

SUPPORTING INFORMATION

Evidence that the C-terminal Domain of a Type B PutA Protein Contributes to Aldehyde Dehydrogenase Activity and Substrate Channeling

Research reported in this publication was supported by the NIGMS of the National Institutes of Health under award numbers GM061068, GM065546, and P30GM103335.

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Table of Contents

Table S1. Primers used for cloning and site-directed mutagenesis	S-3
Figure S1. Sequence alignment of BjPutA and RcPutA.	S-4
Figure S2. Homology models of RcPutA used in rigid body modeling.	S-5
Figure S3. Decoy structures used in rigid body modeling calculations.	S-6

Table S1. Primers used for cloning and site-directed mutagenesis

Cloning of RcPutA	
NdeI fwd	5'-CATGTCCATATGACCGACCTTCCGCCCTT-3'
XhoI rev	5'-TCACTCGAGTCACCCGGCCAGCAAAGC-3'
RcPutA site-directed mutations and deletions	
G1011P fwd	5'-CTGCCCCGCCCCGACGCCGGAGCTGAACCGGCTGACG-3'
G1011P rev	5'-CGTCAGCCGGTTCAGCTCCGGCGTCGGGCCGGGCAG-3'
E1012A fwd	5'-CTGCCCCGCCCCGACGGGCGCGCTGAACCGGCTGACGCGG-3'
E1012A rev	5'-CCGCGTCAGCCGGTTCAGCGCGCCCGTCGGGCCGGGCAG-3'
N1014A fwd	5'-GGCCCCGACGGGCGAGCTGGCCCCGGCTGACGCGGCATC-3'
N1014A rev	5'-GATGCCGCGTCAGCCGGGCCAGCTCGCCCCGTCGGGCC-3'
RcPutAΔ1108-1112 fwd	5'-TGGACGAGATCTTCCTGCCCTGAACCGGCTGACGCGGCATC-3'
RcPutAΔ1108-1112 rev	5'-GATGCCGCGTCAGCCGGTTCAGGGGCAGGAAGATCTCGTCCA-3'
RcPutA1-1116 fwd	5'-CTGCGTCGACACGACGTGAGCGGGCGGCAATGCG-3'
RcPutA1-1116 rev	5'-CGCATTGCCGCCCGCTCACGTCGTGTCGACGCAG-3'
R454M fwd	5'-CTGCTCGCCTATCTGGTGATGCGGCTTTGGAGAACGGC-3'
R454M rev	5'-GCCGTTCTCCAAAAGCCGCATCACCAGATAGGCGAGCAG-3'
C791A fwd	5'-CGCTCGGCCGGGCAACGCGCCTCGGCGCTGCGCTGTC-3'
C791A rev	5'-GACAGCGCAGCGCCGAGGCGCGTTGCCCGGCCGAGCG-3'
BjPutA site-directed mutations and deletions	
G638P fwd	5'-GCGATGCCAGGCCCGACCCAGAGAGCAACGCGCTCAC-3'
G638P rev	5'-GTGAGCGCGTTGCTCTCTGGGGTTCGGGCCTGGCATCGC-3'
E639A fwd	5'-CGATGCCAGGCCCGACCGGCGCGAGCAACGCGC-3'
E639A rev	5'-GCCGGTCGGGCCTGGCATCGCCGTCTCGC-3'
N641A fwd	5'-GGCCCCGACCGGCGAGAGCGCCGCGCTCACCATGCGCGGC-3'
N641A rev	5'-GCCGCGCATGGTGAGCGCGGCGCTCTCGCCGGTCGGGCC-3'
BjPutAΔ635-639 fwd	5'-GCAGCGAGACGGCGATGCCAAGCAACGCGCTCACCATGCGCGG-3'
BjPutAΔ635-639 rev	5'-CCGCGCATGGTGAGCGCGTTGCTTGGCATCGCCGTCTCGCTGC-3'
BjPutA1-986 fwd	5'-AGACCGTAACCATCAACACGGCTTAAGCCGGCGGCAAT-3'
BjPutA1-986 rev	5'-ATTGCCCGCGGCTTAAGCCGTGTTGATGGTTACGGTCT-3'

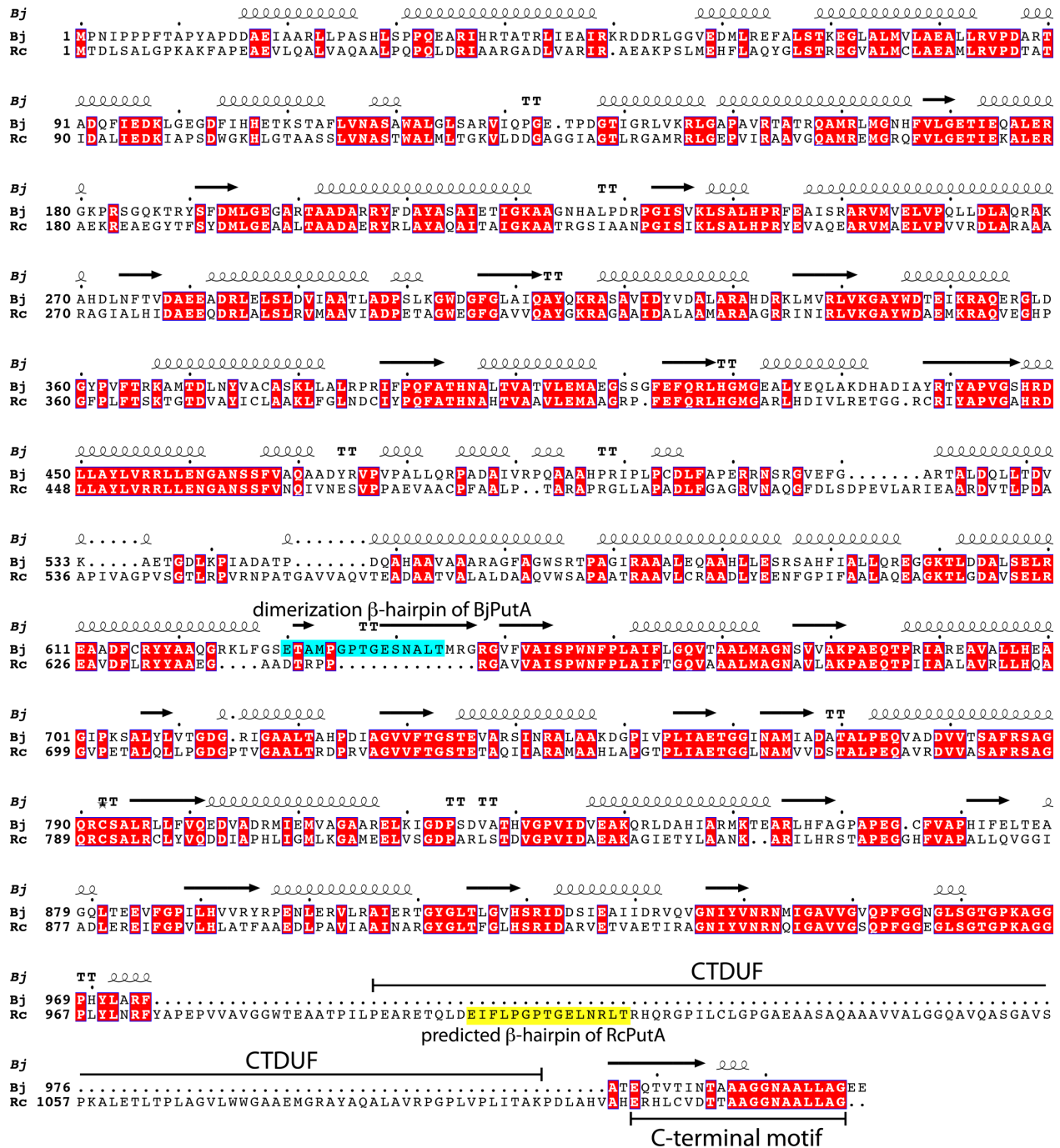


Figure. S1. Sequence alignment of BjPutA and RcPutA. The secondary structure elements are from the BjPutA structure (PDB code 3HAZ). The cyan box indicates residues of the dimerization β -hairpin of BjPutA. Note that these residues are missing in RcPutA. The yellow box indicates the predicted β -hairpin of RcPutA. The overall identity is 52 %.

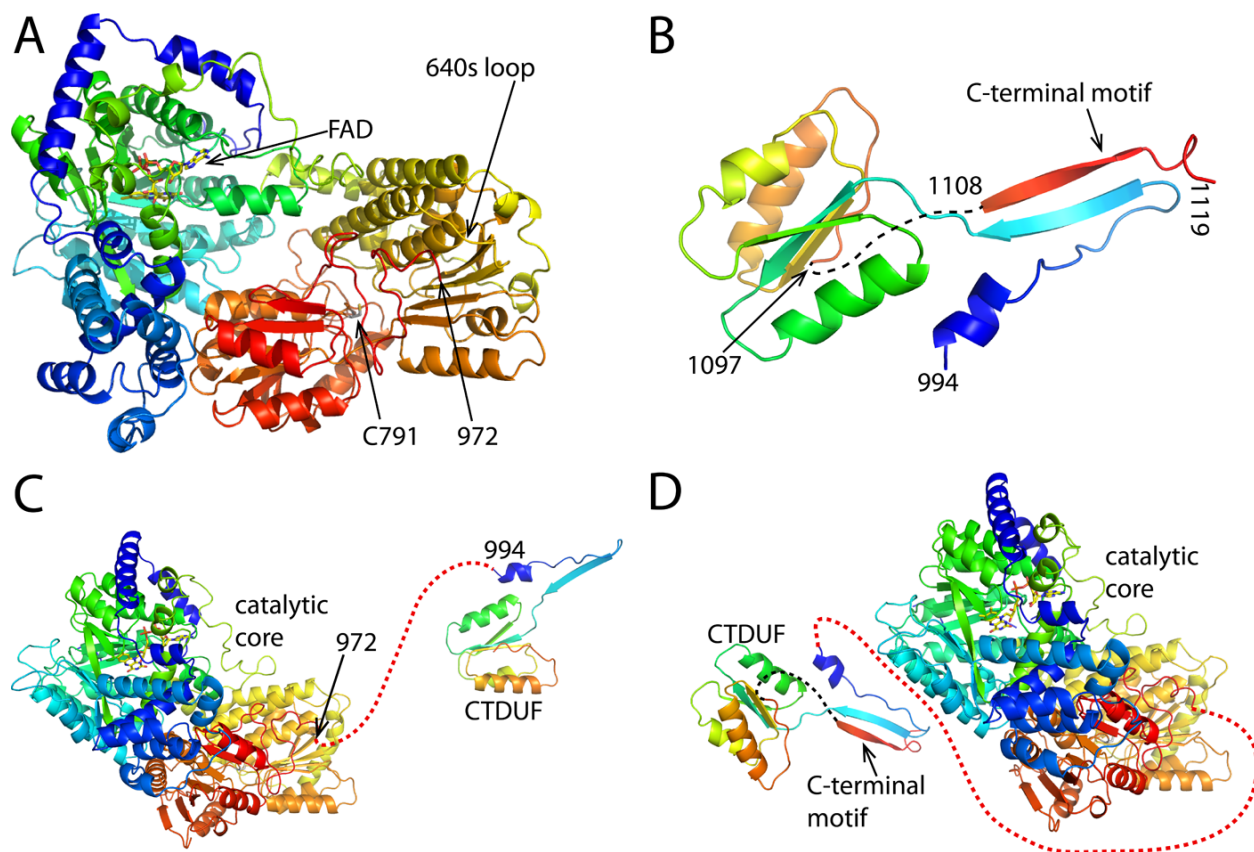


Figure S2. Homology models of RcPutA used in rigid body modeling. (A) Model of the catalytic core created with SWISS-MODEL, colored using a rainbow scheme with blue at the N-terminus and red at the C-terminus. (B) Combined model of the CTDUF (residues 994-1097) and C-terminal motif (residues 1108-1119), colored in the rainbow scheme. Dashes indicate residues that were not modeled. (C) Starting configuration used for CORAL set 1 calculations. The catalytic core (residues 1-972) and CTDUF (residues 994-1097) are each colored with the rainbow scheme. The red dashes denote the region modeled as dummy residues in CORAL (residues 973-993). (D) One of the starting configurations used in CORAL set 2 calculations.

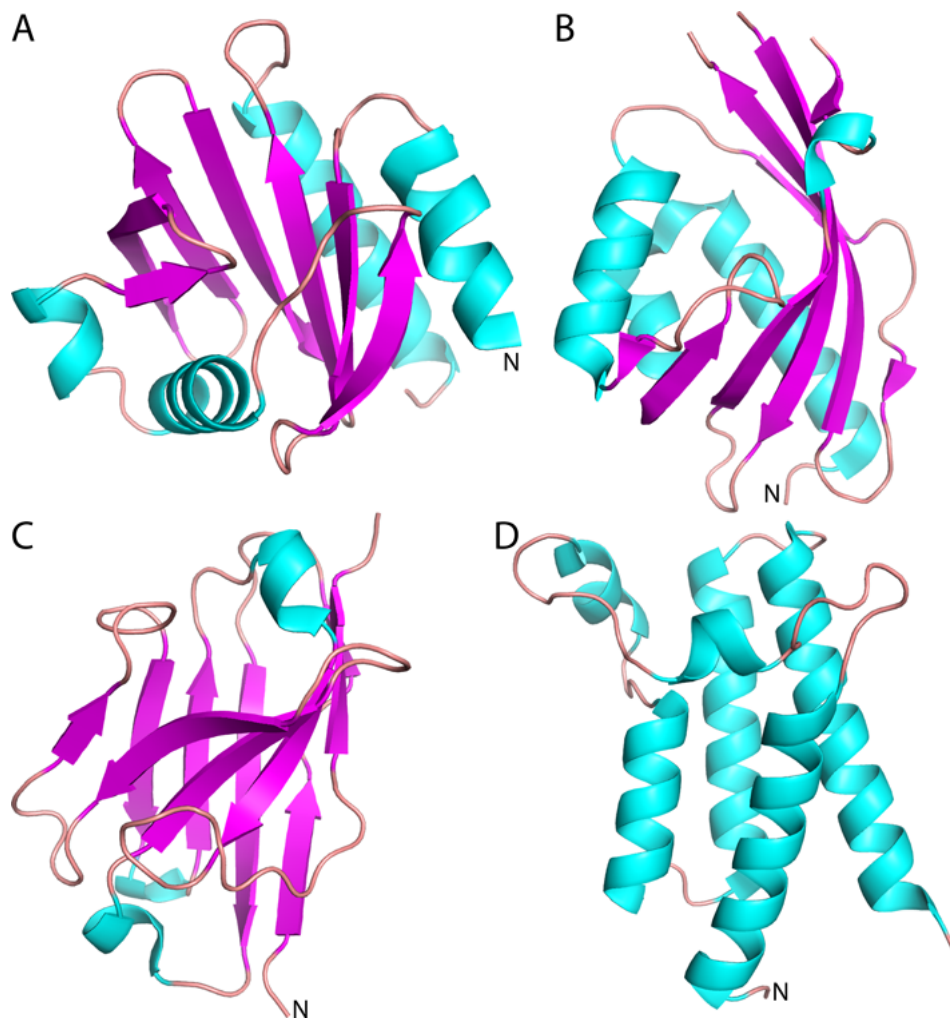


Figure S3. Decoy structures used in rigid body modeling calculations. (A) Profilin IB (125 residues, PDB code 1ACF). (B) Ketosteroid isomerase (126 residues, PDB code 3SED). (C) Human VH domain (116 residues, PDB code 1T2J). (D) Human bromodomain (118 residues, PDB code 3HMF).