

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 19, 2023 – 11:35 PM EDT

PDB ID : 8HGN

Title : Crystal structure of MeaC (Mesaconyl-CoA hydratase)

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Deposited on : 2022-11-15

Resolution : 1.95 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 (i) 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 (1)) 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 : 2.35.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

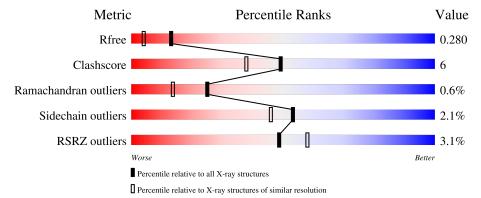
Validation Pipeline (wwPDB-VP) : 2.35.1

## 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 1.95 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	Similar resolution
Metric	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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		
			3%		
1	A	356	84%	15%	••



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2817 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.

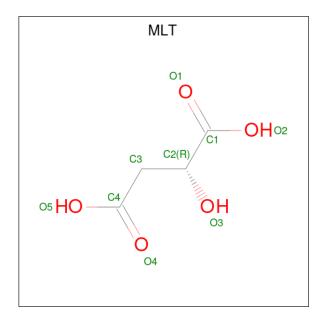
• Molecule 1 is a protein called Beta-methylmalyl-CoA dehydratase.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	Λ	353	Total	С	N	О	S	0	0	0
1	A	393	2718	1726	481	508	3	U	U	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	LEU	-	expression tag	UNP B7KZU4
A	350	GLU	-	expression tag	UNP B7KZU4
A	351	HIS	-	expression tag	UNP B7KZU4
A	352	HIS	-	expression tag	UNP B7KZU4
A	353	HIS	-	expression tag	UNP B7KZU4
A	354	HIS	-	expression tag	UNP B7KZU4
A	355	HIS	-	expression tag	UNP B7KZU4
A	356	HIS	-	expression tag	UNP B7KZU4

• Molecule 2 is D-MALATE (three-letter code: MLT) (formula:  $C_4H_6O_5$ ).





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

## • Molecule 3 is water.

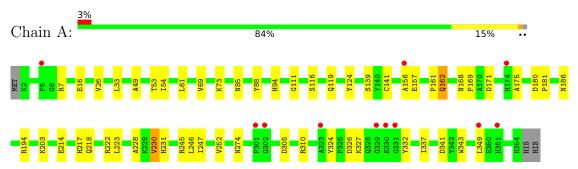
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	90	Total O 90 90	0	0



# 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 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.

• Molecule 1: Beta-methylmalyl-CoA dehydratase





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants	79.22Å 79.22Å 91.01Å	Donositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	32.12 - 1.95	Depositor
Resolution (A)	32.10 - 1.95	EDS
% Data completeness	98.5 (32.12-1.95)	Depositor
(in resolution range)	98.5 (32.10-1.95)	EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	9.18 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D.D.	0.210 , 0.278	Depositor
$R, R_{free}$	0.216 , $0.280$	DCC
$R_{free}$ test set	1180 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36 , 41.3	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.40, < L^2> = 0.23$	Xtriage
Estimated twinning fraction	0.096 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2817	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MLT

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).

Mal	Chain	Bond	lengths	Bo	nd angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.76	0/2788	0.95	$2/3799 \ (0.1\%)$

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	222	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	A	222	ARG	NE-CZ-NH1	7.81	124.21	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	2718	0	2657	32	0
2	A	9	0	4	2	0
3	A	90	0	0	1	0
All	All	2817	0	2661	32	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 6.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash



## magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	overlap (Å)
1:A:162:GLN:OE1	1:A:162:GLN:HA	1.83	0.78
1:A:186:ASN:HD21	1:A:194:ARG:HE	1.42	0.67
1:A:119:GLN:HG3	3:A:507:HOH:O	2.00	0.60
1:A:49:ALA:O	1:A:53:THR:HG23	2.02	0.58
1:A:274:ASN:ND2	1:A:341:ASP:OD2	2.27	0.58
1:A:214:GLU:OE2	1:A:217:HIS:HE1	1.90	0.55
1:A:230:VAL:CG1	1:A:246:LEU:HB3	2.38	0.54
1:A:85:ASN:HB2	2:A:401:MLT:H32	1.89	0.53
1:A:218:GLN:NE2	1:A:245:ARG:HH11	2.06	0.53
1:A:228:ALA:HB3	1:A:231:HIS:CD2	2.44	0.53
1:A:218:GLN:HE22	1:A:245:ARG:HH11	1.56	0.52
1:A:230:VAL:HG13	1:A:246:LEU:HB3	1.93	0.51
1:A:33:LEU:HD23	1:A:223:LEU:HD13	1.93	0.50
1:A:69:VAL:O	1:A:73:LYS:HD2	2.13	0.48
1:A:310:ARG:HB2	1:A:343:TRP:CH2	2.49	0.47
1:A:169:PRO:HD3	1:A:343:TRP:CZ2	2.50	0.46
1:A:310:ARG:HB2	1:A:343:TRP:CZ3	2.51	0.46
1:A:168:ASN:HA	1:A:169:PRO:HD2	1.76	0.46
1:A:7:ARG:HH12	1:A:16:GLU:CD	2.20	0.45
1:A:203:LYS:HB3	1:A:324:TYR:CE1	2.51	0.45
1:A:181:PRO:HB2	1:A:349:LEU:O	2.16	0.45
1:A:252:VAL:HG11	1:A:337:ILE:HG13	1.98	0.45
1:A:26:VAL:HG11	1:A:61:LEU:HD13	1.99	0.44
1:A:181:PRO:HG3	1:A:305:ASP:HA	2.00	0.43
1:A:54:ILE:O	1:A:180:ASP:N	2.43	0.43
1:A:85:ASN:HB2	2:A:401:MLT:C3	2.49	0.42
1:A:327:LYS:HA	1:A:332:TYR:HA	2.02	0.42
1:A:94:HIS:O	1:A:175:ALA:HA	2.20	0.41
1:A:217:HIS:HB2	1:A:247:ILE:HG23	2.02	0.41
1:A:111:GLY:HA3	1:A:161:PRO:HD3	2.03	0.41
1:A:111:GLY:HA3	1:A:124:TYR:HB2	2.03	0.40
1:A:88:TYR:HA	1:A:141:CYS:O	2.22	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	351/356 (99%)	329 (94%)	20 (6%)	2 (1%)	25 14

#### All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	ALA
1	A	326	ASP

#### 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	Analysed Rotameric Outliers		Percentiles
1	A	281/284 (99%)	275 (98%)	6 (2%)	53 46

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	SER
1	A	139	SER
1	A	157	GLU
1	A	162	GLN
1	A	171	ASP
1	A	230	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	119	GLN
1	A	186	ASN
1	A	217	HIS
1	A	218	GLN
1	A	251	HIS
1	A	328	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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

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	Tuno	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Res	Link	В	ond leng	$\operatorname{gths}$	В	ond ang	les
		туре		res L	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2						
	2	MLT	A	401	-	8,8,8	1.43	2 (25%)	10,10,10	1.79	1 (10%)						

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	MLT	A	401	-	-	4/8/8/8	-

#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
2	A	401	MLT	O5-C4	-2.44	1.22	1.30
2	A	401	MLT	O2-C1	-2.19	1.23	1.30

#### All (1) bond angle outliers are listed below:

$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	A	401	MLT	C2-C3-C4	4.24	122.62	112.13

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	MLT	O2-C1-C2-C3
2	A	401	MLT	O1-C1-C2-C3
2	A	401	MLT	O2-C1-C2-O3
2	A	401	MLT	C2-C3-C4-O5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	MLT	2	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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	353/356 (99%)	0.18	11 (3%) 49 58	14, 33, 58, 72	0

All (11) RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	A	174	HIS	4.0
1	A	330	GLU	3.9
1	A	323	ALA	3.6
1	A	302	GLY	2.9
1	A	351	HIS	2.9
1	A	156	ALA	2.8
1	A	301	PRO	2.7
1	A	331	GLY	2.6
1	A	5	PRO	2.4
1	A	349	LEU	2.3
1	A	329	GLY	2.2

## 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 monosaccharides 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. The B-factors column lists the minimum,



median,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	MLT	A	401	9/9	0.94	0.13	24,31,35,35	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

