AN ASYMMETRIC MODEL FOR NA^+-TRANSLOCATING GLUTACONYL-COA DECARBOXYLASES

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SUPPLEMENTAL FIGURES

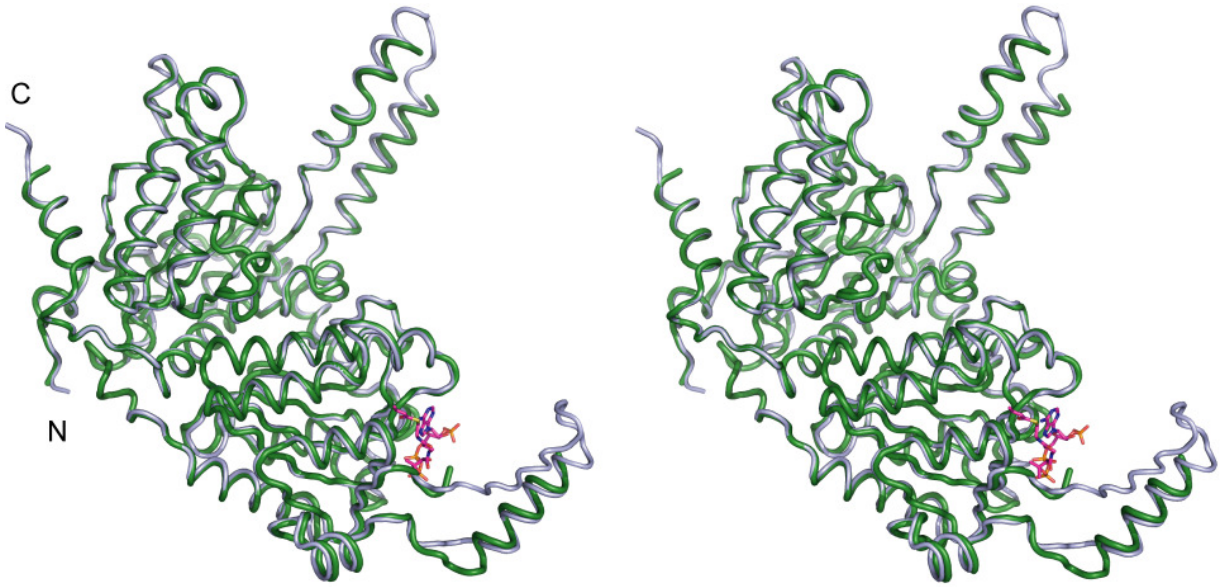

Figure S1: Stereo representation of a superposition of the *C. symbiosum* (dark green) and *A. fermentans* (light blue) GcdA monomer structures. The coloring of the displayed stick model of crotonyl-CoA is in accordance to Fig. 4*A*.

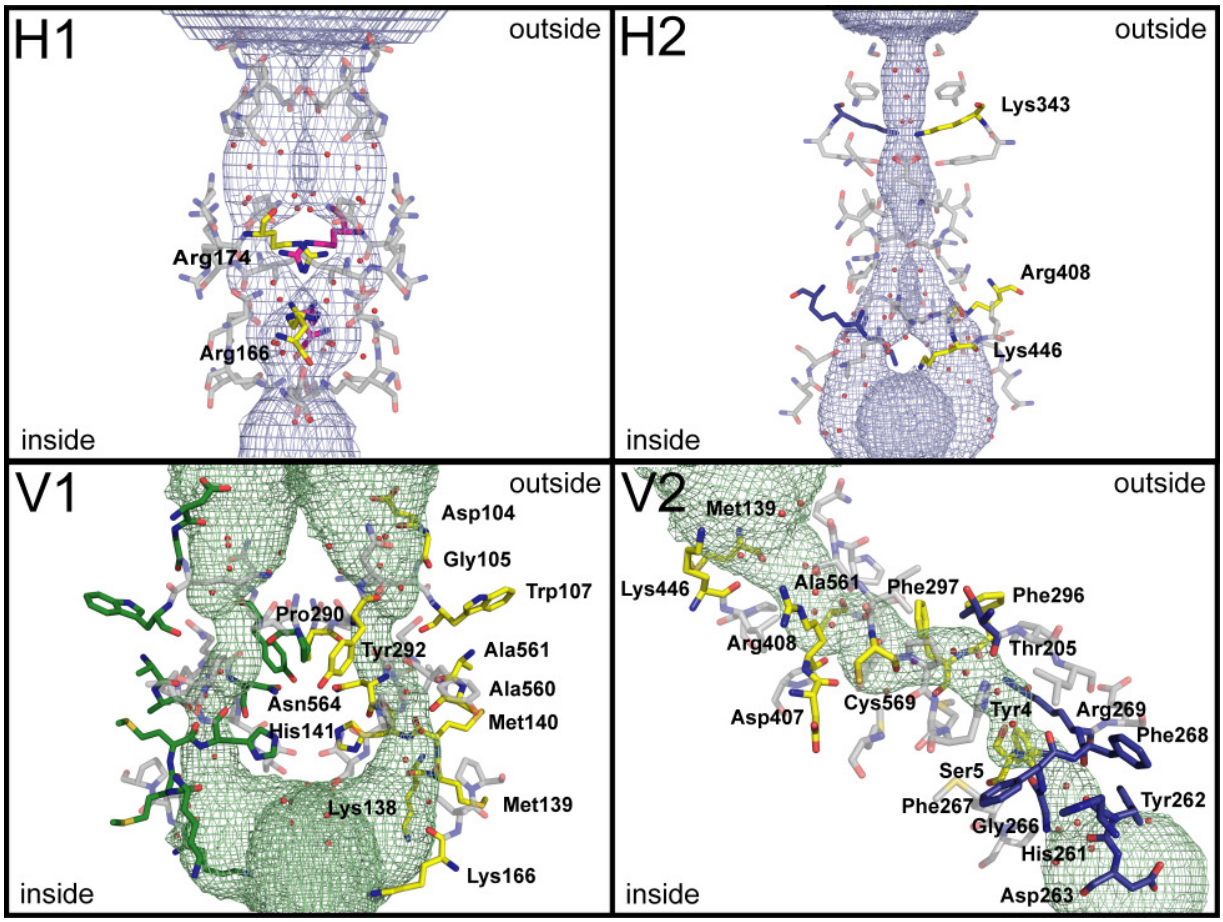

Figure S2: Close-up view of the four different horizontal (H) and vertical (V) channels found in the GcdA tetramer. Residues at a distance of 5 Å from the centers of the tunnels are shown as gray stick models. The bottle neck residues for the horizontal tunnels and residues supposed to permit transient coordination of monovalent cations in case of the vertical channels are displayed in the colors of their respective protein chains (cf. Fig. 6). In case of H1, V1 and V2 only one portion of residues was labeled for clarity reasons. Water molecules are illustrated as red spheres. For this analysis an initial tunnel search using the Molaxis server (2) was further refined using the programs Mole (3) and CAVER (4). The figure was created using the CAVER Plugin for the program Pymol.

SUPPLEMENTAL FIGURES

Table S1. Data collection statistics for *C. symbiosum* GcdA and its complexes. Values in parentheses correspond to the highest resolution shell.

	Apo[1]	**Crotonyl-CoA**[1]	**Glutaryl-CoA**[2]	**Glutaconyl-CoA**[2]
Wavelenght (Å)	0.80150	0.80150	1.54179	1.54179
Resolution (Å)	2.40	2.50	2.70	1.75
Highest resolution shell	2.53 - 2.40	2.64 – 2.50	2.85 - 2.59	1.84 – 1.75
Total reflections	148483	212893	402828	239351
Unique reflections (> 1δ)	24154	79234	61822	60672
Completness (%)	99.9 (100.0)	99.6 (98.9)	98.7 (91.4)	97.9 (99.7)
I/σ	20.9 (5.1)	9.6 (2.1)	16.6 (3.4)	18.9 (4.5)
R_{merge}	0.074 (0.334)	0.097 (0.464)	0.103 (0.455)	0.046 (0.262)
Multiplicity	6.1 (6.2)	2.7 (2.4)	6.5 (6.1)	3.9 (3.7)
Space group	F222	C2	$P3_121$	F222
Unit cell parameters				
a (Å)	102.05	101.50	156.47	102.360
b (Å)	143.53	167.45	156.47	144.360
c (Å)	167.52	138.11	141.40	167.150
α (°)	90.00	90.00	90.00	90.00
β (°)	90.00	89.98	90.00	90.00
γ (°)	90.00	90.00	120.00	90.00
Monomers per asymmetric unit	1	4	2	1

[1] collected at X13 beamline at DESY, EMBL-Hamburg
[2] collected with rotating anode

Table S2. Refinement statistics for *C. symbiosum* GcdA and its complexes.

	Apo	**Crotonyl-CoA**	**Glutaryl-CoA**	**Glutaconyl-CoA**
R_{cryst}/R_{free}	0.185 / 0.225	0.194 / 0.230	0.189 / 0.210	0.163 / 0.176
r.m.s.d. bond length (Å)	0.007	0.009	0.008	0.008
r.m.s.d. bond angles (°)	1.095	1.202	1.155	1.173
Average B factor (Å^2)	31.6	35.7	36.9	23.2
number of protein atoms	4202	17298	8723	4371
number ligand atoms	-	212	112	53
number of ion atoms	5	4	-	1
number of water molecules	201	627	352	466
Ramachandran Plot (%)				
Most favored	90.1	89.6	90.6	91.3
Allowed	9.3	9.3	8.6	7.8
Generously allowed	0.2	0.6	0.4	0.4
Disallowed	0.4	0.4	0.4	0.4
Gaps[1]	G218-K251 L502-Q513	G221-A237 (C) K501-Q513 (C)	A220-A236 (A) K501-Q513 (A)	G221-A237 A505-Q513

[1] In case of the structural models containing more than one chain in the asymmetric unit only the widest gaps are displayed with the respective chain identifier in parenthesis.

SUPPLEMENTAL REFERENCES

1. DeLano, W. L. (2002) *The PyMOL molecular graphics system*. DeLano Scientific LLC, http://www.pymol.org, San Carlos, CA, USA
2. Yaffe, E., Fishelovitch, D., Wolfson, H. J., Halperin, D., and Nussinov, R. (2008) *Nucleic Acids Res.* **36**, W210-215
3. Petrek, M., Kosinova, P., Koca, J., and Otyepka, M. (2007) *Structure* **15**, 1357-1363
4. Petrek, M., Otyepka, M., Banas, P., Kosinova, P., Koca, J., and Damborsky, J. (2006) *BMC Bioinformatics* **7**, 316