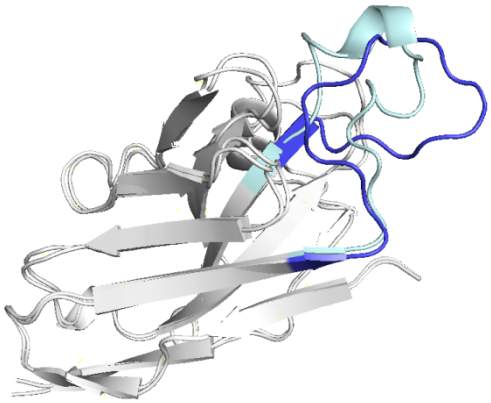
Supplementary Figure 1. High outlier (3k3q) in CDR1 by AlphaFold2



Blue: AlphaFold2 in CDR1.

Cyan: Experimental results in CDR1.

White: Experimental results in other parts.

Supplementary Figure 2. Boxplot of CDR-lengths and correlation on CDR-RMSD, CDR-RMSD_avg and VHH-RMSD

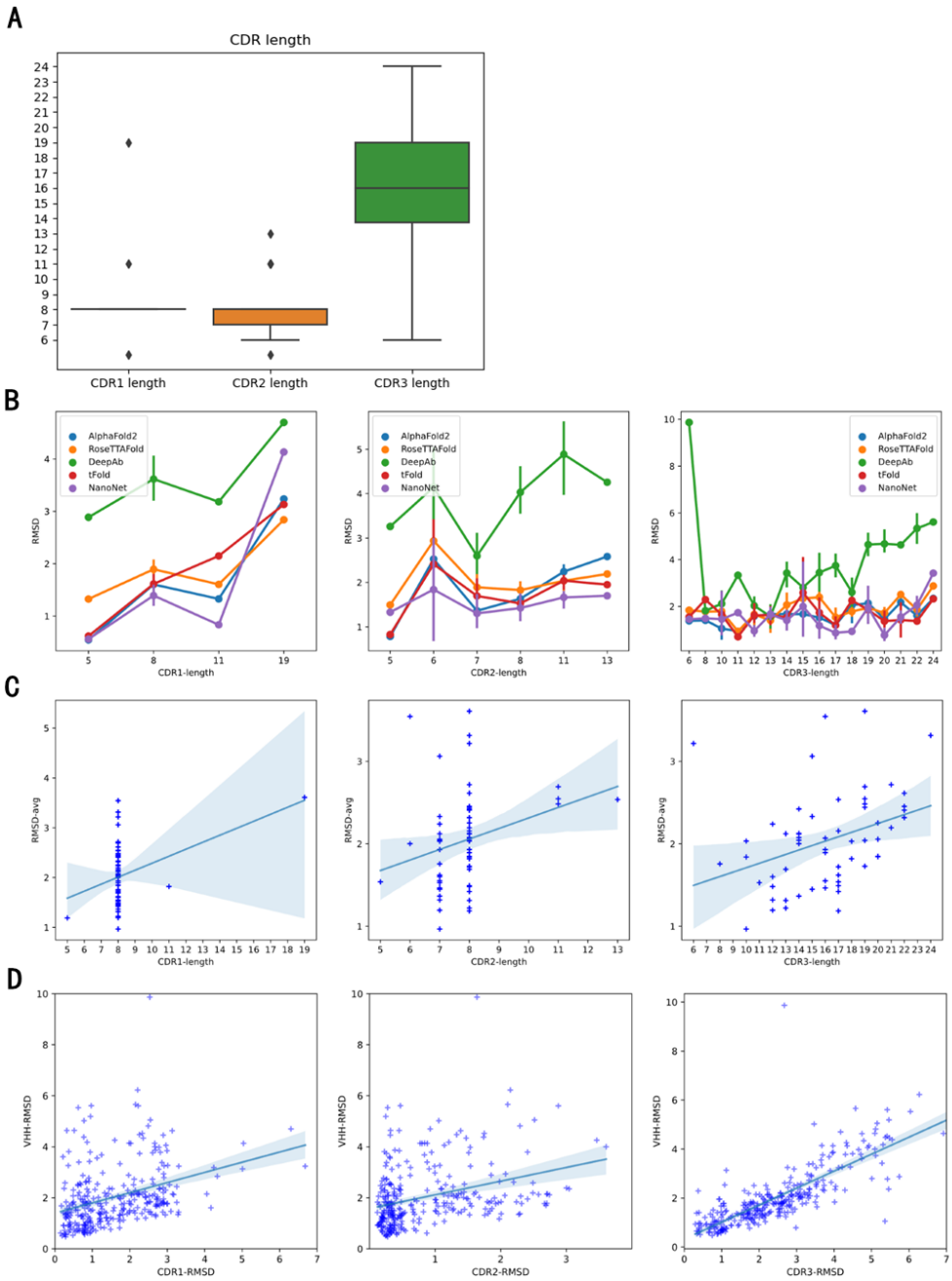


Figure A: Boxplot of the length of CDR1, CDR2 and CDR3.

Figure B: Line graph of the length of each type of CDR with the mean RMSD value of each VHH by the five algorithms.

Figure C: Comparison of the length of each CDR with the average RMSD value of each nanobodies obtained by the five algorithms in the scatter plot.

Figure D: Comparison of the average RMSD value of each CDR obtained by the five algorithms with the average RMSD value of each VHH obtained by the five algorithms in the scatter plot.

Supplementary Figure 3. Visualization comparison

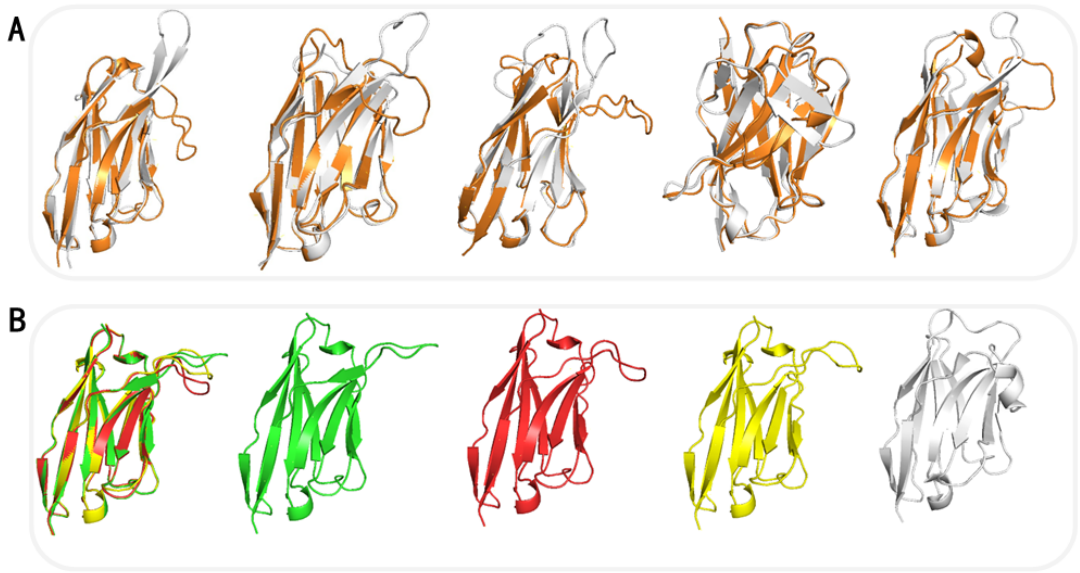
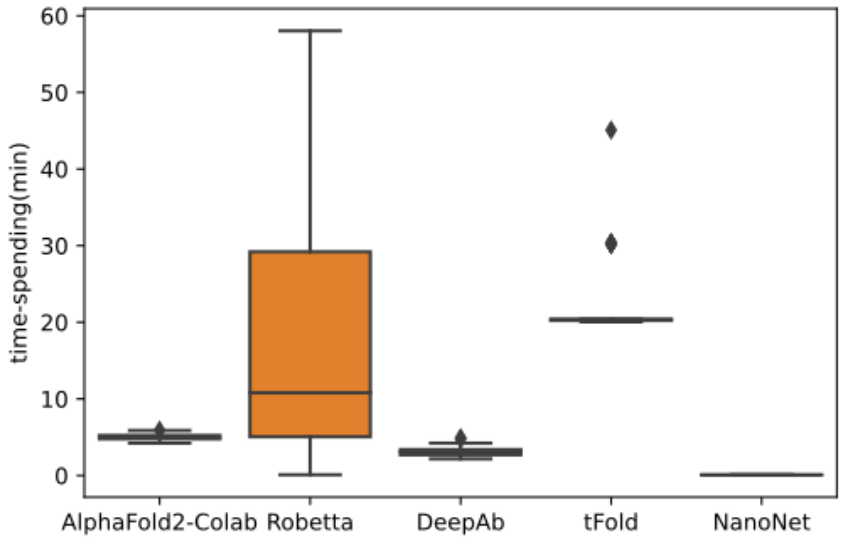


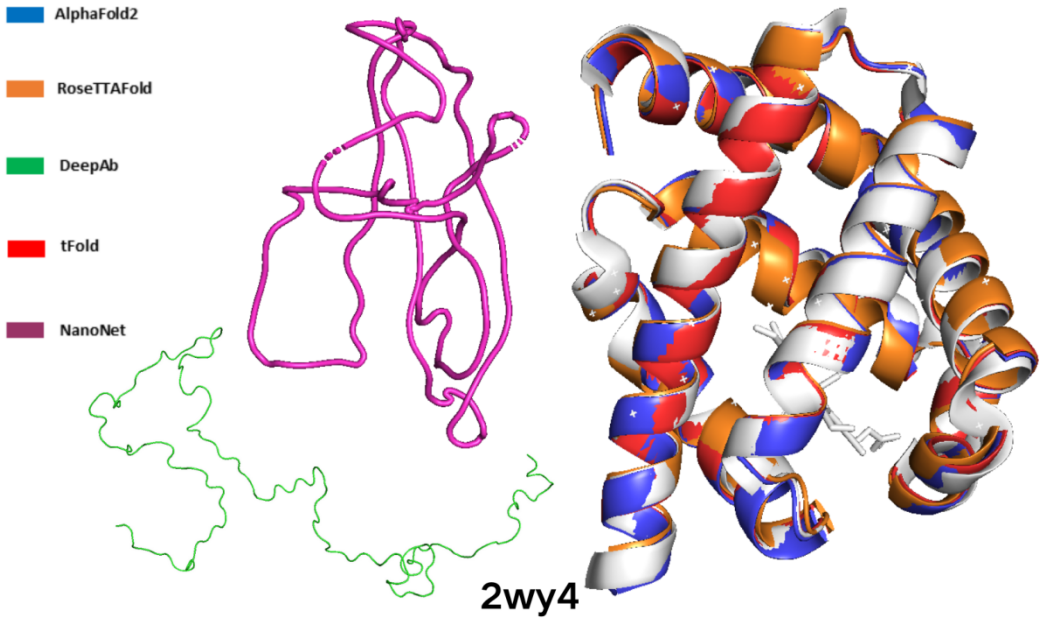
Figure A: Inaccuracy of RoseTTAFold predictions on β-turn structures (or structures similar to the β-turns) of the CDR3 loop (from left to right: 4idl, 4b50, 1kxv, 4hep, 5hvf).

Figure B: Uncertainty of DeepAb's 3 times prediction results for the same sequence (first time in green, second time in red and third time in yellow) compared with the experimental results (white).

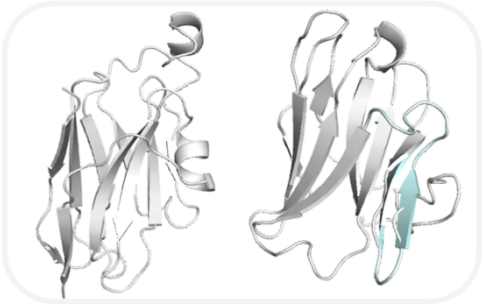
Supplementary Figure 4. Boxplot of time-spending of each platform



Supplementary Figure 5. Haemoglobin (PDB ID: 2wy4) as the input of the five algorithms to test the robustness of each algorithm



Supplementary Figure 6. Comparison of the visualization of the whole-atom structure and the structure with only the Cα atom



In the first picture, the visualization of the two structures overlaps completely. In the second picture, the visualization of the all-atom (white) structure differs in a lesser extent from that of the Cα-only structure in the light cyan area.