



STRUCTURAL
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Supporting information for article:

Binding of hydroxycitrate to human ATP-citrate lyase

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Table S1 Surface areas buried by crystal-packing interactions

DM with citrate, phosphate (5TEQ) chain A with A	$1-x, y-\frac{1}{2}, -z$	$1-x, y+\frac{1}{2}, -z$		
	712.6 Å ²	767.9 Å ²		
DM with citrate, phosphate (5TEQ) chain A with B	x, y, z	$-x, y+\frac{1}{2}, -z$	$x, y+1, z$	$1-x, y+\frac{1}{2}, 1-z$
	1044.6 Å ²	417.9 Å ²	397.8 Å ²	350.1 Å ²
3690.9 Å ² out of 29548.3 Å ² , 12.5%				
DM with citrate, phosphate (5TEQ) chain B with B	$-x, y-\frac{1}{2}, 1-z$	$-x, y+\frac{1}{2}, 1-z$		
	762.7 Å ²	706.6 Å ²		
DM with citrate, phosphate (5TEQ) chain B with A	x, y, z	$-x, y-\frac{1}{2}, -z$	$x, y-1, z$	$1-x, y-\frac{1}{2}, 1-z$
	1022.6 Å ²	397.5 Å ²	395.8 Å ²	330.9 Å ²
3616.1 Å ² out of 29654.6 Å ² , 12.2%				
TEV-Nter hACLY with citrate, phosphate (5TDE)	$1-x, y-\frac{1}{2}, \frac{1}{2}-z$	$1-x, y+\frac{1}{2}, \frac{1}{2}-z$	$x+\frac{1}{2}, \frac{1}{2}-y, -z$	$x-\frac{1}{2}, \frac{1}{2}-y, -z$
	1263.0 Å ²	1292.9 Å ²	474.7 Å ²	444.8 Å ²
	$x+1, y, z$	$x-1, y, z$	$-x, y-\frac{1}{2}, \frac{1}{2}-z$	$-x, y+\frac{1}{2}, \frac{1}{2}-z$
	317.1 Å ²	311.4 Å ²	159.2 Å ²	160.8 Å ²
4423.9 Å ² out of 29586.7 Å ² , 15.0%				