Redefining bacterial Wzy polymerase families via three-dimensional structure-based clustering

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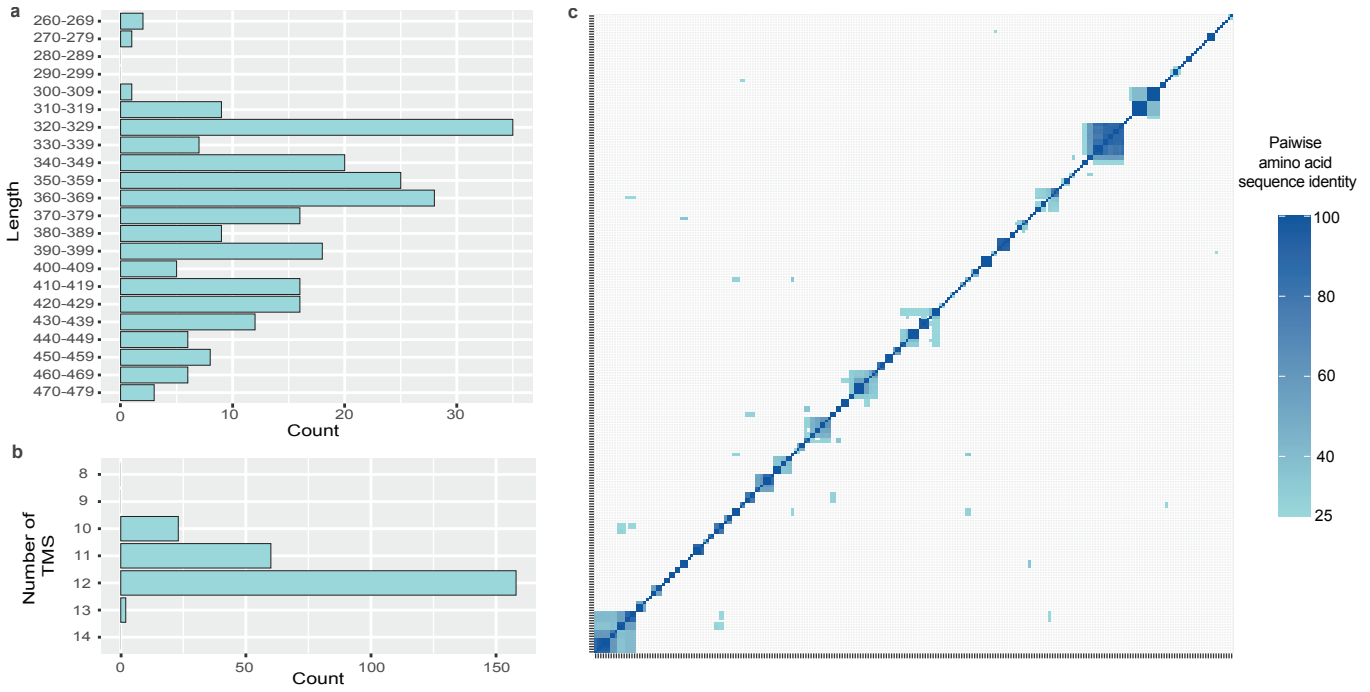
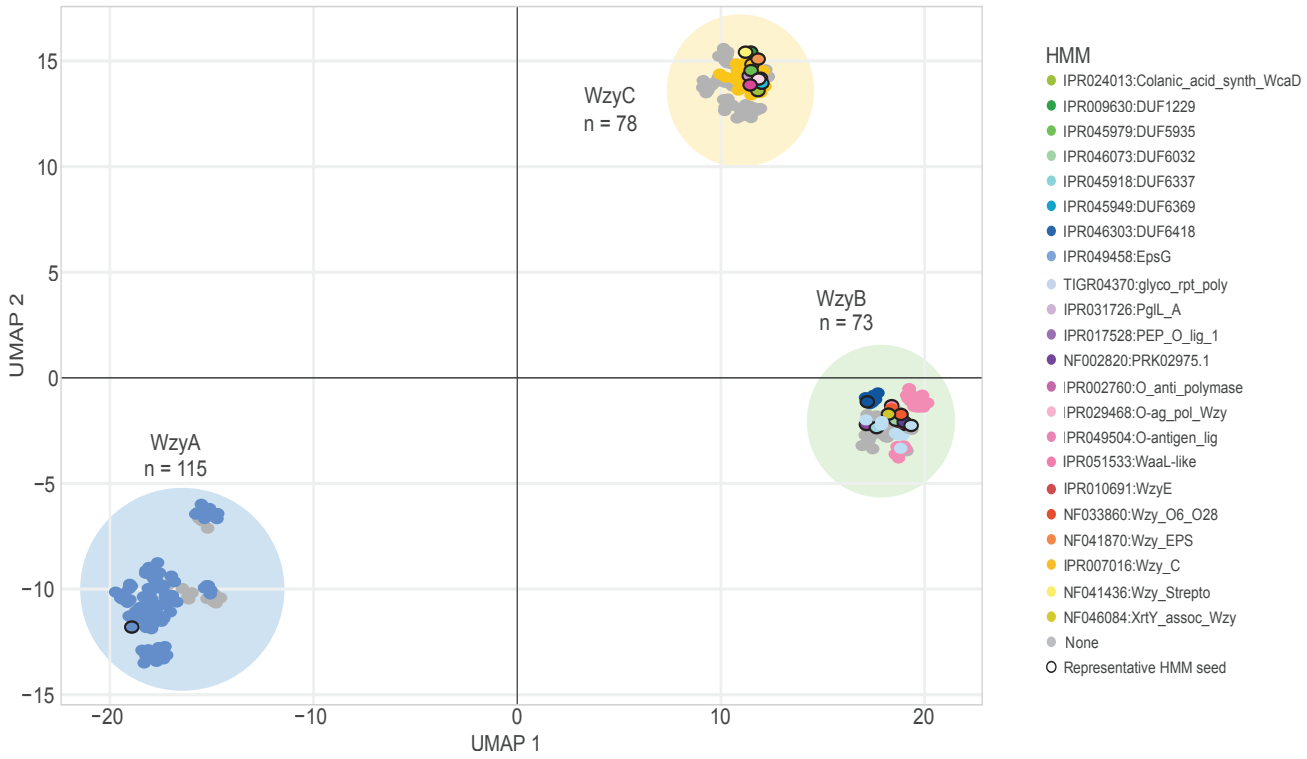
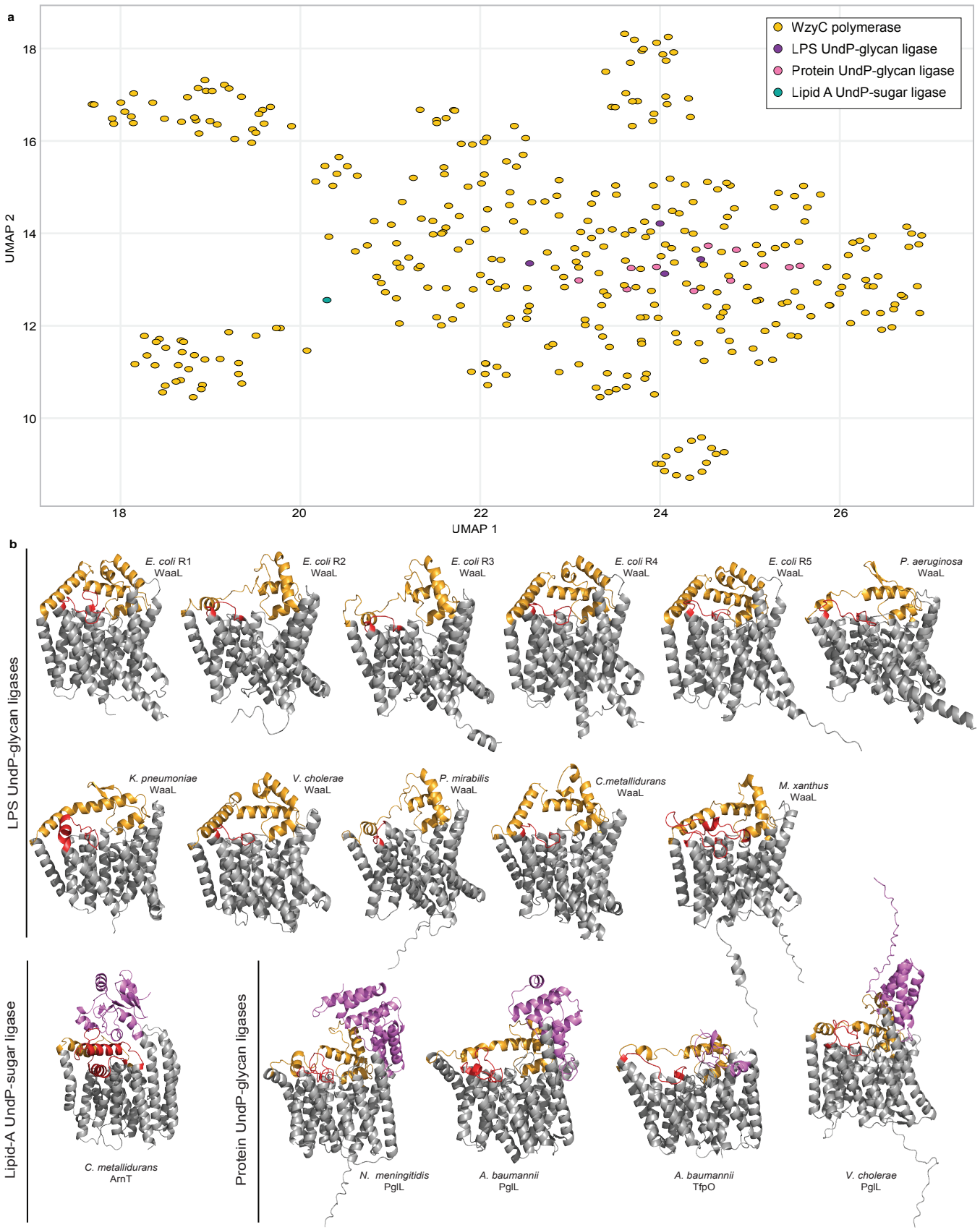


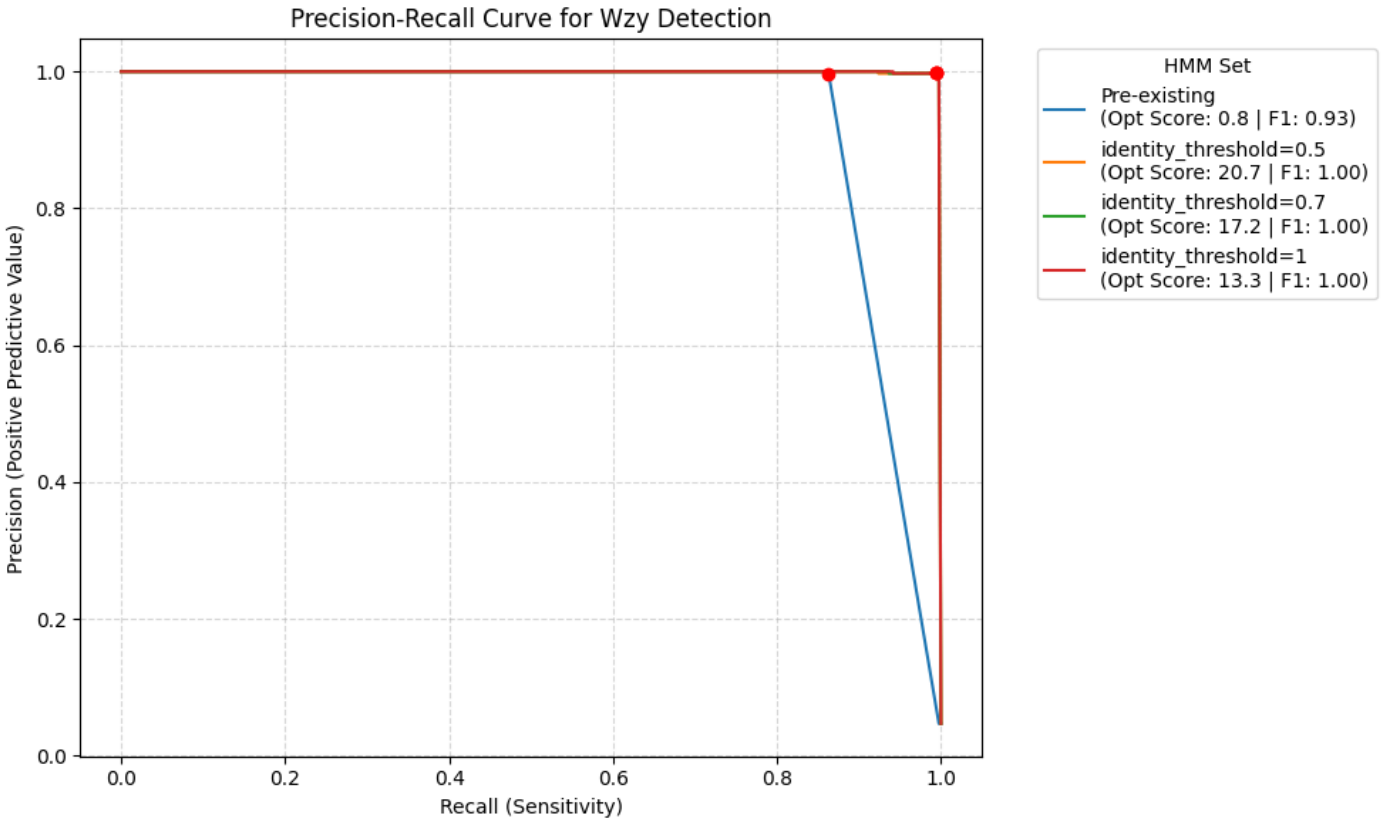
Supplementary Figure 1. General properties and relationships of Wzy polymerases from *A. baumannii*. (a) Distribution of proteins across different length ranges. **(b)** Distribution of proteins by number of predicted transmembrane segments (TMS). **(c)** All-vs-all pairwise sequence identity matrix visualised as a heatmap. Figure generated using ggplot2 in RStudio *v. 3.3.0+*.



Supplementary Figure 2. Clustering of representative seed sequences with *A. baumannii* Wzy. UMAP of Leiden clustering results for *A. baumannii* Wzy and representative seed sequences (bold outline points) from established protein families. Colours of HMM assignments are shown in legend. Circles represent individual proteins.



Supplementary Figure 3. Relationship between WzyC polymerases and UndPP-glycan ligases. **(a)** UMAP projection based on Leiden clustering with key identifying protein types shown top right. **(b)** Visualisation of UndPP-glycan ligase structures showing PL1 (red), PL2 (orange) and PL3 (purple). ArnT does not hit the IPR007016 HMM but is structurally similar to WzyC proteins.



Supplementary Figure 4. Precision recall curves for Wzy detection using generated HMM profiles. HMM profiles (no trimming) were screened against sequences for 8431 CPS biosynthesis proteins extracted from *A. baumannii* and *K. pneumoniae Kaptive* databases. Curves were used to calculate optimal bitscore thresholds for each HMM profile as indicated in the key on the right.

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