



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:05 PM UTC

PDB ID : 2FK7 / pdb_00002fk7
Title : Crystal structure of Hma (MmaA4) from Mycobacterium tuberculosis, apo-form
Authors : Boissier, F.; Guillet, V.; Mourey, L.
Deposited on : 2006-01-04
Resolution : 2.10 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

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	:	4-5-2 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

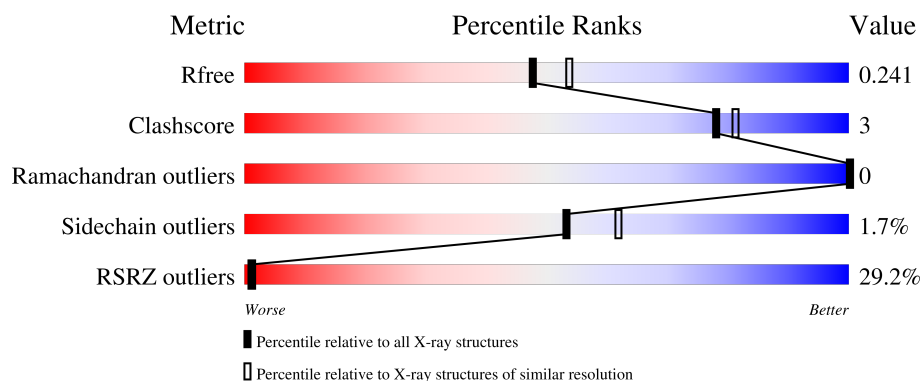
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	318	25% 79% 8% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2342 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 methoxy mycolic acid synthase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	2218	1411	374	418	15	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	GB 13880191
A	-15	GLY	-	expression tag	GB 13880191
A	-14	SER	-	expression tag	GB 13880191
A	-13	SER	-	expression tag	GB 13880191
A	-12	HIS	-	expression tag	GB 13880191
A	-11	TYR	-	expression tag	GB 13880191
A	-10	HIS	-	expression tag	GB 13880191
A	-9	HIS	-	expression tag	GB 13880191
A	-8	HIS	-	expression tag	GB 13880191
A	-7	HIS	-	expression tag	GB 13880191
A	-6	SER	-	expression tag	GB 13880191
A	-5	SER	-	expression tag	GB 13880191
A	-4	GLY	-	expression tag	GB 13880191
A	-3	LEU	-	expression tag	GB 13880191
A	-2	VAL	-	expression tag	GB 13880191
A	-1	PRO	-	expression tag	GB 13880191
A	0	ARG	-	expression tag	GB 13880191
A	1	GLY	-	expression tag	GB 13880191
A	2	SER	-	expression tag	GB 13880191
A	3	HIS	-	expression tag	GB 13880191

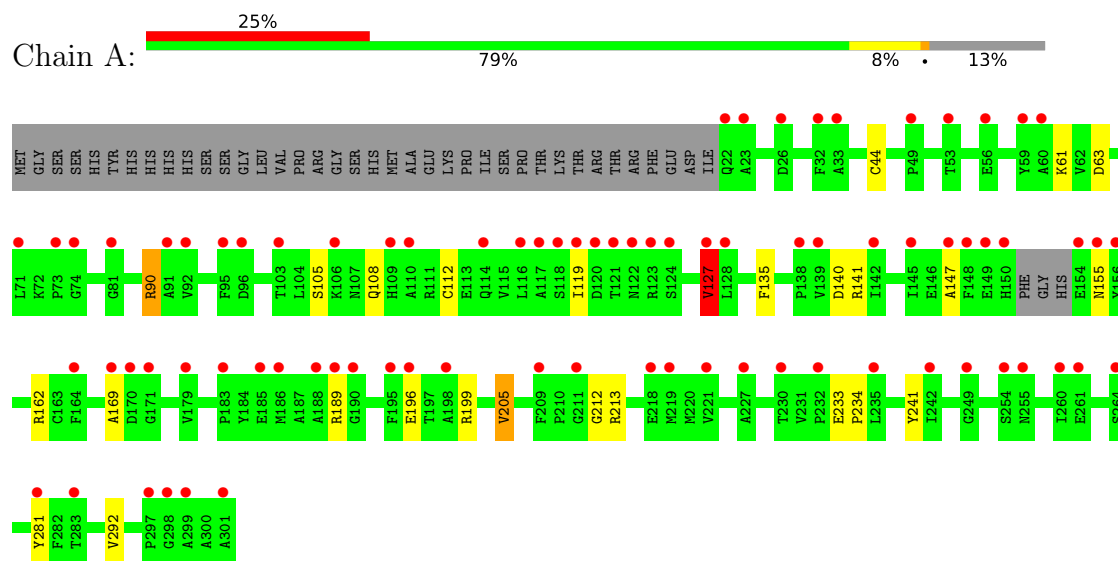
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	124	Total	O	0	0
			124	124		

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: methoxy mycolic acid synthase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	56.72Å 56.72Å 206.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.00-2.10) 96.6 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.31 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.232 0.204 , 0.241	Depositor DCC
R_{free} test set	1170 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2342	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.14	5/2271 (0.2%)	1.10	7/3076 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	ALA	CA-CB	6.65	1.63	1.53
1	A	119	ILE	CA-CB	6.29	1.61	1.54
1	A	189	ARG	CG-CD	6.11	1.70	1.52
1	A	292	VAL	CA-CB	5.50	1.60	1.54
1	A	147	ALA	CA-CB	5.35	1.59	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ARG	CG-CD-NE	-7.61	95.27	112.00
1	A	127	VAL	CB-CA-C	7.48	122.01	110.50
1	A	189	ARG	CB-CG-CD	6.83	127.02	111.30
1	A	189	ARG	CD-NE-CZ	6.45	133.43	124.40
1	A	189	ARG	NE-CZ-NH1	6.07	127.57	121.50
1	A	199	ARG	NE-CZ-NH2	-5.70	114.07	119.20
1	A	90	ARG	NE-CZ-NH2	-5.06	114.65	119.20

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	2218	0	2133	12	0
2	A	124	0	0	1	0
All	All	2342	0	2133	12	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 (12) 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:63:ASP:OD1	1:A:90:ARG:HD3	1.74	0.87
1:A:205:VAL:HG13	2:A:355:HOH:O	1.87	0.73
1:A:196:GLU:HG2	1:A:281:TYR:OH	2.08	0.53
1:A:135:PHE:O	1:A:162:ARG:HD2	2.09	0.53
1:A:61:LYS:HD2	1:A:61:LYS:C	2.36	0.51
1:A:105:SER:HB3	1:A:108:GLN:HB2	1.93	0.51
1:A:212:GLY:O	1:A:213:ARG:HG2	2.14	0.48
1:A:63:ASP:OD1	1:A:90:ARG:CD	2.54	0.47
1:A:44:CYS:O	1:A:61:LYS:HG3	2.18	0.43
1:A:140:ASP:O	1:A:141:ARG:HD3	2.19	0.42
1:A:233:GLU:HA	1:A:234:PRO:HD3	1.92	0.42
1:A:112:CYS:HB3	1:A:127:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	273/318 (86%)	267 (98%)	6 (2%)	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	238/279 (85%)	234 (98%)	4 (2%)	53 62

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
1	A	155	ASN
1	A	205	VAL
1	A	241	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	36	GLN
1	A	65	ASN
1	A	122	ASN
1	A	155	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	277/318 (87%)	1.64	81 (29%) 1 1	56, 64, 76, 89	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	ALA	4.0
1	A	190	GLY	3.8
1	A	148	PHE	3.7
1	A	154	GLU	3.7
1	A	124	SER	3.5
1	A	301	ALA	3.5
1	A	118	SER	3.4
1	A	211	GLY	3.3
1	A	169	ALA	3.2
1	A	227	ALA	3.2
1	A	164	PHE	3.2
1	A	155	ASN	3.2
1	A	149	GLU	3.1
1	A	110	ALA	3.1
1	A	117	ALA	3.1
1	A	242	ILE	3.0
1	A	297	PRO	2.9
1	A	147	ALA	2.8
1	A	299	ALA	2.8
1	A	283	THR	2.8
1	A	189	ARG	2.7
1	A	60	ALA	2.7
1	A	188	ALA	2.7
1	A	156	TYR	2.7
1	A	103	THR	2.6
1	A	73	PRO	2.6
1	A	122	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	219	MET	2.5
1	A	121	THR	2.5
1	A	138	PRO	2.5
1	A	150	HIS	2.5
1	A	91	ALA	2.5
1	A	96	ASP	2.5
1	A	106	LYS	2.5
1	A	170	ASP	2.4
1	A	198	ALA	2.4
1	A	128	LEU	2.4
1	A	281	TYR	2.4
1	A	183	PRO	2.4
1	A	218	GLU	2.4
1	A	123	ARG	2.4
1	A	109	HIS	2.4
1	A	264	SER	2.4
1	A	49	PRO	2.4
1	A	22	GLN	2.3
1	A	254	SER	2.3
1	A	298	GLY	2.3
1	A	32	PHE	2.3
1	A	261	GLU	2.3
1	A	59	TYR	2.3
1	A	116	LEU	2.3
1	A	179	VAL	2.3
1	A	171	GLY	2.3
1	A	95	PHE	2.2
1	A	26	ASP	2.2
1	A	235	LEU	2.2
1	A	195	PHE	2.2
1	A	145	ILE	2.2
1	A	127	VAL	2.2
1	A	33	ALA	2.2
1	A	196	GLU	2.2
1	A	186	MET	2.2
1	A	139	VAL	2.2
1	A	249	GLY	2.2
1	A	255	ASN	2.2
1	A	232	PRO	2.1
1	A	142	ILE	2.1
1	A	92	VAL	2.1
1	A	114	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	56	GLU	2.1
1	A	53	THR	2.1
1	A	119	ILE	2.1
1	A	260	ILE	2.1
1	A	71	LEU	2.1
1	A	221	VAL	2.1
1	A	185	GLU	2.1
1	A	120	ASP	2.1
1	A	74	GLY	2.0
1	A	81	GLY	2.0
1	A	209	PHE	2.0
1	A	230	THR	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 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.