



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 12:34 PM BST

PDB ID : 3TQE
Title : Structure of the malonyl CoA-acyl carrier protein transacylase (fabD) from *Coxiella burnetii*
Authors : Franklin, M.C.; Cheung, J.; Rudolph, M.; Cassidy, M.; Gary, E.; Burshteyn, F.; Love, J.
Deposited on : 2011-09-09
Resolution : 1.50 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

<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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

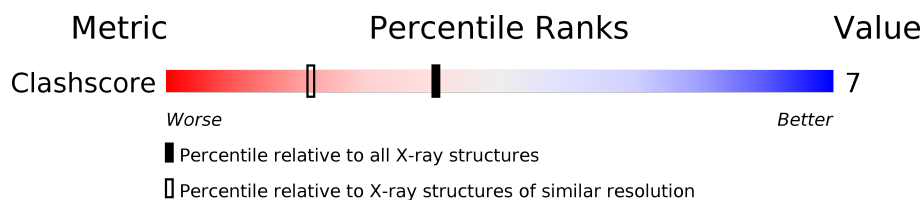
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

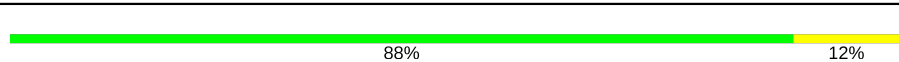
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3144 (1.50-1.50)

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 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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	316	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2915 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.

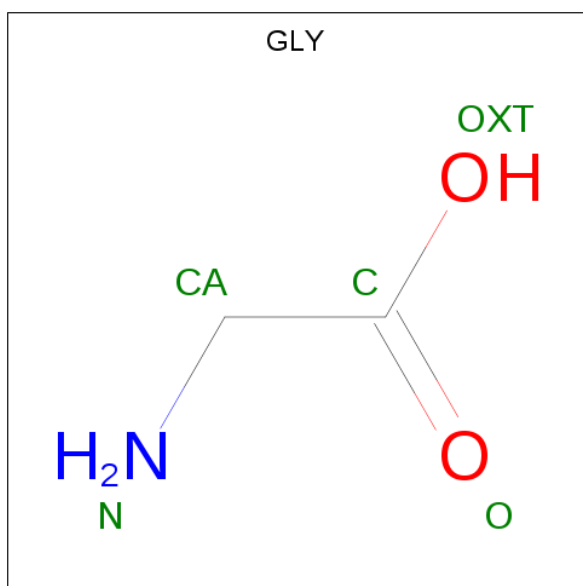
- Molecule 1 is a protein called Malonyl-CoA-[acyl-carrier-protein] transacylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	316	2554	1636	437	465	5	11	0	26	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q83E39
A	-1	TYR	-	EXPRESSION TAG	UNP Q83E39
A	0	VAL	-	EXPRESSION TAG	UNP Q83E39

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	A	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0

- Molecule 4 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	347	Total O 347 347	0	0

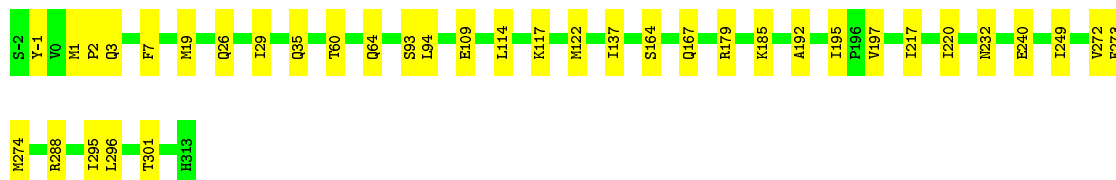
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: Malonyl-CoA-[acyl-carrier-protein] transacylase

Chain A:  88% 12%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.36Å 63.18Å 42.77Å 90.00° 98.81° 90.00°	Depositor
Resolution (Å)	85.66 – 1.50	Depositor
% Data completeness (in resolution range)	99.5 (85.66-1.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 1.50Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.146 , 0.171	Depositor
Wilson B-factor (Å ²)	16.7	Xtrriage
Anisotropy	0.461	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2915	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.71	1/2666 (0.0%)	0.71	2/3599 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	GLU	CD-OE1	5.50	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	MSE	CG-SE-CE	-6.36	84.91	98.90
1	A	179	ARG	NE-CZ-NH1	5.09	122.84	120.30

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	2554	0	2692	38	0
2	A	10	0	4	0	0
3	A	4	0	6	0	0
4	A	347	0	0	9	0
All	All	2915	0	2702	38	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 (38) 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:60[A]:THR:HG23	4:A:436:HOH:O	1.52	1.09
1:A:-1:TYR:OH	1:A:1[B]:MSE:HE3	1.64	0.98
1:A:64:GLN:HE22	1:A:122[A]:MSE:CE	1.92	0.82
1:A:93:SER:H	1:A:232:ASN:HD21	1.25	0.82
1:A:26:GLN:HE22	1:A:301:THR:H	1.30	0.80
1:A:60[A]:THR:HG22	4:A:572:HOH:O	1.83	0.78
1:A:217[A]:ILE:HD12	1:A:249:ILE:HD11	1.67	0.77
1:A:114:LEU:HD22	1:A:220[B]:ILE:HD13	1.69	0.74
1:A:64:GLN:NE2	1:A:122[A]:MSE:CE	2.56	0.68
1:A:217[A]:ILE:HD12	1:A:249:ILE:CD1	2.27	0.64
1:A:288[A]:ARG:NH1	4:A:642:HOH:O	2.30	0.64
1:A:64:GLN:NE2	1:A:122[A]:MSE:HE1	2.13	0.62
1:A:64:GLN:HE22	1:A:122[A]:MSE:HE1	1.64	0.61
1:A:35[B]:GLN:HG3	4:A:514:HOH:O	2.01	0.61
1:A:64:GLN:HE22	1:A:122[A]:MSE:HE2	1.65	0.58
1:A:3:GLN:HG2	1:A:272:VAL:HG21	1.85	0.58
1:A:64:GLN:NE2	1:A:122[A]:MSE:HE2	2.20	0.57
1:A:109:GLU:CD	4:A:381:HOH:O	2.46	0.53
1:A:64:GLN:HA	1:A:94:LEU:HD21	1.91	0.53
1:A:137:ILE:HD13	1:A:167[B]:GLN:HE21	1.73	0.52
1:A:217[B]:ILE:HG13	1:A:220[B]:ILE:HD11	1.91	0.52
1:A:26:GLN:NE2	1:A:301:THR:H	2.04	0.49
1:A:64:GLN:HA	1:A:94:LEU:CD2	2.43	0.49
1:A:29[B]:ILE:CD1	4:A:641:HOH:O	2.60	0.49
1:A:1[A]:MSE:HG3	1:A:2:PRO:N	2.29	0.48
1:A:117[B]:LYS:CE	4:A:591:HOH:O	2.61	0.48
1:A:93:SER:N	1:A:232:ASN:HD21	2.04	0.48
1:A:29[B]:ILE:HD11	4:A:641:HOH:O	2.15	0.47
1:A:-1:TYR:HH	1:A:1[B]:MSE:HE3	1.78	0.46
1:A:7:PHE:CE1	1:A:274[B]:MSE:HG3	2.51	0.45
1:A:185:LYS:HG2	1:A:192:ALA:HB3	2.00	0.44
1:A:117[B]:LYS:NZ	4:A:611:HOH:O	2.51	0.44
1:A:195[B]:ILE:HG13	1:A:197:VAL:HG22	1.99	0.44
1:A:274[A]:MSE:HE3	1:A:296:LEU:HD12	2.00	0.44
1:A:217[B]:ILE:HG13	1:A:220[B]:ILE:CD1	2.48	0.43
1:A:164:SER:OG	1:A:288[B]:ARG:NE	2.51	0.43
1:A:93:SER:H	1:A:232:ASN:ND2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:PHE:O	1:A:295:ILE:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

3 ligands are 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	GLY	A	314	-	1,4,4	0.13	0	0,4,4	0.00	-
2	GLY	A	315	-	1,4,4	0.13	0	0,4,4	0.00	-
3	EDO	A	316	-	3,3,3	0.45	0	2,2,2	0.32	0

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	GLY	A	314	-	-	0/0/2/2	-
2	GLY	A	315	-	-	0/0/2/2	-
3	EDO	A	316	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.