA.1 and BA.2 Variants on its Interaction with ACE2 Receptor Protein

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Abstract: The COVID-19 pandemic started at the onset of 2020 and still thriving due to its continuous mutation and evolution into new strains. Omicron strain has been recently categorized as a variant of concern(VoC) by WHO and based on mutations, it is divided into BA.1 and BA.2. In this study, we compared the interaction profile of RBD of the spike protein of the BA.1 and BA.2 variant of SARS-CoV-2 with ACE2 receptor. From the molecular dynamics simulation study, we observed the spike protein of BA.1, and BA.2 variant utilizes unique strategies to have a stable binding with ACE2. The binding affinity of the spike protein of the BA.2 variant-ACE2 complex is indeed high (GBTOT=-23.87 kcal/mol) in comparison with the spike protein of BA.1 variant-ACE2 complex (GBTOT=5.38 kcal/mol). Stable binding of spike protein to ACE2 is essential for virus entry, and the interactions between them should be understood well for the treatment modalities.

Keywords: BA.1; BA.2; ACE2 receptor; SARS-CoV-2; spike protein; molecular dynamics; COVID-19.

1. Introduction

Strange pneumonia endemic with symptoms including fever, dry cough, lethargy, and gastrointestinal problems first appeared in late December 2019 at the Huainan Seafood Wholesale Market in Wuhan, Hubei, China [1]. However, the virus was hastily named 2019-nCoV, after which renamed SARS-CoV-2. Coronaviruses take their understanding from the precise spikes with rounded pointers that enhance their surface, which reminded virologists of the appeal of the sun's atmosphere as its corona [2]. The earliest recounted infected person fell sick on 1 December 2019. However, that person did not have a reference to the later wet marketplace cluster while within side the preceding case may moreover be handed off on 17 November. Two-thirds of the initial case cluster has been related to the marketplace [3]. Molecular clock evaluation indicates that the index case may have been infected between mid-October and mid-November 2019. As of 6 May 2022, more than 6,272,189 deaths have been attributed to COVID-19, with the primary loss of life in Wuhan on 9th January 2020. These numbers range with the aid of the community and, over time, stimulated via way of means of sorting out the volume, healthcare, treatment options, authorities' response, time for the cause

of the initial outbreak, and population characteristics, including age, sex, and popular health [4,5].

ACE2 was identified as the access receptor for each SARS-CoV-2 and SARS-CoV. Structural research revealed that each SARS-CoV-2 and SARS-CoV spike (S) glycoproteins bind ACE2 with elevated affinity [6]. The shape of SARS-CoV-2 S-protein resembles that of SARS-CoV S-protein with the spike RBD located contacting the extracellular vicinity of ACE2, which is surprisingly a big macromolecule with a diameter of 70 Å. The distinctive features of the SARS spike include its enormous mass (500 kD compatible with trimer) and club-shaped shape; when viewed from the end, this seems to have three blades with a radius of 90 Å [7].

Genetic lineages of SARS-CoV-2 had been growing and circulating around the arena because of the COVID-19 pandemic. CoVs are enveloped viruses with fine sense ssRNA genomes with a cistern of approximately 26-32 kb, the largest genome length for an RNA virus. The four structural domains of the SARS spike (from N to C terminus) can be subdivided; the two large extracellular domains, S1 and S2, are regularly responsible for receptor binding and membrane fusion, respectively. The SARS spike seems to be unaffected by redox conditions [8]. It is suggested that the SARS-CoV virus be absorbed by endocytosis into the cell and then exposed to a low pH environment. It is postulated that the membrane fusion process is started by proteolytic cleavage between the S1 and S2 domains [9-12]. The S protein of the SARS-CoV-2 genome is of leading significance for ACE2 receptor binding and membrane fusion of the virus and running medical research on healing techniques and the formation of the immune response [13-17]. Therefore, mutations that arise within the S protein, specifically the RBD within the S gene, have ended in versions of coronavirus. Some of the massive SARS-CoV-2 versions are Alpha (B.1.1.7, on the start placed within side the United Kingdom), Beta (B.1.351, first determined in South Africa), Epsilon (B.1.427 and B.1.429, first recognized in United States-California), Delta (B.1.617.2, first recognized in India), Gamma (P.1, first identified in Japan/Brazil).

Omicron was as quickly first identified in Botswana and South Africa; scientists were alerted by the World Health Organization (WHO) approximately the version on November 24, 2021. On 26 November 2021, WHO declared the strain as a “Variant of Concern (VOC)” because of its excessive ease of transmission [18]. The genomic series evaluation has shown over 30 mutations in Omicron in difference from the unique SARS-CoV-2 strain. BA.1 is the maximum prolific sub-lineage, detected in maximum international regions worldwide and presently accounting for 99% of instances in the United States. BA.2 is much less prolific, as a substitute has overtaken BA.1 in Denmark, Nepal, and the Philippines as the maximum detected version, and has a minor presence in India, the United Kingdom, and infinite specific countries. The third sub-lineage BA.3 is to take off globally, accounting for numerous hundred conditions on the most [19]. Triad, a grow to be aware of that denotes 3 mutations, the D614G mutation within the Spike protein, the P323L mutation in NSP12 polymerase, and the C241U noncoding mutation within the 5’ end. The Triad is the founding version of all variations of venture viruses. Omicron (BA.1) is already identified to have a few extraordinary innate sojourns relative to the mutated strains [20]. Most strikingly, 2.7-3.7-fold is more transmissible than Delta. Moreover, the affinity of the BA.1 Spike for the ACE2 receptor is absolutely two times more than the Wuhan strain [21]. The first cluster consists of receptor-binding mutations G339D, S371F/L, S373P, and S375F. The second cluster consists of receptor-binding region mutations Q493R, G496S, Q498R, and Y505H. The 1/3 consists of fusion region mutations

N764K, N856K, Q954H, N969K, and L981F. The aggregate of these clusters results in high binding affinity of the S-protein and ACE2 and hence gains access to enter the cell. Out of the three mutations, G496S, N856K, and L981F are determined completely in BA.1, not BA.2 or BA.3 [16]. Henceforth, we aspire to look into the comparative structural evaluation of the two sub-versions of omicron BA.1 and BA.2 binding affinities with ACE2 deploying molecular dynamics and computational programs.

2. Materials and Methods

The 3-D structure of the SARS-CoV-2 receptor-binding domain of BA.1 (Figure 1A) and BA.2 (Figure 1B) variants bound with ACE2 were obtained by inducing punctual mutation in the 3-D structure of SARS-CoV-2 spike receptor-binding domain bound with ACE2 (S protein-ACE2) (PDB ID: 6LZG with a resolution of 2.50 Å retrieved from the Research Collaboratory for Structural Bioinformatics Protein Data bank (www.rcsb.org) [22].) using UCSF Chimera package alpha v.1.12 [23]. The punctual mutations induced in the 6LZG to construct the BA.1 and BA.2 are shown in Table 1. Both the complex structures were then energy minimized using the steepest descents followed by the conjugate gradient minimization technique.

(A) (B)

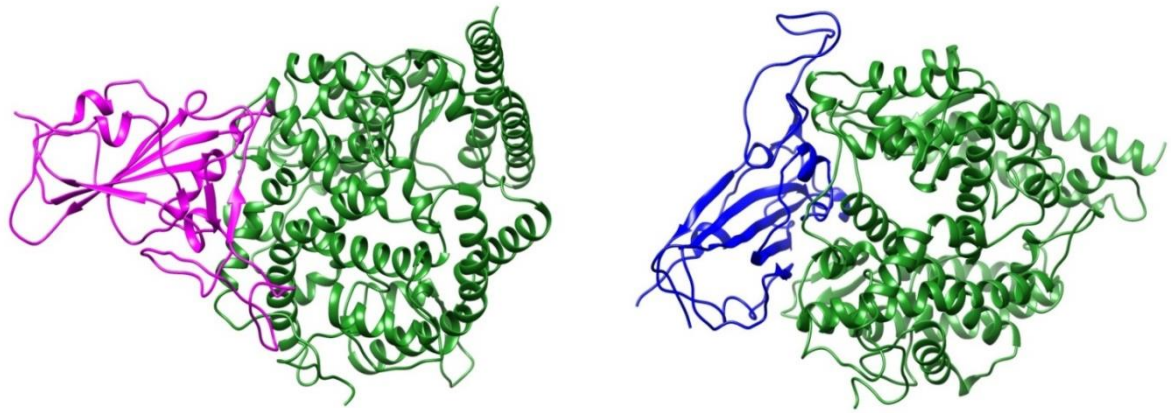

Figure 1. Three-dimensional structure of (**A**) SARS-CoV-2 spike receptor-binding domain of BA.1 variant bound with ACE2 (S protein (BA.1)-ACE2); (**B**) SARS-CoV-2 spike receptor-binding domain of BA.2 variant bound with ACE2 (S protein (BA.2)-ACE2).

Table 1. Showing mutations (in RBD of Spike Protein) of BA.1 and BA.2 lineages.

Mutations of BA.1 lineages	Mutations of BA.2 lineages	Common mutations of BA.1 and BA.2 lineages
G339D, S373P, K417N, N440K, S477N, T478K, E484A, Q493R, Q498R, N501Y, Y505H, **S371L, G446S, G496S,** S375F.	G339D, S373P, K417N, N440K, S477N, T478K, E484A, Q493R, Q498R, N501Y, Y505H, S375F, **S371F, T376A, D405N, R408S.**	G339D, S373P, K417N, N440K, S477N, T478K, E484A, Q493R, Q498R, N501Y, Y505H, S375F.

2.1. Molecular dynamics simulations.

The two complexes, SARS-CoV-2 receptor-binding domain of BA.1 and BA.2 variants bound with ACE2 were then subjected to MD simulations. The MD simulation was carried out using the AMBER ff14SB force field [24] with the AMBER software package. To ensure the overall neutrality of the two complex systems, appropriate numbers of counter ions were added.

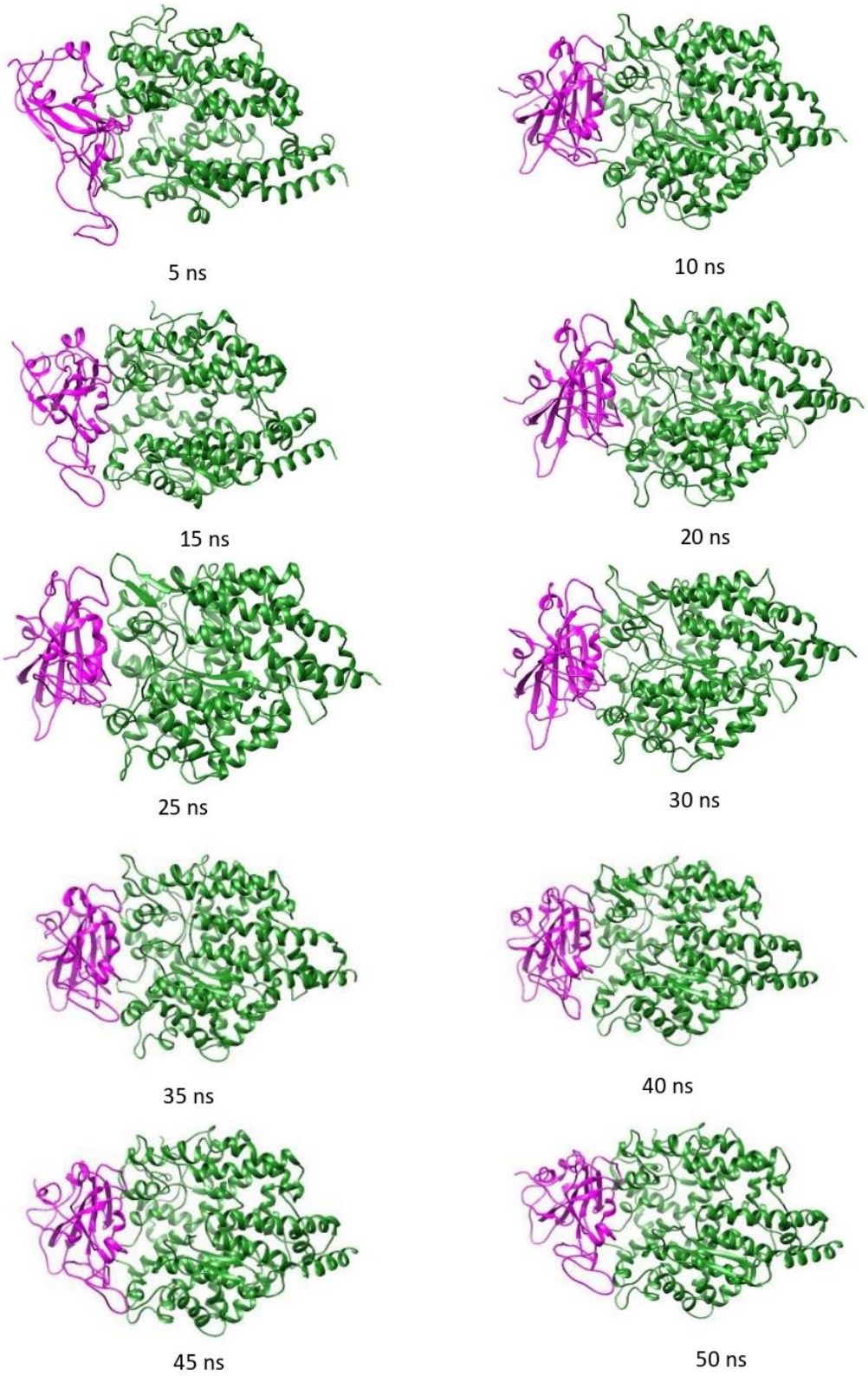

Figure 2. Snapshots of SARS-CoV-2 ACE2-Spike Protein (BA.1 variant) structures at a discrete distance of separation (in Å) between their center of mass.

The two complex systems were subjected to MD simulations in explicit solvent and were solvated with TIP3P [25] water model with a solvent buffer of 10 Å in all directions. In the first step of energy minimization, the steepest descent (SD) of 10000 steps, followed by

10000-steps of conjugate gradient (CG) by holding the complex system using a force constant of 50 kcal/mol/Å^2, allowing the water molecules and counterions to move freely.

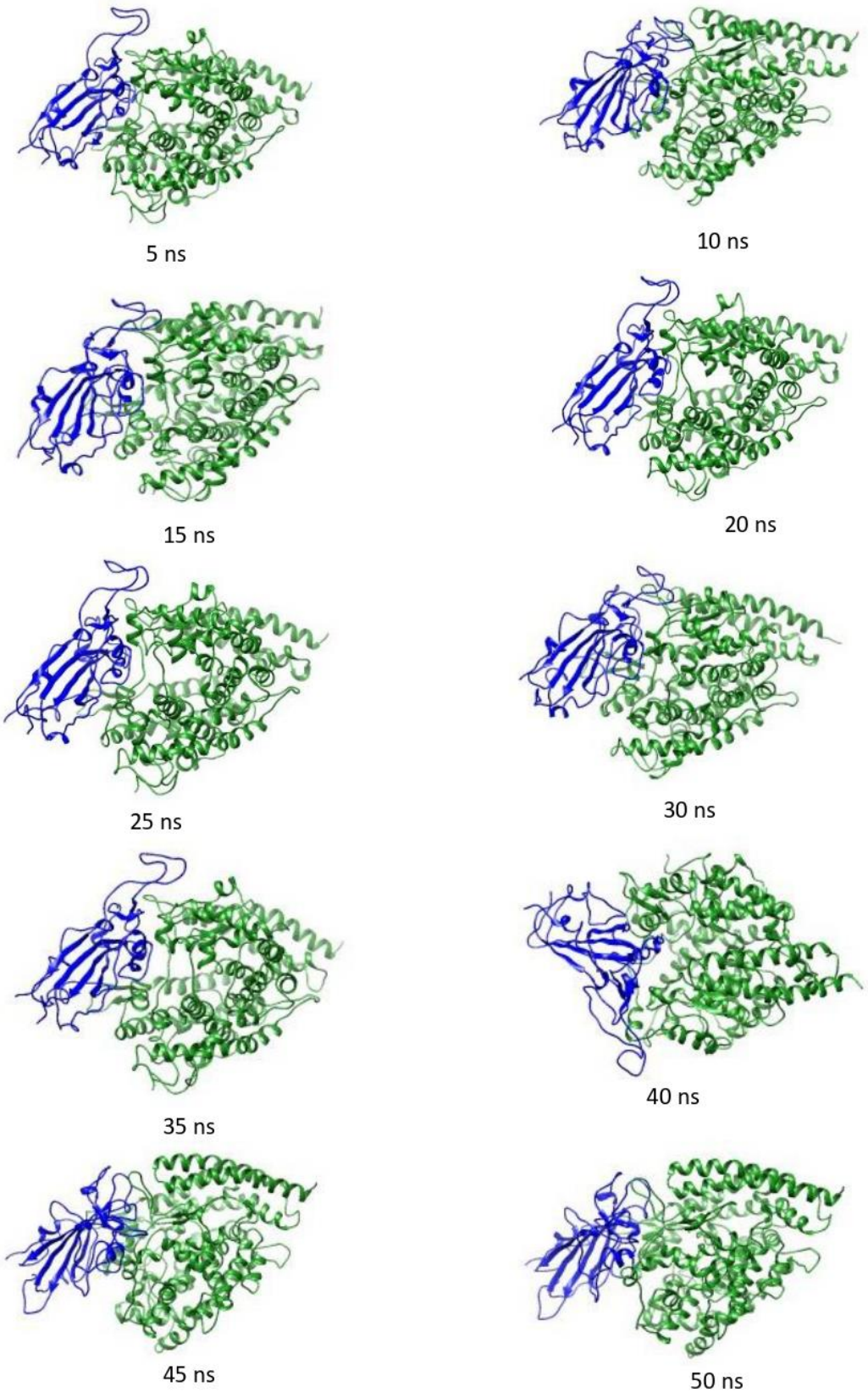

Figure 3. Snapshots of SARS-CoV-2 ACE2-Spike Protein (BA.2 variant) structures at a discrete distance of separation (in Å) between their center of mass.

Then, in the second minimization step, the entire complex system was iterated for 12000 steps of SD minimization and 8000 steps of CG minimization to remove conflicting contacts. Next, both the complex systems were gradually heated from 0-300 K in constant volume (NVT) conditions, thereby applying harmonic restraints with force constant of 10 kcal/mol/Å^2 on the solute atoms. Equilibration was then carried out thrice with 3000 ps using a force constant of 5.0 kcal/mol/Å^2. Finally, 50 ns MD simulations were performed using the NPT ensemble without restraints. In order to tackle the long-range electrostatic interactions, we limited the direct space sum using the Particle Mesh Ewald [26] approach with a non-bonded cutoff of 12.0. The SHAKE method was used to restrict all of the bonds present in the system [27]. The Berendsen weak coupling algorithm [28] maintained a steady pressure and temperature (0.5 ps of heat bath and 0.2 ps of pressure relaxation) throughout the simulation. The time step of MD simulation was set to 2 fs, and sampling was performed every 10 ps into the MD file.

After completion of the 50 ns of production dynamics of the complexes, the lowest energy conformer of the individual complex (S protein (BA.1)-ACE2 and S protein (BA.2)-ACE2) was extracted using the RMSD clustering algorithm from the highly populated clusters and submitted to PDBsum server (http://www.ebi.ac.uk/thorntonsrv/databases/pdbsum/Generate.html) in order to investigate their residue-specific interactions, which are thought to be crucial to understanding the nature of interactions. In the RMSD clustering, the sampled configurations need to be put into a common reference frame before building the centroid (for example, using an RMSd fit to the first frame or a representative structure), or, better yet, separate reference frames need to be made for each cluster, with the frame of reference being the configuration that best represents that cluster. Before calculating the centroid in this method, all the structures in a given cluster are rms fitted to the most representative structure. The structure that has the smallest total of the squared displacements between other structures in the cluster and itself is the representative structure.

Schematic depictions of the nonbonded interactions between amino acid residues at the interface of molecules in a multimer complex are among the things that are displayed in the database PDBsum [29]. Snapshots of SARS-CoV-2 ACE2-Spike Protein (BA.1 and BA.2 variant) structures at a discrete distance of separation (in Å) between their center of mass are shown in Figures 2 and 3.

2.2. Binding free energy calculations.

The Molecular Mechanics Generalized Born Surface Area (MM-GBSA) method [30,31] implemented in the AMBER 16 package was performed to calculate the binding free energy as well as the free energy decomposition of the two complex systems (S protein(BA.1)-ACE2 and S protein(BA.2)-ACE2). 200 snapshots were selected from the last 10 ns of MD trajectories for each complex system to compute the binding energies.

The equations (1-6) display the formulas for computing the BFE and their decomposed energetic components. Where the total BFE (ΔG_{bind}) denotes the difference in free energy between the bound state complex ($G_{complex}$) and the free state individuals of the receptor ($G_{receptor}$) and ligand (G_{ligand}). According to the second law of thermodynamics, ΔG_{bind} can be represented as the difference between the change in enthalpy (ΔH) and the change in temperature times the entropy of the system ($T\Delta S$). Here the enthalpies were calculated by Poisson–Boltzmann or Generalized-Born surface area continuum solvation (MM-PBSA/MM-GBSA) methods with a modest computational effort [32,33]. After taking all the trajectories

for MM-GBSA calculation, analysis was done for three components of the individual two complexes as (i) ligand (S protein) (ii) receptor (ACE2) (iii) complex (S protein-ACE2). Many recent in-silico investigations have employed the methods and protocols we considered in our study to estimate the binding free energy [34-44].

BFE for the two complex systems was calculated using Eqn. (1):

$$\Delta G_{binding} = \Delta G_{complex} - [\Delta G_{receptor} + \Delta G_{ligand}] \quad (1)$$

where, $\Delta_{Gbinding}$ is the total binding free energy.

Thermodynamically,

$$\Delta G = \Delta H - T\Delta S \quad (2)$$

$$\Delta G = \Delta E_{MM} + \Delta G_{sol} - T\Delta S \quad (3)$$

$$\Delta E_{MM} = \Delta E_{int} + \Delta E_{ele} + \Delta E_{vdw} \quad (4)$$

and

$$\Delta G_{sol} = \Delta G_{PB/GB} + \Delta G_{SURF} \quad (5)$$

$$\Delta G_{SURF} = E_{NP} + Edis \quad (6)$$

Calculating enthalpies with MM-GBSA/PBSA: $\Delta G_{complex}$, $\Delta G_{receptor}$, and ΔG_{ligand} indicate free energy contributions from S protein-ACE2 (complex), ACE2 (receptor), and S protein (ligand), respectively, for the two complex systems (S protein (BA.1)-ACE2 and S protein(BA.2)-ACE2), as illustrated in Eqn. (1)

The enthalpy component is derived by adding the change in molecular mechanics components in the gas phase (ΔE_{MM}) and the stabilization energy due to solvation (ΔG_{sol}) as shown in Eqn. (3). ΔE_{MM} indicates the summation of internal energy (ΔE_{int}) (bond, angle, and dihedral energies), electrostatic interaction (ΔEele), and van der Waals interaction (ΔE_{vdw}). The solvation free energy (ΔG_{sol}) is indicated by the summation of electrostatic solvation free energy ($\Delta G_{PB/GB}$) and the non-polar solvation free energy (ΔG_{SURF}) contribution, as mentioned in Eqn. (5). ΔG_{GB} is calculated by Poisson-Boltzmann/Generalized-Boltzmann models, and ΔG_{SURF}, is obtained by the summation of non-polar contribution calculated by PB (E_{NP}) and dispersion energy (E_{dis}) using Solvent accessibility surface area (SASA).

The crucial residues in the two complex systems were found using the method of energy decompositions. The energy contribution of each residue from the combination of the protein (ACE2) and the ligand (S protein) was divided into three terms in this case: van der Waals contribution (ΔE_{vdW}), electrostatic contribution (ΔE_{ele}), and solvation contribution (ΔG_{GB} + ΔG_{SA}). In this case, only per-residue decomposition was included.

3. Results and Discussion

3.1. MD simulation of the BA.1 and B.A.2 structure of SARS-CoV-2 spike receptor-binding domain bound with ACE2.

To study the dynamic properties of the two complexes BA.1 and B.A.2 of SARS-CoV-2 spike receptor-binding domain bound with ACE2, we carried out 50 ns of molecular dynamics simulation.

3.1.1. RMSD analysis.

To test the stability of the (S protein (BA.1)-ACE2) and (S protein (BA.2)-ACE2) complexes, 50 ns of MD simulation studies were carried out. The conformational snapshots of the (S protein (BA.1)-ACE2) and (S protein (BA.2)-ACE2) complexes during the course of 50 ns MD simulation time were depicted in Figure 2 and Figure 3. The average deviations in the

atomic positions and the stability through the trajectory of 50 ns of the MD simulations, the RMSD (root mean square deviation) values of the backbone atoms of the complexes along with the S protein (Apo form) for both BA.1 and BA.2 were calculated (Figure 4 and 5). The RMSD of the BA.1 type and the BA.2 complex appeared stable after 10 ns, revealing that good convergence was achieved for each system. Interestingly, we noticed that the RMSD values of the BA.2 complex were slightly smaller than that of the BA.1type complex. The average RMSD value of S protein (BA.1)-ACE2 and S protein (BA.2)-ACE2 type complex structure were calculated to be 1.41 Å (± 0.62) and 1.07 Å (± 0.62), respectively, which could indicate greater stability of the BA.2 complex structure. We observed significant differences in the conformational dynamics of S protein (BA.1/BA.2)-ACE2 complexes in the region in and around the mutation sites, as shown in Figures S1, S2, and S3. We also noticed that the binding of ACE2 reduced the perturbation of S protein to a significant extent in both complex systems.

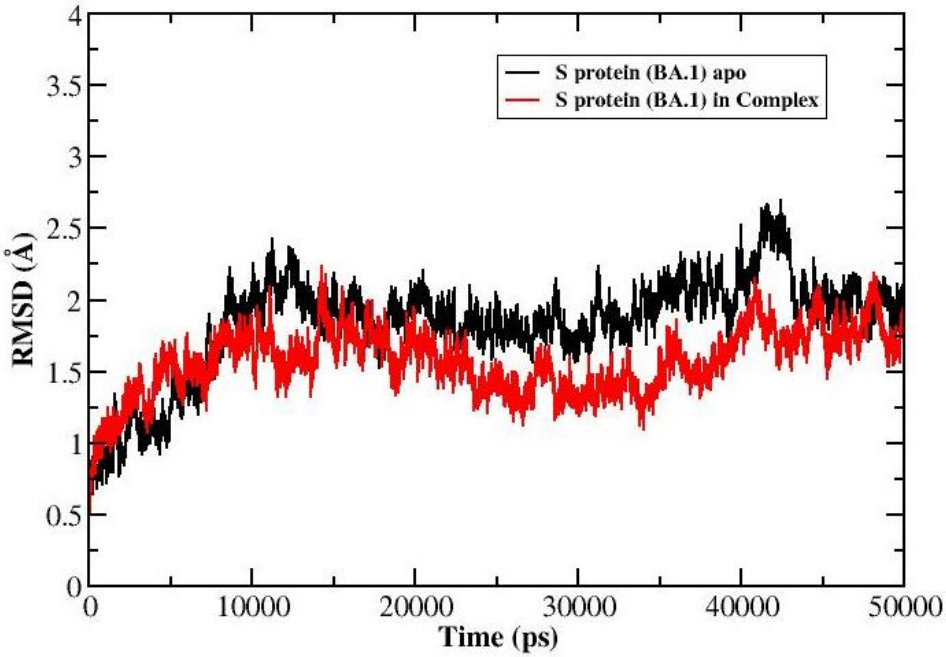

Figure 4. Backbone RMSD's for S protein (BA.1) Apo (black) and S protein (BA.1)-ACE2 complex (red).

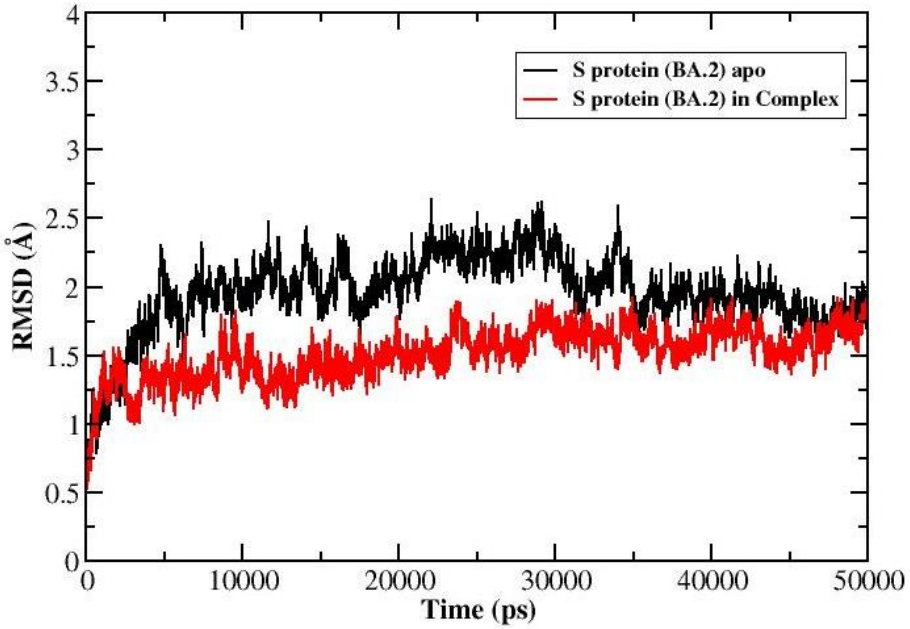

Figure 5. Backbone RMSD's for S protein (BA.2) Apo (black) and S protein (BA.2)-ACE2 complex (red).

3.1.2. RMSF analysis.

We further explored the S protein flexibility by RMSF values of the Cα from the MD simulations of the (S protein (BA.1)-ACE2) and (S protein (BA.2)-ACE2) complexes along with the wild-type complex shown in Figure 6. We observed significant differences in the flexibility of S protein in BA.1, BA.2, and wild-type complexes, particularly at the regions in and around the mutation sites mentioned in Table 1. The RMSF values of Cα atoms of S protein in BA.1 and BA.2 complexes show relatively lower values than in the wild-type complex [45]. From Figure 6, it is more apparent that there is a significant reduction in structural fluctuations and increased stability in the case of BA.1 and BA.2 complexes. Among BA.1 and BA.2 complexes, we found the fluctuations are relatively less in the case of BA.2 complex.

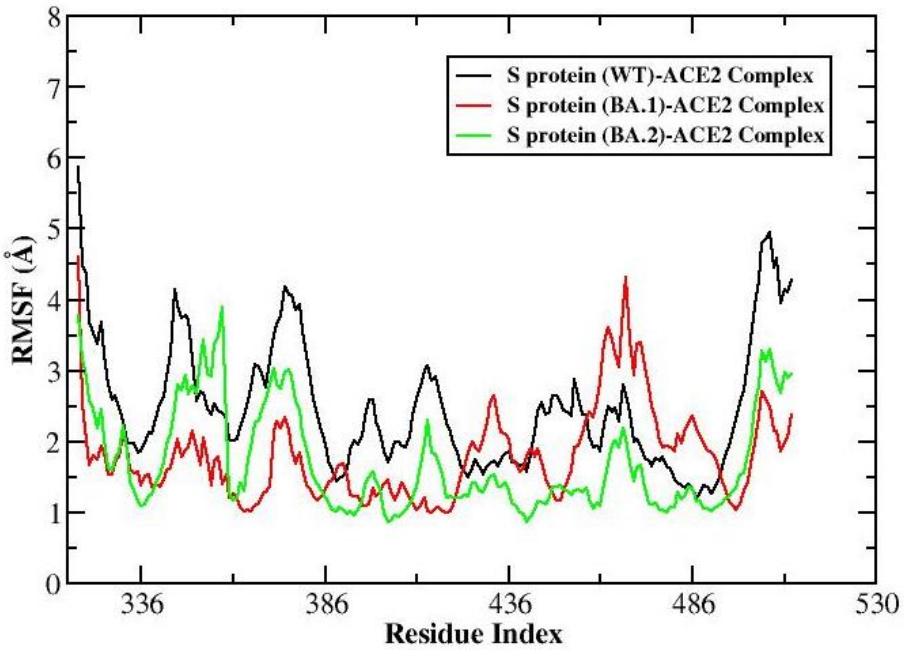

Figure 6. Backbone RMSF's for S protein in (A) S protein (WILD)-ACE2 complex (black) (B) S protein (BA.1)-ACE2 complex (red) and (C) S protein (BA.2)-ACE2 complex (green).

3.1.3. Hydrogen bond analysis.

Additionally, we also calculated and plotted the number of intermolecular hydrogen bonds present in the (S protein (BA.1)-ACE2) and (S protein (BA.2)-ACE2) complexes (Figure 7), as these hydrogen bonds play a crucial role in conferring the stability to the protein complexes. The number of intermolecular hydrogen bonds was found to be higher in S protein (BA.2)-ACE2 complex than in S protein (BA.1)-ACE2 complex. The list of intermolecular hydrogen bonds between the S protein (acceptor/donor) and ACE2 (donor/acceptor) during the last 20 ns of MD simulation of both complexes was summarized in Table S1- S4.

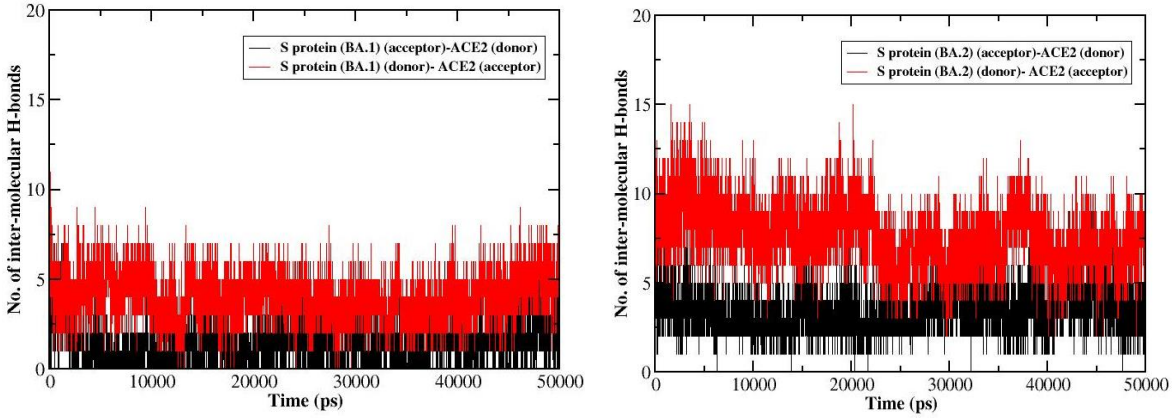

Figure 7. The number of intermolecular hydrogen bonds between S protein and ACE2 in A) S protein (BA.1)-ACE2 complex B) S protein (BA.2)-ACE2 complex.

3.1.4. Determination of the interface interactions of the S protein (BA.1)-ACE2 and (S protein (BA.2)-ACE2 complexes.

Table 2. Interface statistics for the S protein (BA.1)-ACE2 and S protein(BA.2)-ACE2 complexes.

Complex System	Chain	No. of Interface Residues	Interface area(Å^2)	No. of Salt Bridges	No. of Disulphide Bonds	No. of Hydrogen bonds	No. of Non-Bonded Contacts
S Protein(BA1-ACE2)	ACE2	36	1479	3	-	19	246
	SPIKE (BA.1)	31	1574				
S Protein(BA2-ACE2)	ACE2	42	2066	4	-	18	255
	SPIKE (BA.2)	46	2012				

An interface area is usually defined as a region where two sets of proteins come in contact. Surface residues with large surface regions accessible to the solvent available usually characterize them. The interface statistics for the S protein (BA.1)-ACE2 and S protein(BA.2)-ACE2 complexes were obtained upon submitting the corresponding lowest energy structure extracted from the 50 ns MD simulation trajectory using RMSD clustering algorithm to the PDBsum server. The interface statistics for both complexes have been summarised in Table 2.

The summarized intermolecular interactions between S protein and ACE2 in S protein (BA.1)-ACE2 and S protein (BA.2)-ACE2 complexes at the residue levels are shown in Figure 8. The detailed contributions of each interface residue stabilizing the BA.1 and BA.2 complexes were summarized in Table S5 and S6. The total number of interface residues in the S protein (BA.1)-ACE2 and S protein (BA.2)-ACE2 complexes were found to be sixty-seven and eighty-eight, respectively.

In the S protein (BA.1)-ACE2 complex, the interface area for the S protein chain and the ACE2 chain involved in the interaction was observed to be 1479Å2 and 1574Å2, respectively, while in the S protein (BA.2)-ACE2 complex, the S protein chain and the ACE2 chain involved in the interaction was observed to be 2066 Å2 and 2012 Å2 respectively. The BA.1 and BA.2 complexes were stabilized by molecular interactions like salt bridges, hydrogen bonding, and non-bonded contacts. From Table S5 and S6, we can see the presence of two hundred and forty-six non-bonded contacts, three salt bridges, and nineteen hydrogen bonds at the interface of S protein and ACE2 in the S protein (BA.1)-ACE2 complex. However, at the interface of S protein and ACE2 in the S protein (BA.2)-ACE2 complex, we observed two hundred and fifty-five non-bonded contacts, four salt bridges, and eighteen hydrogen bonds. Overall, we see the number of intermolecular interactions and the interface area shared by S

protein and ACE2 in forming complex is larger in BA.2 complex than in the BA.1type complex. Therefore the stability of the BA.2 complex was found to be higher than the BA.1 type complex.

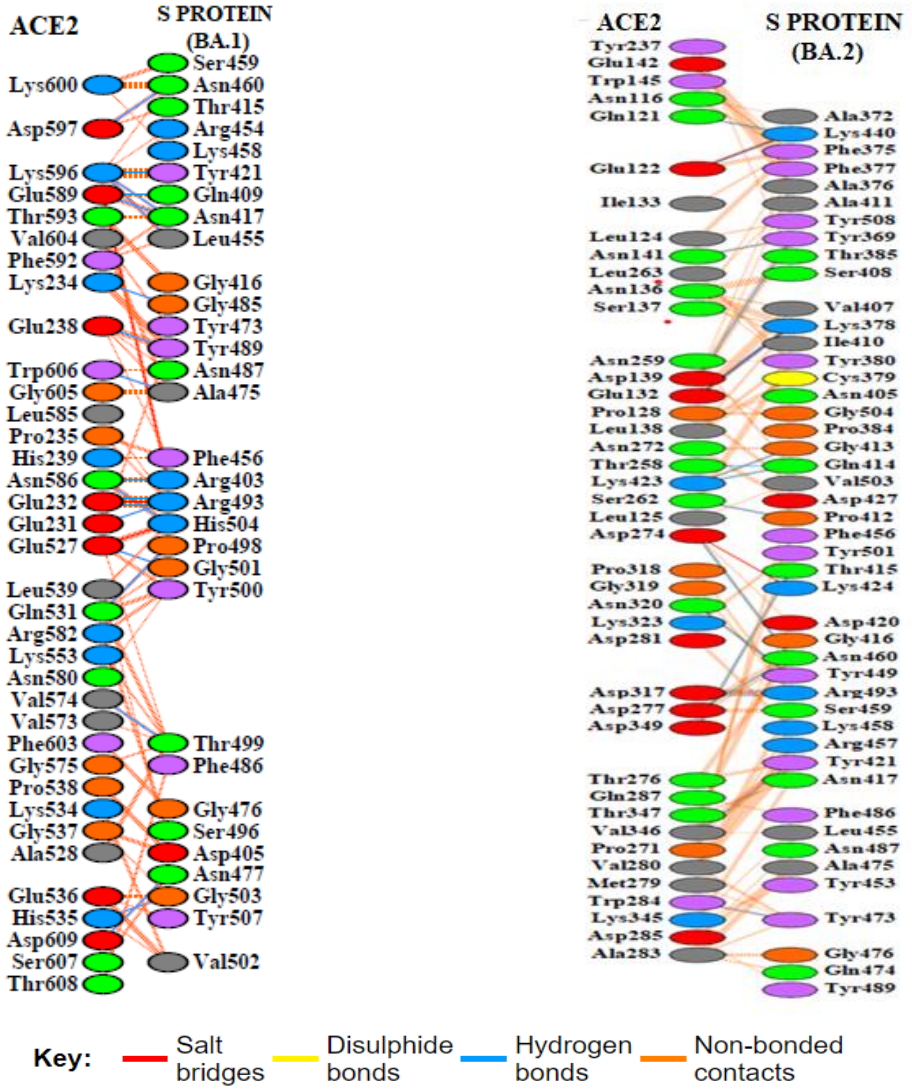

Figure 8. Intermolecular interactions at residue level between ACE2 and S protein in **A)** S protein (BA.1)-ACE2 and **B)** S protein (BA.2)-ACE2 complex.

3.1.5. Binding Free energy and per residue energy decomposition (PRED) analysis.

Using the MM-GBSA approach, the binding free energies of the S protein (BA.1)-ACE2 and S protein (BA.2)-ACE2 complexes were calculated from the last 10 ns of the MD simulation. The binding free energy values here reflect the relative binding free energy rather than absolute or total binding energy, as the MM-GBSA approach uses a continuum solvent approach to determine the binding free energies of a system. The binding free energies were determined for the BA.1, and BA.2 complexes, and the energy terms were summarized in Tables 2 and 3. From Table 3, it can be seen that the S protein(BA.2)-ACE2 (GBTOT=-23.87 kcal/mol) complex was energetically more favorable than the S protein(BA.1)-ACE2 complex (GBTOT=5.38 kcal/mol). Analyzing Tables 3 and 4, we observed that all the derived components for the BFE analysis contributed to the binding of S protein and ACE2 to form the S protein (BA.1 /BA.2)-ACE2 complex.

Table 3. Binding free energies (kcal/mol) and its components of S protein (BA.1)-ACE2 and S protein (BA.2)-ACE2 complexes obtained using the MM-GBSA approach.

Energy components	$\Delta G_{(S\ protein(BA.1)-ACE2)} - [\Delta G_{S\ protein(BA.1)} + \Delta G_{ACE2}]$		$\Delta G_{(S\ protein(BA.2)-ACE2)} - [\Delta G_{S\ protein(BA.2)} + \Delta G_{ACE2}]$	
	Average	std. dev. (±)	Average	std. dev. (±)
VDW	-83.27	3.19	-133.43	6.45
ELE	-1176.79	22.22	-1595.14	34.34
GB	1275.85	21.42	1722.84	31.62
GBSUR	-10.39	0.2904	-18.13	0.43
GAS	-1260.06	21.45	-1728.57	33.18
GBSOL	1265.45	2134	1704.70	31.65
GBTOT	5.38	4.54	-23.87	6.38

To gain insights into the contribution of the individual amino acid residues to the overall PPI of the S protein (BA.1/BA.2)-ACE2 complexes, PRED values were calculated. In this analysis, the total binding energy was decomposed into residues to identify key residues for ACE2 binding to S protein (BA.1/BA.2). Essential residues with the binding energy value below -1.00 kcal/mol were shown in Figures 9 and 10. The highest energy contributions for S protein (BA.1) come from the residues ARG408, TYR501, VAL503, TYR380, PHE377, THR376, ASP428, GLY502, PRO384, PRO499 while in S protein (BA.2) come from the residues LYS417, GLN498, GLN493, TYR505, PHE486, TYR449, TYR489, PHE456, ALA475, PHE490, LEU492, and LEU455.

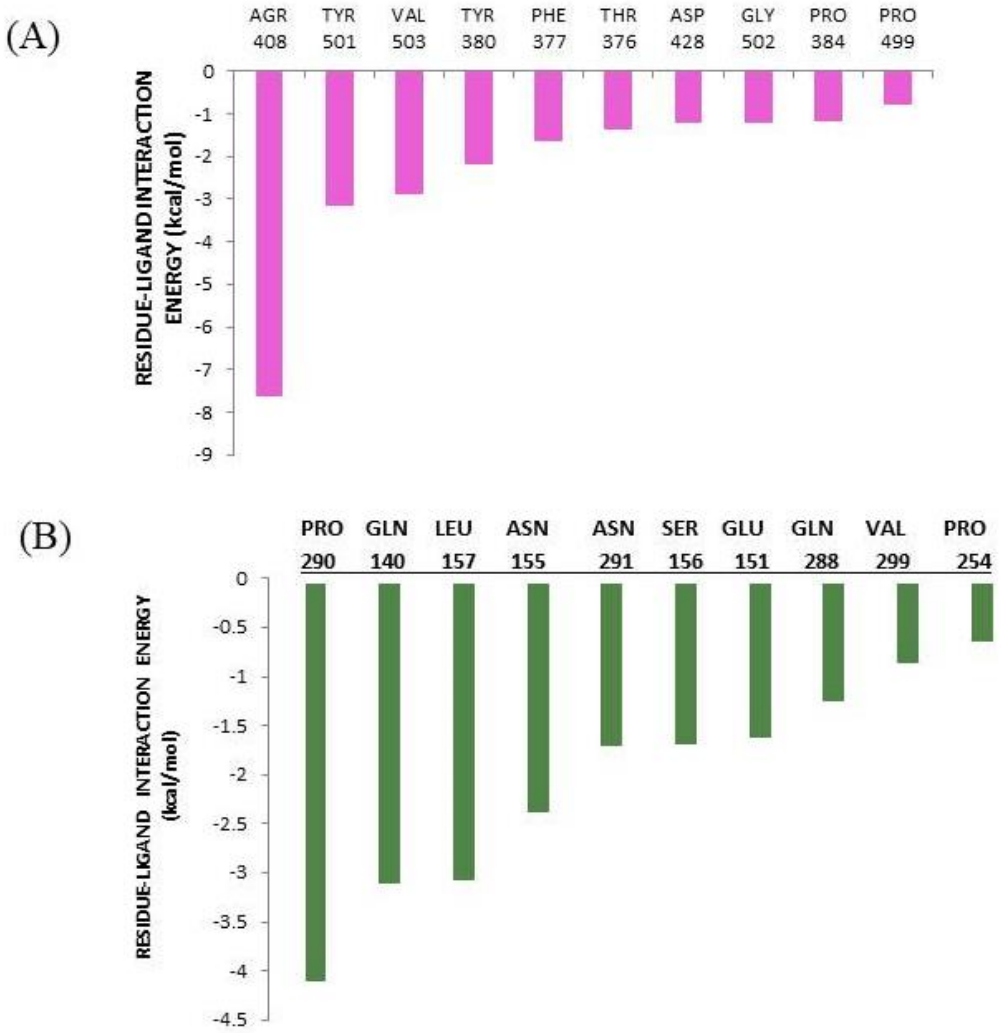

Figure 9. Decomposition of binding free energy (kcal/mol) on a per residue basis for (**A**) SPIKE (BA.1) and (**B**) ACE2 obtained using the MM-GBSA approach.

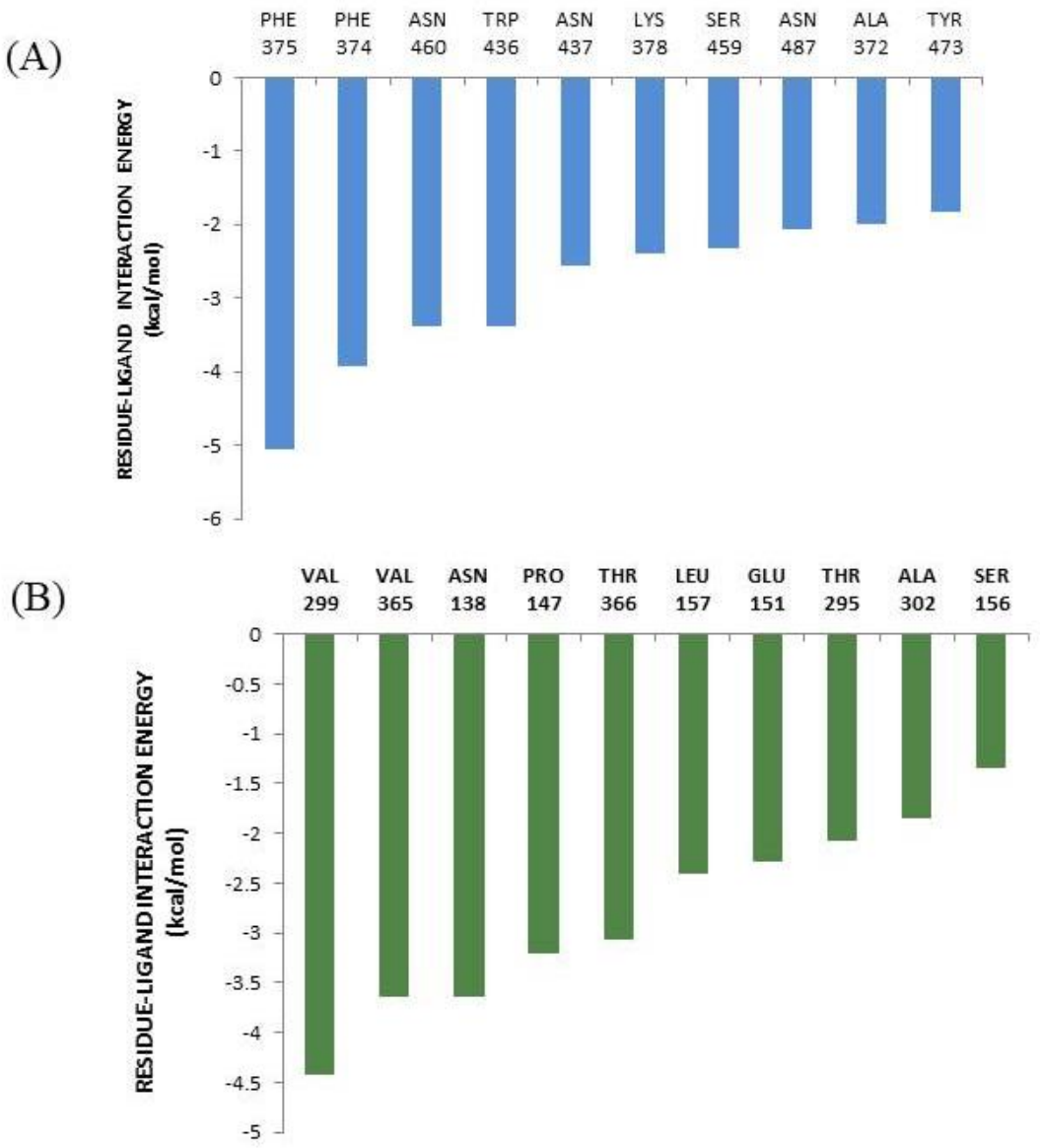

Figure 10. Decomposition of binding free energy (kcal/mol) on a per residue basis for (**A**) SPIKE (BA.2) and (**B**) ACE2 obtained using the MM-GBSA approach.

4. Conclusions

There isn't enough information to establish whether the SARS-CoV-2 BA.1 or BA.2 variant is causing a more severe COVID-19 sickness than during the pandemic's initial wave. It is indistinguishable if the increased fatality is connected to either the variant being deadlier or the inflated volume of infections. The current study uses molecular dynamics and other computational techniques to show the impact of these BA.1 and BA.2 omicron variants on the SARS-CoV-2 RBD's tendency to connect with ACE2. From the MD simulation of S protein (BA.1)-ACE2 and S protein(BA.2)-ACE2 complexes, we found that BA.2 causes extensive structural changes in the mutation region of spike protein in S protein(BA.2)-ACE2 complex. From the RMSD, RMSF, and a number of intermolecular hydrogen bond analyses, we found the S protein (BA.2)-ACE2 complex to have enhanced stability than the S protein (BA.1)-ACE2 complex. The number of non-bonded contacts was also higher in the S protein(BA.2)-ACE2 complex. From the binding free energy calculations of the S protein(BA.1)-ACE2 and S protein(BA.2)-ACE2 complexes, we found that the affinity between S protein and ACE2 is higher in the BA.2 complex. The overall stability of the S protein(BA.2)-ACE2 complex and

the increased affinity between S protein (BA.2) and ACE2 may result in higher virulence of the BA.2 strain than its BA.1 type strain. The salient interactions we have reported across the S protein and ACE2 in the BA.1 type and the BA.2 complexes could be used to design novel inhibitors against the newly emerging coronavirus strains.

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Conflicts of Interest

The authors declare no conflict of interest.

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Supplementary Information

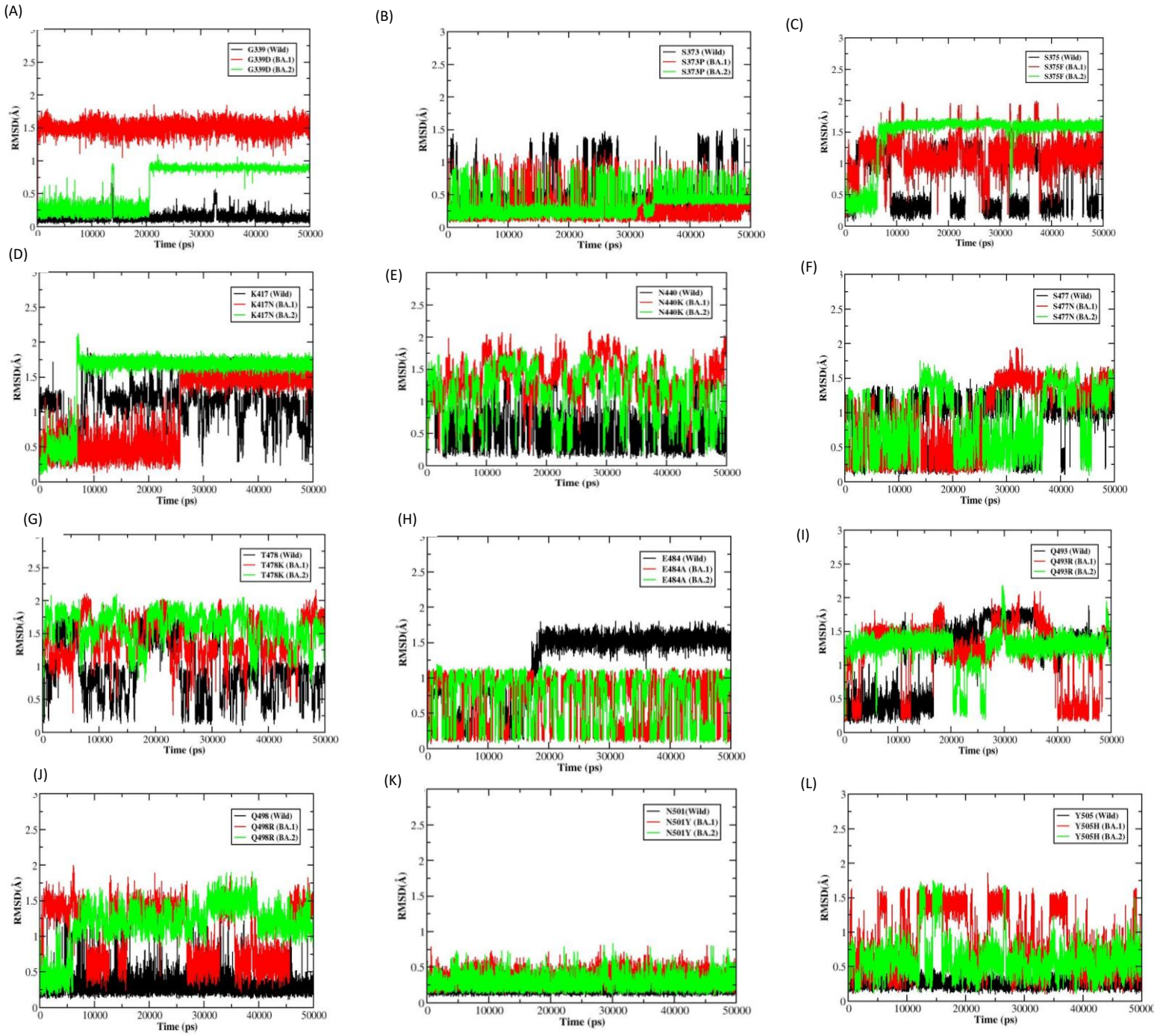

Figure S1. RMSD plot of the common mutated residues at position A) 339 B) 373 C) 375 D) 417 E) 440 F) 477 G)478 H)484 I)493 J)498 K)501 L) 505 in S protein (WILD)-ACE2 complex (black), S protein (BA.1)-ACE2 complex (red) and S protein (BA.2)-ACE2 complex (green).

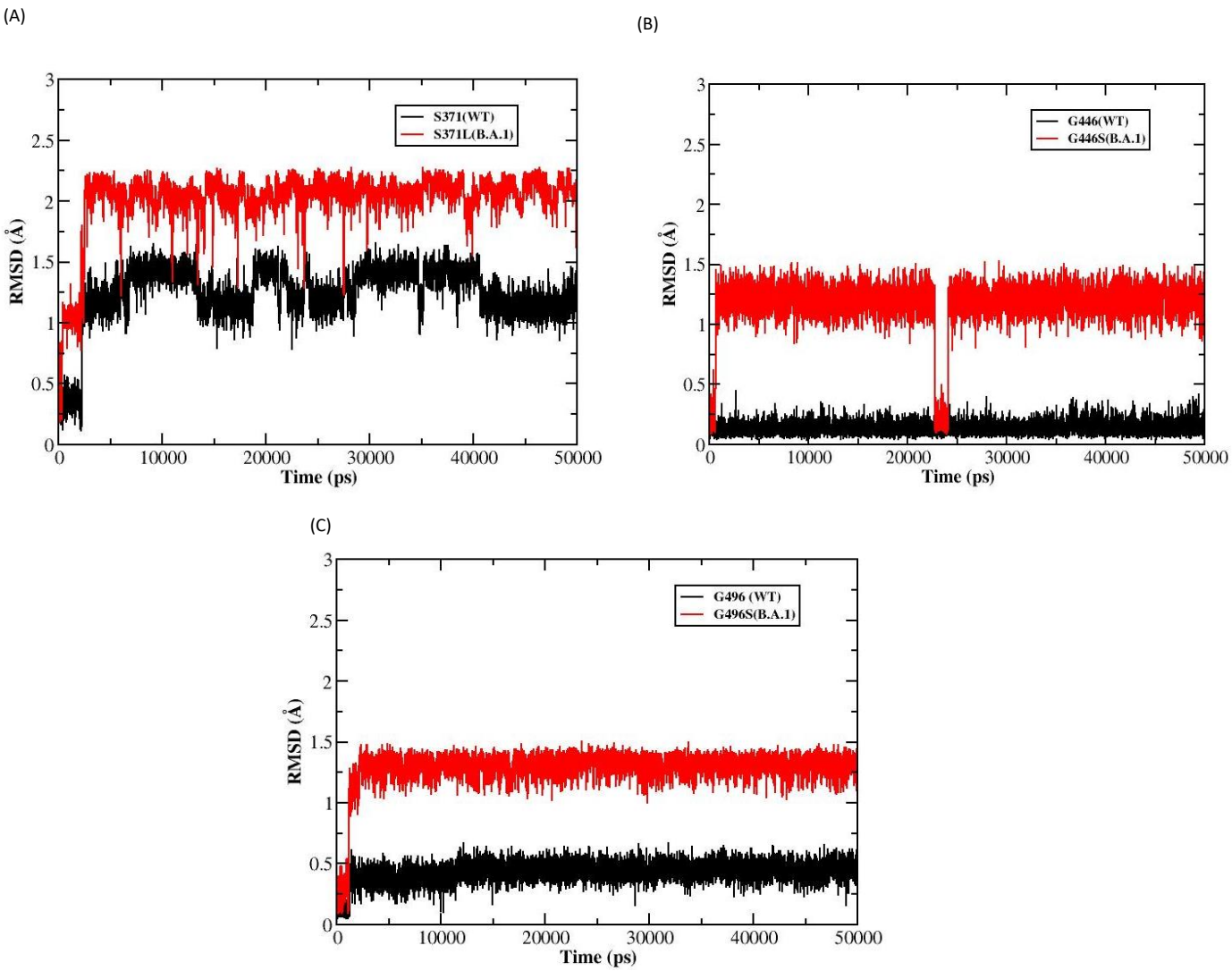

Figure S2. RMSD plot of the residues exclusively present in BA.1at position A) 371 B) 446 C) 496 in S protein (WILD)-ACE2 complex (black), S protein (BA.1)-ACE2 complex (red).

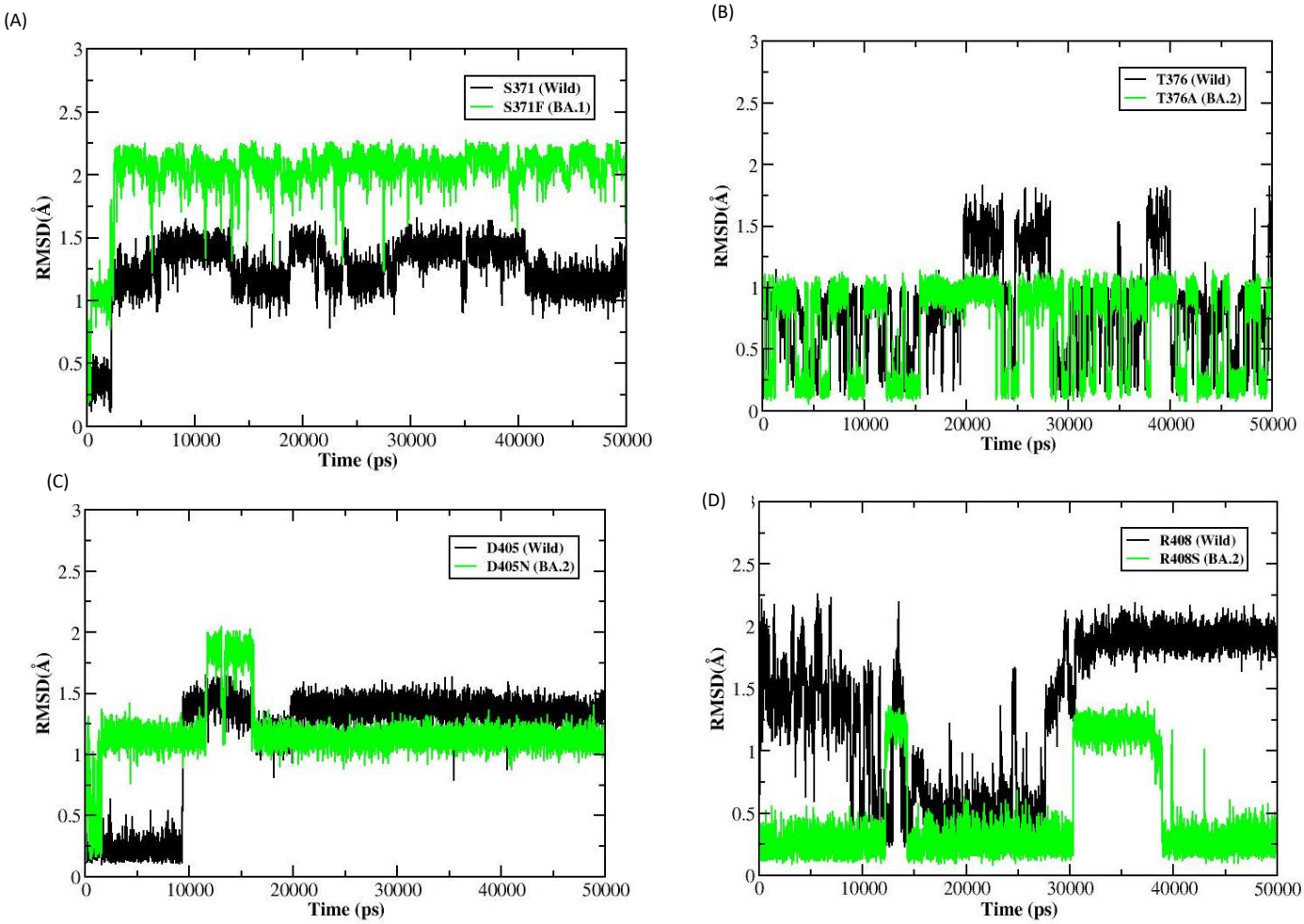

Figure S3. RMSD plot of the residues exclusively present in BA.2 at position A) 371 B) 376 C) 405 D) 408 in S protein (WILD)-ACE2 complex (black), S protein (BA.2)-ACE2 complex (green).

Table S1. Hydrogen bond analysis of S protein (BA.1)-ACE2 complex during the last 20 ns of MD simulation with S protein as acceptor and ACE2 as donor.

#Acceptor	DonorH	Donor	Frames	Frac	AvgDist	AvgAng
GLY_49@O	GLN_464@HE22	GLN_464@NE2	2397	0.2397	2.8640	160.9005
TYR_169@O	GLN_316@HE22	GLN_316@NE2	2082	0.2082	2.8367	159.4083
THR_168@O	GLN_316@HE21	GLN_316@NE2	1570	0.1570	2.8488	158.5888
ASP_95@OD2	ASN_467@H	ASN_467@N	1356	0.1356	2.8779	162.9477
PRO_167@O	GLN_316@HE21	GLN_316@NE2	1101	0.1101	2.8452	150.8264
PHE_43@O	LEU_333@H	LEU_333@N	498	0.0498	2.8725	158.9543
ASP_95@OD1	ASN_467@H	ASN_467@N	443	0.0443	2.8669	163.7890
THR_168@O	GLN_316@HE22	GLN_316@NE2	406	0.0406	2.8536	159.5178
SER_51@OG	ASN_427@HD21	ASN_427@ND2	329	0.0329	2.8969	159.1247
THR_98@OG1	GLN_464@HE22	GLN_464@NE2	284	0.0284	2.8917	161.8117
VAL_171@H	GLU_317@HG2	GLU_317@CG	256	0.0256	2.8624	148.8493
PRO_167@O	ASN_314@HD21	ASN_314@ND2	247	0.0247	2.8500	157.4171
GLY_170@HA2	GLN_316@HB3	GLN_316@CB	184	0.0184	2.9379	144.3039
ARG_76@HB3	ASN_331@HD21	ASN_331@ND2	140	0.0140	2.8186	152.9300
LYS_46@HE3	ASN_331@HA	ASN_331@CA	136	0.0136	2.8803	141.7735
VAL_75@HG13	ASN_331@HD21	ASN_331@ND2	132	0.0132	2.8503	149.1277
ASP_95@O	ASN_467@H	ASN_467@N	130	0.0130	2.8928	159.6823
THR_53@HG1	ALA_428@HA	ALA_428@CA	117	0.0117	2.8968	144.0213
ASP_96@HB3	PRO_466@HD3	PRO_466@CD	112	0.0112	2.9266	140.7922
VAL_75@HG12	ASN_331@HD21	ASN_331@ND2	98	0.0098	2.8589	149.7488
GLN_174@HE22	GLN_316@HE22	GLN_316@NE2	82	0.0082	2.8593	142.0411
ASN_38@OD1	TYR_432@HH	TYR_432@OH	81	0.0081	2.7748	161.4923
CYX_47@O	SER_457@HG	SER_457@OG	81	0.0081	2.7697	159.6387

PRO_80@O	ASN_467@HD22	ASN_467@ND2	77	0.0077	2.8665	163.6005
LEU_58@HD23	GLN_464@HE21	GLN_464@NE2	74	0.0074	2.8469	153.3379
THR_44@HB	ASN_331@HB3	ASN_331@CB	71	0.0071	2.9447	144.2455
VAL_75@HG11	ASN_331@HD21	ASN_331@ND2	65	0.0065	2.8420	149.4356
PHE_45@HB3	LEU_333@HB2	LEU_333@CB	61	0.0061	2.9458	142.1613
PHE_45@H	LEU_333@HD11	LEU_333@CD1	50	0.0050	2.8183	150.3143
GLY_49@HA2	GLY_463@HA3	GLY_463@CA	49	0.0049	2.9320	141.9332
LEU_58@HD22	GLN_464@HE21	GLN_464@NE2	48	0.0048	2.8426	152.5831
ASP_96@HB3	PRO_466@HB3	PRO_466@CB	43	0.0043	2.9506	138.5580
LEU_58@HD21	GLN_464@HE21	GLN_464@NE2	41	0.0041	2.8282	153.2695
GLY_170@HA3	GLN_316@HB3	GLN_316@CB	39	0.0039	2.9488	144.0922
VAL_171@HG13	ASN_314@HD21	ASN_314@ND2	38	0.0038	2.8107	147.9498
PHE_45@H	LEU_333@HD13	LEU_333@CD1	35	0.0035	2.8086	150.7565
SER_51@HB3	ASN_427@HD21	ASN_427@ND2	34	0.0034	2.8505	143.4813
PHE_43@O	SER_332@HG	SER_332@OG	30	0.0030	2.7707	161.5707
TYR_48@HD2	SER_457@HB3	SER_457@CB	30	0.0030	2.9499	141.5948
GLY_49@HA3	GLN_464@HG2	GLN_464@CG	30	0.0030	2.9444	142.1123
PHE_42@HE1	LEU_333@HG	LEU_333@CG	26	0.0026	2.9521	141.9051
SER_51@HB2	ASN_427@HD21	ASN_427@ND2	26	0.0026	2.8404	144.7371
SER_51@HG	ASN_427@HD21	ASN_427@ND2	26	0.0026	2.9053	144.1853
THR_98@OG1	GLN_464@HE21	GLN_464@NE2	24	0.0024	2.8839	156.8871
ASN_128@HD22	VAL_475@HG11	VAL_475@CG1	24	0.0024	2.9064	144.2958
LYS_46@HD2	ASN_331@HA	ASN_331@CA	20	0.0020	2.9619	142.7854
THR_83@HG1	THR_542@HB	THR_542@CB	20	0.0020	2.9449	147.5527
LEU_58@HD11	GLN_464@HE21	GLN_464@NE2	19	0.0019	2.8837	147.7311
TYR_48@HD2	SER_457@HB2	SER_457@CB	18	0.0018	2.9331	142.9105
THR_53@O	ASN_427@HD21	ASN_427@ND2	17	0.0017	2.8920	157.6533
ASP_95@HB3	PRO_466@HB3	PRO_466@CB	17	0.0017	2.9475	139.9677
TYR_48@HE2	SER_457@HB2	SER_457@CB	16	0.0016	2.9313	140.3828
ASN_128@HD22	VAL_475@HG23	VAL_475@CG2	16	0.0016	2.9297	147.5273
PHE_42@HE1	LEU_333@HB3	LEU_333@CB	15	0.0015	2.9321	139.8203
PHE_45@H	LEU_333@HD23	LEU_333@CD2	15	0.0015	2.8588	144.6686
ASN_128@HD21	VAL_475@HG13	VAL_475@CG1	15	0.0015	2.8928	144.3010
THR_44@HG22	ASN_331@HB3	ASN_331@CB	14	0.0014	2.9481	141.4560
PHE_45@H	LEU_333@HD12	LEU_333@CD1	14	0.0014	2.7833	144.1054
TYR_48@HE2	SER_457@HB3	SER_457@CB	14	0.0014	2.9376	139.0274
ASP_95@HB3	ASN_467@H	ASN_467@N	14	0.0014	2.8640	146.7700
ASP_96@HB3	PRO_466@HG3	PRO_466@CG	14	0.0014	2.9378	140.7272
ASN_128@HD21	VAL_475@HG11	VAL_475@CG1	14	0.0014	2.8328	143.0306
ARG_76@HA	ASN_331@HD21	ASN_331@ND2	13	0.0013	2.8863	148.4360
LEU_185@HD21	GLN_464@HE21	GLN_464@NE2	13	0.0013	2.8357	147.5448
THR_44@HA	SER_332@HA	SER_332@CA	12	0.0012	2.9504	149.0557
LYS_46@HE2	ASN_331@HA	ASN_331@CA	12	0.0012	2.9238	143.2173
ASN_128@HD22	VAL_475@HG12	VAL_475@CG1	12	0.0012	2.9159	141.1953
THR_44@HG1	ASN_331@HB3	ASN_331@CB	11	0.0011	2.8829	151.2197
PHE_45@HB3	LEU_333@HG	LEU_333@CG	11	0.0011	2.9703	141.2827
SER_51@HG	ALA_428@HA	ALA_428@CA	11	0.0011	2.8708	140.5887
THR_98@HG22	GLN_464@HE22	GLN_464@NE2	11	0.0011	2.8964	141.2293
THR_98@HG23	GLN_464@HG2	GLN_464@CG	11	0.0011	2.9577	142.4567
VAL_171@H	LEU_319@HG	LEU_319@CG	11	0.0011	2.8597	150.0912
VAL_171@HG22	GLU_317@HA	GLU_317@CA	11	0.0011	2.9290	145.6942
TYR_37@HH	LEU_333@HD22	LEU_333@CD2	10	0.0010	2.9222	144.0308
PHE_42@HE1	LEU_333@HD13	LEU_333@CD1	10	0.0010	2.9450	139.5930
VAL_75@HG22	ASN_331@HD21	ASN_331@ND2	10	0.0010	2.7666	142.7799
VAL_171@HG11	GLU_317@HG3	GLU_317@CG	10	0.0010	2.9361	141.8414
VAL_171@HG13	GLU_317@HG2	GLU_317@CG	10	0.0010	2.9564	140.5828
VAL_171@HG23	GLU_317@HA	GLU_317@CA	10	0.0010	2.9521	147.3366
LEU_185@HD23	GLN_464@HE21	GLN_464@NE2	10	0.0010	2.8325	145.2162
PHE_42@HE1	LEU_333@HD23	LEU_333@CD2	9	0.0009	2.9600	139.2185
THR_44@HG23	ASN_331@HB3	ASN_331@CB	9	0.0009	2.9536	139.5163
THR_83@HG22	THR_471@HG21	THR_471@CG2	9	0.0009	2.9771	142.3336
THR_83@HG1	THR_542@HG21	THR_542@CG2	9	0.0009	2.8391	143.9850
ASN_128@HD21	VAL_475@HG12	VAL_475@CG1	9	0.0009	2.9206	147.5613

ASN_128@HD22	VAL_475@HG22	VAL_475@CG2	9	0.0009	2.9008	139.7042
ASN_128@HD22	VAL_475@HG13	VAL_475@CG1	9	0.0009	2.9206	140.3041
VAL_171@HG21	GLU_317@HG2	GLU_317@CG	9	0.0009	2.9481	142.1209
LEU_185@HD22	GLN_464@HE21	GLN_464@NE2	9	0.0009	2.8238	143.2390
TYR_37@HH	LEU_333@HD12	LEU_333@CD1	8	0.0008	2.9050	144.6657
TYR_37@HH	LEU_333@HD21	LEU_333@CD2	8	0.0008	2.8291	149.0081
TYR_37@HH	LEU_333@HD23	LEU_333@CD2	8	0.0008	2.9180	153.6321
PHE_42@HE1	LEU_333@HD11	LEU_333@CD1	8	0.0008	2.9494	139.8021
PHE_42@HZ	LEU_333@HD23	LEU_333@CD2	8	0.0008	2.9703	139.8677
THR_44@HA	LEU_333@HD21	LEU_333@CD2	8	0.0008	2.9195	144.4069
PHE_45@H	LEU_333@HD22	LEU_333@CD2	8	0.0008	2.7751	146.9952
PHE_45@HB3	LEU_333@HD22	LEU_333@CD2	8	0.0008	2.9504	142.1563
PHE_45@HD2	LEU_333@HD23	LEU_333@CD2	8	0.0008	2.9533	140.1948
LEU_58@HD12	GLN_464@HE21	GLN_464@NE2	8	0.0008	2.9165	146.7030
THR_83@HB	THR_542@HG21	THR_542@CG2	8	0.0008	2.9422	140.3468
THR_98@HG22	GLN_464@HG2	GLN_464@CG	8	0.0008	2.9589	146.1923
VAL_171@HG13	GLU_317@HB2	GLU_317@CB	8	0.0008	2.9709	141.0590
VAL_171@HG21	GLU_317@HA	GLU_317@CA	8	0.0008	2.9684	139.7298
VAL_171@HG22	GLU_317@HG3	GLU_317@CG	8	0.0008	2.9375	142.1650
PHE_42@HZ	LEU_333@HD21	LEU_333@CD2	7	0.0007	2.9493	149.7520
THR_44@HG21	ASN_331@HB3	ASN_331@CB	7	0.0007	2.9326	140.1947
PHE_45@H	LEU_333@HD21	LEU_333@CD2	7	0.0007	2.7460	143.2461
PHE_45@HB3	LEU_333@HD23	LEU_333@CD2	7	0.0007	2.9142	140.0097
LYS_54@HD2	ASN_427@HA	ASN_427@CA	7	0.0007	2.9472	149.3113
ARG_76@HH11	PRO_323@HB2	PRO_323@CB	7	0.0007	2.9254	138.4464
THR_98@HG23	GLN_464@HE22	GLN_464@NE2	7	0.0007	2.8279	147.3584
ASN_128@HD21	VAL_475@HG21	VAL_475@CG2	7	0.0007	2.9479	150.8662
THR_168@HB	GLN_316@HB2	GLN_316@CB	7	0.0007	2.9557	140.6582
VAL_171@HG11	GLU_317@HB2	GLU_317@CB	7	0.0007	2.9553	141.6230
VAL_171@HG12	GLU_317@HG2	GLU_317@CG	7	0.0007	2.9772	145.9541
VAL_171@HG13	GLU_317@HG3	GLU_317@CG	7	0.0007	2.9440	138.6893
VAL_171@HG13	GLU_317@HA	GLU_317@CA	7	0.0007	2.9534	144.3872
TYR_37@HH	LEU_333@HD13	LEU_333@CD1	6	0.0006	2.9088	142.7217
TYR_37@HE2	ALA_428@HA	ALA_428@CA	6	0.0006	2.9489	148.6209
PHE_42@HE1	LEU_333@HD22	LEU_333@CD2	6	0.0006	2.9437	138.1460
PHE_45@HB3	LEU_333@HD21	LEU_333@CD2	6	0.0006	2.9238	137.9579
TYR_48@HE2	SER_457@HA	SER_457@CA	6	0.0006	2.9594	137.7779
LYS_54@HE3	PRO_430@HG3	PRO_430@CG	6	0.0006	2.8924	150.4649
VAL_75@HB	ASN_331@HD21	ASN_331@ND2	6	0.0006	2.8050	141.2380
THR_83@HG1	THR_542@HG22	THR_542@CG2	6	0.0006	2.8891	144.8144
THR_98@HG21	GLN_464@HG2	GLN_464@CG	6	0.0006	2.9473	144.3534
THR_98@HG21	GLN_464@HE22	GLN_464@NE2	6	0.0006	2.8050	148.2003
ASN_128@HD21	VAL_475@HG22	VAL_475@CG2	6	0.0006	2.9075	145.5546
ASN_128@HD22	VAL_475@HG21	VAL_475@CG2	6	0.0006	2.8823	145.4259
PRO_167@O	GLN_316@HE22	GLN_316@NE2	6	0.0006	2.8802	148.1719
GLY_170@HA2	GLU_317@HG2	GLU_317@CG	6	0.0006	2.9437	142.9475
VAL_171@H	LEU_319@HD21	LEU_319@CD2	6	0.0006	2.7884	141.7519
VAL_171@HG12	GLU_317@HB2	GLU_317@CB	6	0.0006	2.9697	141.7803
VAL_171@HG23	GLU_317@HG3	GLU_317@CG	6	0.0006	2.9430	141.1262
PHE_42@HE1	LEU_333@HD21	LEU_333@CD2	5	0.0005	2.9477	139.7728
THR_44@HA	LEU_333@HD23	LEU_333@CD2	5	0.0005	2.9613	142.4802
PHE_45@HD2	LEU_333@HD22	LEU_333@CD2	5	0.0005	2.9491	137.1644
LYS_46@HZ1	ALA_330@HB1	ALA_330@CB	5	0.0005	2.8695	148.5997
TYR_48@HE2	SER_457@HG	SER_457@OG	5	0.0005	2.8897	146.3800
GLY_49@HA2	GLN_464@HG2	GLN_464@CG	5	0.0005	2.9339	144.8389
SER_51@OG	ASN_427@HD22	ASN_427@ND2	5	0.0005	2.9164	146.3764
THR_53@HB	ALA_428@HA	ALA_428@CA	5	0.0005	2.9568	144.4715
THR_53@HG22	ALA_428@HA	ALA_428@CA	5	0.0005	2.9436	144.9762
LYS_54@HE3	ASN_427@HA	ASN_427@CA	5	0.0005	2.9214	158.6571
LEU_58@HD13	GLN_464@HE21	GLN_464@NE2	5	0.0005	2.9232	147.1837
GLY_81@HA3	ASN_467@HB3	ASN_467@CB	5	0.0005	2.9304	137.2197
ASN_128@HD21	VAL_475@HB	VAL_475@CB	5	0.0005	2.8717	140.0067
THR_168@HA	ASN_314@HD21	ASN_314@ND2	5	0.0005	2.8193	150.4138

TYR_169@O	GLN_316@HE21	GLN_316@NE2	5	0.0005	2.8400	143.3367
GLY_170@HA2	GLU_317@HG3	GLU_317@CG	5	0.0005	2.9514	142.1281
VAL_171@HG11	GLU_317@HA	GLU_317@CA	5	0.0005	2.9449	147.5483
VAL_171@HG11	GLU_317@HG2	GLU_317@CG	5	0.0005	2.9356	138.4398
VAL_171@HG23	GLU_317@HG2	GLU_317@CG	5	0.0005	2.9249	140.0572
ASN_38@O	TYR_432@HH	TYR_432@OH	4	0.0004	2.7520	152.4650
ALA_40@HB3	LEU_333@HD12	LEU_333@CD1	4	0.0004	2.9297	141.3815
PHE_42@HE1	LEU_333@HB2	LEU_333@CB	4	0.0004	2.9259	135.5932
THR_44@HA	ASN_331@HB3	ASN_331@CB	4	0.0004	2.9773	144.2615
LYS_46@HE3	SER_457@HB2	SER_457@CB	4	0.0004	2.9361	141.6998
LYS_46@HZ2	ALA_330@HB1	ALA_330@CB	4	0.0004	2.9142	147.3731
LYS_46@HZ2	ALA_330@HB3	ALA_330@CB	4	0.0004	2.9257	145.6782
GLY_49@HA2	GLN_464@HG3	GLN_464@CG	4	0.0004	2.8903	138.1014
VAL_50@HG12	GLN_464@HE22	GLN_464@NE2	4	0.0004	2.9262	139.0295
VAL_75@HG21	ASN_331@HD21	ASN_331@ND2	4	0.0004	2.9336	143.5532
ARG_76@H	ASN_331@HD21	ASN_331@ND2	4	0.0004	2.9124	141.3069
GLY_81@HA3	ASN_467@HD22	ASN_467@ND2	4	0.0004	2.8828	146.5079
THR_83@HG23	THR_471@HG21	THR_471@CG2	4	0.0004	2.9761	145.3320
ASP_96@HB3	PRO_466@HA	PRO_466@CA	4	0.0004	2.8945	139.3901
ASN_128@H	VAL_475@HG12	VAL_475@CG1	4	0.0004	2.9325	145.9643
GLN_174@HE21	GLN_316@HG3	GLN_316@CG	4	0.0004	2.9685	144.1569
TYR_37@HE1	LEU_333@HD22	LEU_333@CD2	3	0.0003	2.9545	139.8017
TYR_37@HE1	LEU_333@HD21	LEU_333@CD2	3	0.0003	2.9600	143.3755
PHE_42@HZ	LEU_333@HD22	LEU_333@CD2	3	0.0003	2.9559	144.4039
THR_44@HG23	SER_332@HA	SER_332@CA	3	0.0003	2.8866	140.9961
THR_44@HG1	SER_332@HA	SER_332@CA	3	0.0003	2.9130	140.9138
PHE_45@H	LEU_333@HG	LEU_333@CG	3	0.0003	2.7765	139.4505
LYS_46@HG2	LEU_458@HD21	LEU_458@CD2	3	0.0003	2.9393	145.0430
LYS_46@HG3	ASN_331@HA	ASN_331@CA	3	0.0003	2.9535	153.8871
LYS_46@HD3	SER_457@HB2	SER_457@CB	3	0.0003	2.8730	138.4584
LYS_46@HE2	ALA_330@HB3	ALA_330@CB	3	0.0003	2.9439	145.8532
LYS_46@HE2	ALA_330@HB2	ALA_330@CB	3	0.0003	2.8801	143.2310
LYS_46@HE2	ALA_330@HB1	ALA_330@CB	3	0.0003	2.9796	142.0502
LYS_46@HZ1	ALA_330@HB2	ALA_330@CB	3	0.0003	2.9606	154.0231
LYS_46@HZ3	SER_457@HG	SER_457@OG	3	0.0003	2.9146	138.4706
VAL_50@HG13	GLN_464@HE22	GLN_464@NE2	3	0.0003	2.8824	148.2517
THR_53@HG21	PRO_430@HG3	PRO_430@CG	3	0.0003	2.9568	144.4437
THR_53@HG21	PRO_430@HD3	PRO_430@CD	3	0.0003	2.9242	137.2533
THR_53@HG23	ALA_428@HA	ALA_428@CA	3	0.0003	2.9049	138.5340
THR_53@OG1	ASN_427@HD21	ASN_427@ND2	3	0.0003	2.8944	143.8703
LYS_54@HB2	ASN_427@HD21	ASN_427@ND2	3	0.0003	2.8614	142.8461
LEU_58@CD2	GLN_464@HE21	GLN_464@NE2	3	0.0003	2.9597	153.6116
ASP_73@HA	GLU_327@HG3	GLU_327@CG	3	0.0003	2.9815	139.6200
THR_83@HG21	THR_471@HG22	THR_471@CG2	3	0.0003	2.9352	139.5947
THR_83@HG21	THR_471@HG21	THR_471@CG2	3	0.0003	2.9624	138.5463
ASP_96@HB2	PRO_466@HD3	PRO_466@CD	3	0.0003	2.9934	139.5179
VAL_171@H	LEU_319@HD23	LEU_319@CD2	3	0.0003	2.8648	144.6345
VAL_171@H	LEU_319@HD22	LEU_319@CD2	3	0.0003	2.8420	136.9852
VAL_171@HG11	ASN_314@HD21	ASN_314@ND2	3	0.0003	2.7684	147.3542
VAL_171@HG11	GLY_324@HA2	GLY_324@CA	3	0.0003	2.9090	141.8482
VAL_171@HG12	GLU_317@HA	GLU_317@CA	3	0.0003	2.9549	140.5270
VAL_171@HG21	LEU_319@HD23	LEU_319@CD2	3	0.0003	2.9704	139.9419
VAL_171@HG23	GLU_317@HB2	GLU_317@CB	3	0.0003	2.9384	136.8943
GLN_174@HE22	GLN_316@HB3	GLN_316@CB	3	0.0003	2.9257	143.9707
GLN_174@HE22	GLN_316@HG3	GLN_316@CG	3	0.0003	2.9283	139.5917
TYR_37@HE1	LEU_333@HG	LEU_333@CG	2	0.0002	2.9729	139.5924
TYR_37@HH	LEU_333@HG	LEU_333@CG	2	0.0002	2.9421	141.4905
TYR_37@HH	LEU_333@HD11	LEU_333@CD1	2	0.0002	2.9858	154.9903
ASN_38@HD21	SER_431@HG	SER_431@OG	2	0.0002	2.8508	138.2651
ALA_40@HB1	LEU_333@HD11	LEU_333@CD1	2	0.0002	2.9697	141.4184
ALA_40@HB2	LEU_333@HB2	LEU_333@CB	2	0.0002	2.9420	136.6643
PHE_42@HE1	LEU_333@HD12	LEU_333@CD1	2	0.0002	2.9845	136.5944
THR_44@HA	LEU_333@HB2	LEU_333@CB	2	0.0002	2.9567	145.8570

THR_44@HG21	ASN_331@HD22	ASN_331@ND2	2	0.0002	2.7790	145.6448
THR_44@HG21	SER_332@HA	SER_332@CA	2	0.0002	2.9631	136.8424
THR_44@HG22	ASN_331@HD22	ASN_331@ND2	2	0.0002	2.9253	140.2961
THR_44@HG22	ASN_331@HD21	ASN_331@ND2	2	0.0002	2.5646	140.1155
THR_44@HG23	ASN_331@HD22	ASN_331@ND2	2	0.0002	2.8467	141.4274
PHE_45@HD2	LEU_333@HD21	LEU_333@CD2	2	0.0002	2.9687	139.6829
LYS_46@HE2	LEU_458@HD23	LEU_458@CD2	2	0.0002	2.9387	146.6443
LYS_46@HE2	LEU_458@HD21	LEU_458@CD2	2	0.0002	2.7458	137.1877
LYS_46@HE2	LEU_458@HD11	LEU_458@CD1	2	0.0002	2.9296	146.5164
LYS_46@HE3	LEU_333@HD12	LEU_333@CD1	2	0.0002	2.9412	138.3178
LYS_46@HE3	ALA_330@HB2	ALA_330@CB	2	0.0002	2.9441	149.8472
LYS_46@HE3	ASN_331@HB2	ASN_331@CB	2	0.0002	2.9134	137.7690
LYS_46@HZ2	ALA_330@HB2	ALA_330@CB	2	0.0002	2.9819	141.4861
LYS_46@HZ3	ASN_331@HD21	ASN_331@ND2	2	0.0002	2.8955	135.7215
TYR_48@HA	SER_457@HB2	SER_457@CB	2	0.0002	2.8856	161.8446
GLY_49@H	GLY_463@HA3	GLY_463@CA	2	0.0002	2.8618	141.5107
GLY_49@O	GLN_464@HE21	GLN_464@NE2	2	0.0002	2.9384	156.2133
VAL_50@HG11	GLN_464@HE22	GLN_464@NE2	2	0.0002	2.8776	138.0050
THR_53@HG21	ALA_428@HA	ALA_428@CA	2	0.0002	2.9674	152.8077
THR_53@HG23	PRO_430@HD3	PRO_430@CD	2	0.0002	2.9388	140.8045
LYS_54@HG3	ASN_427@HD21	ASN_427@ND2	2	0.0002	2.8590	138.5783
LEU_58@HD23	GLN_464@HE22	GLN_464@NE2	2	0.0002	2.7358	151.5236
VAL_75@HG23	ASN_331@HD21	ASN_331@ND2	2	0.0002	2.8915	135.5893
ARG_76@N	ASN_331@HD21	ASN_331@ND2	2	0.0002	2.9704	141.4923
THR_83@HG21	THR_471@HG23	THR_471@CG2	2	0.0002	2.9676	137.3224
THR_83@HG22	THR_471@HG23	THR_471@CG2	2	0.0002	2.9816	140.8253
THR_83@HG22	THR_542@HG23	THR_542@CG2	2	0.0002	2.9613	139.3829
THR_83@HG22	THR_471@HG22	THR_471@CG2	2	0.0002	2.9374	141.6886
THR_83@HG23	THR_542@HG22	THR_542@CG2	2	0.0002	2.9353	142.3712
THR_83@HG23	THR_471@HG22	THR_471@CG2	2	0.0002	2.9521	140.6101
THR_83@OG1	LYS_540@HZ2	LYS_540@NZ	2	0.0002	2.8369	157.4676
THR_83@OG1	LYS_540@HZ3	LYS_540@NZ	2	0.0002	2.9041	159.3562
THR_83@HG1	THR_542@HG23	THR_542@CG2	2	0.0002	2.9745	150.4222
THR_83@HG1	LYS_540@HE2	LYS_540@CE	2	0.0002	2.9156	142.3807
ASP_95@HB3	PRO_466@HG3	PRO_466@CG	2	0.0002	2.9722	139.6324
ASP_95@HB3	PRO_466@HA	PRO_466@CA	2	0.0002	2.9771	142.0372
ASP_96@HA	PRO_466@HD3	PRO_466@CD	2	0.0002	2.9717	146.8923
ASP_96@HB2	LYS_465@HA	LYS_465@CA	2	0.0002	2.9962	141.2575
THR_98@HG21	GLN_464@HG3	GLN_464@CG	2	0.0002	2.9495	138.5911
THR_98@HG1	GLN_464@HE22	GLN_464@NE2	2	0.0002	2.8643	156.7691
SER_127@HA	VAL_475@HG12	VAL_475@CG1	2	0.0002	2.9387	143.3622
ASN_128@HD21	VAL_475@HG23	VAL_475@CG2	2	0.0002	2.8853	150.9022
THR_168@HB	GLN_316@HB3	GLN_316@CB	2	0.0002	2.9684	140.1896
THR_168@HG21	GLN_316@HB2	GLN_316@CB	2	0.0002	2.9744	140.2517
GLY_170@HA2	GLN_316@HE22	GLN_316@NE2	2	0.0002	2.8059	137.4304
GLY_170@HA2	LEU_319@HG	LEU_319@CG	2	0.0002	2.9411	139.0613
GLY_170@HA3	LEU_319@HD23	LEU_319@CD2	2	0.0002	2.9726	135.2089
VAL_171@H	LEU_319@HD12	LEU_319@CD1	2	0.0002	2.6615	141.9125
VAL_171@HB	LEU_319@HD22	LEU_319@CD2	2	0.0002	2.9618	136.7078
VAL_171@HG12	ASN_314@HD21	ASN_314@ND2	2	0.0002	2.8618	143.9082
VAL_171@HG21	CYX_318@H	CYX_318@N	2	0.0002	2.9434	161.2385
VAL_171@HG21	GLU_317@HG3	GLU_317@CG	2	0.0002	2.9635	143.0767
VAL_171@HG22	LEU_319@HD22	LEU_319@CD2	2	0.0002	2.9772	144.0090
VAL_171@HG22	GLU_317@HB2	GLU_317@CB	2	0.0002	2.9806	137.6464
TYR_37@HE1	LEU_333@HD12	LEU_333@CD1	1	0.0001	2.9648	137.3845
TYR_37@HE1	LEU_333@HD23	LEU_333@CD2	1	0.0001	2.9672	138.1247
TYR_37@HE1	LEU_333@HD13	LEU_333@CD1	1	0.0001	2.9794	140.4609
TYR_37@HH	TYR_429@HE2	TYR_429@CE2	1	0.0001	2.9331	137.3926
TYR_37@HH	ALA_428@HB2	ALA_428@CB	1	0.0001	2.9440	136.7401
ASN_38@OD1	SER_431@HG	SER_431@OG	1	0.0001	2.7188	147.8825
ALA_40@HB1	LEU_333@HG	LEU_333@CG	1	0.0001	2.9862	135.5188
ALA_40@HB1	LEU_333@HD13	LEU_333@CD1	1	0.0001	2.9797	138.7059
ALA_40@HB2	LEU_333@HB3	LEU_333@CB	1	0.0001	2.9907	149.4344

ALA_40@HB3	LEU_333@HB3	LEU_333@CB	1	0.0001	2.9598	157.0938
ALA_40@HB3	LEU_333@HD13	LEU_333@CD1	1	0.0001	2.9147	139.9927
ALA_40@HB3	ASP_334@HB2	ASP_334@CB	1	0.0001	2.9748	135.7778
PHE_42@HZ	LEU_333@HB3	LEU_333@CB	1	0.0001	2.9785	136.9596
PHE_43@HD2	ASP_334@HB2	ASP_334@CB	1	0.0001	2.9364	135.6634
THR_44@HA	LEU_333@HG	LEU_333@CG	1	0.0001	2.9934	146.1419
THR_44@HA	LEU_333@HD22	LEU_333@CD2	1	0.0001	2.9958	143.7828
THR_44@HA	LEU_333@HD13	LEU_333@CD1	1	0.0001	2.9351	135.7224
THR_44@HG22	SER_332@HB2	SER_332@CB	1	0.0001	2.9745	141.7555
THR_44@OG1	LEU_333@H	LEU_333@N	1	0.0001	2.7881	146.3879
PHE_45@H	SER_332@HA	SER_332@CA	1	0.0001	2.9849	136.8934
PHE_45@HB3	LEU_333@HD13	LEU_333@CD1	1	0.0001	2.9205	148.2838
PHE_45@HB3	LEU_333@HB3	LEU_333@CB	1	0.0001	2.9753	153.7883
PHE_45@HD2	LEU_333@HB2	LEU_333@CB	1	0.0001	2.9364	136.5219
PHE_45@HD2	LEU_333@HD13	LEU_333@CD1	1	0.0001	2.9419	139.9597
PHE_45@HD2	LEU_333@HG	LEU_333@CG	1	0.0001	2.9989	147.2695
PHE_45@HD2	LEU_333@HD12	LEU_333@CD1	1	0.0001	2.8739	139.5222
LYS_46@HA	LEU_458@HD23	LEU_458@CD2	1	0.0001	2.9302	135.4242
LYS_46@HG2	LEU_333@HD13	LEU_333@CD1	1	0.0001	2.9746	138.0879
LYS_46@HG2	LEU_458@HD22	LEU_458@CD2	1	0.0001	2.9683	137.3943
LYS_46@HG2	LEU_458@HD23	LEU_458@CD2	1	0.0001	2.9566	168.4511
LYS_46@HG3	LEU_333@HD13	LEU_333@CD1	1	0.0001	2.9314	144.4297
LYS_46@HG3	LEU_333@HD12	LEU_333@CD1	1	0.0001	2.9499	152.4369
LYS_46@HD2	SER_457@HG	SER_457@OG	1	0.0001	2.8522	141.8805
LYS_46@HD3	ASN_331@HA	ASN_331@CA	1	0.0001	2.9017	152.1153
LYS_46@HE2	LEU_333@HD13	LEU_333@CD1	1	0.0001	2.9798	159.8868
LYS_46@HE2	LEU_458@HG	LEU_458@CG	1	0.0001	2.9662	142.7082
LYS_46@HE2	LEU_455@HD22	LEU_455@CD2	1	0.0001	2.9303	136.8720
LYS_46@HE2	LEU_333@HD11	LEU_333@CD1	1	0.0001	2.7842	168.6144
LYS_46@HE3	LEU_333@HD21	LEU_333@CD2	1	0.0001	2.9905	164.6514
LYS_46@HE3	SER_457@HG	SER_457@OG	1	0.0001	2.9180	139.6412
LYS_46@HE3	LEU_333@HD13	LEU_333@CD1	1	0.0001	2.9686	137.4369
LYS_46@HZ1	ALA_330@HB3	ALA_330@CB	1	0.0001	2.9635	151.4177
LYS_46@HZ1	ASN_331@HA	ASN_331@CA	1	0.0001	2.9639	148.9968
LYS_46@HZ2	SER_457@HG	SER_457@OG	1	0.0001	2.8841	167.0234
TYR_48@CE2	SER_457@HG	SER_457@OG	1	0.0001	2.9051	141.5949
GLY_49@HA2	GLN_464@HA	GLN_464@CA	1	0.0001	2.8521	137.8046
GLY_49@HA3	GLN_464@HG3	GLN_464@CG	1	0.0001	2.8982	138.4884
SER_51@HA	ASN_427@HD21	ASN_427@ND2	1	0.0001	2.9654	140.5230
SER_51@HB3	ALA_428@HA	ALA_428@CA	1	0.0001	2.9170	143.6892
SER_51@HB3	ALA_428@HB3	ALA_428@CB	1	0.0001	2.8722	135.5885
SER_51@HG	LYS_424@HE2	LYS_424@CE	1	0.0001	2.9222	138.6796
PRO_52@HD2	ALA_428@HA	ALA_428@CA	1	0.0001	2.9483	152.8967
PRO_52@HG2	LEU_458@HD22	LEU_458@CD2	1	0.0001	2.9749	140.6132
PRO_52@HG2	ALA_428@HA	ALA_428@CA	1	0.0001	2.9783	159.2989
PRO_52@HG3	LEU_458@HD22	LEU_458@CD2	1	0.0001	2.9842	145.1514
THR_53@HG21	ASN_427@HA	ASN_427@CA	1	0.0001	2.8952	136.0815
THR_53@HG21	PRO_430@HG2	PRO_430@CG	1	0.0001	2.9392	136.7409
THR_53@HG21	PRO_430@HD2	PRO_430@CD	1	0.0001	2.9894	140.3941
THR_53@HG22	ASN_427@HD21	ASN_427@ND2	1	0.0001	2.8351	140.6144
THR_53@HG22	PRO_430@HD3	PRO_430@CD	1	0.0001	2.9827	137.9776
THR_53@HG22	PRO_430@HG2	PRO_430@CG	1	0.0001	2.9555	136.7280
THR_53@HG22	PRO_430@HG3	PRO_430@CG	1	0.0001	2.9724	143.8391
THR_53@HG22	PRO_430@HB3	PRO_430@CB	1	0.0001	2.9917	135.7267
THR_53@HG23	PRO_430@HG2	PRO_430@CG	1	0.0001	2.9654	139.3097
THR_53@HG23	PRO_430@HG3	PRO_430@CG	1	0.0001	2.9741	148.1172
LYS_54@HB2	ASN_427@HD22	ASN_427@ND2	1	0.0001	2.6934	135.5353
LYS_54@HG3	ASN_427@HA	ASN_427@CA	1	0.0001	2.9815	139.6927
LYS_54@HZ1	ASN_427@HA	ASN_427@CA	1	0.0001	2.8751	140.9215
LYS_54@HZ1	PRO_430@HB3	PRO_430@CB	1	0.0001	2.9282	143.6974
LYS_54@HZ2	ASN_427@HA	ASN_427@CA	1	0.0001	2.8187	147.6891
LYS_54@O	ASN_427@HD21	ASN_427@ND2	1	0.0001	2.8946	170.2383
LEU_58@HG	GLN_464@HE21	GLN_464@NE2	1	0.0001	2.9719	154.8589

PHE_60@HE1	GLN_464@HE21	GLN_464@NE2	1	0.0001	2.9861	151.3496
PHE_60@HZ	GLN_464@HE21	GLN_464@NE2	1	0.0001	2.8920	146.1020
VAL_75@HG21	ASN_331@HD22	ASN_331@ND2	1	0.0001	2.8755	135.7619
ARG_76@HD3	GLU_327@HG3	GLU_327@CG	1	0.0001	2.7997	143.1146
ARG_76@HH12	LYS_540@HE3	LYS_540@CE	1	0.0001	2.9050	140.6078
ARG_76@HH12	PRO_323@HG3	PRO_323@CG	1	0.0001	2.7592	139.3505
ARG_76@HH22	PRO_323@HB3	PRO_323@CB	1	0.0001	2.9824	164.3534
THR_83@HG21	THR_471@HG1	THR_471@OG1	1	0.0001	2.4382	139.8677
THR_83@HG21	VAL_475@HG11	VAL_475@CG1	1	0.0001	2.9727	135.5504
THR_83@HG21	VAL_475@HG12	VAL_475@CG1	1	0.0001	2.9594	139.2657
THR_83@HG21	THR_542@HG21	THR_542@CG2	1	0.0001	2.9585	135.4838
THR_83@HG21	THR_542@HG22	THR_542@CG2	1	0.0001	2.9486	145.0200
THR_83@HG22	THR_542@HG21	THR_542@CG2	1	0.0001	2.8995	147.6632
THR_83@HG22	VAL_475@HG11	VAL_475@CG1	1	0.0001	2.9992	137.5217
THR_83@HG22	VAL_475@HG12	VAL_475@CG1	1	0.0001	2.9737	143.4581
THR_83@HG22	THR_542@HB	THR_542@CB	1	0.0001	2.9291	144.3668
THR_83@HG23	THR_542@HG23	THR_542@CG2	1	0.0001	2.9692	140.1232
THR_83@HG23	THR_542@HG21	THR_542@CG2	1	0.0001	2.9787	140.2887
THR_83@HG23	THR_542@HB	THR_542@CB	1	0.0001	2.8903	138.5073
THR_83@HG23	VAL_475@HG13	VAL_475@CG1	1	0.0001	2.9079	140.3901
THR_83@OG1	LYS_540@HZ1	LYS_540@NZ	1	0.0001	2.9826	135.3224
GLY_84@HA2	LYS_540@HE2	LYS_540@CE	1	0.0001	2.9488	136.1417
ASP_96@HA	PRO_466@HG3	PRO_466@CG	1	0.0001	2.9154	146.4614
THR_98@HG21	GLN_464@HE21	GLN_464@NE2	1	0.0001	2.7756	147.0057
THR_98@HG22	GLN_464@HE21	GLN_464@NE2	1	0.0001	2.9811	139.1968
THR_98@HG22	GLN_464@HG3	GLN_464@CG	1	0.0001	2.9602	142.3728
THR_98@HG23	GLN_464@HB3	GLN_464@CB	1	0.0001	2.9984	139.0967
THR_98@HG23	GLN_464@HE21	GLN_464@NE2	1	0.0001	2.8322	142.8154
THR_98@HG1	GLN_464@HG2	GLN_464@CG	1	0.0001	2.9270	171.4679
THR_98@HG1	GLN_464@HA	GLN_464@CA	1	0.0001	2.9992	153.9134
ASN_107@HD21	GLN_316@HE21	GLN_316@NE2	1	0.0001	2.9136	137.8111
ASN_128@H	VAL_475@HG22	VAL_475@CG2	1	0.0001	2.9616	152.9822
ASN_128@HD22	VAL_475@HB	VAL_475@CB	1	0.0001	2.8959	144.1667
PRO_167@HB2	ASN_314@HD21	ASN_314@ND2	1	0.0001	2.7986	140.5038
THR_168@HA	GLN_316@HB2	GLN_316@CB	1	0.0001	2.9403	139.4214
THR_168@HA	GLU_317@HA	GLU_317@CA	1	0.0001	2.9435	137.7498
THR_168@HA	GLN_316@HG3	GLN_316@CG	1	0.0001	2.8378	138.4911
THR_168@HB	GLN_316@HE21	GLN_316@NE2	1	0.0001	2.8872	135.1611
THR_168@HB	GLN_316@HG3	GLN_316@CG	1	0.0001	2.9787	136.8055
THR_168@HG22	GLN_316@HE21	GLN_316@NE2	1	0.0001	2.9334	136.7724
THR_168@HG22	PRO_315@HG2	PRO_315@CG	1	0.0001	2.9203	138.3521
THR_168@HG23	GLN_316@HE21	GLN_316@NE2	1	0.0001	2.6852	150.7765
GLY_170@HA2	GLN_316@HG2	GLN_316@CG	1	0.0001	2.9997	149.5428
GLY_170@HA2	GLN_316@HG3	GLN_316@CG	1	0.0001	2.9793	136.0356
GLY_170@HA3	GLU_317@HG3	GLU_317@CG	1	0.0001	2.9946	136.3562
VAL_171@H	GLU_317@HA	GLU_317@CA	1	0.0001	2.9628	143.2312
VAL_171@HB	GLY_324@HA2	GLY_324@CA	1	0.0001	2.9909	146.1447
VAL_171@HB	GLU_317@HG2	GLU_317@CG	1	0.0001	2.9912	150.7051
VAL_171@HB	LEU_319@HD23	LEU_319@CD2	1	0.0001	2.9684	137.6138
VAL_171@HG11	LEU_319@HD23	LEU_319@CD2	1	0.0001	2.9770	145.2273
VAL_171@HG11	LEU_319@HD21	LEU_319@CD2	1	0.0001	2.9855	136.5819
VAL_171@HG11	GLU_327@HG3	GLU_327@CG	1	0.0001	2.9389	137.5658
VAL_171@HG12	GLY_324@HA2	GLY_324@CA	1	0.0001	2.7961	138.8938
VAL_171@HG12	GLN_316@HB2	GLN_316@CB	1	0.0001	2.9489	135.8571
VAL_171@HG12	LEU_319@HG	LEU_319@CG	1	0.0001	2.9983	139.0094
VAL_171@HG13	LEU_319@HD21	LEU_319@CD2	1	0.0001	2.9826	151.0507
VAL_171@HG13	GLU_327@HB3	GLU_327@CB	1	0.0001	2.9727	135.4407
VAL_171@HG13	GLY_324@HA2	GLY_324@CA	1	0.0001	2.9366	139.1409
VAL_171@HG21	LEU_319@HD11	LEU_319@CD1	1	0.0001	2.9891	137.0496
VAL_171@HG21	GLU_317@HB3	GLU_317@CB	1	0.0001	2.9837	137.9926
VAL_171@HG21	LEU_319@HG	LEU_319@CG	1	0.0001	2.9139	137.8275
VAL_171@HG22	LEU_319@HD11	LEU_319@CD1	1	0.0001	2.9481	161.4359
VAL_171@HG22	GLU_317@HG2	GLU_317@CG	1	0.0001	2.9615	137.2463

VAL_171@HG22	GLU_317@HB3	GLU_317@CB	1	0.0001	2.9970	136.7952
VAL_171@HG23	LEU_319@HD12	LEU_319@CD1	1	0.0001	2.9726	137.7852
VAL_171@HG23	GLU_317@HB3	GLU_317@CB	1	0.0001	2.9897	145.3844
VAL_171@HG23	LEU_319@HD11	LEU_319@CD1	1	0.0001	2.8481	138.0276
VAL_171@HG23	LEU_319@HD13	LEU_319@CD1	1	0.0001	2.9879	139.8146
VAL_171@HG23	LEU_319@HD22	LEU_319@CD2	1	0.0001	2.8118	135.2234
VAL_171@HG23	LEU_319@HD21	LEU_319@CD2	1	0.0001	2.9492	136.5100
GLY_172@H	GLY_324@HA2	GLY_324@CA	1	0.0001	2.8535	167.9849
GLY_172@HA3	PRO_323@HG2	PRO_323@CG	1	0.0001	2.9825	158.7646
GLN_174@NE2	GLN_316@HE22	GLN_316@NE2	1	0.0001	2.8782	171.6912
GLN_174@HE21	GLN_316@HB2	GLN_316@CB	1	0.0001	2.9637	135.6771
GLN_174@HE21	GLN_316@HB3	GLN_316@CB	1	0.0001	2.9932	136.3368
GLN_174@HE21	GLN_316@HE22	GLN_316@NE2	1	0.0001	2.8226	145.0130

Table S2. Hydrogen bond analysis of S protein (BA.1)-ACE2 complex during the last 20 ns of MD simulation with S protein as donor and ACE2 as acceptor.

#Acceptor	DonorH	Donor	Frames	Frac	AvgDist	AvgAng
GLU_327@OE1	ARG_76@HH11	ARG_76@NH1	7025	0.7025	2.7958	161.2338
GLU_327@OE2	ARG_76@HE	ARG_76@NE	6838	0.6838	2.8227	161.2765
ASN_331@O	PHE_45@H	PHE_45@N	5423	0.5423	2.8656	158.1682
ASN_427@O	THR_53@HG1	THR_53@OG1	4837	0.4837	2.7391	161.9292
ASN_427@OD1	SER_51@HG	SER_51@OG	2479	0.2479	2.7516	160.3904
ASN_331@O	THR_44@HG1	THR_44@OG1	1381	0.1381	2.7299	162.9640
GLN_316@O	VAL_171@H	VAL_171@N	1161	0.1161	2.9052	160.6858
GLU_327@OE2	ARG_76@HH11	ARG_76@NH1	875	0.0875	2.8355	150.6311
GLU_317@OE1	GLN_174@HE21	GLN_174@NE2	833	0.0833	2.8346	160.3588
ASN_427@O	SER_51@HG	SER_51@OG	813	0.0813	2.7699	158.3964
GLU_317@OE2	GLN_174@HE21	GLN_174@NE2	613	0.0613	2.8321	160.4130
ASN_331@OD1	LYS_46@HZ1	LYS_46@NZ	566	0.0566	2.8251	153.3407
GLU_327@OE1	ARG_76@HE	ARG_76@NE	546	0.0546	2.8737	150.8037
ASN_331@OD1	LYS_46@HZ2	LYS_46@NZ	439	0.0439	2.8292	152.0606
ASN_331@OD1	LYS_46@HZ3	LYS_46@NZ	423	0.0423	2.8211	153.1969
GLU_317@HG2	VAL_171@H	VAL_171@N	373	0.0373	2.8540	156.5184
ASN_331@HA	LYS_46@HE3	LYS_46@CE	325	0.0325	2.8989	147.7269
ALA_428@O	THR_53@HG1	THR_53@OG1	300	0.0300	2.7931	158.4839
GLU_327@OE2	ARG_76@HH21	ARG_76@NH2	269	0.0269	2.8163	157.2369
ALA_330@O	LYS_46@HZ2	LYS_46@NZ	215	0.0215	2.8361	152.8299
ALA_330@O	LYS_46@HZ1	LYS_46@NZ	215	0.0215	2.8409	153.4074
ASN_427@OD1	THR_53@HG1	THR_53@OG1	193	0.0193	2.7568	157.1427
ALA_330@O	LYS_46@HZ3	LYS_46@NZ	192	0.0192	2.8427	151.0891
PRO_466@HD3	ASP_96@HB3	ASP_96@CB	154	0.0154	2.9328	140.5884
GLN_316@HB3	GLY_170@HA2	GLY_170@CA	135	0.0135	2.9417	146.5182
GLN_316@HE22	GLN_174@HE22	GLN_174@NE2	135	0.0135	2.8863	141.7449
LEU_333@HD11	PHE_45@H	PHE_45@N	115	0.0115	2.8022	151.1491
LEU_333@HD13	PHE_45@H	PHE_45@N	106	0.0106	2.7901	150.7829
ASN_331@HD21	ARG_76@HB3	ARG_76@CB	91	0.0091	2.8072	147.0750
ASP_472@OD1	LYS_130@HZ2	LYS_130@NZ	91	0.0091	2.8227	158.8880
SER_457@OG	LYS_46@HZ1	LYS_46@NZ	90	0.0090	2.8950	157.0052
LEU_333@HD12	PHE_45@H	PHE_45@N	83	0.0083	2.8029	151.9859
GLY_463@HA3	GLY_49@HA2	GLY_49@CA	82	0.0082	2.9389	146.3336
LEU_333@HD21	PHE_45@H	PHE_45@N	80	0.0080	2.8444	155.0599
ASN_331@HB3	THR_44@HB	THR_44@CB	75	0.0075	2.9383	139.8947
GLN_316@OE1	GLY_170@H	GLY_170@N	72	0.0072	2.8642	152.2153
ASN_427@OD1	LYS_54@HZ2	LYS_54@NZ	72	0.0072	2.8145	155.5906
GLU_327@OE1	ARG_76@HH21	ARG_76@NH2	71	0.0071	2.7995	152.8337
GLN_316@OE1	GLN_174@HE21	GLN_174@NE2	66	0.0066	2.8425	149.1729
SER_457@OG	LYS_46@HZ2	LYS_46@NZ	63	0.0063	2.8702	149.8814
LEU_333@HD22	PHE_45@H	PHE_45@N	59	0.0059	2.8145	154.1179
ASP_476@OD1	LYS_130@HZ2	LYS_130@NZ	59	0.0059	2.7653	158.4283
LEU_333@HB2	PHE_45@HB3	PHE_45@CB	53	0.0053	2.9425	143.5890
SER_457@OG	LYS_46@HZ3	LYS_46@NZ	53	0.0053	2.8910	151.9508
LEU_333@HD23	PHE_45@H	PHE_45@N	52	0.0052	2.8672	151.4475
ASN_427@OD1	LYS_54@HZ3	LYS_54@NZ	48	0.0048	2.8142	157.7675

ASP_472@OD1	LYS_130@HZ1	LYS_130@NZ	46	0.0046	2.8467	154.4640
ASN_427@OD1	LYS_54@HZ1	LYS_54@NZ	45	0.0045	2.7991	153.8497
LEU_333@HG	PHE_42@HE1	PHE_42@CE1	43	0.0043	2.9516	143.5770
ALA_428@O	TYR_37@HH	TYR_37@OH	40	0.0040	2.8183	148.7259
PRO_466@HB3	ASP_96@HB3	ASP_96@CB	37	0.0037	2.9623	144.0466
GLU_317@OE2	ASN_107@HD21	ASN_107@ND2	35	0.0035	2.8222	153.9614
LEU_319@HD21	VAL_171@H	VAL_171@N	33	0.0033	2.8150	155.9262
ASN_331@HD21	VAL_75@HG13	VAL_75@CG1	30	0.0030	2.8500	141.7809
ASN_427@HD21	SER_51@HB2	SER_51@CB	27	0.0027	2.8696	144.2883
GLN_464@HG2	GLY_49@HA3	GLY_49@CA	27	0.0027	2.9393	139.4896
GLU_327@OE1	TYR_176@HH	TYR_176@OH	24	0.0024	2.6819	166.5290
ASN_427@HD21	SER_51@HG	SER_51@OG	24	0.0024	2.8665	143.9469
VAL_475@HG11	ASN_128@HD21	ASN_128@ND2	23	0.0023	2.7923	144.4682
GLU_317@HA	VAL_171@HG22	VAL_171@CG2	22	0.0022	2.9200	140.3879
ALA_428@HA	THR_53@HG1	THR_53@OG1	22	0.0022	2.7893	142.2342
ASP_472@OD2	LYS_130@HZ2	LYS_130@NZ	22	0.0022	2.7822	152.3050
ASP_472@OD2	ASN_128@HD22	ASN_128@ND2	22	0.0022	2.8082	161.9079
GLU_317@OE1	VAL_171@H	VAL_171@N	21	0.0021	2.8815	155.7281
ASN_331@HB2	LYS_46@HE3	LYS_46@CE	20	0.0020	2.9421	147.0610
VAL_475@HG11	ASN_128@HD22	ASN_128@ND2	20	0.0020	2.8522	141.5941
ASN_331@OD1	LYS_46@HE3	LYS_46@CE	19	0.0019	2.9591	141.7372
PRO_466@HG3	ASP_96@HB3	ASP_96@CB	19	0.0019	2.9493	142.0084
GLN_316@HB3	GLY_170@HA3	GLY_170@CA	18	0.0018	2.9303	138.8393
LEU_319@HG	VAL_171@H	VAL_171@N	17	0.0017	2.8774	158.7462
ASP_472@OD1	LYS_130@HZ3	LYS_130@NZ	17	0.0017	2.8136	164.4650
SER_457@HG	LYS_46@HZ1	LYS_46@NZ	16	0.0016	2.8916	146.0712
GLU_317@HA	VAL_171@HG23	VAL_171@CG2	15	0.0015	2.9379	142.0943
LEU_319@HD22	VAL_171@H	VAL_171@N	15	0.0015	2.8976	152.3946
LEU_333@HB3	PHE_42@HE1	PHE_42@CE1	15	0.0015	2.9549	148.5371
LEU_333@HD13	PHE_42@HE1	PHE_42@CE1	15	0.0015	2.9549	140.0400
PRO_466@HB3	ASP_95@HB3	ASP_95@CB	15	0.0015	2.9671	140.5245
LEU_333@HD11	PHE_42@HE1	PHE_42@CE1	14	0.0014	2.9686	141.6854
THR_542@HG21	THR_83@HG1	THR_83@OG1	14	0.0014	2.7721	143.6129
GLU_317@HA	VAL_171@HG21	VAL_171@CG2	13	0.0013	2.9686	145.2795
LEU_319@HD23	VAL_171@H	VAL_171@N	13	0.0013	2.8840	149.6015
SER_457@HB3	TYR_48@HE2	TYR_48@CE2	13	0.0013	2.9503	139.4367
GLN_464@HE21	LEU_58@HD23	LEU_58@CD2	13	0.0013	2.8596	144.8933
ASP_476@OD2	LYS_130@HZ1	LYS_130@NZ	13	0.0013	2.7489	157.2656
ASN_331@HA	LYS_46@HD2	LYS_46@CD	12	0.0012	2.9342	139.8101
ASN_331@HD21	VAL_75@HG11	VAL_75@CG1	12	0.0012	2.8643	140.1737
ASN_427@OD1	THR_53@H	THR_53@N	12	0.0012	2.9111	148.2271
VAL_475@HG12	ASN_128@H	ASN_128@N	12	0.0012	2.7510	144.8835
VAL_475@HG23	ASN_128@HD22	ASN_128@ND2	12	0.0012	2.8926	142.5556
THR_542@HG23	THR_83@HG1	THR_83@OG1	12	0.0012	2.8627	142.9646
ASN_331@HA	LYS_46@HG3	LYS_46@CG	11	0.0011	2.9640	143.6499
LEU_333@HD21	PHE_42@HZ	PHE_42@CZ	11	0.0011	2.9232	141.5742
LEU_333@HD21	PHE_42@HE1	PHE_42@CE1	11	0.0011	2.9527	139.5030
LEU_333@HD22	TYR_37@HE1	TYR_37@CE1	11	0.0011	2.9652	141.9861
ALA_428@HA	THR_53@HB	THR_53@CB	11	0.0011	2.9593	144.4574
SER_457@HB3	TYR_48@HD2	TYR_48@CD2	11	0.0011	2.9123	138.4276
ASN_467@H	ASP_95@HB3	ASP_95@CB	11	0.0011	2.8942	147.5456
VAL_475@HG13	ASN_128@HD21	ASN_128@ND2	11	0.0011	2.8366	144.7026
GLU_317@OE2	VAL_171@H	VAL_171@N	10	0.0010	2.9263	156.8533
ASN_331@HA	LYS_46@HE2	LYS_46@CE	10	0.0010	2.9121	145.1363
LEU_333@HB2	PHE_42@HE1	PHE_42@CE1	10	0.0010	2.9658	143.0629
LEU_333@HD22	PHE_45@HB3	PHE_45@CB	10	0.0010	2.9496	139.9733
LEU_333@HD23	PHE_42@HE1	PHE_42@CE1	10	0.0010	2.9506	138.0161
MET_426@O	LYS_54@HZ1	LYS_54@NZ	10	0.0010	2.8714	158.8839
PRO_466@HA	ASP_96@HB3	ASP_96@CB	10	0.0010	2.9614	146.7698
ASN_467@HD22	GLY_81@HA3	GLY_81@CA	10	0.0010	2.9210	145.4292
VAL_475@HG21	ASN_128@HD22	ASN_128@ND2	10	0.0010	2.9064	141.0225
VAL_541@O	THR_83@HG1	THR_83@OG1	10	0.0010	2.8889	151.7120
GLU_317@HG3	VAL_171@HG22	VAL_171@CG2	9	0.0009	2.9282	139.0174

ASN_331@HB3	THR_44@HG22	THR_44@CG2	9	0.0009	2.9379	141.1840
LEU_333@HD21	TYR_37@HH	TYR_37@OH	9	0.0009	2.7718	143.6960
LEU_333@HD23	PHE_45@HD2	PHE_45@CD2	9	0.0009	2.9382	139.0296
LEU_333@HD23	PHE_42@HZ	PHE_42@CZ	9	0.0009	2.9652	137.8583
LEU_333@HD23	TYR_37@HH	TYR_37@OH	9	0.0009	2.8406	142.3651
GLY_463@O	GLY_49@H	GLY_49@N	9	0.0009	2.9046	143.2821
VAL_475@HG22	ASN_128@HD22	ASN_128@ND2	9	0.0009	2.8975	148.2841
THR_542@HB	THR_83@HG1	THR_83@OG1	9	0.0009	2.8553	140.6088
ASN_314@HD21	VAL_171@HG13	VAL_171@CG1	8	0.0008	2.8246	143.2261
ASN_314@HD21	THR_168@HA	THR_168@CA	8	0.0008	2.8626	143.1758
GLN_316@HA	GLY_170@HA2	GLY_170@CA	8	0.0008	2.9586	144.5592
GLU_317@HA	VAL_171@HG13	VAL_171@CG1	8	0.0008	2.9202	140.8048
GLU_317@HG2	VAL_171@HG11	VAL_171@CG1	8	0.0008	2.9450	140.9028
GLU_317@HG3	VAL_171@HG23	VAL_171@CG2	8	0.0008	2.9301	139.5145
ALA_330@HB1	LYS_46@HZ2	LYS_46@NZ	8	0.0008	2.8651	142.0463
LEU_333@HD12	PHE_42@HE1	PHE_42@CE1	8	0.0008	2.9406	141.2320
PRO_430@HD3	THR_53@HG21	THR_53@CG2	8	0.0008	2.9463	144.1314
PRO_430@HG3	LYS_54@HE3	LYS_54@CE	8	0.0008	2.9057	150.8304
SER_457@HB2	TYR_48@HE2	TYR_48@CE2	8	0.0008	2.9588	142.6388
SER_457@HG	LYS_46@HZ3	LYS_46@NZ	8	0.0008	2.9127	147.3033
SER_457@HG	LYS_46@HZ2	LYS_46@NZ	8	0.0008	2.9246	149.1477
SER_457@HG	LYS_46@HE3	LYS_46@CE	8	0.0008	2.9031	141.0235
GLN_464@HE21	LEU_58@HD22	LEU_58@CD2	8	0.0008	2.8846	156.0419
ASP_472@OD2	LYS_130@HZ1	LYS_130@NZ	8	0.0008	2.8264	146.5028
ASN_331@HD21	LYS_46@HZ2	LYS_46@NZ	7	0.0007	2.9559	150.9037
ASN_331@HD22	THR_44@HG21	THR_44@CG2	7	0.0007	2.9109	139.2347
SER_332@HA	THR_44@HG23	THR_44@CG2	7	0.0007	2.9165	139.3240
LEU_333@HG	PHE_45@HB3	PHE_45@CB	7	0.0007	2.9715	139.6221
LEU_333@HD12	TYR_37@HH	TYR_37@OH	7	0.0007	2.8795	151.2013
LEU_333@HD21	PHE_45@HB3	PHE_45@CB	7	0.0007	2.9544	143.3989
LEU_333@HD21	TYR_37@HE1	TYR_37@CE1	7	0.0007	2.9725	144.5085
SER_457@HB2	LYS_46@HE3	LYS_46@CE	7	0.0007	2.8970	140.4548
SER_457@HG	TYR_48@HE2	TYR_48@CE2	7	0.0007	2.9021	141.5687
GLN_464@HE21	LEU_185@HD21	LEU_185@CD2	7	0.0007	2.8426	150.5971
GLN_464@HE21	LEU_58@HD13	LEU_58@CD1	7	0.0007	2.9383	150.1807
VAL_475@HG13	ASN_128@HD22	ASN_128@ND2	7	0.0007	2.8132	145.3354
ASP_476@OD1	LYS_130@HZ1	LYS_130@NZ	7	0.0007	2.7908	151.7691
THR_542@HG22	THR_83@HG1	THR_83@OG1	7	0.0007	2.7876	143.4959
GLN_316@HE21	THR_168@HA	THR_168@CA	6	0.0006	2.9322	143.4938
GLU_317@HG2	VAL_171@HG21	VAL_171@CG2	6	0.0006	2.9454	142.5419
GLU_317@HG2	VAL_171@HG13	VAL_171@CG1	6	0.0006	2.9451	140.8673
GLU_317@HG3	VAL_171@HG21	VAL_171@CG2	6	0.0006	2.9407	138.3059
GLU_317@HG3	VAL_171@HG11	VAL_171@CG1	6	0.0006	2.9235	140.7732
ALA_330@HB1	LYS_46@HZ1	LYS_46@NZ	6	0.0006	2.8795	145.6459
ALA_330@HB3	LYS_46@HZ2	LYS_46@NZ	6	0.0006	2.9023	137.5282
ALA_330@O	LYS_46@HE2	LYS_46@CE	6	0.0006	2.9760	139.5879
ASN_331@HB3	THR_44@HG23	THR_44@CG2	6	0.0006	2.9444	140.2317
ASN_331@HD21	VAL_75@HG12	VAL_75@CG1	6	0.0006	2.8654	141.3063
ASN_331@HD22	THR_44@HG22	THR_44@CG2	6	0.0006	2.9215	142.3126
SER_332@HA	THR_44@HA	THR_44@CA	6	0.0006	2.9256	148.9829
LEU_333@HD21	THR_44@HA	THR_44@CA	6	0.0006	2.9329	149.5742
LEU_333@HD22	PHE_42@HE1	PHE_42@CE1	6	0.0006	2.9574	142.4228
ASN_427@HA	LYS_54@HD2	LYS_54@CD	6	0.0006	2.9314	145.6203
ASN_427@ND2	SER_51@HG	SER_51@OG	6	0.0006	2.8821	157.8399
GLN_464@HG3	GLY_49@HA2	GLY_49@CA	6	0.0006	2.9435	139.6093
GLN_464@OE1	THR_98@HG1	THR_98@OG1	6	0.0006	2.8238	154.0426
GLN_464@HE22	THR_98@HG23	THR_98@CG2	6	0.0006	2.8524	139.4092
GLN_464@HE22	THR_98@HG21	THR_98@CG2	6	0.0006	2.8342	145.2123
THR_471@HG22	THR_83@HG22	THR_83@CG2	6	0.0006	2.9246	138.9190
ASP_472@OD2	LYS_130@HZ3	LYS_130@NZ	6	0.0006	2.8233	156.4751
GLN_316@HB2	THR_168@HB	THR_168@CB	5	0.0005	2.9520	140.7306
GLU_317@HB2	VAL_171@HG13	VAL_171@CG1	5	0.0005	2.9659	140.8683
GLU_317@HG2	GLY_170@HA2	GLY_170@CA	5	0.0005	2.9356	144.2063

GLU_317@HG2	VAL_171@HG23	VAL_171@CG2	5	0.0005	2.9495	146.5264
GLU_317@HG3	GLY_170@HA2	GLY_170@CA	5	0.0005	2.9767	144.0980
GLU_317@HG3	VAL_171@HG13	VAL_171@CG1	5	0.0005	2.9295	141.8035
LEU_319@HD12	VAL_171@H	VAL_171@N	5	0.0005	2.7904	158.1248
ALA_330@HB2	LYS_46@HZ1	LYS_46@NZ	5	0.0005	2.8554	150.9010
ASN_331@OD1	LYS_46@HE2	LYS_46@CE	5	0.0005	2.9450	143.8856
ASN_331@HD22	THR_44@HG23	THR_44@CG2	5	0.0005	2.9161	139.2761
LEU_333@HG	PHE_45@H	PHE_45@N	5	0.0005	2.8186	144.3606
LEU_333@HD13	TYR_37@HH	TYR_37@OH	5	0.0005	2.8619	148.8638
LEU_333@HD23	THR_44@HA	THR_44@CA	5	0.0005	2.9717	148.9075
LEU_333@HD23	PHE_45@HB3	PHE_45@CB	5	0.0005	2.8927	136.7077
LEU_333@HD23	TYR_37@HE1	TYR_37@CE1	5	0.0005	2.9219	139.0531
ALA_428@HA	THR_53@HG21	THR_53@CG2	5	0.0005	2.9560	144.3660
PRO_430@HD3	THR_53@HG22	THR_53@CG2	5	0.0005	2.9395	143.2486
SER_431@HG	ASN_38@HD21	ASN_38@ND2	5	0.0005	2.9308	140.0468
SER_457@HB2	TYR_48@HA	TYR_48@CA	5	0.0005	2.8910	144.0097
SER_457@HB2	LYS_46@HD3	LYS_46@CD	5	0.0005	2.9710	151.5276
GLN_464@HE21	PHE_60@HZ	PHE_60@CZ	5	0.0005	2.9085	144.3795
GLN_464@HE21	LEU_58@HD11	LEU_58@CD1	5	0.0005	2.9237	145.0133
THR_471@HG23	THR_83@HG23	THR_83@CG2	5	0.0005	2.9571	140.8309
VAL_475@HB	ASN_128@HD21	ASN_128@ND2	5	0.0005	2.9178	140.8591
VAL_475@HG12	ASN_128@HD22	ASN_128@ND2	5	0.0005	2.8397	139.4211
THR_542@HG21	THR_83@HB	THR_83@CB	5	0.0005	2.9776	149.4458
ASP_313@OD1	LYS_108@HZ2	LYS_108@NZ	4	0.0004	2.7474	146.8814
GLN_316@HB3	THR_168@HB	THR_168@CB	4	0.0004	2.9180	139.5475
GLN_316@HB3	VAL_171@H	VAL_171@N	4	0.0004	2.9739	143.3668
GLU_317@HB2	VAL_171@HG21	VAL_171@CG2	4	0.0004	2.9612	143.6590
GLU_317@HB2	VAL_171@HG11	VAL_171@CG1	4	0.0004	2.9569	144.9168
GLU_317@HG2	VAL_171@HG12	VAL_171@CG1	4	0.0004	2.9365	140.5566
GLY_324@HA2	GLY_172@H	GLY_172@N	4	0.0004	2.9202	162.2633
ALA_330@HB2	LYS_46@HZ2	LYS_46@NZ	4	0.0004	2.8892	144.1690
ASN_331@OD1	THR_44@HG1	THR_44@OG1	4	0.0004	2.8331	154.3221
ASN_331@HD21	THR_44@HB	THR_44@CB	4	0.0004	2.9530	142.0494
SER_332@HA	THR_44@HG21	THR_44@CG2	4	0.0004	2.9517	144.0748
LEU_333@HB3	ALA_40@HB2	ALA_40@CB	4	0.0004	2.9762	144.8371
LEU_333@HD21	PHE_45@HD2	PHE_45@CD2	4	0.0004	2.9215	139.4274
ASN_427@HD21	SER_51@HB3	SER_51@CB	4	0.0004	2.9527	149.3227
PRO_430@HG3	THR_53@HG21	THR_53@CG2	4	0.0004	2.9503	140.2380
SER_431@OG	ASN_38@HD21	ASN_38@ND2	4	0.0004	2.9515	158.1391
SER_457@HG	LYS_46@HE2	LYS_46@CE	4	0.0004	2.9217	147.9416
GLN_464@HE21	LEU_58@HD21	LEU_58@CD2	4	0.0004	2.9397	148.7910
GLN_464@HE22	THR_98@HG22	THR_98@CG2	4	0.0004	2.8470	143.9283
ASN_467@HB3	GLY_81@HA3	GLY_81@CA	4	0.0004	2.9493	139.5862
THR_471@HB	THR_83@HG22	THR_83@CG2	4	0.0004	2.9191	143.3105
THR_471@HG23	THR_83@HG21	THR_83@CG2	4	0.0004	2.9805	137.7477
THR_471@HG23	THR_83@HG22	THR_83@CG2	4	0.0004	2.9887	136.4926
VAL_475@HG12	ASN_128@HD21	ASN_128@ND2	4	0.0004	2.7947	138.6200
VAL_475@HG12	SER_127@HA	SER_127@CA	4	0.0004	2.9702	143.9876
VAL_475@HG22	ASN_128@HD21	ASN_128@ND2	4	0.0004	2.8640	141.1822
ASN_314@HD21	PRO_167@HB2	PRO_167@CB	3	0.0003	2.9248	140.9630
GLN_316@HB2	THR_168@HA	THR_168@CA	3	0.0003	2.9700	139.3239
GLN_316@HE22	THR_168@HB	THR_168@CB	3	0.0003	2.8569	146.2317
GLN_316@HE22	THR_168@HA	THR_168@CA	3	0.0003	2.9490	146.3572
GLU_317@HA	VAL_171@HG11	VAL_171@CG1	3	0.0003	2.9165	142.4737
GLU_317@HG2	VAL_171@HG22	VAL_171@CG2	3	0.0003	2.8881	137.8554
LEU_319@HD21	GLY_170@HA2	GLY_170@CA	3	0.0003	2.9540	147.2932
LEU_319@HD23	VAL_171@HG11	VAL_171@CG1	3	0.0003	2.9090	142.9750
PRO_323@HB2	ARG_76@HH11	ARG_76@NH1	3	0.0003	2.9636	139.8213
ALA_330@HB1	LYS_46@HZ3	LYS_46@NZ	3	0.0003	2.9289	138.5206
ALA_330@O	LYS_46@HE3	LYS_46@CE	3	0.0003	2.9890	140.0881
ASN_331@HB3	THR_44@HG1	THR_44@OG1	3	0.0003	2.6624	141.7130
ASN_331@HB3	THR_44@HA	THR_44@CA	3	0.0003	2.9710	144.9116
ASN_331@HD21	LYS_46@HZ1	LYS_46@NZ	3	0.0003	2.9702	149.4963

ASN_331@HD21	VAL_75@HG22	VAL_75@CG2	3	0.0003	2.9911	143.1544
LEU_333@HD11	TYR_37@HH	TYR_37@OH	3	0.0003	2.8889	147.4202
LEU_333@HD12	ALA_40@HB3	ALA_40@CB	3	0.0003	2.9371	144.6480
LEU_333@HD22	PHE_42@HZ	PHE_42@CZ	3	0.0003	2.9303	139.1257
LEU_333@HD22	TYR_37@HH	TYR_37@OH	3	0.0003	2.9694	149.0009
ASN_427@HA	LYS_54@HG3	LYS_54@CG	3	0.0003	2.9574	139.5832
ASN_427@HA	LYS_54@HE3	LYS_54@CE	3	0.0003	2.9257	145.5630
ASN_427@HA	THR_53@HG21	THR_53@CG2	3	0.0003	2.9229	137.0016
ASN_427@HD21	THR_53@HB	THR_53@CB	3	0.0003	2.9442	140.1443
ASN_427@HD22	SER_51@HG	SER_51@OG	3	0.0003	2.8691	140.0844
ALA_428@HA	TYR_37@HE2	TYR_37@CE2	3	0.0003	2.9380	148.2268
PRO_430@HG3	LYS_54@HE2	LYS_54@CE	3	0.0003	2.9354	141.5675
TYR_432@OH	ASN_38@HD21	ASN_38@ND2	3	0.0003	2.9161	139.4336
SER_457@HA	TYR_48@HE2	TYR_48@CE2	3	0.0003	2.9691	164.8430
SER_457@HB2	TYR_48@HD2	TYR_48@CD2	3	0.0003	2.9567	139.3091
LEU_458@HD11	LYS_46@HE2	LYS_46@CE	3	0.0003	2.8761	141.2092
LEU_458@HD21	LYS_46@HG2	LYS_46@CG	3	0.0003	2.9574	145.7684
LEU_458@HD23	LYS_46@HE2	LYS_46@CE	3	0.0003	2.8906	138.7262
GLN_464@HG2	THR_98@HG21	THR_98@CG2	3	0.0003	2.9496	137.1671
GLN_464@HG2	GLY_49@HA2	GLY_49@CA	3	0.0003	2.9777	143.6989
GLN_464@HE21	LEU_185@HD22	LEU_185@CD2	3	0.0003	2.7732	140.6555
GLN_464@HE21	LEU_185@HD23	LEU_185@CD2	3	0.0003	2.8454	152.4389
GLN_464@HE21	LEU_58@HD12	LEU_58@CD1	3	0.0003	2.9498	151.8773
GLN_464@HE22	VAL_50@HG11	VAL_50@CG1	3	0.0003	2.8569	139.0526
LYS_465@HA	ASP_96@HB2	ASP_96@CB	3	0.0003	2.9648	140.3360
THR_471@HG21	THR_83@HG22	THR_83@CG2	3	0.0003	2.9890	139.3537
THR_471@HG22	THR_83@HG23	THR_83@CG2	3	0.0003	2.8903	135.5392
THR_471@HG1	THR_83@HG21	THR_83@CG2	3	0.0003	2.8829	168.6280
THR_542@HG22	THR_83@HG23	THR_83@CG2	3	0.0003	2.8933	136.9603
GLN_316@HB2	THR_168@HG22	THR_168@CG2	2	0.0002	2.9576	140.4310
GLN_316@HB2	GLN_174@HE21	GLN_174@NE2	2	0.0002	2.9677	137.1201
GLN_316@HG3	THR_168@HB	THR_168@CB	2	0.0002	2.9761	141.3238
GLU_317@HA	THR_168@HA	THR_168@CA	2	0.0002	2.9063	135.9771
GLU_317@HA	VAL_171@HG12	VAL_171@CG1	2	0.0002	2.9462	137.2929
GLU_317@HB2	VAL_171@HG23	VAL_171@CG2	2	0.0002	2.9934	142.6089
GLU_317@HB2	THR_168@HA	THR_168@CA	2	0.0002	2.9380	143.1207
GLU_317@CD	GLN_174@HE21	GLN_174@NE2	2	0.0002	2.9815	142.9710
LEU_319@HD12	VAL_171@HG23	VAL_171@CG2	2	0.0002	2.9847	140.4472
LEU_319@HD21	VAL_171@HG22	VAL_171@CG2	2	0.0002	2.9530	137.3514
LEU_319@HD22	VAL_171@HG22	VAL_171@CG2	2	0.0002	2.9586	136.0902
PRO_323@HG2	GLY_172@HA3	GLY_172@CA	2	0.0002	2.9775	143.6151
GLU_327@HG3	ARG_76@HH11	ARG_76@NH1	2	0.0002	2.7967	143.1365
ALA_330@HB2	LYS_46@HE2	LYS_46@CE	2	0.0002	2.8290	140.6498
ALA_330@HB2	LYS_46@HE3	LYS_46@CE	2	0.0002	2.9294	139.5770
ALA_330@HB3	LYS_46@HZ3	LYS_46@NZ	2	0.0002	2.9475	143.0557
ALA_330@HB3	LYS_46@HZ1	LYS_46@NZ	2	0.0002	2.9001	147.2174
ASN_331@HB3	THR_44@HG21	THR_44@CG2	2	0.0002	2.9546	137.6352
ASN_331@HD21	LYS_46@HZ3	LYS_46@NZ	2	0.0002	2.9320	142.4074
ASN_331@HD21	VAL_75@HB	VAL_75@CB	2	0.0002	2.9167	143.7364
ASN_331@HD21	THR_44@HG22	THR_44@CG2	2	0.0002	2.7132	142.1233
ASN_331@HD21	ARG_76@HA	ARG_76@CA	2	0.0002	2.9592	136.1536
SER_332@HA	THR_44@HG22	THR_44@CG2	2	0.0002	2.9508	141.3384
SER_332@HG	PHE_43@HD2	PHE_43@CD2	2	0.0002	2.8828	160.4582
LEU_333@HB2	ALA_40@HB2	ALA_40@CB	2	0.0002	2.9558	138.4625
LEU_333@HB3	PHE_45@HB3	PHE_45@CB	2	0.0002	2.9814	145.0292
LEU_333@HG	PHE_45@HD2	PHE_45@CD2	2	0.0002	2.9315	135.5125
LEU_333@HG	TYR_37@HE1	TYR_37@CE1	2	0.0002	2.9955	141.8260
LEU_333@HD12	LYS_46@HE3	LYS_46@CE	2	0.0002	2.9034	140.3963
LEU_333@HD13	LYS_46@HE2	LYS_46@CE	2	0.0002	2.9837	138.5432
LEU_333@HD13	ALA_40@HB3	ALA_40@CB	2	0.0002	2.9110	138.1453
LEU_333@HD22	PHE_45@HD2	PHE_45@CD2	2	0.0002	2.9373	143.3947
ASP_334@HB2	PHE_43@HD2	PHE_43@CD2	2	0.0002	2.9350	138.7842
MET_426@O	LYS_54@HZ2	LYS_54@NZ	2	0.0002	2.8753	139.6734

ALA_428@HA	THR_53@HG22	THR_53@CG2	2	0.0002	2.9440	142.1014
ALA_428@HA	SER_51@HG	SER_51@OG	2	0.0002	2.9937	150.5870
PRO_430@HG2	THR_53@HG23	THR_53@CG2	2	0.0002	2.9600	136.7225
PRO_430@HG3	THR_53@HG23	THR_53@CG2	2	0.0002	2.9421	136.7664
LEU_458@HD21	LYS_46@HE2	LYS_46@CE	2	0.0002	2.8312	148.7101
GLN_464@HA	GLY_49@HA2	GLY_49@CA	2	0.0002	2.9950	138.5596
GLN_464@HG2	THR_98@HG22	THR_98@CG2	2	0.0002	2.9054	137.1226
GLN_464@HG3	THR_98@HG23	THR_98@CG2	2	0.0002	2.9733	137.0025
GLN_464@HE22	VAL_50@HG12	VAL_50@CG1	2	0.0002	2.8278	135.4827
PRO_466@HG3	ASP_95@HB3	ASP_95@CB	2	0.0002	2.9638	138.5655
THR_471@HB	THR_83@HG21	THR_83@CG2	2	0.0002	2.9322	144.1314
THR_471@HG21	THR_83@HG23	THR_83@CG2	2	0.0002	2.9153	136.2114
THR_471@HG21	THR_83@HG1	THR_83@OG1	2	0.0002	2.9108	139.5232
THR_471@HG22	THR_83@HG21	THR_83@CG2	2	0.0002	2.9136	151.5111
THR_471@HG1	THR_83@HG23	THR_83@CG2	2	0.0002	2.9552	144.0611
THR_471@HG1	THR_83@HG22	THR_83@CG2	2	0.0002	2.9718	149.3647
VAL_475@HG11	THR_83@HG22	THR_83@CG2	2	0.0002	2.9565	139.8079
VAL_475@HG13	ASN_128@H	ASN_128@N	2	0.0002	2.8766	163.2935
VAL_475@HG21	ASN_128@HD21	ASN_128@ND2	2	0.0002	2.9062	151.1710
THR_542@HG21	THR_83@HG22	THR_83@CG2	2	0.0002	2.9346	142.0952
THR_542@HG23	THR_83@HG23	THR_83@CG2	2	0.0002	2.9807	142.1250
THR_542@HG23	THR_83@HG22	THR_83@CG2	2	0.0002	2.9798	137.5712
ASN_314@HD21	VAL_171@HG11	VAL_171@CG1	1	0.0001	2.9982	140.6755
GLN_316@HB2	GLY_170@HA3	GLY_170@CA	1	0.0001	2.9863	137.2009
GLN_316@HB2	VAL_171@HG13	VAL_171@CG1	1	0.0001	2.9103	139.6883
GLN_316@HB2	VAL_171@HG12	VAL_171@CG1	1	0.0001	2.9608	144.2060
GLN_316@HB3	VAL_171@HG22	VAL_171@CG2	1	0.0001	2.9120	137.2040
GLN_316@HG3	THR_168@HG22	THR_168@CG2	1	0.0001	2.9613	139.4982
GLN_316@HG3	THR_168@HG21	THR_168@CG2	1	0.0001	2.9969	138.6888
GLN_316@HG3	GLY_170@HA2	GLY_170@CA	1	0.0001	2.8896	140.5574
GLN_316@NE2	GLN_174@HE22	GLN_174@NE2	1	0.0001	2.9093	135.8156
GLN_316@HE21	TYR_169@HA	TYR_169@CA	1	0.0001	2.8265	135.4067
GLN_316@HE21	ASN_107@HD21	ASN_107@ND2	1	0.0001	2.9575	135.4425
GLN_316@HE21	THR_168@HG22	THR_168@CG2	1	0.0001	2.9109	149.5615
GLN_316@HE21	THR_168@HG23	THR_168@CG2	1	0.0001	2.9529	157.7372
GLU_317@HA	GLY_170@HA2	GLY_170@CA	1	0.0001	2.9905	138.1051
GLU_317@HB2	VAL_171@HG12	VAL_171@CG1	1	0.0001	2.9769	140.6155
GLU_317@HG2	VAL_171@HB	VAL_171@CB	1	0.0001	2.9723	139.3850
GLU_317@HG2	GLN_174@HE21	GLN_174@NE2	1	0.0001	2.8458	138.1292
GLU_317@HG3	VAL_171@H	VAL_171@N	1	0.0001	2.9802	143.5694
GLU_317@HG3	VAL_171@HG12	VAL_171@CG1	1	0.0001	2.9522	137.8494
LEU_319@HG	VAL_171@HG12	VAL_171@CG1	1	0.0001	2.9795	140.1444
LEU_319@HD11	VAL_171@H	VAL_171@N	1	0.0001	2.9986	146.7203
LEU_319@HD11	VAL_171@HG21	VAL_171@CG2	1	0.0001	2.9703	135.0684
LEU_319@HD11	VAL_171@HG22	VAL_171@CG2	1	0.0001	2.9910	146.9642
LEU_319@HD13	GLY_170@HA2	GLY_170@CA	1	0.0001	2.9820	143.7356
LEU_319@HD13	VAL_171@H	VAL_171@N	1	0.0001	2.8165	168.6178
LEU_319@CD2	VAL_171@H	VAL_171@N	1	0.0001	2.9980	151.3019
LEU_319@HD21	VAL_171@HG11	VAL_171@CG1	1	0.0001	2.9675	139.8402
LEU_319@HD21	VAL_171@HB	VAL_171@CB	1	0.0001	2.9919	137.8229
LEU_319@HD22	VAL_171@HG11	VAL_171@CG1	1	0.0001	2.9348	139.1979
LEU_319@HD22	VAL_171@HB	VAL_171@CB	1	0.0001	2.9876	142.0108
LEU_319@HD23	GLY_170@HA3	GLY_170@CA	1	0.0001	2.9984	137.6999
LEU_319@HD23	VAL_171@HB	VAL_171@CB	1	0.0001	2.9675	136.1829
LEU_319@HD23	GLY_170@HA2	GLY_170@CA	1	0.0001	2.8728	144.9153
LEU_319@HD23	VAL_171@HG13	VAL_171@CG1	1	0.0001	2.9968	141.0029
GLU_327@HB2	VAL_171@HG12	VAL_171@CG1	1	0.0001	2.9577	139.2847
GLU_327@HG3	ARG_76@HD3	ARG_76@CD	1	0.0001	2.9238	167.5529
GLU_327@HG3	ARG_76@HE	ARG_76@NE	1	0.0001	2.9242	150.4200
GLU_327@CD	ARG_76@HE	ARG_76@NE	1	0.0001	2.9509	141.8872
GLU_327@CD	ARG_76@HH11	ARG_76@NH1	1	0.0001	2.9785	140.9319
GLU_327@OE2	TYR_176@HH	TYR_176@OH	1	0.0001	2.7615	137.3291
ALA_330@HB2	LYS_46@HZ3	LYS_46@NZ	1	0.0001	2.9409	145.0535

ALA_330@HB3	LYS_46@HE3	LYS_46@CE	1	0.0001	2.9625	135.4087
ASN_331@HA	LYS_46@HD3	LYS_46@CD	1	0.0001	2.9800	136.1174
ASN_331@HB2	LYS_46@HE2	LYS_46@CE	1	0.0001	2.9968	142.3775
ASN_331@HB2	THR_44@HG23	THR_44@CG2	1	0.0001	2.9981	145.2717
ASN_331@HD21	THR_44@HG1	THR_44@OG1	1	0.0001	2.9713	171.9539
ASN_331@HD21	THR_44@HG23	THR_44@CG2	1	0.0001	2.8740	141.3159
ASN_331@HD21	VAL_75@HG21	VAL_75@CG2	1	0.0001	2.9760	153.3532
ASN_331@HD21	LYS_46@HE3	LYS_46@CE	1	0.0001	2.8044	147.6294
ASN_331@HD21	THR_44@HG21	THR_44@CG2	1	0.0001	2.9644	138.8551
ASN_331@HD22	LYS_46@HE3	LYS_46@CE	1	0.0001	2.9817	141.7887
LEU_333@HB3	ALA_40@HB3	ALA_40@CB	1	0.0001	2.8935	146.0806
LEU_333@HG	TYR_37@HH	TYR_37@OH	1	0.0001	2.9075	155.2530
LEU_333@HD11	ALA_40@HB3	ALA_40@CB	1	0.0001	2.9166	137.3499
LEU_333@HD11	PHE_45@HD2	PHE_45@CD2	1	0.0001	2.9790	152.8593
LEU_333@HD11	LYS_46@HE2	LYS_46@CE	1	0.0001	2.6482	141.4952
LEU_333@HD11	THR_44@HA	THR_44@CA	1	0.0001	2.9977	149.1273
LEU_333@HD11	LYS_46@HE3	LYS_46@CE	1	0.0001	2.9647	135.0657
LEU_333@HD12	THR_44@HA	THR_44@CA	1	0.0001	2.9105	136.1688
LEU_333@HD12	LYS_46@HG3	LYS_46@CG	1	0.0001	2.9465	151.7896
LEU_333@HD12	PHE_45@HD2	PHE_45@CD2	1	0.0001	2.8540	138.3393
LEU_333@HD13	PHE_45@HB3	PHE_45@CB	1	0.0001	2.9901	161.4530
LEU_333@HD13	LYS_46@HG3	LYS_46@CG	1	0.0001	2.8583	135.6048
LEU_333@HD13	ALA_40@HB1	ALA_40@CB	1	0.0001	2.9534	136.4061
LEU_333@HD21	LYS_46@HE3	LYS_46@CE	1	0.0001	2.9596	156.8854
LEU_333@HD23	ALA_40@HB1	ALA_40@CB	1	0.0001	2.9654	139.5535
ASP_334@HB2	PHE_43@HB3	PHE_43@CB	1	0.0001	2.9654	136.6347
ASP_334@HB3	PHE_43@HD2	PHE_43@CD2	1	0.0001	2.9813	145.7227
MET_426@O	LYS_54@HZ3	LYS_54@NZ	1	0.0001	2.8190	149.0064
ASN_427@HA	LYS_54@HZ1	LYS_54@NZ	1	0.0001	2.8101	141.8119
ASN_427@HA	LYS_54@HZ2	LYS_54@NZ	1	0.0001	2.7919	156.5380
ASN_427@HB3	LYS_54@HB2	LYS_54@CB	1	0.0001	2.9951	141.5852
ASN_427@CG	SER_51@HG	SER_51@OG	1	0.0001	2.9554	158.7391
ASN_427@HD21	LYS_54@HD2	LYS_54@CD	1	0.0001	2.9509	146.8924
ASN_427@HD22	SER_51@HB2	SER_51@CB	1	0.0001	2.9203	138.6429
ASN_427@HD22	LYS_54@HB2	LYS_54@CB	1	0.0001	2.8732	149.8308
ASN_427@O	THR_53@H	THR_53@N	1	0.0001	2.9768	154.4851
ALA_428@HA	THR_53@HG23	THR_53@CG2	1	0.0001	2.9902	146.0912
ALA_428@HA	PRO_52@HG2	PRO_52@CG	1	0.0001	2.9826	136.4504
ALA_428@HA	PRO_52@HD2	PRO_52@CD	1	0.0001	2.9133	147.3091
ALA_428@HA	TYR_37@HH	TYR_37@OH	1	0.0001	2.7973	138.2806
ALA_428@HA	SER_51@HB3	SER_51@CB	1	0.0001	2.9178	142.6949
ALA_428@HB3	SER_51@HG	SER_51@OG	1	0.0001	2.8667	148.5569
PRO_430@HG2	THR_53@HG21	THR_53@CG2	1	0.0001	2.9273	139.3609
PRO_430@HG2	THR_53@HG22	THR_53@CG2	1	0.0001	2.9800	139.4589
PRO_430@HG2	LYS_54@HE2	LYS_54@CE	1	0.0001	2.9663	151.1400
PRO_430@HB3	LYS_54@HZ2	LYS_54@NZ	1	0.0001	2.7979	139.2362
PRO_430@HB3	LYS_54@HE2	LYS_54@CE	1	0.0001	2.9416	145.1241
PRO_430@HB3	LYS_54@HE3	LYS_54@CE	1	0.0001	2.9967	145.1648
TYR_432@OH	ASN_38@HD22	ASN_38@ND2	1	0.0001	2.8134	170.5454
SER_457@HB2	LYS_46@HE2	LYS_46@CE	1	0.0001	2.9898	138.9481
SER_457@HB3	LYS_46@HZ2	LYS_46@NZ	1	0.0001	2.9865	135.6797
SER_457@HB3	LYS_46@HE2	LYS_46@CE	1	0.0001	2.9455	147.5794
SER_457@OG	LYS_46@HE2	LYS_46@CE	1	0.0001	2.9708	141.5416
SER_457@HG	LYS_46@HD3	LYS_46@CD	1	0.0001	2.7953	156.5179
SER_457@HG	LYS_46@HD2	LYS_46@CD	1	0.0001	2.9987	145.7433
LEU_458@HG	LYS_46@HE2	LYS_46@CE	1	0.0001	2.9176	158.3919
LEU_458@HD13	SER_51@HG	SER_51@OG	1	0.0001	2.9179	140.4071
LEU_458@HD23	LYS_46@HA	LYS_46@CA	1	0.0001	3.0000	143.5629
LEU_458@HD23	LYS_46@HG2	LYS_46@CG	1	0.0001	2.8062	140.1619
GLY_463@HA3	GLY_49@H	GLY_49@N	1	0.0001	2.7215	135.0857
GLN_464@HG2	THR_98@HG23	THR_98@CG2	1	0.0001	2.9998	139.6800
GLN_464@HG3	THR_98@HG22	THR_98@CG2	1	0.0001	2.9445	136.3296
GLN_464@HG3	THR_98@HG21	THR_98@CG2	1	0.0001	2.9304	138.9000

GLN_464@HG3	THR_98@HG1	THR_98@OG1	1	0.0001	2.9154	157.1157
GLN_464@HG3	GLY_49@HA3	GLY_49@CA	1	0.0001	2.8985	138.5334
GLN_464@HE21	LEU_58@HG	LEU_58@CG	1	0.0001	2.9448	144.9363
GLN_464@HE22	LEU_58@HD23	LEU_58@CD2	1	0.0001	2.8811	150.7074
GLN_464@HE22	VAL_50@HG13	VAL_50@CG1	1	0.0001	2.8883	136.7535
GLN_464@HE22	PHE_60@HE1	PHE_60@CE1	1	0.0001	2.7698	148.6707
GLN_464@HE22	LEU_185@HD21	LEU_185@CD2	1	0.0001	2.8852	139.2626
PRO_466@HD3	ASP_96@HA	ASP_96@CA	1	0.0001	2.9133	135.5813
PRO_466@HD3	ASP_96@HB2	ASP_96@CB	1	0.0001	2.8866	135.6158
PRO_466@HB2	ASP_95@HB3	ASP_95@CB	1	0.0001	2.9676	142.3814
ASP_469@OD1	THR_83@HG1	THR_83@OG1	1	0.0001	2.8333	164.3866
THR_471@HB	THR_83@HG23	THR_83@CG2	1	0.0001	2.8690	144.0455
THR_471@HG21	THR_83@HG21	THR_83@CG2	1	0.0001	2.9488	147.4477
THR_471@HG21	THR_83@HB	THR_83@CB	1	0.0001	2.9764	144.1727
THR_471@HG22	ASN_128@HD21	ASN_128@ND2	1	0.0001	2.9261	148.0161
THR_471@HG23	THR_83@HB	THR_83@CB	1	0.0001	2.9917	137.0787
THR_471@OG1	THR_83@HG1	THR_83@OG1	1	0.0001	2.9732	162.7033
ASP_472@OD1	ASN_128@HD22	ASN_128@ND2	1	0.0001	2.8324	143.0917
VAL_475@HB	ASN_128@HD22	ASN_128@ND2	1	0.0001	2.8257	144.6120
VAL_475@HG11	THR_83@HG21	THR_83@CG2	1	0.0001	2.9168	137.3530
VAL_475@HG12	THR_83@HG22	THR_83@CG2	1	0.0001	2.9141	136.4015
VAL_475@HG13	THR_83@HG23	THR_83@CG2	1	0.0001	2.9108	140.7954
VAL_475@HG13	THR_83@HG22	THR_83@CG2	1	0.0001	2.9632	137.3908
VAL_475@HG22	THR_83@HG22	THR_83@CG2	1	0.0001	2.9632	144.1012
VAL_475@HG23	ASN_128@HD21	ASN_128@ND2	1	0.0001	2.8171	144.5997
ASN_515@OD1	ARG_161@HH12	ARG_161@NH1	1	0.0001	2.9402	151.1878
LYS_540@HE2	ARG_76@HH12	ARG_76@NH1	1	0.0001	2.9233	141.7919
THR_542@HG21	THR_83@HG23	THR_83@CG2	1	0.0001	2.9530	142.0541
THR_542@HG22	THR_83@HG21	THR_83@CG2	1	0.0001	2.8724	135.7027
THR_542@HG22	THR_83@HG22	THR_83@CG2	1	0.0001	2.9816	135.0010
THR_542@HG23	THR_83@HG21	THR_83@CG2	1	0.0001	2.9084	137.9127

Table S3. Hydrogen bond analysis of S protein (BA.2)-ACE2 complex during the last 20 ns of MD simulation with S protein as acceptor and ACE2 as donor.

#Acceptor	DonorH	Donor	Frames	Frac	AvgDist	AvgAng
ASP_88@OD1	THR_542@HG1	THR_542@OG1	9647	0.9647	2.6654	164.6703
ASP_88@OD1	THR_471@HG1	THR_471@OG1	5003	0.5003	2.7392	166.4083
ASP_88@OD2	THR_471@HG1	THR_471@OG1	2685	0.2685	2.6938	164.1908
PHE_39@O	GLN_316@HE22	GLN_316@NE2	2621	0.2621	2.8512	158.2493
SER_162@O	ASN_515@HD22	ASN_515@ND2	1687	0.1687	2.8529	158.2120
ALA_40@O	ASN_314@HD22	ASN_314@ND2	1472	0.1472	2.8452	158.2836
HIE_173@ND1	LYS_518@HZ2	LYS_518@NZ	588	0.0588	2.9133	155.6680
TYR_163@O	ASN_515@HD22	ASN_515@ND2	536	0.0536	2.8694	152.5046
ALA_40@O	ASN_311@HD22	ASN_311@ND2	472	0.0472	2.8537	160.6247
HIE_173@ND1	LYS_518@HZ3	LYS_518@NZ	460	0.0460	2.9081	154.2679
HIE_173@ND1	LYS_518@HZ1	LYS_518@NZ	438	0.0438	2.9004	154.6989
SER_162@OG	ASN_515@HD21	ASN_515@ND2	407	0.0407	2.8612	157.9923
PHE_42@O	ASN_311@HD21	ASN_311@ND2	377	0.0377	2.8201	151.4343
SER_76@O	ASN_331@HD22	ASN_331@ND2	343	0.0343	2.8913	144.8645
ALA_79@HB2	ASN_331@HD22	ASN_331@ND2	258	0.0258	2.8367	147.2984
ALA_79@HB1	ASN_331@HD22	ASN_331@ND2	247	0.0247	2.8314	144.9576
PRO_80@O	SER_457@HG	SER_457@OG	236	0.0236	2.7337	161.4115
ASN_38@O	ASN_314@HD21	ASN_314@ND2	229	0.0229	2.8625	155.6036
ALA_79@HB3	ASN_331@HD22	ASN_331@ND2	211	0.0211	2.8432	146.3181
ARG_161@HD3	GLY_514@HA2	GLY_514@CA	170	0.0170	2.9234	146.0214
ALA_143@HA	ALA_478@HB3	ALA_478@CB	161	0.0161	2.9384	144.4056
ALA_143@HA	ALA_478@HB1	ALA_478@CB	155	0.0155	2.9378	145.6210
ALA_143@HA	ALA_478@HB2	ALA_478@CB	151	0.0151	2.9436	145.4799
TYR_37@O	ASN_314@HD21	ASN_314@ND2	147	0.0147	2.8709	145.1977
GLY_114@O	ASN_515@HD22	ASN_515@ND2	139	0.0139	2.8622	161.1175
TYR_117@OH	ASN_515@HD22	ASN_515@ND2	137	0.0137	2.8960	159.6331
ASP_95@OD1	GLN_464@HE22	GLN_464@NE2	123	0.0123	2.8582	160.1229
ASN_128@HD21	THR_471@HB	THR_471@CB	116	0.0116	2.8947	148.8492

GLY_81@O	ASN_467@HD21	ASN_467@ND2	115	0.0115	2.8401	156.3788
GLY_164@HA2	ASN_515@HD22	ASN_515@ND2	107	0.0107	2.8571	145.8386
ASN_85@HD22	LYS_540@HB2	LYS_540@CB	105	0.0105	2.8553	144.2317
PHE_43@HE1	GLU_327@HB3	GLU_327@CB	101	0.0101	2.9407	141.3841
GLU_74@OE2	LYS_540@HZ2	LYS_540@NZ	92	0.0092	2.8468	155.4526
TYR_157@HH	ASP_480@HB2	ASP_480@CB	88	0.0088	2.8974	148.1025
SER_162@OG	ASN_515@HD22	ASN_515@ND2	88	0.0088	2.9119	157.5968
ASN_85@OD1	THR_542@HG1	THR_542@OG1	87	0.0087	2.7628	159.4577
PHE_42@CE1	ASN_311@HD22	ASN_311@ND2	83	0.0083	2.9531	154.1856
LYS_46@HE2	ASN_331@HB3	ASN_331@CB	70	0.0070	2.8815	145.7664
PHE_43@HB2	LEU_319@HG	LEU_319@CG	67	0.0067	2.9407	140.5247
THR_83@HB	ASP_544@HB2	ASP_544@CB	67	0.0067	2.9402	142.0697
PHE_42@HE2	ASN_314@HD21	ASN_314@ND2	64	0.0064	2.8436	146.1362
TYR_48@OH	SER_457@HG	SER_457@OG	57	0.0057	2.8545	160.6670
PHE_43@HE1	GLY_324@HA2	GLY_324@CA	55	0.0055	2.9434	143.1251
ASN_128@HB3	ASP_472@HB2	ASP_472@CB	47	0.0047	2.9562	140.1362
ASN_85@HD22	LYS_540@HE3	LYS_540@CE	45	0.0045	2.8943	149.9352
TYR_176@HH	GLY_324@HA2	GLY_324@CA	44	0.0044	2.8966	148.3841
ARG_161@HH11	ASP_512@HB3	ASP_512@CB	43	0.0043	2.9430	145.0297
ASN_85@HB2	LYS_540@HE2	LYS_540@CE	41	0.0041	2.9164	141.6190
TYR_176@HH	LEU_319@HD12	LEU_319@CD1	41	0.0041	2.8176	143.5894
TYR_117@CD1	ASN_515@HD22	ASN_515@ND2	40	0.0040	2.9534	153.4532
LYS_46@HD2	ASN_331@HB3	ASN_331@CB	39	0.0039	2.9492	140.8174
GLU_74@OE2	LYS_540@HZ1	LYS_540@NZ	39	0.0039	2.8028	154.9426
PRO_41@HB3	GLN_316@HG3	GLN_316@CG	37	0.0037	2.9481	140.9380
TYR_48@OH	ASN_331@HD22	ASN_331@ND2	35	0.0035	2.8930	142.4634
ASN_73@HA	PRO_323@HG3	PRO_323@CG	35	0.0035	2.9545	143.9954
GLN_82@HE21	ASN_331@HD22	ASN_331@ND2	35	0.0035	2.8868	146.9151
ASN_38@O	GLN_316@HE22	GLN_316@NE2	34	0.0034	2.8654	158.2105
GLY_84@HA2	ASP_544@HB2	ASP_544@CB	33	0.0033	2.9332	141.2042
GLU_74@OE1	LYS_540@HZ2	LYS_540@NZ	32	0.0032	2.7996	143.4653
GLU_74@OE2	LYS_540@HZ3	LYS_540@NZ	30	0.0030	2.7930	155.4852
VAL_171@HG21	LEU_320@H	LEU_320@N	29	0.0029	2.8822	149.4553
PHE_43@HZ	GLU_327@HG2	GLU_327@CG	28	0.0028	2.9483	142.9530
TYR_117@HD1	ASN_515@HD22	ASN_515@ND2	28	0.0028	2.8795	145.1970
TYR_117@HE1	ASN_515@HB3	ASN_515@CB	28	0.0028	2.9442	142.2482
ARG_161@HH12	GLY_514@H	GLY_514@N	28	0.0028	2.9381	140.7100
TYR_121@OH	LYS_540@HZ2	LYS_540@NZ	27	0.0027	2.8832	149.6097
LEU_123@HD12	LYS_540@HG2	LYS_540@CG	27	0.0027	2.9421	140.4583
ASN_128@HB2	ASP_472@HB2	ASP_472@CB	27	0.0027	2.9453	139.4898
PHE_42@HE1	ASN_311@HD22	ASN_311@ND2	26	0.0026	2.9160	149.8197
TYR_89@HH	VAL_541@HG22	VAL_541@CG2	26	0.0026	2.9128	145.6042
SER_76@HA	ASN_331@HD21	ASN_331@ND2	25	0.0025	2.8514	139.0097
LEU_123@HD11	LYS_540@HG2	LYS_540@CG	25	0.0025	2.9485	144.8126
HIE_173@CE1	LYS_518@HZ2	LYS_518@NZ	25	0.0025	2.9591	144.4559
ASN_128@HD21	THR_471@HG22	THR_471@CG2	24	0.0024	2.8687	143.4011
ASN_128@HD22	THR_471@HB	THR_471@CB	24	0.0024	2.8977	152.8809
VAL_171@HB	PRO_323@HD2	PRO_323@CD	24	0.0024	2.9267	141.9704
LEU_123@HD13	LYS_540@HG2	LYS_540@CG	23	0.0023	2.9422	141.1247
ASN_128@HD22	THR_471@HG1	THR_471@OG1	23	0.0023	2.8703	140.1777
PHE_42@O	ASN_311@HD22	ASN_311@ND2	22	0.0022	2.8269	152.2872
TYR_89@HH	VAL_541@HG23	VAL_541@CG2	22	0.0022	2.9224	149.4115
TYR_141@HE1	VAL_475@HB	VAL_475@CB	22	0.0022	2.9718	138.4731
GLY_164@HA3	ASN_515@HB3	ASN_515@CB	22	0.0022	2.9290	145.8152
VAL_171@HG22	PRO_323@HD3	PRO_323@CD	22	0.0022	2.9493	141.9495
ASN_38@HA	ASN_314@HB2	ASN_314@CB	21	0.0021	2.9576	138.6894
TYR_89@HH	VAL_541@HG21	VAL_541@CG2	21	0.0021	2.9394	145.2132
TYR_89@HH	VAL_541@HB	VAL_541@CB	21	0.0021	2.9068	140.9454
LYS_108@HE2	GLN_316@HB2	GLN_316@CB	21	0.0021	2.8957	142.9185
ASN_128@HD21	THR_471@HG23	THR_471@CG2	21	0.0021	2.8476	143.2846
VAL_171@HG21	PRO_323@HD3	PRO_323@CD	21	0.0021	2.9411	142.5727
ASP_95@OD2	GLN_464@HE21	GLN_464@NE2	20	0.0020	2.8227	158.8715
TYR_121@OH	LYS_540@HZ1	LYS_540@NZ	20	0.0020	2.9035	147.9032

GLY_84@HA2	THR_542@HG21	THR_542@CG2	19	0.0019	2.9426	141.5210
ARG_161@HG3	ASN_515@HA	ASN_515@CA	19	0.0019	2.9310	146.0337
GLY_172@HA2	PRO_323@HG3	PRO_323@CG	19	0.0019	2.9494	140.0238
LYS_46@HG2	SER_332@HB2	SER_332@CB	18	0.0018	2.9186	140.9608
LYS_46@HE3	ASN_331@HB3	ASN_331@CB	18	0.0018	2.8957	140.2079
CYS_47@HB2	LEU_333@HB3	LEU_333@CB	18	0.0018	2.9544	144.8765
GLY_84@HA2	ASP_544@HB3	ASP_544@CB	18	0.0018	2.9513	138.6809
ASN_85@HB2	LYS_540@HE3	LYS_540@CE	18	0.0018	2.9101	141.0338
PHE_124@HE1	VAL_541@HG21	VAL_541@CG2	18	0.0018	2.9471	139.5552
ALA_143@HB1	ASP_480@HB3	ASP_480@CB	18	0.0018	2.9615	143.6659
VAL_171@HG13	PRO_323@HD2	PRO_323@CD	18	0.0018	2.9320	141.8550
HIE_173@CE1	LYS_518@HZ3	LYS_518@NZ	18	0.0018	2.9550	143.9830
LYS_46@HD3	ASN_331@HB3	ASN_331@CB	17	0.0017	2.9495	141.3550
GLN_82@NE2	ASN_331@HD22	ASN_331@ND2	17	0.0017	2.9236	148.9167
VAL_171@HG11	PRO_323@HD2	PRO_323@CD	17	0.0017	2.9468	142.5240
PRO_41@HA	GLN_316@HG3	GLN_316@CG	16	0.0016	2.9578	138.7748
LYS_46@HB3	SER_332@HA	SER_332@CA	16	0.0016	2.9375	137.2109
LYS_46@HD3	GLU_327@HG3	GLU_327@CG	16	0.0016	2.9478	139.3046
ASN_85@HB3	LYS_540@HE3	LYS_540@CE	16	0.0016	2.9437	141.9553
LYS_108@HE3	GLN_316@HB2	GLN_316@CB	16	0.0016	2.8805	147.2528
TYR_121@OH	LYS_540@HZ3	LYS_540@NZ	16	0.0016	2.8890	149.4556
ASN_128@HB2	ASP_472@HA	ASP_472@CA	16	0.0016	2.9601	141.6737
VAL_75@HG13	GLU_327@HG2	GLU_327@CG	15	0.0015	2.9471	140.5195
ASP_95@OD2	GLN_464@HE22	GLN_464@NE2	15	0.0015	2.8596	157.3975
LYS_46@HD2	GLU_327@HG3	GLU_327@CG	14	0.0014	2.9673	138.9748
THR_83@HG22	ASP_544@HB2	ASP_544@CB	14	0.0014	2.9448	143.5040
THR_83@HG23	ASP_544@HB2	ASP_544@CB	14	0.0014	2.9585	139.9286
SER_127@HA	VAL_475@HG22	VAL_475@CG2	14	0.0014	2.9601	144.1247
ALA_143@HB3	ASP_480@HB3	ASP_480@CB	14	0.0014	2.9577	145.5118
GLU_74@OE1	LYS_540@HZ3	LYS_540@NZ	13	0.0013	2.7705	149.1223
ASN_85@OD1	LYS_540@HZ2	LYS_540@NZ	13	0.0013	2.8768	147.9460
ASP_95@OD1	ASN_467@H	ASN_467@N	13	0.0013	2.9024	164.8175
ASN_128@HD21	ASP_472@HB2	ASP_472@CB	13	0.0013	2.8585	147.3759
LYS_46@HB2	SER_332@HA	SER_332@CA	12	0.0012	2.9585	148.3981
ASN_85@OD1	LYS_540@HZ3	LYS_540@NZ	12	0.0012	2.8217	150.9682
TYR_89@HE2	VAL_475@HG13	VAL_475@CG1	12	0.0012	2.9641	140.5142
ALA_143@HB2	ASP_480@HB3	ASP_480@CB	12	0.0012	2.9624	148.4417
VAL_171@HG22	LEU_320@HB2	LEU_320@CB	12	0.0012	2.9569	142.5805
VAL_171@HG23	LEU_320@H	LEU_320@N	12	0.0012	2.9116	149.9249
PHE_43@HB2	LEU_319@HD13	LEU_319@CD1	11	0.0011	2.9241	138.2701
PHE_43@HD1	LEU_319@HG	LEU_319@CG	11	0.0011	2.9370	138.5582
THR_83@HB	MET_543@HB3	MET_543@CB	11	0.0011	2.9711	143.2973
GLY_84@HA2	THR_542@HG22	THR_542@CG2	11	0.0011	2.9321	140.4000
ASN_85@H	THR_542@HG21	THR_542@CG2	11	0.0011	2.9304	147.0557
ASP_88@HB3	THR_471@HG21	THR_471@CG2	11	0.0011	2.9308	140.4918
TYR_89@HH	VAL_541@HG13	VAL_541@CG1	11	0.0011	2.9139	142.4041
TYR_121@HE1	LYS_540@HE2	LYS_540@CE	11	0.0011	2.9306	148.5435
PHE_124@HE1	VAL_541@HG22	VAL_541@CG2	11	0.0011	2.9501	140.0337
TYR_169@OH	LYS_518@HZ3	LYS_518@NZ	11	0.0011	2.9099	150.6651
VAL_171@HG22	LEU_320@H	LEU_320@N	11	0.0011	2.9430	154.8770
TYR_37@OH	ASN_336@HD21	ASN_336@ND2	10	0.0010	2.9131	162.4383
PHE_39@O	ASN_314@HD22	ASN_314@ND2	10	0.0010	2.9348	147.9482
PHE_43@HB2	LEU_319@HD12	LEU_319@CD1	10	0.0010	2.9776	142.0959
THR_83@HG1	ASP_544@HB2	ASP_544@CB	10	0.0010	2.8751	150.8931
PHE_124@HE1	VAL_541@HG23	VAL_541@CG2	10	0.0010	2.9373	138.9374
SER_127@HA	VAL_475@HG21	VAL_475@CG2	10	0.0010	2.9419	140.6115
ASN_128@HD22	ASP_472@HB2	ASP_472@CB	10	0.0010	2.9622	147.2252
GLY_164@HA3	LYS_518@HE2	LYS_518@CE	10	0.0010	2.9333	141.7968
VAL_171@HG21	PRO_323@HD2	PRO_323@CD	10	0.0010	2.9305	139.3389
VAL_171@HG22	PRO_323@HD2	PRO_323@CD	10	0.0010	2.9233	142.6084
VAL_171@HG23	PRO_323@HD2	PRO_323@CD	10	0.0010	2.9666	140.7728
HIE_173@CG	LYS_518@HZ2	LYS_518@NZ	10	0.0010	2.9686	155.1265
HIE_173@CG	LYS_518@HZ1	LYS_518@NZ	10	0.0010	2.9746	148.9832

PHE_43@HD1	ILE_328@HD12	ILE_328@CD1	9	0.0009	2.9374	143.0825
PHE_43@HD1	GLY_324@HA2	GLY_324@CA	9	0.0009	2.9581	149.1011
GLY_84@HA2	THR_542@HG23	THR_542@CG2	9	0.0009	2.9325	139.1180
ARG_161@HH11	ASP_512@HB2	ASP_512@CB	9	0.0009	2.9282	138.3446
VAL_171@HG22	LEU_320@HD13	LEU_320@CD1	9	0.0009	2.9460	141.7459
HIE_173@CD2	LYS_518@HZ2	LYS_518@NZ	9	0.0009	2.9619	156.1836
TYR_176@HH	LEU_319@HD13	LEU_319@CD1	9	0.0009	2.7516	142.7384
TYR_176@HH	LEU_319@HD11	LEU_319@CD1	9	0.0009	2.8879	144.3410
ALA_40@HB2	ASN_311@HD22	ASN_311@ND2	8	0.0008	2.8151	143.5649
ASN_85@HD22	LYS_540@HE2	LYS_540@CE	8	0.0008	2.9014	148.9932
ASP_88@HB3	THR_471@HG22	THR_471@CG2	8	0.0008	2.9269	139.6748
ASP_88@OD1	MET_543@H	MET_543@N	8	0.0008	2.9354	156.9634
TYR_89@HH	VAL_541@HG12	VAL_541@CG1	8	0.0008	2.9472	144.9756
LYS_108@HE3	GLN_316@HG3	GLN_316@CG	8	0.0008	2.8706	143.4391
SER_162@HB2	ASN_515@HD22	ASN_515@ND2	8	0.0008	2.6919	138.9808
ARG_166@HH21	VAL_516@HG13	VAL_516@CG1	8	0.0008	2.9364	142.6808
HIE_173@CE1	LYS_518@HZ1	LYS_518@NZ	8	0.0008	2.9695	142.5117
ALA_40@HB1	ASN_311@HD22	ASN_311@ND2	7	0.0007	2.8828	143.3312
GLN_82@HG3	ASN_331@HD22	ASN_331@ND2	7	0.0007	2.8768	141.7429
THR_83@HG23	MET_543@HB3	MET_543@CB	7	0.0007	2.9359	141.0998
TYR_89@HE2	VAL_475@HG12	VAL_475@CG1	7	0.0007	2.9443	140.9573
TYR_89@HE2	VAL_475@HG11	VAL_475@CG1	7	0.0007	2.9252	140.6129
TYR_117@HE2	VAL_516@HA	VAL_516@CA	7	0.0007	2.9506	142.8449
TYR_121@HE1	LYS_540@HZ1	LYS_540@NZ	7	0.0007	2.9248	151.0161
LEU_123@HD13	LYS_540@HE3	LYS_540@CE	7	0.0007	2.9243	145.8532
TYR_141@HH	VAL_541@HG13	VAL_541@CG1	7	0.0007	2.9595	162.7448
VAL_171@HG13	LEU_320@HD13	LEU_320@CD1	7	0.0007	2.9643	140.6987
VAL_171@HG23	LEU_320@HB2	LEU_320@CB	7	0.0007	2.9421	139.7796
VAL_171@HG23	PRO_323@HD3	PRO_323@CD	7	0.0007	2.9398	141.0986
PHE_42@CZ	ASN_311@HD22	ASN_311@ND2	6	0.0006	2.9761	160.4348
PHE_43@HA	LEU_319@HD11	LEU_319@CD1	6	0.0006	2.9789	143.4539
PHE_43@HB2	LEU_319@HD22	LEU_319@CD2	6	0.0006	2.9442	140.2513
PHE_43@HD1	ILE_328@HD11	ILE_328@CD1	6	0.0006	2.9389	142.0514
ALA_44@HB3	ILE_328@HG12	ILE_328@CG1	6	0.0006	2.9419	139.0814
LYS_46@HG2	SER_332@HA	SER_332@CA	6	0.0006	2.9566	136.3038
PRO_80@O	ASN_331@HD22	ASN_331@ND2	6	0.0006	2.9049	153.5071
GLN_82@HE22	ASN_331@HD22	ASN_331@ND2	6	0.0006	2.8903	138.7035
ASN_85@H	THR_542@HG22	THR_542@CG2	6	0.0006	2.9328	146.5981
ASN_85@HB2	THR_542@HG22	THR_542@CG2	6	0.0006	2.9226	139.7030
ASN_85@HB2	LYS_540@HD3	LYS_540@CD	6	0.0006	2.9326	143.8476
ASP_88@CG	THR_471@HG1	THR_471@OG1	6	0.0006	2.9676	151.0008
TYR_89@HH	VAL_541@HG11	VAL_541@CG1	6	0.0006	2.9546	143.4421
TYR_117@CE1	ASN_515@HD22	ASN_515@ND2	6	0.0006	2.9446	150.1087
TYR_117@HE1	ASN_515@HD21	ASN_515@ND2	6	0.0006	2.9162	141.9757
TYR_117@HE1	ASN_515@HD22	ASN_515@ND2	6	0.0006	2.8721	147.5173
TYR_121@HE1	LYS_540@HZ2	LYS_540@NZ	6	0.0006	2.9138	142.6650
PHE_124@HE1	ASP_480@HA	ASP_480@CA	6	0.0006	2.9510	149.7804
SER_127@HA	VAL_475@HG23	VAL_475@CG2	6	0.0006	2.9175	140.2971
ASN_128@H	VAL_475@HG21	VAL_475@CG2	6	0.0006	2.9195	149.8948
ASN_128@HD21	THR_471@HG21	THR_471@CG2	6	0.0006	2.8160	141.8221
ASN_128@HD22	THR_471@HG21	THR_471@CG2	6	0.0006	2.8818	151.2487
ARG_161@HD2	GLY_514@HA2	GLY_514@CA	6	0.0006	2.9533	145.4905
ARG_161@HH11	GLY_514@H	GLY_514@N	6	0.0006	2.9459	144.1170
GLY_164@HA3	ASN_515@HD21	ASN_515@ND2	6	0.0006	2.9113	145.7855
TYR_169@HE1	LYS_518@HE2	LYS_518@CE	6	0.0006	2.9058	142.0070
TYR_169@OH	LYS_518@HZ2	LYS_518@NZ	6	0.0006	2.8502	151.7073
VAL_171@HG12	PRO_323@HD2	PRO_323@CD	6	0.0006	2.9051	139.0682
VAL_171@HG13	LEU_320@HD12	LEU_320@CD1	6	0.0006	2.9473	142.6242
PHE_42@CE2	ASN_314@HD21	ASN_314@ND2	5	0.0005	2.9224	142.8091
PHE_42@CE2	ASN_311@HD22	ASN_311@ND2	5	0.0005	2.9564	149.1971
PHE_43@HB2	LEU_319@HD11	LEU_319@CD1	5	0.0005	2.9494	137.1598
PHE_43@HD1	LEU_319@HD23	LEU_319@CD2	5	0.0005	2.9272	140.4508
PHE_43@HE1	CYS_318@HA	CYS_318@CA	5	0.0005	2.9474	138.4642

PHE_43@HD2	ILE_328@HD12	ILE_328@CD1	5	0.0005	2.9682	141.6884
LYS_46@HA	SER_332@HA	SER_332@CA	5	0.0005	2.9656	148.1894
CYS_47@HB2	LEU_333@HD21	LEU_333@CD2	5	0.0005	2.9443	140.2786
TYR_48@HE2	LEU_333@HD12	LEU_333@CD1	5	0.0005	2.9326	145.9520
TYR_48@HE2	LEU_333@HD11	LEU_333@CD1	5	0.0005	2.9477	140.1833
ASN_73@HA	PRO_323@HG2	PRO_323@CG	5	0.0005	2.9233	137.7334
THR_83@HG21	ASP_544@HB2	ASP_544@CB	5	0.0005	2.9654	139.4086
ASN_85@HB2	LYS_540@HD2	LYS_540@CD	5	0.0005	2.9546	141.3643
ASN_85@HD22	LYS_540@HD2	LYS_540@CD	5	0.0005	2.9387	140.0532
ASN_85@HD22	THR_542@HG22	THR_542@CG2	5	0.0005	2.8813	141.0976
ASN_85@HD22	THR_542@HB	THR_542@CB	5	0.0005	2.8344	141.6080
LYS_108@HE3	GLN_316@HA	GLN_316@CA	5	0.0005	2.8552	146.4168
LYS_108@HZ1	GLN_316@HB2	GLN_316@CB	5	0.0005	2.8788	145.6454
TYR_117@HH	VAL_516@HA	VAL_516@CA	5	0.0005	2.8909	154.7263
PHE_124@HZ	ASP_480@HA	ASP_480@CA	5	0.0005	2.9637	144.2061
ASN_128@H	VAL_475@HG23	VAL_475@CG2	5	0.0005	2.8944	144.9304
ASN_128@H	ASP_472@HB2	ASP_472@CB	5	0.0005	2.9626	152.5117
ARG_161@HH12	GLY_514@HA2	GLY_514@CA	5	0.0005	2.9388	147.0974
ARG_166@HH21	VAL_516@HB	VAL_516@CB	5	0.0005	2.8817	148.8589
TYR_169@OH	LYS_518@HZ1	LYS_518@NZ	5	0.0005	2.8863	155.0536
VAL_171@HG12	LEU_320@HD13	LEU_320@CD1	5	0.0005	2.9698	141.2474
VAL_171@HG12	LEU_320@HD12	LEU_320@CD1	5	0.0005	2.9543	137.1051
VAL_171@HG23	LEU_320@HD12	LEU_320@CD1	5	0.0005	2.9399	141.0131
HIE_173@HB3	LYS_518@HZ2	LYS_518@NZ	5	0.0005	2.9304	146.3238
HIE_173@CG	LYS_518@HZ3	LYS_518@NZ	5	0.0005	2.9496	155.0586
HIE_173@NE2	LYS_518@HZ2	LYS_518@NZ	5	0.0005	2.9536	149.1133
ALA_40@O	GLN_316@HE22	GLN_316@NE2	4	0.0004	2.7784	140.3804
PHE_43@HD1	ILE_328@HD13	ILE_328@CD1	4	0.0004	2.9550	147.1599
PHE_43@HE1	GLU_317@HG3	GLU_317@CG	4	0.0004	2.9393	139.3523
ALA_44@HB1	ILE_328@HG12	ILE_328@CG1	4	0.0004	2.9660	141.2961
ALA_44@HB2	ILE_328@HG12	ILE_328@CG1	4	0.0004	2.9300	142.5483
LYS_46@HG2	ASN_331@HB3	ASN_331@CB	4	0.0004	2.9523	141.6547
LYS_46@HG3	SER_332@HA	SER_332@CA	4	0.0004	2.9006	137.5527
TYR_48@HE2	SER_457@HB2	SER_457@CB	4	0.0004	2.9695	141.8322
GLU_74@OE1	LYS_540@HZ1	LYS_540@NZ	4	0.0004	2.7665	139.9338
THR_83@HG21	MET_543@HB3	MET_543@CB	4	0.0004	2.9395	141.9388
ASN_85@H	THR_542@HG23	THR_542@CG2	4	0.0004	2.8980	150.7197
ASN_85@HD21	LYS_540@HZ1	LYS_540@NZ	4	0.0004	2.9346	144.9952
ASN_85@HD22	THR_542@HG23	THR_542@CG2	4	0.0004	2.9009	137.5776
ASN_85@HD22	THR_542@HG21	THR_542@CG2	4	0.0004	2.8792	150.8589
TYR_89@HH	THR_471@HG21	THR_471@CG2	4	0.0004	2.9326	139.0106
ASP_96@OD1	GLN_464@HE22	GLN_464@NE2	4	0.0004	2.8859	164.9287
TYR_117@CD2	ASN_515@HD22	ASN_515@ND2	4	0.0004	2.9448	161.4845
LEU_123@HD12	VAL_541@H	VAL_541@N	4	0.0004	2.8956	154.3589
LEU_123@HD12	LYS_540@HE3	LYS_540@CE	4	0.0004	2.9034	145.8053
LEU_123@HD13	LYS_540@HD2	LYS_540@CD	4	0.0004	2.9528	142.0416
LYS_126@HE3	ASP_476@HA	ASP_476@CA	4	0.0004	2.9182	147.2705
ASN_128@HB3	ASP_472@HA	ASP_472@CA	4	0.0004	2.9661	136.8607
ALA_143@HB3	ASP_480@HA	ASP_480@CA	4	0.0004	2.9412	147.4224
TYR_157@HE1	ASP_480@HB2	ASP_480@CB	4	0.0004	2.9571	140.4676
TYR_169@HE2	LYS_518@HD2	LYS_518@CD	4	0.0004	2.9497	142.4421
VAL_171@HG21	LEU_320@HD22	LEU_320@CD2	4	0.0004	2.9669	145.8487
HIE_173@HB3	LYS_518@HZ1	LYS_518@NZ	4	0.0004	2.9155	137.4996
ALA_40@H	ASN_314@HD22	ASN_314@ND2	3	0.0003	2.8515	139.4694
PRO_41@HB2	GLU_317@HB2	GLU_317@CB	3	0.0003	2.9684	136.9188
PRO_41@HA	GLN_316@HE21	GLN_316@NE2	3	0.0003	2.7610	138.2636
PHE_43@HB2	LEU_319@HD21	LEU_319@CD2	3	0.0003	2.9785	137.2741
PHE_43@HD1	LEU_319@HD13	LEU_319@CD1	3	0.0003	2.9673	140.4060
PHE_43@HE1	GLU_327@HG2	GLU_327@CG	3	0.0003	2.9025	143.4972
PHE_43@HE1	GLU_317@HG2	GLU_317@CG	3	0.0003	2.9831	143.9408
PHE_43@HD2	ILE_328@HD11	ILE_328@CD1	3	0.0003	2.9348	137.8911
LYS_46@HZ3	ASN_331@HB3	ASN_331@CB	3	0.0003	2.9875	138.4651
ARG_71@HH22	CYS_521@HG	CYS_521@SG	3	0.0003	2.8443	149.3491

VAL_75@HG12	GLU_327@HG3	GLU_327@CG	3	0.0003	2.9635	137.9469
SER_76@HB3	GLU_327@HG2	GLU_327@CG	3	0.0003	2.9888	142.0423
GLN_82@OE1	LYS_618@HZ1	LYS_618@NZ	3	0.0003	2.9700	159.5951
GLN_82@HE21	ASN_454@HD21	ASN_454@ND2	3	0.0003	2.8502	143.5296
THR_83@HG21	ASP_544@H	ASP_544@N	3	0.0003	2.9457	142.1084
GLY_84@O	THR_542@HG1	THR_542@OG1	3	0.0003	2.8688	154.3476
ASP_88@HB3	THR_471@HG23	THR_471@CG2	3	0.0003	2.9512	138.9333
TYR_89@HE1	THR_542@HB	THR_542@CB	3	0.0003	2.9497	149.4600
TYR_89@HH	THR_471@HG23	THR_471@CG2	3	0.0003	2.9730	135.9773
ASP_96@OD2	GLN_464@HE22	GLN_464@NE2	3	0.0003	2.8050	162.0971
ASN_105@HB2	LEU_319@HD23	LEU_319@CD2	3	0.0003	2.9853	139.4406
TYR_117@HE1	ASN_515@HB2	ASN_515@CB	3	0.0003	2.9862	141.7911
TYR_117@HH	VAL_516@HG13	VAL_516@CG1	3	0.0003	2.8189	143.2608
TYR_117@HH	VAL_516@HG12	VAL_516@CG1	3	0.0003	2.9490	153.9230
TYR_121@HE1	LYS_540@HZ3	LYS_540@NZ	3	0.0003	2.9513	147.0390
LEU_123@HD12	LYS_540@HD3	LYS_540@CD	3	0.0003	2.9514	138.6093
PHE_124@HD1	VAL_541@HG23	VAL_541@CG2	3	0.0003	2.9047	138.7898
LYS_126@HA	VAL_475@HB	VAL_475@CB	3	0.0003	2.9368	138.6630
ASN_128@H	ASP_472@HA	ASP_472@CA	3	0.0003	2.9479	145.4384
ASN_128@HB3	THR_471@HG21	THR_471@CG2	3	0.0003	2.9612	141.8486
ASN_128@HD22	THR_471@HG23	THR_471@CG2	3	0.0003	2.7926	138.5924
ASN_128@HD22	THR_471@HG22	THR_471@CG2	3	0.0003	2.8185	150.9376
SER_162@H	ASN_515@HD22	ASN_515@ND2	3	0.0003	2.8712	139.1386
SER_162@HB2	ASN_515@HD21	ASN_515@ND2	3	0.0003	2.8340	138.9550
TYR_163@C	ASN_515@HD22	ASN_515@ND2	3	0.0003	2.9486	146.0160
ARG_166@HH21	VAL_516@HG12	VAL_516@CG1	3	0.0003	2.9424	143.6891
TYR_169@HD2	LYS_518@HZ3	LYS_518@NZ	3	0.0003	2.8505	140.2417
VAL_171@HG11	LEU_320@HD11	LEU_320@CD1	3	0.0003	2.9242	138.5239
VAL_171@HG11	LEU_320@HD12	LEU_320@CD1	3	0.0003	2.9295	141.4815
VAL_171@HG13	GLY_324@HA3	GLY_324@CA	3	0.0003	2.9666	139.5419
VAL_171@HG13	LEU_320@HD11	LEU_320@CD1	3	0.0003	2.9718	140.2398
VAL_171@HG22	LEU_320@HD23	LEU_320@CD2	3	0.0003	2.9036	139.6611
VAL_171@HG23	LEU_320@HD23	LEU_320@CD2	3	0.0003	2.9289	141.0693
VAL_171@HG23	LEU_320@HD22	LEU_320@CD2	3	0.0003	2.9214	142.1838
VAL_171@HG23	LEU_320@HD13	LEU_320@CD1	3	0.0003	2.8742	142.7806
VAL_171@HG23	LEU_320@HD11	LEU_320@CD1	3	0.0003	2.9384	143.0190
HIE_173@HE1	CYS_521@HG	CYS_521@SG	3	0.0003	2.9389	140.6136
HIE_173@HD2	LYS_518@HZ2	LYS_518@NZ	3	0.0003	2.9706	149.0863
TYR_37@HH	ASN_336@HD21	ASN_336@ND2	2	0.0002	2.9527	139.0019
ASN_38@HD21	ASN_314@HB2	ASN_314@CB	2	0.0002	2.9318	152.2347
PHE_42@H	GLU_317@HB3	GLU_317@CB	2	0.0002	2.9692	143.1596
PHE_42@CD1	ASN_311@HD22	ASN_311@ND2	2	0.0002	2.9935	144.5099
PHE_43@HA	LEU_319@HD13	LEU_319@CD1	2	0.0002	2.9528	143.1043
PHE_43@HA	LEU_319@HD12	LEU_319@CD1	2	0.0002	2.9608	140.3077
PHE_43@HB2	LEU_319@HD23	LEU_319@CD2	2	0.0002	2.9886	138.6706
PHE_43@HD1	GLU_317@HG3	GLU_317@CG	2	0.0002	2.9621	140.9140
PHE_43@HD1	LEU_319@HD22	LEU_319@CD2	2	0.0002	2.9521	138.8646
PHE_43@HD1	LEU_319@HD11	LEU_319@CD1	2	0.0002	2.9811	139.7792
PHE_43@HE1	ASN_311@HB2	ASN_311@CB	2	0.0002	2.9519	146.2387
PHE_43@HZ	GLU_327@HB3	GLU_327@CB	2	0.0002	2.9628	137.6305
PHE_43@HE2	TRP_340@HH2	TRP_340@CH2	2	0.0002	2.9366	138.7315
ALA_44@HA	ILE_328@HD13	ILE_328@CD1	2	0.0002	2.9825	140.9641
ALA_44@HB1	ILE_328@HD12	ILE_328@CD1	2	0.0002	2.9863	138.4068
ALA_44@HB1	ILE_328@HD13	ILE_328@CD1	2	0.0002	2.9279	138.5278
PHE_45@O	SER_332@HG	SER_332@OG	2	0.0002	2.7538	173.3028
LYS_46@HB3	SER_332@HB2	SER_332@CB	2	0.0002	2.9759	140.7434
VAL_75@HG11	GLU_327@HG2	GLU_327@CG	2	0.0002	2.9122	141.2750
VAL_75@HG13	GLU_327@HG3	GLU_327@CG	2	0.0002	2.9366	141.5066
VAL_75@HG22	PRO_323@HB2	PRO_323@CB	2	0.0002	2.9499	136.1237
VAL_75@HG22	GLU_327@HG2	GLU_327@CG	2	0.0002	2.9599	142.7222
PRO_80@HG2	SER_457@HB2	SER_457@CB	2	0.0002	2.9058	136.7032
GLY_81@HA3	SER_457@HB3	SER_457@CB	2	0.0002	2.9528	156.1116
THR_83@HG22	MET_543@HE2	MET_543@CE	2	0.0002	2.9131	140.0542

GLY_84@HA2	THR_542@HG1	THR_542@OG1	2	0.0002	2.8143	149.9849
ASN_85@HB2	THR_542@HG21	THR_542@CG2	2	0.0002	2.9221	139.1176
ASN_85@HB2	THR_542@HG23	THR_542@CG2	2	0.0002	2.9664	144.4564
ASN_85@HB3	LYS_540@HZ3	LYS_540@NZ	2	0.0002	2.9455	152.4241
ASN_85@HD21	LYS_540@HE3	LYS_540@CE	2	0.0002	2.9748	155.5298
TYR_89@HE1	VAL_541@HG22	VAL_541@CG2	2	0.0002	2.9392	149.2137
TYR_89@HE1	VAL_541@HG21	VAL_541@CG2	2	0.0002	2.9468	146.2764
ASP_95@OD1	GLN_464@HE21	GLN_464@NE2	2	0.0002	2.8983	166.9875
ASN_105@HB2	LEU_319@HD13	LEU_319@CD1	2	0.0002	2.9896	145.9982
ASN_105@HB2	LEU_319@HD11	LEU_319@CD1	2	0.0002	2.9715	139.2396
ASN_105@HB3	GLU_317@HG2	GLU_317@CG	2	0.0002	2.9773	138.6387
ASN_105@HB3	LEU_319@HD11	LEU_319@CD1	2	0.0002	2.9624	146.2555
ASN_105@HD21	LEU_319@HD23	LEU_319@CD2	2	0.0002	2.9764	145.8618
LYS_108@HE2	GLN_316@HG3	GLN_316@CG	2	0.0002	2.9470	139.4976
LYS_108@HE3	GLN_316@HG2	GLN_316@CG	2	0.0002	2.9778	140.5831
TYR_117@HH	VAL_516@HG11	VAL_516@CG1	2	0.0002	2.9029	159.5536
TYR_117@HD2	ASN_515@HD22	ASN_515@ND2	2	0.0002	2.9272	139.0094
TYR_121@HE1	LYS_540@HD2	LYS_540@CD	2	0.0002	2.9064	136.9321
LEU_123@HD11	LYS_540@HE3	LYS_540@CE	2	0.0002	2.8755	157.0066
LEU_123@HD13	LYS_540@HE2	LYS_540@CE	2	0.0002	2.8928	151.1546
LEU_123@HD13	LYS_540@HD3	LYS_540@CD	2	0.0002	2.9579	137.5583
LEU_123@HD13	LYS_540@HG3	LYS_540@CG	2	0.0002	2.9426	149.7307
PHE_124@HD1	VAL_541@HG22	VAL_541@CG2	2	0.0002	2.9322	137.4886
TYR_141@HE1	VAL_475@HG13	VAL_475@CG1	2	0.0002	2.9485	137.5636
TYR_141@HH	TRP_479@H	TRP_479@N	2	0.0002	2.7570	142.2877
ALA_143@HB1	ASP_480@HA	ASP_480@CA	2	0.0002	2.8980	138.3797
ALA_143@HB2	ASP_480@HB2	ASP_480@CB	2	0.0002	2.9147	138.1725
ASN_155@HD22	ASP_480@HB3	ASP_480@CB	2	0.0002	2.8210	139.6607
TYR_157@HH	GLN_482@HE21	GLN_482@NE2	2	0.0002	2.8994	143.5331
ARG_161@HH22	ASP_512@HB3	ASP_512@CB	2	0.0002	2.9804	137.0288
SER_162@HG	ASN_515@HD21	ASN_515@ND2	2	0.0002	2.8496	150.9437
GLY_164@HA3	LYS_518@HE3	LYS_518@CE	2	0.0002	2.8964	147.7282
ARG_166@HH21	VAL_516@HG11	VAL_516@CG1	2	0.0002	2.9611	144.5321
ARG_166@HH22	VAL_516@HG12	VAL_516@CG1	2	0.0002	2.9006	152.1468
TYR_169@HH	LYS_518@HD2	LYS_518@CD	2	0.0002	2.9513	153.9894
VAL_171@HB	PRO_323@HD3	PRO_323@CD	2	0.0002	2.9628	135.5073
VAL_171@HG12	PRO_323@HD3	PRO_323@CD	2	0.0002	2.9598	139.1612
VAL_171@HG12	LEU_320@HD11	LEU_320@CD1	2	0.0002	2.9784	143.5943
VAL_171@HG13	LEU_320@HD22	LEU_320@CD2	2	0.0002	2.9590	144.4647
VAL_171@HG13	LEU_319@HD22	LEU_319@CD2	2	0.0002	2.9801	142.1179
VAL_171@HG21	LEU_320@HD23	LEU_320@CD2	2	0.0002	2.9418	140.0618
VAL_171@HG21	LEU_320@HD21	LEU_320@CD2	2	0.0002	2.9412	144.7761
VAL_171@HG21	LEU_320@HD13	LEU_320@CD1	2	0.0002	2.8885	137.3264
VAL_171@HG21	LEU_320@HB2	LEU_320@CB	2	0.0002	2.9875	155.6008
VAL_171@HG22	LEU_320@HD21	LEU_320@CD2	2	0.0002	2.8982	141.6263
VAL_171@HG22	LEU_320@HD12	LEU_320@CD1	2	0.0002	2.9655	142.5880
HIE_173@HB3	LYS_518@HZ3	LYS_518@NZ	2	0.0002	2.9082	145.7465
HIE_173@HE1	LYS_518@HZ2	LYS_518@NZ	2	0.0002	2.9517	141.9114
HIE_173@NE2	LYS_518@HZ3	LYS_518@NZ	2	0.0002	2.9562	145.9284
HIE_173@CD2	LYS_518@HZ1	LYS_518@NZ	2	0.0002	2.9567	156.4237
TYR_176@HH	PRO_323@HG2	PRO_323@CG	2	0.0002	2.9120	140.1685
TYR_37@OH	ASN_336@HD22	ASN_336@ND2	1	0.0001	2.9105	142.4580
TYR_37@HH	ASN_336@HD22	ASN_336@ND2	1	0.0001	2.9196	135.6392
ASN_38@OD1	ASN_314@HD21	ASN_314@ND2	1	0.0001	2.8831	155.5677
ASN_38@HD22	ASP_313@HB3	ASP_313@CB	1	0.0001	2.9420	145.1877
PHE_39@HA	GLN_316@HE22	GLN_316@NE2	1	0.0001	2.8042	139.9387
PHE_39@C	GLN_316@HE22	GLN_316@NE2	1	0.0001	2.9850	146.7598
ALA_40@HB1	PRO_312@HB2	PRO_312@CB	1	0.0001	2.9272	140.2130
ALA_40@HB2	PRO_312@HD2	PRO_312@CD	1	0.0001	2.9057	136.5669
ALA_40@O	GLN_316@HE21	GLN_316@NE2	1	0.0001	2.7608	136.6708
PRO_41@HB2	GLU_317@HB3	GLU_317@CB	1	0.0001	2.8933	137.4148
PRO_41@O	ASN_311@HD22	ASN_311@ND2	1	0.0001	2.9323	137.0609
PHE_42@H	ASN_311@HD21	ASN_311@ND2	1	0.0001	2.9727	138.4194

PHE_43@HB3	LEU_319@HD12	LEU_319@CD1	1	0.0001	2.9651	139.3697
PHE_43@HB3	LEU_319@HD13	LEU_319@CD1	1	0.0001	2.9715	138.5745
PHE_43@CD1	ASN_311@HD21	ASN_311@ND2	1	0.0001	2.9565	153.0673
PHE_43@HD1	ASN_311@HD21	ASN_311@ND2	1	0.0001	2.7871	140.6232
PHE_43@HD1	LEU_319@HD21	LEU_319@CD2	1	0.0001	2.9739	144.2645
PHE_43@HD1	LEU_319@HD12	LEU_319@CD1	1	0.0001	2.9098	135.0457
PHE_43@HE1	ILE_328@HG13	ILE_328@CG1	1	0.0001	2.9763	136.9769
PHE_43@HZ	GLY_324@HA2	GLY_324@CA	1	0.0001	2.9866	145.1627
PHE_43@HZ	LEU_325@HD21	LEU_325@CD2	1	0.0001	2.9944	137.7815
PHE_43@HZ	LEU_325@HD22	LEU_325@CD2	1	0.0001	2.9290	143.1147
PHE_43@HE2	ILE_328@HD11	ILE_328@CD1	1	0.0001	2.9744	140.4322
PHE_43@HE2	LEU_325@HD23	LEU_325@CD2	1	0.0001	2.8925	137.0278
PHE_43@HE2	LEU_325@HD21	LEU_325@CD2	1	0.0001	2.9303	137.3902
PHE_43@HE2	LEU_325@HD22	LEU_325@CD2	1	0.0001	2.9757	137.3084
ALA_44@HA	ILE_328@HD12	ILE_328@CD1	1	0.0001	2.9846	144.3814
ALA_44@HA	ILE_328@HD11	ILE_328@CD1	1	0.0001	2.9939	139.4801
ALA_44@HB2	ILE_328@HD13	ILE_328@CD1	1	0.0001	2.9554	157.3078
ALA_44@HB3	ILE_328@HD13	ILE_328@CD1	1	0.0001	2.9557	137.9928
ALA_44@HB3	ILE_328@HD11	ILE_328@CD1	1	0.0001	2.9866	136.8990
LYS_46@HG3	SER_332@HB2	SER_332@CB	1	0.0001	2.9680	140.8539
LYS_46@HE2	GLU_327@HG3	GLU_327@CG	1	0.0001	2.9242	142.3901
LYS_46@HZ1	ASN_331@HB3	ASN_331@CB	1	0.0001	2.9821	150.4884
CYS_47@HB2	LEU_333@HD23	LEU_333@CD2	1	0.0001	2.9695	145.2042
CYS_47@HB2	LEU_333@HD22	LEU_333@CD2	1	0.0001	2.8614	147.0204
CYS_47@HG	LEU_333@HD23	LEU_333@CD2	1	0.0001	2.7384	138.2784
CYS_47@HG	LEU_333@HD22	LEU_333@CD2	1	0.0001	2.9932	163.2474
TYR_48@HD1	LEU_333@HD22	LEU_333@CD2	1	0.0001	2.9930	137.6277
TYR_48@HH	ASN_331@HB3	ASN_331@CB	1	0.0001	2.8164	138.2600
TYR_48@HE2	ASN_331@HD22	ASN_331@ND2	1	0.0001	2.7365	142.8227
TYR_48@HE2	LEU_333@HD23	LEU_333@CD2	1	0.0001	2.8808	137.0908
TYR_48@HE2	SER_457@HG	SER_457@OG	1	0.0001	2.7441	136.4205
TYR_48@HE2	LEU_333@HD13	LEU_333@CD1	1	0.0001	2.9887	137.2564
TYR_48@HD2	LEU_333@HD21	LEU_333@CD2	1	0.0001	2.9892	144.1898
ARG_71@HH11	LYS_540@HZ2	LYS_540@NZ	1	0.0001	2.9499	137.3163
ARG_71@HH11	LYS_540@HZ3	LYS_540@NZ	1	0.0001	2.9809	146.8214
GLY_72@HA3	PRO_323@HG2	PRO_323@CG	1	0.0001	2.9533	136.2671
ASN_73@HA	PRO_323@HB3	PRO_323@CB	1	0.0001	2.9515	140.4965
ASN_73@HD21	PRO_323@HG3	PRO_323@CG	1	0.0001	2.9659	159.3360
GLU_74@CD	LYS_540@HZ2	LYS_540@NZ	1	0.0001	2.9730	141.9065
VAL_75@HG11	GLU_327@HG3	GLU_327@CG	1	0.0001	2.8889	141.4490
VAL_75@HG11	PRO_323@HB3	PRO_323@CB	1	0.0001	2.9926	143.8680
VAL_75@HG12	PRO_323@HB3	PRO_323@CB	1	0.0001	2.9876	136.6074
VAL_75@HG12	GLU_327@HG2	GLU_327@CG	1	0.0001	2.9456	144.4544
VAL_75@HG21	PRO_323@HB2	PRO_323@CB	1	0.0001	2.9732	139.7795
ALA_79@CB	ASN_331@HD22	ASN_331@ND2	1	0.0001	2.9469	167.0771
PRO_80@HG2	SER_457@HG	SER_457@OG	1	0.0001	2.9913	139.5157
GLY_81@O	ASN_467@HD22	ASN_467@ND2	1	0.0001	2.8349	144.2469
GLN_82@OE1	ASN_331@HD21	ASN_331@ND2	1	0.0001	2.7621	141.9905
GLN_82@OE1	ASN_331@HD22	ASN_331@ND2	1	0.0001	2.7309	138.3744
GLN_82@HE21	SER_457@HB3	SER_457@CB	1	0.0001	2.9590	168.9383
GLN_82@HE22	ASN_454@HB3	ASN_454@CB	1	0.0001	2.9183	139.2999
GLN_82@HE22	ASN_454@HA	ASN_454@CA	1	0.0001	2.8513	159.3379
GLN_82@HE22	ASN_454@HD21	ASN_454@ND2	1	0.0001	2.8911	148.0488
GLN_82@HE22	TYR_456@HB3	TYR_456@CB	1	0.0001	2.9160	159.8198
GLN_82@HE22	SER_457@HB3	SER_457@CB	1	0.0001	2.8804	136.1402
GLN_82@HE22	ASN_331@HD21	ASN_331@ND2	1	0.0001	2.7718	140.3144
THR_83@HG21	ASN_467@HD22	ASN_467@ND2	1	0.0001	2.9738	136.7960
THR_83@HG21	MET_543@HG2	MET_543@CG	1	0.0001	2.9373	137.0765
THR_83@HG21	MET_543@HE1	MET_543@CE	1	0.0001	2.7980	135.6456
THR_83@HG21	ASP_469@HB2	ASP_469@CB	1	0.0001	2.9724	143.8318
THR_83@HG21	MET_543@HE2	MET_543@CE	1	0.0001	2.9323	135.1794
THR_83@HG22	MET_543@HB3	MET_543@CB	1	0.0001	2.9394	137.6230
THR_83@HG22	MET_543@HG3	MET_543@CG	1	0.0001	2.9931	145.2234

THR_83@HG22	MET_543@HE1	MET_543@CE	1	0.0001	2.9823	139.3663
THR_83@HG22	ASP_469@HB2	ASP_469@CB	1	0.0001	2.9907	138.1319
THR_83@HG23	MET_543@HB2	MET_543@CB	1	0.0001	2.9931	137.2305
THR_83@HG23	MET_543@HE2	MET_543@CE	1	0.0001	2.9543	141.4349
THR_83@HG23	ASP_544@H	ASP_544@N	1	0.0001	2.8724	141.8484
THR_83@OG1	ASP_544@H	ASP_544@N	1	0.0001	2.8400	145.9328
THR_83@HG1	MET_543@HE1	MET_543@CE	1	0.0001	2.9116	140.6363
ASN_85@HA	THR_542@HB	THR_542@CB	1	0.0001	2.9507	142.4222
ASN_85@HB2	LYS_540@HZ2	LYS_540@NZ	1	0.0001	2.7429	135.0283
ASN_85@HB2	LYS_540@HG2	LYS_540@CG	1	0.0001	2.9216	144.0460
ASN_85@HB3	LYS_540@HE2	LYS_540@CE	1	0.0001	2.9359	141.0983
ASN_85@HB3	LYS_540@HZ1	LYS_540@NZ	1	0.0001	2.8892	157.9799
ASN_85@OD1	VAL_541@H	VAL_541@N	1	0.0001	2.9471	150.2361
ASN_85@OD1	LYS_540@HZ1	LYS_540@NZ	1	0.0001	2.9378	142.8320
ASN_85@ND2	LYS_540@HZ1	LYS_540@NZ	1	0.0001	2.9978	136.4974
ASN_85@HD21	THR_542@HB	THR_542@CB	1	0.0001	2.9789	139.9341
ASN_85@HD21	LYS_540@HE2	LYS_540@CE	1	0.0001	2.8311	154.7508
TYR_89@HH	THR_471@HG22	THR_471@CG2	1	0.0001	2.9111	135.1126
TYR_89@HE2	VAL_475@HG23	VAL_475@CG2	1	0.0001	2.9452	139.5963
ASN_105@HB2	LEU_319@HD21	LEU_319@CD2	1	0.0001	2.9270	138.2858
ASN_105@HD21	LEU_319@HD21	LEU_319@CD2	1	0.0001	2.8852	138.8015
ASN_105@HD21	LEU_319@HD22	LEU_319@CD2	1	0.0001	2.9964	143.0219
LYS_108@HD3	GLN_316@HE22	GLN_316@NE2	1	0.0001	2.8942	137.9136
LYS_108@HD3	GLN_316@HB2	GLN_316@CB	1	0.0001	2.9924	137.8726
LYS_108@HE2	GLU_317@HG2	GLU_317@CG	1	0.0001	2.9273	146.3238
LYS_108@HE3	GLU_317@HG2	GLU_317@CG	1	0.0001	2.8908	137.9007
LYS_108@HZ1	GLN_316@HA	GLN_316@CA	1	0.0001	2.8554	143.5161
LYS_108@HZ1	GLN_316@HG3	GLN_316@CG	1	0.0001	2.9168	136.3911
LYS_108@HZ2	GLN_316@HB2	GLN_316@CB	1	0.0001	2.8941	142.3919
LYS_108@HZ3	GLU_317@HA	GLU_317@CA	1	0.0001	2.9695	138.9288
LYS_108@HZ3	GLN_316@HA	GLN_316@CA	1	0.0001	2.8895	158.1800
LYS_108@HZ3	GLN_316@HB2	GLN_316@CB	1	0.0001	2.8960	154.2790
TYR_117@HB3	ASN_515@HD22	ASN_515@ND2	1	0.0001	2.8336	154.3920
TYR_117@CG	ASN_515@HD22	ASN_515@ND2	1	0.0001	2.9967	142.5790
TYR_117@CD1	ASN_515@HD21	ASN_515@ND2	1	0.0001	2.9128	139.6719
TYR_117@HD1	ASN_515@HD21	ASN_515@ND2	1	0.0001	2.9374	143.1539
TYR_117@CE1	ASN_515@HD21	ASN_515@ND2	1	0.0001	2.9353	168.1685
TYR_117@HE1	VAL_516@HG22	VAL_516@CG2	1	0.0001	2.9759	140.1048
TYR_117@HH	VAL_516@HG22	VAL_516@CG2	1	0.0001	2.9245	148.8706
TYR_117@HH	ASN_515@HD22	ASN_515@ND2	1	0.0001	2.9946	154.7193
TYR_117@HH	VAL_516@HG21	VAL_516@CG2	1	0.0001	2.9993	171.7275
TYR_117@HH	VAL_516@HG23	VAL_516@CG2	1	0.0001	2.8699	157.3766
TYR_117@HE2	ASN_515@HD22	ASN_515@ND2	1	0.0001	2.8658	139.8544
TYR_117@HD2	ASN_515@HB3	ASN_515@CB	1	0.0001	2.9465	147.2367
TYR_121@OH	LYS_540@HE2	LYS_540@CE	1	0.0001	2.9506	139.7318
TYR_121@HH	LYS_540@HZ3	LYS_540@NZ	1	0.0001	2.9918	149.2831
LEU_123@HD11	VAL_541@H	VAL_541@N	1	0.0001	2.9282	153.5286
LEU_123@HD11	LYS_540@HE2	LYS_540@CE	1	0.0001	2.8815	135.3909
LEU_123@HD12	LYS_540@HE2	LYS_540@CE	1	0.0001	2.9816	154.4352
LEU_123@HD13	VAL_541@H	VAL_541@N	1	0.0001	2.7920	155.8528
LEU_123@HD22	ASP_512@HB3	ASP_512@CB	1	0.0001	2.9358	141.6303
PHE_124@HD1	VAL_541@HG21	VAL_541@CG2	1	0.0001	2.9746	136.3248
PHE_124@HE1	VAL_541@HG12	VAL_541@CG1	1	0.0001	2.9602	137.8015
PHE_124@HE1	VAL_541@HG11	VAL_541@CG1	1	0.0001	2.9846	136.4139
PHE_124@HZ	ALA_481@HB3	ALA_481@CB	1	0.0001	2.9367	146.0455
LYS_126@HE2	ASP_476@HA	ASP_476@CA	1	0.0001	2.9390	143.9284
LYS_126@HZ3	ASP_476@HA	ASP_476@CA	1	0.0001	2.9816	136.5968
ASN_128@H	VAL_475@HG22	VAL_475@CG2	1	0.0001	2.9899	139.7951
ASN_128@HD21	ASP_472@H	ASP_472@N	1	0.0001	2.8403	148.4327
ASN_128@HD21	THR_471@HG1	THR_471@OG1	1	0.0001	2.9545	138.9416
ASN_128@HD22	ASP_472@HA	ASP_472@CA	1	0.0001	2.8674	139.9688
TYR_141@HE1	ALA_478@HA	ALA_478@CA	1	0.0001	2.9757	144.7148
TYR_141@HE1	VAL_475@HA	VAL_475@CA	1	0.0001	2.9375	145.8561

TYR_141@OH	TRP_479@H	TRP_479@N	1	0.0001	2.8644	155.7309
TYR_141@HH	VAL_541@HG12	VAL_541@CG1	1	0.0001	2.9936	155.2720
ALA_143@HB1	ALA_478@HB3	ALA_478@CB	1	0.0001	2.9951	135.3721
ALA_143@HB2	ASP_480@HA	ASP_480@CA	1	0.0001	2.9712	138.3799
ALA_143@HB3	ASP_480@HB2	ASP_480@CB	1	0.0001	2.9670	138.4641
ASN_155@HD22	ASP_480@HB2	ASP_480@CB	1	0.0001	2.8470	141.1473
ARG_161@HG2	ASN_515@HD22	ASN_515@ND2	1	0.0001	2.7571	142.4608
ARG_161@NH1	GLY_514@H	GLY_514@N	1	0.0001	2.9959	138.5110
ARG_161@HH11	THR_511@HG23	THR_511@CG2	1	0.0001	2.6897	138.9009
ARG_161@HH21	ASP_512@HB3	ASP_512@CB	1	0.0001	2.9557	138.0570
ARG_161@HH22	THR_511@HG22	THR_511@CG2	1	0.0001	2.9649	141.1395
ARG_161@HH22	ASP_512@HB2	ASP_512@CB	1	0.0001	2.8458	142.8885
SER_162@O	ASN_515@HD21	ASN_515@ND2	1	0.0001	2.9540	164.5197
TYR_163@HA	ASN_515@HD22	ASN_515@ND2	1	0.0001	2.8015	144.1544
GLY_164@N	ASN_515@HD22	ASN_515@ND2	1	0.0001	2.9916	147.9608
GLY_164@H	LYS_518@HZ1	LYS_518@NZ	1	0.0001	2.8767	150.1174
GLY_164@HA3	LYS_518@HZ1	LYS_518@NZ	1	0.0001	2.9289	136.2379
ARG_166@HH21	VAL_516@HA	VAL_516@CA	1	0.0001	2.8608	164.3073
ARG_166@HH22	VAL_516@HA	VAL_516@CA	1	0.0001	2.9977	152.8251
ARG_166@HH22	VAL_516@HG11	VAL_516@CG1	1	0.0001	2.9930	135.9233
ARG_166@HH22	VAL_516@HG13	VAL_516@CG1	1	0.0001	2.9729	135.3996
TYR_169@HE1	LYS_518@HE3	LYS_518@CE	1	0.0001	2.9476	142.9731
TYR_169@HE2	LYS_518@HE3	LYS_518@CE	1	0.0001	2.9865	142.8656
VAL_171@HG12	LEU_320@HD23	LEU_320@CD2	1	0.0001	2.9250	136.3747
VAL_171@HG12	LEU_319@HD23	LEU_319@CD2	1	0.0001	2.9323	147.4804
VAL_171@HG12	GLY_324@HA3	GLY_324@CA	1	0.0001	2.9840	139.0960
VAL_171@HG12	LEU_319@HD22	LEU_319@CD2	1	0.0001	2.9728	135.3363
VAL_171@HG12	LEU_319@HD21	LEU_319@CD2	1	0.0001	2.9755	149.8647
VAL_171@HG12	LEU_320@HD21	LEU_320@CD2	1	0.0001	2.9514	145.4456
VAL_171@HG13	LEU_320@HG	LEU_320@CG	1	0.0001	2.9640	136.0659
VAL_171@HG21	LEU_320@HD12	LEU_320@CD1	1	0.0001	2.9615	144.6225
VAL_171@HG21	LEU_320@HD11	LEU_320@CD1	1	0.0001	2.9158	136.9363
VAL_171@HG22	LEU_320@HD22	LEU_320@CD2	1	0.0001	2.9955	145.1856
VAL_171@HG22	LEU_320@HD11	LEU_320@CD1	1	0.0001	2.9617	135.7401
VAL_171@HG23	LEU_320@HD21	LEU_320@CD2	1	0.0001	2.9425	141.2425
GLY_172@HA2	PRO_323@HG2	PRO_323@CG	1	0.0001	2.9983	137.9834
GLY_172@HA2	PRO_323@HD3	PRO_323@CD	1	0.0001	2.8692	146.9202
HIE_173@HB2	LYS_518@HE3	LYS_518@CE	1	0.0001	2.9941	144.0338
HIE_173@HB3	LYS_518@HE3	LYS_518@CE	1	0.0001	2.8682	136.1987
HIE_173@HE1	LYS_518@HE3	LYS_518@CE	1	0.0001	2.9117	139.6295
HIE_173@HE1	LYS_518@HZ3	LYS_518@NZ	1	0.0001	2.9426	137.8560
HIE_173@NE2	LYS_518@HZ1	LYS_518@NZ	1	0.0001	2.9933	164.7036
HIE_173@HE2	LYS_518@HZ1	LYS_518@NZ	1	0.0001	2.8038	145.0723
HIE_173@HE2	CYS_521@HG	CYS_521@SG	1	0.0001	2.7521	158.3879
HIE_173@HE2	LYS_518@HB3	LYS_518@CB	1	0.0001	2.9839	141.0212
HIE_173@CD2	LYS_518@HZ3	LYS_518@NZ	1	0.0001	2.9616	171.9251
TYR_176@HH	PRO_323@HD2	PRO_323@CD	1	0.0001	2.9060	136.8964

Table S4. Hydrogen bond analysis of S protein (BA.2)-ACE2 complex during the last 20 ns of MD simulation with S protein as donor and ACE2 as acceptor.

#Acceptor	DonorH	Donor	Frames	Frac	AvgDist	AvgAng
VAL_541@O	TYR_89@HH	TYR_89@OH	9229	0.9229	2.7453	165.5502
TRP_479@O	TYR_141@HH	TYR_141@OH	8523	0.8523	2.7577	165.5495
ASN_331@OD1	TYR_48@HH	TYR_48@OH	5694	0.5694	2.7781	155.9643
ASP_480@OD1	ASN_155@HD22	ASN_155@ND2	4299	0.4299	2.8563	165.0414
ASP_512@OD1	ARG_161@HH12	ARG_161@NH1	4242	0.4242	2.7798	156.2918
ASP_472@OD2	ASN_128@H	ASN_128@N	2538	0.2538	2.8659	164.1645
ASP_544@OD1	THR_83@HG1	THR_83@OG1	2297	0.2297	2.7074	163.2369
GLU_327@OE2	LYS_46@HZ2	LYS_46@NZ	2001	0.2001	2.7305	159.8604
GLU_327@OE1	LYS_46@HZ3	LYS_46@NZ	1975	0.1975	2.7326	159.3155
ASP_472@OD1	ASN_128@H	ASN_128@N	1954	0.1954	2.8657	161.9071
GLU_327@OE2	LYS_46@HZ3	LYS_46@NZ	1953	0.1953	2.7282	158.1404
GLU_327@OE1	LYS_46@HZ1	LYS_46@NZ	1764	0.1764	2.7224	158.4546

ASP_334@OD2	TYR_37@HH	TYR_37@OH	1652	0.1652	2.6888	162.7179
GLU_337@OE2	PHE_45@H	PHE_45@N	1606	0.1606	2.8781	157.8172
ASN_331@O	TYR_48@HH	TYR_48@OH	1573	0.1573	2.7641	155.8226
GLU_317@OE2	ASN_105@H	ASN_105@N	1556	0.1556	2.8427	165.4033
ASN_331@OD1	LYS_46@HZ1	LYS_46@NZ	1555	0.1555	2.8224	155.0685
GLU_327@OE1	SER_76@HG	SER_76@OG	1478	0.1478	2.6963	164.0958
ASP_512@O	ARG_161@HH11	ARG_161@NH1	1142	0.1142	2.8459	147.1124
ASN_515@OD1	SER_162@H	SER_162@N	1040	0.1040	2.8644	158.9792
GLU_317@OE1	ASN_105@H	ASN_105@N	1021	0.1021	2.8386	164.6936
GLU_327@OE2	LYS_46@HZ1	LYS_46@NZ	976	0.0976	2.7265	158.5452
ASP_472@OD2	ASN_128@HD21	ASN_128@ND2	808	0.0808	2.8236	163.1318
GLU_327@OE1	LYS_46@HZ2	LYS_46@NZ	778	0.0778	2.7222	157.7996
ASP_313@O	ASN_38@HD22	ASN_38@ND2	709	0.0709	2.8422	151.9465
ASN_331@OD1	LYS_46@HZ2	LYS_46@NZ	703	0.0703	2.8289	155.8814
ASN_331@OD1	LYS_46@HZ3	LYS_46@NZ	696	0.0696	2.8277	155.9213
GLN_316@O	LYS_108@HZ2	LYS_108@NZ	584	0.0584	2.8119	153.9518
THR_471@OG1	ASN_128@HD21	ASN_128@ND2	459	0.0459	2.8750	159.1622
ASP_313@OD1	ASN_38@HD22	ASN_38@ND2	425	0.0425	2.8348	153.9379
GLU_317@OE1	LYS_108@HZ1	LYS_108@NZ	420	0.0420	2.7905	157.4565
ASP_512@OD2	ARG_161@HH12	ARG_161@NH1	406	0.0406	2.7851	157.1577
GLN_316@O	LYS_108@HZ1	LYS_108@NZ	389	0.0389	2.8193	152.6150
GLU_327@OE2	SER_76@HG	SER_76@OG	385	0.0385	2.6778	165.7468
ASP_480@OD2	ASN_155@HD22	ASN_155@ND2	376	0.0376	2.8213	163.0243
ASP_472@OD1	SER_127@HG	SER_127@OG	364	0.0364	2.6356	165.7015
GLU_337@OE1	PHE_45@H	PHE_45@N	360	0.0360	2.9015	162.0898
GLN_316@O	LYS_108@HZ3	LYS_108@NZ	347	0.0347	2.8138	152.5818
GLU_317@OE1	LYS_108@HZ3	LYS_108@NZ	322	0.0322	2.7970	157.0850
GLU_317@OE1	LYS_108@HZ2	LYS_108@NZ	262	0.0262	2.7885	157.4804
LYS_540@HB2	ASN_85@HD22	ASN_85@ND2	259	0.0259	2.8187	146.9217
GLU_317@OE2	LYS_108@HZ2	LYS_108@NZ	245	0.0245	2.7841	157.9416
GLN_316@OE1	LYS_108@HZ3	LYS_108@NZ	229	0.0229	2.8066	153.6982
GLN_316@OE1	LYS_108@HZ1	LYS_108@NZ	226	0.0226	2.8089	155.1187
ASN_331@HD21	SER_76@HA	SER_76@CA	218	0.0218	2.9237	152.6790
GLU_317@OE2	LYS_108@HZ1	LYS_108@NZ	168	0.0168	2.7941	155.7396
ASN_331@ND2	LYS_46@HZ1	LYS_46@NZ	165	0.0165	2.9079	148.1849
GLY_514@HA2	ARG_161@HD3	ARG_161@CD	164	0.0164	2.9166	143.3700
GLU_317@OE2	LYS_108@HZ3	LYS_108@NZ	160	0.0160	2.7927	153.9583
GLN_316@OE1	LYS_108@HZ2	LYS_108@NZ	151	0.0151	2.8211	155.0515
VAL_475@O	LYS_126@HZ3	LYS_126@NZ	147	0.0147	2.8358	157.5360
ASN_515@OD1	SER_162@HG	SER_162@OG	142	0.0142	2.7313	156.5555
LEU_319@HD12	TYR_176@HH	TYR_176@OH	133	0.0133	2.7621	146.4185
ALA_478@HB1	ALA_143@HA	ALA_143@CA	129	0.0129	2.9414	148.1254
ASP_469@OD2	ASN_128@HD22	ASN_128@ND2	127	0.0127	2.8249	157.5205
ALA_478@HB3	ALA_143@HA	ALA_143@CA	118	0.0118	2.9479	147.9682
ASP_334@OD1	TYR_37@HH	TYR_37@OH	113	0.0113	2.7762	161.0213
ALA_478@HB2	ALA_143@HA	ALA_143@CA	113	0.0113	2.9431	148.5557
ASP_544@HB3	GLY_84@HA2	GLY_84@CA	113	0.0113	2.9453	143.1727
GLU_327@HB3	PHE_43@HE1	PHE_43@CE1	111	0.0111	2.9586	146.1893
VAL_475@O	LYS_126@HZ1	LYS_126@NZ	110	0.0110	2.8406	157.8559
ASN_331@HB3	LYS_46@HE3	LYS_46@CE	101	0.0101	2.9208	146.1572
ALA_519@O	HIE_173@HE2	HIE_173@NE2	86	0.0086	2.9141	161.7022
THR_471@HG1	ASN_128@HD21	ASN_128@ND2	84	0.0084	2.8994	149.1190
ASN_331@OD1	LYS_46@HE3	LYS_46@CE	71	0.0071	2.9644	143.3018
THR_471@HG23	ASN_128@HD21	ASN_128@ND2	67	0.0067	2.8375	146.0775
ASN_331@HB3	LYS_46@HE2	LYS_46@CE	66	0.0066	2.8803	148.0042
VAL_516@O	TYR_169@HH	TYR_169@OH	66	0.0066	2.8191	146.4795
ASP_334@OD2	LYS_54@HZ1	LYS_54@NZ	56	0.0056	2.8035	155.9428
GLN_316@HG3	PRO_41@HB3	PRO_41@CB	55	0.0055	2.9540	141.3549
THR_471@HG22	ASN_128@HD21	ASN_128@ND2	55	0.0055	2.8199	146.2541
ASP_544@HB2	GLY_84@HA2	GLY_84@CA	54	0.0054	2.9282	141.0426
ASN_331@HD22	ALA_79@HB1	ALA_79@CB	53	0.0053	2.8313	142.4231
ASP_544@HB2	THR_83@HB	THR_83@CB	53	0.0053	2.9388	142.0956
THR_471@O	ASN_128@HD21	ASN_128@ND2	51	0.0051	2.8938	156.0918

ASN_515@OD1	TYR_117@HH	TYR_117@OH	49	0.0049	2.7572	159.6136
ASP_334@OD1	LYS_54@HZ1	LYS_54@NZ	48	0.0048	2.8147	157.7252
ASN_331@HD22	ALA_79@HB2	ALA_79@CB	45	0.0045	2.8618	143.5598
ASN_331@HD21	LYS_46@HZ3	LYS_46@NZ	42	0.0042	2.8723	148.8670
ASN_331@HD21	LYS_46@HZ1	LYS_46@NZ	42	0.0042	2.8896	146.8180
ASN_515@HB3	TYR_117@HE1	TYR_117@CE1	41	0.0041	2.9346	141.5653
LEU_319@HD13	TYR_176@HH	TYR_176@OH	38	0.0038	2.7926	146.2066
THR_471@HB	ASN_128@HD21	ASN_128@ND2	37	0.0037	2.7961	141.9411
GLU_327@HG2	PHE_43@HZ	PHE_43@CZ	36	0.0036	2.9470	141.1631
ASN_331@HD22	ALA_79@HB3	ALA_79@CB	36	0.0036	2.8366	141.1552
ASN_515@HD22	GLY_164@HA2	GLY_164@CA	36	0.0036	2.8560	141.3223
LEU_319@HG	PHE_43@HB2	PHE_43@CB	35	0.0035	2.9636	146.5823
ASP_512@O	ARG_161@HH22	ARG_161@NH2	35	0.0035	2.8645	153.4804
ASP_480@HB2	TYR_157@HH	TYR_157@OH	34	0.0034	2.8303	142.5693
ASN_515@HD22	SER_162@HB2	SER_162@CB	34	0.0034	2.9031	145.6085
ASN_515@O	TYR_117@HH	TYR_117@OH	34	0.0034	2.8225	155.8960
VAL_475@HG22	SER_127@HA	SER_127@CA	33	0.0033	2.9419	139.9848
VAL_475@HG23	SER_127@HA	SER_127@CA	33	0.0033	2.9301	140.8669
ASP_472@HB2	ASN_128@HB3	ASN_128@CB	32	0.0032	2.9472	139.4292
ASP_512@OD1	ARG_161@HH11	ARG_161@NH1	32	0.0032	2.7606	156.1972
ASN_515@HD21	SER_162@HB2	SER_162@CB	32	0.0032	2.9292	143.4778
CYS_521@HG	HIE_173@HE2	HIE_173@NE2	32	0.0032	2.8284	144.7035
LYS_540@HE3	ASN_85@HB2	ASN_85@CB	32	0.0032	2.9034	142.6290
ASN_515@O	ARG_166@HH22	ARG_166@NH2	31	0.0031	2.8430	151.2300
LYS_540@HB3	ASN_85@HD22	ASN_85@ND2	31	0.0031	2.8345	140.8462
CYS_521@HG	HIE_173@HE1	HIE_173@CE1	30	0.0030	2.8487	149.6786
ASN_314@HD21	PHE_42@HE2	PHE_42@CE2	28	0.0028	2.8857	140.0951
ASN_331@CG	TYR_48@HH	TYR_48@OH	27	0.0027	2.9598	139.2511
VAL_541@HB	TYR_89@HH	TYR_89@OH	27	0.0027	2.8551	144.9296
VAL_475@O	LYS_126@HZ2	LYS_126@NZ	26	0.0026	2.8457	159.9295
ASP_480@HB3	ASN_155@HD22	ASN_155@ND2	26	0.0026	2.8656	142.6375
LYS_540@HE2	ASN_85@HB2	ASN_85@CB	26	0.0026	2.9101	144.7857
VAL_541@HG21	PHE_124@HE1	PHE_124@CE1	26	0.0026	2.9613	140.2385
ASN_331@ND2	LYS_46@HZ2	LYS_46@NZ	25	0.0025	2.9126	148.9130
VAL_516@O	ARG_166@HH21	ARG_166@NH2	25	0.0025	2.8446	148.1430
VAL_516@O	TYR_117@HH	TYR_117@OH	25	0.0025	2.8024	157.5670
LYS_540@HG2	LEU_123@HD13	LEU_123@CD1	25	0.0025	2.9483	140.1259
THR_542@HG23	ASN_85@HD22	ASN_85@ND2	25	0.0025	2.8530	141.8540
GLU_337@OE1	LYS_46@H	LYS_46@N	24	0.0024	2.9464	157.0218
PRO_323@HD2	VAL_171@HB	VAL_171@CB	23	0.0023	2.9421	140.7465
PRO_323@HD3	VAL_171@HG21	VAL_171@CG2	23	0.0023	2.9389	140.2554
PRO_323@HG3	ASN_73@HA	ASN_73@CA	23	0.0023	2.9461	143.7192
PRO_323@HG3	GLY_172@HA2	GLY_172@CA	23	0.0023	2.9467	143.8965
ASN_331@ND2	LYS_46@HZ3	LYS_46@NZ	23	0.0023	2.9140	148.8365
THR_471@HG21	ASN_128@HD21	ASN_128@ND2	23	0.0023	2.8145	147.0784
ASP_469@OD1	ASN_128@HD22	ASN_128@ND2	22	0.0022	2.9194	160.1775
ASP_544@HB2	THR_83@HG1	THR_83@OG1	22	0.0022	2.7592	145.1275
ASN_331@HB3	LYS_46@HD2	LYS_46@CD	21	0.0021	2.9601	143.9109
VAL_475@HG21	SER_127@HA	SER_127@CA	21	0.0021	2.9566	141.9469
ASN_515@HB3	GLY_164@HA3	GLY_164@CA	21	0.0021	2.9421	145.9427
LYS_540@HG2	LEU_123@HD11	LEU_123@CD1	21	0.0021	2.9558	141.3499
MET_543@HB3	THR_83@HB	THR_83@CB	21	0.0021	2.9479	141.1959
GLN_316@HB2	LYS_108@HE2	LYS_108@CE	20	0.0020	2.8702	143.3183
LEU_319@HD11	TYR_176@HH	TYR_176@OH	20	0.0020	2.7641	152.6718
ASN_331@HD21	LYS_46@HZ2	LYS_46@NZ	20	0.0020	2.8911	150.1725
SER_457@OG	GLN_82@HE21	GLN_82@NE2	20	0.0020	2.9051	161.4428
THR_471@HB	ASN_128@HD22	ASN_128@ND2	20	0.0020	2.8187	144.1972
LYS_540@HG2	LEU_123@HD12	LEU_123@CD1	20	0.0020	2.9481	141.1535
GLN_316@HB2	LYS_108@HE3	LYS_108@CE	19	0.0019	2.8812	144.9370
GLY_324@HA2	TYR_176@HH	TYR_176@OH	19	0.0019	2.8929	141.0070
GLU_327@HG3	LYS_46@HD3	LYS_46@CD	18	0.0018	2.9617	141.4255
THR_471@HG21	ASN_128@HD22	ASN_128@ND2	18	0.0018	2.8435	142.6600
VAL_475@HG12	TYR_89@HE2	TYR_89@CE2	18	0.0018	2.9595	142.7604

ASN_515@HD22	TYR_117@HD1	TYR_117@CD1	18	0.0018	2.8749	145.9126
VAL_541@HG23	PHE_124@HE1	PHE_124@CE1	18	0.0018	2.9592	142.2585
THR_542@HG21	GLY_84@HA2	GLY_84@CA	18	0.0018	2.9511	146.3151
ASN_331@HD22	LYS_46@HZ1	LYS_46@NZ	17	0.0017	2.9212	144.4266
ASP_472@HA	ASN_128@HB2	ASN_128@CB	17	0.0017	2.9513	145.8543
VAL_475@HB	TYR_141@HE1	TYR_141@CE1	17	0.0017	2.9718	141.9103
ASP_476@OD2	LYS_126@HZ3	LYS_126@NZ	17	0.0017	2.7775	157.6579
THR_542@HG22	GLY_84@HA2	GLY_84@CA	17	0.0017	2.9375	145.8437
LEU_319@HG	PHE_43@HD1	PHE_43@CD1	16	0.0016	2.9457	139.9284
ASP_472@HB2	ASN_128@HB2	ASN_128@CB	16	0.0016	2.9578	139.5966
ASN_515@OD1	ARG_166@HH22	ARG_166@NH2	16	0.0016	2.8405	147.9694
THR_542@HG22	ASN_85@HD22	ASN_85@ND2	16	0.0016	2.8576	142.4397
ASP_544@OD2	THR_83@HG1	THR_83@OG1	16	0.0016	2.6518	164.7970
ASN_331@OD1	GLN_82@HE21	GLN_82@NE2	15	0.0015	2.8738	150.7245
THR_471@HG23	ASN_128@HD22	ASN_128@ND2	15	0.0015	2.8076	147.2106
VAL_541@HG22	PHE_124@HE1	PHE_124@CE1	15	0.0015	2.9436	144.8802
GLN_316@HE21	PRO_41@HA	PRO_41@CA	14	0.0014	2.9288	144.4343
LYS_518@HE2	GLY_164@HA3	GLY_164@CA	14	0.0014	2.9271	146.5358
PRO_315@O	LYS_108@HZ3	LYS_108@NZ	13	0.0013	2.8377	157.3589
GLN_316@HG3	LYS_108@HE3	LYS_108@CE	13	0.0013	2.8796	147.2000
GLN_316@HG3	PRO_41@HA	PRO_41@CA	13	0.0013	2.9428	138.2682
LEU_319@HD13	PHE_43@HB2	PHE_43@CB	13	0.0013	2.9194	141.3627
THR_471@HG1	ASN_128@HD22	ASN_128@ND2	13	0.0013	2.8972	139.5625
LEU_320@H	VAL_171@HG21	VAL_171@CG2	12	0.0012	2.8700	151.5885
PRO_323@HD3	VAL_171@HG23	VAL_171@CG2	12	0.0012	2.9287	144.7265
VAL_475@HB	LYS_126@HA	LYS_126@CA	12	0.0012	2.9514	142.3197
VAL_475@HG13	TYR_89@HE2	TYR_89@CE2	12	0.0012	2.9636	140.2939
LEU_319@HD12	PHE_43@HB2	PHE_43@CB	11	0.0011	2.9625	142.0874
ILE_328@HG12	ALA_44@HB2	ALA_44@CB	11	0.0011	2.9626	140.1355
ASN_331@HB3	LYS_46@HD3	LYS_46@CD	11	0.0011	2.9353	142.4427
SER_332@HB2	LYS_46@HG2	LYS_46@CG	11	0.0011	2.9385	147.4037
LYS_540@HD2	ASN_85@HB2	ASN_85@CB	11	0.0011	2.9478	139.3069
GLU_317@HB3	PHE_42@H	PHE_42@N	10	0.0010	2.9285	142.3313
ASN_331@HD22	TYR_48@HH	TYR_48@OH	10	0.0010	2.8970	141.3542
ASP_472@HB2	ASN_128@HD21	ASN_128@ND2	10	0.0010	2.7400	146.5143
VAL_475@HG11	TYR_89@HE2	TYR_89@CE2	10	0.0010	2.9712	143.3908
THR_542@HG1	GLY_84@H	GLY_84@N	10	0.0010	2.8730	140.4149
ASN_311@HD22	ALA_40@HB2	ALA_40@CB	9	0.0009	2.8984	142.8411
ASP_313@OD1	ASN_38@HD21	ASN_38@ND2	9	0.0009	2.8614	158.2723
LEU_320@HD13	VAL_171@HG13	VAL_171@CG1	9	0.0009	2.9506	139.4960
PRO_323@HD3	VAL_171@HG22	VAL_171@CG2	9	0.0009	2.9313	140.0813
GLU_327@HG2	PHE_43@HE1	PHE_43@CE1	9	0.0009	2.8879	140.5615
THR_471@O	ASN_128@HD22	ASN_128@ND2	9	0.0009	2.8696	152.9703
ASP_472@HA	ASN_128@H	ASN_128@N	9	0.0009	2.9593	144.1286
ASP_472@HB2	ASN_128@HD22	ASN_128@ND2	9	0.0009	2.8878	138.4897
ASP_472@HB2	ASN_128@H	ASN_128@N	9	0.0009	2.9200	149.6907
ASN_515@HB2	TYR_117@HE1	TYR_117@CE1	9	0.0009	2.9461	140.8424
GLN_316@HG3	LYS_108@HE2	LYS_108@CE	8	0.0008	2.8916	149.7902
LEU_320@HB2	VAL_171@HG22	VAL_171@CG2	8	0.0008	2.9650	139.6913
LEU_320@HB2	VAL_171@HG21	VAL_171@CG2	8	0.0008	2.9531	141.1251
PRO_323@HD2	VAL_171@HG11	VAL_171@CG1	8	0.0008	2.9393	139.3466
GLU_327@HG2	VAL_75@HG13	VAL_75@CG1	8	0.0008	2.9508	139.0695
ASN_331@HD22	GLN_82@HE21	GLN_82@NE2	8	0.0008	2.8303	142.9574
SER_332@HA	LYS_46@HG2	LYS_46@CG	8	0.0008	2.9383	143.9257
LEU_333@HB3	CYS_47@HB2	CYS_47@CB	8	0.0008	2.9495	146.5078
ASP_480@HA	PHE_124@HE1	PHE_124@CE1	8	0.0008	2.9341	142.8078
ASN_515@HD22	SER_162@H	SER_162@N	8	0.0008	2.9030	152.5982
VAL_541@HG21	PHE_124@HD1	PHE_124@CD1	8	0.0008	2.9837	136.7884
GLN_316@HE21	LYS_108@HE3	LYS_108@CE	7	0.0007	2.8825	147.6224
LEU_320@HB2	VAL_171@HG23	VAL_171@CG2	7	0.0007	2.9369	142.0633
LEU_320@HD23	VAL_171@HG23	VAL_171@CG2	7	0.0007	2.9443	142.3263
GLU_327@HG3	LYS_46@HZ3	LYS_46@NZ	7	0.0007	2.9008	142.7106
ILE_328@HD11	PHE_43@HD1	PHE_43@CD1	7	0.0007	2.9298	140.1784

ILE_328@HD13	PHE_43@HD1	PHE_43@CD1	7	0.0007	2.9471	144.6247
ASN_331@ND2	TYR_48@HH	TYR_48@OH	7	0.0007	2.9050	147.7079
LEU_333@HD21	CYS_47@HB2	CYS_47@CB	7	0.0007	2.9483	140.8704
ASN_454@O	GLN_82@HE22	GLN_82@NE2	7	0.0007	2.8987	154.4595
GLY_514@HA2	ARG_161@HD2	ARG_161@CD	7	0.0007	2.9235	137.7478
LYS_540@HD3	ASN_85@HB2	ASN_85@CB	7	0.0007	2.9286	139.4779
VAL_541@HG22	TYR_89@HH	TYR_89@OH	7	0.0007	2.7941	139.5340
VAL_541@HG23	PHE_124@HD1	PHE_124@CD1	7	0.0007	2.9378	140.3438
THR_542@HB	TYR_89@HE1	TYR_89@CE1	7	0.0007	2.9426	142.4992
THR_542@HG21	ASN_85@H	ASN_85@N	7	0.0007	2.8923	144.1100
THR_542@HG22	ASN_85@HB2	ASN_85@CB	7	0.0007	2.9421	143.7140
THR_542@HG23	ASN_85@HB2	ASN_85@CB	7	0.0007	2.9435	140.1971
ASP_544@HB2	THR_83@HG21	THR_83@CG2	7	0.0007	2.9498	138.5213
ASP_544@HB2	THR_83@HG23	THR_83@CG2	7	0.0007	2.9670	140.6778
ASN_314@HB2	ASN_38@HA	ASN_38@CA	6	0.0006	2.9737	143.7027
GLU_317@HG3	PHE_43@HE1	PHE_43@CE1	6	0.0006	2.9270	139.3555
LEU_319@HD23	PHE_43@HB2	PHE_43@CB	6	0.0006	2.9604	140.6928
LEU_320@H	VAL_171@HG23	VAL_171@CG2	6	0.0006	2.8954	146.0696
PRO_323@HD2	VAL_171@HG21	VAL_171@CG2	6	0.0006	2.9235	142.4945
PRO_323@HD2	VAL_171@HG12	VAL_171@CG1	6	0.0006	2.9391	144.4584
PRO_323@HD3	VAL_171@HB	VAL_171@CB	6	0.0006	2.9115	139.5601
GLY_324@HA3	VAL_171@HG13	VAL_171@CG1	6	0.0006	2.9377	139.8527
ILE_328@HG12	ALA_44@HB1	ALA_44@CB	6	0.0006	2.9408	138.6502
ASN_331@HD22	LYS_46@HZ2	LYS_46@NZ	6	0.0006	2.9145	144.0194
ASN_331@HD22	GLN_82@HG3	GLN_82@CG	6	0.0006	2.9191	144.9652
THR_471@HG22	ASN_128@HD22	ASN_128@ND2	6	0.0006	2.7888	148.4216
THR_471@HG23	ASP_88@HB3	ASP_88@CB	6	0.0006	2.9424	136.3164
ASP_480@HA	ALA_143@HB1	ALA_143@CB	6	0.0006	2.9090	141.7474
ASP_480@HA	PHE_124@HZ	PHE_124@CZ	6	0.0006	2.9392	141.6319
ASN_515@HD21	SER_162@HG	SER_162@OG	6	0.0006	2.8660	142.5888
ASN_515@O	ARG_166@HH21	ARG_166@NH2	6	0.0006	2.8485	145.8067
VAL_516@HA	TYR_117@HE2	TYR_117@CE2	6	0.0006	2.9621	140.2797
ASP_544@HB2	THR_83@HG22	THR_83@CG2	6	0.0006	2.9524	143.6474
ASP_313@HB3	ASN_38@HD22	ASN_38@ND2	5	0.0005	2.8661	139.3713
PRO_315@O	LYS_108@HZ2	LYS_108@NZ	5	0.0005	2.8300	154.1115
GLN_316@HA	LYS_108@HE3	LYS_108@CE	5	0.0005	2.8611	145.7963
LEU_319@HD12	PHE_43@HA	PHE_43@CA	5	0.0005	2.9476	136.9986
LEU_319@HD23	PHE_43@HD1	PHE_43@CD1	5	0.0005	2.9622	148.2494
LEU_320@HD13	VAL_171@HG22	VAL_171@CG2	5	0.0005	2.9144	141.4911
LEU_320@HD13	VAL_171@HG23	VAL_171@CG2	5	0.0005	2.9412	140.3607
PRO_323@HD2	VAL_171@HG23	VAL_171@CG2	5	0.0005	2.9236	138.6633
PRO_323@HD2	VAL_171@HG13	VAL_171@CG1	5	0.0005	2.9299	138.8464
LEU_325@HD21	PHE_43@HE2	PHE_43@CE2	5	0.0005	2.9691	138.3471
ILE_328@HG12	ALA_44@HB3	ALA_44@CB	5	0.0005	2.9588	139.7056
ILE_328@HG13	ALA_44@HB2	ALA_44@CB	5	0.0005	2.9561	141.4110
ILE_328@HD12	PHE_43@HD1	PHE_43@CD1	5	0.0005	2.9619	159.4453
ILE_328@HD13	PHE_43@HD2	PHE_43@CD2	5	0.0005	2.9806	143.2343
SER_457@HB2	TYR_48@HE2	TYR_48@CE2	5	0.0005	2.9503	146.2392
ASP_480@HA	ALA_143@HB3	ALA_143@CB	5	0.0005	2.9505	146.7512
ASP_480@HB2	ASN_155@HD22	ASN_155@ND2	5	0.0005	2.7954	150.5205
ASP_480@HB2	TYR_157@HE1	TYR_157@CE1	5	0.0005	2.9663	142.5232
ASP_480@HB3	ALA_143@HB2	ALA_143@CB	5	0.0005	2.9276	137.4180
ASN_515@HA	ARG_161@HG3	ARG_161@CG	5	0.0005	2.8950	139.9595
ASN_515@HD21	TYR_117@HE1	TYR_117@CE1	5	0.0005	2.9337	140.7213
LYS_518@HE3	GLY_164@HA3	GLY_164@CA	5	0.0005	2.9079	152.0988
CYS_521@SG	HIE_173@HE2	HIE_173@NE2	5	0.0005	2.9657	150.3254
THR_542@HG21	ASN_85@HD22	ASN_85@ND2	5	0.0005	2.7755	142.2976
THR_542@HG21	ASN_85@HB2	ASN_85@CB	5	0.0005	2.9467	136.7653
THR_542@HG23	GLY_84@HA2	GLY_84@CA	5	0.0005	2.9609	145.2990
GLN_316@HB2	LYS_108@HZ1	LYS_108@NZ	4	0.0004	2.7953	143.2549
GLN_316@HB2	LYS_108@HD3	LYS_108@CD	4	0.0004	2.9512	140.9583
GLN_316@HB2	LYS_108@HZ2	LYS_108@NZ	4	0.0004	2.9697	140.0395
GLU_317@HG2	LYS_108@HE3	LYS_108@CE	4	0.0004	2.9666	153.4242

GLU_317@HG3	PHE_43@HB3	PHE_43@CB	4	0.0004	2.9593	138.5944
CYS_318@HA	PHE_43@HE1	PHE_43@CE1	4	0.0004	2.9626	138.2543
LEU_319@HD11	PHE_43@HB2	PHE_43@CB	4	0.0004	2.9591	140.0974
LEU_320@H	VAL_171@HG22	VAL_171@CG2	4	0.0004	2.9259	144.8447
LEU_320@HD11	VAL_171@HG23	VAL_171@CG2	4	0.0004	2.9492	141.7471
LEU_320@HD13	VAL_171@HG12	VAL_171@CG1	4	0.0004	2.9551	140.9426
GLU_322@OE2	ASN_73@HD22	ASN_73@ND2	4	0.0004	2.8407	158.9213
PRO_323@HG2	ASN_73@HA	ASN_73@CA	4	0.0004	2.9464	145.8485
GLU_327@HG3	LYS_46@HZ1	LYS_46@NZ	4	0.0004	2.8999	149.3220
ASN_331@HB3	LYS_46@HG2	LYS_46@CG	4	0.0004	2.9825	140.7247
SER_332@HA	LYS_46@HG3	LYS_46@CG	4	0.0004	2.9424	145.8842
THR_471@HG21	TYR_89@HH	TYR_89@OH	4	0.0004	2.9218	137.7771
THR_471@HG21	ASP_88@HB3	ASP_88@CB	4	0.0004	2.9115	136.5073
ASP_476@HA	LYS_126@HE3	LYS_126@CE	4	0.0004	2.9320	141.8896
ASP_480@HA	ALA_143@HB2	ALA_143@CB	4	0.0004	2.9407	141.1416
VAL_516@HA	TYR_117@HH	TYR_117@OH	4	0.0004	2.9203	154.2732
VAL_516@O	ARG_166@HH22	ARG_166@NH2	4	0.0004	2.8594	149.3750
LYS_540@HE2	TYR_121@HE1	TYR_121@CE1	4	0.0004	2.8089	137.3724
THR_542@HG22	ASN_85@H	ASN_85@N	4	0.0004	2.8814	145.7209
MET_543@HB3	THR_83@HG23	THR_83@CG2	4	0.0004	2.9437	137.6695
ASP_544@OD2	GLN_77@HE22	GLN_77@NE2	4	0.0004	2.7693	146.9359
ASP_313@O	ASN_38@HD21	ASN_38@ND2	3	0.0003	2.7867	142.8640
ASN_314@HD22	ALA_40@H	ALA_40@N	3	0.0003	2.9770	143.7268
GLN_316@OE1	LYS_108@HE3	LYS_108@CE	3	0.0003	2.9930	140.0663
GLU_317@HG2	PHE_43@HB3	PHE_43@CB	3	0.0003	2.9955	137.7751
GLU_317@HG2	PHE_43@HE1	PHE_43@CE1	3	0.0003	2.9464	141.2869
GLU_317@CD	LYS_108@HZ3	LYS_108@NZ	3	0.0003	2.9667	145.4342
LEU_319@HD11	PHE_43@HA	PHE_43@CA	3	0.0003	2.9396	138.9445
LEU_319@HD22	VAL_171@HG13	VAL_171@CG1	3	0.0003	2.9606	138.7974
LEU_319@HD22	PHE_43@HB2	PHE_43@CB	3	0.0003	2.9379	137.7424
LEU_319@HD23	ASN_105@HB2	ASN_105@CB	3	0.0003	2.9652	137.4078
LEU_320@HD11	VAL_171@HG12	VAL_171@CG1	3	0.0003	2.9249	139.3650
LEU_320@HD11	VAL_171@HG13	VAL_171@CG1	3	0.0003	2.9351	142.8258
LEU_320@HD11	VAL_171@HG22	VAL_171@CG2	3	0.0003	2.9590	137.4855
LEU_320@HD12	VAL_171@HG21	VAL_171@CG2	3	0.0003	2.9849	140.0485
LEU_320@HD12	VAL_171@HG11	VAL_171@CG1	3	0.0003	2.9835	148.9546
LEU_320@HD12	VAL_171@HG13	VAL_171@CG1	3	0.0003	2.9408	142.6798
LEU_320@HD21	VAL_171@HG22	VAL_171@CG2	3	0.0003	2.9500	141.3029
PRO_323@HD2	VAL_171@HG22	VAL_171@CG2	3	0.0003	2.9110	138.9647
PRO_323@HG2	GLY_172@HA2	GLY_172@CA	3	0.0003	2.9523	141.7239
PRO_323@HB2	VAL_75@HG22	VAL_75@CG2	3	0.0003	2.9237	136.4428
LEU_325@HD23	PHE_43@HE2	PHE_43@CE2	3	0.0003	2.9342	137.2847
GLU_327@HG3	VAL_75@HG13	VAL_75@CG1	3	0.0003	2.9637	136.1470
GLU_327@HG3	LYS_46@HD2	LYS_46@CD	3	0.0003	2.9806	145.2273
ILE_328@HD12	ALA_44@HB3	ALA_44@CB	3	0.0003	2.9767	140.9669
ILE_328@HD12	PHE_43@HD2	PHE_43@CD2	3	0.0003	2.9171	137.2979
ILE_328@HD13	ALA_44@HB3	ALA_44@CB	3	0.0003	2.9685	150.5842
SER_332@HG	ALA_44@HB2	ALA_44@CB	3	0.0003	2.9268	148.5896
LEU_333@HD12	TYR_48@HE2	TYR_48@CE2	3	0.0003	2.9732	137.1453
ASP_334@OD1	LYS_54@HZ2	LYS_54@NZ	3	0.0003	2.8254	161.2474
ASN_454@HA	GLN_82@HE22	GLN_82@NE2	3	0.0003	2.8328	138.6779
SER_457@HB3	TYR_48@HE2	TYR_48@CE2	3	0.0003	2.9277	142.4980
THR_471@HG21	ASN_128@HB3	ASN_128@CB	3	0.0003	2.9606	141.0678
THR_471@HG22	ASP_88@HB3	ASP_88@CB	3	0.0003	2.8806	137.8332
ASP_472@HA	ASN_128@HB3	ASN_128@CB	3	0.0003	2.9228	142.7528
ASP_472@CG	ASN_128@HD21	ASN_128@ND2	3	0.0003	2.9680	143.5044
ASP_480@HB2	ALA_143@HB2	ALA_143@CB	3	0.0003	2.9461	140.0141
GLY_514@H	ARG_161@HH12	ARG_161@NH1	3	0.0003	2.7669	137.7015
ASN_515@ND2	SER_162@HG	SER_162@OG	3	0.0003	2.8423	148.8047
ASN_515@HD21	SER_162@H	SER_162@N	3	0.0003	2.7594	137.3292
ASN_515@HD21	GLY_164@HA3	GLY_164@CA	3	0.0003	2.8784	137.9574
ASN_515@HD22	GLY_115@HA3	GLY_115@CA	3	0.0003	2.9122	149.7611
ASN_515@HD22	ARG_166@HH22	ARG_166@NH2	3	0.0003	2.9064	141.1941

VAL_516@HG12	ARG_166@HH21	ARG_166@NH2	3	0.0003	2.9565	140.3024
VAL_516@HG13	ARG_166@HH21	ARG_166@NH2	3	0.0003	2.7995	138.1895
VAL_541@HG23	TYR_89@HH	TYR_89@OH	3	0.0003	2.8662	138.7140
ASP_545@OD1	ASN_85@HD22	ASN_85@ND2	3	0.0003	2.8929	143.3814
ASN_311@HB2	PHE_43@HE1	PHE_43@CE1	2	0.0002	2.9536	136.8301
ASN_311@HD22	ALA_40@HB1	ALA_40@CB	2	0.0002	2.8441	148.2710
ASN_314@HD21	ASN_38@HA	ASN_38@CA	2	0.0002	2.9674	143.1302
GLN_316@HG2	LYS_108@HE3	LYS_108@CE	2	0.0002	2.9565	138.1588
GLN_316@HG2	LYS_108@HE2	LYS_108@CE	2	0.0002	2.9236	151.2068
GLU_317@HB2	PRO_41@HB3	PRO_41@CB	2	0.0002	2.9851	143.5952
GLU_317@OE1	LYS_108@HE2	LYS_108@CE	2	0.0002	2.9600	138.7349
CYS_318@HA	PHE_43@HZ	PHE_43@CZ	2	0.0002	2.9485	147.9223
LEU_319@CD1	TYR_176@HH	TYR_176@OH	2	0.0002	2.9781	157.2708
LEU_319@HD21	PHE_43@HD1	PHE_43@CD1	2	0.0002	2.9875	143.1315
LEU_319@HD21	PHE_43@HB2	PHE_43@CB	2	0.0002	2.9662	140.7298
LEU_319@HD21	ASN_105@HB2	ASN_105@CB	2	0.0002	2.9554	140.3835
LEU_319@HD21	ASN_105@HD21	ASN_105@ND2	2	0.0002	2.9075	150.0962
LEU_319@HD22	PHE_43@HD1	PHE_43@CD1	2	0.0002	2.9502	137.7671
LEU_320@HD11	VAL_171@HG11	VAL_171@CG1	2	0.0002	2.9866	146.7109
LEU_320@HD11	VAL_171@HG21	VAL_171@CG2	2	0.0002	2.9991	145.2494
LEU_320@HD12	VAL_171@HG23	VAL_171@CG2	2	0.0002	2.9046	138.6973
LEU_320@HD12	VAL_171@HG22	VAL_171@CG2	2	0.0002	2.9430	140.1595
LEU_320@HD13	VAL_171@HG11	VAL_171@CG1	2	0.0002	2.9948	148.0165
LEU_320@HD21	VAL_171@HG21	VAL_171@CG2	2	0.0002	2.9609	140.1375
LEU_320@HD22	VAL_171@HG21	VAL_171@CG2	2	0.0002	2.9924	146.8159
LEU_320@HD22	VAL_171@HG23	VAL_171@CG2	2	0.0002	2.9423	136.0423
GLY_324@H	VAL_171@HG13	VAL_171@CG1	2	0.0002	2.9188	141.4055
GLY_324@HA2	PHE_43@HE1	PHE_43@CE1	2	0.0002	2.9538	138.5107
GLU_327@HG2	VAL_75@HG22	VAL_75@CG2	2	0.0002	2.9832	137.1777
GLU_327@HG2	VAL_75@HG12	VAL_75@CG1	2	0.0002	2.9770	144.8560
ILE_328@HD11	PHE_43@HD2	PHE_43@CD2	2	0.0002	2.9201	138.4535
ILE_328@HD11	ALA_44@HB2	ALA_44@CB	2	0.0002	2.9892	142.6059
ASN_331@HA	TYR_48@HH	TYR_48@OH	2	0.0002	2.9162	140.9223
ASN_331@HD22	LYS_46@HZ3	LYS_46@NZ	2	0.0002	2.9593	153.2400
SER_332@HA	LYS_46@HB3	LYS_46@CB	2	0.0002	2.9812	138.3789
SER_332@HA	LYS_46@HB2	LYS_46@CB	2	0.0002	2.9296	138.5484
SER_332@HA	LYS_46@HA	LYS_46@CA	2	0.0002	2.9538	147.0476
SER_332@OG	LYS_46@H	LYS_46@N	2	0.0002	2.9676	144.4017
SER_332@HG	LYS_46@HG2	LYS_46@CG	2	0.0002	2.9298	144.7690
LEU_333@HD11	TYR_48@HE2	TYR_48@CE2	2	0.0002	2.9894	139.5764
LEU_333@HD13	TYR_48@HE2	TYR_48@CE2	2	0.0002	2.9549	142.0540
LEU_333@HD23	CYS_47@HB2	CYS_47@CB	2	0.0002	2.9517	141.1324
ASP_334@CG	TYR_37@HH	TYR_37@OH	2	0.0002	2.9770	151.3688
ASP_334@OD2	LYS_54@HZ3	LYS_54@NZ	2	0.0002	2.8587	159.0679
SER_457@HG	GLN_82@HE21	GLN_82@NE2	2	0.0002	2.9138	151.0896
SER_457@HG	GLN_82@HG2	GLN_82@CG	2	0.0002	2.9578	143.4883
THR_471@HG22	TYR_89@HH	TYR_89@OH	2	0.0002	2.7713	135.3620
THR_471@HG23	TYR_89@HH	TYR_89@OH	2	0.0002	2.9414	135.7697
VAL_475@HA	TYR_141@HE1	TYR_141@CE1	2	0.0002	2.9234	139.2735
VAL_475@HG13	TYR_141@HE1	TYR_141@CE1	2	0.0002	2.9420	136.4731
VAL_475@HG21	ASN_128@H	ASN_128@N	2	0.0002	2.9126	136.3133
VAL_475@HG23	ASN_128@H	ASN_128@N	2	0.0002	2.7634	148.7031
ASP_476@O	LYS_126@HZ2	LYS_126@NZ	2	0.0002	2.8726	138.3339
ASP_480@HB3	ALA_143@HB3	ALA_143@CB	2	0.0002	2.9619	155.1252
ASP_480@HB3	ALA_143@HB1	ALA_143@CB	2	0.0002	2.9819	140.1100
ASP_480@HB3	TYR_157@HH	TYR_157@OH	2	0.0002	2.9156	146.9233
ASP_480@CG	ASN_155@HD22	ASN_155@ND2	2	0.0002	2.9846	150.7542
ASP_480@OD2	TYR_157@HH	TYR_157@OH	2	0.0002	2.8956	140.1375
THR_511@HG22	ARG_161@HH22	ARG_161@NH2	2	0.0002	2.8666	142.4775
ASN_515@HD21	GLY_164@H	GLY_164@N	2	0.0002	2.9643	150.6703
VAL_516@HG12	TYR_117@HH	TYR_117@OH	2	0.0002	2.9123	141.4273
VAL_516@HG13	TYR_117@HH	TYR_117@OH	2	0.0002	2.9373	149.0747
VAL_516@HG23	TYR_117@HH	TYR_117@OH	2	0.0002	2.8611	146.3617

VAL_516@O	ARG_166@HH11	ARG_166@NH1	2	0.0002	2.9660	144.2844
LYS_518@HE2	HIE_173@HD2	HIE_173@CD2	2	0.0002	2.9764	149.1865
LYS_518@HZ2	HIE_173@HB3	HIE_173@CB	2	0.0002	2.9054	135.6951
CYS_521@HG	ARG_71@HH11	ARG_71@NH1	2	0.0002	2.8911	140.8122
CYS_521@HG	ARG_71@HH21	ARG_71@NH2	2	0.0002	2.7627	138.1684
LYS_540@HE3	ASN_85@HB3	ASN_85@CB	2	0.0002	2.9624	145.2187
VAL_541@H	LEU_123@HD12	LEU_123@CD1	2	0.0002	2.8774	139.1573
VAL_541@HG11	PHE_124@HE1	PHE_124@CE1	2	0.0002	2.9344	135.5619
VAL_541@HG22	PHE_124@HD1	PHE_124@CD1	2	0.0002	2.9284	139.0939
VAL_541@HG22	TYR_89@HE1	TYR_89@CE1	2	0.0002	2.8822	141.9673
THR_542@HB	ASN_85@HA	ASN_85@CA	2	0.0002	2.9165	138.0766
THR_542@OG1	ASN_85@H	ASN_85@N	2	0.0002	2.8949	143.6151
THR_542@HG1	GLY_84@HA2	GLY_84@CA	2	0.0002	2.8870	138.7980
MET_543@HB3	THR_83@HG21	THR_83@CG2	2	0.0002	2.9348	137.7837
MET_543@HE1	THR_83@HG21	THR_83@CG2	2	0.0002	2.9324	144.4364
GLU_233@OE2	ARG_166@HH11	ARG_166@NH1	1	0.0001	2.9029	152.2325
ASN_311@HD21	PHE_42@H	PHE_42@N	1	0.0001	2.9809	146.5215
ASN_311@HD22	ALA_40@HB3	ALA_40@CB	1	0.0001	2.9879	138.3808
PRO_312@HD2	ALA_40@HB2	ALA_40@CB	1	0.0001	2.9327	138.0264
PRO_312@HG3	ALA_40@HB1	ALA_40@CB	1	0.0001	2.9625	135.5852
PRO_312@HB2	ALA_40@HB1	ALA_40@CB	1	0.0001	2.9005	137.1359
ASN_314@HD21	PHE_39@HA	PHE_39@CA	1	0.0001	2.9928	137.3614
GLN_316@HA	LYS_108@HZ2	LYS_108@NZ	1	0.0001	2.9383	145.6123
GLN_316@HA	LYS_108@HZ1	LYS_108@NZ	1	0.0001	2.7764	142.6746
GLN_316@HA	LYS_108@HZ3	LYS_108@NZ	1	0.0001	2.6962	139.3050
GLN_316@HB2	LYS_108@HZ3	LYS_108@NZ	1	0.0001	2.8980	143.7617
GLN_316@HB3	LYS_108@HZ3	LYS_108@NZ	1	0.0001	2.9641	136.1594
GLN_316@HB3	LYS_108@HD3	LYS_108@CD	1	0.0001	2.9649	145.7909
GLN_316@HB3	LYS_108@HE3	LYS_108@CE	1	0.0001	2.9848	139.6813
GLN_316@HG3	LYS_108@HZ1	LYS_108@NZ	1	0.0001	2.9361	138.8281
GLN_316@HE21	PRO_41@HB3	PRO_41@CB	1	0.0001	2.9240	150.5129
GLN_316@HE21	LYS_108@HZ1	LYS_108@NZ	1	0.0001	2.9797	163.1389
GLN_316@HE22	PRO_41@HD3	PRO_41@CD	1	0.0001	2.8633	146.4506
GLN_316@HE22	LYS_108@HZ3	LYS_108@NZ	1	0.0001	2.9912	144.2115
GLN_316@HE22	LYS_108@HZ2	LYS_108@NZ	1	0.0001	2.8014	177.9866
GLN_316@O	LYS_108@HE3	LYS_108@CE	1	0.0001	3.0000	146.9489
GLU_317@HB2	PRO_41@HB2	PRO_41@CB	1	0.0001	2.9665	136.6267
GLU_317@HG2	LYS_108@HE2	LYS_108@CE	1	0.0001	2.8795	140.2124
GLU_317@HG3	PHE_43@HD1	PHE_43@CD1	1	0.0001	2.9496	147.3923
GLU_317@CD	LYS_108@HZ2	LYS_108@NZ	1	0.0001	2.9394	138.1176
GLU_317@CD	LYS_108@HZ1	LYS_108@NZ	1	0.0001	2.9733	147.7819
GLU_317@OE2	LYS_108@HE2	LYS_108@CE	1	0.0001	2.9428	146.5169
GLU_317@OE2	ASN_105@HD21	ASN_105@ND2	1	0.0001	2.7448	156.6039
LEU_319@H	PHE_43@HZ	PHE_43@CZ	1	0.0001	2.9847	147.0669
LEU_319@HD11	PHE_43@HD1	PHE_43@CD1	1	0.0001	2.9448	136.1947
LEU_319@HD12	PHE_43@HB3	PHE_43@CB	1	0.0001	2.9935	135.5922
LEU_319@HD13	ASN_105@HD21	ASN_105@ND2	1	0.0001	2.8274	135.9027
LEU_319@HD13	PHE_43@HA	PHE_43@CA	1	0.0001	2.9854	135.8544
LEU_319@HD13	PHE_43@HB3	PHE_43@CB	1	0.0001	2.8279	137.9417
LEU_319@HD13	PHE_43@HD1	PHE_43@CD1	1	0.0001	2.9807	138.1793
LEU_319@HD22	ASN_105@HD21	ASN_105@ND2	1	0.0001	2.9731	172.4572
LEU_319@HD23	ASN_105@HD21	ASN_105@ND2	1	0.0001	2.8658	140.8739
LEU_319@HD23	VAL_171@HG12	VAL_171@CG1	1	0.0001	2.9535	135.9177
LEU_319@HD23	PHE_43@HA	PHE_43@CA	1	0.0001	2.9603	146.8659
LEU_319@HD23	TYR_176@HH	TYR_176@OH	1	0.0001	2.6872	149.1094
LEU_320@HD12	VAL_171@HG12	VAL_171@CG1	1	0.0001	2.9957	140.1656
LEU_320@HD13	VAL_171@HG21	VAL_171@CG2	1	0.0001	2.9330	137.2327
LEU_320@HD21	VAL_171@HG23	VAL_171@CG2	1	0.0001	2.9925	143.6906
LEU_320@HD21	VAL_171@HG11	VAL_171@CG1	1	0.0001	2.9768	135.2093
LEU_320@HD23	VAL_171@HG22	VAL_171@CG2	1	0.0001	2.9666	139.0622
PRO_323@HD2	TYR_176@HH	TYR_176@OH	1	0.0001	2.9252	137.2885
PRO_323@HG3	GLY_72@HA3	GLY_72@CA	1	0.0001	2.9891	135.6117
PRO_323@HG3	ASN_73@HD21	ASN_73@ND2	1	0.0001	2.8037	144.2320

PRO_323@HB2	PHE_43@HZ	PHE_43@CZ	1	0.0001	2.9621	135.9517
PRO_323@HB2	VAL_75@HG23	VAL_75@CG2	1	0.0001	2.9007	140.1882
PRO_323@HB2	VAL_75@HG11	VAL_75@CG1	1	0.0001	2.9675	137.8510
PRO_323@HB2	PHE_43@HE1	PHE_43@CE1	1	0.0001	2.9495	137.6558
PRO_323@HB3	ASN_73@HA	ASN_73@CA	1	0.0001	2.9883	147.1814
GLY_324@H	VAL_171@HG12	VAL_171@CG1	1	0.0001	2.9868	138.3686
GLY_324@HA2	PHE_43@HD1	PHE_43@CD1	1	0.0001	2.8927	136.7875
LEU_325@HD22	PHE_43@HZ	PHE_43@CZ	1	0.0001	2.9579	148.4140
GLU_327@HG2	VAL_75@HG11	VAL_75@CG1	1	0.0001	2.9684	140.6802
GLU_327@HG2	SER_76@HB3	SER_76@CB	1	0.0001	2.9852	141.6260
GLU_327@HG2	LYS_46@HZ2	LYS_46@NZ	1	0.0001	2.9061	138.6663
GLU_327@HG3	VAL_75@HG11	VAL_75@CG1	1	0.0001	2.8725	139.4855
GLU_327@HG3	LYS_46@HZ2	LYS_46@NZ	1	0.0001	2.9505	162.2957
GLU_327@CD	SER_76@HG	SER_76@OG	1	0.0001	2.9832	169.0655
ILE_328@HG13	PHE_43@HE1	PHE_43@CE1	1	0.0001	2.9776	139.5697
ILE_328@HD11	PHE_43@HE2	PHE_43@CE2	1	0.0001	2.9710	142.1757
ILE_328@HD11	ALA_44@HB3	ALA_44@CB	1	0.0001	2.8681	148.5659
ILE_328@HD12	PHE_43@HE2	PHE_43@CE2	1	0.0001	2.8914	141.1282
ILE_328@HD13	ALA_44@HB1	ALA_44@CB	1	0.0001	2.9422	136.8626
ASN_331@HB3	TYR_48@HH	TYR_48@OH	1	0.0001	2.6832	136.1013
ASN_331@HB3	LYS_46@HZ3	LYS_46@NZ	1	0.0001	2.9562	136.4417
ASN_331@HB3	LYS_46@HZ2	LYS_46@NZ	1	0.0001	2.7980	138.5093
ASN_331@CG	LYS_46@HZ1	LYS_46@NZ	1	0.0001	2.9900	146.5362
ASN_331@ND2	GLN_82@HE21	GLN_82@NE2	1	0.0001	2.9545	137.0665
ASN_331@HD21	SER_76@HB3	SER_76@CB	1	0.0001	2.6622	137.2042
ASN_331@HD22	LYS_46@HE3	LYS_46@CE	1	0.0001	2.9441	142.8781
ASN_331@O	LYS_46@HE3	LYS_46@CE	1	0.0001	2.9885	137.8854
SER_332@HB2	LYS_46@HB3	LYS_46@CB	1	0.0001	2.9739	152.4128
SER_332@HG	PHE_45@H	PHE_45@N	1	0.0001	2.9886	141.6553
LEU_333@HD22	CYS_47@HG	CYS_47@SG	1	0.0001	2.9163	139.2584
LEU_333@HD22	CYS_47@HB2	CYS_47@CB	1	0.0001	2.9962	142.5790
LEU_333@HD23	TYR_48@HE2	TYR_48@CE2	1	0.0001	2.9342	144.6585
ASN_454@HB3	GLN_82@HE22	GLN_82@NE2	1	0.0001	2.8388	138.3075
SER_457@HB3	GLY_81@HA3	GLY_81@CA	1	0.0001	2.8013	143.6017
SER_457@OG	GLN_82@HE22	GLN_82@NE2	1	0.0001	2.8499	174.8874
SER_457@HG	GLY_81@HA3	GLY_81@CA	1	0.0001	2.8256	136.8973
ASN_467@HD22	THR_83@HG23	THR_83@CG2	1	0.0001	2.9293	135.8573
ASN_467@HD22	THR_83@HG22	THR_83@CG2	1	0.0001	2.8670	137.5710
ASP_469@HB2	THR_83@HG23	THR_83@CG2	1	0.0001	2.9491	151.9254
THR_471@HG23	ASN_128@HB3	ASN_128@CB	1	0.0001	2.9887	149.7254
ASP_472@H	ASN_128@HD22	ASN_128@ND2	1	0.0001	2.8747	140.0852
ASP_472@HA	ASN_128@HD21	ASN_128@ND2	1	0.0001	2.9591	155.3869
ASP_472@OD1	ASN_128@HD21	ASN_128@ND2	1	0.0001	2.9994	145.7490
ASP_472@OD2	LYS_130@HZ3	LYS_130@NZ	1	0.0001	2.9071	147.7968
ASP_476@HA	LYS_126@HZ1	LYS_126@NZ	1	0.0001	2.9719	143.5877
ASP_476@OD1	LYS_126@HZ2	LYS_126@NZ	1	0.0001	2.9932	142.1239
ASP_476@O	LYS_126@HZ3	LYS_126@NZ	1	0.0001	2.9901	164.3143
ASP_476@O	LYS_126@HZ1	LYS_126@NZ	1	0.0001	2.8765	142.8460
ALA_478@HB3	ALA_143@HB3	ALA_143@CB	1	0.0001	2.9804	135.9348
ASP_480@HB2	ALA_143@HB3	ALA_143@CB	1	0.0001	2.9558	135.1339
ASP_480@HB3	TYR_157@HE1	TYR_157@CE1	1	0.0001	2.9635	139.8989
ALA_481@HB2	TYR_157@HH	TYR_157@OH	1	0.0001	2.9709	135.8797
ALA_481@HB3	PHE_124@HZ	PHE_124@CZ	1	0.0001	2.9286	146.2297
GLN_482@HE22	PHE_154@HZ	PHE_154@CZ	1	0.0001	2.9240	153.9188
THR_511@HG21	ARG_161@HH11	ARG_161@NH1	1	0.0001	2.9429	140.2363
THR_511@HG22	ARG_161@HH11	ARG_161@NH1	1	0.0001	2.8952	138.5775
THR_511@HG23	ARG_161@HH11	ARG_161@NH1	1	0.0001	2.7794	177.1379
ASP_512@HB2	ARG_161@HH11	ARG_161@NH1	1	0.0001	2.8949	136.3561
ASP_512@OD2	TYR_121@HH	TYR_121@OH	1	0.0001	2.7455	137.7975
GLY_514@HA2	ARG_161@HH12	ARG_161@NH1	1	0.0001	2.7606	146.4420
ASN_515@ND2	SER_162@H	SER_162@N	1	0.0001	2.8341	163.8811
ASN_515@HD21	TYR_117@HD1	TYR_117@CD1	1	0.0001	2.9261	135.5002
ASN_515@HD21	TYR_117@HD2	TYR_117@CD2	1	0.0001	2.9958	135.2130

ASN_515@HD22	TYR_117@HH	TYR_117@OH	1	0.0001	2.8461	136.9474
ASN_515@HD22	SER_162@HG	SER_162@OG	1	0.0001	2.6495	148.1738
ASN_515@HD22	ARG_161@HG2	ARG_161@CG	1	0.0001	2.8609	146.7015
ASN_515@HD22	ARG_161@HE	ARG_161@NE	1	0.0001	2.9399	140.8870
ASN_515@O	SER_162@HG	SER_162@OG	1	0.0001	2.9481	144.8002
VAL_516@HA	ARG_166@HH22	ARG_166@NH2	1	0.0001	2.9155	140.6883
VAL_516@HG11	TYR_117@HH	TYR_117@OH	1	0.0001	2.9644	135.5859
VAL_516@HG11	ARG_166@HH21	ARG_166@NH2	1	0.0001	2.9747	136.8056
VAL_516@HG12	ARG_166@HH22	ARG_166@NH2	1	0.0001	2.9157	137.7097
VAL_516@HG12	TYR_117@HE2	TYR_117@CE2	1	0.0001	2.9335	141.3058
VAL_516@HG21	TYR_117@HH	TYR_117@OH	1	0.0001	2.9123	170.8249
VAL_516@HG22	TYR_117@HH	TYR_117@OH	1	0.0001	2.7330	138.9442
LYS_518@HD2	TYR_169@HE2	TYR_169@CE2	1	0.0001	2.9288	138.3652
LYS_518@HE3	TYR_169@HE1	TYR_169@CE1	1	0.0001	2.8208	150.8502
LYS_518@HZ2	GLY_164@HA3	GLY_164@CA	1	0.0001	2.8849	135.9306
LYS_518@HZ3	GLY_164@H	GLY_164@N	1	0.0001	2.9897	143.1619
CYS_521@HB2	ARG_71@HH21	ARG_71@NH2	1	0.0001	2.9482	135.2989
CYS_521@HB3	HIE_173@HE2	HIE_173@NE2	1	0.0001	2.9537	141.0947
CYS_521@HG	ARG_71@HH22	ARG_71@NH2	1	0.0001	2.6542	149.8314
CYS_538@HG	ARG_161@HH11	ARG_161@NH1	1	0.0001	2.9702	154.6324
LYS_540@HB3	ASN_85@HB2	ASN_85@CB	1	0.0001	2.9321	135.6155
LYS_540@HG2	ASN_85@HB2	ASN_85@CB	1	0.0001	2.8731	138.0778
LYS_540@HG3	LEU_123@HD11	LEU_123@CD1	1	0.0001	2.9370	136.6169
LYS_540@HD2	TYR_121@HE1	TYR_121@CE1	1	0.0001	2.9340	145.1137
LYS_540@HD2	LEU_123@HD12	LEU_123@CD1	1	0.0001	2.9618	140.4479
LYS_540@HD2	LEU_123@HD13	LEU_123@CD1	1	0.0001	2.9001	139.2540
LYS_540@HD3	LEU_123@HD11	LEU_123@CD1	1	0.0001	2.9322	135.8651
LYS_540@HE3	LEU_123@HD13	LEU_123@CD1	1	0.0001	2.9366	160.7197
LYS_540@HZ1	ASN_85@HB3	ASN_85@CB	1	0.0001	2.8270	137.3214
VAL_541@H	LEU_123@HD11	LEU_123@CD1	1	0.0001	2.8724	135.7601
VAL_541@H	LEU_123@HD13	LEU_123@CD1	1	0.0001	2.8094	145.9932
VAL_541@HB	PHE_124@HE1	PHE_124@CE1	1	0.0001	2.9996	135.6875
VAL_541@HG11	TYR_141@HH	TYR_141@OH	1	0.0001	2.9730	138.7000
VAL_541@HG12	PHE_124@HE1	PHE_124@CE1	1	0.0001	2.9810	141.2303
VAL_541@HG13	TYR_89@HH	TYR_89@OH	1	0.0001	2.7514	144.6160
VAL_541@HG21	TYR_89@HH	TYR_89@OH	1	0.0001	2.7652	141.9695
VAL_541@HG21	TYR_89@HE1	TYR_89@CE1	1	0.0001	2.9424	135.5924
VAL_541@O	ASN_85@HD22	ASN_85@ND2	1	0.0001	2.9040	140.0754
THR_542@HB	ASN_85@HD22	ASN_85@ND2	1	0.0001	2.7750	136.3189
THR_542@HG22	GLY_84@HA3	GLY_84@CA	1	0.0001	2.9523	140.7182
THR_542@HG23	ASN_85@H	ASN_85@N	1	0.0001	2.8759	136.8398
THR_542@HG23	ASN_85@HD21	ASN_85@ND2	1	0.0001	2.7951	135.3373
THR_542@OG1	GLY_84@HA2	GLY_84@CA	1	0.0001	2.9712	135.2667
MET_543@HB3	THR_83@HG1	THR_83@OG1	1	0.0001	2.6998	137.0193
MET_543@HB3	THR_83@HG22	THR_83@CG2	1	0.0001	2.9383	136.3038
MET_543@HG2	THR_83@HG22	THR_83@CG2	1	0.0001	2.9900	145.6628
MET_543@HG3	THR_83@HG22	THR_83@CG2	1	0.0001	2.9259	136.9345
MET_543@HE2	THR_83@HG22	THR_83@CG2	1	0.0001	2.9824	140.3868
MET_543@HE3	THR_83@HG23	THR_83@CG2	1	0.0001	2.9406	141.6963
ASP_544@H	THR_83@HG22	THR_83@CG2	1	0.0001	2.9107	144.5875
ASP_544@HB2	GLY_84@H	GLY_84@N	1	0.0001	2.9220	137.0047

Table S5A. List of atom-atom interactions (Hydrogen bonds) across protein-ligand interface in ACE2(chain A)-Spike Protein(Chain B) (BA.1variant) complex from PDBsum server.

Sl. No.	Atom no.	Atom name	Residue name	Residue no.	Chain Id	Hydrogen bonds	Atom no.	Atom name	Residue name	Residue no.	Chain Id	Distance (Å)
1	2136	O	GLU	231	A	<-->	7489	NH2	ARG	493	B	3.29
2	2146	O	GLU	232	A	<-->	7486	NH1	ARG	493	B	3.02
3	2143	OE1	GLU	232	A	<-->	7486	NH1	ARG	493	B	2.67
4	2163	NZ	LYS	234	A	<-->	7404	O	GLY	485	B	3.02
5	2206	OE2	GLU	238	A	<-->	7445	OH	TYR	489	B	2.54
6	5047	O	GLU	527	A	<-->	7566	N	GLY	501	B	3.27

Sl. No.	Atom no.	Atom name	Residue name	Residue no.	Chain Id	Hydrogen bonds	Atom no.	Atom name	Residue name	Residue no.	Chain Id	Distance (Å)
7	5077	NE2	GLN	531	A	<-->	7542	O	PRO	498	B	2.77
8	5118	O	HIS	535	A	<-->	7579	N	GLY	503	B	3.31
9	5486	O	VAL	574	A	<-->	7547	OG1	THR	499	B	2.75
10	5602	O	ASN	586	A	<-->	6598	NH2	ARG	403	B	3.07
11	5597	OD1	ASN	586	A	<-->	7589	ND1	HIS	504	B	2.65
12	5636	OE2	GLU	589	A	<-->	6659	NE2	GLN	409	B	3
13	5636	OE2	GLU	589	A	<-->	6723	ND2	ASN	417	B	2.76
14	5713	O	LYS	596	A	<-->	6762	OH	TYR	421	B	2.82
15	5708	NZ	LYS	596	A	<-->	6722	OD1	ASN	417	B	2.66
16	5708	NZ	LYS	596	A	<-->	7111	O	LEU	455	B	2.72
17	5719	OD1	ASP	597	A	<-->	7168	ND2	ASN	460	B	2.66
18	5803	N	TRP	606	A	<-->	7326	O	ALA	475	B	3.22
19	5842	OD2	ASP	609	A	<-->	7338	ND2	ASN	477	B	2.74

Table S5B. List of atom-atom interactions (Non-bonded contacts) across protein-ligand interface in ACE2(chain A)-Spike Protein(Chain B) (BA.1variant) complex from PDBsum server.

Sl.No.	Atom no.	Atom name	Residue name	Residue no.	Chain	Non-bonded contacts	Atom no.	Atom name	Residue name	Residue no.	Chain	Distance
					Id						Id	(Å)
1	2136	O	GLU	231	A	<-->	7489	NH2	ARG	493	B	3.29
2	2133	OE1	GLU	231	A	<-->	7441	CD2	TYR	489	B	3.49
3	2133	OE1	GLU	231	A	<-->	7443	CE2	TYR	489	B	3.31
4	2139	CA	GLU	232	A	<-->	7485	CZ	ARG	493	B	3.69
5	2139	CA	GLU	232	A	<-->	7486	NH1	ARG	493	B	3.33
6	2139	CA	GLU	232	A	<-->	7489	NH2	ARG	493	B	3.4
7	2145	C	GLU	232	A	<-->	7486	NH1	ARG	493	B	3.59
8	2146	O	GLU	232	A	<-->	7485	CZ	ARG	493	B	3.78
9	2146	O	GLU	232	A	<-->	7486	NH1	ARG	493	B	3.02
10	2146	O	GLU	232	A	<-->	7489	NH2	ARG	493	B	3.63
11	2140	CB	GLU	232	A	<-->	7486	NH1	ARG	493	B	3.45
12	2141	CG	GLU	232	A	<-->	7485	CZ	ARG	493	B	3.83
13	2141	CG	GLU	232	A	<-->	7486	NH1	ARG	493	B	3.5
14	2142	CD	GLU	232	A	<-->	7486	NH1	ARG	493	B	3.49
15	2143	OE1	GLU	232	A	<-->	7482	CD	ARG	493	B	3.24
16	2143	OE1	GLU	232	A	<-->	7483	NE	ARG	493	B	3.57
17	2143	OE1	GLU	232	A	<-->	7485	CZ	ARG	493	B	3.35
18	2143	OE1	GLU	232	A	<-->	7486	NH1	ARG	493	B	2.67
19	2159	CB	LYS	234	A	<-->	7443	CE2	TYR	489	B	3.85
20	2159	CB	LYS	234	A	<-->	7444	CZ	TYR	489	B	3.76
21	2159	CB	LYS	234	A	<-->	7445	OH	TYR	489	B	3.4
22	2162	CE	LYS	234	A	<-->	7443	CE2	TYR	489	B	3.43
23	2162	CE	LYS	234	A	<-->	7444	CZ	TYR	489	B	3.7
24	2162	CE	LYS	234	A	<-->	7445	OH	TYR	489	B	3.05
25	2163	NZ	LYS	234	A	<-->	7404	O	GLY	485	B	3.02
26	2163	NZ	LYS	234	A	<-->	7443	CE2	TYR	489	B	3.19
27	2163	NZ	LYS	234	A	<-->	7444	CZ	TYR	489	B	3.85
28	2163	NZ	LYS	234	A	<-->	7445	OH	TYR	489	B	3.6
29	2170	CA	PRO	235	A	<-->	7121	CZ	PHE	456	B	3.84
30	2171	CB	PRO	235	A	<-->	7120	CE2	PHE	456	B	3.58
31	2171	CB	PRO	235	A	<-->	7121	CZ	PHE	456	B	3.46
32	2172	CG	PRO	235	A	<-->	7120	CE2	PHE	456	B	3.85
33	2172	CG	PRO	235	A	<-->	7489	NH2	ARG	493	B	3.34
34	2173	CD	PRO	235	A	<-->	7489	NH2	ARG	493	B	3.85
35	2204	CD	GLU	238	A	<-->	7324	CB	ALA	475	B	3.89
36	2204	CD	GLU	238	A	<-->	7442	CE1	TYR	489	B	3.35
37	2204	CD	GLU	238	A	<-->	7444	CZ	TYR	489	B	3.78
38	2204	CD	GLU	238	A	<-->	7445	OH	TYR	489	B	3.35
39	2205	OE1	GLU	238	A	<-->	7121	CZ	PHE	456	B	3.61
40	2205	OE1	GLU	238	A	<-->	7440	CD1	TYR	489	B	3.89
41	2205	OE1	GLU	238	A	<-->	7442	CE1	TYR	489	B	3.09
42	2205	OE1	GLU	238	A	<-->	7444	CZ	TYR	489	B	3.88
43	2205	OE1	GLU	238	A	<-->	7445	OH	TYR	489	B	3.89
44	2206	OE2	GLU	238	A	<-->	7324	CB	ALA	475	B	3.69
45	2206	OE2	GLU	238	A	<-->	7419	CA	ASN	487	B	3.66

Sl.No.	Atom no.	Atom name	Residue name	Residue no.	Chain	Non-bonded contacts	Atom no.	Atom name	Residue name	Residue no.	Chain	Distance
46	2206	OE2	GLU	238	A	<-->	7442	CE1	TYR	489	B	2.97
47	2206	OE2	GLU	238	A	<-->	7444	CZ	TYR	489	B	3.17
48	2206	OE2	GLU	238	A	<-->	7445	OH	TYR	489	B	2.54
49	2215	CD2	HIS	239	A	<-->	7119	CE1	PHE	456	B	3.77
50	2217	NE2	HIS	239	A	<-->	7119	CE1	PHE	456	B	3.37
51	5047	O	GLU	527	A	<-->	7551	O	THR	499	B	3.9
52	5047	O	GLU	527	A	<-->	7566	N	GLY	501	B	3.27
53	5042	CG	GLU	527	A	<-->	7588	CG	HIS	504	B	3.87
54	5042	CG	GLU	527	A	<-->	7591	CD2	HIS	504	B	3.7
55	5042	CG	GLU	527	A	<-->	7593	NE2	HIS	504	B	3.81
56	5043	CD	GLU	527	A	<-->	7557	CD1	TYR	500	B	3.82
57	5043	CD	GLU	527	A	<-->	7588	CG	HIS	504	B	3.71
58	5043	CD	GLU	527	A	<-->	7589	ND1	HIS	504	B	3.74
59	5045	OE2	GLU	527	A	<-->	7555	CB	TYR	500	B	3.26
60	5045	OE2	GLU	527	A	<-->	7556	CG	TYR	500	B	3.42
61	5045	OE2	GLU	527	A	<-->	7557	CD1	TYR	500	B	3.19
62	5045	OE2	GLU	527	A	<-->	7587	CB	HIS	504	B	3.37
63	5045	OE2	GLU	527	A	<-->	7588	CG	HIS	504	B	3.43
64	5045	OE2	GLU	527	A	<-->	7589	ND1	HIS	504	B	3.76
65	5048	N	ALA	528	A	<-->	7551	O	THR	499	B	3.78
66	5050	CA	ALA	528	A	<-->	7551	O	THR	499	B	2.96
67	5052	C	ALA	528	A	<-->	7551	O	THR	499	B	3.89
68	5053	O	ALA	528	A	<-->	7551	O	THR	499	B	3.84
69	5051	CB	ALA	528	A	<-->	7551	O	THR	499	B	3.38
70	5072	CA	GLN	531	A	<-->	7568	CA	GLY	501	B	3.67
71	5073	CB	GLN	531	A	<-->	7550	C	THR	499	B	3.74
72	5073	CB	GLN	531	A	<-->	7551	O	THR	499	B	3.58
73	5073	CB	GLN	531	A	<-->	7564	C	TYR	500	B	3.58
74	5073	CB	GLN	531	A	<-->	7565	O	TYR	500	B	3.58
75	5073	CB	GLN	531	A	<-->	7566	N	GLY	501	B	3.8
76	5074	CG	GLN	531	A	<-->	7542	O	PRO	498	B	3.71
77	5074	CG	GLN	531	A	<-->	7550	C	THR	499	B	3.67
78	5074	CG	GLN	531	A	<-->	7552	N	TYR	500	B	3.83
79	5074	CG	GLN	531	A	<-->	7564	C	TYR	500	B	3.82
80	5074	CG	GLN	531	A	<-->	7565	O	TYR	500	B	3.37
81	5075	CD	GLN	531	A	<-->	7542	O	PRO	498	B	3.67
82	5075	CD	GLN	531	A	<-->	7545	CA	THR	499	B	3.74
83	5077	NE2	GLN	531	A	<-->	7541	C	PRO	498	B	3.68
84	5077	NE2	GLN	531	A	<-->	7542	O	PRO	498	B	2.77
85	5077	NE2	GLN	531	A	<-->	7545	CA	THR	499	B	3.35
86	5096	CA	LYS	534	A	<-->	7576	CG2	VAL	502	B	3.47
87	5105	C	LYS	534	A	<-->	7576	CG2	VAL	502	B	3.62
88	5106	O	LYS	534	A	<-->	7576	CG2	VAL	502	B	3.84
89	5097	CB	LYS	534	A	<-->	7576	CG2	VAL	502	B	3.75
90	5118	O	HIS	535	A	<-->	7571	N	VAL	502	B	3.58
91	5118	O	HIS	535	A	<-->	7579	N	GLY	503	B	3.31
92	5124	CD	GLU	536	A	<-->	7574	CB	VAL	502	B	3.49
93	5124	CD	GLU	536	A	<-->	7575	CG1	VAL	502	B	3.63
94	5125	OE1	GLU	536	A	<-->	7574	CB	VAL	502	B	3.35
95	5125	OE1	GLU	536	A	<-->	7575	CG1	VAL	502	B	3.5
96	5125	OE1	GLU	536	A	<-->	7579	N	GLY	503	B	3.88
97	5125	OE1	GLU	536	A	<-->	7626	OH	TYR	507	B	3.41
98	5126	OE2	GLU	536	A	<-->	7574	CB	VAL	502	B	3.36
99	5126	OE2	GLU	536	A	<-->	7575	CG1	VAL	502	B	3.13
100	5126	OE2	GLU	536	A	<-->	7576	CG2	VAL	502	B	3.71
101	5129	N	GLY	537	A	<-->	7581	CA	GLY	503	B	3.86
102	5132	C	GLY	537	A	<-->	6612	CG	ASP	405	B	3.63
103	5132	C	GLY	537	A	<-->	6613	OD1	ASP	405	B	3.22
104	5133	O	GLY	537	A	<-->	6612	CG	ASP	405	B	3.58
105	5133	O	GLY	537	A	<-->	6613	OD1	ASP	405	B	2.99
106	5133	O	GLY	537	A	<-->	6614	OD2	ASP	405	B	3.74
107	5134	N	PRO	538	A	<-->	6612	CG	ASP	405	B	3.59
108	5134	N	PRO	538	A	<-->	6613	OD1	ASP	405	B	3.65
109	5134	N	PRO	538	A	<-->	6614	OD2	ASP	405	B	3.72

Sl.No.	Atom no.	Atom name	Residue name	Residue no.	Chain	Non-bonded contacts	Atom no.	Atom name	Residue name	Residue no.	Chain	Distance
110	5135	CA	PRO	538	A	<-->	6612	CG	ASP	405	B	3.52
111	5135	CA	PRO	538	A	<-->	6614	OD2	ASP	405	B	3.14
112	5139	C	PRO	538	A	<-->	6614	OD2	ASP	405	B	3.78
113	5141	N	LEU	539	A	<-->	6614	OD2	ASP	405	B	3.38
114	5144	CB	LEU	539	A	<-->	7592	CE1	HIS	504	B	3.46
115	5144	CB	LEU	539	A	<-->	7593	NE2	HIS	504	B	3.54
116	5146	CD1	LEU	539	A	<-->	7593	NE2	HIS	504	B	3.42
117	5275	CE	LYS	553	A	<-->	7549	CG2	THR	499	B	3.71
118	5276	NZ	LYS	553	A	<-->	7549	CG2	THR	499	B	3.15
119	5478	O	VAL	573	A	<-->	7549	CG2	THR	499	B	3.61
120	5485	C	VAL	574	A	<-->	7546	CB	THR	499	B	3.65
121	5485	C	VAL	574	A	<-->	7547	OG1	THR	499	B	3.45
122	5486	O	VAL	574	A	<-->	7546	CB	THR	499	B	3.18
123	5486	O	VAL	574	A	<-->	7547	OG1	THR	499	B	2.75
124	5487	N	GLY	575	A	<-->	7547	OG1	THR	499	B	3.73
125	5489	CA	GLY	575	A	<-->	7547	OG1	THR	499	B	3.37
126	5537	ND2	ASN	580	A	<-->	7562	OH	TYR	500	B	3.2
127	5554	CG	ARG	582	A	<-->	7519	CB	SER	496	B	3.58
128	5556	NE	ARG	582	A	<-->	7523	O	SER	496	B	3.85
129	5556	NE	ARG	582	A	<-->	7519	CB	SER	496	B	3.61
130	5562	NH2	ARG	582	A	<-->	7523	O	SER	496	B	3.67
131	5562	NH2	ARG	582	A	<-->	7556	CG	TYR	500	B	3.54
132	5562	NH2	ARG	582	A	<-->	7557	CD1	TYR	500	B	3.5
133	5562	NH2	ARG	582	A	<-->	7558	CD2	TYR	500	B	3.81
134	5562	NH2	ARG	582	A	<-->	7559	CE1	TYR	500	B	3.75
135	5588	CD1	LEU	585	A	<-->	7486	NH1	ARG	493	B	3.23
136	5602	O	ASN	586	A	<-->	6598	NH2	ARG	403	B	3.07
137	5596	CG	ASN	586	A	<-->	7589	ND1	HIS	504	B	3.45
138	5596	CG	ASN	586	A	<-->	7592	CE1	HIS	504	B	3.77
139	5597	OD1	ASN	586	A	<-->	6592	NE	ARG	403	B	3.25
140	5597	OD1	ASN	586	A	<-->	6594	CZ	ARG	403	B	3.19
141	5597	OD1	ASN	586	A	<-->	6598	NH2	ARG	403	B	3.13
142	5597	OD1	ASN	586	A	<-->	7588	CG	HIS	504	B	3.89
143	5597	OD1	ASN	586	A	<-->	7589	ND1	HIS	504	B	2.65
144	5597	OD1	ASN	586	A	<-->	7592	CE1	HIS	504	B	3.15
145	5598	ND2	ASN	586	A	<-->	7589	ND1	HIS	504	B	3.59
146	5598	ND2	ASN	586	A	<-->	7592	CE1	HIS	504	B	3.57
147	5638	O	GLU	589	A	<-->	6723	ND2	ASN	417	B	3.86
148	5632	CB	GLU	589	A	<-->	6595	NH1	ARG	403	B	3.67
149	5632	CB	GLU	589	A	<-->	6598	NH2	ARG	403	B	3.52
150	5633	CG	GLU	589	A	<-->	6595	NH1	ARG	403	B	3.23
151	5633	CG	GLU	589	A	<-->	6723	ND2	ASN	417	B	3.44
152	5634	CD	GLU	589	A	<-->	6595	NH1	ARG	403	B	3.83
153	5634	CD	GLU	589	A	<-->	6659	NE2	GLN	409	B	3.45
154	5634	CD	GLU	589	A	<-->	6723	ND2	ASN	417	B	3.49
155	5635	OE1	GLU	589	A	<-->	6598	NH2	ARG	403	B	3.89
156	5635	OE1	GLU	589	A	<-->	6659	NE2	GLN	409	B	3.19
157	5636	OE2	GLU	589	A	<-->	6659	NE2	GLN	409	B	3
158	5636	OE2	GLU	589	A	<-->	6717	N	ASN	417	B	3.58
159	5636	OE2	GLU	589	A	<-->	6720	CB	ASN	417	B	3.12
160	5636	OE2	GLU	589	A	<-->	6721	CG	ASN	417	B	3.41
161	5636	OE2	GLU	589	A	<-->	6723	ND2	ASN	417	B	2.76
162	5661	CD2	PHE	592	A	<-->	6722	OD1	ASN	417	B	3.5
163	5661	CD2	PHE	592	A	<-->	6723	ND2	ASN	417	B	3.46
164	5663	CE2	PHE	592	A	<-->	6722	OD1	ASN	417	B	3.66
165	5663	CE2	PHE	592	A	<-->	7107	CG	LEU	455	B	3.66
166	5663	CE2	PHE	592	A	<-->	7108	CD1	LEU	455	B	3.53
167	5670	CB	THR	593	A	<-->	6712	N	GLY	416	B	3.76
168	5670	CB	THR	593	A	<-->	6714	CA	GLY	416	B	3.06
169	5670	CB	THR	593	A	<-->	6715	C	GLY	416	B	3.62
170	5670	CB	THR	593	A	<-->	6717	N	ASN	417	B	3.66
171	5671	OG1	THR	593	A	<-->	6714	CA	GLY	416	B	3.88
172	5673	CG2	THR	593	A	<-->	6714	CA	GLY	416	B	3.34
173	5673	CG2	THR	593	A	<-->	6715	C	GLY	416	B	3.75

Sl.No.	Atom no.	Atom name	Residue name	Residue no.	Chain	Non-bonded contacts	Atom no.	Atom name	Residue name	Residue no.	Chain	Distance
174	5673	CG2	THR	593	A	<-->	6717	N	ASN	417	B	3.32
175	5712	C	LYS	596	A	<-->	6762	OH	TYR	421	B	3.63
176	5713	O	LYS	596	A	<-->	6759	CE1	TYR	421	B	3.76
177	5713	O	LYS	596	A	<-->	6761	CZ	TYR	421	B	3.6
178	5713	O	LYS	596	A	<-->	6762	OH	TYR	421	B	2.82
179	5713	O	LYS	596	A	<-->	7167	OD1	ASN	460	B	3.82
180	5704	CB	LYS	596	A	<-->	6759	CE1	TYR	421	B	3.85
181	5704	CB	LYS	596	A	<-->	6761	CZ	TYR	421	B	3.69
182	5704	CB	LYS	596	A	<-->	6762	OH	TYR	421	B	3.87
183	5706	CD	LYS	596	A	<-->	6760	CE2	TYR	421	B	3.86
184	5706	CD	LYS	596	A	<-->	7111	O	LEU	455	B	3.17
185	5707	CE	LYS	596	A	<-->	6722	OD1	ASN	417	B	3.14
186	5707	CE	LYS	596	A	<-->	6756	CG	TYR	421	B	3.71
187	5707	CE	LYS	596	A	<-->	6758	CD2	TYR	421	B	3.68
188	5707	CE	LYS	596	A	<-->	7111	O	LEU	455	B	3.5
189	5708	NZ	LYS	596	A	<-->	6721	CG	ASN	417	B	3.66
190	5708	NZ	LYS	596	A	<-->	6722	OD1	ASN	417	B	2.66
191	5708	NZ	LYS	596	A	<-->	6755	CB	TYR	421	B	3.45
192	5708	NZ	LYS	596	A	<-->	6756	CG	TYR	421	B	3.47
193	5708	NZ	LYS	596	A	<-->	6758	CD2	TYR	421	B	3.41
194	5708	NZ	LYS	596	A	<-->	7102	O	ARG	454	B	3.61
195	5708	NZ	LYS	596	A	<-->	7105	CA	LEU	455	B	3.73
196	5708	NZ	LYS	596	A	<-->	7110	C	LEU	455	B	3.48
197	5708	NZ	LYS	596	A	<-->	7111	O	LEU	455	B	2.72
198	5716	CA	ASP	597	A	<-->	7167	OD1	ASN	460	B	3.55
199	5722	O	ASP	597	A	<-->	7167	OD1	ASN	460	B	3.78
200	5718	CG	ASP	597	A	<-->	6709	CG2	THR	415	B	3.89
201	5718	CG	ASP	597	A	<-->	7168	ND2	ASN	460	B	3.67
202	5719	OD1	ASP	597	A	<-->	6709	CG2	THR	415	B	3.86
203	5719	OD1	ASP	597	A	<-->	7166	CG	ASN	460	B	3.65
204	5719	OD1	ASP	597	A	<-->	7168	ND2	ASN	460	B	2.66
205	5748	CA	LYS	600	A	<-->	7156	CA	SER	459	B	3.88
206	5758	O	LYS	600	A	<-->	7153	O	LYS	458	B	3.59
207	5758	O	LYS	600	A	<-->	7156	CA	SER	459	B	3.8
208	5758	O	LYS	600	A	<-->	7157	CB	SER	459	B	3.11
209	5749	CB	LYS	600	A	<-->	7156	CA	SER	459	B	3.67
210	5749	CB	LYS	600	A	<-->	7157	CB	SER	459	B	3.76
211	5749	CB	LYS	600	A	<-->	7162	N	ASN	460	B	3.56
212	5749	CB	LYS	600	A	<-->	7167	OD1	ASN	460	B	3.05
213	5750	CG	LYS	600	A	<-->	7167	OD1	ASN	460	B	3.6
214	5751	CD	LYS	600	A	<-->	7165	CB	ASN	460	B	3.77
215	5751	CD	LYS	600	A	<-->	7166	CG	ASN	460	B	3.37
216	5751	CD	LYS	600	A	<-->	7167	OD1	ASN	460	B	3.25
217	5751	CD	LYS	600	A	<-->	7168	ND2	ASN	460	B	3.9
218	5753	NZ	LYS	600	A	<-->	7168	ND2	ASN	460	B	3.65
219	5785	CE1	PHE	603	A	<-->	7331	O	GLY	476	B	3.64
220	5787	CZ	PHE	603	A	<-->	7327	N	GLY	476	B	3.88
221	5787	CZ	PHE	603	A	<-->	7329	CA	GLY	476	B	3.71
222	5787	CZ	PHE	603	A	<-->	7330	C	GLY	476	B	3.59
223	5787	CZ	PHE	603	A	<-->	7331	O	GLY	476	B	3.5
224	5796	C	VAL	604	A	<-->	7324	CB	ALA	475	B	3.86
225	5797	O	VAL	604	A	<-->	7323	CA	ALA	475	B	3.08
226	5797	O	VAL	604	A	<-->	7325	C	ALA	475	B	3.34
227	5797	O	VAL	604	A	<-->	7326	O	ALA	475	B	3.39
228	5797	O	VAL	604	A	<-->	7324	CB	ALA	475	B	3.34
229	5793	CB	VAL	604	A	<-->	7305	OH	TYR	473	B	3.35
230	5795	CG2	VAL	604	A	<-->	7305	OH	TYR	473	B	3.31
231	5800	CA	GLY	605	A	<-->	7325	C	ALA	475	B	3.74
232	5800	CA	GLY	605	A	<-->	7326	O	ALA	475	B	2.86
233	5800	CA	GLY	605	A	<-->	7324	CB	ALA	475	B	3.7
234	5801	C	GLY	605	A	<-->	7326	O	ALA	475	B	3.48
235	5803	N	TRP	606	A	<-->	7326	O	ALA	475	B	3.22
236	5803	N	TRP	606	A	<-->	7423	ND2	ASN	487	B	3.52
237	5818	O	TRP	606	A	<-->	7423	ND2	ASN	487	B	3.68

Sl.No.	Atom no.	Atom name	Residue name	Residue no.	Chain	Non-bonded contacts	Atom no.	Atom name	Residue name	Residue no.	Chain	Distance
238	5823	OG	SER	607	A	<-->	7336	CG	ASN	477	B	3.38
239	5823	OG	SER	607	A	<-->	7337	OD1	ASN	477	B	3.8
240	5823	OG	SER	607	A	<-->	7338	ND2	ASN	477	B	3.15
241	5831	OG1	THR	608	A	<-->	7413	CE2	PHE	486	B	3.77
242	5831	OG1	THR	608	A	<-->	7414	CZ	PHE	486	B	3.29
243	5833	CG2	THR	608	A	<-->	7414	CZ	PHE	486	B	3.87
244	5840	CG	ASP	609	A	<-->	7338	ND2	ASN	477	B	3.76
245	5842	OD2	ASP	609	A	<-->	7336	CG	ASN	477	B	3.88
246	5842	OD2	ASP	609	A	<-->	7338	ND2	ASN	477	B	2.74

Table S5C. List of atom-atom interactions (Salt bridges) across protein-ligand interface in ACE2(chain A)-Spike Protein(Chain B) (BA.1variant) complex from PDBsum server.

Sl.No.	Atom no.	Atom name	Residue name	Residue no.	Chain	Salt bridges	Atom no.	Atom name	Residue name	Residue no.	Chain	Distance
					Id						Id	(Å)
1	2143	OE1	GLU	232	A	<-->	7486	NH1	ARG	493	B	2.67
2	5044	OE1	GLU	527	A	<-->	7589	ND1	HIS	504	B	3.76
3	5635	OE1	GLU	589	A	<-->	6598	NH2	ARG	403	B	3.89

Table S6A. List of atom-atom interactions(Hydrogen bonds) across protein-ligand interface in ACE2 (Chain A)-Spike Protein (Chain B) (BA.2 variant) complex from PDBsum server.

Sl.No.	Atom no.	Atom name	Residue name	Residue no.	Chain	Hydrogen bonds	Atom no.	Atom name	Residue name	Residue no.	Chain	Distance
					Id						Id	(Å)
1	258	NH1	ARG	357	A	<-->	5932	O	GLU	430	B	2.65
2	261	NH2	ARG	357	A	<-->	5917	OE1	GLN	429	B	3.11
3	261	NH2	ARG	357	A	<-->	5932	O	GLU	430	B	2.93
4	611	ND2	ASN	394	A	<-->	5917	OE1	GLN	429	B	2.92
5	922	OD1	ASP	427	A	<-->	7003	NZ	LYS	534	B	2.59
6	931	OD1	ASP	428	A	<-->	7003	NZ	LYS	534	B	2.59
7	947	N	THR	430	A	<-->	7029	OE2	GLU	536	B	2.68
8	1242	NZ	LYS	458	A	<-->	4045	OE2	GLU	232	B	2.57
9	1252	OG	SER	459	A	<-->	7440	ND2	ASN	580	B	3.1
10	1275	O	LEU	461	A	<-->	6979	NE2	GLN	531	B	2.87
11	1283	NZ	LYS	462	A	<-->	6946	OE1	GLU	527	B	2.58
12	1315	OE2	GLU	465	A	<-->	7462	NH1	ARG	582	B	2.8
13	1344	N	ILE	468	A	<-->	7539	OE2	GLU	589	B	3.02
14	1388	O	ILE	472	A	<-->	4003	NE2	HIS	228	B	2.79
15	1410	NE2	GLN	474	A	<-->	3965	OE2	GLU	224	B	2.64
16	1795	N	PHE	515	A	<-->	7028	OE1	GLU	536	B	3.32
17	1846	O	HIS	519	A	<-->	5829	NZ	LYS	419	B	2.76

Table S6B. List of atom-atom interactions(Non-bonded contacts) across protein-ligand interface in ACE2 (Chain A)-Spike Protein (Chain B) (BA.2 variant) complex from PDBsum server.

Sl.No.	Atom no.	Atom name	Residue name	Residue no.	Chain	Non-bonded contacts	Atom no.	Atom name	Residue name	Residue no.	Chain	Distance
					Id						Id	(Å)
1	228	NH1	ARG	355	A	<-->	7041	CD	PRO	538	B	3.63
2	257	CZ	ARG	357	A	<-->	5932	O	GLU	430	B	3.21
3	258	NH1	ARG	357	A	<-->	5931	C	GLU	430	B	3.72
4	258	NH1	ARG	357	A	<-->	5932	O	GLU	430	B	2.65
5	258	NH1	ARG	357	A	<-->	5935	CA	ASP	431	B	3.63
6	261	NH2	ARG	357	A	<-->	5915	CG	GLN	429	B	3.75
7	261	NH2	ARG	357	A	<-->	5916	CD	GLN	429	B	3.52
8	261	NH2	ARG	357	A	<-->	5917	OE1	GLN	429	B	3.11
9	261	NH2	ARG	357	A	<-->	5932	O	GLU	430	B	2.93
10	609	CG	ASN	394	A	<-->	5917	OE1	GLN	429	B	3.65
11	610	OD1	ASN	394	A	<-->	5916	CD	GLN	429	B	3.79
12	610	OD1	ASN	394	A	<-->	5917	OE1	GLN	429	B	3.54
13	610	OD1	ASN	394	A	<-->	5918	NE2	GLN	429	B	3.84
14	611	ND2	ASN	394	A	<-->	5916	CD	GLN	429	B	3.73
15	611	ND2	ASN	394	A	<-->	5917	OE1	GLN	429	B	2.92

Sl.No.	Atom no.	Atom name	Residue name	Residue no.	Chain	Non-bonded contacts	Atom no.	Atom name	Residue name	Residue no.	Chain	Distance
16	913	CG	PRO	426	A	<-->	7026	CG	GLU	536	B	3.72
17	921	CG	ASP	427	A	<-->	7003	NZ	LYS	534	B	3.77
18	922	OD1	ASP	427	A	<-->	7002	CE	LYS	534	B	3.54
19	922	OD1	ASP	427	A	<-->	7003	NZ	LYS	534	B	2.59
20	930	CG	ASP	428	A	<-->	7001	CD	LYS	534	B	3.8
21	930	CG	ASP	428	A	<-->	7002	CE	LYS	534	B	3.86
22	930	CG	ASP	428	A	<-->	7003	NZ	LYS	534	B	3.42
23	931	OD1	ASP	428	A	<-->	7001	CD	LYS	534	B	3.73
24	931	OD1	ASP	428	A	<-->	7002	CE	LYS	534	B	3.46
25	931	OD1	ASP	428	A	<-->	7003	NZ	LYS	534	B	2.59
26	932	OD2	ASP	428	A	<-->	6999	CB	LYS	534	B	3.47
27	932	OD2	ASP	428	A	<-->	7001	CD	LYS	534	B	3.63
28	937	CA	PHE	429	A	<-->	7029	OE2	GLU	536	B	3.17
29	945	C	PHE	429	A	<-->	7029	OE2	GLU	536	B	3.4
30	938	CB	PHE	429	A	<-->	7029	OE2	GLU	536	B	3.81
31	939	CG	PHE	429	A	<-->	7029	OE2	GLU	536	B	3.7
32	940	CD1	PHE	429	A	<-->	7027	CD	GLU	536	B	3.59
33	940	CD1	PHE	429	A	<-->	7029	OE2	GLU	536	B	3.01
34	942	CE1	PHE	429	A	<-->	7029	OE2	GLU	536	B	3.76
35	947	N	THR	430	A	<-->	7029	OE2	GLU	536	B	2.68
36	949	CA	THR	430	A	<-->	7029	OE2	GLU	536	B	3.72
37	955	O	THR	430	A	<-->	7029	OE2	GLU	536	B	3.72
38	953	CG2	THR	430	A	<-->	7029	OE2	GLU	536	B	3.36
39	1222	CG	ARG	457	A	<-->	7458	CD	ARG	582	B	3.87
40	1224	NE	ARG	457	A	<-->	7458	CD	ARG	582	B	3.26
41	1226	CZ	ARG	457	A	<-->	7458	CD	ARG	582	B	3.26
42	1226	CZ	ARG	457	A	<-->	7459	NE	ARG	582	B	3.87
43	1230	NH2	ARG	457	A	<-->	7458	CD	ARG	582	B	3.27
44	1247	O	LYS	458	A	<-->	7398	CB	ALA	576	B	3.61
45	1238	CB	LYS	458	A	<-->	7438	CG	ASN	580	B	3.77
46	1238	CB	LYS	458	A	<-->	7440	ND2	ASN	580	B	3.52
47	1241	CE	LYS	458	A	<-->	4045	OE2	GLU	232	B	3.51
48	1241	CE	LYS	458	A	<-->	7438	CG	ASN	580	B	3.58
49	1241	CE	LYS	458	A	<-->	7439	OD1	ASN	580	B	3.15
50	1242	NZ	LYS	458	A	<-->	4043	CD	GLU	232	B	3.15
51	1242	NZ	LYS	458	A	<-->	4044	OE1	GLU	232	B	3.28
52	1242	NZ	LYS	458	A	<-->	4045	OE2	GLU	232	B	2.57
53	1242	NZ	LYS	458	A	<-->	7439	OD1	ASN	580	B	3.65
54	1251	CB	SER	459	A	<-->	7461	CZ	ARG	582	B	3.89
55	1251	CB	SER	459	A	<-->	7465	NH2	ARG	582	B	3.06
56	1252	OG	SER	459	A	<-->	7440	ND2	ASN	580	B	3.1
57	1252	OG	SER	459	A	<-->	7459	NE	ARG	582	B	3.68
58	1252	OG	SER	459	A	<-->	7461	CZ	ARG	582	B	3.66
59	1252	OG	SER	459	A	<-->	7465	NH2	ARG	582	B	2.78
60	1275	O	LEU	461	A	<-->	6979	NE2	GLN	531	B	2.87
61	1280	CG	LYS	462	A	<-->	6949	O	GLU	527	B	3.32
62	1280	CG	LYS	462	A	<-->	6975	CB	GLN	531	B	3.61
63	1281	CD	LYS	462	A	<-->	6949	O	GLU	527	B	3.68
64	1281	CD	LYS	462	A	<-->	6943	CB	GLU	527	B	3.86
65	1281	CD	LYS	462	A	<-->	6945	CD	GLU	527	B	3.88
66	1281	CD	LYS	462	A	<-->	6946	OE1	GLU	527	B	3.79
67	1282	CE	LYS	462	A	<-->	6949	O	GLU	527	B	3.89
68	1282	CE	LYS	462	A	<-->	6943	CB	GLU	527	B	3.38
69	1282	CE	LYS	462	A	<-->	6946	OE1	GLU	527	B	3.51
70	1283	NZ	LYS	462	A	<-->	6943	CB	GLU	527	B	3.43
71	1283	NZ	LYS	462	A	<-->	6945	CD	GLU	527	B	3.43
72	1283	NZ	LYS	462	A	<-->	6946	OE1	GLU	527	B	2.58
73	1283	NZ	LYS	462	A	<-->	7462	NH1	ARG	582	B	3.84
74	1295	O	PRO	463	A	<-->	7021	O	HIS	535	B	3.68
75	1295	O	PRO	463	A	<-->	7036	O	GLY	537	B	3.35
76	1291	CB	PRO	463	A	<-->	7021	O	HIS	535	B	3.37
77	1307	O	PHE	464	A	<-->	7036	O	GLY	537	B	3.82
78	1302	CD2	PHE	464	A	<-->	7030	C	GLU	536	B	3.72
79	1302	CD2	PHE	464	A	<-->	7032	N	GLY	537	B	3.14

Sl.No.	Atom no.	Atom name	Residue name	Residue no.	Chain	Non-bonded contacts	Atom no.	Atom name	Residue name	Residue no.	Chain	Distance
80	1302	CD2	PHE	464	A	<-->	7034	CA	GLY	537	B	3.78
81	1304	CE2	PHE	464	A	<-->	7024	CA	GLU	536	B	3.78
82	1304	CE2	PHE	464	A	<-->	7025	CB	GLU	536	B	3.85
83	1304	CE2	PHE	464	A	<-->	7026	CG	GLU	536	B	3.34
84	1304	CE2	PHE	464	A	<-->	7027	CD	GLU	536	B	3.6
85	1304	CE2	PHE	464	A	<-->	7028	OE1	GLU	536	B	3.49
86	1304	CE2	PHE	464	A	<-->	7032	N	GLY	537	B	3.78
87	1305	CZ	PHE	464	A	<-->	7028	OE1	GLU	536	B	3.81
88	1312	CG	GLU	465	A	<-->	7499	CG	ASN	586	B	3.67
89	1312	CG	GLU	465	A	<-->	7500	OD1	ASN	586	B	3.16
90	1313	CD	GLU	465	A	<-->	7462	NH1	ARG	582	B	3.81
91	1315	OE2	GLU	465	A	<-->	7462	NH1	ARG	582	B	2.8
92	1315	OE2	GLU	465	A	<-->	7498	CB	ASN	586	B	3.77
93	1315	OE2	GLU	465	A	<-->	7499	CG	ASN	586	B	3.79
94	1333	C	ARG	466	A	<-->	7539	OE2	GLU	589	B	3.48
95	1334	O	ARG	466	A	<-->	7498	CB	ASN	586	B	3.4
96	1334	O	ARG	466	A	<-->	7539	OE2	GLU	589	B	3.8
97	1321	CB	ARG	466	A	<-->	7536	CG	GLU	589	B	3.68
98	1321	CB	ARG	466	A	<-->	7537	CD	GLU	589	B	3.47
99	1321	CB	ARG	466	A	<-->	7538	OE1	GLU	589	B	3.84
100	1321	CB	ARG	466	A	<-->	7539	OE2	GLU	589	B	3.58
101	1322	CG	ARG	466	A	<-->	7537	CD	GLU	589	B	3.66
102	1322	CG	ARG	466	A	<-->	7538	OE1	GLU	589	B	3.63
103	1322	CG	ARG	466	A	<-->	7539	OE2	GLU	589	B	3.72
104	1323	CD	ARG	466	A	<-->	7537	CD	GLU	589	B	3.52
105	1323	CD	ARG	466	A	<-->	7538	OE1	GLU	589	B	3
106	1327	NH1	ARG	466	A	<-->	7535	CB	GLU	589	B	3.27
107	1327	NH1	ARG	466	A	<-->	7538	OE1	GLU	589	B	3.41
108	1335	N	ASP	467	A	<-->	7539	OE2	GLU	589	B	3.25
109	1337	CA	ASP	467	A	<-->	7539	OE2	GLU	589	B	3.45
110	1342	C	ASP	467	A	<-->	7539	OE2	GLU	589	B	3.43
111	1339	CG	ASP	467	A	<-->	7457	CG	ARG	582	B	3.66
112	1339	CG	ASP	467	A	<-->	7458	CD	ARG	582	B	3.77
113	1340	OD1	ASP	467	A	<-->	7457	CG	ARG	582	B	3.47
114	1341	OD2	ASP	467	A	<-->	7457	CG	ARG	582	B	3.42
115	1341	OD2	ASP	467	A	<-->	7458	CD	ARG	582	B	3.05
116	1344	N	ILE	468	A	<-->	7539	OE2	GLU	589	B	3.02
117	1346	CA	ILE	468	A	<-->	7539	OE2	GLU	589	B	3.85
118	1347	CB	ILE	468	A	<-->	7539	OE2	GLU	589	B	3.6
119	1348	CG1	ILE	468	A	<-->	7489	CB	LEU	585	B	3.51
120	1348	CG1	ILE	468	A	<-->	7537	CD	GLU	589	B	3.88
121	1348	CG1	ILE	468	A	<-->	7539	OE2	GLU	589	B	3.23
122	1349	CG2	ILE	468	A	<-->	7537	CD	GLU	589	B	3.7
123	1349	CG2	ILE	468	A	<-->	7538	OE1	GLU	589	B	3.42
124	1349	CG2	ILE	468	A	<-->	7539	OE2	GLU	589	B	3.3
125	1350	CD1	ILE	468	A	<-->	7494	O	LEU	585	B	3.66
126	1350	CD1	ILE	468	A	<-->	7489	CB	LEU	585	B	3.81
127	1350	CD1	ILE	468	A	<-->	7562	CG	PHE	592	B	3.85
128	1350	CD1	ILE	468	A	<-->	7564	CD2	PHE	592	B	3.59
129	1353	N	SER	469	A	<-->	7491	CD1	LEU	585	B	3.85
130	1355	CA	SER	469	A	<-->	7491	CD1	LEU	585	B	3.57
131	1356	CB	SER	469	A	<-->	7491	CD1	LEU	585	B	3.78
132	1357	OG	SER	469	A	<-->	7491	CD1	LEU	585	B	3.78
133	1365	OG1	THR	470	A	<-->	4073	CG	PRO	235	B	3.54
134	1373	CB	GLU	471	A	<-->	4042	CG	GLU	232	B	3.33
135	1373	CB	GLU	471	A	<-->	4043	CD	GLU	232	B	3.75
136	1373	CB	GLU	471	A	<-->	4045	OE2	GLU	232	B	3.76
137	1387	C	ILE	472	A	<-->	4003	NE2	HIS	228	B	3.89
138	1388	O	ILE	472	A	<-->	4002	CE1	HIS	228	B	3.48
139	1388	O	ILE	472	A	<-->	4003	NE2	HIS	228	B	2.79
140	1406	CB	GLN	474	A	<-->	4003	NE2	HIS	228	B	3.87
141	1408	CD	GLN	474	A	<-->	3965	OE2	GLU	224	B	3.68
142	1409	OE1	GLN	474	A	<-->	4001	CD2	HIS	228	B	3.69
143	1410	NE2	GLN	474	A	<-->	3963	CD	GLU	224	B	3.49

Sl.No.	Atom no.	Atom name	Residue name	Residue no.	Chain	Non-bonded contacts	Atom no.	Atom name	Residue name	Residue no.	Chain	Distance
144	1410	NE2	GLN	474	A	<-->	3965	OE2	GLU	224	B	2.64
145	1428	CA	ASN	477	A	<-->	3965	OE2	GLU	224	B	3.61
146	1435	C	ASN	477	A	<-->	3964	OE1	GLU	224	B	3.48
147	1435	C	ASN	477	A	<-->	3965	OE2	GLU	224	B	3.62
148	1436	O	ASN	477	A	<-->	3964	OE1	GLU	224	B	3.82
149	1437	N	LYS	478	A	<-->	3963	CD	GLU	224	B	3.44
150	1437	N	LYS	478	A	<-->	3964	OE1	GLU	224	B	3.17
151	1437	N	LYS	478	A	<-->	3965	OE2	GLU	224	B	3.3
152	1439	CA	LYS	478	A	<-->	3963	CD	GLU	224	B	3.78
153	1439	CA	LYS	478	A	<-->	3964	OE1	GLU	224	B	3.25
154	1448	C	LYS	478	A	<-->	3964	OE1	GLU	224	B	3.85
155	1450	N	PRO	479	A	<-->	3964	OE1	GLU	224	B	3.78
156	1454	CD	PRO	479	A	<-->	3962	CG	GLU	224	B	3.63
157	1454	CD	PRO	479	A	<-->	3963	CD	GLU	224	B	3.64
158	1454	CD	PRO	479	A	<-->	3964	OE1	GLU	224	B	3.2
159	1789	CA	SER	514	A	<-->	7028	OE1	GLU	536	B	3.9
160	1790	CB	SER	514	A	<-->	7028	OE1	GLU	536	B	3.57
161	1795	N	PHE	515	A	<-->	7028	OE1	GLU	536	B	3.32
162	1806	O	PHE	515	A	<-->	7028	OE1	GLU	536	B	3.56
163	1814	OE2	GLU	516	A	<-->	7072	NZ	LYS	541	B	3.81
164	1832	CD2	LEU	518	A	<-->	5793	CD	LYS	416	B	3.74
165	1845	C	HIS	519	A	<-->	5889	O	PRO	426	B	3.5
166	1846	O	HIS	519	A	<-->	5827	CD	LYS	419	B	3.17
167	1846	O	HIS	519	A	<-->	5828	CE	LYS	419	B	3.21
168	1846	O	HIS	519	A	<-->	5829	NZ	LYS	419	B	2.76
169	1846	O	HIS	519	A	<-->	5889	O	PRO	426	B	3.1
170	1838	CB	HIS	519	A	<-->	5825	CB	LYS	419	B	3.55
171	1838	CB	HIS	519	A	<-->	5827	CD	LYS	419	B	3.72
172	1839	CG	HIS	519	A	<-->	5825	CB	LYS	419	B	3.77
173	1840	ND1	HIS	519	A	<-->	5800	O	LYS	416	B	3.88
174	1841	CD2	HIS	519	A	<-->	5837	CA	SER	420	B	3.87
175	1842	CE1	HIS	519	A	<-->	5838	CB	SER	420	B	3.54
176	1842	CE1	HIS	519	A	<-->	5839	OG	SER	420	B	3.44
177	1843	NE2	HIS	519	A	<-->	5835	N	SER	420	B	3.81
178	1843	NE2	HIS	519	A	<-->	5837	CA	SER	420	B	3.43
179	1843	NE2	HIS	519	A	<-->	5838	CB	SER	420	B	3.35
180	1843	NE2	HIS	519	A	<-->	5839	OG	SER	420	B	3.76
181	1847	N	ALA	520	A	<-->	5889	O	PRO	426	B	3.49
182	1849	CA	ALA	520	A	<-->	5889	O	PRO	426	B	2.98
183	1851	C	ALA	520	A	<-->	5889	O	PRO	426	B	3.78
184	1853	N	PRO	521	A	<-->	5889	O	PRO	426	B	3.83
185	1856	CG	PRO	521	A	<-->	5892	CA	ASP	427	B	3.5
186	1857	CD	PRO	521	A	<-->	5889	O	PRO	426	B	3.27
187	1857	CD	PRO	521	A	<-->	5892	CA	ASP	427	B	3.52
188	1857	CD	PRO	521	A	<-->	5897	C	ASP	427	B	3.87
189	1857	CD	PRO	521	A	<-->	5898	O	ASP	427	B	3.83
190	1870	OG1	THR	523	A	<-->	5918	NE2	GLN	429	B	3.49

Table S6C. List of atom-atom interactions(Salt bridges) across protein-ligand interface in ACE2 (Chain A)-Spike Protein (Chain B) (BA.2 variant) complex from PDBsum server.

Sl.No.	Atom no.	Atom name	Residue name	Residue no.	Chain	Salt bridges	Atom no.	Atom name	Residue name	Residue no.	Chain	Distance
					Id						Id	(Å)
1	923	OD2	ASP	427	A	<-->	7003	NZ	LYS	534	B	2.59
2	931	OD1	ASP	428	A	<-->	7003	NZ	LYS	534	B	2.59
3	1242	NZ	LYS	458	A	<-->	4045	OE2	GLU	232	B	2.57
4	1283	NZ	LYS	462	A	<-->	6947	OE2	GLU	527	B	2.58
5	1315	OE2	GLU	465	A	<-->	7462	NH1	ARG	582	B	2.8
6	1327	NH1	ARG	466	A	<-->	7539	OE2	GLU	589	B	3.41
7	1813	OE1	GLU	516	A	<-->	7072	NZ	LYS	541	B	3.81