

Supplementary Figure S2

a

| Docking peptide: | | mAb 2219 conformation: | | | | | | |
|------------------|-----|------------------------|------|------|--------------|--------------|--------------|----------------------|
| Start | End | 2B0S | 2B1A | 2B1H | 2B0S 2B1A | 2B1A 2B1H | 2B0S 2B1H | 2B0S 2B1A 2B1H |
| 10 | 21 | 0.95 | 0.87 | 0.92 | 0.94 | 0.91 | 0.96 | 0.95 |
| 10 | 20 | 0.93 | 0.87 | 0.89 | 0.90 | 0.87 | 0.91 | 0.89 |
| 10 | 19 | 0.93 | 0.87 | 0.89 | 0.91 | 0.88 | 0.92 | 0.91 |
| 10 | 18 | 0.95 | 0.91 | 0.91 | 0.94 | 0.92 | 0.94 | 0.94 |
| 10 | 17 | 0.94 | 0.91 | 0.86 | 0.93 | 0.90 | 0.94 | 0.93 |
| 10 | 16 | 0.94 | 0.92 | 0.91 | 0.95 | 0.93 | 0.94 | 0.95 |
| 10 | 15 | 0.94 | 0.93 | 0.92 | 0.95 | 0.94 | 0.95 | 0.95 |
| 10 | 14 | 0.94 | 0.93 | 0.93 | 0.95 | 0.94 | 0.95 | 0.95 |
| 10 | 13 | 0.96 | 0.92 | 0.92 | 0.94 | 0.91 | 0.94 | 0.93 |
| 9 | 20 | 0.91 | 0.89 | 0.88 | 0.90 | 0.89 | 0.91 | 0.91 |
| 9 | 19 | 0.91 | 0.87 | 0.90 | 0.90 | 0.88 | 0.91 | 0.90 |
| 9 | 18 | 0.91 | 0.90 | 0.91 | 0.91 | 0.91 | 0.92 | 0.92 |
| 9 | 17 | 0.91 | 0.89 | 0.89 | 0.91 | 0.90 | 0.92 | 0.92 |
| 9 | 16 | 0.90 | 0.89 | 0.89 | 0.90 | 0.90 | 0.91 | 0.91 |
| 9 | 15 | 0.91 | 0.90 | 0.89 | 0.91 | 0.91 | 0.91 | 0.91 |
| 9 | 14 | 0.90 | 0.90 | 0.89 | 0.91 | 0.90 | 0.91 | 0.91 |
| 9 | 13 | 0.94 | 0.91 | 0.92 | 0.92 | 0.91 | 0.93 | 0.92 |
| 8 | 19 | 0.92 | 0.91 | 0.88 | 0.92 | 0.91 | 0.91 | 0.92 |
| 8 | 18 | 0.91 | 0.91 | 0.90 | 0.91 | 0.91 | 0.91 | 0.91 |
| 8 | 17 | 0.91 | 0.91 | 0.86 | 0.92 | 0.91 | 0.91 | 0.92 |
| 8 | 16 | 0.91 | 0.91 | 0.85 | 0.92 | 0.91 | 0.91 | 0.91 |
| 8 | 15 | 0.90 | 0.91 | 0.87 | 0.91 | 0.91 | 0.90 | 0.91 |
| 8 | 14 | 0.91 | 0.92 | 0.89 | 0.92 | 0.92 | 0.91 | 0.92 |
| 8 | 13 | 0.95 | 0.93 | 0.90 | 0.94 | 0.93 | 0.94 | 0.94 |
| 7 | 18 | 0.91 | 0.90 | 0.86 | 0.92 | 0.91 | 0.91 | 0.92 |
| 7 | 17 | 0.91 | 0.88 | 0.81 | 0.92 | 0.89 | 0.91 | 0.92 |
| 7 | 16 | 0.91 | 0.87 | 0.85 | 0.92 | 0.91 | 0.91 | 0.91 |
| 7 | 15 | 0.90 | 0.87 | 0.85 | 0.91 | 0.90 | 0.91 | 0.92 |
| 7 | 14 | 0.90 | 0.88 | 0.83 | 0.91 | 0.90 | 0.90 | 0.91 |
| 7 | 13 | 0.94 | 0.87 | 0.88 | 0.94 | 0.91 | 0.94 | 0.94 |
| 6 | 17 | 0.90 | 0.88 | 0.77 | 0.91 | 0.87 | 0.90 | 0.91 |
| 6 | 16 | 0.91 | 0.87 | 0.79 | 0.91 | 0.87 | 0.91 | 0.91 |
| 6 | 15 | 0.90 | 0.88 | 0.81 | 0.91 | 0.89 | 0.91 | 0.91 |
| 6 | 14 | 0.92 | 0.88 | 0.83 | 0.92 | 0.90 | 0.92 | 0.93 |
| 6 | 13 | 0.94 | 0.81 | 0.87 | 0.93 | 0.85 | 0.94 | 0.93 |
| 5 | 16 | 0.92 | 0.86 | 0.79 | 0.92 | 0.86 | 0.92 | 0.92 |
| 5 | 15 | 0.91 | 0.82 | 0.80 | 0.92 | 0.87 | 0.91 | 0.92 |
| 5 | 14 | 0.91 | 0.85 | 0.79 | 0.92 | 0.87 | 0.91 | 0.92 |
| 5 | 13 | 0.93 | 0.79 | 0.81 | 0.92 | 0.82 | 0.93 | 0.92 |
| 4 | 15 | 0.88 | 0.84 | 0.77 | 0.89 | 0.85 | 0.89 | 0.90 |
| 4 | 14 | 0.90 | 0.81 | 0.76 | 0.90 | 0.84 | 0.90 | 0.90 |
| 4 | 13 | 0.92 | 0.86 | 0.76 | 0.93 | 0.87 | 0.93 | 0.93 |
| 3 | 14 | 0.81 | 0.78 | 0.75 | 0.85 | 0.78 | 0.85 | 0.86 |
| 3 | 13 | 0.82 | 0.69 | 0.71 | 0.83 | 0.71 | 0.85 | 0.84 |
| 2 | 13 | 0.73 | 0.57 | 0.70 | 0.70 | 0.62 | 0.75 | 0.74 |

b

| Docking peptide: | | mAb 2219 conformation: | | | | | | |
|------------------|-----|------------------------|------|------|--------------|--------------|--------------|----------------------|
| Start | End | 2B0S | 2B1A | 2B1H | 2B0S 2B1A | 2B1A 2B1H | 2B0S 2B1H | 2B0S 2B1A 2B1H |
| 10 | 21 | 0.03 | 0.05 | 0.04 | 0.03 | 0.04 | 0.03 | 0.03 |
| 10 | 20 | 0.04 | 0.07 | 0.06 | 0.05 | 0.07 | 0.05 | 0.06 |
| 10 | 19 | 0.04 | 0.06 | 0.05 | 0.04 | 0.05 | 0.04 | 0.04 |
| 10 | 18 | 0.03 | 0.04 | 0.04 | 0.03 | 0.04 | 0.03 | 0.03 |
| 10 | 17 | 0.03 | 0.05 | 0.06 | 0.04 | 0.05 | 0.03 | 0.04 |
| 10 | 16 | 0.03 | 0.04 | 0.04 | 0.03 | 0.04 | 0.03 | 0.03 |
| 10 | 15 | 0.03 | 0.03 | 0.04 | 0.03 | 0.03 | 0.03 | 0.03 |
| 10 | 14 | 0.03 | 0.03 | 0.03 | 0.03 | 0.03 | 0.03 | 0.03 |
| 10 | 13 | 0.03 | 0.04 | 0.04 | 0.03 | 0.04 | 0.03 | 0.03 |
| 9 | 20 | 0.04 | 0.05 | 0.05 | 0.04 | 0.05 | 0.04 | 0.04 |
| 9 | 19 | 0.04 | 0.05 | 0.04 | 0.04 | 0.05 | 0.04 | 0.04 |
| 9 | 18 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 |
| 9 | 17 | 0.04 | 0.05 | 0.05 | 0.04 | 0.04 | 0.04 | 0.04 |
| 9 | 16 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 |
| 9 | 15 | 0.04 | 0.04 | 0.05 | 0.04 | 0.04 | 0.04 | 0.04 |
| 9 | 14 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 |
| 9 | 13 | 0.03 | 0.04 | 0.04 | 0.03 | 0.04 | 0.03 | 0.03 |
| 8 | 19 | 0.04 | 0.04 | 0.05 | 0.04 | 0.04 | 0.04 | 0.04 |
| 8 | 18 | 0.04 | 0.04 | 0.05 | 0.04 | 0.04 | 0.04 | 0.04 |
| 8 | 17 | 0.04 | 0.04 | 0.06 | 0.04 | 0.04 | 0.04 | 0.04 |
| 8 | 16 | 0.04 | 0.04 | 0.06 | 0.04 | 0.04 | 0.04 | 0.04 |
| 8 | 15 | 0.04 | 0.04 | 0.06 | 0.04 | 0.04 | 0.04 | 0.04 |
| 8 | 14 | 0.04 | 0.04 | 0.05 | 0.04 | 0.04 | 0.04 | 0.04 |
| 8 | 13 | 0.03 | 0.03 | 0.05 | 0.03 | 0.03 | 0.03 | 0.03 |
| 7 | 18 | 0.04 | 0.04 | 0.06 | 0.04 | 0.04 | 0.04 | 0.04 |
| 7 | 17 | 0.04 | 0.05 | 0.08 | 0.04 | 0.05 | 0.05 | 0.04 |
| 7 | 16 | 0.04 | 0.05 | 0.06 | 0.04 | 0.04 | 0.04 | 0.04 |
| 7 | 15 | 0.04 | 0.05 | 0.06 | 0.04 | 0.05 | 0.04 | 0.04 |
| 7 | 14 | 0.04 | 0.05 | 0.07 | 0.04 | 0.05 | 0.04 | 0.04 |
| 7 | 13 | 0.03 | 0.05 | 0.05 | 0.03 | 0.04 | 0.03 | 0.03 |
| 6 | 17 | 0.05 | 0.05 | 0.09 | 0.04 | 0.06 | 0.05 | 0.04 |
| 6 | 16 | 0.04 | 0.05 | 0.08 | 0.04 | 0.05 | 0.04 | 0.04 |
| 6 | 15 | 0.05 | 0.04 | 0.08 | 0.04 | 0.04 | 0.04 | 0.04 |
| 6 | 14 | 0.04 | 0.05 | 0.07 | 0.04 | 0.05 | 0.04 | 0.04 |
| 6 | 13 | 0.03 | 0.06 | 0.05 | 0.03 | 0.06 | 0.03 | 0.03 |
| 5 | 16 | 0.04 | 0.05 | 0.08 | 0.04 | 0.06 | 0.04 | 0.04 |
| 5 | 15 | 0.04 | 0.06 | 0.07 | 0.04 | 0.06 | 0.04 | 0.04 |
| 5 | 14 | 0.04 | 0.06 | 0.08 | 0.04 | 0.06 | 0.04 | 0.04 |
| 5 | 13 | 0.03 | 0.07 | 0.07 | 0.04 | 0.07 | 0.03 | 0.04 |
| 4 | 15 | 0.05 | 0.06 | 0.09 | 0.05 | 0.06 | 0.05 | 0.05 |
| 4 | 14 | 0.04 | 0.06 | 0.09 | 0.04 | 0.06 | 0.04 | 0.04 |
| 4 | 13 | 0.04 | 0.05 | 0.08 | 0.03 | 0.05 | 0.04 | 0.03 |
| 3 | 14 | 0.06 | 0.08 | 0.09 | 0.06 | 0.08 | 0.06 | 0.06 |
| 3 | 13 | 0.06 | 0.08 | 0.09 | 0.06 | 0.08 | 0.05 | 0.05 |
| 2 | 13 | 0.08 | 0.11 | 0.09 | 0.07 | 0.10 | 0.08 | 0.07 |