



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 03:52 PM EDT

PDB ID : 3HLK
Title : Crystal structure of human mitochondrial acyl-CoA thioesterase (ACOT2)
Authors : Mandel, C.R.; Tweel, B.; Tong, L.
Deposited on : 2009-05-27
Resolution : 2.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

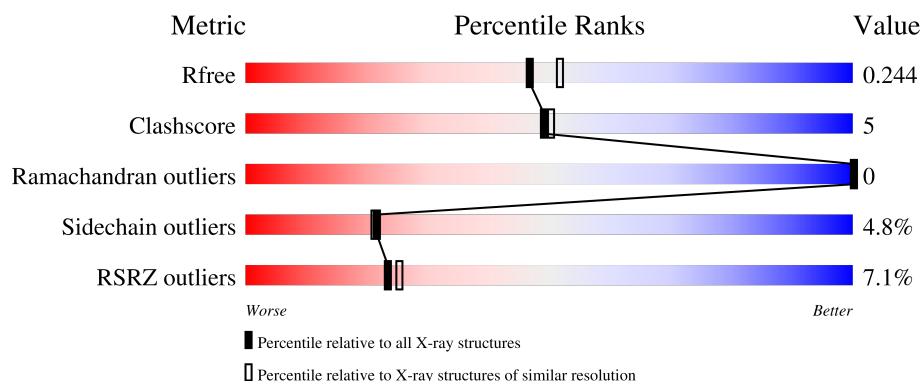
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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 $\leq 5\%$. 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	446	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	446	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>•</div> <div>8%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6829 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 Acyl-coenzyme A thioesterase 2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	Se	0	0	0
			3183	2038	564	566	7	8			
1	B	411	Total	C	N	O	S	Se	0	0	0
			3205	2053	567	570	7	8			

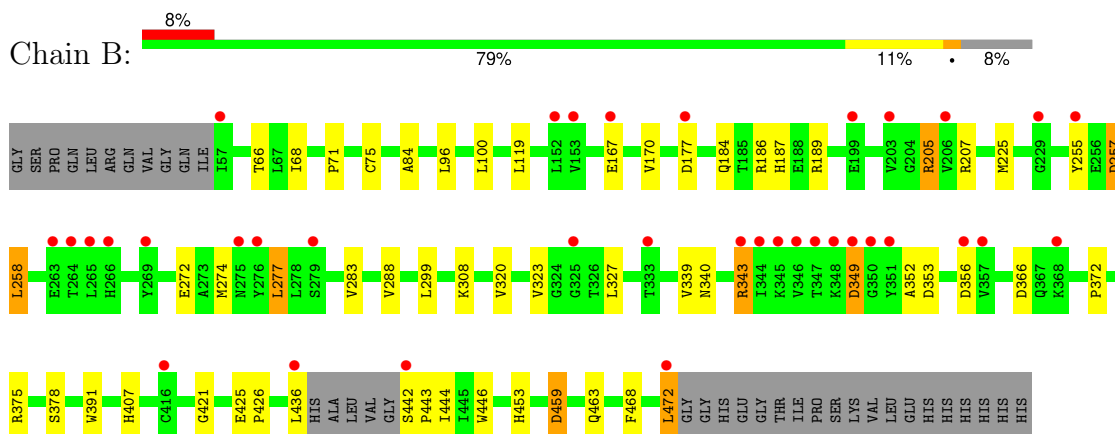
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	484	LEU	-	expression tag	UNP P49753
A	485	GLU	-	expression tag	UNP P49753
A	486	HIS	-	expression tag	UNP P49753
A	487	HIS	-	expression tag	UNP P49753
A	488	HIS	-	expression tag	UNP P49753
A	489	HIS	-	expression tag	UNP P49753
A	490	HIS	-	expression tag	UNP P49753
A	491	HIS	-	expression tag	UNP P49753
B	484	LEU	-	expression tag	UNP P49753
B	485	GLU	-	expression tag	UNP P49753
B	486	HIS	-	expression tag	UNP P49753
B	487	HIS	-	expression tag	UNP P49753
B	488	HIS	-	expression tag	UNP P49753
B	489	HIS	-	expression tag	UNP P49753
B	490	HIS	-	expression tag	UNP P49753
B	491	HIS	-	expression tag	UNP P49753

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	224	Total	O	0	0
			224	224		
2	B	217	Total	O	0	0
			217	217		

- Molecule 1: Acyl-coenzyme A thioesterase 2, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.56Å 124.56Å 131.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.6 (30.00-2.10) 95.6 (30.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.194 , 0.236 0.248 , 0.244	Depositor DCC
R_{free} test set	5152 reflections (7.47%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6829	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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	0.53	0/3259	0.73	8/4411 (0.2%)
1	B	0.52	0/3281	0.74	8/4442 (0.2%)
All	All	0.53	0/6540	0.73	16/8853 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	353	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	100	LEU	CA-CB-CG	6.47	130.18	115.30
1	B	353	ASP	CB-CG-OD2	6.45	124.11	118.30
1	B	366	ASP	CB-CG-OD2	6.15	123.84	118.30
1	B	459	ASP	CB-CG-OD2	6.01	123.70	118.30
1	A	175	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	356	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	349	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	459	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	177	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	257	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	366	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	387	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	177	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	257	ASP	CB-CG-OD2	5.15	122.94	118.30

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	3183	0	3191	35	0
1	B	3205	0	3217	37	0
2	A	224	0	0	8	0
2	B	217	0	0	3	0
All	All	6829	0	6408	68	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 5.

All (68) 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:407:HIS:HE1	1:B:407:HIS:HE1	1.14	0.95
1:A:416:CYS:SG	2:A:686:HOH:O	2.24	0.94
1:A:416:CYS:HB3	2:A:686:HOH:O	1.73	0.88
1:A:416:CYS:CB	2:A:686:HOH:O	2.21	0.87
1:A:407:HIS:HE1	1:B:407:HIS:CE1	1.94	0.85
1:B:274:MSE:HE1	1:B:308:LYS:O	1.76	0.85
1:A:187:HIS:HE1	1:A:189:ARG:HH11	1.24	0.83
1:B:421:GLY:H	1:B:453:HIS:HD2	1.30	0.80
1:A:407:HIS:CE1	1:B:407:HIS:HE1	2.00	0.76
1:A:421:GLY:H	1:A:453:HIS:HD2	1.33	0.76
1:B:343:ARG:HB2	1:B:343:ARG:HH11	1.52	0.75
1:B:205:ARG:CB	1:B:205:ARG:HH11	2.00	0.74
1:A:277:LEU:HD22	1:A:283:VAL:HG21	1.70	0.73
1:B:340:ASN:HB3	1:B:343:ARG:NH1	2.03	0.73
1:B:421:GLY:H	1:B:453:HIS:CD2	2.08	0.72
1:B:187:HIS:HE1	1:B:189:ARG:HH11	1.38	0.70
1:A:376:ALA:O	2:A:685:HOH:O	2.11	0.67
1:B:186:ARG:HH11	1:B:186:ARG:HG3	1.60	0.67
1:B:352:ALA:HB3	1:B:444:ILE:HG22	1.80	0.64
1:B:277:LEU:HD22	1:B:283:VAL:HG21	1.81	0.62
1:B:75:CYS:HB2	2:B:675:HOH:O	2.00	0.61
1:B:343:ARG:HH11	1:B:343:ARG:CB	2.14	0.61
1:A:187:HIS:CE1	1:A:189:ARG:HH11	2.13	0.60
1:A:205:ARG:HD3	1:A:272:GLU:OE1	2.00	0.60
1:B:205:ARG:HH11	1:B:205:ARG:HB2	1.64	0.60
1:A:143:LEU:HD21	1:A:166:VAL:HG21	1.84	0.58
1:B:468:PHE:O	1:B:472:LEU:HB2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:NH1	1:B:272:GLU:OE1	2.37	0.57
1:A:278:LEU:HD13	1:A:288:VAL:HG13	1.88	0.56
1:B:343:ARG:HH11	1:B:343:ARG:CG	2.19	0.56
1:A:421:GLY:H	1:A:453:HIS:CD2	2.18	0.56
1:A:248:MSE:HE3	1:A:277:LEU:HG	1.87	0.55
1:B:187:HIS:HD2	2:B:535:HOH:O	1.89	0.54
1:B:187:HIS:CE1	1:B:189:ARG:HH11	2.22	0.53
1:A:274:MSE:HE1	1:A:310:ILE:HD11	1.91	0.52
1:B:442:SER:N	1:B:443:PRO:HD2	2.25	0.52
1:B:207:ARG:HD2	1:B:257:ASP:OD1	2.09	0.52
1:A:407:HIS:CE1	1:B:407:HIS:CE1	2.84	0.51
1:A:158:ARG:NE	1:A:233:LEU:HD22	2.26	0.51
1:A:248:MSE:HE1	1:A:276:TYR:CD2	2.47	0.50
1:B:340:ASN:HB3	1:B:343:ARG:HH12	1.74	0.49
1:A:248:MSE:HE1	1:A:276:TYR:HD2	1.77	0.48
1:B:96:LEU:HD22	1:B:170:VAL:HG22	1.96	0.48
1:B:459:ASP:O	1:B:463:GLN:HG2	2.15	0.47
1:A:97:ARG:HH12	1:A:178:PRO:HG3	1.80	0.47
1:A:459:ASP:O	1:A:463:GLN:HG2	2.15	0.46
1:B:68:ILE:CG2	1:B:84:ALA:HB3	2.46	0.46
1:B:255:TYR:O	1:B:258:LEU:HB2	2.16	0.46
1:B:372:PRO:HB2	1:B:375:ARG:HD3	1.98	0.46
1:A:215:GLU:HB3	1:A:216:PRO:HA	1.98	0.45
1:B:225:MSE:HE1	1:B:299:LEU:HD13	1.97	0.45
1:A:178:PRO:HA	2:A:690:HOH:O	2.15	0.44
1:A:220:PRO:HB3	1:A:472:LEU:HB3	2.00	0.44
1:A:320:VAL:CG1	1:A:400:ALA:HB2	2.48	0.44
1:A:401:CYS:HB2	2:A:672:HOH:O	2.18	0.43
1:B:339:VAL:HG12	1:B:340:ASN:N	2.34	0.43
1:B:425:GLU:HB3	1:B:426:PRO:HD2	2.00	0.43
1:B:444:ILE:HD11	1:B:446:TRP:CH2	2.53	0.43
1:A:472:LEU:HG	2:A:689:HOH:O	2.19	0.42
1:A:444:ILE:HD11	1:A:446:TRP:CZ3	2.54	0.42
1:A:347:THR:HA	1:A:348:LYS:HA	1.84	0.42
1:B:186:ARG:HH11	1:B:186:ARG:CG	2.31	0.42
1:A:151:PRO:O	1:A:152:LEU:HB2	2.20	0.42
1:A:150:LYS:HA	1:A:151:PRO:HD2	1.92	0.41
1:B:205:ARG:HH12	1:B:272:GLU:CD	2.23	0.41
1:B:71:PRO:HG2	2:B:675:HOH:O	2.20	0.41
1:A:372:PRO:HB2	1:A:375:ARG:HD3	2.03	0.40
1:A:455:MSE:SE	2:A:691:HOH:O	2.90	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	404/446 (91%)	394 (98%)	10 (2%)	0	100	100
1	B	407/446 (91%)	393 (97%)	14 (3%)	0	100	100
All	All	811/892 (91%)	787 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	332/355 (94%)	317 (96%)	15 (4%)	23	24
1	B	335/355 (94%)	318 (95%)	17 (5%)	20	19
All	All	667/710 (94%)	635 (95%)	32 (5%)	21	21

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	67	LEU
1	A	96	LEU
1	A	119	LEU
1	A	143	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	260	LYS
1	A	274	MSE
1	A	277	LEU
1	A	294	SER
1	A	320	VAL
1	A	323	VAL
1	A	348	LYS
1	A	384	VAL
1	A	391	TRP
1	A	444	ILE
1	B	66	THR
1	B	119	LEU
1	B	167	GLU
1	B	184	GLN
1	B	205	ARG
1	B	258	LEU
1	B	277	LEU
1	B	288	VAL
1	B	320	VAL
1	B	323	VAL
1	B	327	LEU
1	B	343	ARG
1	B	349	ASP
1	B	378	SER
1	B	391	TRP
1	B	436	LEU
1	B	472	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
1	A	407	HIS
1	A	453	HIS
1	A	469	HIS
1	B	184	GLN
1	B	187	HIS
1	B	407	HIS
1	B	453	HIS
1	B	463	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 oligosaccharides 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

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, 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	400/446 (89%)	0.51	21 (5%) 33 35	19, 30, 50, 74	0
1	B	403/446 (90%)	0.74	36 (8%) 17 18	20, 32, 52, 72	0
All	All	803/892 (90%)	0.63	57 (7%) 23 25	19, 31, 51, 74	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	GLY	6.0
1	B	57	ILE	4.2
1	A	177	ASP	4.2
1	B	346	VAL	3.9
1	B	347	THR	3.8
1	A	347	THR	3.7
1	B	206	VAL	3.6
1	A	351	TYR	3.6
1	B	276	TYR	3.6
1	B	177	ASP	3.4
1	A	352	ALA	3.2
1	B	279	SER	3.1
1	B	265	LEU	3.1
1	B	351	TYR	3.0
1	B	348	LYS	3.0
1	B	344	ILE	2.9
1	B	263	GLU	2.9
1	B	345	LYS	2.9
1	B	350	GLY	2.8
1	A	416	CYS	2.8
1	B	275	ASN	2.7
1	B	436	LEU	2.7
1	B	442	SER	2.7
1	B	153	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	152	LEU	2.6
1	B	416	CYS	2.6
1	B	356	ASP	2.5
1	B	255	TYR	2.5
1	A	58	ARG	2.5
1	B	333	THR	2.5
1	B	167	GLU	2.4
1	B	349	ASP	2.4
1	A	348	LYS	2.4
1	A	445	ILE	2.4
1	A	255	TYR	2.4
1	A	356	ASP	2.4
1	A	261	THR	2.4
1	A	346	VAL	2.4
1	A	276	TYR	2.4
1	B	199	GLU	2.3
1	A	205	ARG	2.3
1	B	266	HIS	2.3
1	B	343	ARG	2.3
1	A	344	ILE	2.3
1	B	472	LEU	2.3
1	B	203	VAL	2.2
1	B	229	GLY	2.2
1	A	73	GLY	2.2
1	B	264	THR	2.2
1	B	269	TYR	2.2
1	A	343	ARG	2.2
1	A	355	VAL	2.2
1	B	368	LYS	2.1
1	A	217	GLY	2.1
1	B	357	VAL	2.0
1	B	325	GLY	2.0
1	A	158	ARG	2.0

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 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.