



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:45 PM GMT

PDB ID : 4MOC
Title : Human Acyl-coenzyme A Thioesterase 12
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Deposited on : 2013-09-12
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/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
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

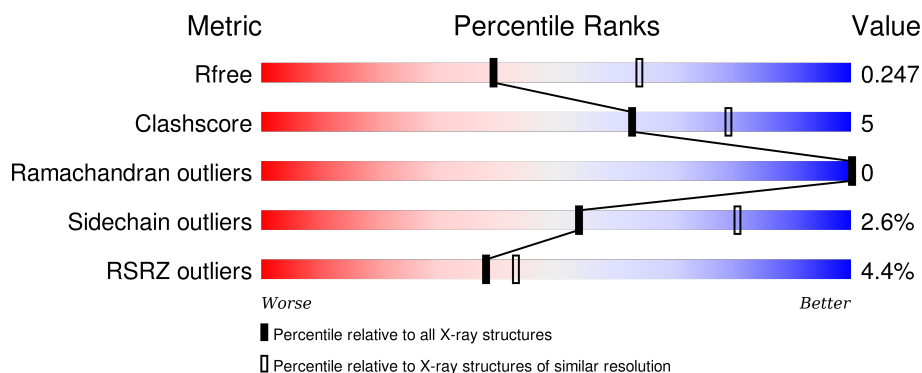
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	332	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2240 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.

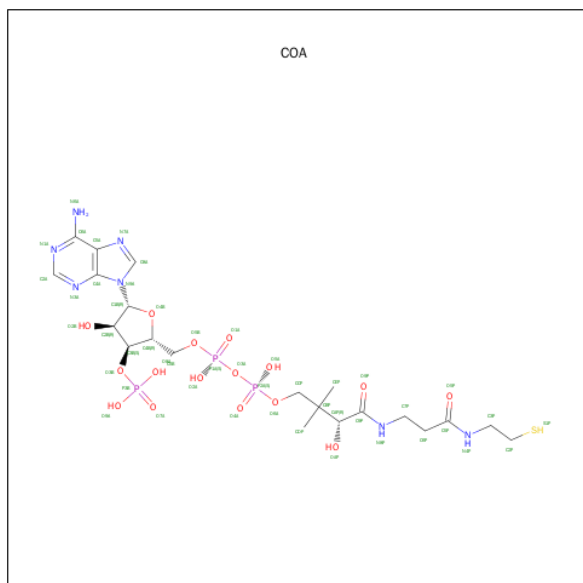
- Molecule 1 is a protein called Acyl-coenzyme A thioesterase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	2121	1337	377	394	13	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	SER	-	EXPRESSION TAG	UNP Q8WYK0
A	6	MET	-	EXPRESSION TAG	UNP Q8WYK0

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).

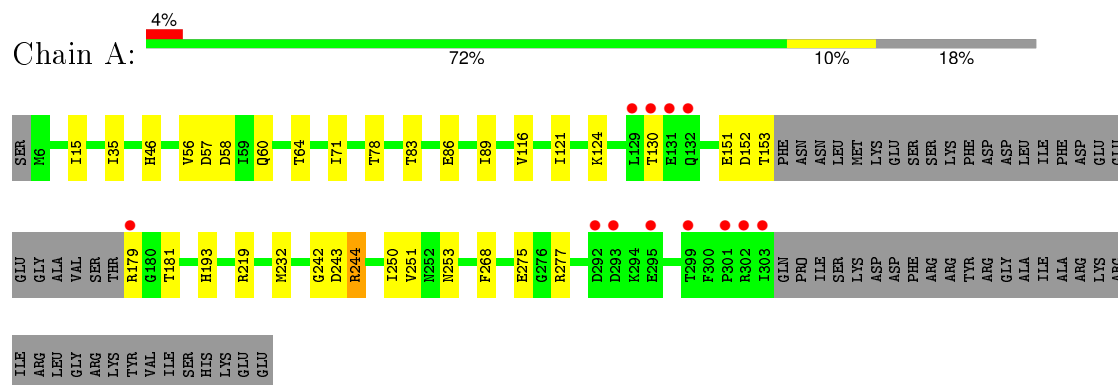


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	48	21	7	16	3	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		

- Molecule 1: Acyl-coenzyme A thioesterase 12



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.56 Å 123.56 Å 49.75 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.38 – 2.50 31.38 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.2 (31.38-2.50) 87.7 (31.38-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.51 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.247 0.207 , 0.247	Depositor DCC
R_{free} test set	720 reflections (5.62%)	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.5	EDS
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 14329 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2240	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.27	0/2160	0.47	0/2925

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

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	2121	0	2126	23	0
2	A	48	0	32	1	0
3	A	71	0	0	1	0
All	All	2240	0	2158	23	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 (23) 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:179:ARG:HH21	1:A:251:VAL:H	1.21	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLY:O	1:A:244:ARG:NH1	2.20	0.74
1:A:179:ARG:HE	1:A:251:VAL:HB	1.55	0.71
1:A:181:THR:OG1	1:A:219:ARG:HB3	1.95	0.67
1:A:179:ARG:HH12	1:A:181:THR:N	2.03	0.57
1:A:179:ARG:NH2	1:A:251:VAL:H	1.99	0.54
1:A:58:ASP:OD1	1:A:232:MET:N	2.39	0.54
1:A:179:ARG:HH21	1:A:251:VAL:N	1.99	0.53
1:A:179:ARG:NH1	1:A:181:THR:H	2.08	0.52
1:A:179:ARG:NE	1:A:251:VAL:HB	2.25	0.50
1:A:179:ARG:HH12	1:A:181:THR:H	1.58	0.50
1:A:83:THR:HG22	1:A:121:ILE:HG23	1.93	0.49
1:A:152:ASP:OD1	1:A:153:THR:N	2.45	0.49
1:A:275:GLU:OE1	1:A:277:ARG:NH1	2.46	0.49
1:A:179:ARG:NH2	1:A:250:ILE:HG13	2.27	0.48
1:A:46:HIS:NE2	1:A:124:LYS:O	2.45	0.47
1:A:78:THR:OG1	1:A:86:GLU:OE1	2.25	0.46
1:A:15:ILE:HD11	1:A:71:ILE:HG12	1.97	0.45
1:A:56:VAL:HG12	1:A:57:ASP:O	2.17	0.45
1:A:193:HIS:HA	3:A:551:HOH:O	2.18	0.44
1:A:243:ASP:HB2	1:A:268:PHE:O	2.18	0.44
1:A:151:GLU:OE2	2:A:401:COA:N6A	2.44	0.43
1:A:35:ILE:HG23	1:A:89:ILE:HG21	2.00	0.43

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	270/332 (81%)	258 (96%)	12 (4%)	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	230 / 282 (82%)	223 (97%)	7 (3%)	48 76

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60[A]	GLN
1	A	60[B]	GLN
1	A	64	THR
1	A	116	VAL
1	A	130	THR
1	A	244	ARG
1	A	253	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	224	HIS

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

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	COA	A	401	-	40,50,50	1.89	9 (22%)	50,75,75	2.08	6 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	A	401	-	-	0/44/64/64	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	COA	C2B-C3B	-2.77	1.46	1.53
2	A	401	COA	C3B-C4B	-2.32	1.46	1.52
2	A	401	COA	C6A-N6A	2.07	1.41	1.34
2	A	401	COA	C6P-C5P	2.43	1.56	1.51
2	A	401	COA	C2A-N3A	2.52	1.36	1.32
2	A	401	COA	O4B-C4B	2.91	1.51	1.45
2	A	401	COA	C5P-N4P	4.86	1.45	1.33
2	A	401	COA	O4B-C1B	5.64	1.48	1.41
2	A	401	COA	C9P-N8P	5.70	1.45	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	COA	N3A-C2A-N1A	-10.90	120.55	128.89
2	A	401	COA	C4B-O4B-C1B	-4.80	104.44	109.72
2	A	401	COA	P2A-O3A-P1A	-3.10	124.03	132.73
2	A	401	COA	C4A-C5A-N7A	-2.57	107.12	109.48
2	A	401	COA	O3A-P2A-O6A	2.69	110.08	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	COA	O3A-P1A-O5B	2.88	110.59	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	COA	1	0

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	273/332 (82%)	-0.06	12 (4%) 38 43	18, 33, 68, 93	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	302	ARG	6.6
1	A	179	ARG	4.9
1	A	301	PRO	4.8
1	A	129	LEU	4.4
1	A	303	ILE	4.1
1	A	293	ASP	4.1
1	A	131	GLU	3.5
1	A	295	GLU	3.2
1	A	130	THR	2.9
1	A	292	ASP	2.9
1	A	132	GLN	2.2
1	A	299	THR	2.1

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	COA	A	401	48/48	0.97	0.10	-1.26	14,27,41,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.