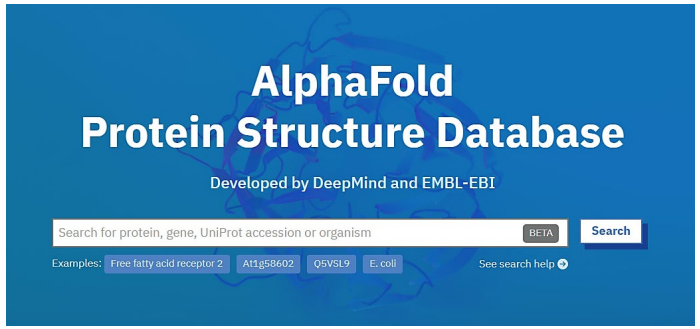
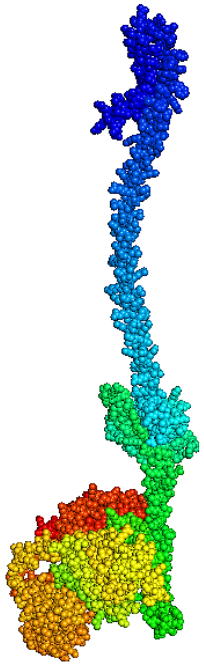
A https://alphafold.ebi.ac.uk/

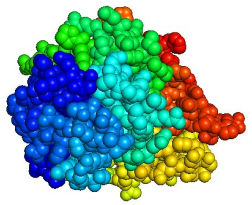


Monomeric structures



ArcB

ArcB full model docking



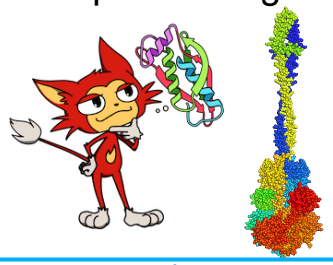
ArcA

Sequence analysis, leucine zipper.

ArcA or ArcB sequence

C

D AlphaFold2 in collaborative environment
Generation of multimer models and protein fragments



PAS domain docking

E Structural alignment of proteins, protein fragments and protein motif analysis

F Visualization

B Cavity-detection docking using anaerobic metabolites

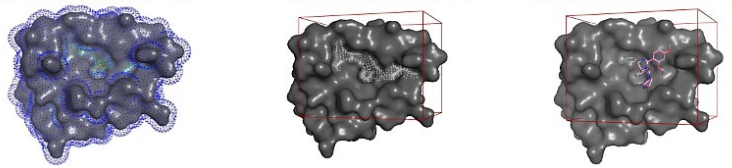
PubChem

http://clab.labshare.cn/cb-dock/php/blinddock.php

CB-Dock

Cavity-detection guided Blind Docking

Curvature of protein surface *Cavity detected by clustering* *Docking with AutoDock Vina*

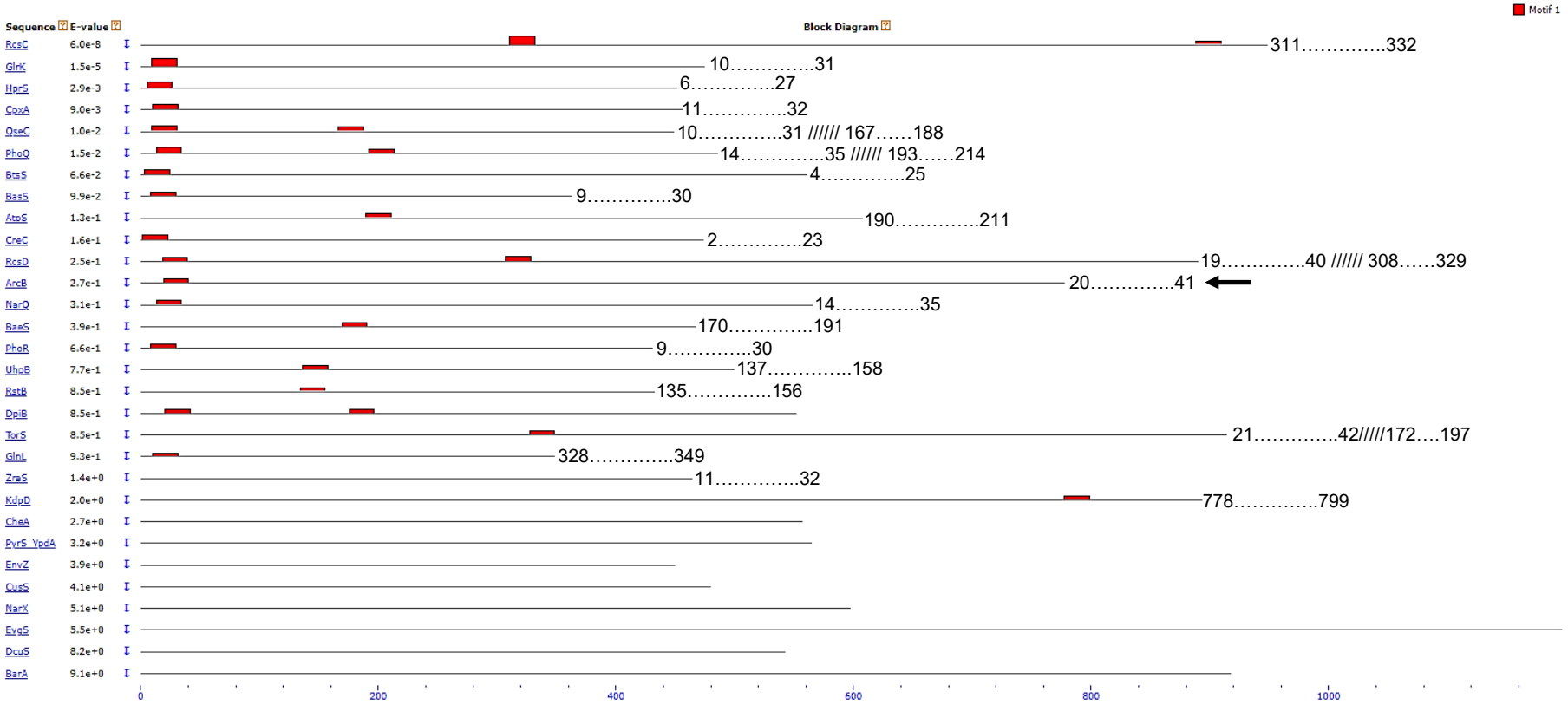


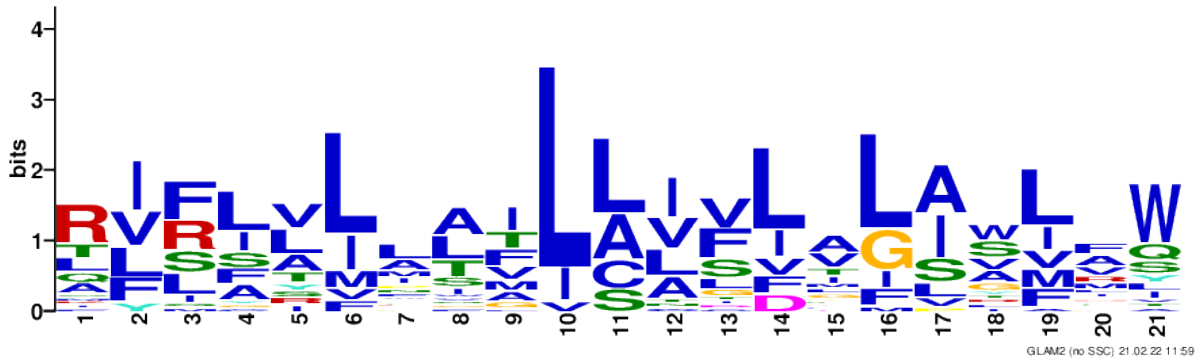
Anaerobic metabolites physiochemical characteristics

MolCalc

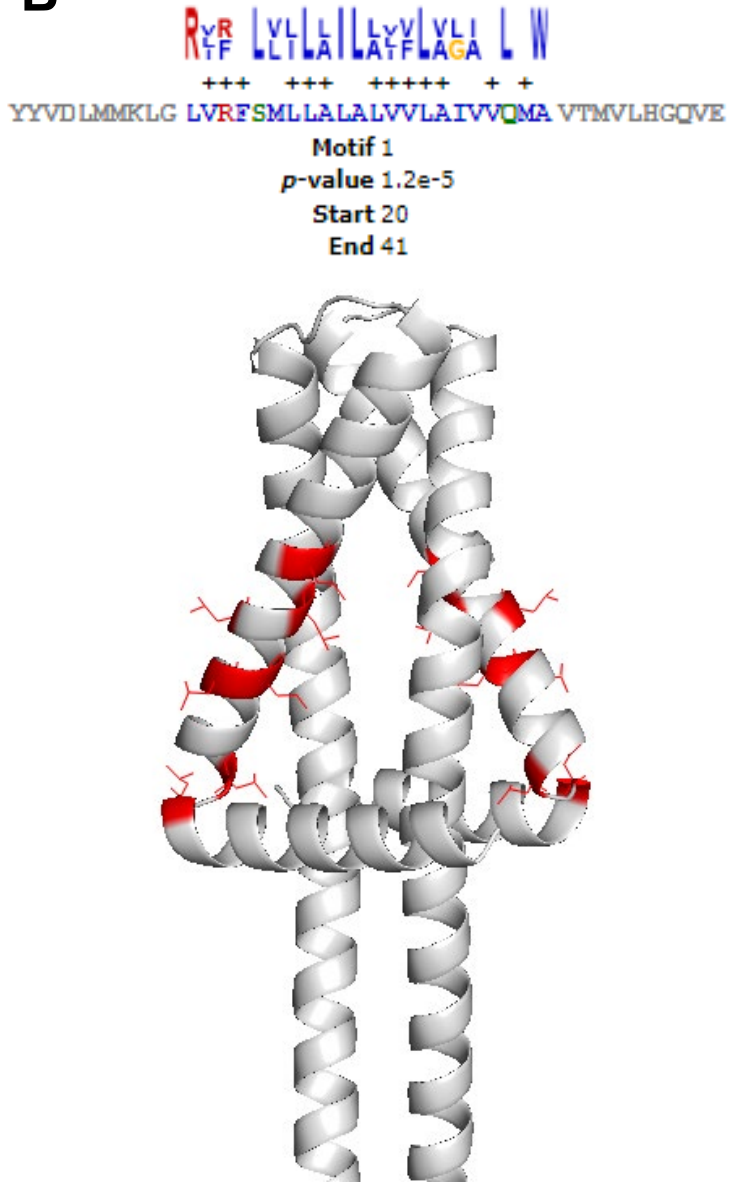
Supplementary Figure 1

A

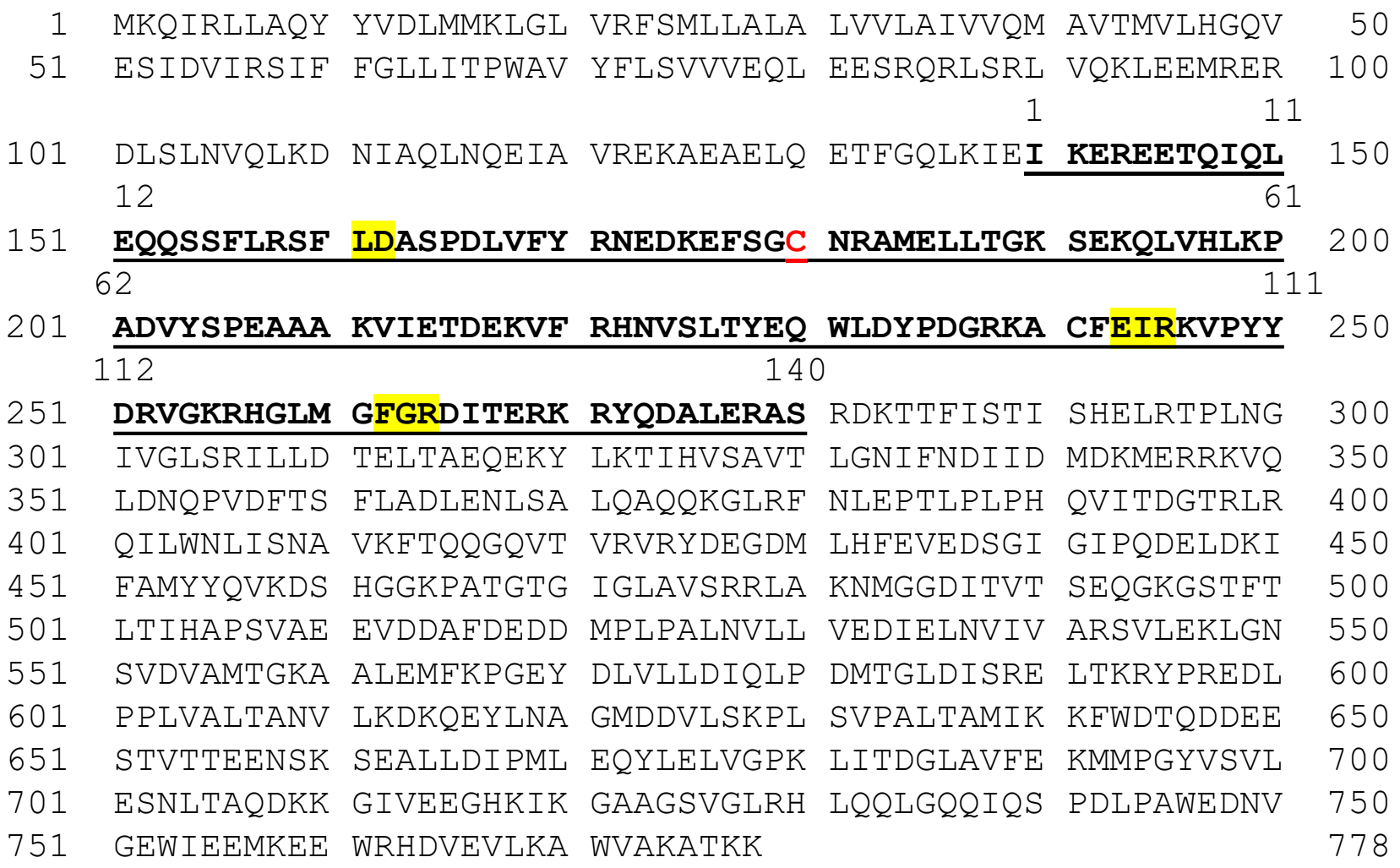




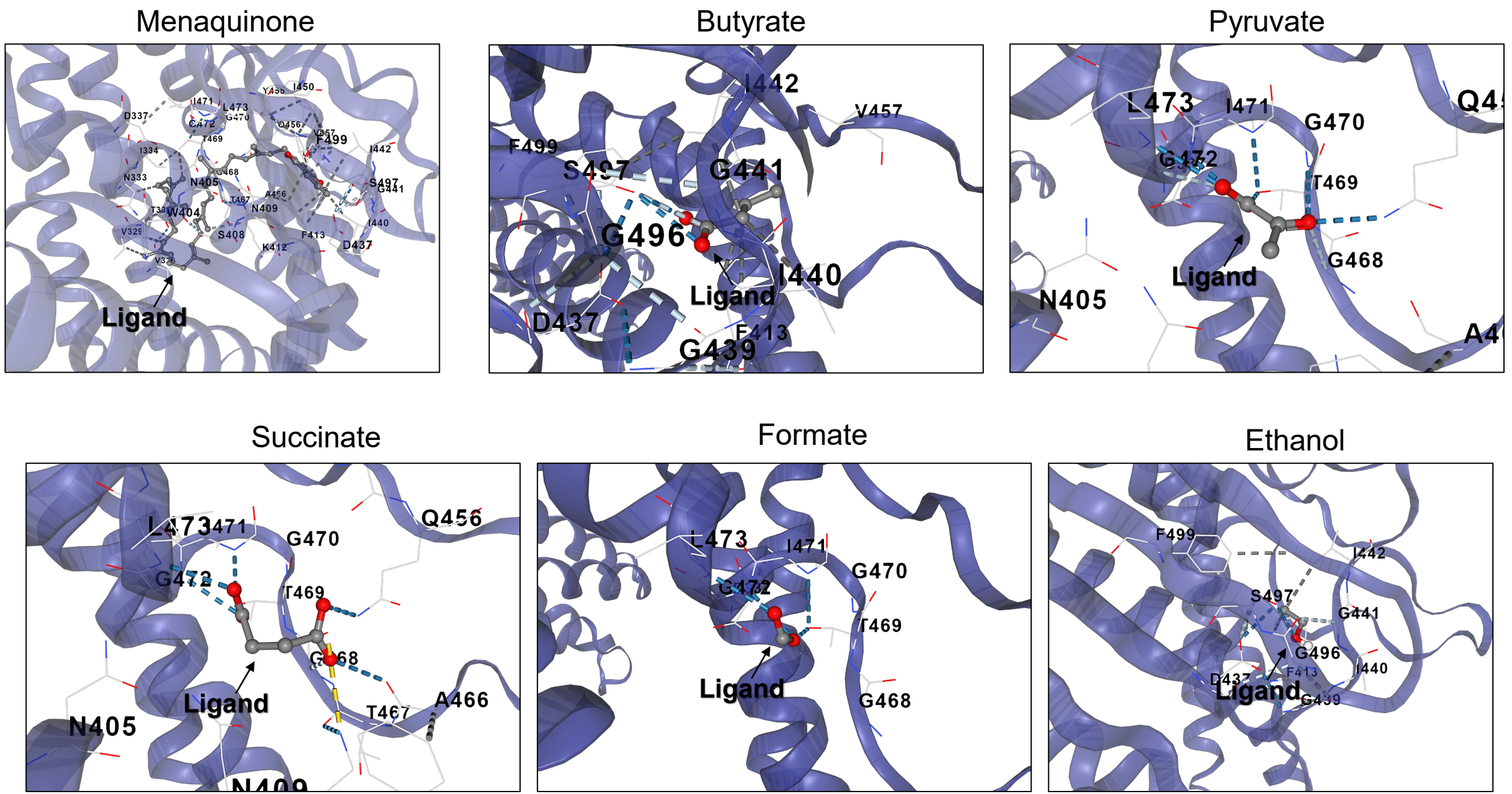
B



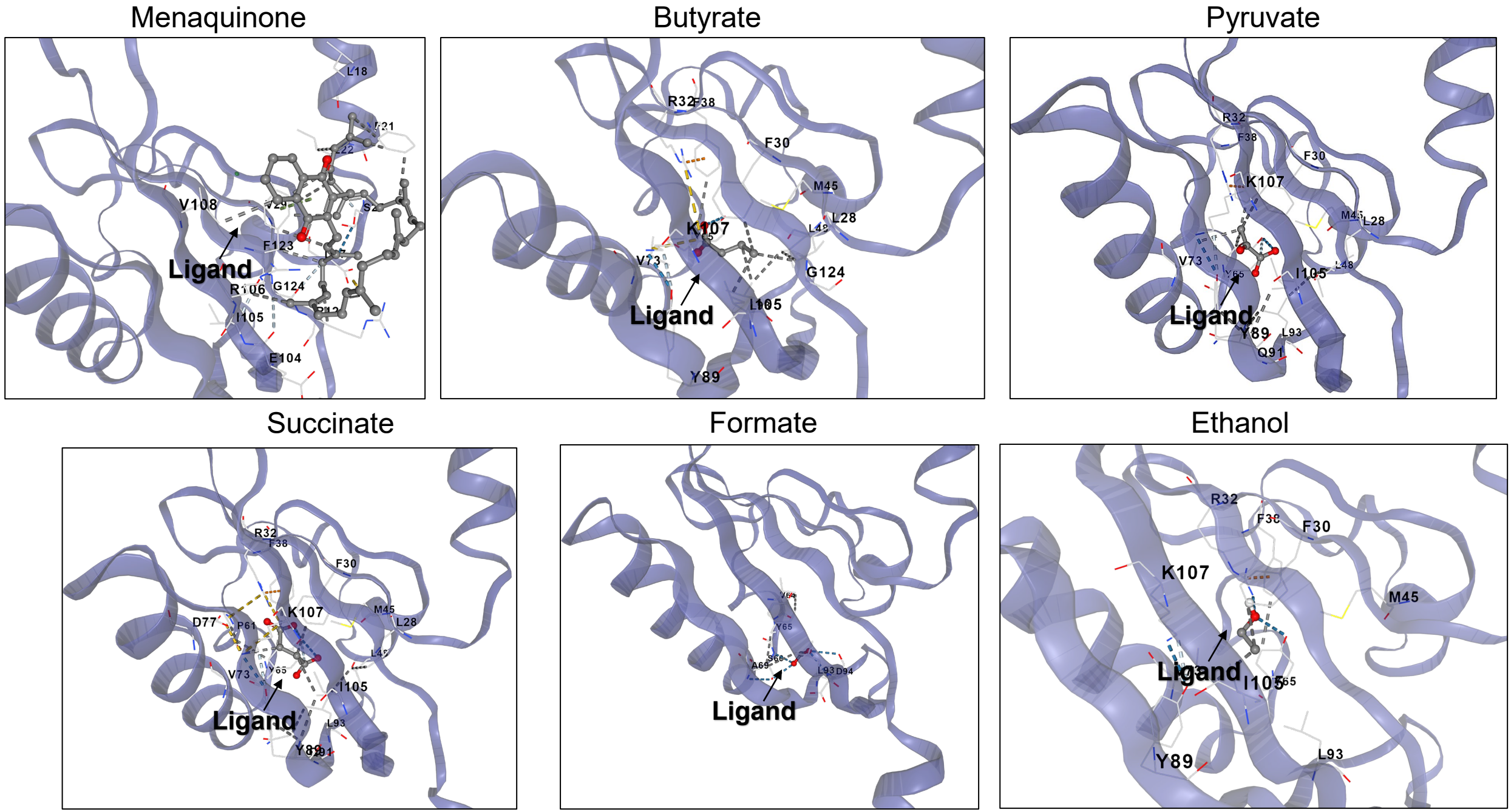
Supplementary Figure 2



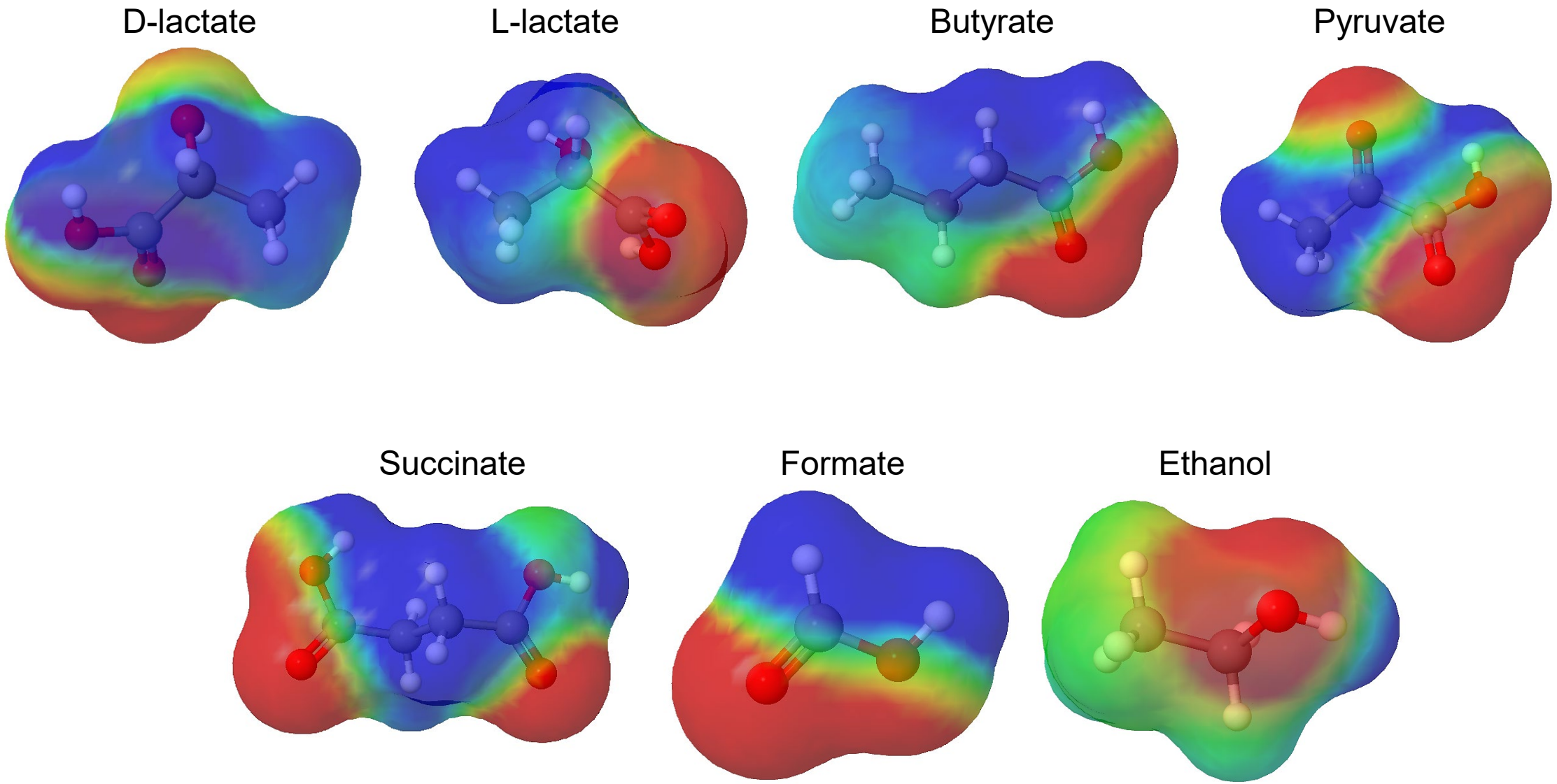
Supplementary Figure 3



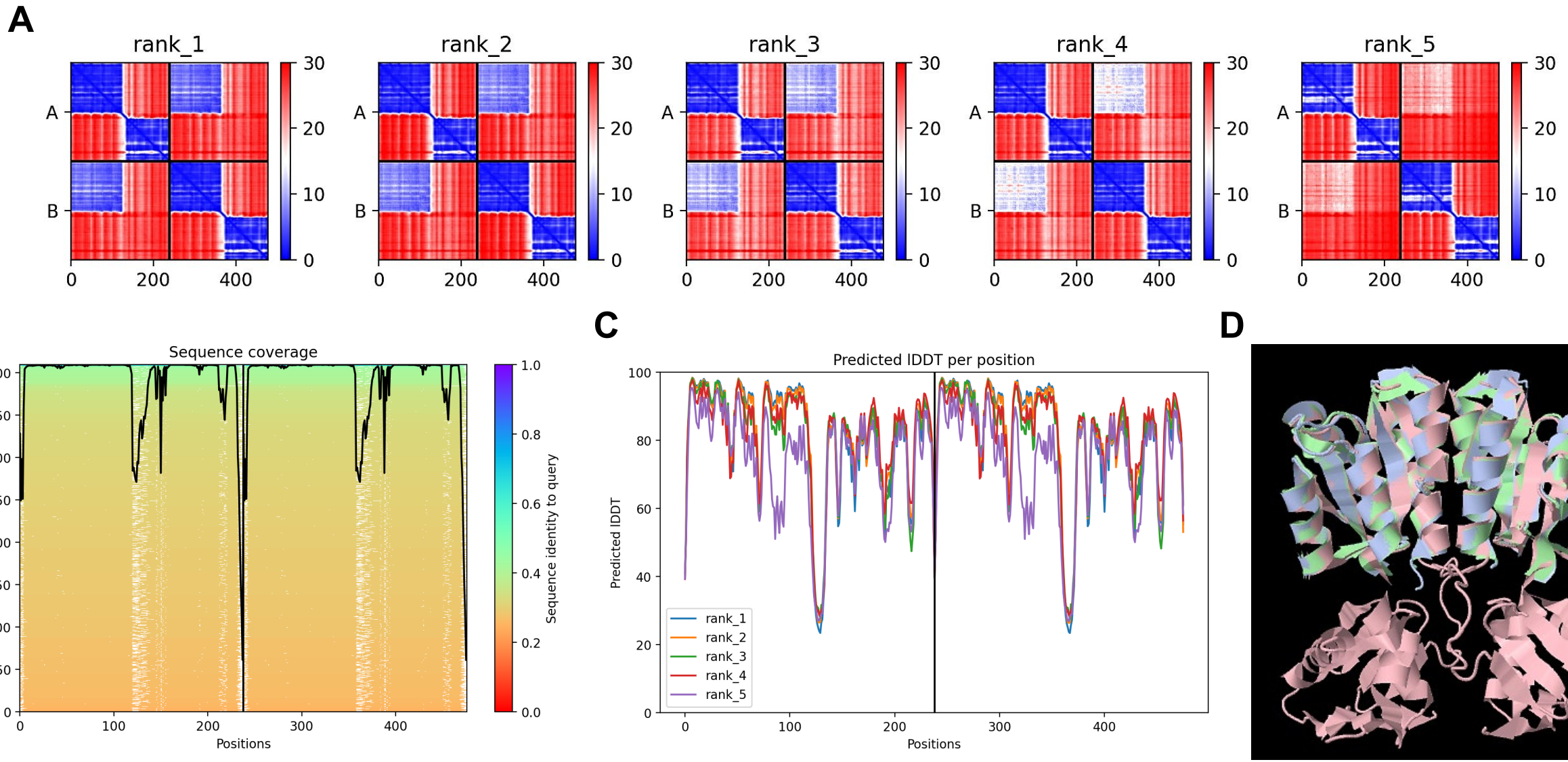
Supplementary Figure 4



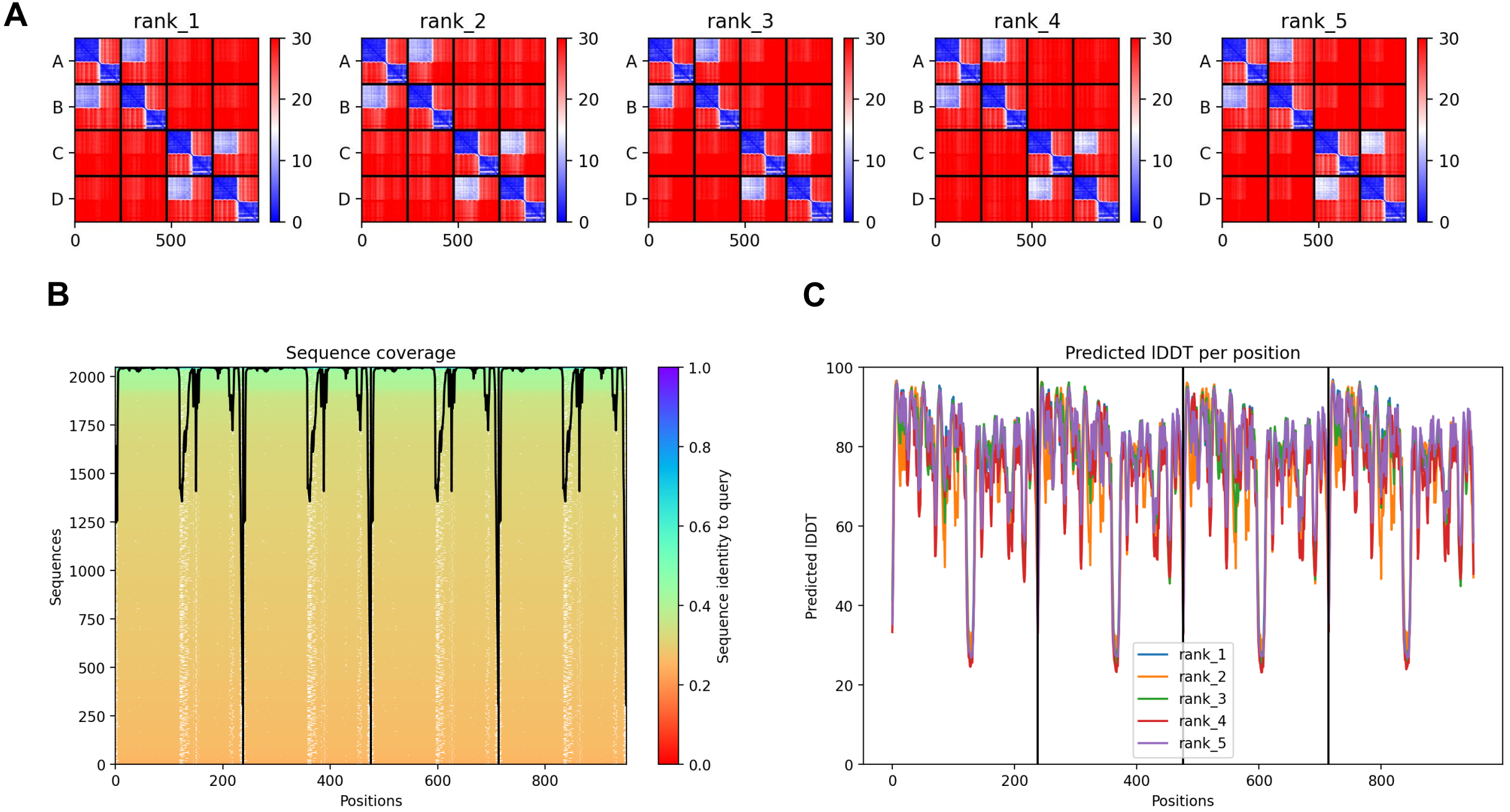
Supplementary Figure 5



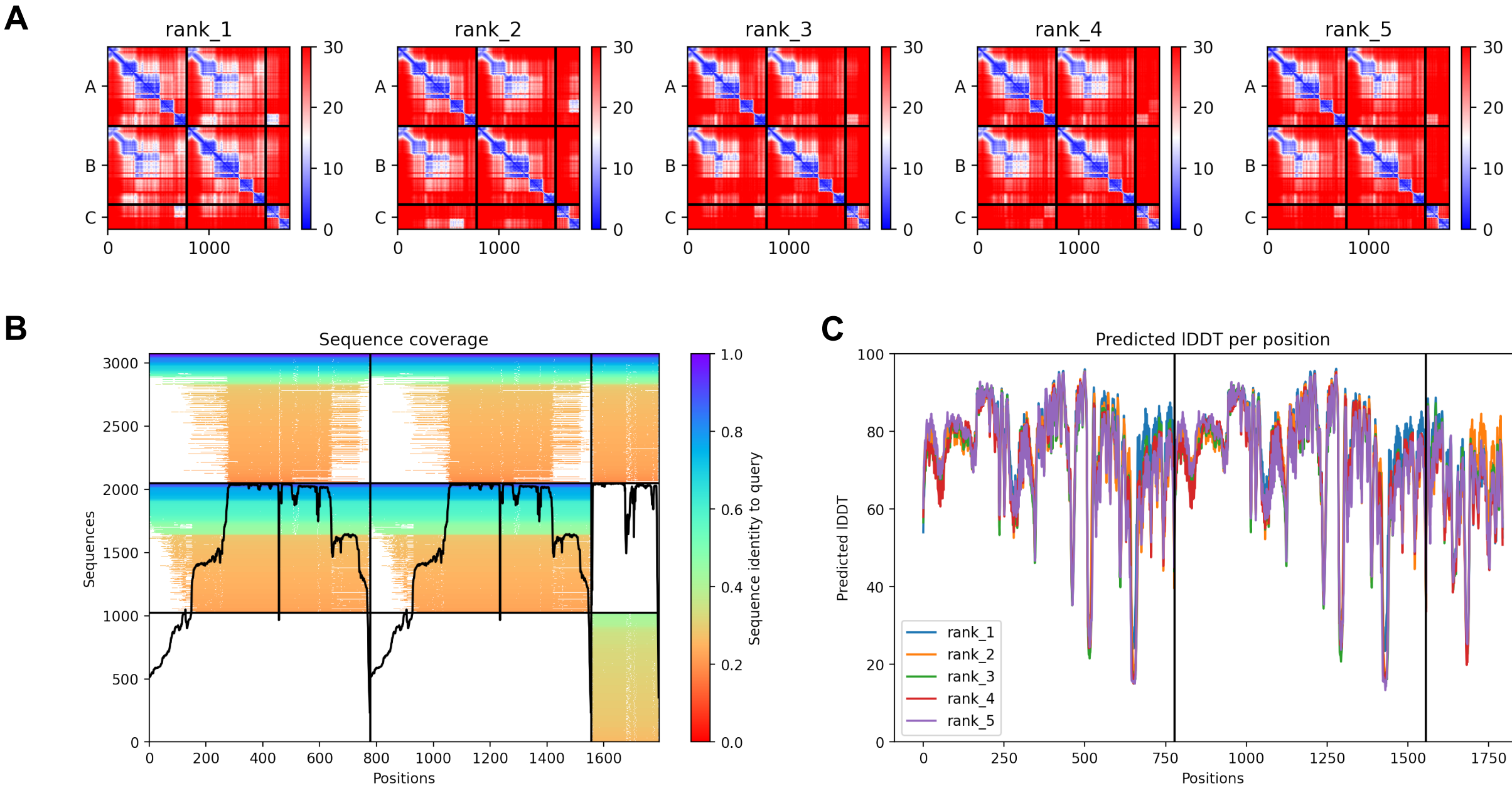
Supplementary Figure 6



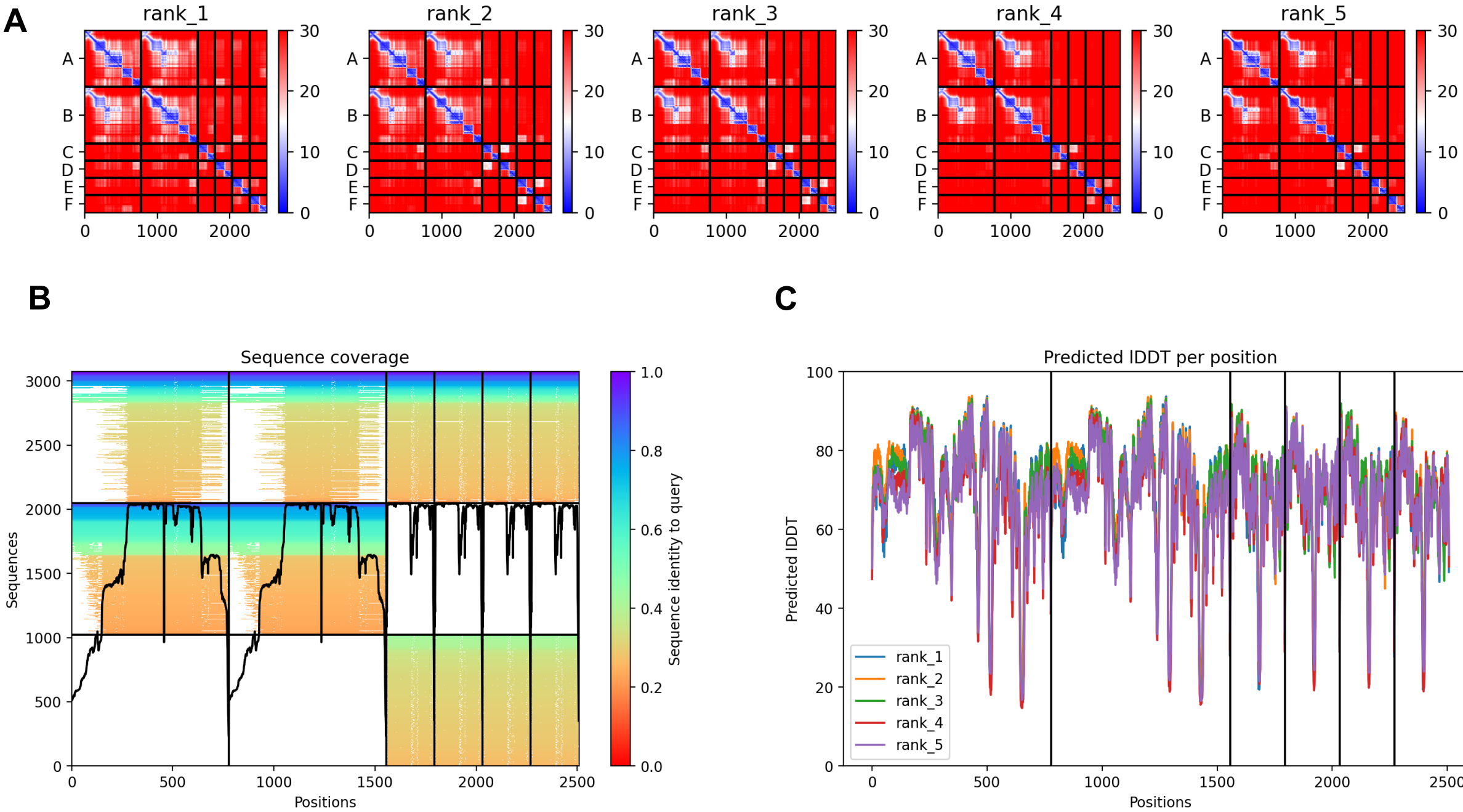
Supplementary Figure 7



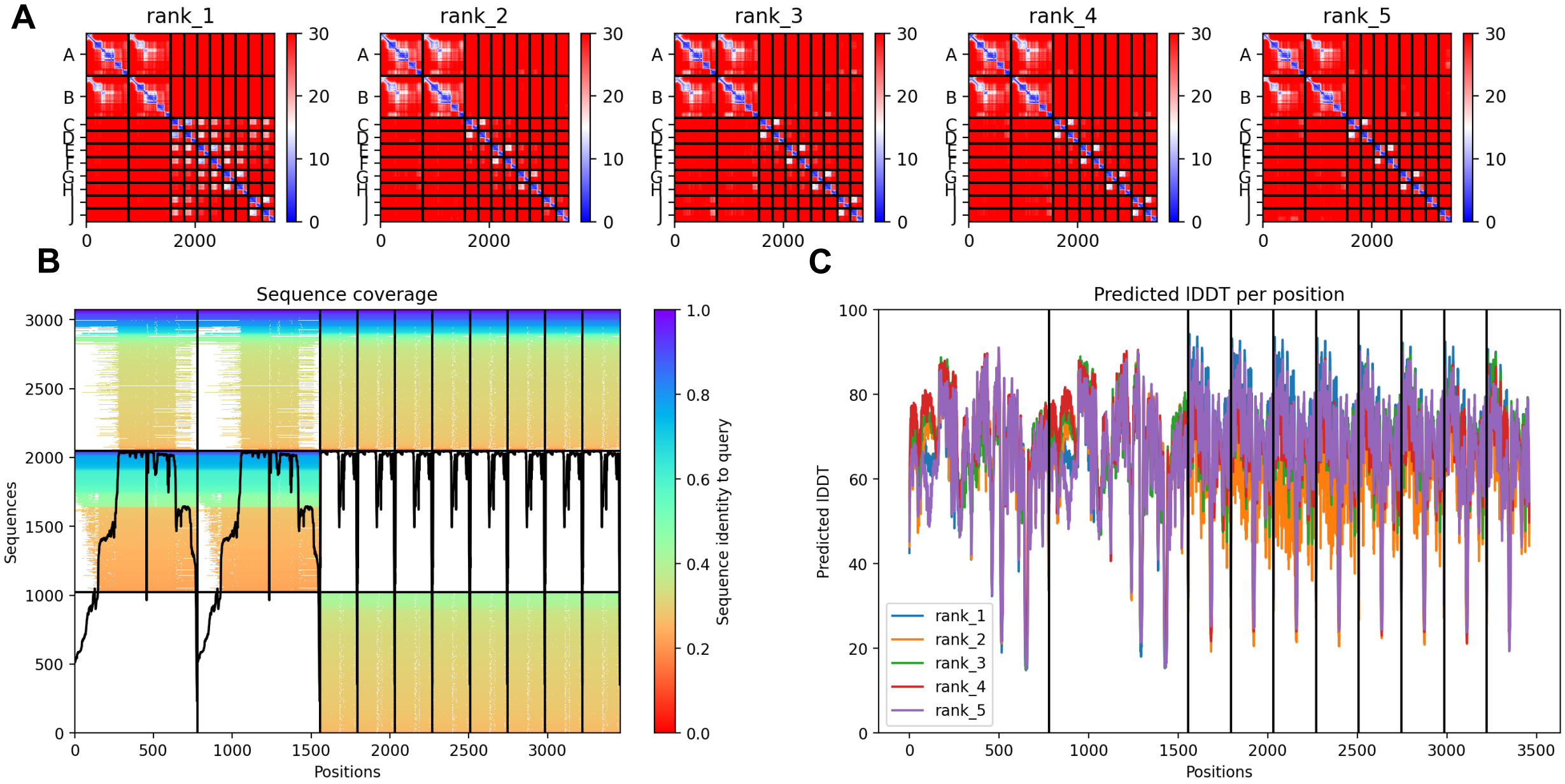
Supplementary Figure 8



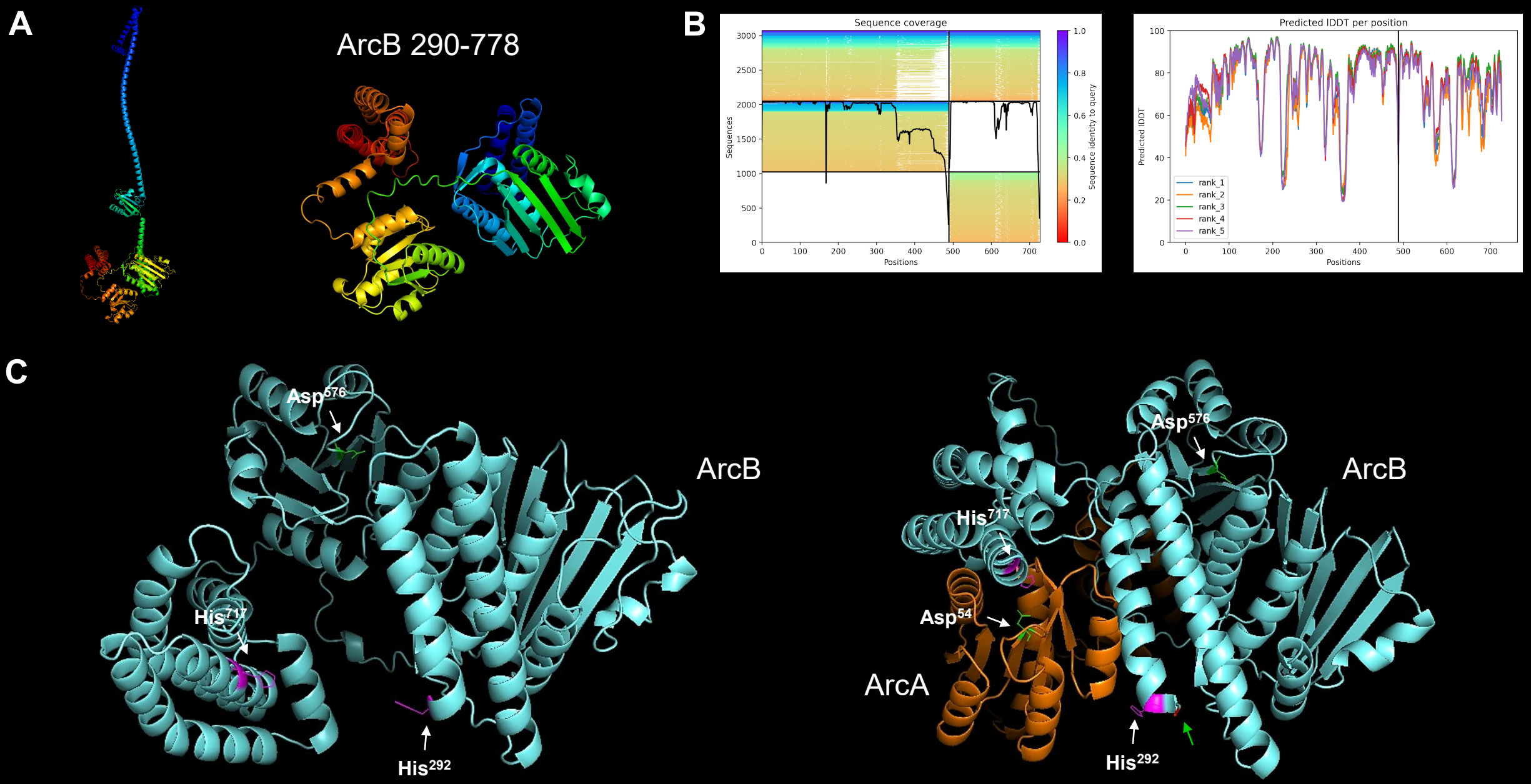
Supplementary Figure 9



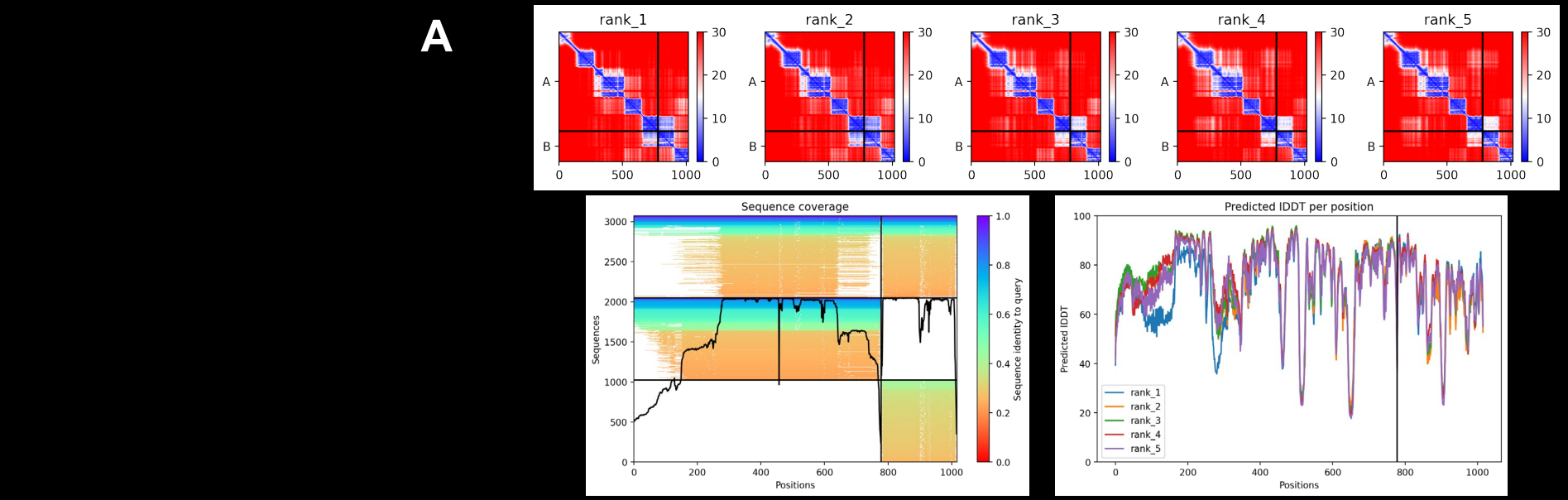
Supplementary Figure 10

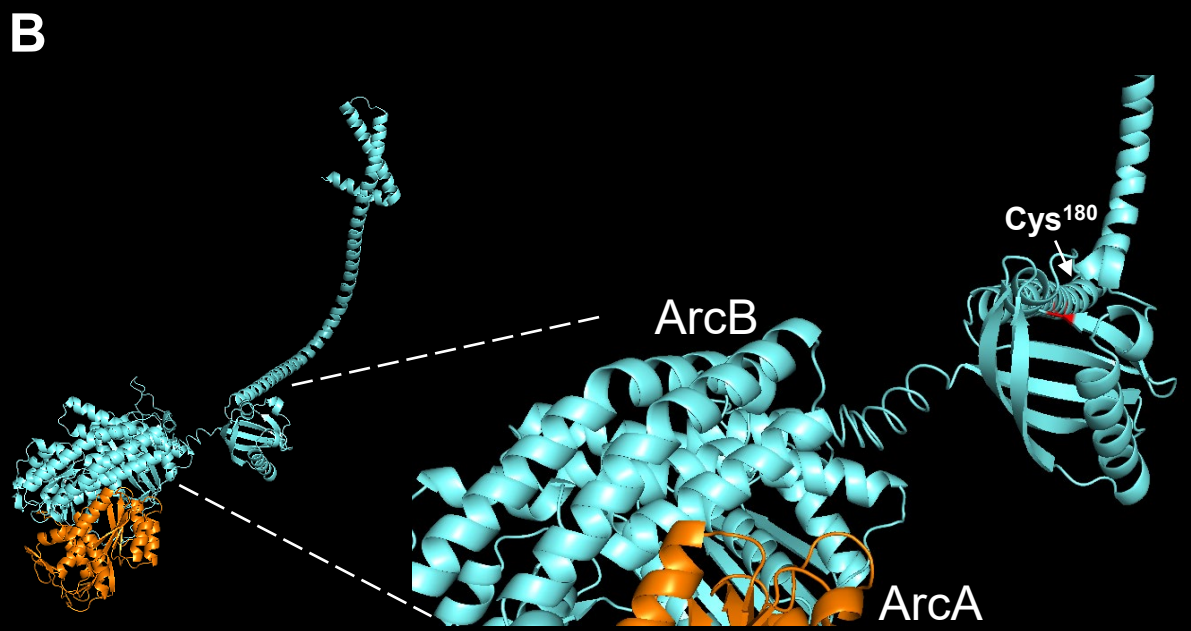


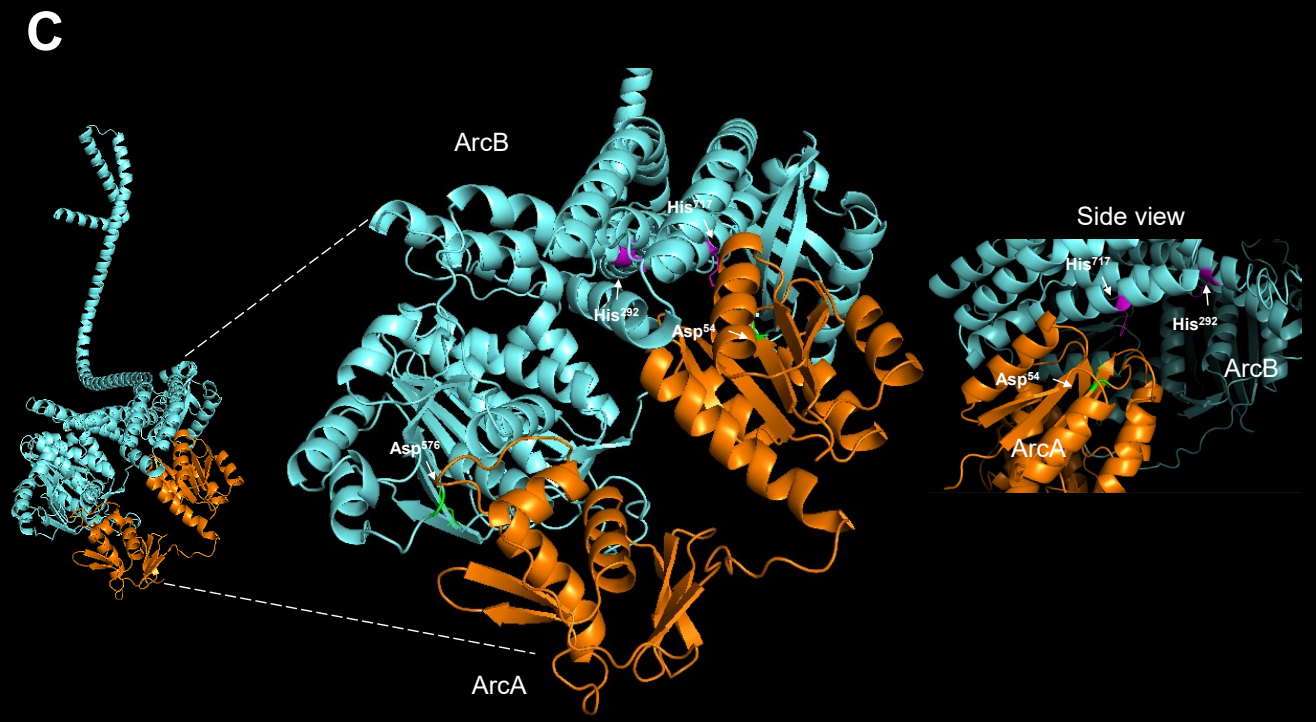
Supplementary Figure 11



Supplementary Figure 12







Supplementary Figure 13