



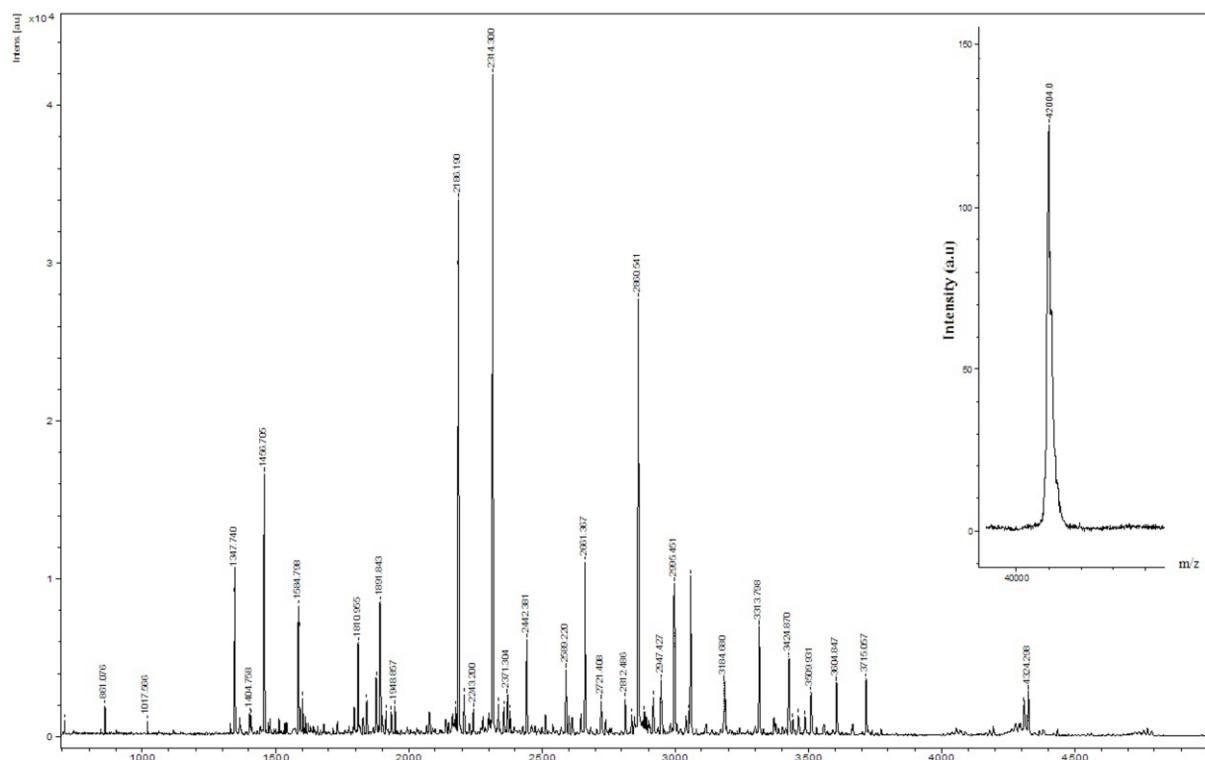
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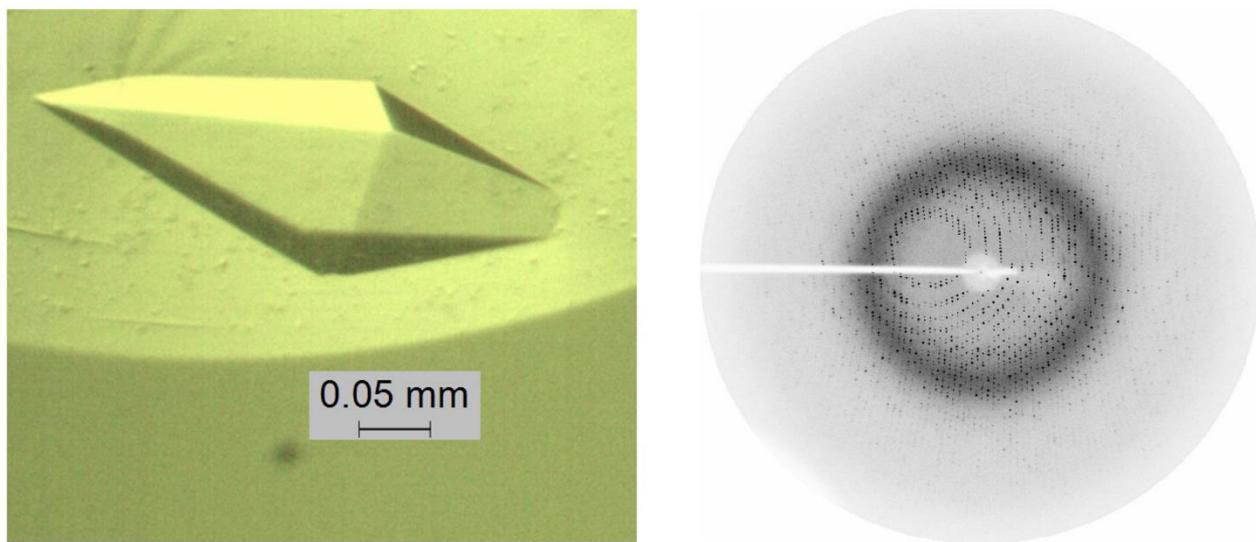
**Supporting information for article:**

**Crystal structure of a thiolase from *Escherichia coli* at 1.8 Å resolution**

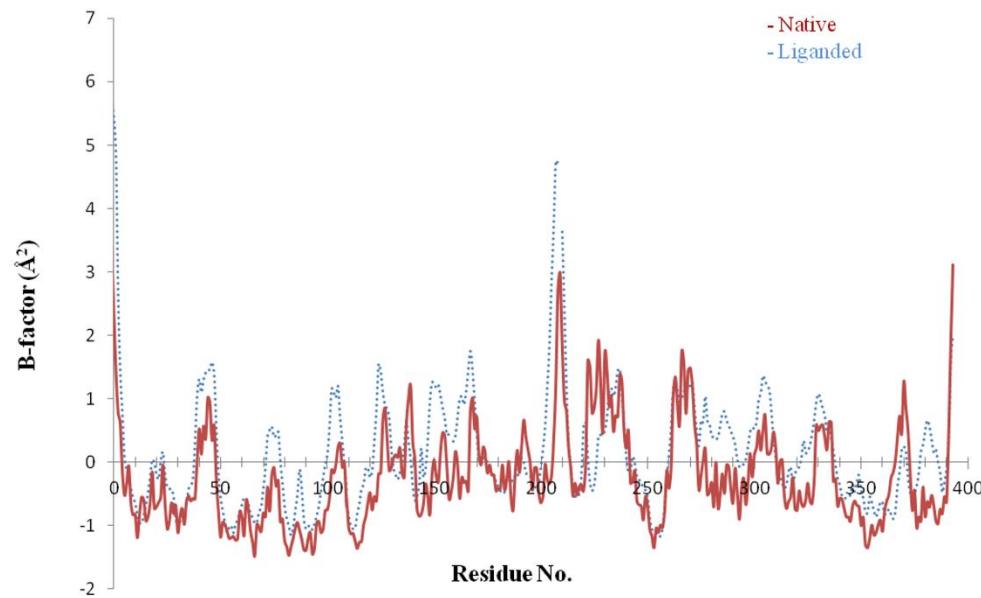
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**Figure S1** (a) MS spectrum for purified protein. (b) MALDI spectra for peptides of trypsin digested protein.



**Figure S2** (a) A crystal of the *E. coli* thiolase obtained by co-crystallization in the presence of avetyl-CoA. (b) A typical oscillation diffraction image acquired using the home X-ray source.



**Figure S3** B-factor plot for the A-chain of both native and liganded (CoA bound) structures.

**Table S1** Peptide mass fingerprinting of trypsin digested peptides and mass of individual peptides

S. No	Residue No.	Observed mass	Mr (Expt)	Mr (Calc)	Delta	Peptide sequence
1.	3 – 11	1017.57	1016.56	1016.54	0.02	NCVIVSAVR
2.	12 – 40	2834.54	2833.53	2833.52	0.01	TAIGSFNGSLASTSAIDLGATVIKAAIER
3.	41 – 67	2860.54	2859.53	2859.47	0.07	AKIDSQHVDEVIMGNVLQAGLGQNPAR
4.	43 – 67	2661.37	2660.36	2660.33	0.03	IDSQHVDEVIMGNVLQAGLGQNPAR
5.	94 – 128	3487.93	3486.93	3486.78	0.14	SVALAAQAIQAGQAQSIVAGGMENMSLAPYLLDAK
6.	94 – 130	3715.06	3714.05	3713.92	0.13	SVALAAQAIQAGQAQSIVAGGMENMSLAPYLLDAKAR
7.	131 – 146	1810.95	1809.95	1809.94	0.01	SGYRLGDGQVYDVILR
8.	135 – 146	1347.74	1346.73	1346.72	0.01	LGDGQVYDVILR
9.	135 – 167	3604.85	3603.84	3603.73	0.11	LGDGQVYDVILRDGLMCATHGYHMGITAENVAK
10	147 – 173	2995.45	2994.44	2994.38	0.07	DGLMCATHGYHMGITAENVAKEYGITR
11	168 – 185	2176.05	2175.04	2175.04	0.00	EYGITREMQDELALHSQR
12	174 – 185	1456.70	1455.70	1455.68	0.02	EMQDELALHSQR
13	174 – 186	1584.80	1583.79	1583.77	0.02	EMQDELALHSQRK
14	174 – 186	1600.85	1599.84	1599.77	0.07	EMQDELALHSQRK
15	187 – 208	2186.19	2185.18	2185.17	0.01	AAAAIESGAFTAEIVPVNVVTR
16	187 – 209	2314.30	2313.29	2313.27	0.02	AAAAIESGAFTAEIVPVNVVTRK
17	211 – 221	1344.67	1343.66	1343.64	0.02	TFVFSQDEFPK
18	211 – 238	3057.60	3056.60	3056.52	0.07	TFVFSQDEFPKANSTAEALGALRPAFDK
19	239 – 275	3424.87	3423.86	3423.77	0.10	AGTVTAGNASGINDGAAALVIMEESAALAAGLTPLAR
20	330 – 357	2721.41	2720.40	2720.40	0.00	NLGFDSEKVNNGAIALGHPIGASGAR
21	372 – 394	2357.26	2356.25	2356.26	-0.01	TLGLATLCIGGGQGIAMVIERLN