Structure and topology prediction of phage adhesion devices using AlphaFold2: the case of two *Oenococcus oeni* phages

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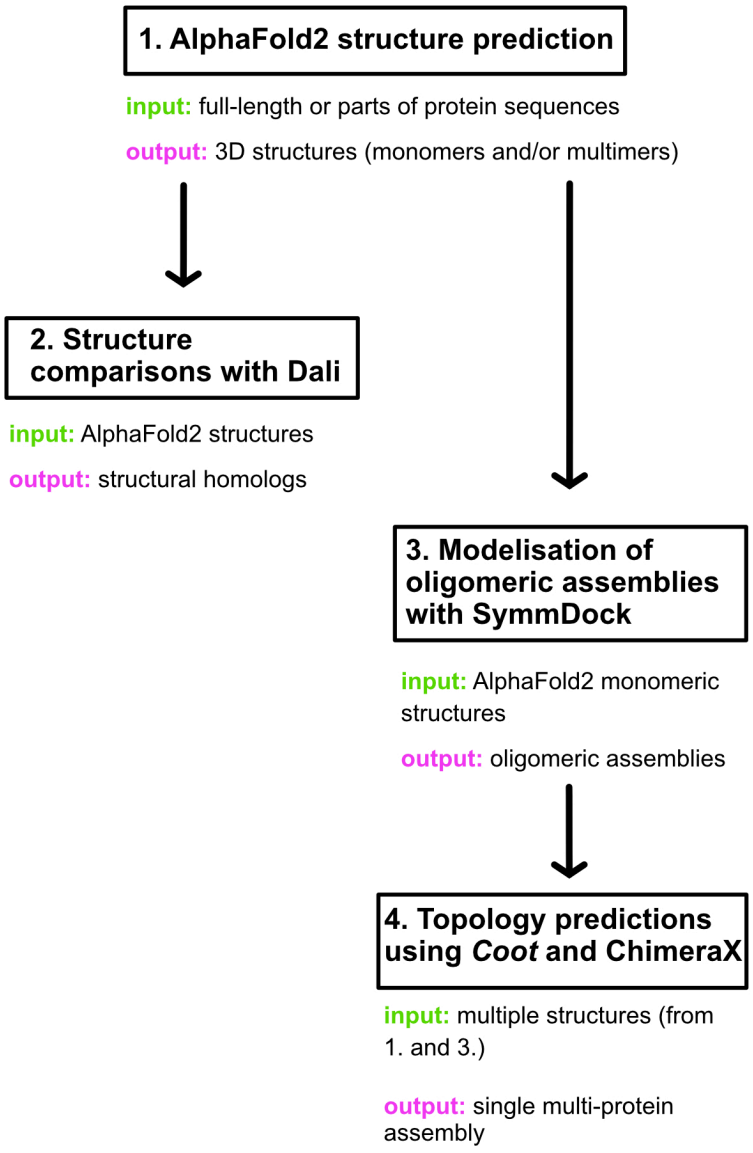
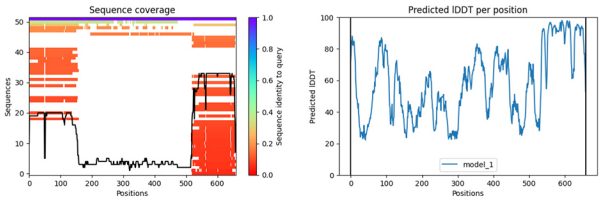


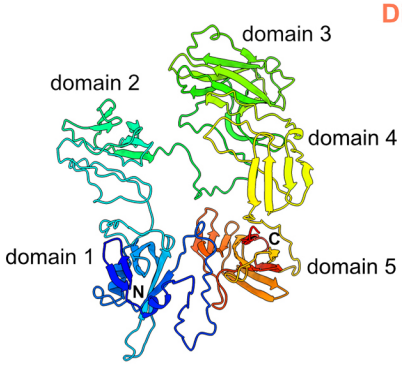
Figure S1. Workflow for structure and topology predictions. The different steps carried out for the structure and topology predictions are presented. The software used as well as their inputs and outputs are indicated.

A

full-length sequence (1-659)



Dit OE33PA



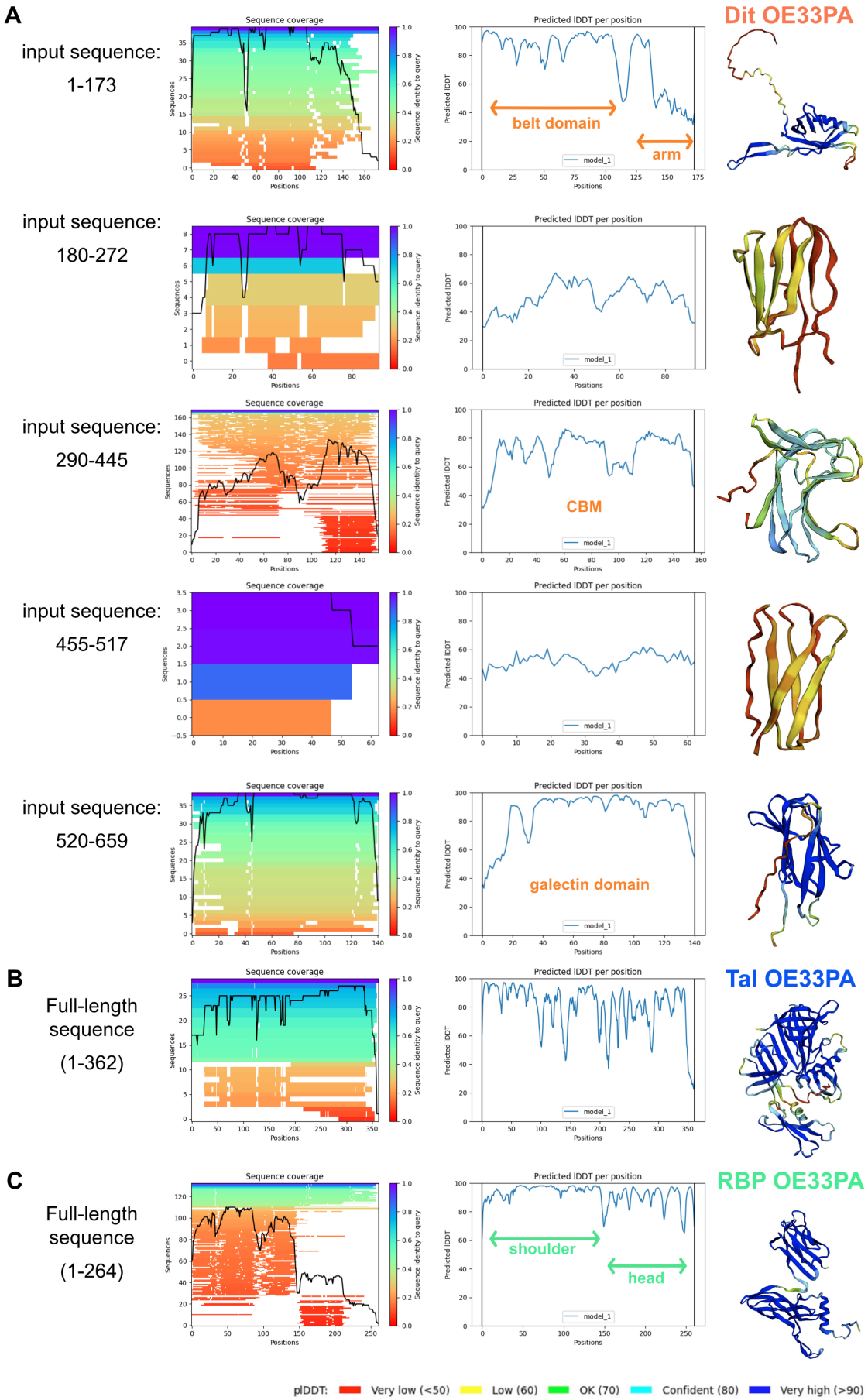


Figure S3. AlphaFold2 confidence measures for OE33PA Dit domains, Tal and RBP. of AlphaFold2 structure predictions of OE33PA Dit, Tal, and RBP. A. The Dit sequence was split into five parts and each of them were submitted to AlphaFold2. Left. The plots report the number of sequences, sequence coverage, and sequence identity to query. Right. Predicted

lDDT per position. AlphaFold2 predicted 3D structures are shown (the color code is indicated). B. The full-length Tal sequence was submitted to AlphaFold2. Left. This plot reports the number of sequences, sequence coverage, and sequence identity to query. Right. Predicted lDDT per position. The AlphaFold2 predicted 3D structure is shown (the color code is indicated). C. The full-length RBP sequence was submitted to AlphaFold2. Left. This plot reports the number of sequences, sequence coverage, and sequence identity to query. Right. Predicted plDDT per position. The AlphaFold2 predicted 3D structures is shown (the color code is indicated).

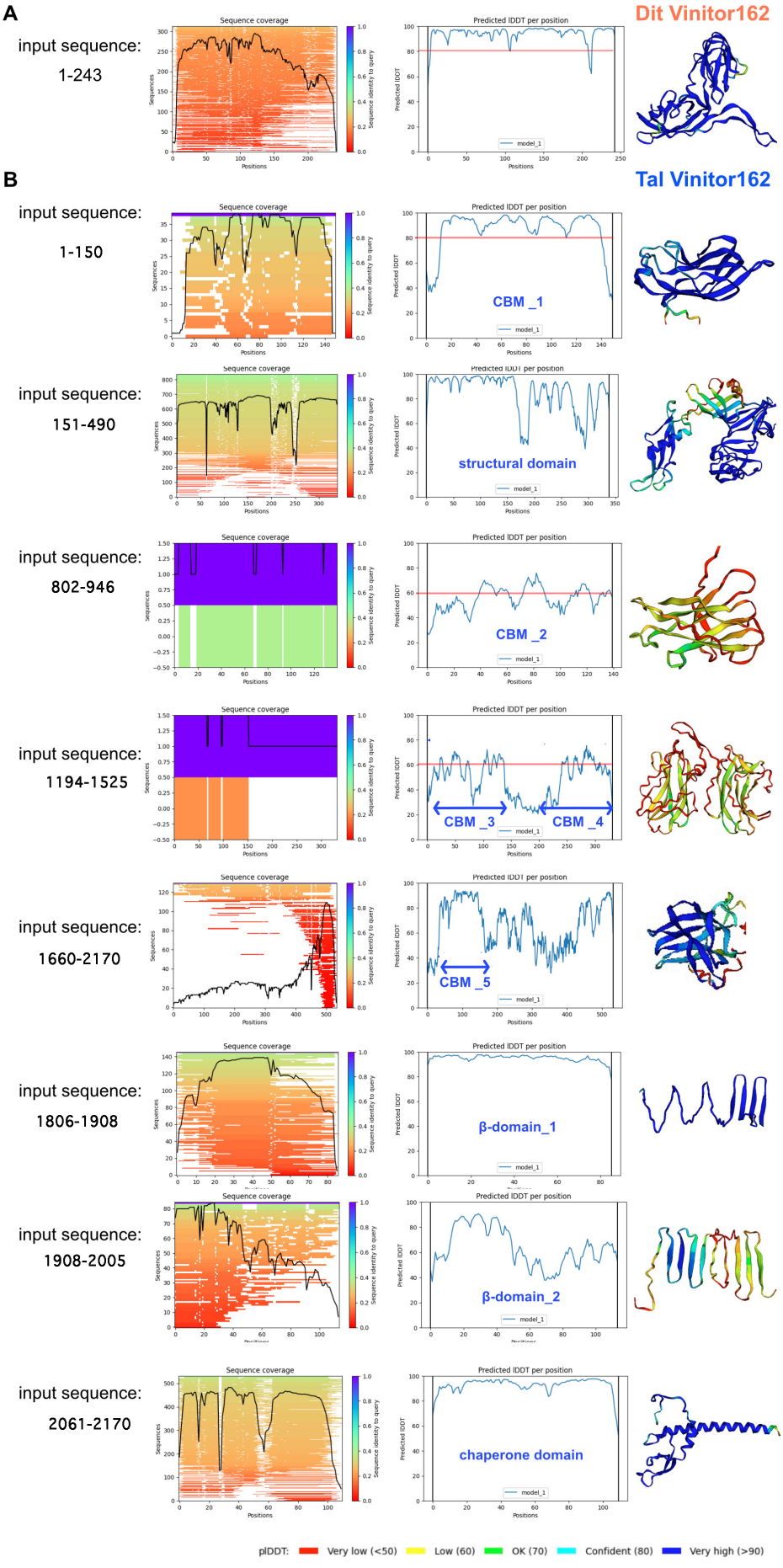


Figure S4. AlphaFold2 confidence measures for Vinitor162 Dit and Tal domains. A. The full-length Dit sequence was submitted to AlphaFold2. Left. This plot reports the number of sequences, sequence coverage, and sequence identity to query. Right. Predicted lDDT per

position. The AlphaFold2 predicted 3D structure is shown (the color code is indicated). B. The Tal sequence was split into eight parts and each of them were submitted to AlphaFold2. Left. The plots report the number of sequences, sequence coverage, and sequence identity to query. Right. Predicted lDDT per position. AlphaFold2 predicted 3D structures are shown (the color code is indicated).

Table S1. Comparison of domain predictions by HHpred and AlphaFold2.

Domains	HHpred boundaries (PDB ID; probability)	AlphaFold2 boundaries	Dali PDB ID•Z-score• rmsd (Å)•aligned residues
OE33PA Dit			
belt	1-166 (2wzp, *L. lactis* phage p2; 99.9%) 43-281 (2x8k, *B. subtilis* phage SPP1; 92.9%)	1-131	2wzp (*L. lactis* phage p2)• Z=13.4•rmsd=2.3•121 2x8k (*B. subtilis* phage SPP1)• Z=9.5•rmsd=3.4•112
unknown β-fold	n.i	199-270	2x5p (fibronectin-binding domain)• Z=6•rmsd=3•75
CBM	286-438 (2w5f, CBM22 CAZyDB; 95.1%)	305-445	5w6h (tail spike protein)• Z=12.2•rmsd=2.6•131 1gui (CBM4 CAZyDB)• Z=11.8•rmsd=2.3•130
unknown β-fold	n.i	455-517	nd
galectin	554-657 (2x8k, *B. subtilis* phage SPP1; 96.2%)	527-659	2x8k (*B. subtilis* phage SPP1)• •Z=12.3•rmsd=2.6•119 2wzp (*L. lactis* phage p2)• •Z=11.9•rmsd=2.6•121
OE33PA Tal			
structural domain (phage T4 gp27-like)	2-359 (3gs9, *Listeria* phage; 99.6%) 27-348 (3d37, *Neisseria* phage; 99.4%) 5-351 (6v8i, *Staphylococcus* phage 80α; 99.2%) 1-347 (1wru, phage Mu; 99.1%) 1-349 (3cdd, phage MuSo2; 99.1%)	1-362	2wzp (*L. lactis* phage p2)• Z=19.7•rmsd=4.4•300 3d37 (*Neisseria* phage)• Z=16.3•rmsd=4•267 3cdd (phage MuSo2)• Z=14.9•rmsd=4.1•246 3gs9 (*Listeria* phage)• Z=13.9•rmsd=3.8•263
OE33PA RBP			
shoulder	1-147 (4l9b, *L. lactis* phage 1358; 99.94%)	1-148	4l92 (*L. lactis* phage 1358)• Z=14.9•rmsd=2.2•144
head	155-261 (6r5w, *Listeria* phage PSA; 98.4%) 167-260 (4ios, *L. lactis* phage TP-901; 98.4%) 130-260	173-261	2fsd (*L. lactis* phage Bil170)• Z=11.9•rmsd=2.5•97 6r5w (*Listeria* phage PSA)• Z=10.7•rmsd=2.3•96

	(2fsd, *L. lactis* phage Bil170; 97.7%)		
	1-260 (1zru, *L. lactis* phage; 99.98%)		
Vinitor162 Dit			
belt and galectin	1-243 (2x8k, *B. subtilis* phage SPP1; 100%)	1-242	2x53 (*L. lactis* phage p2)• Z=12.9•rmsd=3.2•210
Vinitor162 Tal			
CBM_1	n.i	1-150	1us2 (CBM15 CAZyDB)• Z=8.3•rmsd=2.6•104
structural domain (phage T4 gp27-like)	129-489 (3gs9 *Listeria* phage; 99.9%) (6v8i, *Staphylococcus* phage 80α; 99.7%)	151-489	3gs9 (*Listeria* phage)• Z=18.3•rmsd=3.8•270
α-helix_1	490-708 (7boz, phage T7 tail fiber; 95.8%)	490-801	nd
CBM_2	827-940 (4xup, CBM22 CAZyDB; 69%) (5w6h, coliphage CBA120 tail spike; 50.6%)	802-946	4csb (bacterial β-barrel)• Z=4.1•rmsd=3•113
unknown β-fold	n.i	947-1193	nd
CBM_3	1194-1333 (4xup, CBM22 CAZyDB; 96.9%) (6zpv, GH51 CAZyDB; 95.6%)	1194-1333	5w6h (coliphage CBA120 tail spike)• Z=14.3•rmsd=2.3•126 2wze (CBM22 CAZyDB)• Z=12.5•rmsd= 2.5•125
linker_2		1334-1407	
CBM_4	1407-1525 (4xup, CBM22 CAZyDB; 96.9%)	1408-1524	4bjo (CBM4 CAZyDB)• Z=8.8 • rmsd=2.0•97
unknown β-fold	n.i	1525-1636	nd
CBM_5	1681-1784 (4d0q, CBM; 76.1%) (1dyo, CBM22 CAZyDB; 49.2%)	1637-1791	1dyo (CBM22 CAZyDB)• Z=9.4• rmsd=2.8•116
β-domain_1	n.i	1806-1891	4s37 (membrane-piercing spike)• Z=5.1• rmsd=1.5•52
β-domain_2	n.i	1908-2005	4bxq• Z=5.7• rmsd=3.7•86
C-term	2065-2170 (6f45, phage S16 tail fiber; 96.6%) (3gw6, tail spike; 94.8%)	2061-2170	4uw8 (phage T5 tail fiber)• Z=5.4• rmsd=3.1•81 3gw6 (tail spike)• Z=5.8• rmsd=2.8•90