A Furin Cleavage Site Inserted into the Spike Protein of SARS-CoV-2: A Structural Implication? Supplementary Materials

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Supporting Material

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
MODEL	A_ARG_34	NH1	A_GLU_191	OE2	2.674
MODEL	A_ARG_44	NH1	A_ASP_40	OD1	2.695
MODEL	A_ARG_44	NH1	A_ASP_40	OD2	3.232
MODEL	A_ARG_44	NH2	A_ASP_40	OD1	3.625
MODEL	A_ARG_44	NH2	A_ASP_40	OD2	2.635
MODEL	A_ARG_78	NH1	A_ASP_138	OD2	2.688
MODEL	A_ARG_102	NH1	A_GLU_96	OE1	3.329
MODEL	A_LYS_195	NZ	A_ASP_53	OD1	2.683
MODEL	A_LYS_195	NZ	A_ASP_53	OD2	2.722
MODEL	A_LYS_206	NZ	A_GLU_224	OE1	2.749
MODEL	A_LYS_206	NZ	A_GLU_224	OE2	2.697
MODEL	A_ARG_214	NH1	A_ASP_215	OD1	2.721
MODEL	A_ARG_214	NH1	A_ASP_215	OD2	3.669
MODEL	A_ARG_273	NH2	A_ASP_290	OD1	2.616
MODEL	A_ARG_273	NH2	A_ASP_290	OD2	3.058
MODEL	A_LYS_278	NZ	A_ASP_287	OD2	3.755
MODEL	A_LYS_310	NZ	A_ASP_663	OD1	2.628
MODEL	A_LYS_310	NZ	A_ASP_663	OD2	2.667
MODEL	A_ARG_319	NH1	B_ASP_737	OD2	2.735
MODEL	A_ARG_319	NH1	B_ASP_745	OD1	3.587
MODEL	A_ARG_319	NH2	B_ASP_737	OD2	3.982
MODEL	A_ARG_328	NH1	A_ASP_578	OD2	3.263
MODEL	A_ARG_328	NH2	A_ASP_578	OD2	3.964
MODEL	A_ARG_355	NH2	A_ASP_398	OD1	3.101
MODEL	A_ARG_355	NH2	A_ASP_398	OD2	2.632
MODEL	A_LYS_356	NZ	A_GLU_340	OE1	2.636
MODEL	A_ARG_403	NH1	A_GLU_406	OE2	3.089
MODEL	A_LYS_458	NZ	A_GLU_471	OE1	2.430
MODEL	A_ARG_466	NH1	A_ASP_467	OD1	3.188
MODEL	A_ARG_466	NH1	A_ASP_467	OD2	2.659
MODEL	A_ARG_509	NH1	A_ASP_442	OD1	2.803
MODEL	A_ARG_509	NH1	A_ASP_442	OD2	3.407
MODEL	A_LYS_537	NZ	A_GLU_324	OE1	2.730
MODEL	A_LYS_537	NZ	A_GLU_324	OE2	2.652
MODEL	A_LYS_557	NZ	A_ASP_568	OD1	2.715
MODEL	A_LYS_557	NZ	A_ASP_568	OD2	2.782
MODEL	A_LYS_557	NZ	A_ASP_574	OD1	2.869
MODEL	A_LYS_557	NZ	A_ASP_574	OD2	2.649
MODEL	A_ARG_567	NH1	A_ASP_571	OD1	2.606
MODEL	A_ARG_567	NH2	A_ASP_571	OD1	2.720
MODEL	A_LYS_733	NZ	A_ASP_775	OD1	3.202
MODEL	A_LYS_733	NZ	A_ASP_775	OD2	2.601
MODEL	A_LYS_790	NZ	C_GLU_702	OE1	2.623
MODEL	A_LYS_790	NZ	C_GLU_702	OE2	2.744
MODEL	A_LYS_811	NZ	A_ASP_820	OD2	2.461
MODEL	A_ARG_815	NH1	A_ASP_820	OD1	2.649
MODEL	A_LYS_986	NZ	A_GLU_748	OE2	2.597
MODEL	A_ARG_995	NH1	B_ASP_994	OD1	3.497
MODEL	A_ARG_995	NH1	B_ASP_994	OD2	2.691
MODEL	A_ARG_995	NH2	B_ASP_994	OD1	2.657
MODEL	A_ARG_995	NH2	B_ASP_994	OD2	3.473
MODEL	A_ARG_1019	NH1	A_GLU_773	OE1	2.777
MODEL	A_ARG_1019	NH2	A_GLU_780	OE1	3.073
MODEL	A_ARG_1019	NH2	A_GLU_780	OE2	3.823
MODEL	A_LYS_1028	NZ	A_GLU_725	OE1	2.878
MODEL	A_LYS_1028	NZ	A_GLU_725	OE2	2.589
MODEL	A_ARG_1039	NH1	A_GLU_1031	OE1	2.697

MODEL	A_ARG_1039	NH1	A_GLU_1031	OE2	3.642
MODEL	A_ARG_1039	NH2	B_GLU_1031	OE1	3.621
MODEL	A_ARG_1039	NH2	B_GLU_1031	OE2	2.620
MODEL	A_HIS_1064	NE2	A_GLU_725	OE1	2.720
MODEL	A_HIS_1083	ND1	A_ASP_1084	OD1	3.726
MODEL	A_HIS_1083	NE2	A_ASP_1084	OD1	2.954
MODEL	A_HIS_1083	NE2	A_ASP_1084	OD2	3.064
MODEL	A_LYS_1086	NZ	A_ASP_1084	OD2	2.860
MODEL	B_ARG_34	NH1	B_GLU_191	OE2	2.594
MODEL	B_ARG_78	NH2	B_ASP_80	OD1	3.853
MODEL	B_ARG_78	NH2	B_ASP_80	OD2	3.115
MODEL	B_LYS_195	NZ	B_ASP_53	OD1	2.671
MODEL	B_LYS_195	NZ	B_ASP_53	OD2	2.656
MODEL	B_LYS_206	NZ	B_GLU_224	OE1	3.459
MODEL	B_LYS_206	NZ	B_GLU_224	OE2	2.611
MODEL	B_ARG_273	NH2	B_ASP_290	OD1	2.633
MODEL	B_ARG_273	NH2	B_ASP_290	OD2	3.259
MODEL	B_LYS_278	NZ	B_ASP_287	OD2	2.604
MODEL	B_LYS_310	NZ	B_ASP_663	OD1	2.691
MODEL	B_LYS_310	NZ	B_ASP_663	OD2	2.615
MODEL	B_ARG_319	NH1	C_ASP_745	OD1	2.606
MODEL	B_ARG_319	NH1	C_ASP_745	OD2	3.565
MODEL	B_ARG_319	NH2	C_ASP_745	OD1	3.325
MODEL	B_ARG_319	NH2	C_ASP_745	OD2	2.636
MODEL	B_ARG_328	NH1	B_ASP_578	OD2	3.286
MODEL	B_ARG_328	NH2	B_ASP_578	OD1	3.906
MODEL	B_ARG_328	NH2	B_ASP_578	OD2	2.659
MODEL	B_ARG_355	NH2	B_ASP_398	OD2	2.596
MODEL	B_ARG_403	NH1	B_GLU_406	OE2	2.630
MODEL	B_ARG_403	NH2	B_GLU_406	OE2	3.754
MODEL	B_ARG_408	NH1	B_ASP_405	OD1	2.895
MODEL	B_ARG_408	NH1	B_ASP_405	OD2	2.755
MODEL	B_ARG_408	NH2	B_ASP_405	OD2	3.887
MODEL	B_ARG_454	NH1	B_ASP_467	OD2	2.590
MODEL	B_LYS_462	NZ	B_GLU_465	OE2	3.504
MODEL	B_ARG_509	NH1	B_ASP_442	OD1	2.673
MODEL	B_ARG_509	NH1	B_ASP_442	OD2	3.881
MODEL	B_LYS_528	NZ	B_ASP_389	OD2	2.658
MODEL	B_LYS_535	NZ	B_GLU_554	OE2	2.577
MODEL	B_LYS_537	NZ	B_GLU_324	OE1	2.634
MODEL	B_LYS_537	NZ	B_GLU_324	OE2	2.706
MODEL	B_LYS_557	NZ	B_ASP_586	OD1	2.689
MODEL	B_LYS_557	NZ	B_ASP_586	OD2	2.627
MODEL	B_ARG_567	NH1	B_ASP_571	OD1	2.826
MODEL	B_ARG_567	NH1	B_ASP_571	OD2	2.786
MODEL	B_ARG_567	NH2	B_ASP_571	OD1	3.551
MODEL	B_HIS_625	ND1	B_ASP_627	OD2	3.516
MODEL	B_HIS_625	NE2	B_ASP_627	OD2	3.967
MODEL	B_ARG_646	NH1	B_ASP_614	OD2	2.839
MODEL	B_LYS_733	NZ	B_ASP_775	OD1	3.016
MODEL	B_LYS_733	NZ	B_ASP_775	OD2	2.582
MODEL	B_LYS_776	NZ	B_GLU_780	OE1	2.710
MODEL	B_LYS_776	NZ	B_GLU_780	OE2	2.672
MODEL	B_LYS_790	NZ	A_GLU_702	OE1	2.570
MODEL	B_LYS_790	NZ	A_GLU_702	OE2	3.570
MODEL	B_ARG_815	NH1	B_ASP_820	OD1	2.696
MODEL	B_ARG_815	NH2	B_ASP_867	OD1	2.920
MODEL	B_ARG_815	NH2	B_GLU_868	OE2	3.311

MODEL	B_LYS_854	NZ	A_ASP_614	OD1	3.487
MODEL	B_ARG_983	NH2	B_ASP_979	OD1	2.614
MODEL	B_ARG_983	NH2	B_ASP_979	OD2	3.538
MODEL	B_LYS_986	NZ	C_ASP_427	OD2	3.985
MODEL	B_ARG_995	NH1	C_ASP_994	OD1	2.636
MODEL	B_ARG_995	NH1	C_ASP_994	OD2	3.371
MODEL	B_ARG_995	NH2	C_ASP_994	OD1	3.182
MODEL	B_ARG_995	NH2	C_ASP_994	OD2	2.637
MODEL	B_ARG_1019	NH1	B_GLU_773	OE1	3.284
MODEL	B_ARG_1019	NH1	B_GLU_773	OE2	2.600
MODEL	B_LYS_1028	NZ	B_GLU_725	OE1	2.732
MODEL	B_LYS_1028	NZ	B_GLU_725	OE2	2.670
MODEL	B_ARG_1039	NH1	B_GLU_1031	OE1	2.669
MODEL	B_ARG_1039	NH1	B_GLU_1031	OE2	3.057
MODEL	B_ARG_1039	NH2	C_GLU_1031	OE1	2.711
MODEL	B_ARG_1039	NH2	C_GLU_1031	OE2	3.989
MODEL	B_LYS_1045	NZ	B_ASP_1041	OD1	2.637
MODEL	B_HIS_1064	NE2	B_GLU_725	OE2	2.768
MODEL	B_LYS_1086	NZ	B_ASP_1084	OD2	2.620
MODEL	C_LYS_97	NZ	C_GLU_96	OE2	2.761
MODEL	C_LYS_97	NZ	C_ASP_253	OD1	2.693
MODEL	C_LYS_97	NZ	C_ASP_253	OD2	2.866
MODEL	C_LYS_113	NZ	B_GLU_471	OE2	2.679
MODEL	C_LYS_129	NZ	C_GLU_169	OE1	2.582
MODEL	C_LYS_129	NZ	C_GLU_169	OE2	2.463
MODEL	C_LYS_150	NZ	C_GLU_154	OE1	2.608
MODEL	C_LYS_150	NZ	C_GLU_154	OE2	2.752
MODEL	C_ARG_158	NH2	C_GLU_154	OE2	3.189
MODEL	C_LYS_187	NZ	C_GLU_180	OE2	2.873
MODEL	C_LYS_202	NZ	C_ASP_228	OD2	2.762
MODEL	C_ARG_246	NH1	C_GLU_156	OE1	2.756
MODEL	C_ARG_246	NH1	C_GLU_156	OE2	3.170
MODEL	C_ARG_246	NH2	C_GLU_156	OE1	3.528
MODEL	C_ARG_246	NH2	C_GLU_156	OE2	2.612
MODEL	C_ARG_273	NH1	C_ASP_290	OD1	2.966
MODEL	C_ARG_273	NH1	C_ASP_290	OD2	3.840
MODEL	C_ARG_273	NH2	C_ASP_290	OD1	2.966
MODEL	C_ARG_273	NH2	C_ASP_290	OD2	2.552
MODEL	C_LYS_310	NZ	C_ASP_663	OD1	3.129
MODEL	C_ARG_319	NH1	A_ASP_745	OD1	3.819
MODEL	C_ARG_328	NH1	C_ASP_578	OD2	2.598
MODEL	C_ARG_328	NH2	C_ASP_578	OD1	3.708
MODEL	C_ARG_328	NH2	C_ASP_578	OD2	2.801
MODEL	C_ARG_355	NH2	C_ASP_398	OD1	3.407
MODEL	C_ARG_355	NH2	C_ASP_398	OD2	2.579
MODEL	C_LYS_356	NZ	C_GLU_340	OE1	2.568
MODEL	C_ARG_403	NH1	C_GLU_406	OE1	3.581
MODEL	C_ARG_403	NH1	C_GLU_406	OE2	2.672
MODEL	C_ARG_403	NH2	C_GLU_406	OE2	2.658
MODEL	C_LYS_458	NZ	A_ASP_389	OD2	3.696
MODEL	C_LYS_462	NZ	C_GLU_465	OE1	2.614
MODEL	C_LYS_462	NZ	C_GLU_465	OE2	2.647
MODEL	C_ARG_509	NH1	C_ASP_442	OD1	2.578
MODEL	C_LYS_528	NZ	C_ASP_389	OD1	3.189
MODEL	C_LYS_528	NZ	C_ASP_389	OD2	3.148
MODEL	C_LYS_535	NZ	C_GLU_554	OE1	2.654
MODEL	C_LYS_535	NZ	C_GLU_554	OE2	2.723
MODEL	C_LYS_537	NZ	C_GLU_324	OE2	2.535

MODEL	C_LYS_557	NZ	C_ASP_568	OD1	2.816
MODEL	C_LYS_557	NZ	C_ASP_568	OD2	2.819
MODEL	C_LYS_557	NZ	C_ASP_574	OD1	3.661
MODEL	C_LYS_557	NZ	C_ASP_574	OD2	2.584
MODEL	C_ARG_567	NH1	C_ASP_571	OD1	3.523
MODEL	C_ARG_567	NH1	C_ASP_571	OD2	2.610
MODEL	C_ARG_567	NH2	C_ASP_571	OD1	2.539
MODEL	C_ARG_567	NH2	C_ASP_571	OD2	3.300
MODEL	C_ARG_646	NH1	A_ASP_848	OD2	3.643
MODEL	C_ARG_646	NH2	A_ASP_848	OD1	3.695
MODEL	C_ARG_646	NH2	A_ASP_848	OD2	2.627
MODEL	C_LYS_733	NZ	C_ASP_775	OD1	3.066
MODEL	C_LYS_733	NZ	C_ASP_775	OD2	2.575
MODEL	C_LYS_811	NZ	C_ASP_820	OD2	3.817
MODEL	C_ARG_815	NH1	C_ASP_820	OD1	2.929
MODEL	C_ARG_815	NH1	C_ASP_820	OD2	2.916
MODEL	C_ARG_815	NH2	C_ASP_820	OD1	3.727
MODEL	C_ARG_847	NH1	B_GLU_619	OE1	3.034
MODEL	C_LYS_854	NZ	B_ASP_614	OD1	2.686
MODEL	C_LYS_986	NZ	C_GLU_748	OE1	2.531
MODEL	C_ARG_995	NH1	A_ASP_994	OD1	2.647
MODEL	C_ARG_995	NH1	A_ASP_994	OD2	3.498
MODEL	C_ARG_995	NH2	A_ASP_994	OD1	3.382
MODEL	C_ARG_995	NH2	A_ASP_994	OD2	2.636
MODEL	C_ARG_1019	NH1	B_GLU_1017	OE2	2.726
MODEL	C_ARG_1019	NH1	C_GLU_773	OE2	2.647
MODEL	C_ARG_1019	NH2	B_GLU_1017	OE2	3.415
MODEL	C_LYS_1028	NZ	C_GLU_725	OE1	2.678
MODEL	C_LYS_1028	NZ	C_GLU_725	OE2	2.787
MODEL	C_ARG_1039	NH1	C_GLU_1031	OE1	3.735
MODEL	C_ARG_1039	NH1	C_GLU_1031	OE2	2.669
MODEL	C_ARG_1039	NH2	A_GLU_1031	OE1	3.509
MODEL	C_ARG_1039	NH2	A_GLU_1031	OE2	2.596
MODEL	C_HIS_1064	NE2	C_GLU_725	OE1	2.774
MODEL	C_LYS_1086	NZ	C_ASP_1084	OD2	2.855

Table 1: Salt bridging networks within the PDB entries. In this table, the residue naming scheme is **Chain ID_residue name_residue number**.

Count	Residue A	Residue B
12	ARG995	ASP994
12	ARG1039	GLU1031
9	ARG567	ASP571
8	ARG328	ASP578
8	ARG273	ASP290
6	ARG403	GLU406
6	LYS733	ASP775
6	LYS1028	GLU725
6	ARG319	ASP745
5	LYS310	ASP663
5	ARG815	ASP820
5	ARG355	ASP398
5	ARG509	ASP442
5	LYS537	GLU324
4	LYS790	GLU702
4	LYS206	GLU224
4	ARG1019	GLU773
4	LYS557	ASP568
4	ARG246	GLU156
4	LYS557	ASP574
4	LYS195	ASP53
4	ARG44	ASP40
3	LYS1086	ASP1084
3	ARG408	ASP405
3	LYS528	ASP389
3	LYS462	GLU465
3	LYS535	GLU554
3	ARG646	ASP848
3	HIS1064	GLU725
3	HIS1083	ASP1084
2	ARG214	ASP215
2	ARG34	GLU191
2	ARG1019	GLU780
2	LYS150	GLU154
2	LYS811	ASP820
2	LYS854	ASP614
2	LYS986	GLU748
2	ARG466	ASP467
2	ARG319	ASP737
2	LYS278	ASP287
2	LYS557	ASP586
2	LYS97	ASP253
2	HIS625	ASP627
2	ARG1019	GLU1017
2	ARG78	ASP80
2	LYS356	GLU340
2	LYS129	GLU169
2	LYS776	GLU780
2	ARG983	ASP979
1	ARG78	ASP138
1	ARG102	GLU96
1	ARG158	GLU154
1	LYS458	ASP389
1	LYS187	GLU180
1	ARG815	GLU868
1	ARG646	ASP614
1	LYS202	ASP228

1	LYS458	GLU471
1	ARG454	ASP467
1	LYS986	ASP427
1	LYS97	GLU96
1	ARG815	ASP867
1	LYS113	GLU471
1	ARG847	GLU619
1	LYS1045	ASP1041

Table 2: Counting of salt bridges within the PDB entries in Table 1.

PDB	Acceptor (A)	Donor (D)	Hydrogen (H)	D-A (Å)	H-A (Å)	$\angle ADH(°)$

Table 3: The side chain and main chain hydrogen bonding networks.In this table, the names of the PDB files correspond to the single NMR structural model split from the NMR ensemble, the residue naming scheme is **Chain ID_residue name_residue number**, $\angle ADH$ represents the angle formed by acceptor (A), donor (D) and hydrogen (H) ($\angle ADH$).

PDB	Acceptor (A)	Donor (D)	Hydrogen (H)	D-A (Å)	H-A (Å)	$\angle ADH(°)$

Table 4: Side chain hydrogen bonding network analysis. In this table, the names of the PDB files correspond to the single NMR structural model split from the NMR ensemble, the residue naming scheme is **Chain ID_residue name_residue number**, $\angle ADH$ represents the angle formed by acceptor (A), donor (D) and hydrogen (H) ($\angle ADH$).

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
MODEL	A_ARG_319	NH1	B_ASP_737	OD2	2.735
MODEL	A_ARG_319	NH1	B_ASP_745	OD1	3.587
MODEL	A_ARG_319	NH2	B_ASP_737	OD2	3.982
MODEL	A_LYS_790	NZ	C_GLU_702	OE1	2.623
MODEL	A_LYS_790	NZ	C_GLU_702	OE2	2.744
MODEL	A_ARG_995	NH1	B_ASP_994	OD1	3.497
MODEL	A_ARG_995	NH1	B_ASP_994	OD2	2.691
MODEL	A_ARG_995	NH2	B_ASP_994	OD1	2.657
MODEL	A_ARG_995	NH2	B_ASP_994	OD2	3.473
MODEL	A_ARG_1039	NH2	B_GLU_1031	OE1	3.621
MODEL	A_ARG_1039	NH2	B_GLU_1031	OE2	2.620
MODEL	B_ARG_319	NH1	C_ASP_745	OD1	2.606
MODEL	B_ARG_319	NH1	C_ASP_745	OD2	3.565
MODEL	B_ARG_319	NH2	C_ASP_745	OD1	3.325
MODEL	B_ARG_319	NH2	C_ASP_745	OD2	2.636
MODEL	B_LYS_790	NZ	A_GLU_702	OE1	2.570
MODEL	B_LYS_790	NZ	A_GLU_702	OE2	3.570
MODEL	B_LYS_854	NZ	A_ASP_614	OD1	3.487
MODEL	B_LYS_986	NZ	C_ASP_427	OD2	3.985
MODEL	B_ARG_995	NH1	C_ASP_994	OD1	2.636
MODEL	B_ARG_995	NH1	C_ASP_994	OD2	3.371
MODEL	B_ARG_995	NH2	C_ASP_994	OD1	3.182
MODEL	B_ARG_995	NH2	C_ASP_994	OD2	2.637
MODEL	B_ARG_1039	NH2	C_GLU_1031	OE1	2.711
MODEL	B_ARG_1039	NH2	C_GLU_1031	OE2	3.989
MODEL	C_LYS_113	NZ	B_GLU_471	OE2	2.679
MODEL	C_ARG_319	NH1	A_ASP_745	OD1	3.819
MODEL	C_LYS_458	NZ	A_ASP_389	OD2	3.696
MODEL	C_ARG_646	NH1	A_ASP_848	OD2	3.643
MODEL	C_ARG_646	NH2	A_ASP_848	OD1	3.695
MODEL	C_ARG_646	NH2	A_ASP_848	OD2	2.627
MODEL	C_ARG_847	NH1	B_GLU_619	OE1	3.034
MODEL	C_LYS_854	NZ	B_ASP_614	OD1	2.686
MODEL	C_ARG_995	NH1	A_ASP_994	OD1	2.647
MODEL	C_ARG_995	NH1	A_ASP_994	OD2	3.498
MODEL	C_ARG_995	NH2	A_ASP_994	OD1	3.382
MODEL	C_ARG_995	NH2	A_ASP_994	OD2	2.636
MODEL	C_ARG_1019	NH1	B_GLU_1017	OE2	2.726
MODEL	C_ARG_1019	NH2	B_GLU_1017	OE2	3.415
MODEL	C_ARG_1039	NH2	A_GLU_1031	OE1	3.509
MODEL	C_ARG_1039	NH2	A_GLU_1031	OE2	2.596

Table 5: Interfacial salt bridging network analysis within the PDB entries. In this table, the residue naming scheme is **Chain ID_residue name_residue number**.

Count	Residue A	Residue B
12	ARG995	ASP994
6	ARG319	ASP745
6	ARG1039	GLU1031
4	LYS790	GLU702
3	ARG646	ASP848
2	ARG319	ASP737
2	LYS854	ASP614
2	ARG1019	GLU1017
1	LYS986	ASP427
1	ARG847	GLU619
1	LYS113	GLU471
1	LYS458	ASP389

Table 6: Counting of interfacial salt bridges within the PDB entries in Table 5.