



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:55 pm BST

PDB ID : 3RSI  
Title : The structure of a putative enoyl-CoA hydratase/isomerase from *Mycobacterium abscessus* ATCC 19977 / DSM 44196  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2011-05-02  
Resolution : 2.00 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](mailto: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.

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 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) : 2.11

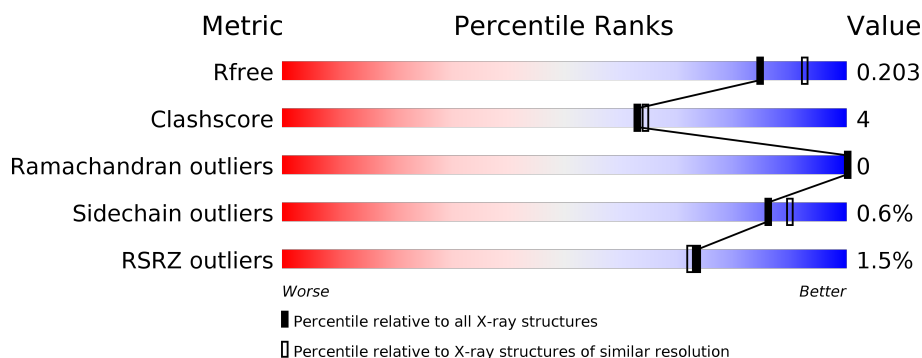
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	265	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>8%</div> </div> </div>
1	B	265	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>
1	C	265	<div> <div></div> <div> <div></div> <div>86%</div> <div>5%</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	A	265	-	-	X	-
3	IOD	A	267	-	-	-	X
3	IOD	B	264	-	-	-	X
3	IOD	B	265	-	-	X	X
3	IOD	B	268	-	-	X	-
3	IOD	C	262	-	-	-	X
3	IOD	C	264	-	-	X	-
3	IOD	C	267	-	-	X	-
3	IOD	C	270	-	-	-	X
3	IOD	C	271	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5950 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 Putative enoyl-CoA hydratase/isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	2	0
			1812	1128	337	338	9			
1	B	244	Total	C	N	O	S	0	1	0
			1806	1125	331	341	9			
1	C	241	Total	C	N	O	S	0	0	0
			1780	1112	329	330	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP B1MIA8
A	-2	PRO	-	EXPRESSION TAG	UNP B1MIA8
A	-1	GLY	-	EXPRESSION TAG	UNP B1MIA8
A	0	SER	-	EXPRESSION TAG	UNP B1MIA8
B	-3	GLY	-	EXPRESSION TAG	UNP B1MIA8
B	-2	PRO	-	EXPRESSION TAG	UNP B1MIA8
B	-1	GLY	-	EXPRESSION TAG	UNP B1MIA8
B	0	SER	-	EXPRESSION TAG	UNP B1MIA8
C	-3	GLY	-	EXPRESSION TAG	UNP B1MIA8
C	-2	PRO	-	EXPRESSION TAG	UNP B1MIA8
C	-1	GLY	-	EXPRESSION TAG	UNP B1MIA8
C	0	SER	-	EXPRESSION TAG	UNP B1MIA8

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

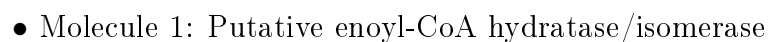
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	9	Total	I	0	0
			9	9		
3	A	5	Total	I	0	0
			5	5		
3	C	11	Total	I	0	0
			11	11		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	182	Total	O	0	0
			182	182		
4	B	164	Total	O	0	0
			164	164		
4	C	175	Total	O	0	0
			175	175		



- Molecule 1: Putative enoyl-CoA hydratase/isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.85Å 121.67Å 64.55Å 90.00° 96.65° 90.00°	Depositor
Resolution (Å)	19.97 – 2.00 19.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.97-2.00) 95.2 (19.97-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.32 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.150 , 0.195 0.161 , 0.203	Depositor DCC
$R_{free}$ test set	2371 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.8	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 51.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5950	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

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

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	0.57	0/1846	0.65	0/2500
1	B	0.59	0/1837	0.67	0/2491
1	C	0.56	0/1808	0.68	0/2451
All	All	0.57	0/5491	0.67	0/7442

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	251	LYS	Peptide
1	B	64	VAL	Peptide

### 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	1812	0	1818	14	0
1	B	1806	0	1798	17	0
1	C	1780	0	1781	10	0
2	A	6	0	8	0	0
3	A	5	0	0	4	0
3	B	9	0	0	7	0
3	C	11	0	0	8	0
4	A	182	0	0	3	0
4	B	164	0	0	3	0
4	C	175	0	0	4	0
All	All	5950	0	5405	46	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 4.

All (46) 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:64:VAL:HG23	1:B:64:VAL:O	1.64	0.98
1:A:5:ARG:O	3:A:265:IOD:I	2.53	0.97
1:B:43:GLU:OE1	3:B:270:IOD:I	2.60	0.89
1:B:64:VAL:CG2	1:B:64:VAL:O	2.28	0.80
3:A:267:IOD:I	4:A:642:HOH:O	2.69	0.79
3:B:262:IOD:I	4:B:399:HOH:O	2.71	0.78
1:B:66:GLY:HA2	4:C:511:HOH:O	1.83	0.78
1:A:82:LEU:HD12	1:A:87:ILE:HD11	1.72	0.71
1:B:153:GLN:NE2	3:B:268:IOD:I	2.92	0.70
4:A:278:HOH:O	3:C:267:IOD:I	2.80	0.68
4:B:281:HOH:O	3:C:267:IOD:I	2.84	0.66
3:C:270:IOD:I	4:C:638:HOH:O	2.84	0.66
1:C:32:ASN:OD1	3:C:266:IOD:I	2.84	0.65
1:B:249:ALA:O	1:B:251:LYS:HA	1.96	0.65
1:C:43:GLU:OE1	3:C:264:IOD:I	2.85	0.65
1:C:227:ARG:NH1	4:C:584:HOH:O	2.37	0.58
1:C:11:ARG:NH1	1:C:47:ASP:OD2	2.37	0.58
1:B:16:VAL:HG11	1:B:44:ILE:HG12	1.85	0.58
1:A:82:LEU:HD12	1:A:87:ILE:CD1	2.34	0.56
1:A:31:THR:HG23	1:A:82:LEU:HG	1.87	0.55
1:A:6:GLU:OE1	1:A:22:ARG:HD2	2.07	0.55
1:B:29:LEU:O	1:B:67:ASP:HB3	2.07	0.55
1:B:238:ILE:HD11	4:C:405:HOH:O	2.06	0.54
1:A:21:ASN:ND2	3:A:265:IOD:I	3.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ARG:HB2	1:A:201:VAL:HG22	1.92	0.52
1:C:40:ALA:HA	3:C:264:IOD:I	2.82	0.49
1:A:51:ARG:NH1	1:A:205:PRO:HG3	2.28	0.48
3:B:265:IOD:I	4:B:749:HOH:O	2.90	0.47
1:A:6:GLU:OE1	1:A:30:SER:OG	2.27	0.47
1:A:8:LEU:HD21	3:A:265:IOD:I	2.84	0.47
1:A:51:ARG:HG2	1:A:51:ARG:HH11	1.81	0.46
4:A:310:HOH:O	3:B:268:IOD:I	2.92	0.46
1:A:51:ARG:CZ	1:A:205:PRO:HG3	2.45	0.46
1:A:17:ILE:N	1:A:17:ILE:HD12	2.30	0.46
1:B:235:ARG:HB2	1:B:236:PRO:HD3	1.98	0.45
1:B:138:ARG:CB	3:B:265:IOD:I	3.35	0.45
1:B:63:CYS:SG	1:B:65:GLY:HA2	2.58	0.44
1:B:149:ARG:HG2	3:B:268:IOD:I	2.88	0.43
1:C:153:GLN:NE2	3:C:267:IOD:I	3.13	0.43
1:C:213:GLU:O	1:C:217:ARG:HG2	2.21	0.41
1:C:17:ILE:CD1	1:C:54:ILE:HD12	2.51	0.41
1:B:92:LEU:O	1:B:119:GLN:HG3	2.20	0.41
1:B:249:ALA:C	1:B:251:LYS:HA	2.41	0.40
1:A:211:ALA:HA	1:B:147:MET:SD	2.62	0.40
1:B:14:PRO:HG2	1:C:201:VAL:HG21	2.03	0.40
1:C:64:VAL:O	3:C:265:IOD:I	3.09	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	241/265 (91%)	233 (97%)	8 (3%)	0	100	100
1	B	241/265 (91%)	229 (95%)	12 (5%)	0	100	100
1	C	237/265 (89%)	231 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	719/795 (90%)	693 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	181/201 (90%)	180 (99%)	1 (1%)	86	90
1	B	180/201 (90%)	178 (99%)	2 (1%)	73	78
1	C	176/201 (88%)	176 (100%)	0	100	100
All	All	537/603 (89%)	534 (99%)	3 (1%)	86	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	GLU
1	B	84	PRO
1	B	223	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 26 ligands modelled in this entry, 25 are monoatomic - leaving 1 for Mogul analysis.

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	GOL	A	262	-	5,5,5	0.45	0	5,5,5	0.46	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	GOL	A	262	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	262	GOL	O1-C1-C2-C3
2	A	262	GOL	C1-C2-C3-O3
2	A	262	GOL	O2-C2-C3-O3
2	A	262	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	243/265 (91%)	-0.57	4 (1%) 72 70	9, 14, 31, 51	0
1	B	244/265 (92%)	-0.50	6 (2%) 57 56	8, 15, 31, 40	0
1	C	241/265 (90%)	-0.54	1 (0%) 92 92	9, 15, 27, 37	0
All	All	728/795 (91%)	-0.53	11 (1%) 73 72	8, 14, 30, 51	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	PHE	4.0
1	A	81	PRO	3.1
1	A	250	PHE	2.7
1	A	253	LYS	2.5
1	B	82	LEU	2.4
1	B	251	LYS	2.3
1	B	66	GLY	2.3
1	B	172	PHE	2.2
1	A	66	GLY	2.2
1	C	4	ALA	2.1
1	B	4	ALA	2.0

### 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 ⓘ

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<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	IOD	C	263	1/1	0.06	0.34	271,271,271,271	0
3	IOD	C	272	1/1	0.28	0.34	173,173,173,173	0
3	IOD	A	263	1/1	0.34	0.20	191,191,191,191	0
3	IOD	A	265	1/1	0.41	0.21	200,200,200,200	0
3	IOD	C	262	1/1	0.42	0.53	219,219,219,219	0
3	IOD	B	267	1/1	0.45	0.36	166,166,166,166	0
3	IOD	C	271	1/1	0.47	0.41	251,251,251,251	0
3	IOD	C	265	1/1	0.48	0.14	168,168,168,168	0
3	IOD	B	270	1/1	0.52	0.33	200,200,200,200	0
3	IOD	A	267	1/1	0.54	0.43	231,231,231,231	0
3	IOD	B	265	1/1	0.56	0.50	220,220,220,220	0
3	IOD	A	266	1/1	0.61	0.26	174,174,174,174	0
3	IOD	B	264	1/1	0.64	0.57	235,235,235,235	0
3	IOD	A	264	1/1	0.69	0.34	244,244,244,244	0
3	IOD	B	266	1/1	0.71	0.12	210,210,210,210	0
3	IOD	B	262	1/1	0.74	0.30	199,199,199,199	0
3	IOD	C	270	1/1	0.74	0.51	236,236,236,236	0
3	IOD	C	268	1/1	0.76	0.24	183,183,183,183	0
3	IOD	B	269	1/1	0.76	0.23	203,203,203,203	0
3	IOD	B	263	1/1	0.78	0.21	180,180,180,180	0
3	IOD	C	269	1/1	0.82	0.28	209,209,209,209	0
3	IOD	C	266	1/1	0.89	0.18	136,136,136,136	0
2	GOL	A	262	6/6	0.89	0.16	39,40,41,41	0
3	IOD	C	264	1/1	0.91	0.15	202,202,202,202	0
3	IOD	B	268	1/1	0.99	0.27	55,55,55,55	1
3	IOD	C	267	1/1	0.99	0.18	56,56,56,56	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.