

wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 12:53 PM EDT

PDB ID : 1XK7

Title : Crystal Structure- C2 form- of Escherichia coli Crotonobetainyl-CoA: carnitine

CoA transferase (CaiB)

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Deposited on : 2004-09-27

Resolution : 1.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

Mol Probity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

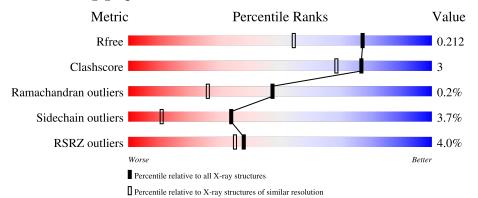
Validation Pipeline (wwPDB-VP) : 2.35

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 1.60 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	Whole archive	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	Δ	408	92%	7% •
1	11	400	3%	7% •
1	В	408	92%	6% •
1	C	400	6%	
1		408	93%	6% •



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10735 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 Crotonobetainyl-CoA:carnitine CoA-transferase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	Λ	407	Total	С	N	О	S	Se	0	0	0
1	A	407	3187	2038	531	594	7	17	0	U	U
1	D	407	Total	С	N	О	S	Se	0	0	0
1	Ъ	407	3187	2038	531	594	7	17	0	U	U
1	С	407	Total	С	N	О	S	Se	0	0	0
1		407	3187	2038	531	594	7	17		U	U

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P31572
A	-1	SER	-	cloning artifact	UNP P31572
A	0	HIS	-	cloning artifact	UNP P31572
В	-2	GLY	-	cloning artifact	UNP P31572
В	-1	SER	-	cloning artifact	UNP P31572
В	0	HIS	-	cloning artifact	UNP P31572
С	-2	GLY	-	cloning artifact	UNP P31572
С	-1	SER	-	cloning artifact	UNP P31572
С	0	HIS	-	cloning artifact	UNP P31572

• Molecule 2 is water.

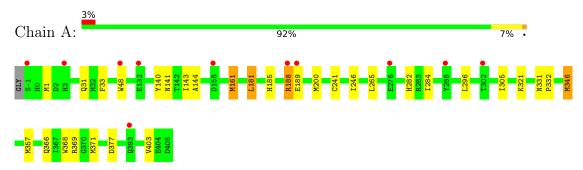
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	381	Total O 381 381	0	0
2	В	383	Total O 383 383	0	0
2	С	410	Total O 410 410	0	0



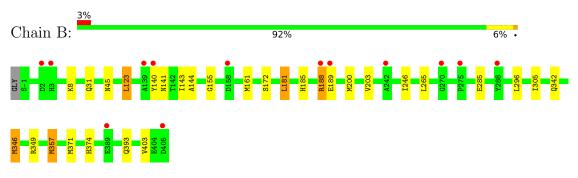
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

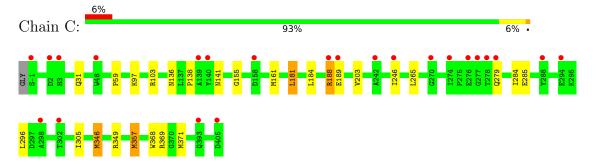
• Molecule 1: Crotonobetainyl-CoA:carnitine CoA-transferase



• Molecule 1: Crotonobetainyl-CoA:carnitine CoA-transferase



• Molecule 1: Crotonobetainyl-CoA:carnitine CoA-transferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	184.28Å 106.17Å 69.68Å	Depositor
a, b, c, α , β , γ	90.00° 107.45° 90.00°	Depositor
Resolution (Å)	45.44 - 1.60	Depositor
rtesolution (A)	45.44 - 1.60	EDS
% Data completeness	99.7 (45.44-1.60)	Depositor
(in resolution range)	99.9 (45.44-1.60)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	4.86 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1, REFMAC 5.1.24	Depositor
D.D.	0.187 , 0.213	Depositor
R, R_{free}	0.187 , 0.212	DCC
R_{free} test set	8476 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 48.9	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10735	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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	Mol Chain		lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.33	0/3251	0.63	1/4380 (0.0%)	
1	В	0.33	0/3251	0.63	0/4380	
1	С	0.34	0/3251	0.63	0/4380	
All	All	0.34	0/9753	0.63	1/13140 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
1	A	377	ASP	CB-CG-OD2	5.21	122.99	118.30

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	3187	0	3122	19	0
1	В	3187	0	3122	24	0
1	С	3187	0	3122	25	0
2	A	381	0	0	1	0
2	В	383	0	0	1	0
2	С	410	0	0	3	0
All	All	10735	0	9366	56	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 3.

The worst 5 of 56 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:B:185:HIS:HA	1:B:188:ARG:HH22	1.02	1.18
1:A:185:HIS:HA	1:A:188:ARG:HH22	1.08	1.15
1:B:161:MSE:HE1	1:C:155:GLY:HA2	1.32	1.11
1:B:155:GLY:HA2	1:C:161:MSE:HE1	1.35	1.04
1:B:185:HIS:HA	1:B:188:ARG:NH2	1.77	0.99

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	Percent	iles
1	A	405/408~(99%)	395 (98%)	9 (2%)	1 (0%)	47 2	6
1	В	405/408~(99%)	395 (98%)	9 (2%)	1 (0%)	47 2	6
1	С	405/408 (99%)	397 (98%)	8 (2%)	0	100 1	00
All	All	1215/1224 (99%)	1187 (98%)	26 (2%)	2 (0%)	47 2	6

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	VAL
1	В	403	VAL

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 o	of residues	for	which	the	${\rm sidechain}$	conformation	was
analysed, and the total number of	residues.							

Mol	Chain	Analysed	Rotameric	Outliers	Percen	tiles
1	A	$334/317 \ (105\%)$	322 (96%)	12 (4%)	35	12
1	В	$334/317 \ (105\%)$	321 (96%)	13 (4%)	32	10
1	С	334/317 (105%)	322 (96%)	12 (4%)	35	12
All	All	$1002/951\ (105\%)$	965 (96%)	37 (4%)	34	11

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

Mol	Chain	Res	Type
1	С	188	ARG
1	С	349	ARG
1	С	189	GLU
1	С	285	GLU
1	В	8	LYS

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

Mol	Chain	Res	Type
1	С	55	GLN
1	С	384	ASN
1	С	374	HIS
1	В	267	HIS
1	С	31	GLN

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 monosaccharides in this entry.



5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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>	$\# \mathrm{RSRZ} {>} 2$	2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	A	390/408~(95%)	0.12	11 (2%) 53	50	10, 18, 33, 39	0
1	В	390/408 (95%)	0.04	13 (3%) 46	43	10, 15, 30, 37	0
1	С	390/408 (95%)	0.18	23 (5%) 22	20	9, 16, 29, 35	0
All	All	1170/1224 (95%)	0.11	47 (4%) 38	35	9, 16, 32, 39	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	TRP	6.4
1	С	188	ARG	4.9
1	В	140	TYR	4.5
1	С	189	GLU	3.8
1	A	188	ARG	3.8

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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.



6.5 Other polymers (i)

There are no such residues in this entry.

