

Source File	Job Name	docking score	glide gscore	glide emodel	IMGBSA dG Bind	Structure of SARS-CoV-2 chimeric receptor-binding domain complexed with its receptor human ACE2
6VW1	glide-dock_SP_6VW1_A_Anti-HIV_site_1					6VW1_ACE2
Ritonavir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-6.127	-6.127	-69.366		
Abacavir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-5.287	-5.292	-51.265		
Emtricitabine.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-5.193	-5.193	-38.015		
Lamivudine.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-4.556	-4.556	-38.259		
cobicistat.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-4.406	-4.717	-56.379		
tenofovir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-4.306	-4.584	-42.961		
Elvitegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-3.974	-4.111	-36.652		
cobicistat.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-3.872	-4.402	-63.140		
lopinavir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-3.520	-3.520	-43.943		
tenofovir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-3.425	-4.006	-37.242		
Dolutegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-3.406	-3.693	-36.990		
Elvitegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-3.065	-4.021	-36.433		
Dolutegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-2.840	-3.465	-34.927		
Raltegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-2.703	-3.296	-43.888		
Raltegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-2.280	-2.552	-36.542		
Dolutegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_1	-2.115	-4.083	-50.419		
	glide-dock_SP_6VW1_A_Anti-HIV_site_2					
Ritonavir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-7.812	-7.812	-105.758		
cobicistat.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-6.129	-6.659	-101.345		
Lamivudine.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-5.678	-5.678	-39.797		
cobicistat.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-5.329	-5.641	-87.245		
lopinavir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-4.953	-4.953	-63.682		
Emtricitabine.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-4.888	-4.888	-41.986		
Dolutegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-4.841	-5.128	-61.090		
Abacavir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-4.744	-4.749	-41.797		
tenofovir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-4.095	-4.676	-42.292		
tenofovir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-3.626	-3.904	-40.276		
Raltegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-3.501	-3.772	-48.039		
Elvitegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-3.488	-3.625	-46.865		
Dolutegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-3.434	-4.059	-50.924		
Raltegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-3.393	-3.986	-59.777		
Elvitegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-3.311	-4.267	-51.378		
Dolutegravir.sdf	glide-dock_SP_6VW1_A_Anti-HIV_site_2	-2.564	-4.533	-54.879		

lopinavir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_1	-6.660	-6.660	-75.558	
Raltegravir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_1	-4.587	-5.180	-60.883	
Lamivudine.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_1	-4.411	-4.411	-36.402	
Elvitegravir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_1	-3.967	-4.103	-45.357	
Emtricitabine.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_1	-3.919	-3.919	-39.613	
Ritonavir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_1	-3.603	-3.603	-65.629	
Elvitegravir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_1	-3.251	-4.207	-40.640	
Raltegravir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_1	-2.574	-2.845	-51.644	
	glide-dock_XP_6VW1_A_Anti-HIV_site_2				
cobicistat.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-6.458	-6.988	-98.644	
Ritonavir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-6.210	-6.210	-98.377	
Lamivudine.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-5.966	-5.966	-34.283	
lopinavir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-5.122	-5.122	-75.550	
tenofovir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-4.646	-5.228	-34.548	
tenofovir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-4.308	-4.586	-41.685	
Dolutegravir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-4.016	-4.303	-54.867	
Elvitegravir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-3.896	-4.033	-44.460	
Abacavir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-3.621	-3.627	-42.602	
cobicistat.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-3.611	-3.922	-99.797	
Emtricitabine.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-3.297	-3.297	-39.747	
Raltegravir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-2.985	-3.257	-60.223	
Elvitegravir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-2.835	-3.791	-53.769	
Raltegravir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-2.560	-3.153	-66.488	
Dolutegravir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-2.126	-2.752	-53.987	
Dolutegravir.sdf	glide-dock_XP_6VW1_A_Anti-HIV_site_2	-1.007	-2.975	-60.330	
	prime_mmgsbsa_Anti-HIV_ACE2_site_2				
cobicistat.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-6.458	-6.988	-98.644	-60.92
Ritonavir.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-6.210	-6.210	-98.377	-50.42
Lamivudine.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-5.966	-5.966	-34.283	-29.36
lopinavir.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-5.122	-5.122	-75.550	-49.56
tenofovir.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-4.646	-5.228	-34.548	
tenofovir.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-4.308	-4.586	-41.685	-10.88
Dolutegravir.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-4.016	-4.303	-54.867	-44.11
Elvitegravir.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-3.896	-4.033	-44.460	-26.01
Abacavir.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-3.621	-3.627	-42.602	-38.86
cobicistat.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-3.611	-3.922	-99.797	-63.61
Emtricitabine.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-3.297	-3.297	-39.747	-35.62
Raltegravir.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-2.985	-3.257	-60.223	-25.79
Elvitegravir.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-2.835	-3.791	-53.769	-50.24
Raltegravir.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-2.560	-3.153	-66.488	-45.94
Dolutegravir.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-2.126	-2.752	-53.987	-26.75
Dolutegravir.sdf	prime_mmgsbsa_Anti-HIV_ACE2_site_2	-1.007	-2.975	-60.330	-38.78
	prime_mmgsbsa_SP_Anti-HIV_ACE2_site_2				
Ritonavir.sdf	prime_mmgsbsa_SP_Anti-HIV_ACE2_site_2	-7.812	-7.812	-105.758	-73.16
cobicistat.sdf	prime_mmgsbsa_SP_Anti-HIV_ACE2_site_2	-6.129	-6.659	-101.345	-72.12
Lamivudine.sdf	prime_mmgsbsa_SP_Anti-HIV_ACE2_site_2	-5.678	-5.678	-39.797	-27.15

cobicistat.sdf	prime_mmgbbsa_SP_Anti-HIV_ACE2_site_2	-5.329	-5.641	-87.245	-63.66
lopinavir.sdf	prime_mmgbbsa_SP_Anti-HIV_ACE2_site_2	-4.953	-4.953	-63.682	-15.94
Emtricitabine.sdf	prime_mmgbbsa_SP_Anti-HIV_ACE2_site_2	-4.888	-4.888	-41.986	-35.50
Dolutegravir.sdf	prime_mmgbbsa_SP_Anti-HIV_ACE2_site_2	-4.841	-5.128	-61.090	-33.07
Abacavir.sdf	prime_mmgbbsa_SP_Anti-HIV_ACE2_site_2	-4.744	-4.749	-41.797	-42.79
tenofovir.sdf	prime_mmgbbsa_SP_Anti-HIV_ACE2_site_2	-4.095	-4.676	-42.292	Eyl.37
tenofovir.sdf	prime_mmgbbsa_SP_Anti-HIV_ACE2_site_2	-3.626	-3.904	-40.276	-14.67
Raltegravir.sdf	prime_mmgbbsa_SP_Anti-HIV_ACE2_site_2	-3.501	-3.772	-48.039	-29.18
Elvitegravir.sdf	prime_mmgbbsa_SP_Anti-HIV_ACE2_site_2	-3.488	-3.625	-46.865	-25.10
Dolutegravir.sdf	prime_mmgbbsa_SP_Anti-HIV_ACE2_site_2	-3.434	-4.059	-50.924	-14.62
Raltegravir.sdf	prime_mmgbbsa_SP_Anti-HIV_ACE2_site_2	-3.393	-3.986	-59.777	-55.35
Elvitegravir.sdf	prime_mmgbbsa_SP_Anti-HIV_ACE2_site_2	-3.311	-4.267	-51.378	-50.73
Dolutegravir.sdf	prime_mmgbbsa_SP_Anti-HIV_ACE2_site_2	-2.564	-4.533	-54.879	-36.04

6VW1	glide-dock_SP_antiHIV_6VW1_E_site_1				
Emtricitabine.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-5.147	-5.147	-38.170	
tenofovir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-5.048	-5.326	-51.956	
Lamivudine.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-4.918	-4.918	-43.857	
cobicistat.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-4.874	-5.185	-77.979	
Ritonavir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-4.852	-4.852	-55.564	
Abacavir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-4.595	-4.601	-40.428	
cobicistat.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-4.332	-4.862	-76.455	
lopinavir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-3.638	-3.638	-45.639	
tenofovir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-3.478	-4.060	-45.706	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-3.437	-3.724	-48.605	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-3.436	-3.573	-43.484	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-3.207	-4.163	-51.717	
Raltegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-3.110	-3.381	-51.496	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-2.794	-3.419	-49.185	
Raltegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-2.692	-3.285	-45.553	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_1	-1.594	-3.563	-49.833	
	glide-dock_SP_antiHIV_6VW1_E_site_2				
cobicistat.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-6.488	-7.018	-77.326	
Ritonavir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-6.044	-6.044	-70.310	
Emtricitabine.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-5.664	-5.664	-35.387	
Abacavir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-5.401	-5.407	-39.857	

6VW1_spike S1 protein

Structure
of SARS-
CoV-2
chimeric
receptor-
binding
domain
complex
d with its
receptor
human
ACE2

Lamivudine.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-5.172	-5.172	-34.899
tenofovir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-5.167	-5.445	-48.898
Raltegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-4.909	-5.502	-52.500
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-4.787	-5.074	-50.181
cobicistat.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-4.699	-5.010	-64.246
lopinavir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-4.639	-4.639	-43.924
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-4.567	-4.704	-44.736
Raltegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-4.050	-4.322	-48.781
tenofovir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-4.034	-4.615	-42.886
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-3.670	-4.295	-45.569
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-2.839	-3.795	-41.539
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VW1_E_site_2	-2.172	-4.141	-43.589

6VYB	glide-dock_SP_antiHIV_6VYB_site_1			
Ritonavir.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-6.470	-6.470	-87.550
lopinavir.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-6.347	-6.347	-66.614
Abacavir.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-6.186	-6.191	-51.544
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-6.019	-6.645	-67.274
tenofovir.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-5.898	-6.176	-55.827
Emtricitabine.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-5.437	-5.437	-45.106
Raltegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-5.430	-5.702	-65.256
Lamivudine.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-5.427	-5.427	-45.808
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-5.410	-5.697	-62.166
cobicistat.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-5.379	-5.691	-74.588
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-4.826	-6.794	-69.245
tenofovir.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-4.666	-5.248	-48.120
Raltegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-4.578	-5.171	-58.361
cobicistat.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-4.410	-4.940	-67.087
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-4.036	-4.173	-41.265
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_1	-3.830	-4.786	-53.586
	glide-dock_SP_antiHIV_6VYB_site_2			
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-6.708	-6.845	-63.344
Ritonavir.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-6.140	-6.140	-64.936
cobicistat.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-6.026	-6.337	-81.471
Emtricitabine.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-5.834	-5.834	-42.725
Lamivudine.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-5.656	-5.656	-38.606
tenofovir.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-5.652	-5.930	-57.072
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-5.304	-6.260	-57.699
Abacavir.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-5.296	-5.301	-43.888
cobicistat.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-5.257	-5.787	-75.241

SARS-CoV-2 spike ectodomain in structure (open state)

6VYB

lopinavir.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-5.192	-5.192	-55.229
tenofovir.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-5.083	-5.665	-55.348
Raltegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-4.691	-4.962	-63.819
Raltegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-4.444	-5.037	-63.192
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-4.347	-4.635	-48.183
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-3.657	-4.282	-45.283
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_2	-2.834	-4.803	-47.464
	glide-dock_SP_antiHIV_6VYB_site_3			
tenofovir.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-6.113	-6.391	-60.389
Lamivudine.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-6.075	-6.075	-39.340
Ritonavir.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-5.515	-5.515	-65.898
tenofovir.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-5.244	-5.826	-51.030
cobicistat.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-4.983	-5.295	-58.351
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-4.858	-5.145	-51.334
Raltegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-4.742	-5.013	-54.741
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-4.410	-5.036	-47.424
Raltegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-4.333	-4.926	-49.891
Abacavir.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-4.287	-4.292	-36.629
cobicistat.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-4.252	-4.782	-65.560
lopinavir.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-4.224	-4.224	-46.569
Emtricitabine.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-3.921	-3.921	-31.438
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-3.584	-3.721	-42.066
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-2.744	-3.700	-42.444
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_3	-2.498	-4.467	-46.616
	glide-dock_SP_antiHIV_6VYB_site_4			
lopinavir.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-5.346	-5.346	-59.907
Lamivudine.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-5.324	-5.324	-42.844
Ritonavir.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-5.272	-5.272	-69.019
Emtricitabine.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-5.039	-5.039	-40.516
Abacavir.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-4.942	-4.947	-43.857
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-4.928	-5.065	-47.373
cobicistat.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-4.868	-5.180	-65.707
tenofovir.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-4.459	-4.737	-47.377
Raltegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-4.179	-4.450	-50.593
tenofovir.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-4.139	-4.721	-47.371
cobicistat.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-3.955	-4.485	-64.596
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-3.949	-4.236	-49.269
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-3.927	-4.883	-47.246
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-3.737	-4.362	-50.710
Raltegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-3.688	-4.281	-55.142
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VYB_site_4	-3.185	-5.154	-53.973
	glide-dock_XP_antiHIV_6VYB_site_2			
Elvitegravir.sdf	glide-dock_XP_antiHIV_6VYB_site_2	-6.713	-6.850	-53.503
tenofovir.sdf	glide-dock_XP_antiHIV_6VYB_site_2	-6.058	-6.336	-44.080
Emtricitabine.sdf	glide-dock_XP_antiHIV_6VYB_site_2	-6.035	-6.035	-36.081
Ritonavir.sdf	glide-dock_XP_antiHIV_6VYB_site_2	-5.967	-5.967	-85.041
Abacavir.sdf	glide-dock_XP_antiHIV_6VYB_site_2	-4.734	-4.739	-40.713

Lamivudine.sdf	glide-dock_XP_antiHIV_6VYB_site_2	-4.476	-4.476	-36.271	
Elvitegravir.sdf	glide-dock_XP_antiHIV_6VYB_site_2	-4.474	-5.430	-54.335	
cobicistat.sdf	glide-dock_XP_antiHIV_6VYB_site_2	-4.084	-4.614	-90.522	
cobicistat.sdf	glide-dock_XP_antiHIV_6VYB_site_2	-3.479	-3.790	-77.333	
	glide-dock_XP_antiHIV_6VYB_site_1				
Abacavir.sdf	glide-dock_XP_antiHIV_6VYB_site_1	-5.364	-5.370	-49.072	
lopinavir.sdf	glide-dock_XP_antiHIV_6VYB_site_1	-5.256	-5.256	-82.486	
Emtricitabine.sdf	glide-dock_XP_antiHIV_6VYB_site_1	-4.411	-4.411	-37.708	
Dolutegravir.sdf	glide-dock_XP_antiHIV_6VYB_site_1	-4.382	-4.669	-61.308	
Lamivudine.sdf	glide-dock_XP_antiHIV_6VYB_site_1	-4.287	-4.287	-38.954	
Dolutegravir.sdf	glide-dock_XP_antiHIV_6VYB_site_1	-3.952	-5.921	-65.296	
tenofovir.sdf	glide-dock_XP_antiHIV_6VYB_site_1	-3.825	-4.103	-46.309	
Ritonavir.sdf	glide-dock_XP_antiHIV_6VYB_site_1	-2.391	-2.391	-88.786	
cobicistat.sdf	glide-dock_XP_antiHIV_6VYB_site_1	-1.915	-2.226	-83.104	
Raltegravir.sdf	glide-dock_XP_antiHIV_6VYB_site_1	-1.741	-2.012	-69.307	
Dolutegravir.sdf	glide-dock_XP_antiHIV_6VYB_site_1	-0.709	-1.334	-61.917	
	prime_mmgsbsa_antiHIV_6VYB_site_2				
Elvitegravir.sdf	prime_mmgsbsa_antiHIV_6VYB_site_2	-6.713	-6.850	-53.503	-67.76
tenofovir.sdf	prime_mmgsbsa_antiHIV_6VYB_site_2	-6.058	-6.336	-44.080	-40.59
Emtricitabine.sdf	prime_mmgsbsa_antiHIV_6VYB_site_2	-6.035	-6.035	-36.081	-43.17
Ritonavir.sdf	prime_mmgsbsa_antiHIV_6VYB_site_2	-5.967	-5.967	-85.041	-67.29

6VXX	glide-dock_SP_antiHIV_6VXX_site_4				
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-6.103	-6.240	-47.848	
lopinavir.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-6.087	-6.087	-60.232	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-5.899	-6.524	-52.296	
Lamivudine.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-5.833	-5.833	-33.146	
Emtricitabine.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-5.704	-5.704	-32.385	
cobicistat.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-5.536	-6.066	-70.338	
cobicistat.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-5.361	-5.673	-63.235	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-5.135	-5.422	-43.387	
Abacavir.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-4.908	-4.914	-36.517	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-4.876	-5.832	-47.858	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-4.631	-6.599	-52.162	
Ritonavir.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-4.442	-4.442	-54.999	
Raltegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-4.017	-4.289	-46.042	
tenofovir.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-3.947	-4.225	-34.310	
Raltegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-3.772	-4.365	-46.597	
tenofovir.sdf	glide-dock_SP_antiHIV_6VXX_site_4	-2.812	-3.394	-30.636	

Structure
of the
SARS-CoV-
2 spike
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6VXX

	glide-dock_SP_antiHIV_6VXX_site_2				
lopinavir.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-6.028	-6.028	-68.843	
Emtricitabine.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-5.484	-5.484	-42.164	
cobicistat.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-5.433	-5.963	-84.205	
Ritonavir.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-5.293	-5.293	-60.962	
Abacavir.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-5.250	-5.255	-42.513	
cobicistat.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-4.931	-5.243	-74.720	
Lamivudine.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-4.451	-4.451	-42.211	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-4.067	-4.204	-42.369	
tenofovir.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-4.054	-4.332	-42.088	
Raltegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-3.861	-4.454	-56.261	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-3.698	-3.985	-50.760	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-3.512	-4.468	-46.743	
Raltegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-3.309	-3.580	-47.090	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-3.172	-3.798	-45.233	
tenofovir.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-3.135	-3.717	-40.452	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_2	-2.649	-4.618	-49.004	
	glide-dock_SP_antiHIV_6VXX_site_1				
cobicistat.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-6.108	-6.420	-79.990	
Ritonavir.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-5.432	-5.432	-60.903	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-5.243	-5.531	-63.709	
Lamivudine.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-5.104	-5.104	-41.866	
Abacavir.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-5.102	-5.108	-43.880	
cobicistat.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-5.028	-5.558	-71.139	
Emtricitabine.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-4.924	-4.924	-41.924	
lopinavir.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-4.614	-4.614	-50.924	
tenofovir.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-4.541	-4.820	-47.882	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-4.472	-5.097	-50.742	
Raltegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-4.393	-4.665	-59.607	
tenofovir.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-4.251	-4.832	-49.825	
Raltegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-4.153	-4.746	-57.109	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-4.012	-4.149	-45.894	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-3.348	-5.317	-60.072	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6VXX_site_1	-2.914	-3.870	-45.809	
	glide-dock_XP_antiHIV_6VXX_site_1				
Ritonavir.sdf	glide-dock_XP_antiHIV_6VXX_site_1	-6.283	-6.283	-80.927	
Dolutegravir.sdf	glide-dock_XP_antiHIV_6VXX_site_1	-4.026	-4.313	-65.762	
cobicistat.sdf	glide-dock_XP_antiHIV_6VXX_site_1	-3.904	-4.215	-82.443	
	prime_mmgsa_antiHIV_6VXX_site_2				
lopinavir.sdf	prime_mmgsa_antiHIV_6VXX_site_2	-6.028	-6.028	-68.843	-42.90
cobicistat.sdf	prime_mmgsa_antiHIV_6VXX_site_2	-5.433	-5.963	-84.205	-77.04

					Structure of post fusion core of 2019- nCoV S2 subunit
6LXT	glide-dock_SP_antiHIV_6LXT_site_1				6LXT
Lamivudine.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-5.368	-5.368	-38.568	
Emtricitabine.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-5.307	-5.307	-38.394	
Ritonavir.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-4.510	-4.510	-54.038	
cobicistat.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-4.272	-4.802	-60.364	
Abacavir.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-4.162	-4.167	-36.398	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-3.983	-4.120	-37.736	
cobicistat.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-3.961	-4.273	-48.259	
tenofovir.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-3.903	-4.181	-37.084	
lopinavir.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-3.394	-3.394	-34.228	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-3.077	-3.365	-40.336	
Raltegravir.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-3.066	-3.338	-41.117	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-3.042	-3.998	-41.085	
tenofovir.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-2.769	-3.351	-29.869	
Raltegravir.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-2.714	-3.307	-41.075	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-2.436	-3.061	-37.522	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6LXT_site_1	-1.447	-3.415	-39.452	
					SARS-Cov- 2 RNA- dependen t RNA polymeras e in complex with cofactors
6M71	glide-dock_SP_antiHIV_6M71_site_1				6M71
cobicistat.sdf	glide-dock_SP_antiHIV_6M71_site_1	-5.898	-6.428	-88.747	
Ritonavir.sdf	glide-dock_SP_antiHIV_6M71_site_1	-5.499	-5.499	-78.144	
Emtricitabine.sdf	glide-dock_SP_antiHIV_6M71_site_1	-5.066	-5.066	-40.366	
Abacavir.sdf	glide-dock_SP_antiHIV_6M71_site_1	-4.926	-4.931	-37.650	
Lamivudine.sdf	glide-dock_SP_antiHIV_6M71_site_1	-4.864	-4.864	-37.396	
cobicistat.sdf	glide-dock_SP_antiHIV_6M71_site_1	-4.706	-5.018	-82.457	
tenofovir.sdf	glide-dock_SP_antiHIV_6M71_site_1	-4.445	-4.723	-43.034	
lopinavir.sdf	glide-dock_SP_antiHIV_6M71_site_1	-4.407	-4.407	-62.070	
Raltegravir.sdf	glide-dock_SP_antiHIV_6M71_site_1	-3.983	-4.254	-51.587	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6M71_site_1	-3.924	-4.060	-44.284	
Raltegravir.sdf	glide-dock_SP_antiHIV_6M71_site_1	-3.805	-4.398	-52.260	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6M71_site_1	-3.770	-4.057	-49.137	
tenofovir.sdf	glide-dock_SP_antiHIV_6M71_site_1	-3.738	-4.319	-45.239	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6M71_site_1	-3.734	-4.690	-51.832	

Dolutegravir.sdf	glide-dock_SP_antiHIV_6M71_site_1	-3.717	-4.343	-51.587	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6M71_site_1	-2.599	-4.567	-55.915	
	glide-dock_SP_antiHIV_6M71_site_2				
cobicistat.sdf	glide-dock_SP_antiHIV_6M71_site_2	-7.109	-7.639	-91.419	
cobicistat.sdf	glide-dock_SP_antiHIV_6M71_site_2	-6.989	-7.301	-89.509	
Ritonavir.sdf	glide-dock_SP_antiHIV_6M71_site_2	-5.973	-5.973	-76.862	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6M71_site_2	-5.721	-6.009	-56.704	
Abacavir.sdf	glide-dock_SP_antiHIV_6M71_site_2	-5.667	-5.672	-47.393	
Lamivudine.sdf	glide-dock_SP_antiHIV_6M71_site_2	-5.548	-5.548	-38.965	
Emtricitabine.sdf	glide-dock_SP_antiHIV_6M71_site_2	-5.516	-5.516	-38.136	
lopinavir.sdf	glide-dock_SP_antiHIV_6M71_site_2	-5.251	-5.251	-56.065	
Raltegravir.sdf	glide-dock_SP_antiHIV_6M71_site_2	-4.767	-5.360	-63.801	
tenofovir.sdf	glide-dock_SP_antiHIV_6M71_site_2	-4.553	-4.832	-46.538	
Raltegravir.sdf	glide-dock_SP_antiHIV_6M71_site_2	-4.456	-4.728	-51.332	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6M71_site_2	-4.351	-4.977	-51.164	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6M71_site_2	-4.067	-5.023	-56.055	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6M71_site_2	-3.761	-3.898	-44.423	
tenofovir.sdf	glide-dock_SP_antiHIV_6M71_site_2	-3.464	-4.046	-36.292	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6M71_site_2	-3.368	-5.336	-53.728	
	glide-dock_SP_antiHIV_6M71_site_3				
lopinavir.sdf	glide-dock_SP_antiHIV_6M71_site_3	-6.524	-6.524	-67.408	
Lamivudine.sdf	glide-dock_SP_antiHIV_6M71_site_3	-5.459	-5.459	-35.715	
Emtricitabine.sdf	glide-dock_SP_antiHIV_6M71_site_3	-5.344	-5.344	-34.254	
Raltegravir.sdf	glide-dock_SP_antiHIV_6M71_site_3	-4.972	-5.565	-64.772	
Abacavir.sdf	glide-dock_SP_antiHIV_6M71_site_3	-4.963	-4.968	-42.069	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6M71_site_3	-4.848	-5.135	-17.502	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6M71_site_3	-4.820	-5.776	-45.343	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6M71_site_3	-4.625	-4.762	-39.676	
tenofovir.sdf	glide-dock_SP_antiHIV_6M71_site_3	-3.591	-4.172	-33.923	
tenofovir.sdf	glide-dock_SP_antiHIV_6M71_site_3	-3.543	-3.821	-38.155	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6M71_site_3	-3.364	-3.989	-42.035	
Raltegravir.sdf	glide-dock_SP_antiHIV_6M71_site_3	-3.129	-3.400	-42.111	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6M71_site_3	-1.864	-3.833	-44.562	
	glide-dock_XP_antiHIV_6M71_site_2				
cobicistat.sdf	glide-dock_XP_antiHIV_6M71_site_2	-6.012	-6.542	-89.919	
Ritonavir.sdf	glide-dock_XP_antiHIV_6M71_site_2	-5.983	-5.983	-76.970	
Dolutegravir.sdf	glide-dock_XP_antiHIV_6M71_site_2	-5.550	-5.837	-58.526	
cobicistat.sdf	glide-dock_XP_antiHIV_6M71_site_2	-1.719	-2.031	-72.688	
	prime_mmgsa_antiHIV_6M71_site_2				
cobicistat.sdf	prime_mmgsa_antiHIV_6M71_site_2	-6.012	-6.542	-89.919	-110.11
Ritonavir.sdf	prime_mmgsa_antiHIV_6M71_site_2	-5.983	-5.983	-76.970	-82.81
Dolutegravir.sdf	prime_mmgsa_antiHIV_6M71_site_2	-5.550	-5.837	-58.526	-54.63
cobicistat.sdf	prime_mmgsa_antiHIV_6M71_site_2	-1.719	-2.031	-72.688	-75.28

					The crystal structure of COVID- 19 main protease in complex with an inhibitor
6LU7					6LU7 N3
cobicistat.sdf	glide-dock_SP_antiHIV_6LU7	-8.122	-8.652	-112.282	
lopinavir.sdf	glide-dock_SP_antiHIV_6LU7	-7.407	-7.407	-86.370	
Ritonavir.sdf	glide-dock_SP_antiHIV_6LU7	-7.266	-7.266	-90.587	
cobicistat.sdf	glide-dock_SP_antiHIV_6LU7	-6.439	-6.751	-90.527	
Emtricitabine.sdf	glide-dock_SP_antiHIV_6LU7	-6.005	-6.005	-42.449	
Lamivudine.sdf	glide-dock_SP_antiHIV_6LU7	-5.992	-5.992	-41.670	
Abacavir.sdf	glide-dock_SP_antiHIV_6LU7	-5.649	-5.654	-48.435	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6LU7	-5.446	-6.072	-59.344	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6LU7	-5.379	-5.515	-56.966	
Raltegravir.sdf	glide-dock_SP_antiHIV_6LU7	-5.267	-5.860	-63.518	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6LU7	-5.082	-5.369	-54.234	
Raltegravir.sdf	glide-dock_SP_antiHIV_6LU7	-4.815	-5.087	-57.953	
Dolutegravir.sdf	glide-dock_SP_antiHIV_6LU7	-4.729	-6.698	-62.243	
tenofovir.sdf	glide-dock_SP_antiHIV_6LU7	-4.538	-4.816	-49.613	
tenofovir.sdf	glide-dock_SP_antiHIV_6LU7	-4.033	-4.614	-47.015	
Elvitegravir.sdf	glide-dock_SP_antiHIV_6LU7	-3.988	-4.944	-59.337	
	glide-dock_XP_antiHIV_5LU7				
cobicistat.sdf	glide-dock_XP_antiHIV_5LU7	-7.233	-7.763	-124.242	
lopinavir.sdf	glide-dock_XP_antiHIV_5LU7	-6.867	-6.867	-86.508	
Ritonavir.sdf	glide-dock_XP_antiHIV_5LU7	-6.858	-6.858	-89.094	
cobicistat.sdf	glide-dock_XP_antiHIV_5LU7	-5.297	-5.608	-106.326	
	prime_mmgsbsa_antiHIV_6LU7				
cobicistat.sdf	prime_mmgsbsa_antiHIV_6LU7	-7.233	-7.763	-124.242	-105.13
lopinavir.sdf	prime_mmgsbsa_antiHIV_6LU7	-6.867	-6.867	-86.508	-71.35
Ritonavir.sdf	prime_mmgsbsa_antiHIV_6LU7	-6.858	-6.858	-89.094	-100.77
cobicistat.sdf	prime_mmgsbsa_antiHIV_6LU7	-5.297	-5.608	-106.326	-99.68