Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information
for
Computational Investigation of Increased Virulence and Pathogenesis of SARS-CoV-2 Lineage B.1.1.7

N. Arul Murugan[†], Prashanth S. Javali[γ] , Chitra Jeyaraj Pandian[‡], Muhammad Akhtar Ali[∂], Vaibhav Srivastava[∂], Jeyakanthan Jeyaraman[γ]
[†]Department of Theoretical Chemistry and Biology,
School of Engineering Sciences in Chemistry, Biotechnology and Health,
KTH Royal Institute of Technology, S-106 91, Stockholm, Sweden
Present address : Department Computational Biology,
Indraprastha Institute of
Information Technology (IIIT-D), New Delhi-110020, India;
arul.murugan@iiitd.ac.in.

[‡] Department of Biotechnology,
Dr. Umayal Ramanathan College for Women, Karaikudi, India

[∂]Division of Glycoscience, Department of Chemistry,
School of Chemistry, Biotechnology and Health,
KTH Royal Institute of Technology, Stockholm, Sweden

[γ] Department of Bioinformatics,
Alagappa University, Karaikudi, Tamilnadu, India

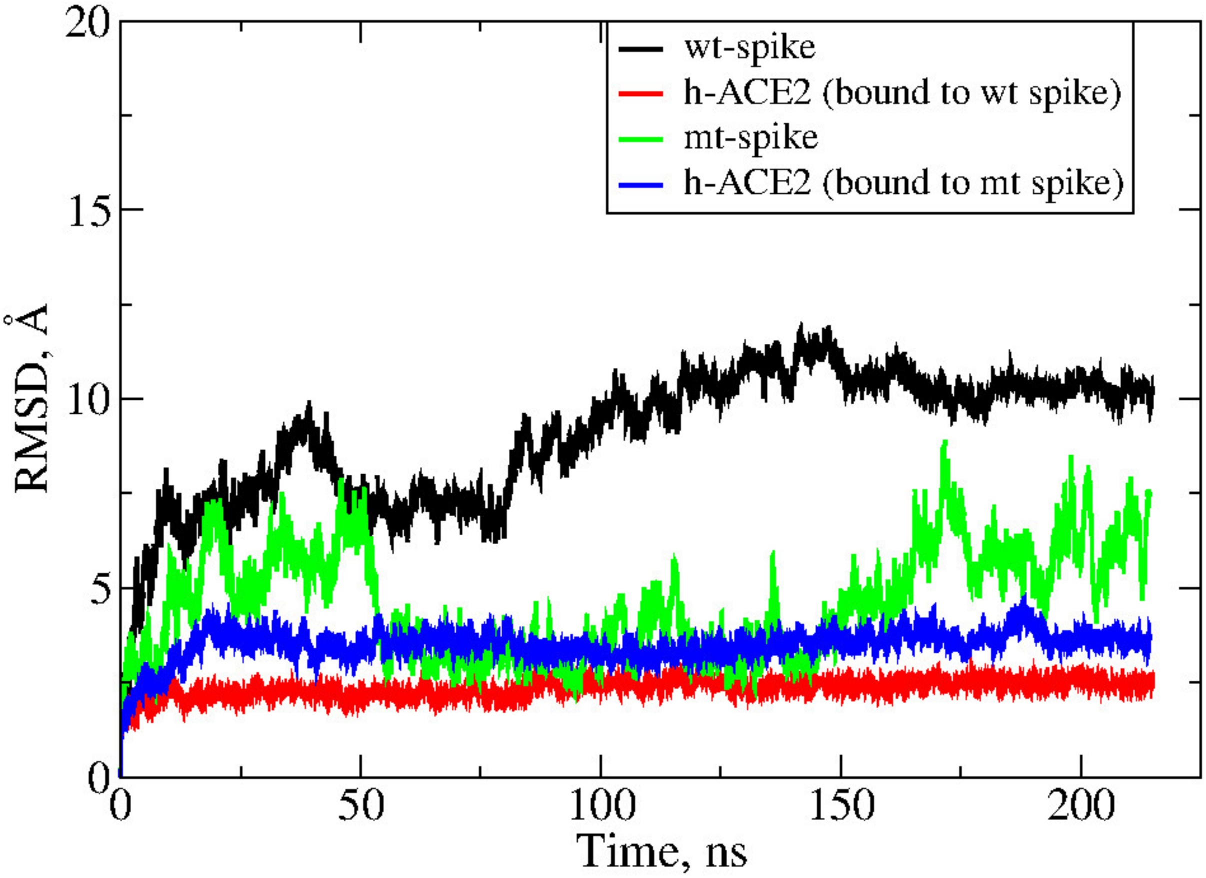

Figure S1: RMSD as a function of time computed for wild type and mutant variants of spike protein and their ACE-2 counterparts in the respective protein-protein complexes. The results correspond to continuation run for a time scale of 210 ns.

The spike glycoprotein sequence (P0DTC2) from the unmutated Wuhan coronavirus strain, was obtained from UniprotKB. The crystal structure of this version of the spike protein has been solved by x-ray diffraction and electron microscope with several structures available in protein data bank (PDB). Four mutations are reported in the receptor binding domain (RBD) of the spike protein in different viral strains found in the UK (Table S1). The eight mutant versions of the spike protein sequences with two harboring mutations in the receptor binding domain (RBD) found in UK mutant strains B.1.1.7 (Table S2) were prepared by substituting all the eight corresponding amino acids with their mutant counterparts before building their structure. All 23 mutations found in the strain B.1.1.7 (Andrew R., *et al.*, https://virological.org/t/preliminary-genomic-characterisation-of-an-emergent-sars-cov-2-lineage-in-the-uk-defined-by-a-novel-set-of-spike-mutations/563) with their mutation type and location are summarized in supplementary table S2.

Supplementary table S.1

Strains found in UK with mutation in the RBD of spike protein			
Sr.No	**Strain**	**gisaid_epi_isl**	**Mutation at RBD domain**
1	England/QEUH-AE4A64/2020	EPI_ISL_633162	S477N

2	England/MILK-99CD63/2020	EPI_ISL_549878	S477N
3	England/CAMC-B355F9/2020	EPI_ISL_659432	N439K
4	Scotland/EDB7745/2020	EPI_ISL_540884	N439K
5	Wales/PHWC-488752/2020	EPI_ISL_638115	N439K
6	England/CAMC-C479AC/2020	EPI_ISL_718708	N501Y
7	England/CAMC-BFBCAF/2020	EPI_ISL_708999	N501Y
8	England/CAMC-C3F43D/2020	EPI_ISL_719418	N501Y
9	England/ALDP-C3B63B/2020	EPI_ISL_730684	N501Y
10	England/CAMC-BFB780/2020	EPI_ISL_709146	N501Y
11	Scotland/EDB11122/2020	EPI_ISL_742218	N501Y
12	England/CAMC-C478EB/2020	EPI_ISL_718834	N501Y
13	England/CAMC-C479AC/2020	EPI_ISL_718708	A570D
14	England/CAMC-BFBCAF/2020	EPI_ISL_708999	A570D
15	England/CAMC-C3F43D/2020	EPI_ISL_719418	A570D
16	England/ALDP-C3B63B/2020	EPI_ISL_730684	A570D
17	England/CAMC-BFB780/2020	EPI_ISL_709146	A570D
18	Scotland/EDB11122/2020	EPI_ISL_742218	A570D
19	England/CAMC-C478EB/2020	EPI_ISL_718834	A570D

Supplementary table S.2

All 23 mutations found in UK strain B.1.1.7.						
Sr. No	**Gene**	**Nucleotide change**	**Amino Acid change**	**Mutation type**	**RBD**	**Sequence**
1	ORF1ab	C3267T	T1001I	Non-synonymous	No	acaactactattcaa
2		C5388A	A1708D	Non-synonymous	No	gaagctgctaacttt
3		T6954C	I2230T	Non-synonymous	No	aatattataatttgg
4		11288-11296 deletion	SGF 3675-3677	Deletion	No	ttgtctggttttaag
5		C913T	-	Synonymous	No	actttgtccgaacaa
6		C5986T	-	Synonymous	No	tcttatttcacagag
7		C14676T	-	Synonymous	No	gtcaaacccggtaat
8		C15279T	-	Synonymous	No	aaccctcaccttatg
9		C16176T	-	Synonymous	No	gataacacttcaagg
10	spike	21765-21770 deletion	HV 69-70	Deletion	No	ctatacatgtct
11		21991-21993 deletion	Y144	Deletion	No	gggtgtttattacca
12		A23063T	N501Y	Non-synonymous	yes	cccactaatggtgtt
13		C23271A	A570D	Non-synonymous	yes	gacattgctgacact
14		C23604A	P681H	Non-synonymous	No	aattctcctcggcgg
15		C23709T	T716I	Non-synonymous	No	atacccacaaatttt
16		T24506G	S982A	Non-synonymous	No	atcctttcacgtctt
17		G24914C	D1118H	Non-	No	actacagacaacaca

				synonymous		
18	Orf8	C27972T	Q27*	Stop	No	tgtactcaacatcaa
19		G28048T	R52I	Non-synonymous	No	ggagctagaaaatca
20		A28111G	Y73C	Non-synonymous	No	attcagtacatcgat
21	N	28280 GAT->CTA	D3L	Non-synonymous	No	atgtctgataatgga
22		C28977T	S235F	Non-synonymous	No	aaaatgtctggtaaa
23	M	T26801C	-	Synonymous	No	atgtggctcagctac

This is sequence contains all the 8 mutations of spike protein of B.1.1.7 strain from UK.
MFVFLVLLPLVSSQCVNLTTRTQLPPAYTNSFRGVYYPDKVFRSSVLHSTQDLFLPFFSNVTWFHAISGTN
GTKRFDNPVLPFNDGVYFASTEKSNIIRGWIFGTTLDSKTQSLLIVNNATNVVIKVCEFQFCNDPFLGVYH
KNNKSWMESEFRVYSSANNCTFEYVSQPFLMDLEGKQGNFKNLREFVFKNIDGYFKIYSKHTPINLVRDL
PQGFSALEPLVDLPIGINITRFQTLLALHRSYLTPGDSSSGWTAGAAAYYVGYLQPRTFLLKYNENGTITDA
VDCALDPLSETKCTLKSFTVEKGIYQTSNFRVQPTESIVRFPNITNLCPFGEVFNATRFASVYAWNRKRISN
CVADYSVLYNSASFSTFKCYGVSPTKLNDLCFTNVYADSFVIRGDEVRQIAPGQTGKIADYNYKLPDDFTG
CVIAWNSNNLDSKVGGNYNYLYRLFRKSNLKPFERDISTEIYQAGSTPCNGVEGFNCYFPLQSYGFQPTY
GVGYQPYRVVVLSFELLHAPATVCGPKKSTNLVKNKCVNFNFNGLTGTGVLTESNKKFLPFQQFGRDIDD
TTDAVRDPQTLEILDITPCSFGGVSVITPGTNTSNQVAVLYQDVNCTEVPVAIHADQLTPTWRVYSTGSN
VFQTRAGCLIGAEHVNNSYECDIPIGAGICASYQTQTNSHRRARSVASQSIIAYTMSLGAENSVAYSNNSI
AIPINFTISVTTEILPVSMTKTSVDCTMYICGDSTECSNLLLQYGSFCTQLNRALTGIAVEQDKNTQEVFAQ
VKQIYKTPPIKDFGGFNFSQILPDPSKPSKRSFIEDLLFNKVTLADAGFIKQYGDCLGDIAARDLICAQKFNG
LTVLPPLLTDEMIAQYTSALLAGTITSGWTFGAGAALQIPFAMQMAYRFNGIGVTQNVLYENQKLIANQ
FNSAIGKIQDSLSSTASALGKLQDVVNQNAQALNTLVKQLSSNFGAISSVLNDILARLDKVEAEVQIDRLIT
GRLQSLQTYVTQQLIRAAEIRASANLAATKMSECVLGQSKRVDFCGKGYHLMSFPQSAPHGVVFLHVTY
VPAQEKNFTTAPAICHDGKAHFPREGVFVSNGTHWFVTQRNFYEPQIITTHNTFVSGNCDVVIGIVNNT
VYDPLQPELDSFKEELDKYFKNHTSPDVDLGDISGINASVVNIQKEIDRLNEVAKNLNESLIDLQELGKYEQ
YIKWPWYIWLGFIAGLIAIVMVTIMLCCMTSCCSCLKGCCSCGSCCKFDEDDSEPVLKGVKLHYT*

These are all the mutant spike protein versions of B.1.1.7 strain from the UK. Each sequence has one mutation.

21765-21770 deletion   HV 69-70
MFVFLVLLPLVSSQCVNLTTRTQLPPAYTNSFTRGVYYPDKVFRSSVLHSTQDLFLPF
FSNVTWFHAISGTNGTKRFDNPVLPFNDGVYFASTEKSNIIRGWIFGTTLDSKTQSLLI
VNNATNVVIKVCEFQFCNDPFLGVYYHKNNKSWMESEFRVYSSANNCTFEYVSQPF
LMDLEGKQGNFKNLREFVFKNIDGYFKIYSKHTPINLVRDLPQGFSALEPLVDLPIGIN
ITRFQTLLALHRSYLTPGDSSSGWTAGAAAYYVGYLQPRTFLLKYNENGTITDAVDC
ALDPLSETKCTLKSFTVEKGIYQTSNFRVQPTESIVRFPNITNLCPFGEVFNATRFASV
YAWNRKRISNCVADYSVLYNSASFSTFKCYGVSPTKLNDLCFTNVYADSFVIRGDEV

RQIAPGQTGKIADYNYKLPDDFTGCVIAWNSNNLDSKVGGNYNYLYRLFRKSNLKP
FERDISTEIYQAGSTPCNGVEGFNCYFPLQSYGFQPTNGVGYQPYRVVVLSFELLHAP
ATVCGPKKSTNLVKNKCVNFNFNGLTGTGVLTESNKKFLPFQQFGRDIADTTDAVR
DPQTLEILDITPCSFGGVSVITPGTNTSNQVAVLYQDVNCTEVPVAIHADQLTPTWRV
YSTGSNVFQTRAGCLIGAEHVNNSYECDIPIGAGICASYQTQTNSPRRARSVASQSIIA
YTMSLGAENSVAYSNNSIAIPTNFTISVTTEILPVSMTKTSVDCTMYICGDSTECSNLL
LQYGSFCTQLNRALTGIAVEQDKNTQEVFAQVKQIYKTPPIKDFGGFNFSQILPDPSK
PSKRSFIEDLLFNKVTLADAGFIKQYGDCLGDIAARDLICAQKFNGLTVLPPLLTDEMI
AQYTSALLAGTITSGWTFGAGAALQIPFAMQMAYRFNGIGVTQNVLYENQKLIANQ
FNSAIGKIQDSLSSTASALGKLQDVVNQNAQALNTLVKQLSSNFGAISSVLNDILSRL
DKVEAEVQIDRLITGRLQSLQTYVTQQLIRAAEIRASANLAATKMSECVLGQSKRVD
FCGKGYHLMSFPQSAPHGVVFLHVTYVPAQEKNFTTAPAICHDGKAHFPREGVFVS
NGTHWFVTQRNFYEPQIITTDNTFVSGNCDVVIGIVNNTVYDPLQPELDSFKEELDKY
FKNHTSPDVDLGDISGINASVVNIQKEIDRLNEVAKNLNESLIDLQELGKYEQYIKWP
WYIWLGFIAGLIAIVMVTIMLCCMTSCCSCLKGCCSCGSCCKFDEDDSEPVLKGVKL
HYT*

21991-21993 deletion   Y144
MFVFLVLLPLVSSQCVNLTTRTQLPPAYTNSFTRGVYYPDKVFRSSVLHSTQDLFLPF
FSNVTWFHAIHVSGTNGTKRFDNPVLPFNDGVYFASTEKSNIIRGWIFGTTLDSKTQS
LLIVNNATNVVIKVCEFQFCNDPFLGVYHKNNKSWMESEFRVYSSANNCTFEYVSQP
FLMDLEGKQGNFKNLREFVFKNIDGYFKIYSKHTPINLVRDLPQGFSALEPLVDLPIGI
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CALDPLSETKCTLKSFTVEKGIYQTSNFRVQPTESIVRFPNITNLCPFGEVFNATRFAS
VYAWNRKRISNCVADYSVLYNSASFSTFKCYGVSPTKLNDLCFTNVYADSFVIRGDE
VRQIAPGQTGKIADYNYKLPDDFTGCVIAWNSNNLDSKVGGNYNYLYRLFRKSNLK
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LQYGSFCTQLNRALTGIAVEQDKNTQEVFAQVKQIYKTPPIKDFGGFNFSQILPDPSK
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DKVEAEVQIDRLITGRLQSLQTYVTQQLIRAAEIRASANLAATKMSECVLGQSKRVD
FCGKGYHLMSFPQSAPHGVVFLHVTYVPAQEKNFTTAPAICHDGKAHFPREGVFVS
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FKNHTSPDVDLGDISGINASVVNIQKEIDRLNEVAKNLNESLIDLQELGKYEQYIKWP
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HYT*

A23063T N501Y
MFVFLVLLPLVSSQCVNLTTRTQLPPAYTNSFTRGVYYPDKVFRSSVLHSTQDLFLPF
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VKLHYT*

C23271A A570D
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QPFLMDLEGKQGNFKNLREFVFKNIDGYFKIYSKHTPINLVRDLPQGFSALEPLVDLP
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QSIIAYTMSLGAENSVAYSNNSIAIPTNFTISVTTEILPVSMTKTSVDCTMYICGDSTEC
SNLLLQYGSFCTQLNRALTGIAVEQDKNTQEVFAQVKQIYKTPPIKDFGGFNFSQILP
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SRLDKVEAEVQIDRLITGRLQSLQTYVTQQLIRAAEIRASANLAATKMSECVLGQSK
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ASVYAWNRKRISNCVADYSVLYNSASFSTFKCYGVSPTKLNDLCFTNVYADSFVIRG
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WRVYSTGSNVFQTRAGCLIGAEHVNNSYECDIPIGAGICASYQTQTNSPRRARSVAS
QSIIAYTMSLGAENSVAYSNNSIAIPINFTISVTTEILPVSMTKTSVDCTMYICGDSTEC
SNLLLQYGSFCTQLNRALTGIAVEQDKNTQEVFAQVKQIYKTPPIKDFGGFNFSQILP
DPSKPSKRSFIEDLLFNKVTLADAGFIKQYGDCLGDIAARDLICAQKFNGLTVLPPLLT
DEMIAQYTSALLAGTITSGWTFGAGAALQIPFAMQMAYRFNGIGVTQNVLYENQKLI
ANQFNSAIGKIQDSLSSTASALGKLQDVVNQNAQALNTLVKQLSSNFGAISSVLNDIL
SRLDKVEAEVQIDRLITGRLQSLQTYVTQQLIRAAEIRASANLAATKMSECVLGQSK
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FVSNGTHWFVTQRNFYEPQIITTDNTFVSGNCDVVIGIVNNTVYDPLQPELDSFKEEL
DKYFKNHTSPDVDLGDISGINASVVNIQKEIDRLNEVAKNLNESLIDLQELGKYEQYI
KWPWYIWLGFIAGLIAIVMVTIMLCCMTSCCSCLKGCCSCGSCCKFDEDDSEPVLKG
VKLHYT*

T24506G S982A
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LLIVNNATNVVIKVCEFQFCNDPFLGVYYHKNNKSWMESEFRVYSSANNCTFEYVS
QPFLMDLEGKQGNFKNLREFVFKNIDGYFKIYSKHTPINLVRDLPQGFSALEPLVDLP

IGINITRFQTLLALHRSYLTPGDSSSGWTAGAAAYYVGYLQPRTFLLKYNENGTITDA
VDCALDPLSETKCTLKSFTVEKGIYQTSNFRVQPTESIVRFPNITNLCPFGEVFNATRF
ASVYAWNRKRISNCVADYSVLYNSASFSTFKCYGVSPTKLNDLCFTNVYADSFVIRG
DEVRQIAPGQTGKIADYNYKLPDDFTGCVIAWNSNNLDSKVGGNYNYLYRLFRKSN
LKPFERDISTEIYQAGSTPCNGVEGFNCYFPLQSYGFQPTNGVGYQPYRVVVLSFELL
HAPATVCGPKKSTNLVKNKCVNFNFNGLTGTGVLTESNKKFLPFQQFGRDIADTTD
AVRDPQTLEILDITPCSFGGVSVITPGTNTSNQVAVLYQDVNCTEVPVAIHADQLTPT
WRVYSTGSNVFQTRAGCLIGAEHVNNSYECDIPIGAGICASYQTQTNSPRRARSVAS
QSIIAYTMSLGAENSVAYSNNSIAIPTNFTISVTTEILPVSMTKTSVDCTMYICGDSTEC
SNLLLQYGSFCTQLNRALTGIAVEQDKNTQEVFAQVKQIYKTPPIKDFGGFNFSQILP
DPSKPSKRSFIEDLLFNKVTLADAGFIKQYGDCLGDIAARDLICAQKFNGLTVLPPLLT
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VKLHYT*

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VKLHYT*