



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2023 – 02:10 PM JST

PDB ID : 8HCZ  
Title : N-terminal domain structure of mycobacterium tuberculosis FadD23  
Authors : Yan, M.R.; Liu, X.; Zhang, W.; Rao, Z.H.  
Deposited on : 2022-11-03  
Resolution : 1.48 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.

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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.32.1  
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) : 2.32.1

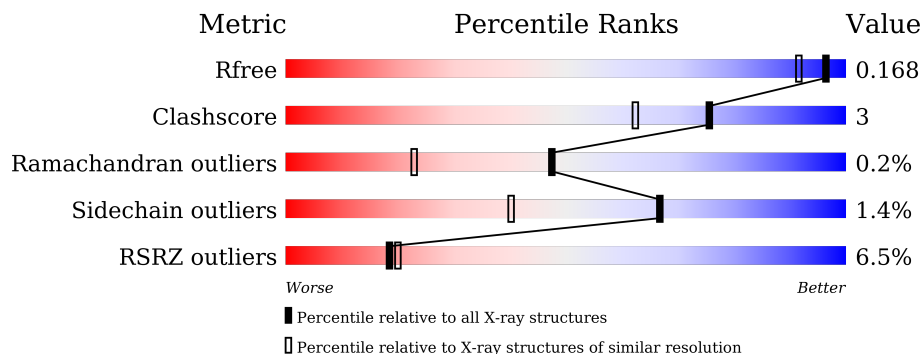
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.48 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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  $\geq 3$ , 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	486	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 3754 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 Long-chain-fatty-acid--AMP ligase FadD23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	443	3364	2150	571	630	13	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P9WQ47
A	-19	GLY	-	expression tag	UNP P9WQ47
A	-18	SER	-	expression tag	UNP P9WQ47
A	-17	SER	-	expression tag	UNP P9WQ47
A	-16	HIS	-	expression tag	UNP P9WQ47
A	-15	HIS	-	expression tag	UNP P9WQ47
A	-14	HIS	-	expression tag	UNP P9WQ47
A	-13	HIS	-	expression tag	UNP P9WQ47
A	-12	HIS	-	expression tag	UNP P9WQ47
A	-11	HIS	-	expression tag	UNP P9WQ47
A	-10	SER	-	expression tag	UNP P9WQ47
A	-9	SER	-	expression tag	UNP P9WQ47
A	-8	GLY	-	expression tag	UNP P9WQ47
A	-7	LEU	-	expression tag	UNP P9WQ47
A	-6	VAL	-	expression tag	UNP P9WQ47
A	-5	PRO	-	expression tag	UNP P9WQ47
A	-4	ARG	-	expression tag	UNP P9WQ47
A	-3	GLY	-	expression tag	UNP P9WQ47
A	-2	SER	-	expression tag	UNP P9WQ47
A	-1	HIS	-	expression tag	UNP P9WQ47
A	0	MET	-	expression tag	UNP P9WQ47

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	390	Total	O	0	0
			390	390		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.92Å 72.59Å 90.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.40 – 1.48 45.40 – 1.48	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.40-1.48) 97.7 (45.40-1.48)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 1.48Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.145 , 0.169 0.149 , 0.168	Depositor DCC
$R_{free}$ test set	3650 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.9	Xtrriage
Anisotropy	0.148	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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 [i](#)

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

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	0.58	0/3445	0.71	0/4706

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	3364	0	3332	21	0
2	A	390	0	0	5	0
All	All	3754	0	3332	21	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 3.

All (21) 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:302:ARG:NE	1:A:302:ARG:HA	2.16	0.60
1:A:193:GLN:NE2	2:A:503:HOH:O	2.35	0.58
1:A:171:THR:HB	2:A:711:HOH:O	2.06	0.55
1:A:4:LEU:HD13	1:A:163:GLN:OE1	2.07	0.54

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HG12	1:A:117:LEU:HD21	1.91	0.53
1:A:350:ARG:NH1	1:A:350:ARG:HG3	2.24	0.52
1:A:9:MET:HE1	1:A:189:LEU:HD21	1.91	0.50
1:A:462:LYS:HE2	2:A:720:HOH:O	2.11	0.49
1:A:9:MET:CE	1:A:189:LEU:HD21	2.43	0.49
1:A:312:VAL:HG11	1:A:322:GLU:HG3	1.98	0.45
1:A:353:GLU:HG2	1:A:365:CYS:HB3	2.00	0.44
1:A:350:ARG:HG3	1:A:350:ARG:HH11	1.81	0.44
1:A:92:LEU:HD21	1:A:107:VAL:HG11	2.00	0.44
1:A:302:ARG:HA	1:A:302:ARG:CZ	2.49	0.43
1:A:48:THR:HG21	2:A:504:HOH:O	2.17	0.43
1:A:138:SER:N	1:A:139:PRO:HD2	2.34	0.42
1:A:350:ARG:HA	1:A:350:ARG:HD2	1.86	0.42
1:A:460:ARG:HB3	1:A:462:LYS:HE2	2.02	0.42
1:A:55:VAL:CG1	1:A:117:LEU:HD21	2.49	0.41
1:A:420:GLU:OE1	2:A:501:HOH:O	2.22	0.41
1:A:232:PRO:HG3	1:A:239:ALA:HB2	2.03	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	435/486 (90%)	429 (99%)	5 (1%)	1 (0%)	47 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	VAL

### 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	A	355/392 (91%)	350 (99%)	5 (1%)	67 40

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	171	THR
1	A	177	THR
1	A	214	MET
1	A	223	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	15	ASN

### 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](#)

There are no ligands in this entry.

## 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

### 6.1 Protein, DNA and RNA chains

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	443/486 (91%)	0.25	29 (6%) <b>18</b> <b>20</b>	9, 16, 37, 47	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	THR	9.9
1	A	127	VAL	6.7
1	A	99	ALA	6.2
1	A	153	ILE	6.2
1	A	367	THR	4.9
1	A	178	PRO	4.7
1	A	126	VAL	4.7
1	A	102	GLU	4.5
1	A	369	ALA	4.3
1	A	177	THR	4.2
1	A	98	GLY	4.0
1	A	128	PRO	4.0
1	A	130	VAL	3.9
1	A	138	SER	3.8
1	A	462	LYS	3.8
1	A	159	ASP	3.5
1	A	125	ASP	3.1
1	A	366	ALA	3.1
1	A	453	ASP	3.0
1	A	96	LEU	2.8
1	A	4	LEU	2.7
1	A	124	GLY	2.7
1	A	463	ASP	2.5
1	A	129	ARG	2.4
1	A	97	GLY	2.3
1	A	350	ARG	2.2
1	A	103	ARG	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	29	GLU	2.1
1	A	160	ASP	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.