



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 26, 2017 – 07:16 PM EDT

PDB ID : 1EF8  
Title : CRYSTAL STRUCTURE OF METHYLMALONYL COA DECARBOXY-  
LASE  
Authors : Benning, M.M.; Haller, T.; Gerlt, J.A.; Holden, H.M.  
Deposited on : unknown  
Resolution : 1.85 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345



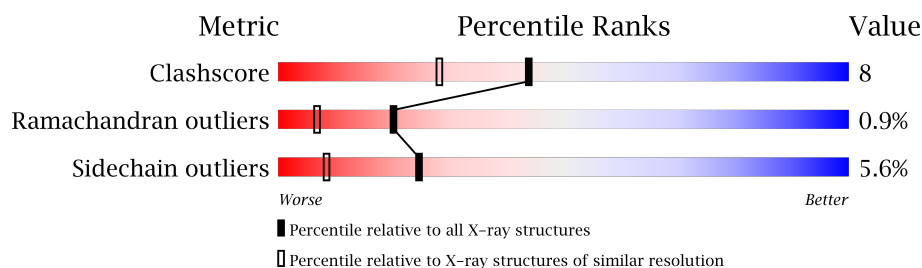
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	261	 77% 18% ...
1	B	261	 68% 25% ...
1	C	261	 69% 23% . .



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6570 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 METHYLMALONYL COA DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2013	1282	343	376	12			
1	B	253	Total	C	N	O	S	0	0	0
			1985	1262	340	371	12			
1	C	250	Total	C	N	O	S	0	0	0
			1968	1253	337	366	12			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	221	Total	O	0	0
			221	221		
3	B	189	Total	O	0	0
			189	189		
3	C	193	Total	O	0	0
			193	193		

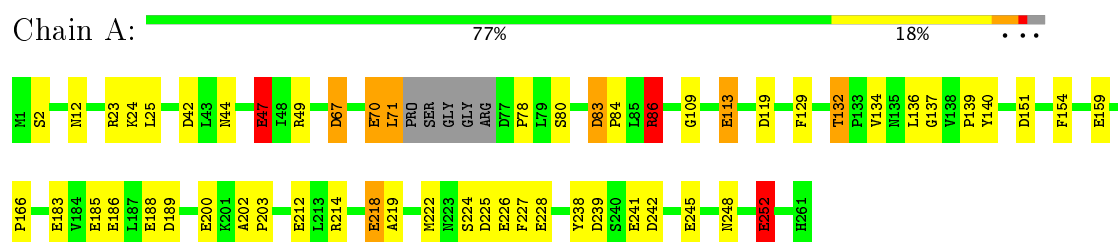


### 3 Residue-property plots

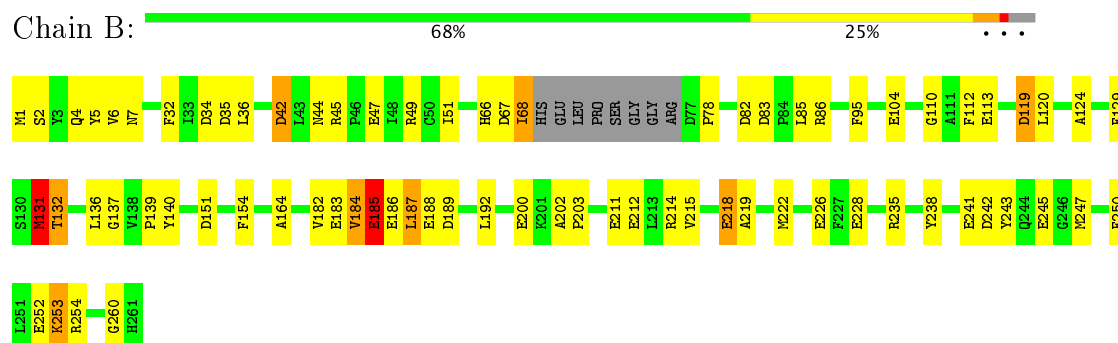
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

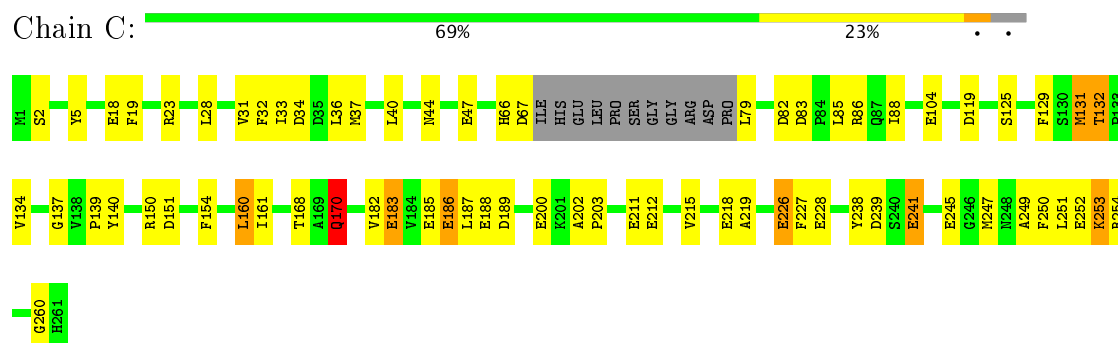
#### • Molecule 1: METHYLMALONYL COA DECARBOXYLASE



#### • Molecule 1: METHYLMALONYL COA DECARBOXYLASE



#### • Molecule 1: METHYLMALONYL COA DECARBOXYLASE





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.30 Å   115.40 Å   80.30 Å 90.00°   127.80°   90.00°	Depositor
Resolution (Å)	30.00 – 1.85	Depositor
% Data completeness (in resolution range)	89.0 (30.00-1.85)	Depositor
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, $R_{free}$	0.178 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6570	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.06	15/2051 (0.7%)	1.12	20/2773 (0.7%)
1	B	1.04	17/2022 (0.8%)	1.11	20/2734 (0.7%)
1	C	1.04	17/2005 (0.8%)	1.11	21/2709 (0.8%)
All	All	1.05	49/6078 (0.8%)	1.12	61/8216 (0.7%)

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	GLU	CD-OE2	7.73	1.34	1.25
1	B	226	GLU	CD-OE2	7.50	1.33	1.25
1	C	218	GLU	CD-OE2	7.49	1.33	1.25
1	A	47	GLU	CD-OE2	7.35	1.33	1.25
1	B	104	GLU	CD-OE2	7.23	1.33	1.25

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	ARG	NE-CZ-NH2	-11.33	114.63	120.30
1	A	86	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	B	86	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	B	86	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	C	227	PHE	CB-CG-CD1	-7.14	115.80	120.80

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	2013	0	2021	28	0
1	B	1985	0	1995	40	0
1	C	1968	0	1980	31	0
2	A	1	0	0	0	0
3	A	221	0	0	5	0
3	B	189	0	0	3	0
3	C	193	0	0	3	0
All	All	6570	0	5996	91	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 8.

The worst 5 of 91 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:ILE:HD11	1:B:250:PHE:CE1	2.04	0.93
1:B:68:ILE:HD11	1:B:250:PHE:HE1	1.38	0.88
1:C:28:LEU:HB3	1:C:33:ILE:HD11	1.61	0.81
1:B:66:HIS:CE1	1:B:85:LEU:HD22	2.16	0.81
1:C:131:MET:SD	1:C:161:ILE:HG12	2.28	0.73

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	252/261 (97%)	242 (96%)	7 (3%)	3 (1%)	15	4
1	B	249/261 (95%)	240 (96%)	7 (3%)	2 (1%)	22	8
1	C	246/261 (94%)	234 (95%)	10 (4%)	2 (1%)	22	8
All	All	747/783 (95%)	716 (96%)	24 (3%)	7 (1%)	20	7

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	219	ALA
1	A	219	ALA
1	C	219	ALA
1	B	132	THR
1	A	132	THR

### 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	221/225 (98%)	212 (96%)	9 (4%)	35	16
1	B	218/225 (97%)	204 (94%)	14 (6%)	20	5
1	C	216/225 (96%)	202 (94%)	14 (6%)	20	5
All	All	655/675 (97%)	618 (94%)	37 (6%)	25	8

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	140	TYR
1	B	187	LEU
1	C	247	MET
1	B	154	PHE
1	B	184	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:



Mol	Chain	Res	Type
1	B	66	HIS
1	B	248	ASN
1	C	66	HIS
1	B	44	ASN
1	C	44	ASN

### 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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.