



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2022 – 08:02 PM EDT

PDB ID : 7ULH  
Title : Crystal Structure of a Short chain dehydrogenase from Mycobacterium avium 104  
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2022-04-04  
Resolution : 2.60 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	:	<b>FAILED</b>
Xtriage (Phenix)	:	1.13
EDS	:	<b>FAILED</b>
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

## 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 2.60 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15788 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 Short chain dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	1	0
			2122	1318	389	412	3			
1	B	289	Total	C	N	O	S	0	0	0
			2121	1319	388	411	3			
1	C	284	Total	C	N	O	S	0	1	0
			2091	1303	383	402	3			
1	D	282	Total	C	N	O	S	0	0	0
			2051	1280	379	389	3			
1	E	272	Total	C	N	O	S	0	0	0
			1958	1223	355	377	3			
1	F	282	Total	C	N	O	S	0	2	0
			2056	1283	374	396	3			
1	G	286	Total	C	N	O	S	0	3	0
			2112	1315	389	405	3			

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A0H2ZRP4
A	-19	ALA	-	expression tag	UNP A0A0H2ZRP4
A	-18	HIS	-	expression tag	UNP A0A0H2ZRP4
A	-17	HIS	-	expression tag	UNP A0A0H2ZRP4
A	-16	HIS	-	expression tag	UNP A0A0H2ZRP4
A	-15	HIS	-	expression tag	UNP A0A0H2ZRP4
A	-14	HIS	-	expression tag	UNP A0A0H2ZRP4
A	-13	HIS	-	expression tag	UNP A0A0H2ZRP4
A	-12	MET	-	expression tag	UNP A0A0H2ZRP4
A	-11	GLY	-	expression tag	UNP A0A0H2ZRP4
A	-10	THR	-	expression tag	UNP A0A0H2ZRP4
A	-9	LEU	-	expression tag	UNP A0A0H2ZRP4
A	-8	GLU	-	expression tag	UNP A0A0H2ZRP4
A	-7	ALA	-	expression tag	UNP A0A0H2ZRP4
A	-6	GLN	-	expression tag	UNP A0A0H2ZRP4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	THR	-	expression tag	UNP A0A0H2ZRP4
A	-4	GLN	-	expression tag	UNP A0A0H2ZRP4
A	-3	GLY	-	expression tag	UNP A0A0H2ZRP4
A	-2	PRO	-	expression tag	UNP A0A0H2ZRP4
A	-1	GLY	-	expression tag	UNP A0A0H2ZRP4
A	0	SER	-	expression tag	UNP A0A0H2ZRP4
B	-20	MET	-	initiating methionine	UNP A0A0H2ZRP4
B	-19	ALA	-	expression tag	UNP A0A0H2ZRP4
B	-18	HIS	-	expression tag	UNP A0A0H2ZRP4
B	-17	HIS	-	expression tag	UNP A0A0H2ZRP4
B	-16	HIS	-	expression tag	UNP A0A0H2ZRP4
B	-15	HIS	-	expression tag	UNP A0A0H2ZRP4
B	-14	HIS	-	expression tag	UNP A0A0H2ZRP4
B	-13	HIS	-	expression tag	UNP A0A0H2ZRP4
B	-12	MET	-	expression tag	UNP A0A0H2ZRP4
B	-11	GLY	-	expression tag	UNP A0A0H2ZRP4
B	-10	THR	-	expression tag	UNP A0A0H2ZRP4
B	-9	LEU	-	expression tag	UNP A0A0H2ZRP4
B	-8	GLU	-	expression tag	UNP A0A0H2ZRP4
B	-7	ALA	-	expression tag	UNP A0A0H2ZRP4
B	-6	GLN	-	expression tag	UNP A0A0H2ZRP4
B	-5	THR	-	expression tag	UNP A0A0H2ZRP4
B	-4	GLN	-	expression tag	UNP A0A0H2ZRP4
B	-3	GLY	-	expression tag	UNP A0A0H2ZRP4
B	-2	PRO	-	expression tag	UNP A0A0H2ZRP4
B	-1	GLY	-	expression tag	UNP A0A0H2ZRP4
B	0	SER	-	expression tag	UNP A0A0H2ZRP4
C	-20	MET	-	initiating methionine	UNP A0A0H2ZRP4
C	-19	ALA	-	expression tag	UNP A0A0H2ZRP4
C	-18	HIS	-	expression tag	UNP A0A0H2ZRP4
C	-17	HIS	-	expression tag	UNP A0A0H2ZRP4
C	-16	HIS	-	expression tag	UNP A0A0H2ZRP4
C	-15	HIS	-	expression tag	UNP A0A0H2ZRP4
C	-14	HIS	-	expression tag	UNP A0A0H2ZRP4
C	-13	HIS	-	expression tag	UNP A0A0H2ZRP4
C	-12	MET	-	expression tag	UNP A0A0H2ZRP4
C	-11	GLY	-	expression tag	UNP A0A0H2ZRP4
C	-10	THR	-	expression tag	UNP A0A0H2ZRP4
C	-9	LEU	-	expression tag	UNP A0A0H2ZRP4
C	-8	GLU	-	expression tag	UNP A0A0H2ZRP4
C	-7	ALA	-	expression tag	UNP A0A0H2ZRP4
C	-6	GLN	-	expression tag	UNP A0A0H2ZRP4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	THR	-	expression tag	UNP A0A0H2ZRP4
C	-4	GLN	-	expression tag	UNP A0A0H2ZRP4
C	-3	GLY	-	expression tag	UNP A0A0H2ZRP4
C	-2	PRO	-	expression tag	UNP A0A0H2ZRP4
C	-1	GLY	-	expression tag	UNP A0A0H2ZRP4
C	0	SER	-	expression tag	UNP A0A0H2ZRP4
D	-20	MET	-	initiating methionine	UNP A0A0H2ZRP4
D	-19	ALA	-	expression tag	UNP A0A0H2ZRP4
D	-18	HIS	-	expression tag	UNP A0A0H2ZRP4
D	-17	HIS	-	expression tag	UNP A0A0H2ZRP4
D	-16	HIS	-	expression tag	UNP A0A0H2ZRP4
D	-15	HIS	-	expression tag	UNP A0A0H2ZRP4
D	-14	HIS	-	expression tag	UNP A0A0H2ZRP4
D	-13	HIS	-	expression tag	UNP A0A0H2ZRP4
D	-12	MET	-	expression tag	UNP A0A0H2ZRP4
D	-11	GLY	-	expression tag	UNP A0A0H2ZRP4
D	-10	THR	-	expression tag	UNP A0A0H2ZRP4
D	-9	LEU	-	expression tag	UNP A0A0H2ZRP4
D	-8	GLU	-	expression tag	UNP A0A0H2ZRP4
D	-7	ALA	-	expression tag	UNP A0A0H2ZRP4
D	-6	GLN	-	expression tag	UNP A0A0H2ZRP4
D	-5	THR	-	expression tag	UNP A0A0H2ZRP4
D	-4	GLN	-	expression tag	UNP A0A0H2ZRP4
D	-3	GLY	-	expression tag	UNP A0A0H2ZRP4
D	-2	PRO	-	expression tag	UNP A0A0H2ZRP4
D	-1	GLY	-	expression tag	UNP A0A0H2ZRP4
D	0	SER	-	expression tag	UNP A0A0H2ZRP4
E	-20	MET	-	initiating methionine	UNP A0A0H2ZRP4
E	-19	ALA	-	expression tag	UNP A0A0H2ZRP4
E	-18	HIS	-	expression tag	UNP A0A0H2ZRP4
E	-17	HIS	-	expression tag	UNP A0A0H2ZRP4
E	-16	HIS	-	expression tag	UNP A0A0H2ZRP4
E	-15	HIS	-	expression tag	UNP A0A0H2ZRP4
E	-14	HIS	-	expression tag	UNP A0A0H2ZRP4
E	-13	HIS	-	expression tag	UNP A0A0H2ZRP4
E	-12	MET	-	expression tag	UNP A0A0H2ZRP4
E	-11	GLY	-	expression tag	UNP A0A0H2ZRP4
E	-10	THR	-	expression tag	UNP A0A0H2ZRP4
E	-9	LEU	-	expression tag	UNP A0A0H2ZRP4
E	-8	GLU	-	expression tag	UNP A0A0H2ZRP4
E	-7	ALA	-	expression tag	UNP A0A0H2ZRP4
E	-6	GLN	-	expression tag	UNP A0A0H2ZRP4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	THR	-	expression tag	UNP A0A0H2ZRP4
E	-4	GLN	-	expression tag	UNP A0A0H2ZRP4
E	-3	GLY	-	expression tag	UNP A0A0H2ZRP4
E	-2	PRO	-	expression tag	UNP A0A0H2ZRP4
E	-1	GLY	-	expression tag	UNP A0A0H2ZRP4
E	0	SER	-	expression tag	UNP A0A0H2ZRP4
F	-20	MET	-	initiating methionine	UNP A0A0H2ZRP4
F	-19	ALA	-	expression tag	UNP A0A0H2ZRP4
F	-18	HIS	-	expression tag	UNP A0A0H2ZRP4
F	-17	HIS	-	expression tag	UNP A0A0H2ZRP4
F	-16	HIS	-	expression tag	UNP A0A0H2ZRP4
F	-15	HIS	-	expression tag	UNP A0A0H2ZRP4
F	-14	HIS	-	expression tag	UNP A0A0H2ZRP4
F	-13	HIS	-	expression tag	UNP A0A0H2ZRP4
F	-12	MET	-	expression tag	UNP A0A0H2ZRP4
F	-11	GLY	-	expression tag	UNP A0A0H2ZRP4
F	-10	THR	-	expression tag	UNP A0A0H2ZRP4
F	-9	LEU	-	expression tag	UNP A0A0H2ZRP4
F	-8	GLU	-	expression tag	UNP A0A0H2ZRP4
F	-7	ALA	-	expression tag	UNP A0A0H2ZRP4
F	-6	GLN	-	expression tag	UNP A0A0H2ZRP4
F	-5	THR	-	expression tag	UNP A0A0H2ZRP4
F	-4	GLN	-	expression tag	UNP A0A0H2ZRP4
F	-3	GLY	-	expression tag	UNP A0A0H2ZRP4
F	-2	PRO	-	expression tag	UNP A0A0H2ZRP4
F	-1	GLY	-	expression tag	UNP A0A0H2ZRP4
F	0	SER	-	expression tag	UNP A0A0H2ZRP4
G	-20	MET	-	initiating methionine	UNP A0A0H2ZRP4
G	-19	ALA	-	expression tag	UNP A0A0H2ZRP4
G	-18	HIS	-	expression tag	UNP A0A0H2ZRP4
G	-17	HIS	-	expression tag	UNP A0A0H2ZRP4
G	-16	HIS	-	expression tag	UNP A0A0H2ZRP4
G	-15	HIS	-	expression tag	UNP A0A0H2ZRP4
G	-14	HIS	-	expression tag	UNP A0A0H2ZRP4
G	-13	HIS	-	expression tag	UNP A0A0H2ZRP4
G	-12	MET	-	expression tag	UNP A0A0H2ZRP4
G	-11	GLY	-	expression tag	UNP A0A0H2ZRP4
G	-10	THR	-	expression tag	UNP A0A0H2ZRP4
G	-9	LEU	-	expression tag	UNP A0A0H2ZRP4
G	-8	GLU	-	expression tag	UNP A0A0H2ZRP4
G	-7	ALA	-	expression tag	UNP A0A0H2ZRP4
G	-6	GLN	-	expression tag	UNP A0A0H2ZRP4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-5	THR	-	expression tag	UNP A0A0H2ZRP4
G	-4	GLN	-	expression tag	UNP A0A0H2ZRP4
G	-3	GLY	-	expression tag	UNP A0A0H2ZRP4
G	-2	PRO	-	expression tag	UNP A0A0H2ZRP4
G	-1	GLY	-	expression tag	UNP A0A0H2ZRP4
G	0	SER	-	expression tag	UNP A0A0H2ZRP4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	195	Total O 195 195	0	0
2	B	219	Total O 219 219	0	0
2	C	211	Total O 211 211	0	0
2	D	169	Total O 171 171	0	2
2	E	82	Total O 82 82	0	0
2	F	121	Total O 121 121	0	0
2	G	277	Total O 278 278	0	1

MolProbity and EDS failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	241.81Å 241.81Å 241.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.37 – 2.60	Depositor
% Data completeness (in resolution range)	100.0 (48.37-2.60)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, $R_{free}$	0.158 , 0.193	Depositor
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtriage
Anisotropy	0.014	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15788	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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.



## 4 Model quality [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 5 Fit of model and data ⓘ

### 5.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.