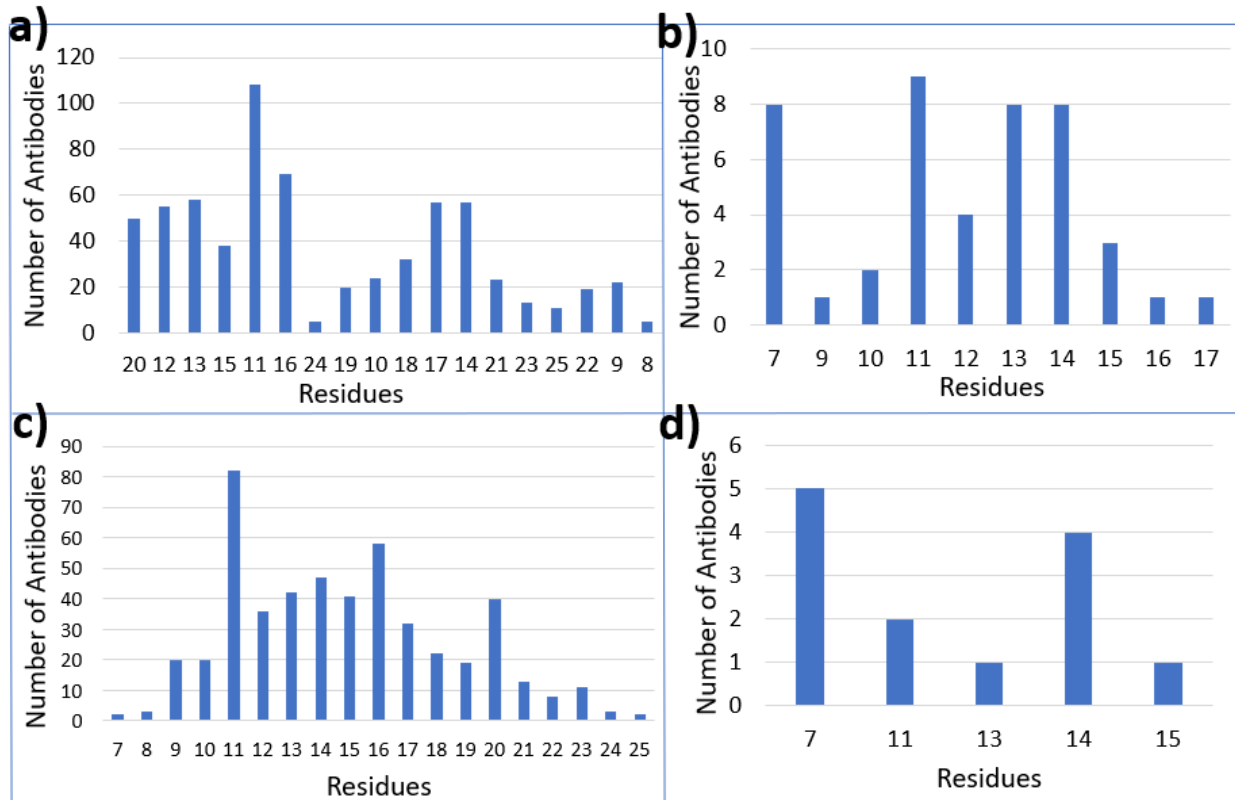


# Structural, Sequence, and Germline Analysis of SARS-CoV-2 Antibodies Across Humans and Mice

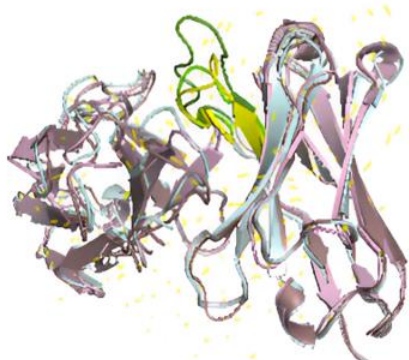
Saanvi Dogra\*

## SUPPORTING INFORMATION



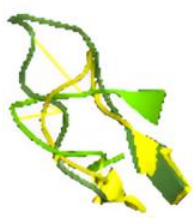
**Figure S1.** Comparing CDRH3 residue length of the natural **a)** human or **b)** mouse antibodies binding to the RBD from the heavy V gene (IGHV1), as well as the CDRH3 residue length of natural **c)** human or **d)** mouse antibodies binding to the RBD from the light V gene (IGKV3)

RMSD Value from Superimposition of Heavy Chain of C112, 4A3, and Ab\_510H2



|          | 4A3   | Ab_510H2 | C112  |
|----------|-------|----------|-------|
| 4A3      | —     | 0.713    | 1.025 |
| Ab_510H2 | 0.713 | —        | 0.813 |
| C112     | 1.025 | 0.813    | —     |

RMSD Value from Superimposition of CDRH3 of C112, 4A3, and Ab\_510H2



|          | 4A3   | Ab_510H2 | C112  |
|----------|-------|----------|-------|
| 4A3      | —     | 0.449    | 3.333 |
| Ab_510H2 | 0.449 | —        | 1.056 |
| C112     | 3.333 | 1.056    | —     |

**Figure S2.** Matrix and model comparing structural similarity of the heavy chains (top) and CDRH3s (bottom) through RMSD value (in Å) of human antibodies C112, 4A3, and AB\_510H2.

Heavy Chain Sequence Alignment Identity Matrix of C112, 4A3, and Ab\_510H2

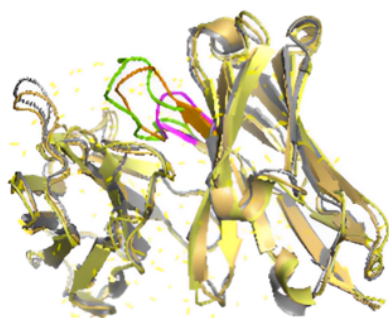
|          | C112  | 4A3   | Ab_510H2 |
|----------|-------|-------|----------|
| C112     | —     | 83.62 | 82.91    |
| 4A3      | 83.62 | —     | 87.83    |
| Ab_510H2 | 82.91 | 87.83 | —        |

CDRH3 Sequence Alignment Identity Matrix of C112, 4A3, and Ab\_510H2

|          | C112  | 4A3   | Ab_510H2 |
|----------|-------|-------|----------|
| C112     | —     | 44.44 | 36.36    |
| 4A3      | 44.44 | —     | 44.44    |
| Ab_510H2 | 36.36 | 44.44 | —        |

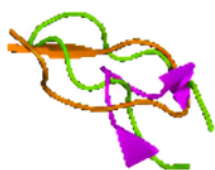
**Figure S3.** Matrix comparing the percent similarity of the heavy chain (top) and CDRH3 (bottom) sequences of human antibodies C112, 4A3, Ab\_510H2.

RMSD Value from Heavy Chain Superimposition of 1E02, 1H06, and 2C02



|      | 1E02  | 1H06  | 2C02  |
|------|-------|-------|-------|
| 1E02 | —     | 0.800 | 1.024 |
| 1H06 | 0.800 | —     | 0.598 |
| 2C02 | 1.024 | 0.598 | —     |

RMSD Value from Superimposition of CDRH3 of 1E02, 1H06, and 2C02



|      | 1E02  | 1H06  | 2C02  |
|------|-------|-------|-------|
| 1E02 | —     | 2.316 | 0.908 |
| 1H06 | 2.316 | —     | 0.011 |
| 2C02 | 0.908 | 0.011 | —     |

**Figure S4.** Matrix and model comparing structural similarity of the heavy chains (top) and CDRH3s (bottom) through RMSD value (in Å) of mouse antibodies 1E02, 1H06, and 2C02.

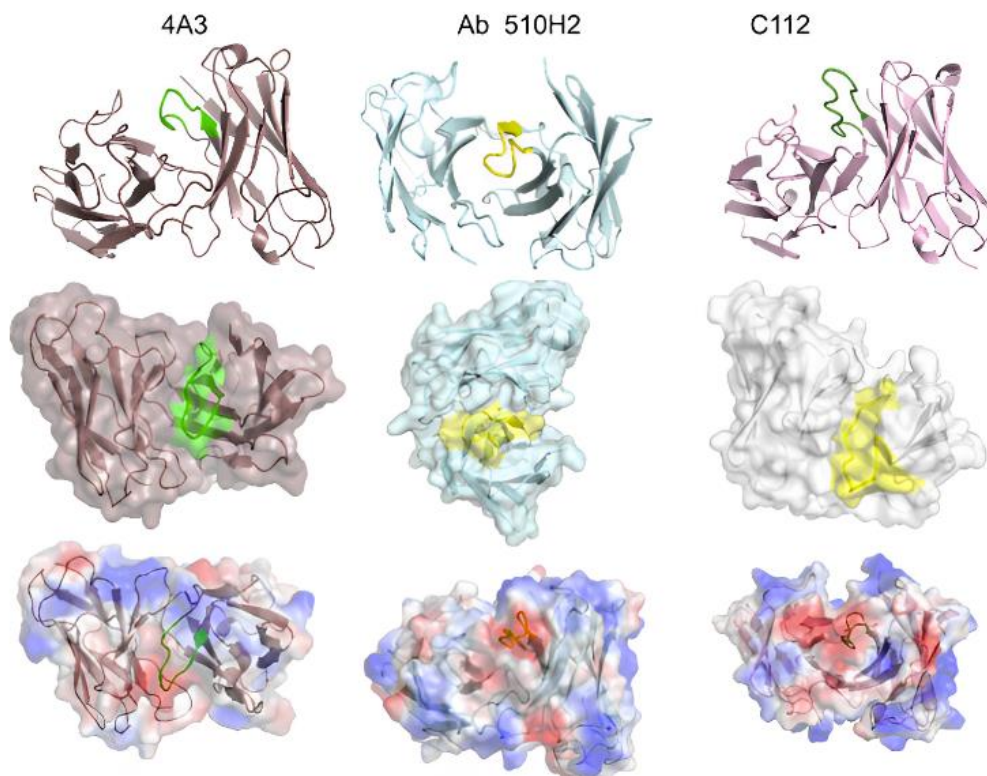
Heavy Chain Sequence Alignment Identity Matrix of 1E02, 1H06, and 2C02

|      | 2C02  | 1E02  | 1H06  |
|------|-------|-------|-------|
| 2C02 | —     | 76.27 | 73.68 |
| 1E02 | 76.27 | —     | 87.72 |
| 1H06 | 73.68 | 87.72 | —     |

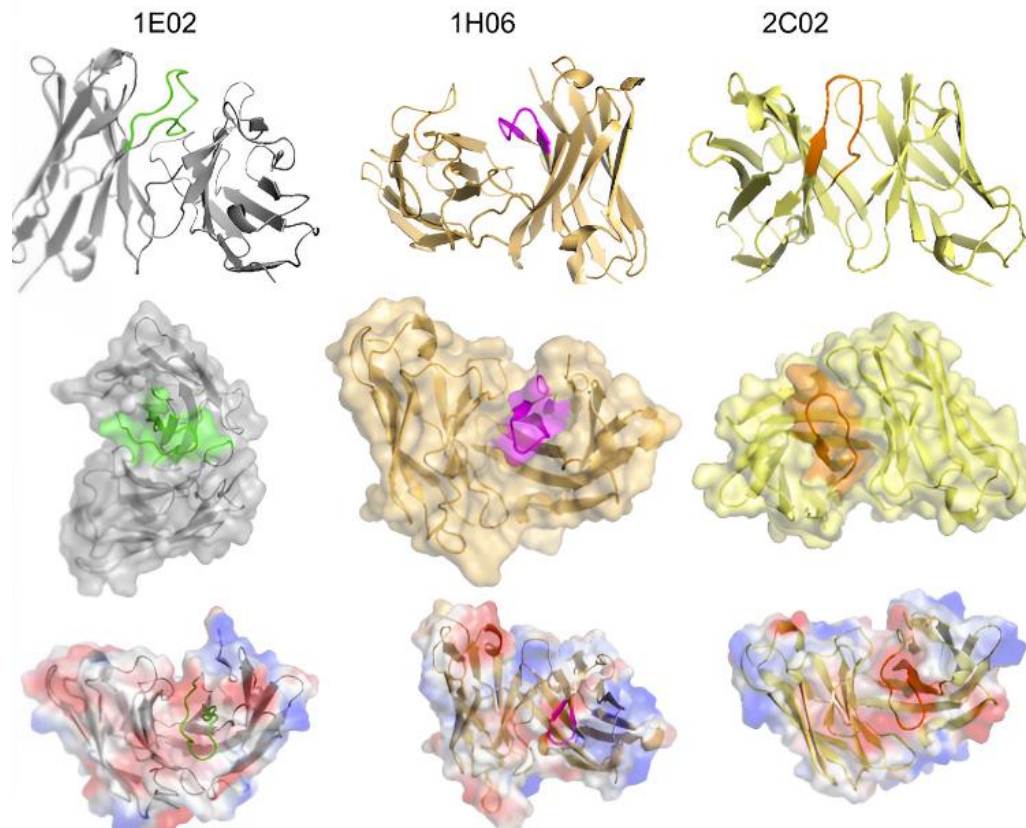
CDRH3 Sequence Alignment Identity Matrix of 1E02, 1H06, and 2C02

|      | 2C02  | 1E02  | 1H06  |
|------|-------|-------|-------|
| 2C02 | —     | 27.27 | 16.67 |
| 1E02 | 27.27 | —     | 28.57 |
| 1H06 | 16.67 | 28.57 | —     |

**Figure S5.** Matrix comparing the percent similarity of the heavy chain (top) and CDRH3 (bottom) sequences of mouse antibodies 1E02, 1H06, and 2C02.



**Figure S6.** The heavy chain structures of three human antibodies binding to RBD with the IGHV3 germline (4A3, Ab\_510H2, and C112) were modeled and the CDRH3 of each was highlighted in a different color. It is known that the CDRH3 length of 4A3 is 9 residues, of Ab\_510H2 is 11 residues, and of C112 is 14 residues. The basic structure, surface structure, and the electrostatic potential structure of the antibodies are shown.



**Figure S7.** The heavy chain structures of three mouse antibodies binding to RBD with the IGHV1 germline (1E02, 1H06, and 2C02) were modeled and the CDRH3 of each was highlighted in a different color. It is known that the CDRH3 length of 1E02 is 14 residues, of 1H06 is 7 residues, and of 2C02 is 11 residues. The basic structure, surface structure, and the electrostatic potential structure of the antibodies are shown.