Published in final edited form as:

Nat Struct Mol Biol. 2020 May ; 27(5): 511–513. doi:10.1038/s41594-020-0421-9.

Author Correction: Molecular Basis for Acetyl-CoA Production by ATP-Citrate Lyase

Xuepeng Wei[1,2], **Kollin Schultz**[2,3], **Gleb A. Bazilevsky**[2,4], **Austin Vogt**[1,2], **Ronen Marmorstein**[1,2]

[1]Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA 19104, USA

[2]Abramson Family Cancer Research Institute, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA 19104, USA

[3]Gradaute Group in Biochemistry and Molecular Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA 19104, USA

[4]Graduate Group in Cell and Molecular Biology, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA 19104, USA

Correction notice:

In the version of the article initially published, the phospho-citryl-CoA intermediate in the ACLY-E599Q–ATP-citrate-CoA structure (PDB 6UUW) was modelled incorrectly. Specifically, the citryl-CoA linkage was modelled with a thioether bond instead of a thioester bond and the phosphate group was connected to the OH of the citryl moiety in the phospho-citryl portion instead of via an ester bond with the carboxylate group as supported by Walsh and Spector (J. Biol Chem. 243, 446–448, 1968). Thus, the intermediate shown in Figure 6 and Extended Date Figure 7c, d was incorrect. The PDB coordinate file has been revised and Figure 6 and Extended Data Figure 7c,d have been replaced in the HTML and PDF versions of the article. Original and corrected Figures are shown below. The text has not been changed but given the inherent instability of the modelled phospho-citryl-CoA intermediate and the limited resolution of the current structure, the modelled intermediate could represent phospho-citrate + CoA, citryl-CoA + PO4 or a mixture of the two. Given this possibility, the precise catalytic role if E599 is unknown and E599 may not be directly involved in cleavage of the citryl-CoA adduct as implied in the article.

Additional corrections that should be made are as follows:

1. In table 1, the ligand number of "E599Q" should be 8 instead of 4
2. In table 1, the rmsd bond length of With citrateCoA (C1 asymm. open) (EMDB-20784,PDB-6uiA) should be 0.008 instead of 0.0008.
3. On page 38, "We therefore mixed the ACLY-E599A mutant" should be "….ACLY-E599Q…."
4. On page 39, " Interestingly, citrate was added to both ACLY-citrate-CoA and ACLY-E599A…" should be "….ACLY-E599Q"

5. On page 40, " This conclusion is further supported by our….. ACLY-E599A catalytic mutant" should be "….ACLY-E599Q"

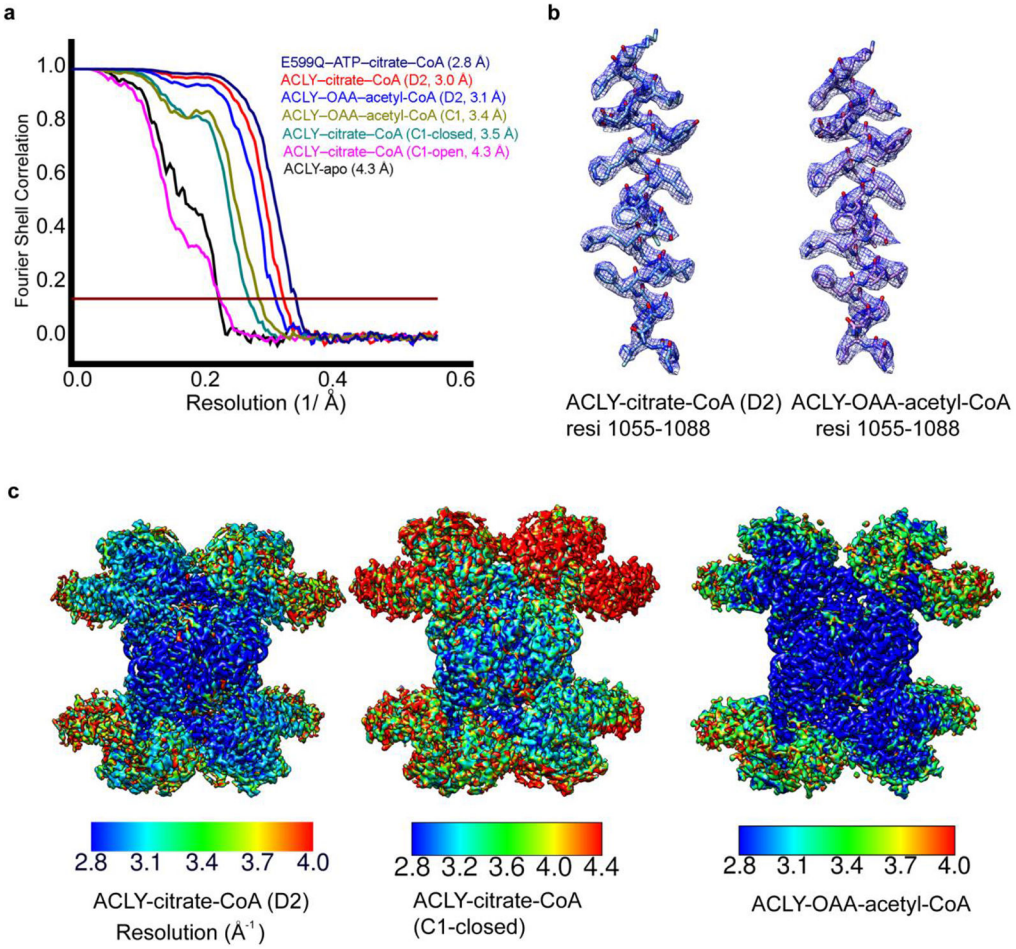
6. **Methods** - "For 3D reconstruction of the ACLY-E599–citrate-ATP-CoA structure, 746,030 particles were picked from 5,600 micrograph" should be "… ACLY-E599Q–citrate-ATP-CoA structure…."

7. Extended Figure 4b -

   ACLY-citrate-CoA (D2) resi 1055-1088 should be "residue 1055-1077"

   ACLY-OAA-acetly-CoA resi 1055-1088 should be "ACLY-OAA-acetly-CoA (D2) residue 1055-1077"

Extended Data



Extended Data Fig. 4.

Analysis of single particle cryo-EM reconstructions. (a) Fourier Shell Correlation (FSC) curves for 3D reconstructions of reported structures, marked with resolutions corresponding to FSC = 0.143. (b) Cryo-EM density of representative helical segments (residues 1055-1077) from ACLY–citrate–CoA (left) and ACLY–OAA–acetyl-CoA structures. (c)

Local resolution estimation of cryo-EM maps of ACLY–citrate–CoA-D2 (left), ACLY–citrate-CoA-C1 asymm closed (middle) and ACLY–OAA–acetyl-CoA (right) by Resmap.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

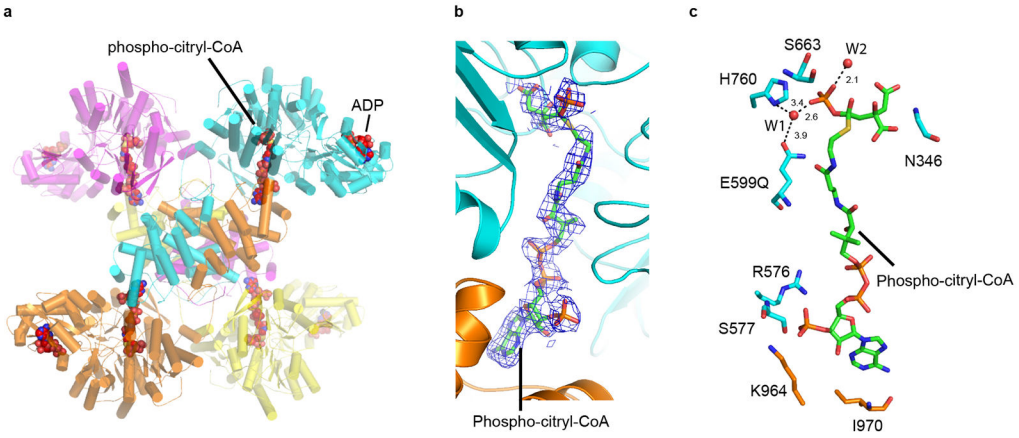


Table 1 |

Cryo-EM data collection, refinement, and validation statistics

	Apo (EMDB-20414, PDB-6POF)	With citrate–CoA (D2) (EMDB-20903, PDB-6UUZ)	With citrate–CoA (C1 asymm closed) (EMDB-20413, PDB-6POE)	With citrate–CoA (C1 asymm open) (EMDB-20784, PDB-6UIA)	With OAA–acetyl-CoA (D2) (EMDB-20783, PDB-6UI9)	With OAA–acetyl-CoA (C1) (EMDB-20904, PDB-6UV5)	E599Q With ATP–citrate–CoA (D2) (EMDB-20902, PDB-6UUW)
Data collection and processing							
Magnification	28,000	45,000	45,000	45,000	45,000	45,000	45,000
Voltage (kV)	200	200	200	200	200	200	200
Electron exposure (e–/Å^2)	40	37	37	37	37	37	40
Defocus range (μm)	1.5-3.5	0.9-2.8	0.9-2.8	0.9-2.8	0.9-2.8	0.9-2.8	1.0-2.0
Pixel size (Å)	1.485	0.87	0.87	0.87	0.87	0.87	0.87
Symmetry imposed	D2	D2	C1	C1	D2	C1	D2
Initial particle images (no.)	398,391	716,394	716,394	716,394	719,613	719,613	770,837
Final particle images (no.)	20,677	129,563	129,563	73,969	108,738	108,738	207,653
Map resolution (Å)	4.3	3.0	3.5	4.3	3.1	3.4	2.9
FSC threshold	0.143	0.143	0.143	0.143	0.143	0.143	0.143
Map resolution Range (Å)	4.1-5.3	2.8-4.0	2.8-4.4	4.0-5.3	2.8-4.0	2.8-4.4	2.7-3.6
Refinement							
Initial model used (PDB code)	3MWD	3MWD	3MWD	3MWD	3MWD	3MWD	5TDF
Model resolution (Å)	4.4	3.1	3.6	4.4	3.2	3.5	2.9
Model resolution Range (Å)	-	-	-	-	-	-	-
Map sharpening *B* factor (Å^2)	−138	−95	−100	−122	−98	−101	−80
Model composition							
Nonhydrogen atoms	31,624	31,816	31,810	31,720	31,900	31,951	32,532
Protein residues	4,084	4,084	4,084	4,084	4,084	4,084	4,136
Ligands	0	4	4	2	12	12	8
R.m.s. deviations							
Bond lengths (Å)	0.009	0.01	0.008	0.012	0.009	0.014	0.01
Bond angles (°)	1.234	1.114	0.946	1.673	1.102	1.202	1.155
Validation							
MolProbity score	1.95	1.90	2.51	2.20	1.77	1.77	1.56
Clashscore	9.80	8.06	6.34	14.17	6.03	6.26	3.11
Poor rotamers (%)	0.27	0.24	0.12	0.86	0.27	0.15	0.55
Ramachandran plot (%)							
Favored (%)	93.16	93.25	93.20	90.44	93.23	93.05	94.27
Allowed (%)	6.64	6.65	6.48	9.02	6.27	6.75	5.29
Disallowed (%)	0.2	0.1	0.32	0.54	0.1	0.2	0.4