



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 03:33 pm BST

PDB ID : 4P4L  
Title : Crystal Structure of Mycobacterium tuberculosis Shikimate Dehydrogenase  
Authors : Lalgondar, M.; Sacchettini, J.C.; TB Structural Genomics Consortium (TB-SGC)  
Deposited on : 2014-03-12  
Resolution : 2.01 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

<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

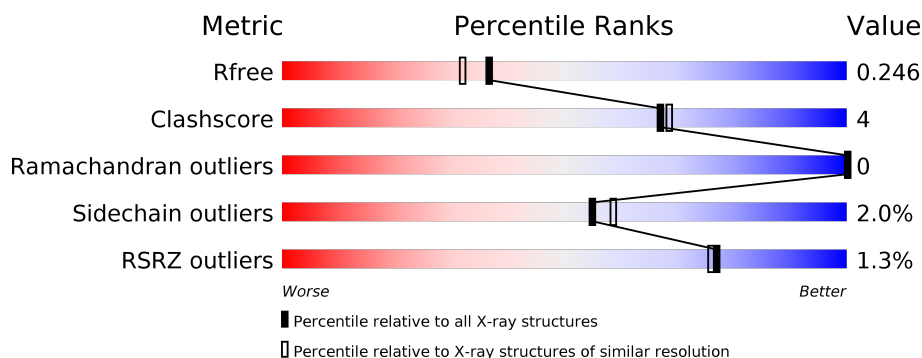
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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	277	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	277	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>7%</div> </div> </div>
1	C	277	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</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
2	SKM	A	301	X	-	-	-
2	SKM	B	301	X	-	-	-
2	SKM	C	301	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5759 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 Shikimate 5-dehydrogenase AroE (5-dehydroshikimate reductase).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			1880	1191	334	349	6			
1	B	257	Total	C	N	O	S	0	0	0
			1840	1168	327	339	6			
1	C	263	Total	C	N	O	S	0	0	0
			1876	1189	333	348	6			

There are 24 discrepancies between the modelled and reference sequences:

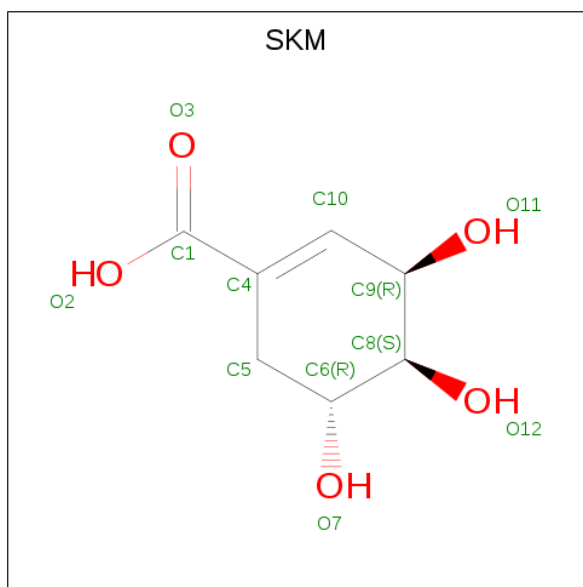
Chain	Residue	Modelled	Actual	Comment	Reference
A	270	LEU	-	expression tag	UNP P95001
A	271	ASP	-	expression tag	UNP P95001
A	272	HIS	-	expression tag	UNP P95001
A	273	HIS	-	expression tag	UNP P95001
A	274	HIS	-	expression tag	UNP P95001
A	275	HIS	-	expression tag	UNP P95001
A	276	HIS	-	expression tag	UNP P95001
A	277	HIS	-	expression tag	UNP P95001
B	270	LEU	-	expression tag	UNP P95001
B	271	ASP	-	expression tag	UNP P95001
B	272	HIS	-	expression tag	UNP P95001
B	273	HIS	-	expression tag	UNP P95001
B	274	HIS	-	expression tag	UNP P95001
B	275	HIS	-	expression tag	UNP P95001
B	276	HIS	-	expression tag	UNP P95001
B	277	HIS	-	expression tag	UNP P95001
C	270	LEU	-	expression tag	UNP P95001
C	271	ASP	-	expression tag	UNP P95001
C	272	HIS	-	expression tag	UNP P95001
C	273	HIS	-	expression tag	UNP P95001
C	274	HIS	-	expression tag	UNP P95001
C	275	HIS	-	expression tag	UNP P95001

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Chain	Residue	Modelled	Actual	Comment	Reference
C	276	HIS	-	expression tag	UNP P95001
C	277	HIS	-	expression tag	UNP P95001

- Molecule 2 is (3R,4S,5R)-3,4,5-TRIHIDROXYCYCLOHEX-1-ENE-1-CARBOXYLIC ACID (three-letter code: SKM) (formula: C<sub>7</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	7	5		
2	B	1	Total	C	O	0	0
			12	7	5		
2	C	1	Total	C	O	0	0
			12	7	5		

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



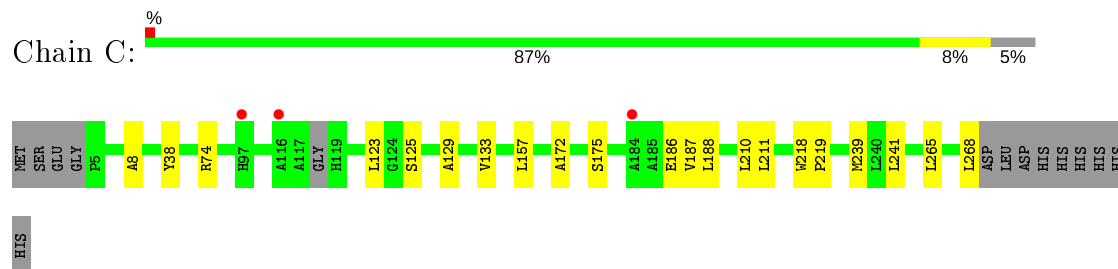
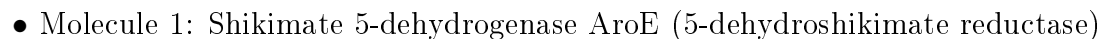
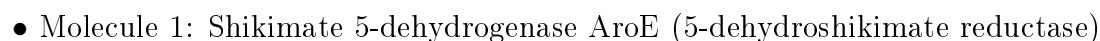
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	23	Total	O	0	0
			23	23		
4	C	48	Total	O	0	0
			48	48		



- Molecule 1: Shikimate 5-dehydrogenase AroE (5-dehydroshikimate reductase)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.70Å 132.31Å 38.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.31 – 2.01 46.31 – 2.01	Depositor EDS
% Data completeness (in resolution range)	94.6 (46.31-2.01) 93.6 (46.31-2.01)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.203 , 0.249 0.203 , 0.246	Depositor DCC
$R_{free}$ test set	1999 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5759	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7184e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SKM, SO4

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	0.39	0/1919	0.53	0/2625
1	B	0.36	0/1877	0.51	0/2565
1	C	0.43	0/1914	0.53	0/2617
All	All	0.39	0/5710	0.52	0/7807

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	A	1880	0	1891	14	0
1	B	1840	0	1853	17	0
1	C	1876	0	1887	13	0
2	A	12	0	9	0	0
2	B	12	0	9	0	0
2	C	12	0	9	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
4	A	31	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	23	0	0	0	0
4	C	48	0	0	0	2
All	All	5759	0	5658	44	2

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 44 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:11:LEU:HD13	1:A:62:VAL:HG21	1.63	0.79
1:B:116:ALA:O	1:B:118:GLY:N	2.20	0.74
1:B:95:THR:HG22	1:B:97:HIS:H	1.60	0.65
1:C:172:ALA:HB3	1:C:175:SER:HB3	1.81	0.61
1:A:265:LEU:HD12	1:A:268:LEU:HD12	1.82	0.61

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:403:HOH:O	4:C:406:HOH:O[1_554]	1.94	0.26
4:A:406:HOH:O	4:C:416:HOH:O[4_475]	2.15	0.05

## 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	262/277 (95%)	256 (98%)	6 (2%)	0	100	100
1	B	251/277 (91%)	250 (100%)	1 (0%)	0	100	100
1	C	259/277 (94%)	254 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	772/831 (93%)	760 (98%)	12 (2%)	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	181/193 (94%)	176 (97%)	5 (3%)	43	44
1	B	178/193 (92%)	172 (97%)	6 (3%)	37	36
1	C	181/193 (94%)	181 (100%)	0	100	100
All	All	540/579 (93%)	529 (98%)	11 (2%)	55	58

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	PHE
1	B	35	ASP
1	B	143	ASP
1	A	158	VAL
1	B	79	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	238	GLN

### 5.3.3 RNA ⓘ

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](#)

8 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	$\# Z  > 2$
3	SO4	B	302	-	4,4,4	0.16	0	6,6,6	0.12	0
3	SO4	C	303	-	4,4,4	0.17	0	6,6,6	0.15	0
3	SO4	A	303	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	A	302	-	4,4,4	0.16	0	6,6,6	0.22	0
3	SO4	C	302	-	4,4,4	0.14	0	6,6,6	0.37	0
2	SKM	A	301	-	9,12,12	6.60	4 (44%)	12,17,17	3.30	5 (41%)
2	SKM	C	301	-	9,12,12	6.50	4 (44%)	12,17,17	3.09	3 (25%)
2	SKM	B	301	-	9,12,12	6.53	5 (55%)	12,17,17	3.30	4 (33%)

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	SKM	C	301	-	1/1/5/6	0/0/20/20	0/1/1/1
2	SKM	B	301	-	1/1/5/6	0/0/20/20	0/1/1/1
2	SKM	A	301	-	1/1/5/6	0/0/20/20	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	SKM	C10-C4	15.35	1.55	1.34
2	C	301	SKM	C10-C4	15.20	1.55	1.34
2	B	301	SKM	C10-C4	15.18	1.55	1.34
2	A	301	SKM	C5-C4	-10.37	1.33	1.50
2	B	301	SKM	C5-C4	-10.34	1.33	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	SKM	C6-C5-C4	7.86	127.12	111.78
2	A	301	SKM	C6-C5-C4	7.68	126.76	111.78
2	B	301	SKM	C6-C5-C4	7.58	126.56	111.78
2	B	301	SKM	C9-C10-C4	-7.21	105.06	123.50
2	A	301	SKM	C9-C10-C4	-6.78	106.15	123.50

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	SKM	C8
2	C	301	SKM	C8
2	B	301	SKM	C8

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 [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	264/277 (95%)	-0.19	2 (0%) 86 85	25, 40, 73, 95	0
1	B	257/277 (92%)	-0.01	5 (1%) 66 65	29, 50, 87, 103	0
1	C	263/277 (94%)	-0.22	3 (1%) 80 79	28, 40, 68, 84	0
All	All	784/831 (94%)	-0.14	10 (1%) 77 76	25, 43, 80, 103	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	97	HIS	5.0
1	A	97	HIS	4.4
1	C	97	HIS	4.0
1	B	50	VAL	3.9
1	C	116	ALA	3.2

### 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 carbohydrates 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<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( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	302	5/5	0.96	0.09	77,77,78,79	0
2	SKM	A	301	12/12	0.96	0.12	26,31,35,37	0
2	SKM	C	301	12/12	0.96	0.10	28,32,35,38	0
3	SO4	A	303	5/5	0.97	0.10	59,60,61,61	0
3	SO4	A	302	5/5	0.97	0.10	51,51,56,56	0
2	SKM	B	301	12/12	0.97	0.10	35,40,44,45	0
3	SO4	C	302	5/5	0.99	0.10	41,43,46,46	0
3	SO4	C	303	5/5	0.99	0.06	48,49,50,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.