DATA sheet

Predict the effect of spike mutations on antibody binding

1. What is the PDB ID for your assigned antibody?
2. What is the name of your assigned antibody?
3. What is the name of the drug that contains your antibody?
4. What is the sequence ID for your variant protein sequence?
5. Paste images below showing the highlighted amino acids in the antibody binding site in the aligned structures.
6. For each mutation in the antibody binding site, what is the original amino acid and position and the amino acid at that position. Example: E484 is replaced by an A
7. Investigate the potential impact of each mutation listed above on antibody binding.
8. For pair of original and mutant amino acids, paste images below that show the interactions that would be found between the original amino acid and the antibodies, spike protein, and oxygens and the interactions that would be found when the original is replace by the mutant amino acid.

Example:

|  |  |
| --- | --- |
| Original amino acid | Mutant amino acid |
| Picture |  |

1. Prepare a table as shown below and complete the information for each mutated amino acid in the antibody binding site.

Example table:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | E484 | Kind of bond | A484 | Kind of bond |
| Amino acid name | Glutamic acid |  | Alanine |  |
| Heavy chain interaction(s) | R50 | Salt bridge and contacts | None |  |
|  | Y101 | Contacts | None |  |
| Light chain interaction(s) | R96 | Salt bridge | None |  |
| Oxygen interactions | O97 | Hydrogen bond, contacts | None |  |

1. Discuss how each antibody-binding site mutation is likely to impact the ability of the antibody to bind to the SARS-CoV-2 spike protein.