

wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2021 – 02:08 pm BST

PDB ID	:	701I
Title	:	Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme
		alpha-E141A mutant
Authors	:	Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on		
$\operatorname{Resolution}$:	2.30 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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

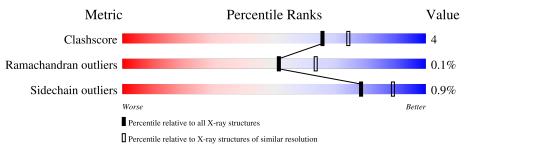
:	4.02b-467
:	1.8.5 (274361), CSD as541be (2020)
:	NOT EXECUTED
:	NOT EXECUTED
:	1.1.7(2018)
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.23.1
	::

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 2.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575(2.30-2.30)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain	
1	D	403	91%	8%
2	А	736	87%	11% •



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8303 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 acyltransferase Rv0859.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	D	401	Total 2931	C 1835	N 522	O 559	S 15	0	0	0

• Molecule 2 is a protein called 3-hydroxyacyl-CoA dehydrogenase.

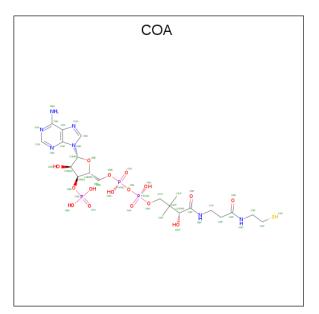
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	А	726	Total 5218	C 3312	N 895	O 991	S 20	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-11	MET	-	initiating methionine	UNP 053872
A	-10	GLY	-	expression tag	UNP 053872
А	-9	SER	-	expression tag	UNP O53872
А	-8	SER	-	expression tag	UNP 053872
A	-7	HIS	-	expression tag	UNP 053872
А	-6	HIS	-	expression tag	UNP O53872
A	-5	HIS	-	expression tag	UNP 053872
A	-5A	HIS	-	expression tag	UNP 053872
A	-5B	HIS	-	expression tag	UNP 053872
А	-5C	HIS	-	expression tag	UNP O53872
A	-5D	SER	-	expression tag	UNP 053872
А	-5E	GLN	-	expression tag	UNP O53872
А	-5F	ASP	-	expression tag	UNP O53872
А	-5G	PRO	-	expression tag	UNP O53872
А	-5H	ASN	-	expression tag	UNP 053872
А	-5I	SER	-	expression tag	UNP 053872
А	141	ALA	GLU	engineered mutation	UNP 053872

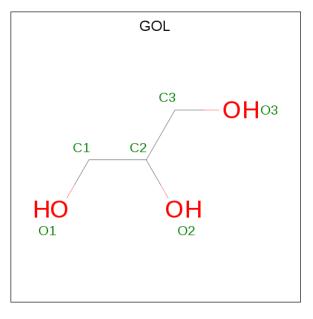
• Molecule 3 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
3	D	1	Total					S	0	0
		-	48	21	7	16	3	1	Ŭ	0

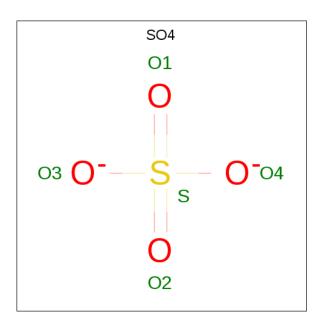
• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 6 & 3 & 3 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	22	$\begin{array}{cc} \text{Total} & \text{O} \\ 22 & 22 \end{array}$	0	0
6	А	22	TotalO2222	0	0

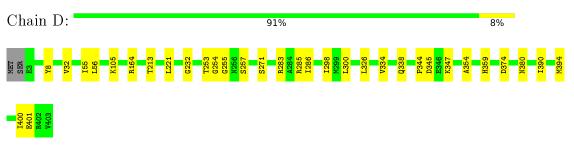


3 Residue-property plots (i)

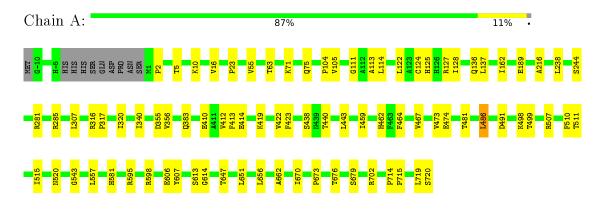
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 was not executed.

• Molecule 1: Putative acyltransferase Rv0859



• Molecule 2: 3-hydroxyacyl-CoA dehydrogenase





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	102.02Å 205.87Å 133.80Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.04 - 2.30	Depositor
% Data completeness	99.4 (48.04-2.30)	Depositor
(in resolution range)	· · · · · · · · · · · · · · · · · · ·	-
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.237 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8303	wwPDB-VP
Average B, all atoms $(Å^2)$	94.0	wwPDB-VP



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: SO4, GOL, CSO, 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	D	0.24	0/2968	0.43	0/4023	
2	А	0.25	0/5318	0.41	0/7228	
All	All	0.25	0/8286	0.42	0/11251	

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 (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	D	2931	0	2941	19	0
2	А	5218	0	5129	48	0
3	D	48	0	32	3	0
4	А	6	0	8	0	0
4	D	6	0	8	0	0
5	А	25	0	0	0	0
5	D	25	0	0	0	0
6	А	22	0	0	1	0
6	D	22	0	0	0	0
All	All	8303	0	8118	66	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.

The worst 5 of 66 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)
2:A:114:LEU:HD11	2:A:136:GLN:HB2	1.72	0.70
2:A:515:ILE:HG13	2:A:670:ILE:HD12	1.76	0.66
1:D:338:GLN:NE2	1:D:345:ASP:OD1	2.28	0.65
2:A:462:HIS:HB3	2:A:474:GLU:HB3	1.79	0.64
1:D:285:ARG:NH1	1:D:401:GLU:OE1	2.30	0.63

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	D	398/403~(99%)	386~(97%)	12 (3%)	0	100	100	
2	А	722/736~(98%)	697~(96%)	24 (3%)	1 (0%)	51	64	
All	All	1120/1139~(98%)	1083~(97%)	36 (3%)	1 (0%)	51	64	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	А	2	PRO

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	D	299/309~(97%)	298~(100%)	1 (0%)	92 97		
2	А	511/565~(90%)	505~(99%)	6 (1%)	71 84		
All	All	810/874~(93%)	803~(99%)	7(1%)	78 89		

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	А	467	VAL
2	А	486	LEU
2	А	557	LEU
2	А	507	ARG
2	А	383	GLN

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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).

М	പ	Type	Chain	Chain	Chain	Res	Link	B	ond leng	gths	В	ond ang	gles
Mol	01	туре		nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2		
1	_	CSO	D	92	1	3,6,7	0.56	0	$0,\!6,\!8$	0.00	-		

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
1	CSO	D	92	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	
1	D	92	CSO	N-CA-CB-SG	

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	Turne	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
MOI	Type	Cham	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
5	SO4	А	803	-	4,4,4	0.14	0	6, 6, 6	0.08	0
5	SO4	А	806	-	4,4,4	0.18	0	$6,\!6,\!6$	0.26	0
3	COA	D	501	-	41,50,50	0.59	0	52,75,75	0.67	1 (1%)
5	SO4	D	506	-	4,4,4	0.14	0	6, 6, 6	0.05	0
4	GOL	А	801	-	$5,\!5,\!5$	0.92	0	5, 5, 5	0.99	0
5	SO4	D	504	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
4	GOL	D	502	-	$5,\!5,\!5$	0.95	0	5, 5, 5	0.95	0
5	SO4	D	507	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
5	SO4	А	804	-	4,4,4	0.14	0	6, 6, 6	0.05	0
5	SO4	D	503	-	4,4,4	0.14	0	$6,\!6,\!6$	0.07	0



Mol	Type	Chain	Res	Link	Bo	Bond lengths			Bond angles		
WIOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
5	SO4	D	505	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.04	0	
5	SO4	А	805	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.05	0	
5	SO4	А	802	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	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
4	GOL	А	801	-	-	2/4/4/4	-
4	GOL	D	502	-	-	0/4/4/4	-
3	COA	D	501	-	_	15/44/64/64	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	D	501	COA	C5A-C6A-N6A	2.16	123.64	120.35

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	COA	C5B-O5B-P1A-O2A
3	D	501	COA	CDP-CBP-CCP-O6A
3	D	501	COA	CEP-CBP-CCP-O6A
3	D	501	COA	CAP-CBP-CCP-O6A
3	D	501	COA	C9P-CAP-CBP-CCP

There are no ring outliers.

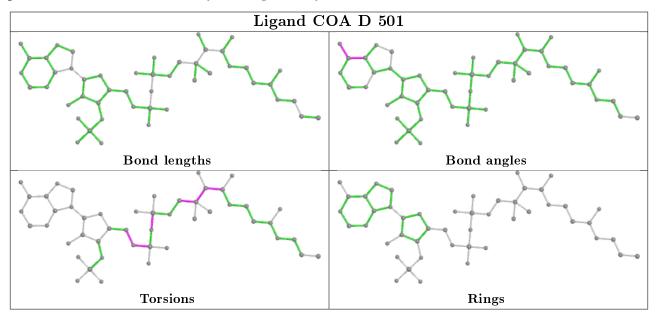
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	COA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is



within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

