SUPPORTING INFORMATION FOR:

Crystal structure of ALD1, a plant-specific homologue of the universal diaminopimelate amino transferase enzyme of lysine biosynthesis

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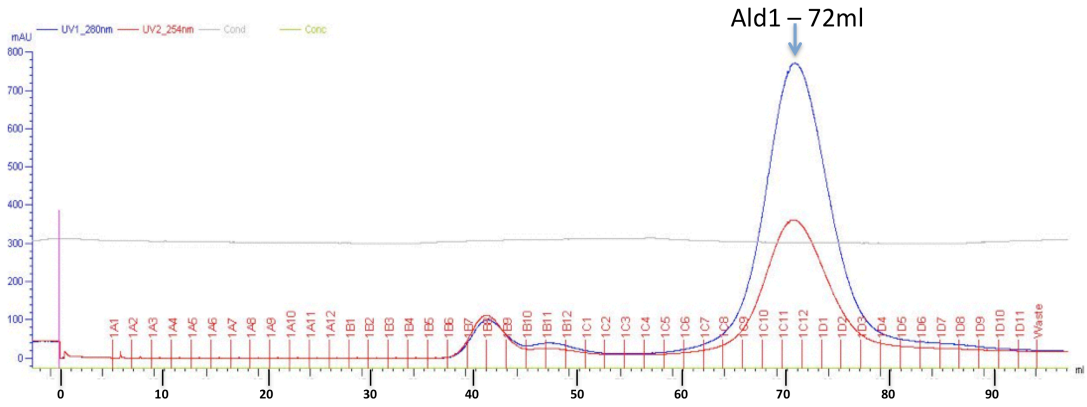
Ald1 on GF HiLoad_16/60 Superdex 200



Protein standards on this column:
Aldolase 158kDa- 65.6ml
Albumin 67kDa -74.2ml
Ovalbumin 43kDa – 80.6ml

72ml corresponds to a MW close to 100kDa which agrees to ALD1 dimer.

Figure S1. Gel-filtration data.

Table S1a. Residues in contact with PLP complexed to *At*ALD1

Residue		Dist,Å	Surf,Å^2
141A	GLY	3.4	5.0
142A	ALA	2.8	35.3
143A	GLN	3.0	23.2
166A	PHE	3.9	50.1
219A	CYS	3.6	24.2
223A	ASN	2.9	24.1
251A	ASP	2.7	29.6
253A	ALA	3.9	17.9
254A	TYR	2.7	37.3
281A	SER	2.6	37.7
283A	SER	2.8	20.3
284A	LYS	3.8	18.7
292A	ARG	2.8	29.8
108B	TYR	2.4	52.5
323B	ASN	3.7	10.8

Residues in contact with PLP belonging to chains A and B. Nearest atom-atom distances (Dist) and contact surface area (Surf) between PLP and the residues were defined using LPC software (http://sgedg.weizmann.ac.il/lpc).

Table S1b. Residues in contact with PLP in PDB entry 2Z20 (malate free)

Residue		Dist,Å	Surf,Å^2
127A	GLY	3.2	8.3
128A	ALA	2.8	40.7
129A	LYS	3.0	44.0
152A	TYR	3.7	44.5
205A	CYS	3.8	15.5
209A	ASN	2.7	52.4
237A	ASP	2.8	33.4
239A	ALA	4.3	8.7
240A	TYR	3.4	19.5
267A	SER	2.6	27.0
269A	SER	2.7	24.6
270A	LYS	3.2	35.8
278A	ARG	3.0	27.4
94B	TYR	3.4	14.8
309B	ASN	2.8	27.9

See legend to Table S1a

Table S1c. Residues in contact with PLP in PDB entry 2Z1Z (malate bound)

Residue		Dist,Å	Surf,Å^2
127A	GLY	3.7	8.5
128A	ALA	3.0	39.3
129A	LYS	3.7	25.2
152A	TYR	3.9	42.8
205A	CYS	3.3	33.4
209A	ASN	2.8	24.9
237A	ASP	2.9	23.9
239A	ALA	3.9	14.1
240A	TYR	2.8	31.3
267A	SER	2.4	37.4
269A	SER	3.0	9.9
270A	LYS	2.8	42.4
278A	ARG	2.9	24.8
94B	TYR	2.7	22.8
309B	ASN	3.2	17.2

See legend to Table S1a

Table S2a. Residues in contact with malate in PDB entry 2Z1Z

Residue	Dist,Å	Surf,Å^2
39A PHE	3.5	39.6
63A ILE	3.3	27.5
64A GLY	3.1	15.3
129A LYS	4.1	16.8
152A TYR	2.9	29.1
209A ASN	2.7	29.1
270A LYS	3.9	9.4
404A ARG	2.8	32.7
94B TYR	3.5	15.7
309B ASN	3.2	25.0

Residues in contact with malate belonging to chains A and B. Nearest atom-atom distances (Dist) and contact surface area (Surf) between malate and the residues were defined using LPC software (http://sgedg.weizmann.ac.il/lpc).

Table S2b. Residues from the *At*ALD1 structure that would be in contact with malate if malate would be placed similar to its position in the *At*DAPAT structure

Residue	Dist,Å	Surf,Å^2
53A PHE	3.9	23.9
78A GLY	3.6	16.2
166A PHE	4.3	11.6
223A ASN	2.6	30.5
284A LYS	3.9	16.6
418A ARG	2.8	35.9
108B TYR	3.6	29.0
323B ASN	4.4	10.5

See legend to Table S2a.