

Supplementary Figure 1. (**A**) Folding energy changes for $\Delta\Delta G$ of substitutions to Alanine (left) and $\Delta\Delta G$ mean of residues (right) in SARS-CoV-2 S trimer and monomer. (**B**) Line charts summarize the folding energy changes for $\Delta\Delta G$ mean of residues (bar) and $\Delta\Delta G$ of substitutions to alanine (circle) in SARS-CoV-2 S trimer and monomer.



Supplementary Figure 2. Folding energy changes for $\Delta\Delta G$ of substitutions to Alanine (left) and $\Delta\Delta G$ mean of residues (right) in (**A**) the cryo-EM structures of SARS-CoV-2 S in closed state and open state and (**B**) the crystal structure of RBD and cryo-EM structure of SARS-Cov-2 S RBD. The folding energy change ($\Delta\Delta G$) is computed based on the A chains of 6VYB and 6VXX.



Supplementary Figure 3. Comparisons of 2P mutations among MERS-Cov, SARS-Cov-2 and SARS-Cov. The folding energy change ($\Delta\Delta G$) is computed based on the monomer.

KRI)												- 0		Maxi	mum	Ì		Min	imur	n	
	0.628	-0.229	1.816	0.81	6.491	2.11	0.002	8.731	1.071	-0.022	1.83	2.198	-0.377	0.017	0.365	17.418	-0.465	-0.459	3.118	2.394	-0.74	W
	-1.268	-0.157			4.23	1.672		7.663	0.173	-0.017	-0.06	0.826		-0.013	3.314	13.42	0.627	-0.181	4.55	1.707		Y
	0 152	0.013	1.539	0.812	2.494	3 570	0.308	2.832	0.092	-0.012	2 008	0.637	-0.597 3 271	0.032	0.193	1.037	0.411	-0.4 0.371	3.986	1.744	-0.529	F
	0.667	0.139	1.922	1.049	2.010	3 4 17	0.27	1 706	0.634	0.052	2.990	0.461	3 1 16	0.032	2 167	7 278	1.045	1 188	-2.49	3.0 3.628	0.676	F
	0.177	0.077	0.036	1.575	2.802	2.513	-0.018	1.422	0.513	-0.009	3.358	0.479	1.038	-0.015	0.645	5.654	0.402	0.043	0.949	2.428	1.096	Н
	0.183	-0.905	0.961	-0.488	2.541	2.091	0.248	5.046	0.276	0.101	3.166	-0.038	2.042	-0.017	-0.571	3.781	0.373	0.795	2.094	1.653	-0.166	R
		-0.01	1.114	1.059	1.914	1.767	-0.146	3.266	0.834	-0.059	2.791	0.128	1.956	0.021	0.704	41	0.313	0.79	-2.134	1.641	0.474	K
	0.492	-0.025	1.889	1.556	2.425	2.88	0.555	0.282	0.291	0.002	3.261	0.755	2.593	0.082	0.791	-0.119	-0.56	0.436	-1.04	11.767	-0.051	Р
	0.545	0.009	1.703	1.502	2 427	3 814	0.100	0.808	0.003	-0.008	3.055	0.579	2.507	0.019	1 182	1 451	-0 221	0.516	-0.413	2 528	0.994	S
	0.481	0.041	1.7	1.568	1.889	3.145	0.223	1.119	0.777	-0.019	3.615	0.010	2.73	0.011	0.679	4.164	0.681	0.551	0.110	2.322	-0.083	N
	0.418	0.05	1.876	1.157	0.968	3.124	0.118	1.456	0.503	-0.01	3.323	-0.032	2.104	0.037		5.502		0.069	-1.528	2.401	0.158	Q
	0.465	0.028	1.758	1.573	1.169	2.891	0.108	-0.031	0.425	-0.019	3.245	0.247	2.101	0.031	0.956	3.578	0.942	0.556	-1.041	2.233	0.382	С
	0.506	0.052	1.762	1.271	0.966	2.414	0.104	0.288	0.237	-0.014	3.046	-0.075	1.121	-0.007	0.621	4.593	-1.527	0.078	-1.29	3.136	-0.188	V
	0.450	0.057	1.703	1.025	0.192	1 522	-0.004	0.99	0.494	-0.014	1 216	-0.362	0.581	-0.041	0.700	2 665	-1.561	-0.328	-0.423	3.00 1.601	-0.341	1
	0.606	-0.199	1.533	1.266	0.458	0.792	-0.28	0.651	0.465	0.004	1.204	-0.106	0.117	-0.006	-0.3	2.305	0.057	-0.304	-2.273	1.709	-0.571	M
	0.597		1.821	1.243	2.667	3.288	0.301	0.521		0.006	3.924	0.805	2.913	0.043	1.19		1.284	1.209	-0.149		1.741	G
	0.483	0.251	1.805	1.641	2.612	3.31	0.191		0.109	-0.025	3.903	0.513	2.559	0.009	0.957	0.756	0.727	0.683	-0.68	1.881	0.569	Α
	0.404	-0.033	1.601	1.263	2.249	2.606	0.103	2.046	0.595	-0.016	2.808	0.301	1.838	0.01	0.867	4.694	0.181	0.299	-0.15	2.922	0.27	Mean
	117	146	149	153	155	156	173	175	9/1	184	186	187	189	190	193	196	198	200	501	502	505	
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610 0.189	0.008	0.481	82 0.293	0.953	0.521	1.156	98 1.399	LEE 0.095	8°C	1.708	270	64FJ 0.391	0.09	0.765	1.704		0.28	0.486	6.681	Line 10.664	0.177	w
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0.189 0.653 0.654 0.864	-0.008 3.353 0.917 1.451	0.481 0.738 1839 0.843	82 0.293 0.126	0.953 0.559 1.117	0.521 0.521 0.724 0.724	1.156 0.22 0.255 0.147	1.399 0.985 0.927 0.778	LEE 0.095 0.968 0.215 0.967	1.331 0.415 1.985	11708 0.279 1.387	1.464 1.537 1.538 1.748	64 0.391 0.71 0.181 0.669	0.09 0.134 0.433 1 159	0.765 1.129 1.077 0.923			0.28 1676 1937 0.313	0.486 0.218 0.876 1.668	6.681 7.284	0.664 3.43 1.154 0.536	0.177 0.2 0.249 0.167	W Y F D
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0.189 0.653 0.654 0.864 0.802 0.101 0.933 0.763 0.962 0.375	-0.008 3.353 0.917 1.451 0.348 0.271 -0.006 0.647 -0.173 0.293	0.481 0.738 1 839 0.843 0.103 0.066 0.252 0.392 0.817 0.817 0.817	82 0.293 0.126 0.052 0.022 1.048 0.055 0.027 1.059 0.445 0.036	0.953 0.953 0.559 1.117 0.834 1.688 0.084 1.063 0.25 1.28	0.521 0.521 0.724 0.724 0.701 2.054 1.915 1.269 0.173 4.036 0.626 2.248	1.156 0.22 0.255 -0.147 0.463 -0.421 1.285 1.861 0.873 1.428	1.399 0.985 0.927 0.778 1.031 1.014 0.854 0.879 1.034 1.034 1.087	255 0.095 0.968 0.215 0.967 0.038 0.447 0.437 0.563 0.148 0.102	1.331 0.415 1.985 2.106 1.129 2.295 2.026 2.463 2.017 2.008	1.708 0.279 1.387 0.652 0.773 0.652 0.773 0.419 0.807 1.808 1.293 1.173	1.464 1.537 1.538 1.748 1.644 0.562 0.069 1.437 1.73 1.375 1.562	0.391 0.071 0.181 0.669 0.54 0.541 0.253 0.431 0.654 0.405 0.521	0.09 0.134 0.433 1.159 1.018 0.751 0.381 0.413 0.964 0.443 1.099	0.765 1.129 1.077 0.923 0.651 1.509 1.037 0.576 1.548 1.36 1.54	1.704 0.873 0.839 0.233 0.845 0.229 0.415 0.749 0.665	1118 0.774 1.326 0.471 0.251 0.301 0.358 0.523 0.034 0.496 0.044	0.28 1 676 1 937 0.313 -0.619 -0.392 0.167 -1 129 -0.383 -1 328	0.486 0.218 0.876 1.668 1.191 0.618 1.457 1.005 0.052 3.141 1.885	6.681 7.284 1.01 1.755 2.535 4.139 1.308 2.154 1.639 1.788	0.664 3.43 1.154 0.536 1.176 0.426 0.505 0.462 0.4 0.241	0.177 0.2 0.249 0.167 0.29 0.25 0.317 0.251 0.317 0.251 0.3183 0.183	ΨΥ F D E H R K P T S
0.189 0.653 0.654 0.864 0.802 0.101 0.933 0.763 0.962 0.375 0.106	-0.008 3.353 0.917 1.451 0.348 0.271 -0.006 0.647 -0.173 0.293 0.061	0.481 0.738 1839 0.843 0.103 0.066 0.252 0.392 0.817 1.419 0.933	0.293 0.126 0.052 0.022 1.048 0.055 0.027 1.059 0.445 0.036 1.069	0.953 0.559 1.117 0.337 0.834 1.688 0.084 1.063 0.25 1.28 0.458	0.521 0.521 0.724 0.701 2.054 1.915 1.269 0.173 4.036 0.626 2.248 0.869	1.156 0.22 0.255 0.147 0.463 0.421 1.285 1.861 0.873 1.428 0.464	1.399 0.985 0.927 0.778 1.031 1.014 0.854 0.879 1.034 1.087 1.034 1.087 -0.454	25 0.095 0.968 0.215 0.967 0.038 0.447 0.437 0.563 0.148 0.102 0.252	1.331 0.415 1.985 2.106 1.129 2.295 2.026 2.463 2.017 2.008 0.343	1.708 0.279 1.387 0.652 0.773 0.652 0.773 0.419 0.807 1.808 1.293 1.173 1.676	1.464 1.537 1.538 1.748 1.644 0.562 0.069 1.437 1.73 1.375 1.562 1.339	0.391 0.071 0.181 0.253 0.431 0.654 0.541 0.654 0.521 0.67	0.09 0.134 0.433 1.159 1.018 0.751 0.381 0.413 0.964 0.443 1.099 0.936	0.765 1.129 1.077 0.923 0.651 1.509 1.037 0.576 1.548 1.36 1.54 1.436	1.704 0.873 0.839 0.233 0.845 0.229 0.415 0.749 0.665 0.617	1.118 0.774 1.326 0.471 0.251 0.301 0.358 0.034 0.034 0.044	0.28 -1.676 -1.937 0.313 -0.619 -0.392 0.167 -1.129 -0.383 -1.328 -1.328 -1.415	0.486 0.218 0.876 1.668 1.191 0.618 1.457 1.005 0.052 3.141 1.885 1.881	6.681 7.284 1.01 1.755 2.535 4.139 1.308 2.154 1.639 1.788 1.338	0.664 3.43 1.154 0.536 1.176 0.426 0.402 0.4 0.241 0.388	0.177 0.2 0.249 0.167 0.199 0.25 0.317 0.251 0.317 0.251 0.183 0.183 0.183 0.183	W Y F D E H R K P T S N
0.189 0.653 0.654 0.802 0.933 0.763 0.962 0.375 0.106 0.846	-0.008 3.353 0.917 1.451 0.348 0.271 -0.006 0.647 -0.173 0.293 0.061	0.481 0.738 1.839 0.843 0.066 0.252 0.392 0.392 0.392 0.392 0.392 0.393 0.091	0.293 0.126 0.052 0.022 1.048 0.055 0.027 1.059 0.445 0.036 1.069 0.165	0.953 0.559 1.117 0.337 0.834 1.063 0.25 1.28 0.458 0.458	0.521 0.521 0.724 0.724 0.724 0.724 0.724 0.724 0.724 0.724 0.724 0.724 0.724 0.724 0.724 0.724 0.724 0.626 2.248 0.869 1.09	1.156 0.22 0.255 0.147 0.463 0.421 1.285 1.861 0.873 1.428 0.873 1.428 0.464 0.796	1.399 0.985 0.927 0.778 1.031 1.014 0.854 0.857 1.034 - 1.034 - 0.454 0.055	0.095 0.968 0.215 0.967 0.437 0.563 0.447 0.563 0.148 0.122 0.252 0.325	1.331 0.415 1.985 2.106 1.129 2.295 2.026 2.463 2.017 2.008 0.343 2.017	1.708 0.279 1.387 0.652 0.773 0.419 0.807 1.808 1.293 1.173 1.676 0.777	1.464 1.537 1.538 1.644 0.562 1.437 1.73 1.375 1.562 1.339	0.391 0.071 0.081 0.541 0.541 0.669 0.54 0.541 0.654 0.405 0.521 0.67 0.120	0.09 0.134 0.433 1.159 1.018 0.751 0.381 0.413 0.964 0.443 1.099 0.936 0.94	0.765 1.129 1.077 0.923 0.651 1.509 1.037 0.576 1.548 1.36 1.54 1.436 1.54	1.704 0.431 0.873 0.839 0.233 0.845 0.229 0.415 0.249 0.665 0.665 0.649	1118 0.774 1326 0.471 0.251 0.301 0.358 0.034 0.496 0.034 0.496	0.28 1.676 1.937 0.313 0.619 0.313 0.619 0.3167 1.129 0.367 1.129 0.383 1.328 1.328 1.415 0.311	0.486 0.218 0.876 1.668 1.191 0.618 1.457 1.005 3.141 1.885 1.881 1.498 1.498	6.681 7.284 1.01 1.755 2.555 4.139 1.308 2.154 1.639 1.308 1.926 2.535 4.139 1.308 2.154 1.639 1.308	0.664 3.43 1.154 0.536 1.176 0.505 0.462 0.4 0.241 0.388 0.473 0.273	0.177 0.2 0.249 0.167 0.29 0.25 0.317 0.251 0.317 0.251 0.183 0.183 0.183 0.184 0.226	WYFDEHRKPTSNQC
0.189 0.653 0.654 0.864 0.864 0.862 0.101 0.933 0.763 0.962 0.375 0.106 0.846 0.789 0.945	-0.008 3.353 0.917 1.451 0.348 0.271 -0.006 0.647 -0.173 0.293 0.061 -0.019 -0.107	21 0.481 0.738 1.839 0.843 0.003 0.043 0.052 0.817 1.419 0.933 0.091 0.015 0.015 0.0702	0.293 0.126 0.052 0.022 1.048 0.055 0.027 1.059 0.445 0.036 1.069 0.165 -0.06	0.953 0.559 1.117 0.834 1.688 0.084 1.063 0.25 1.28 0.458 0.089 0.465 0.069	0.521 0.521 0.724 0.701 2.054 1.915 1.269 0.173 4.036 0.626 2.248 0.869 1.09 1.312 0.993	1.156 0.22 0.255 -0.147 0.463 1.285 1.861 0.873 1.428 0.464 0.796 1.003 0.295	1.399 0.985 0.927 0.778 1.031 1.014 0.854 0.879 1.034 1.034 1.034 1.034 1.034 1.034 0.879 0.454 0.085 0.562 0.553	255 0.095 0.968 0.215 0.967 0.325 0.148 0.102 0.325 0.283 0.148 0.102 0.325 0.283 0.128	2.106 1.331 0.415 1.985 2.106 1.129 2.295 2.026 2.463 2.017 2.008 0.343 2.078 2.304 2.304 2.304	1.708 0.279 1.387 0.652 0.773 0.652 0.773 0.419 0.807 1.808 1.293 1.173 1.676 0.777 0.96 1.071	1.464 1.537 1.538 1.748 1.644 0.562 0.069 1.437 1.73 1.375 1.562 1.339 1.578 1.451	64 0.391 0.071 0.669 0.54 0.654 0.405 0.654 0.405 0.521 0.67 0.112 0.67 0.120 0.335	0.09 0.134 0.433 1.159 1.018 0.751 0.381 0.413 0.964 0.443 1.096 0.94 0.675 0.399	0.765 1.129 1.077 0.923 0.651 1.509 1.037 0.576 1.548 1.36 1.54 1.436 1.54 1.436 1.54 1.436	1.704 0.873 0.839 0.233 0.845 0.229 0.415 0.749 0.665 0.617 0.349 0.663 0.436	1.118 0.774 1.326 0.471 0.251 0.301 0.358 0.523 0.034 0.523 0.034 0.496 0.0441 0.364 0.364	0.28 1676 1937 0.313 0.619 0.313 0.313 1.129 0.383 1.328 1.415 0.311 1.87 2.26	0.486 0.218 0.876 1.668 1.191 0.618 1.457 1.005 0.052 3.141 1.885 1.881 1.498 1.357 2.176	6.681 7.284 1.01 1.755 2.535 4.139 1.308 2.154 1.639 1.308 1.308 1.328 1.338 1.3388 1.338 1.338 1.338 1.338 1.338 1.3388 1.3388 1.3388 1.3388 1.3388 1.3388 1.3388 1.3388 1.3388 1.3388 1.	0.664 3.43 1.154 0.536 1.176 0.426 0.505 0.462 0.4 0.241 0.388 0.473 0.377 0.439	0.177 0.2 0.249 0.167 0.29 0.25 0.317 0.251 0.183 0.183 0.183 0.183 0.184 0.226 0.183 0.183 0.183	WYFDEHRKPTSNQCV
0.189 0.653 0.654 0.864 0.802 0.101 0.933 0.763 0.962 0.375 0.106 0.846 0.789 0.945 0.916	-0.008 3.353 0.917 1.451 0.348 0.271 -0.006 0.647 -0.173 0.293 0.061 -0.019 -0.107 0.3	2L 0.481 0.738 1.839 0.843 0.103 0.066 0.252 0.392 0.817 1.419 0.933 0.091 0.015 0.091 0.015 0.091 0.015	82 0.293 0.126 0.052 0.022 1.048 0.055 0.027 1.059 0.445 0.036 1.069 0.165 -0.06 0.068 0.068 0.111	0.953 0.953 0.559 1.117 0.834 1.688 0.084 1.063 0.25 1.28 0.458 0.458 0.455 0.069 0.465 0.069 0.465	0.521 0.521 0.724 0.701 2.054 1.915 1.269 0.173 4.036 0.626 2.248 0.869 1.09 1.312 0.993 0.697	1.156 0.22 0.255 0.147 0.463 0.463 0.464 0.796 1.003 0.295 1.347	1.399 0.985 0.927 0.778 1.031 1.014 0.854 0.879 1.034 1.087 1.034 1.087 0.454 0.085 0.562 0.553 1.431	0.095 0.968 0.215 0.967 0.038 0.447 0.437 0.563 0.148 0.102 0.252 0.325 0.283 0.108 0.998	1.331 0.415 1.985 2.106 1.129 2.295 2.026 2.463 2.017 2.008 0.343 2.078 2.304 2.304 2.304 2.304 2.304 2.304	1.708 0.279 1.387 0.652 0.773 0.652 0.773 0.652 0.773 1.676 0.777 -0.96 1.071 0.852	1.464 1.537 1.538 1.748 1.644 0.562 0.069 1.437 1.73 1.375 1.562 1.339 1.578 1.451 1.258	0.391 0.071 0.181 0.669 0.54 0.541 0.654 0.405 0.521 0.67 0.67 0.67 0.112 0.67 0.67 0.67 0.67 0.335 0.352	0.09 0.134 0.433 1.159 1.018 0.751 0.381 0.413 0.964 0.443 1.099 0.936 0.94 0.675 0.399 0.249	0.765 1.129 1.077 0.923 0.651 1.509 1.037 0.576 1.548 1.36 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.436 1.54	1.704 0.873 0.839 0.233 0.845 0.229 0.415 0.665 0.617 0.349 0.665 0.617 0.349 0.663 0.436 0.4	1118 0.774 1.326 0.471 0.251 0.301 0.358 0.523 0.034 0.496 0.044 0.612 0.364 0.612 0.393	0.28 -1676 -1937 0.313 -0.619 -0.392 0.167 -1.129 -0.383 -1.328 -1.328 -1.415 0.311 -1.87 2.26 2.737	0.486 0.218 0.876 1.668 1.191 0.618 1.457 1.005 0.052 3.141 1.885 1.881 1.498 1.357 2.176 1.886	6.681 7.284 1.01 1.755 2.535 4.139 1.308 2.154 1.639 1.338 1.926 0.203 0.285 2.245	0.664 3.43 1.154 0.536 1.176 0.426 0.505 0.462 0.4 0.241 0.388 0.473 0.377 0.439 0.477	0.177 0.2 0.249 0.167 0.25 0.317 0.251 0.317 0.251 0.183 0.183 0.183 0.183 0.226	W Y F D E H R K P T S N Q C V I
0.189 0.653 0.654 0.864 0.802 0.101 0.933 0.763 0.962 0.375 0.106 0.846 0.789 0.945 0.945 0.916 0.945	-0.008 3.353 0.917 1.451 0.348 0.271 -0.006 0.647 -0.173 0.293 0.061 -0.107 0.3 -0.107 -0.3 -0.3	0.481 0.738 1.839 0.843 0.103 0.066 0.252 0.392 0.817 1.419 0.933 0.091 0.015 0.091 0.015 0.702 0.968 0.77	82 0.293 0.126 0.052 0.022 1.048 0.055 0.027 1.059 0.445 0.036 1.069 0.165 -0.06 0.068 0.111 0.085	0.953 0.559 1.117 0.834 1.688 0.084 1.063 0.25 1.28 0.458 0.089 0.465 0.069 0.465 0.069 0.118 0.472	0.521 0.521 0.724 0.701 2.054 1.915 1.269 0.173 4.036 0.626 2.248 0.869 1.09 1.312 0.993 0.697 0.255	1.156 0.22 0.255 0.147 0.463 0.421 1.285 1.861 0.873 1.428 0.464 0.796 1.003 0.295 1.347 0.427	1.399 0.985 0.927 0.778 1.031 1.014 0.854 0.879 1.034 1.087 0.454 0.085 0.562 0.553 0.553 0.553	250 0.095 0.968 0.215 0.967 0.252 0.325 0.252 0.325 0.283 0.108 0.252 0.325 0.283 0.108 0.325 0.283 0.108 0.325 0.325	1.331 0.415 1.985 2.106 1.129 2.295 2.026 2.463 2.017 2.008 0.343 2.008 0.343 2.008 0.00800000000	1.708 0.279 1.387 0.652 0.773 0.652 0.773 0.652 0.773 1.676 0.777 -0.96 1.071 0.852 1.09	1.464 1.537 1.538 1.748 1.644 0.562 0.069 1.437 1.73 1.375 1.562 1.339 1.578 1.451 1.258 1.458	0.391 0.071 0.181 0.669 0.54 0.541 0.654 0.521 0.67 0.112 0.67 0.112 0.67 0.335 0.352	0.09 0.134 0.433 1.159 1.018 0.751 0.381 0.413 0.964 0.443 1.099 0.936 0.94 0.675 0.399 0.249	0.765 1.129 1.077 0.923 0.651 1.509 1.037 0.576 1.548 1.36 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.574 1.653 1.653 1.653 1.654411.654 1.654411.654411.654411.6555411.655411.655411.6555411.65555555555	1.704 0.431 0.873 0.839 0.233 0.845 0.229 0.415 0.749 0.665 0.617 0.349 0.663 0.436 0.4 0.63 0.436 0.4 0.4 0.302	1118 0.774 1.326 0.471 0.251 0.301 0.358 0.523 0.034 0.496 0.044 0.411 0.364 0.612 0.393 0.612 0.393 0.878	0.28 1 676 1 937 0.313 -0.619 -0.392 0.167 -1.129 -0.383 -1.328 -1.415 0.311 -1.87 2.26 2.737 -1.521	0.486 0.218 0.876 1.668 1.191 0.618 1.457 1.005 3.141 1.885 1.881 1.498 1.357 2.176 1.886 1.14	6.681 7.284 1.01 1.755 2.535 4.139 1.308 2.154 1.639 1.308 2.154 1.639 1.308 2.154 1.639 1.308 2.154 1.338 1.926 0.203 0.285 2.245 1.502	0.664 3.43 1.154 0.536 1.176 0.426 0.505 0.462 0.4 0.241 0.388 0.473 0.377 0.439 0.477 0.496	0.177 0.2 0.249 0.167 0.29 0.25 0.317 0.251 0.317 0.251 0.183 0.183 0.183 0.183 0.183 0.2 0.183 0.2 0.183	ΨΥFDEHRКРTSNQCVIL
0. 189 0. 653 0. 654 0. 864 0. 802 0. 101 0. 933 0. 962 0. 375 0. 106 0. 846 0. 789 0. 945 0. 916 0. 723 0. 476	-0.008 3.353 0.917 1.451 0.348 0.271 -0.006 0.647 -0.173 0.293 0.061 -0.019 -0.107 0.3 -0.107 -0.3 -0.54	0.481 0.738 1839 0.843 0.066 0.252 0.392 0.817 1.419 0.933 0.091 0.015 0.091 0.015 0.702 0.968 -0.77 -1.078	0.293 0.126 0.052 0.022 1.048 0.055 0.027 1.059 0.445 0.036 1.069 0.165 -0.06 0.068 0.111 0.085 0.101	0.953 0.559 1.117 0.337 0.834 1.063 0.25 1.28 0.084 1.063 0.25 1.28 0.465 0.069 0.465 0.069 0.465 0.069	0.521 0.521 0.724 0.724 0.724 0.724 0.724 0.701 2.054 1.915 1.269 0.173 4.036 0.626 2.248 0.869 1.09 1.312 0.993 0.697 0.255 0.34	1.156 0.22 0.255 0.147 0.463 0.421 1.285 1.861 0.873 1.428 0.464 0.796 1.003 0.295 1.347 0.427 0.955	1.399 0.985 0.927 0.778 1.031 1.014 0.854 0.879 1.034 1.034 1.037 0.454 0.8879 1.034 1.037 0.454 0.085 0.553 0.553 0.553 0.927 0.553 0.927	0.095 0.968 0.215 0.967 0.437 0.437 0.563 0.148 0.148 0.102 0.325 0.283 0.108 0.998 0.485 0.485 0.472	1.331 0.415 1.985 2.106 1.129 2.295 2.026 2.463 2.017 2.008 0.343 2.017 2.008 0.343 2.078 2.304 2 1.981 1.873 2.091	1.708 0.279 1.387 0.652 0.773 0.419 0.807 1.293 1.1676 0.777 -0.96 1.071 0.852 1.109 1.192	1.464 1.537 1.538 1.748 1.644 0.562 1.437 1.73 1.375 1.562 1.339 1.578 1.451 1.258 1.451 1.258 1.458 1.458	0.391 0.071 0.181 0.669 0.54 0.541 0.654 0.431 0.654 0.431 0.654 0.431 0.654 0.405 0.521 0.6521 0.6112 0.429 0.335 0.352 0.011	0.09 0.134 0.433 1.159 1.018 0.751 0.381 0.413 0.964 0.94 0.94 0.94 0.94 0.94 0.94 0.94 0.9	0.765 1.129 1.077 0.923 0.651 1.509 1.037 0.576 1.548 1.36 1.54 1.436 1.54 1.436 1.574 1.863 0.533 0.488	1.704 0.431 0.873 0.839 0.233 0.845 0.229 0.415 0.749 0.665 0.617 0.349 0.663 0.436 0.4 0.302 0.436	1118 0.774 1326 0.471 0.251 0.301 0.358 0.0358 0.034 0.496 0.0364 0.496 0.0364 0.0411 0.364 0.0411 0.364 0.612 0.393 0.878 0.971	0.28 1.676 1.937 0.313 0.619 0.313 0.619 0.312 0.311 1.29 0.311 1.328 1.415 0.311 1.87 2.26 2.737 1.521 0.851 0.851	0.486 0.218 0.876 1.668 1.191 0.618 1.457 1.0052 3.141 1.885 1.881 1.498 1.357 2.176 1.886 1.14 1.141	6.681 7.284 1.01 1.755 2.535 4.139 1.308 2.154 1.639 1.308 1.309 1.308 1	0.664 3.43 1.154 0.536 1.176 0.426 0.4 0.241 0.377 0.439 0.477 0.496 0.284 0.284	0.177 0.2 0.249 0.167 0.251 0.251 0.251 0.251 0.251 0.183 0.226 0.183 0.226 0.183 0.2 0.183 0.2 0.183 0.2 0.183 0.2 0.183	W Y F D E H R K P T S N Q C V I L M C
0.189 0.653 0.654 0.864 0.864 0.862 0.101 0.933 0.962 0.375 0.962 0.375 0.965 0.945 0.945 0.945 0.945 0.945 0.946 1.119 0.661	-0.008 3.353 0.917 1.451 0.348 0.271 -0.006 0.647 -0.173 0.293 0.061 -0.107 0.3 -1.267 -0.554 0.674 0.482	21 0.481 0.738 1.839 0.843 0.103 0.066 0.252 0.392 0.817 0.817 0.933 0.091 0.015 0.091 0.015 0.091 0.015 0.091 0.015 0.702 0.968 0.091 0.015 0.77 0.968 0.071 0.015 0.772 0.968 0.071 0.015 0.772 0.968 0.07100 0.0710000000000	0.293 0.293 0.126 0.052 0.022 1.048 0.055 0.027 1.059 0.445 0.027 1.059 0.445 0.026 1.069 0.165 -0.06 0.165 -0.06 0.165 0.102 0.124 0.124	0.953 0.953 0.559 1.117 0.834 1.688 0.084 1.063 0.25 1.28 0.458 0.089 0.465 0.069 0.455 0.069 0.457 0.077 0.457 0.077 0.457 0.077 0.457 0.0777 0.457 0.0777 0.457 0.0777 0.457 0.07777 0.4577 0.07777 0.45777777777777777777777777777777777777	0.521 0.521 0.724 0.701 2.054 1.915 1.269 0.173 4.036 0.626 2.248 0.869 1.09 1.312 0.993 0.697 0.255 0.34 2.659 1.638	1.156 0.22 0.255 -0.147 0.463 0.463 1.285 1.861 0.873 1.428 0.464 0.796 1.003 0.295 1.347 0.427 0.959 2.376 1.488	1.399 0.985 0.927 0.778 1.031 1.014 0.854 0.879 1.034 1.034 1.034 1.037 0.854 0.553 0.553 0.553 0.553 0.553 0.553 0.553 0.553 0.927 0.312 0.312 0.312 0.312	255 0.095 0.968 0.215 0.967 0.038 0.447 0.437 0.563 0.447 0.563 0.447 0.563 0.148 0.102 0.252 0.325 0.283 0.148 0.102 0.325 0.283 0.108 0.109 0.125 0.283 0.485 0.472 0.425 0.425 0.212	2.106 1.331 0.415 1.985 2.106 1.129 2.295 2.026 2.463 2.017 2.008 0.343 2.017 2.008 0.343 2.304 2.304 2.304 2.304 2.304 2.304 2.304	1.708 0.279 1.387 0.652 0.773 0.652 0.777 0.966 1.173 1.676 0.777 0.966 1.071 0.852 0.773 0.072 0.071 0.852 0.773 0.071 0.852 0.071 0.852 0.071 0.852 0.071 0.852 0.071 0.852 0.071 0.852 0.071 0.852 0.073 0.071 0.852 0.073 0.096 0.0771 0.966 0.0771 0.966 0.0771 0.975 0.097	1.464 1.537 1.538 1.748 1.644 0.562 0.069 1.437 1.73 1.375 1.562 1.339 1.578 1.451 1.258 1.451 1.258 1.451 1.458 1.457 1.67 1.568	64 0.391 0.071 0.181 0.669 0.54 0.541 0.654 0.405 0.521 0.67 0.112 0.429 0.335 0.352 0.352 0.011 0.544 0.521 0.352 0.352 0.352 0.011 0.544 0.544 0.524 0.521 0.545 0.521 0.545 0.521 0.545 0.521 0.545 0.521 0.545 0.552 0.552 0.552 0.552 0.552 0.552 0.552 0.552 0.555	0.09 0.134 0.433 1.159 1.018 0.751 0.381 0.413 0.964 0.443 1.099 0.936 0.94 0.675 0.399 0.249 0.249 0.249 0.249 0.249 1.065	0.765 1.129 1.077 0.923 0.651 1.509 1.037 0.576 1.548 1.36 1.54 1.436 1.54 1.436 1.54 1.574 1.436 1.54 1.574	1.704 0.873 0.839 0.233 0.845 0.229 0.415 0.749 0.663 0.436 0.436 0.436 0.436 0.436 0.4302 0.4302 0.4371 1.142 0.609	1.118 0.774 1.326 0.471 0.251 0.301 0.358 0.523 0.034 0.523 0.034 0.523 0.034 0.523 0.034 0.523 0.034 0.523 0.034 0.523 0.034 0.523 0.034 0.523 0.034 0.523 0.034 0.523 0.034 0.523 0.034 0.533 0.034 0.533 0.034 0.533 0.034 0.533 0.034 0.035 0.035 0.037 0.035 0.037 0.035 0.037 0.035 0.037 0.035 0.037 0.035 0.037 0.035 0.037 0.035 0.037 0.035 0.037 0.035 0.037 0.035 0.037 0.035 0.037 0.035 0.037 0.035 0.037 0.037 0.035 0.0370000000000	0.28 1676 1937 0.313 0.619 0.313 0.312 0.167 1.129 0.383 1.328 1.415 0.311 1.87 2.26 2.737 1.521 0.8511 0.876 0.992	0.486 0.218 0.876 1.668 1.191 0.618 1.457 1.005 0.052 3.141 1.485 1.881 1.498 1.357 2.176 1.886 1.149 1.357 2.176 1.886 1.141 1.491	6.681 7.284 1.01 1.755 2.535 4.139 1.308 2.154 1.639 1.308 1.308 2.154 1.639 1.388 1.926 0.203 0.285 2.245 1.502 1.144 0.382 0.043	0.664 3.43 1.154 0.536 1.176 0.426 0.420 0.420 0.421 0.387 0.439 0.477 0.496 0.284 0.397	0.177 0.2 0.249 0.167 0.29 0.25 0.317 0.251 0.183 0.183 0.183 0.183 0.183 0.183 0.183 0.203 0.246 0.183	W Y F D E H R K P T S N Q C V I L M G A
0.189 0.653 0.654 0.864 0.802 0.101 0.933 0.763 0.962 0.375 0.106 0.789 0.945 0.945 0.945 0.945 0.945 0.945 0.945 0.945 0.945	-0.008 3.353 0.917 1.451 0.348 0.271 -0.006 0.647 -0.006 0.647 -0.173 0.293 0.061 -0.007 -0.107 -0.33 -1.267 -0.554 0.674 0.308	2L 0.481 0.738 1.839 0.843 0.103 0.066 0.252 0.392 0.817 1.419 0.933 0.091 0.015 0.091 0.015 0.091 0.015 0.091 0.015 0.091 0.015 0.091 0.015 0.091 0.015 0.091 0.015 0.091 0.015 0.022 0.968 -0.77 1.078 1.943 0.021 0.048 1.043 0.025 0.0480 0.0480 0.0480 0.0480000000000	821 0.293 0.126 0.052 0.022 1.048 0.055 0.027 1.059 0.445 0.065 0.027 1.059 0.445 0.066 0.068 0.101 0.068 0.111 0.085 0.102 0.124 0.124 0.124 0.124 0.124 0.124	0.953 0.953 0.559 1.117 0.834 1.688 0.084 1.063 0.25 1.28 0.458 0.089 0.465 0.069 0.465 0.069 0.465 0.069 0.465 0.069 0.465 0.069 0.465	0.521 0.521 0.724 -0.701 2.054 1.915 1.269 0.173 4.036 0.626 2.248 0.869 1.09 1.312 0.993 0.697 0.255 -0.34 2.659 1.638 1.084	1.156 0.22 0.255 0.147 0.463 0.463 0.464 0.796 1.003 0.295 1.347 0.427 0.959 2.376 1.488 0.849	1.399 0.985 0.927 0.778 0.778 1.031 1.014 0.854 0.879 1.034 1.037 0.454 0.879 1.034 1.087 0.553 0.553 0.553 0.553 0.553 0.553 0.553 0.553 0.553 0.553 0.927 0.312 0.553 0.927 0.312 0.407 0.312 0.407	0.095 0.968 0.215 0.967 0.038 0.447 0.437 0.563 0.447 0.563 0.148 0.102 0.252 0.252 0.283 0.108 0.998 0.485 0.425 0.485 0.425 0.425 0.425 0.212 0.212	1.331 0.415 1.985 2.106 1.129 2.295 2.026 2.463 2.017 2.008 0.343 2.017 2.008 0.343 2.017 2.008 0.343 2.017 2.008 0.343 2.017 2.008 0.343 2.017 2.008 0.343 2.017 2.008 0.343 2.017 2.008 0.343 2.017 2.008 0.343 2.017 2.008 0.343 2.017 2.008 0.343 2.017 2.008 0.343 2.017 2.008 0.343 2.017 2.008 0.343 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.345 2.007 2.008 0.007 2.008 0.007 2.008 0.007 2.008 0.007 0.00800000000	1.708 0.279 1.387 0.652 0.773 0.652 0.773 0.652 0.773 1.808 1.293 1.173 1.676 0.777 -0.96 1.071 0.852 1.109 1.192 1.492 0.937 0.742	1.464 1.537 1.538 1.748 1.644 0.562 0.069 1.437 1.73 1.375 1.562 1.339 1.578 1.451 1.258 1.451 1.258 1.451 1.258 1.451 1.258 1.451 1.258 1.451 1.568 1.467 1.568 1.392	0.391 0.071 0.181 0.669 0.54 0.541 0.654 0.541 0.654 0.405 0.521 0.67 0.429 0.335 0.352 0.352 0.352 0.011 0.544 0.523 0.352	0.09 0.134 0.433 1.159 1.018 0.751 0.381 0.413 0.964 0.443 1.099 0.936 0.94 0.675 0.399 0.249 0.249 0.249 1.065 1.02 0.59	0.765 1.129 1.077 0.923 0.651 1.509 1.037 0.576 1.548 1.36 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.436 1.54 1.574 1.776 1.574	1.704 0.873 0.839 0.233 0.845 0.229 0.415 0.665 0.617 0.349 0.665 0.617 0.349 0.665 0.617 0.349 0.665 0.436 0.436 0.4 0.302 0.436 0.436 0.4 0.302 0.436 0.436 0.4 0.4 0.302 0.436 0.4 0.4 0.4 0.4 0.4 0.4 0.4 0.4 0.4 0.4		0.28 -1676 -1937 0.313 -0.619 -0.392 0.167 -1.129 -0.383 -1.328 -1.415 0.311 -1.87 2.26 2.737 -1.521 -0.851 -0.851 -0.876 -0.993 -0.47	0.486 0.218 0.876 1.668 1.191 0.618 1.457 1.005 3.141 1.885 1.881 1.498 1.357 2.176 1.886 1.14 1.141 1.097 1.298	6.681 7.284 1.01 1.755 2.535 4.139 1.308 2.154 1.639 1.308 2.154 1.639 1.338 1.926 0.203 0.285 2.245 1.502 1.144 -0.382 0.043 2.031	0.664 3.43 1.154 0.536 1.176 0.426 0.505 0.462 0.4 0.241 0.388 0.473 0.377 0.439 0.477 0.439 0.477 0.439 0.284 0.397 0.397 0.67	0.177 0.2 0.249 0.167 0.25 0.317 0.251 0.183 0.183 0.183 0.183 0.226 0.183 0.226 0.183 0.220 0.183 0.203 0.246 0.183 0.209	W Y F D E H R K P T S N Q C V I L M G A Mean

ACE2

Supplementary Figure 4. Heatmaps show the $\Delta\Delta\Delta G$ of the mutations in RBD residues and ACE2 residues that make van der Waals contacts. Maximum (yellow) and Minimum (magenta) $\Delta\Delta\Delta G$ values are labelled for each residue position.

A. Full-Length S Stability					Viral Variatio	on	Max	kimum [Minimum			
			,		Vanado							
	0.095	-0.253	-0.23	-3.068	1.953	1.483	-1.595	-0.107	0.495	21.688	w	
	-0.241	-0.304	-0.326	-1.902	2.252	0.124	-1.221	-0.489	1.792	22,163	Y	
	-0.407	-0.393	-0.395	-2.639	1.988	-0.29	-1.015	-0.459	1.919	18.399	F	
			-0.021	0.193	2.083	2.806	-0.19	1.45	1.418	1.249	D	
	0.063	-0.373	-0.122	-1.309	2.664	3.066	-0.864	1.122	0.538	-0.949	E	
	-0.122	0.196	-0.035		2.943	1.685	-0.474	0.775	0.764	11.675	н	
	-0.382	-0.333	-0.385	-0.72	1.971	2.821	-1.136	-1.001	-1 116	2.872	R	
	-0.683	-0.281	-0.435	-1 149	1.895	2.128	-1.482	-0.342	-0.197	7.218	ĸ	
	4.419	2.127	-0.26	3,498	4.969	3.573	-1.862	1.378	1.692	4.499	Р	
	0.757	-0.28	0.426	-0.214	3.681	1.76	-0.418		1.095	-0.268	Т	
	0.392	-0.301		0.357	2.986	2.678		1.326	1.312		S	
	-0.285	0.062	-0.07	0.041	2.296	2.174	-0.518	1.047		0.864	N	
	-0.192	-0.251	-0.207	-0.766	2.674	1.192	-1.014	-0.245	0.446	0.803	Q	
	0.239	0.475	0.157	-0.702	2 353	2.249	-1.192	0.284	0.31	-1.881	С	
	1.694	0.176	0.582	-1.855	3.595		-1.395	-1.989	-0.754	-2.182	V	
	1.809	-0.296	0.299	-2.007	3.085	-1.005	-1.513	-2.59	-1.628	0.036		
	0.212	-0.378	-0.288	-2.216	2 404	-0.419	-2.614	-1.063	-0.75	2.275	L	
	0.226	-0.36	-0.353	-2.828	1.507	0.478	-2.058	-3.422	-0.616	2.897	M	
	-0.784	0.363	0.272	0.571		2.623	-0.073	1.797	0.951	-0.51	G	
	0.506	-0.255	-0.026	-0.473	2.515	1.933	-0.71	0.526	-0.09	-1.987	А	
	0.386	-0.035	-0.075	-0.905	2.622	1.635	-1.123	-0.105	0.399	4.677	Mean	
	4	92	53	of	2	두	00	2	5	89		
	Det	ĕ	26S	Ť	112	A34	S	122	ž	SAS		
					0							

B. RBD Stability

0.088	-0.44	5.33	-0.049	0.837	6.622	0.715	-0.101	0.08	14.724	W
-0.069	-0.558	2.91	-0.134	0.992	4.627	0.583	-0.252	-0.14	15.249	Y
-0.14	-0.597	2.371	-0.22	0.819	7.216	0.5	-0.251	-0.356	10.98	F
0.359	-0.03	3.932	2.116	-0.212	3.514	3.317	0.521	0.876	5.317	D
-0.026	-0.262	2.529	0.914	-0.078	2.9	1.27	-0.273	0.472	3.086	E
0.199	-0.031	4.716	1.208	-0.198	6.123	1.875	0.843	0.633	21.956	н
-0 779	-0.492	3.457	0.109	-0.241	2.939	0.021	-0.302	-0.669	4.207	R
-0.851	-0.551	2.687	-0.197	0.708	3.607	0.862	-0.341	-0.91	5.743	ĸ
3.162	0.937	6.207	3.914	6.477	2.714	4.085	-1.241	1.566	7.929	Р
-0.318	-0.679	4 234	-0.06	2.805	0.918	1.855	0.258	-0.203	2.112	Т
-0.55	-0.698	2.122	0.624	0.904	2.054	2.88	0.357	-0.003		S
-0.242	-0 735	4.267	1.286	-0.27	2.198	2.26	0.249		7.467	N
-0.399	-0.829	3.703		-0.241	1.979	1.635	-0.149	-0.073	6 788	Q
-0.314	-0.259	3.177	0.585	-0.224	1.452	2.162	0.414	0.166	-0.671	C
		4.642	-0.035	2.25		1.96		-0.474	0.717	V
0.175	-0.168	4.642	0.227	3.053	-1.256	1.752	-0.352	-0.659	2.812	1
0.204	-0.543	2.429	0.268	-0.462	0.433		-0.107	-1.081	2.705	L
-0.104	-0.803	3.006	0.054	0 241	0.256	0.374	-0.625	-0.964	3.954	M
-0.046	-0.036		1.299	-0.882	3.023	2.935	0.03	0.586	0.72	G
-0.196	-0.711	3.191	0.554		1.95	2.022	0.259	-0.33	-0.566	A
0.008	-0.394	3.661	0.604	0.857	2.804	1.74	-0.056	-0.078	6.065	Mean
0	~	60	ব	0	~	8	e	თ	m	
8	39.	47	4	22	25	42	õ	433	433	
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C. RBD-ACE2 Binding



Supplementary Figure 5. Heatmaps of viral mutations (green) for (**A**) Full-length S stability ($\Delta\Delta$ G), (**B**) RBD stability $\Delta\Delta$ G and (**C**) RBD-ACE2 binding affinity ($\Delta\Delta\Delta$ G). Maximum (yellow) and Minimum (magenta) $\Delta\Delta$ G / $\Delta\Delta\Delta$ G values are labelled for each residue position. The folding energy change ($\Delta\Delta$ G) is computed based on the monomer.



Supplementary Figure 6. Boxplots for the $|\Delta\Delta G|$ of mean of residues with and without viral mutations (upper) and $|\Delta\Delta G|$ of viral mutations and other computationally predicted mutations in the same positions (lower). The mean values are shown as red dots. The folding energy change ($\Delta\Delta G$) is computed based on the monomer.