



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 5, 2026 – 10:08 pm BST

PDB ID : 9R33 / pdb\_00009r33  
Title : Improved crystallization and diffraction quality of Mycobacterium tuberculosis OmamC/Rv1363c upon heat treatment  
Authors : Hynonen, M.J.; Venkatesan, R.  
Deposited on : 2025-05-02  
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](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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

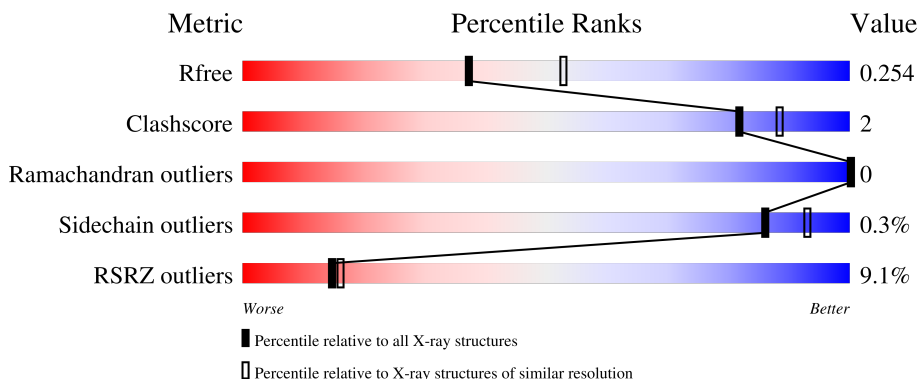
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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  $\geq 3$ , 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	161	<div> <div>10%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div></div> </div> </div>
1	B	161	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>7%</div> </div> </div>
1	C	161	<div> <div>8%</div> <div> <div></div> <div>88%</div> <div></div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3596 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 OmamC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1195	736	214	240	5			
1	B	149	Total	C	N	O	S	0	2	0
			1164	718	206	235	5			
1	C	148	Total	C	N	O	S	0	1	0
			1159	717	210	227	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	MET	-	initiating methionine	UNP P9WLZ9
A	102	LYS	-	expression tag	UNP P9WLZ9
A	103	HIS	-	expression tag	UNP P9WLZ9
A	104	HIS	-	expression tag	UNP P9WLZ9
A	105	HIS	-	expression tag	UNP P9WLZ9
A	106	HIS	-	expression tag	UNP P9WLZ9
A	107	HIS	-	expression tag	UNP P9WLZ9
A	108	HIS	-	expression tag	UNP P9WLZ9
A	109	PRO	-	expression tag	UNP P9WLZ9
A	110	MET	-	expression tag	UNP P9WLZ9
A	111	SER	-	expression tag	UNP P9WLZ9
A	112	ASP	-	expression tag	UNP P9WLZ9
A	113	TYR	-	expression tag	UNP P9WLZ9
A	114	ASP	-	expression tag	UNP P9WLZ9
A	115	ILE	-	expression tag	UNP P9WLZ9
A	116	PRO	-	expression tag	UNP P9WLZ9
A	117	THR	-	expression tag	UNP P9WLZ9
A	118	THR	-	expression tag	UNP P9WLZ9
A	119	GLU	-	expression tag	UNP P9WLZ9
A	120	ASN	-	expression tag	UNP P9WLZ9
A	121	LEU	-	expression tag	UNP P9WLZ9
A	122	TYR	-	expression tag	UNP P9WLZ9
A	123	PHE	-	expression tag	UNP P9WLZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	124	GLN	-	expression tag	UNP P9WLZ9
A	125	GLY	-	expression tag	UNP P9WLZ9
A	126	ALA	-	expression tag	UNP P9WLZ9
A	127	MET	-	expression tag	UNP P9WLZ9
A	128	ALA	-	expression tag	UNP P9WLZ9
B	101	MET	-	initiating methionine	UNP P9WLZ9
B	102	LYS	-	expression tag	UNP P9WLZ9
B	103	HIS	-	expression tag	UNP P9WLZ9
B	104	HIS	-	expression tag	UNP P9WLZ9
B	105	HIS	-	expression tag	UNP P9WLZ9
B	106	HIS	-	expression tag	UNP P9WLZ9
B	107	HIS	-	expression tag	UNP P9WLZ9
B	108	HIS	-	expression tag	UNP P9WLZ9
B	109	PRO	-	expression tag	UNP P9WLZ9
B	110	MET	-	expression tag	UNP P9WLZ9
B	111	SER	-	expression tag	UNP P9WLZ9
B	112	ASP	-	expression tag	UNP P9WLZ9
B	113	TYR	-	expression tag	UNP P9WLZ9
B	114	ASP	-	expression tag	UNP P9WLZ9
B	115	ILE	-	expression tag	UNP P9WLZ9
B	116	PRO	-	expression tag	UNP P9WLZ9
B	117	THR	-	expression tag	UNP P9WLZ9
B	118	THR	-	expression tag	UNP P9WLZ9
B	119	GLU	-	expression tag	UNP P9WLZ9
B	120	ASN	-	expression tag	UNP P9WLZ9
B	121	LEU	-	expression tag	UNP P9WLZ9
B	122	TYR	-	expression tag	UNP P9WLZ9
B	123	PHE	-	expression tag	UNP P9WLZ9
B	124	GLN	-	expression tag	UNP P9WLZ9
B	125	GLY	-	expression tag	UNP P9WLZ9
B	126	ALA	-	expression tag	UNP P9WLZ9
B	127	MET	-	expression tag	UNP P9WLZ9
B	128	ALA	-	expression tag	UNP P9WLZ9
C	101	MET	-	initiating methionine	UNP P9WLZ9
C	102	LYS	-	expression tag	UNP P9WLZ9
C	103	HIS	-	expression tag	UNP P9WLZ9
C	104	HIS	-	expression tag	UNP P9WLZ9
C	105	HIS	-	expression tag	UNP P9WLZ9
C	106	HIS	-	expression tag	UNP P9WLZ9
C	107	HIS	-	expression tag	UNP P9WLZ9
C	108	HIS	-	expression tag	UNP P9WLZ9
C	109	PRO	-	expression tag	UNP P9WLZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	110	MET	-	expression tag	UNP P9WLZ9
C	111	SER	-	expression tag	UNP P9WLZ9
C	112	ASP	-	expression tag	UNP P9WLZ9
C	113	TYR	-	expression tag	UNP P9WLZ9
C	114	ASP	-	expression tag	UNP P9WLZ9
C	115	ILE	-	expression tag	UNP P9WLZ9
C	116	PRO	-	expression tag	UNP P9WLZ9
C	117	THR	-	expression tag	UNP P9WLZ9
C	118	THR	-	expression tag	UNP P9WLZ9
C	119	GLU	-	expression tag	UNP P9WLZ9
C	120	ASN	-	expression tag	UNP P9WLZ9
C	121	LEU	-	expression tag	UNP P9WLZ9
C	122	TYR	-	expression tag	UNP P9WLZ9
C	123	PHE	-	expression tag	UNP P9WLZ9
C	124	GLN	-	expression tag	UNP P9WLZ9
C	125	GLY	-	expression tag	UNP P9WLZ9
C	126	ALA	-	expression tag	UNP P9WLZ9
C	127	MET	-	expression tag	UNP P9WLZ9
C	128	ALA	-	expression tag	UNP P9WLZ9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	23	Total O 23 23	0	0
2	B	32	Total O 32 32	0	0
2	C	23	Total O 23 23	0	0

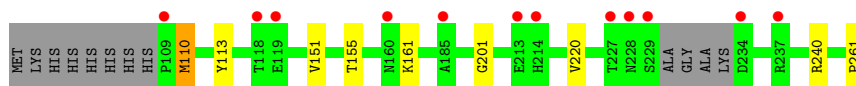
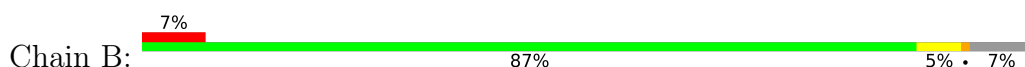
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

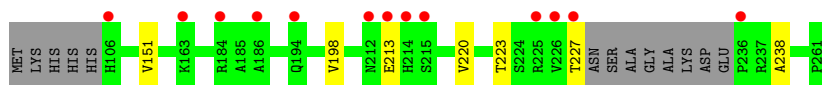
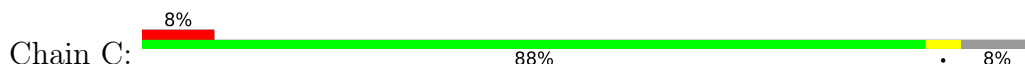
- Molecule 1: OmamC



- Molecule 1: OmamC



- Molecule 1: OmamC



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.12Å 111.89Å 75.24Å 90.00° 117.83° 90.00°	Depositor
Resolution (Å)	66.54 – 2.30 66.54 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (66.54-2.30) 96.9 (66.54-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.228 , 0.253 0.232 , 0.254	Depositor DCC
$R_{free}$ test set	1175 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3596	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% 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

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	0.09	0/1215	0.23	0/1643
1	B	0.08	0/1188	0.20	0/1605
1	C	0.08	0/1182	0.21	0/1596
All	All	0.08	0/3585	0.21	0/4844

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

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	1195	0	1150	6	0
1	B	1164	0	1123	7	0
1	C	1159	0	1123	4	0
2	A	23	0	0	0	0
2	B	32	0	0	0	0
2	C	23	0	0	0	0
All	All	3596	0	3396	17	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 2.

The worst 5 of 17 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:228:ASN:HB3	1:A:232:ALA:HB3	1.79	0.64
1:A:164:GLU:OE1	1:A:164:GLU:N	2.38	0.52
1:B:240:ARG:NH2	1:B:261:PRO:O	2.47	0.47
1:A:151:VAL:HG21	1:A:220:VAL:HG11	1.97	0.46
1:A:163:LYS:HD2	1:A:189:THR:HG21	1.98	0.45

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	153/161 (95%)	147 (96%)	6 (4%)	0	100	100
1	B	147/161 (91%)	143 (97%)	4 (3%)	0	100	100
1	C	145/161 (90%)	141 (97%)	4 (3%)	0	100	100
All	All	445/483 (92%)	431 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	126/132 (96%)	126 (100%)	0	100	100
1	B	125/132 (95%)	124 (99%)	1 (1%)	73	86
1	C	123/132 (93%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	374/396 (94%)	373 (100%)	1 (0%)	86	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	110	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	B	124	GLN
1	C	149	GLN

### 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 oligosaccharides 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 [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	155/161 (96%)	0.82	16 (10%)	12 13	39, 62, 105, 140	0
1	B	149/161 (92%)	0.81	12 (8%)	18 19	28, 62, 104, 126	2 (1%)
1	C	148/161 (91%)	0.91	13 (8%)	15 17	35, 74, 106, 115	1 (0%)
All	All	452/483 (93%)	0.85	41 (9%)	15 16	28, 65, 106, 140	3 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	227	THR	4.4
1	B	109	PRO	4.3
1	A	230	ALA	3.3
1	A	226	VAL	3.1
1	C	226	VAL	3.0

### 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 oligosaccharides 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.