WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:10 PM GMT

PDB ID : 4KS9

Title : Crystal Structure of Malonyl-CoA decarboxylase (Rmet_2797) from Cupriavidus metallidurans, Northeast Structural Genomics Consortium Target CrR76

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Deposited on : 2013-05-17

Resolution : 2.30 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

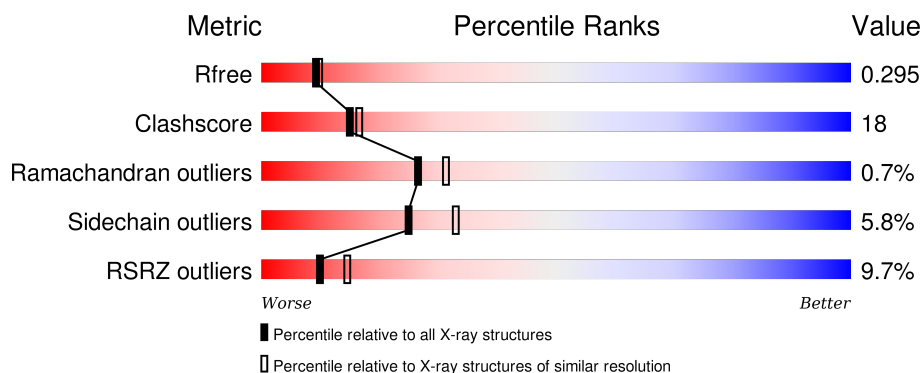|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.295
Clashscore		18
Ramachandran outliers		0.7%
Sidechain outliers		5.8%
RSRZ outliers		9.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	428	8% / 62% / 28% / • / 8%
1	B	428	9% / 60% / 30% / • / 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6535 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Malonyl-CoA decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3118	1971	582	553	12			
1	B	395	Total	C	N	O	S	0	0	0
			3140	1985	585	558	12			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	ALA	-	EXPRESSION TAG	UNP Q1LJK6
A	475	ALA	-	EXPRESSION TAG	UNP Q1LJK6
A	476	ALA	-	EXPRESSION TAG	UNP Q1LJK6
A	477	LEU	-	EXPRESSION TAG	UNP Q1LJK6
A	478	GLU	-	EXPRESSION TAG	UNP Q1LJK6
A	479	HIS	-	EXPRESSION TAG	UNP Q1LJK6
A	480	HIS	-	EXPRESSION TAG	UNP Q1LJK6
A	481	HIS	-	EXPRESSION TAG	UNP Q1LJK6
A	482	HIS	-	EXPRESSION TAG	UNP Q1LJK6
A	483	HIS	-	EXPRESSION TAG	UNP Q1LJK6
A	484	HIS	-	EXPRESSION TAG	UNP Q1LJK6
B	474	ALA	-	EXPRESSION TAG	UNP Q1LJK6
B	475	ALA	-	EXPRESSION TAG	UNP Q1LJK6
B	476	ALA	-	EXPRESSION TAG	UNP Q1LJK6
B	477	LEU	-	EXPRESSION TAG	UNP Q1LJK6
B	478	GLU	-	EXPRESSION TAG	UNP Q1LJK6
B	479	HIS	-	EXPRESSION TAG	UNP Q1LJK6
B	480	HIS	-	EXPRESSION TAG	UNP Q1LJK6
B	481	HIS	-	EXPRESSION TAG	UNP Q1LJK6
B	482	HIS	-	EXPRESSION TAG	UNP Q1LJK6
B	483	HIS	-	EXPRESSION TAG	UNP Q1LJK6
B	484	HIS	-	EXPRESSION TAG	UNP Q1LJK6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

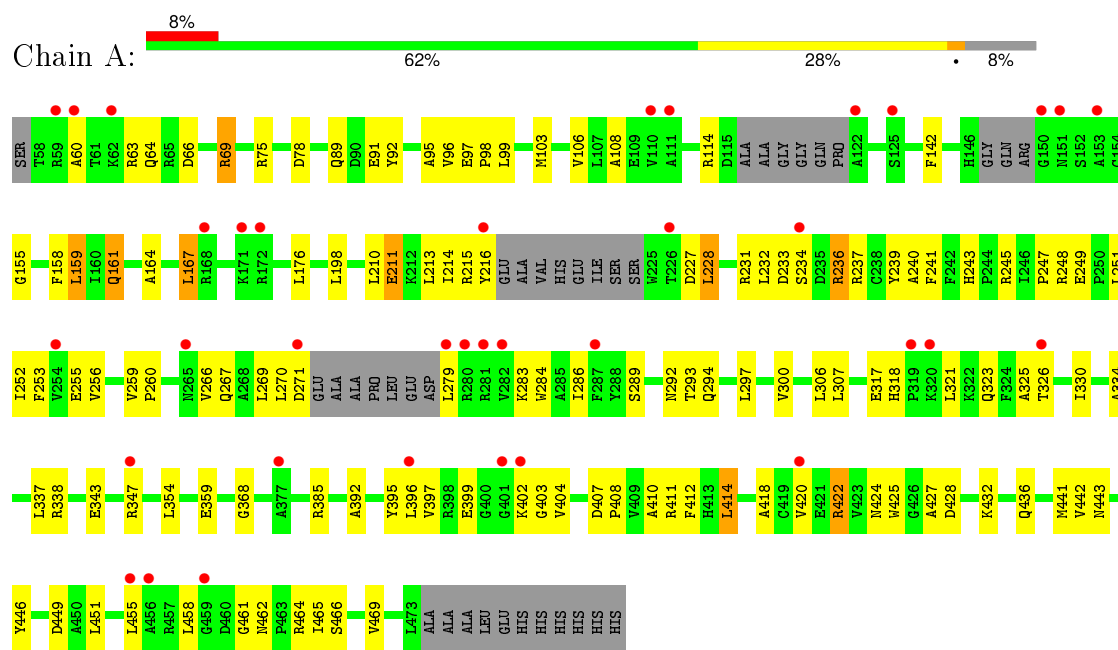| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

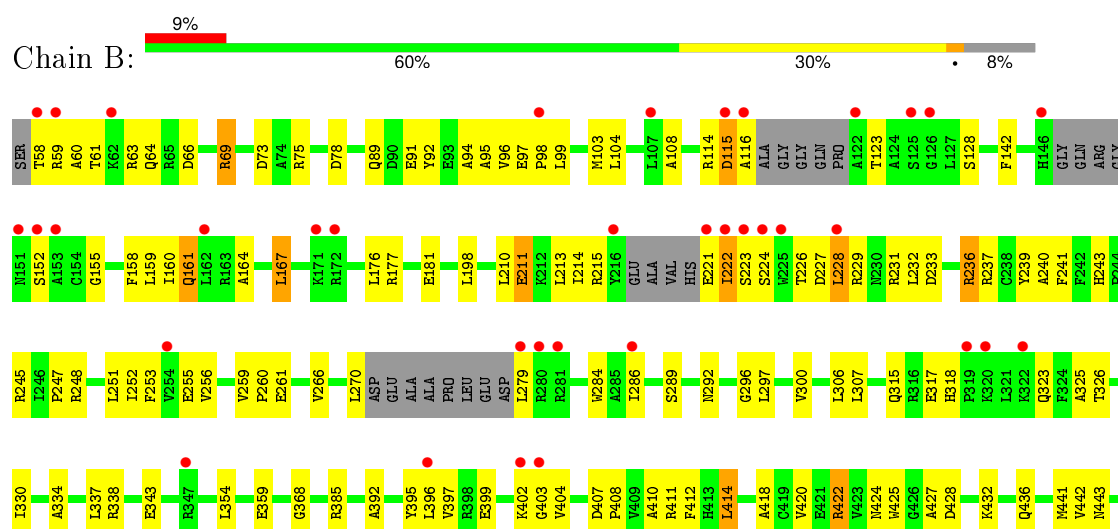| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total 127	O 127	0	0
3	B	149	Total 149	O 149	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Malonyl-CoA decarboxylase

- Molecule 1: Malonyl-CoA decarboxylase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	191.01Å 69.39Å 74.36Å 90.00° 103.80° 90.00°	Depositor
Resolution (Å)	28.75 – 2.30 28.75 – 2.24	Depositor EDS
% Data completeness (in resolution range)	89.1 (28.75-2.30) 92.1 (28.75-2.24)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$<I/\sigma(I)>$ [1]	2.96 (at 2.24Å)	Xtriage
Refinement program	CNS 1.3 & XtalView	Depositor
R, R_{free}	0.239 , 0.286 0.250 , 0.295	Depositor DCC
R_{free} test set	4032 reflections (10.01%)	DCC
Wilson B-factor (Å²)	37.8	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 40.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning [2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Outliers	1 of 44261 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6535	wwPDB-VP
Average B, all atoms (Å²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.37	0/3182	0.58	0/4302
1	B	0.38	0/3204	0.58	0/4332
All	All	0.37	0/6386	0.58	0/8634

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3118	0	3107	110	0
1	B	3140	0	3132	110	0
2	B	1	0	0	0	0
3	A	127	0	0	6	0
3	B	149	0	0	5	0
All	All	6535	0	6239	220	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 220 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ALA:HB1	1:A:63:ARG:HH12	1.37	0.89
1:B:60:ALA:HB1	1:B:63:ARG:HH12	1.41	0.85
1:A:408:PRO:HA	1:A:411:ARG:HH12	1.42	0.84
1:B:247:PRO:O	1:B:248:ARG:HB2	1.78	0.83
1:B:408:PRO:HA	1:B:411:ARG:HH12	1.44	0.81

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	382/428 (89%)	361 (94%)	20 (5%)	1 (0%)	46	57
1	B	385/428 (90%)	360 (94%)	21 (6%)	4 (1%)	19	21
All	All	767/856 (90%)	721 (94%)	41 (5%)	5 (1%)	26	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	ASP
1	B	222	ILE
1	A	402	LYS
1	B	402	LYS
1	B	123	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/342 (93%)	299 (94%)	18 (6%)	25	34
1	B	320/342 (94%)	301 (94%)	19 (6%)	24	32
All	All	637/684 (93%)	600 (94%)	37 (6%)	25	33

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	449	ASP
1	B	69	ARG
1	B	422	ARG
1	A	462	ASN
1	B	59	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	67	GLN
1	B	101	GLN
1	B	315	GLN
1	A	323	GLN
1	A	462	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6   Fit of model and data (i)

6.1   Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	392/428 (91%)	0.55	36 (9%)	11	16	23, 43, 70, 97	0
1	B	395/428 (92%)	0.66	40 (10%)	9	13	22, 43, 72, 91	0
All	All	787/856 (91%)	0.60	76 (9%)	10	14	22, 43, 71, 97	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	ILE	7.0
1	B	223	SER	6.6
1	B	116	ALA	6.6
1	B	125	SER	6.5
1	B	280	ARG	5.4

6.2   Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3   Carbohydrates (i)

There are no carbohydrates in this entry.

6.4   Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	B	501	1/1	0.97	0.11	-0.91	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.