



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 12:37 pm GMT

PDB ID : 4J0F
Title : Crystal structure of 3-hydroxyacyl-CoA dehydrogenase from *Caenorhabditis elegans* in P212121 space group
Authors : Xu, Y.; Sun, F.; Zhai, Y.
Deposited on : 2013-01-30
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

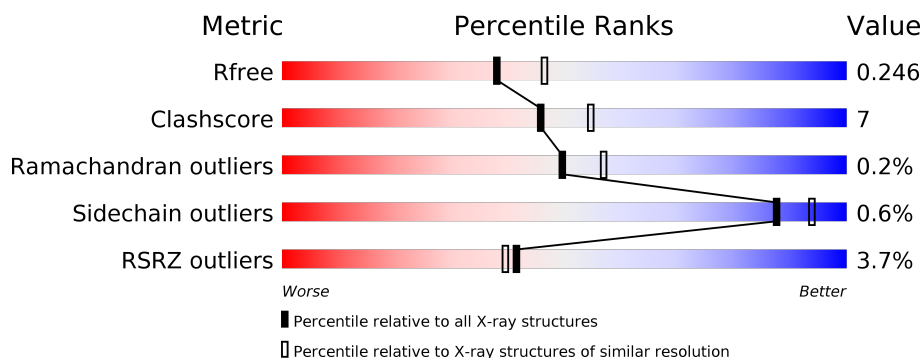
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (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 ≥ 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 $\leq 5\%$. 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	320	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>10%</div> </div> </div>
1	B	320	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>11%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4535 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 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

Continued on next page...

Continued from previous page...

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.187 , 0.246 0.188 , 0.246	Depositor DCC
R_{free} test set	1765 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4535	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

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%)

All (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
1	A	65	GLN	CD-NE2	-5.04	1.20	1.32

All (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
1	B	18	GLY	N-CA-C	-5.21	100.08	113.10
1	A	97	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	71	GLU	OE1-CD-OE2	5.06	129.38	123.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	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

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 7.

All (59) 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: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
1:B:21:GLN:CD	1:B:156:ASN:HD21	1.88	0.77
1:A:130:ASN:HB2	2:A:477:HOH:O	1.88	0.72
1:A:13:ASN:HD21	1:A:36:ASN:HD22	1.37	0.71
1:A:13:ASN:HD22	1:A:36:ASN:HB2	1.56	0.71
1:B:68:THR:HB	1:B:71:GLU:CB	2.20	0.69
1:B:144:GLN:HB3	2:B:407:HOH:O	1.92	0.69
1:B:21:GLN:OE1	1:B:156:ASN:ND2	2.26	0.68
1:A:132:SER:HB2	2:A:415:HOH:O	1.95	0.66
1:B:218:GLU:OE2	1:B:275:LEU:HB2	1.99	0.63
1:A:268:GLN:HE22	1:B:267:VAL:HA	1.65	0.62
1:B:136:LEU:HD22	1:B:167:ILE:HG22	1.79	0.62
1:A:132:SER:HB3	1:A:153:HIS:CE1	2.36	0.60
1:A:237:HIS:ND1	1:B:237:HIS:CD2	2.69	0.60
1:B:22:MET:SD	1:B:156:ASN:HB2	2.43	0.59
1:B:251:ASP:HB3	1:B:285:LEU:HD22	1.87	0.56
1:B:136:LEU:CD2	1:B:167:ILE:HG22	2.35	0.56
1:A:64:LYS:O	1:A:65:GLN:C	2.43	0.55
1:A:153:HIS:HD2	1:A:165:GLU:OE1	1.90	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LYS:HE3	1:B:131:THR:HB	1.89	0.55
1:B:286:GLY:N	1:B:291:ASP:O	2.33	0.54
1:B:21:GLN:CD	1:B:156:ASN:ND2	2.61	0.53
1:B:145:ASP:OD2	1:B:148:ARG:HD2	2.08	0.53
1:A:76:VAL:O	1:A:80:MET:HG2	2.08	0.52
1:B:153:HIS:CD2	1:B:165:GLU:OE1	2.52	0.52
1:B:223:SER:O	1:B:227:ILE:HG13	2.10	0.52
1:B:156:ASN:OD1	1:B:157:PRO:HA	2.09	0.52
1:B:136:LEU:HD22	1:B:167:ILE:CG2	2.40	0.51
1:B:21:GLN:NE2	1:B:156:ASN:HD21	2.08	0.51
1:B:86:CYS:SG	1:B:91:THR:HB	2.51	0.51
1:A:268:GLN:H	1:B:268:GLN:NE2	2.11	0.48
1:B:70:LYS:O	1:B:71:GLU:C	2.54	0.47
1:B:58:VAL:HG12	1:B:76:VAL:HG22	1.98	0.46
1:A:260:TRP:HB3	1:A:270:PHE:CD2	2.51	0.46
1:B:224[A]:MET:CE	1:B:294:TYR:CE1	3.00	0.45
1:A:68:THR:O	1:A:71:GLU:HB3	2.16	0.45
1:B:38:MET:SD	1:B:86:CYS:HB2	2.57	0.45
1:A:146:LYS:HE3	2:A:434:HOH:O	2.17	0.44
1:B:218:GLU:OE2	1:B:275:LEU:CB	2.66	0.44
1:B:41:ASP:O	1:B:87:ASN:HA	2.18	0.44
1:B:168:ARG:HB3	1:B:177:TYR:CD1	2.52	0.44
1:B:265:PRO:HD2	1:B:266:GLU:OE1	2.17	0.43
1:B:114:PHE:HB3	1:B:143:LEU:HD21	1.99	0.43
1:A:153:HIS:CD2	1:A:165:GLU:OE1	2.70	0.43
1:A:147:THR:HA	1:A:171:ASP:O	2.19	0.42
1:A:157:PRO:HG2	1:A:160:VAL:HB	2.00	0.42
1:A:143:LEU:HD23	1:A:143:LEU:HA	1.79	0.42
1:A:243:GLU:HB3	2:A:492:HOH:O	2.18	0.41
1:B:224[A]:MET:HE3	1:B:293:PHE:HB3	2.01	0.41
1:B:45:LYS:O	1:B:49:ARG:HG3	2.20	0.41
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.83	0.41
1:A:117:ILE:HG21	1:A:127:LEU:HD22	2.03	0.40
1:A:257:MET:SD	1:A:270:PHE:HA	2.62	0.40
1:B:128:THR:HA	1:B:150:GLY:O	2.22	0.40
1:B:8:MET:N	2:B:437:HOH:O	2.55	0.40

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	283/320 (88%)	276 (98%)	7 (2%)	0	100	100
1	B	283/320 (88%)	276 (98%)	6 (2%)	1 (0%)	36	39
All	All	566/640 (88%)	552 (98%)	13 (2%)	1 (0%)	49	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	287	ARG

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	237/264 (90%)	236 (100%)	1 (0%)	92	96
1	B	238/264 (90%)	236 (99%)	2 (1%)	83	91
All	All	475/528 (90%)	472 (99%)	3 (1%)	87	94

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. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	153	HIS
1	A	156	ASN
1	A	268	GLN
1	B	13	ASN
1	B	144	GLN
1	B	153	HIS
1	B	237	HIS
1	B	268	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 carbohydrates 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, 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	287/320 (89%)	-0.28	10 (3%) 44 42	23, 35, 61, 95	14 (4%)
1	B	285/320 (89%)	-0.20	11 (3%) 39 37	21, 37, 67, 104	18 (6%)
All	All	572/640 (89%)	-0.24	21 (3%) 41 39	21, 36, 65, 104	32 (5%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	GLU	4.3
1	B	70	LYS	3.9
1	A	68	THR	3.7
1	A	69	ASP	3.6
1	B	74	ASP	3.4
1	A	10	ASN	3.1
1	B	296	TYR	2.9
1	B	75	PHE	2.7
1	B	290	GLY	2.6
1	A	64	LYS	2.5
1	A	65	GLN	2.5
1	B	69	ASP	2.4
1	B	77	THR	2.4
1	B	59	THR	2.4
1	A	61	LEU	2.4
1	A	62	SER	2.3
1	A	266	GLU	2.2
1	A	67	GLY	2.2
1	A	72	LYS	2.0
1	B	294	TYR	2.0
1	B	292	GLY	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.