

Supporting information

Comparison of L-Threonine aldolase variants in the aldol and retro-aldol reactions

Kateryna Fesko¹

¹Institute of Organic Chemistry, Graz University of Technology, Graz, Austria

kateryna.lypetska@tugraz.at

SI content:

Figure S1. Sequence of the wild-type LTAaj..... 2

Figure S2. Sequence alignment of the LTAaj used in this study with the template sequence ... 2

Figure S3. Crystal structure alignment of template PDB:3WGB with the LTAaj model..... 3

MRYIDLRSDTVTQPTDAMRQAMLHAEVGDDVYGEDPSVNLEAYGAKLLGKQAALFVPSGT
 SNLLAVMSHCQRGEGAILGAGAHIYRFEAQGSVALGSVALQPLPMQRDGTLAFDEIKAALAPDD
 AHFVQTRLICLENTHNGKVLPLSYLQEMGAFVAKHGLKLHLDGARLFNAAVASDTPAEAIAAPFD
 SISICLSKGAPVGSLLVGDRDFIARARRLRKMVGGMRQAGMLAQAGLFALEQHVRLADDH
 RRAKRLAEGLAALPGIGLDSLVSQSNMVFRLAKGEPAQLLAFMKERGILFGYGYELRLVTHLQIND
 DDIEEVIDAFTEYLGA

Figure S1. Protein sequence analysis of the wild-type L-threonine aldolase from *Aeromonas jandaei* (LTAaj) used in this study.

3WGB_A PDBID CHAIN SEQUENCE LTAaj_study	MRYIDLRSDTVTQPTDAMRQAMLHAEVGDDVYGEDPGVNLEAYGADLLG MRYIDLRSDTVTQPTDAMRQAMLHAEVGDDVYGEDPSVNLEAYGAKLLG *****.*****.*****.*****.*****.*****.***
3WGB_A PDBID CHAIN SEQUENCE LTAaj_study	KEAALFVPSTGMSNLLAVMSHCQRGEGAVLGSAAHYRYEAQGSVALGSV KQAALFVPSTGMSNLLAVMSHCQRGEGAILGAGAHIYRFEAQGSVALGSV *:*****.*****;*:****;*****;*****
3WGB_A PDBID CHAIN SEQUENCE LTAaj_study	ALQPVPMQADGSLALADVRAAIAPDDVHFTPTRLVCLENTHNGKVLPLPY ALQPLPMQRDGTLAFDEIKAALAPDDAHFVQTRLICLENTHNGKVLPLSY ****;*** **;*** : ;:****;****.**. ***;*****.*
3WGB_A PDBID CHAIN SEQUENCE LTAaj_study	LREMRELVDEHGLQLHLDGARLFNAVVASGHTVRELVAPFDSVSICLSKG LQEMGAFVAKHGLKLHLDGARLFNAAVASDTPAEAIAAPFDSISICLSKG *:*** . * :****;*****.***. ... :.*****;*****
3WGB_A PDBID CHAIN SEQUENCE LTAaj_study	LGAPVGSLLVGSHAFIARARRLRKMVGGMRQAGILAQAGLFALQQHVVR LGAPVGSLLVGDRDFIARARRLRKMVGGMRQAGMLAQAGLFALEQHVVAR *****. : *****.*****;*****;*****;****.*
3WGB_A PDBID CHAIN SEQUENCE LTAaj_study	LADDHRRARQLAEGLAALPGIRLDLAQVQTNMVFLQLTSGESAPLLAFMK LADDHRRAKRLAEGLAALPGIGLDSLVSQSNMVFRLAKGEPAQLLAFMK *****;*****. ***; **;****;*:***.* *****
3WGB_A PDBID CHAIN SEQUENCE LTAaj_study	ARGILFSGYGYELRLVTHLQIHDDDIEEVIDAFTEYLGA ERGILFSGYGYELRLVTHLQINDDIEEVIDAFTEYLGA *****;*****

Figure S2. Sequence alignment of the LTAaj used in this study with the template sequence (UniProtKB O07051; PDB: 3WGB)

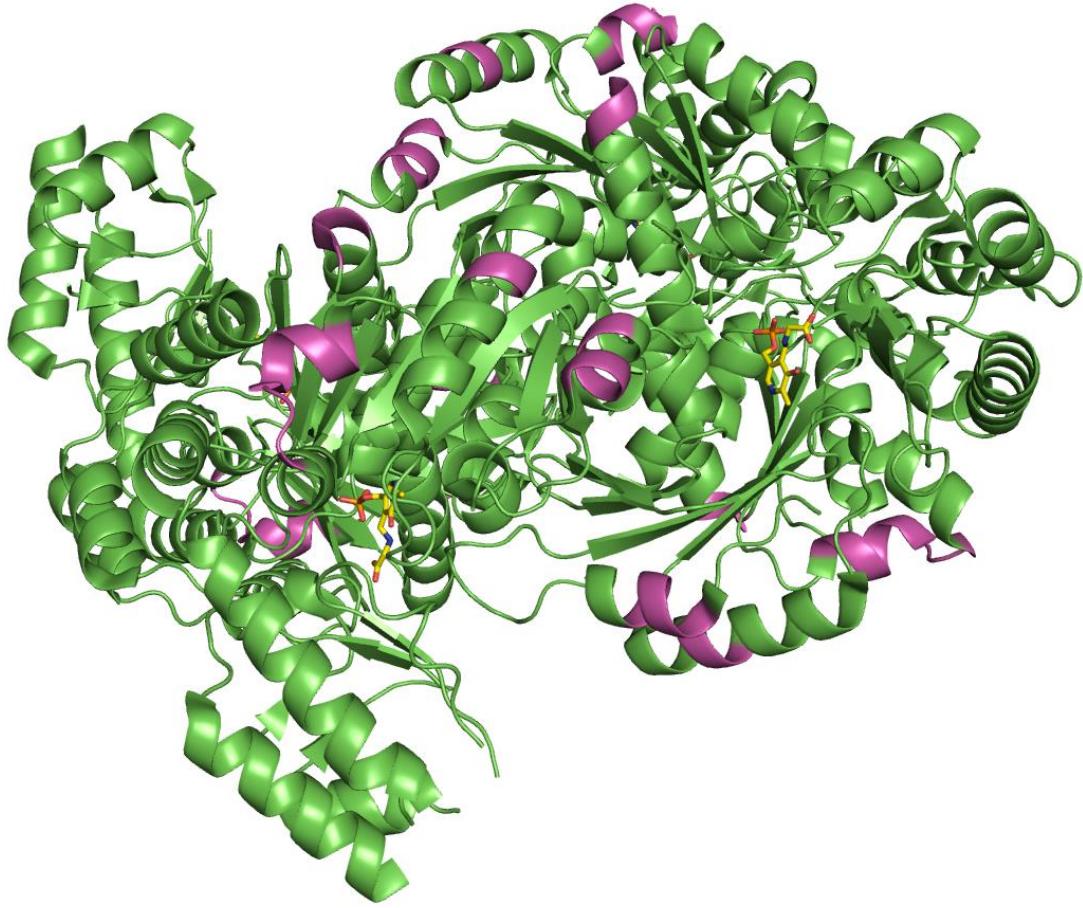


Figure S3. Crystal structure alignment of template PDB:3WGB with the LTAaj model. Pink – not-conserved residues of LTAaj used in study with the template sequence. Not-conserved residues are located in the surface of crystal structure of the protein and do not have significant impact on the active site structure and properties.