



# wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 02:19 PM BST

PDB ID : 4J0F  
Title : Crystal structure of 3-hydroxyacyl-CoA dehydrogenase from *Caenorhabditis elegans* in P212121 space group  
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Deposited on : 2013-01-30  
Resolution : 2.20 Å (reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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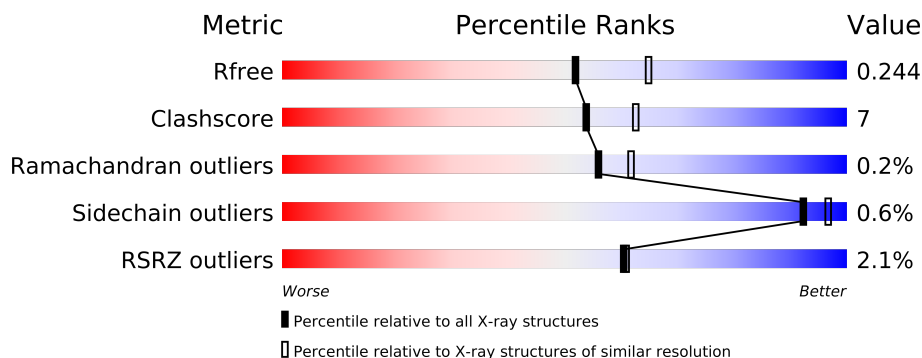
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable23004
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23004

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	320	
1	B	320	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4535 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Probable 3-hydroxyacyl-CoA dehydrogenase F54C8.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	46	0	0
			2189	1385	366	425	13			
1	B	285	Total	C	N	O	S	56	2	0
			2186	1384	363	423	16			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP P34439
A	-1	GLY	-	EXPRESSION TAG	UNP P34439
A	0	SER	-	EXPRESSION TAG	UNP P34439
A	299	GLU	-	EXPRESSION TAG	UNP P34439
A	300	PHE	-	EXPRESSION TAG	UNP P34439
A	301	GLY	-	EXPRESSION TAG	UNP P34439
A	302	THR	-	EXPRESSION TAG	UNP P34439
A	303	SER	-	EXPRESSION TAG	UNP P34439
A	304	SER	-	EXPRESSION TAG	UNP P34439
A	305	THR	-	EXPRESSION TAG	UNP P34439
A	306	GLY	-	EXPRESSION TAG	UNP P34439
A	307	SER	-	EXPRESSION TAG	UNP P34439
A	308	SER	-	EXPRESSION TAG	UNP P34439
A	309	GLY	-	EXPRESSION TAG	UNP P34439
A	310	SER	-	EXPRESSION TAG	UNP P34439
A	311	SER	-	EXPRESSION TAG	UNP P34439
A	312	LEU	-	EXPRESSION TAG	UNP P34439
A	313	GLU	-	EXPRESSION TAG	UNP P34439
A	314	VAL	-	EXPRESSION TAG	UNP P34439
A	315	LEU	-	EXPRESSION TAG	UNP P34439
A	316	PHE	-	EXPRESSION TAG	UNP P34439
A	317	GLN	-	EXPRESSION TAG	UNP P34439
B	-2	MET	-	EXPRESSION TAG	UNP P34439
B	-1	GLY	-	EXPRESSION TAG	UNP P34439
B	0	SER	-	EXPRESSION TAG	UNP P34439

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Chain	Residue	Modelled	Actual	Comment	Reference
B	299	GLU	-	EXPRESSION TAG	UNP P34439
B	300	PHE	-	EXPRESSION TAG	UNP P34439
B	301	GLY	-	EXPRESSION TAG	UNP P34439
B	302	THR	-	EXPRESSION TAG	UNP P34439
B	303	SER	-	EXPRESSION TAG	UNP P34439
B	304	SER	-	EXPRESSION TAG	UNP P34439
B	305	THR	-	EXPRESSION TAG	UNP P34439
B	306	GLY	-	EXPRESSION TAG	UNP P34439
B	307	SER	-	EXPRESSION TAG	UNP P34439
B	308	SER	-	EXPRESSION TAG	UNP P34439
B	309	GLY	-	EXPRESSION TAG	UNP P34439
B	310	SER	-	EXPRESSION TAG	UNP P34439
B	311	SER	-	EXPRESSION TAG	UNP P34439
B	312	LEU	-	EXPRESSION TAG	UNP P34439
B	313	GLU	-	EXPRESSION TAG	UNP P34439
B	314	VAL	-	EXPRESSION TAG	UNP P34439
B	315	LEU	-	EXPRESSION TAG	UNP P34439
B	316	PHE	-	EXPRESSION TAG	UNP P34439
B	317	GLN	-	EXPRESSION TAG	UNP P34439

- Molecule 2 is water.

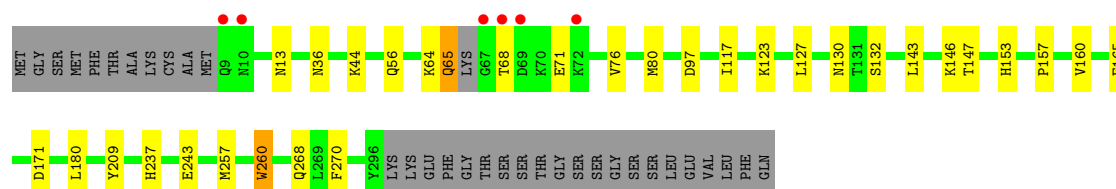
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	92	Total O 92 92	0	0
2	B	68	Total O 68 68	0	0

### 3 Residue-property plots

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.

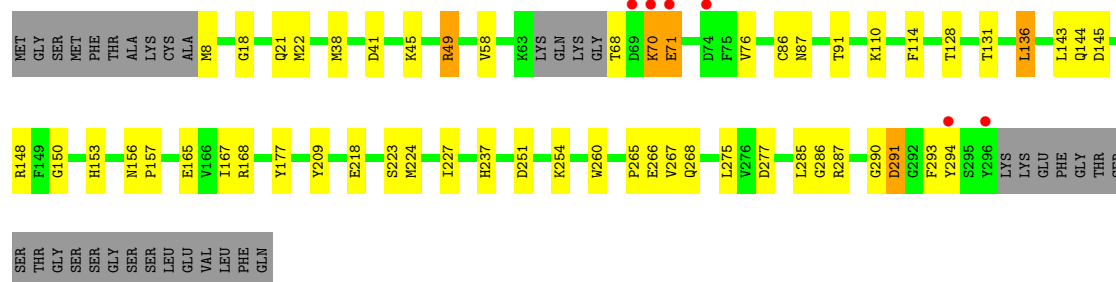
- Molecule 1: Probable 3-hydroxyacyl-CoA dehydrogenase F54C8.1

Chain A: 



- Molecule 1: Probable 3-hydroxyacyl-CoA dehydrogenase F54C8.1

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.56Å 96.37Å 114.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.66 – 2.20 31.28 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (73.66-2.20) 98.7 (31.28-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.71 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.187 , 0.246 0.187 , 0.244	Depositor DCC
$R_{free}$ test set	1765 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 35279 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4535	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.89	4/2222 (0.2%)	0.96	3/2994 (0.1%)
1	B	0.87	2/2222 (0.1%)	0.99	5/2994 (0.2%)
All	All	0.88	6/4444 (0.1%)	0.97	8/5988 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	LYS	CE-NZ	-7.39	1.30	1.49
1	A	56	GLN	CG-CD	-5.79	1.37	1.51
1	B	70	LYS	CD-CE	5.57	1.65	1.51
1	B	260	TRP	CD2-CE2	5.46	1.48	1.41
1	A	260	TRP	CD2-CE2	5.39	1.47	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	ARG	NE-CZ-NH2	-15.30	112.65	120.30
1	B	49	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	A	123	LYS	CD-CE-NZ	6.71	127.14	111.70
1	B	136	LEU	CA-CB-CG	5.82	128.67	115.30
1	A	44	LYS	CD-CE-NZ	5.78	124.99	111.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2189	0	2205	23	0
1	B	2186	0	2203	39	0
2	A	92	0	0	4	0
2	B	68	0	0	2	0
All	All	4535	0	4408	59	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 59 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:68:THR:HB	1:B:71:GLU:HB2	1.43	0.98
1:B:254:LYS:HE2	1:B:277:ASP:OD1	1.76	0.85
1:B:153:HIS:HD2	1:B:165:GLU:OE1	1.61	0.83
1:B:290:GLY:O	1:B:291:ASP:OD1	2.01	0.78
1:A:13:ASN:ND2	1:A:36:ASN:HD22	1.81	0.77

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	283/320 (88%)	276 (98%)	7 (2%)	0	100	100
1	B	283/320 (88%)	276 (98%)	6 (2%)	1 (0%)	43	45
All	All	566/640 (88%)	552 (98%)	13 (2%)	1 (0%)	56	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	287	ARG



### 5.3.2 Protein sidechains ⓘ

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	237/264 (90%)	236 (100%)	1 (0%)	95	98
1	B	238/264 (90%)	236 (99%)	2 (1%)	89	95
All	All	475/528 (90%)	472 (99%)	3 (1%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	TYR
1	B	209	TYR
1	B	291	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	ASN
1	B	268	GLN
1	B	153	HIS
1	A	156	ASN
1	B	144	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	287/320 (89%)	-0.26	6 (2%) 60 61	23, 35, 61, 95	14 (4%)
1	B	285/320 (89%)	-0.25	6 (2%) 60 61	21, 37, 67, 104	18 (6%)
All	All	572/640 (89%)	-0.26	12 (2%) 60 61	21, 36, 65, 104	32 (5%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	THR	4.6
1	B	71	GLU	4.0
1	B	70	LYS	3.6
1	A	69	ASP	3.5
1	B	74	ASP	3.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.