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Data API

3O8J

Crystal structure of 2-methylcitrate synthase (PrpC) from Salmonella typhimurium

PDB DOI: <https://doi.org/10.2210/pdb3O8J/pdb>

Classification: TRANSFERASE
Organism(s): Salmonella enterica subsp. enterica serovar Typhimurium
Expression System: Escherichia coli
Mutation(s): No

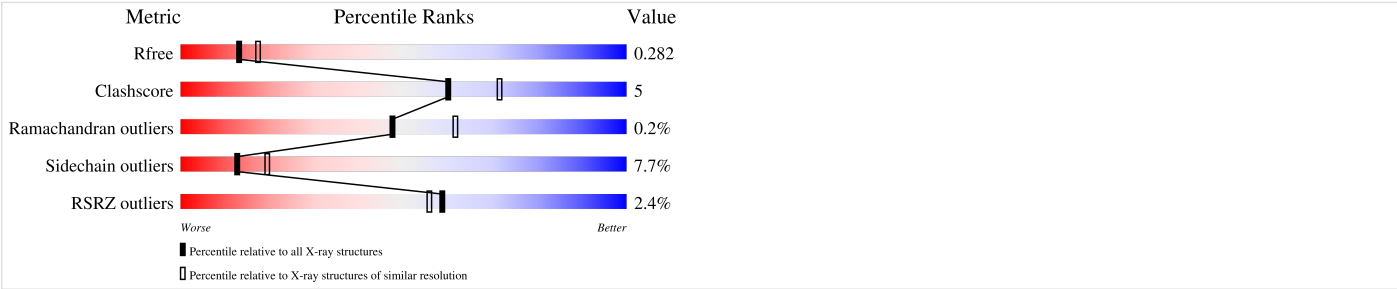
Deposited: 2010-08-03 Released: 2011-04-13
Deposition Author(s): Chittori, S., Savithri, H.S., Murthy, M.R.N.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 2.41 Å
R-Value Free: 0.282
R-Value Work: 0.218
R-Value Observed: 0.221

wwPDB Validation

3D Report Full Report



This is version 1.2 of the entry. See complete history.

Literature

Crystal structure of Salmonella typhimurium 2-methylcitrate synthase: Insights on domain movement and substrate specificity

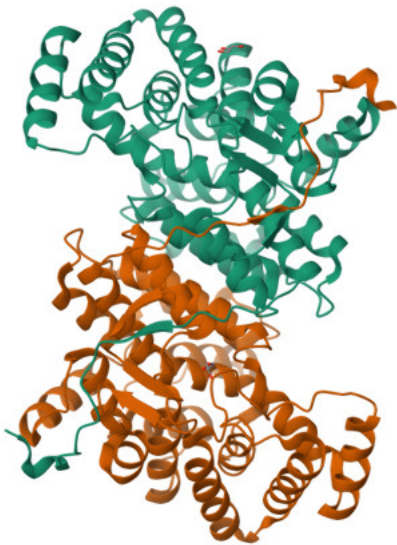
Chittori, S. Savithri, H.S., Murthy, M.R.N.
(2011) J Struct Biol 174: 58-68

PubMed: 20970504
DOI: <https://doi.org/10.1016/j.jsb.2010.10.008>
Primary Citation of Related Structures:
3O8J

PubMed Abstract:
2-Methylcitric acid (2-MCA) cycle is one of the well studied pathways for the utilization of propionate as a source of carbon and energy in bacteria such as Salmonella typhimurium and Escherichia coli. 2-Methylcitrate synthase (2-MCS) catalyzes the conversion of oxaloacetate and propionyl-CoA to 2-methylcitrate and CoA in the second step of 2-MCA cycle. Here, we report the X-ray crystal structure of S. typhimurium 2-MCS (StPrpC) at 2.4Å resolution and its functional...

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Organizational Affiliation:
Molecular Biophysics Unit, Indian Institute of Science, Bangalore, Karnataka 560012, India.



Explore in 3D: Structure | Sequence Annotations | Electron Density | Validation Report | Ligand Interaction (GOL)

Global Symmetry: Cyclic - C2 (Explore in 3D)
Global Stoichiometry: Homo 2-mer - A2

Find Similar Assemblies

Biological assembly 1 assigned by authors and generated by PISA (software)

Macromolecules

Find similar proteins by: Sequence ▾ (by identity cutoff) | 3D Structure

Entity ID: 1					
Molecule	Chains	Sequence Length	Organism	Details	Id
2-methylcitrate synthase	A, B, C, D, E ⊕	404	<u>Salmonella enterica subsp. enterica serovar Typhimurium</u>	Mutation(s): 0 Gene Names: <u>prpC</u> , <u>STM 0369</u> EC: <u>2.3.3.5</u>	

UniProt

Find proteins for [Q56063](#) (*Salmonella typhimurium* (strain LT2 / SGSC1412 / ATCC 700720))
Explore [Q56063](#)

Go to UniProt

Entity Groups

Sequence Clusters	30% Identity	50% Identity	70% Identity	90% Identity	95% Identity	100% Identity
UniProt Group	Q56063					

Sequence Annotations



Small Molecules

Ligands 1 Unique				
ID	Chains	Name / Formula / InChI Key	2D Diagram	3D Interactions
GOL		GLYCEROL C ₃ H ₈ O ₃ PEDCQBHIVMGVHV-UHFFFAOYSA-N		<div>Interactions</div> <div>Interactions & Density</div>
<div>Download Instance Coordinates</div>				

Experimental Data & Validation

Experimental Data

Method: X-RAY DIFFRACTION
Resolution: 2.41 Å
R-Value Free: 0.282
R-Value Work: 0.218
R-Value Observed: 0.221
Space Group: P1

Unit Cell:

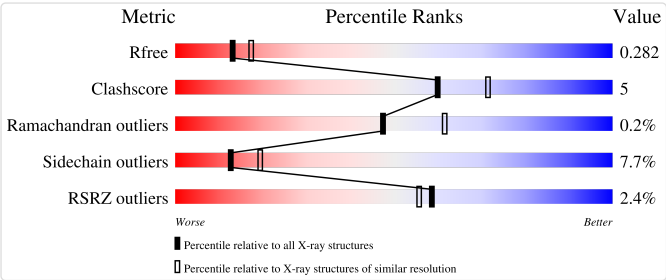
Length (Å)	Angle (°)
a = 92.068	α = 60.84
b = 118.159	β = 67.77
c = 120.659	γ = 81.92

Software Package:

Software Name	Purpose
MAR345dtb	data collection
PHASER	phasing
REFMAC	refinement
HKL-2000	data reduction
SCALEPACK	data scaling

Structure Validation

[View Full Validation Report](#)



Entry History

Deposition Data

Released Date: 2011-04-13
Deposition Author(s): Chittori, S., Savithri, H.S., Murthy, M.R.N.

Revision History (Full details and data files)

- **Version 1.0: 2011-04-13**
Type: Initial release
- **Version 1.1: 2011-07-13**
Changes: Version format compliance
- **Version 1.2: 2023-11-01**
Changes: Data collection, Database references, Derived calculations, Refinement description

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