



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:54 PM UTC

PDB ID : 4Z0M / pdb_00004z0m
Title : EchA5 Mycobacterium tuberculosis
Authors : Chaudhary, S.; Gokhale, R.S.
Deposited on : 2015-03-26
Resolution : 1.97 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

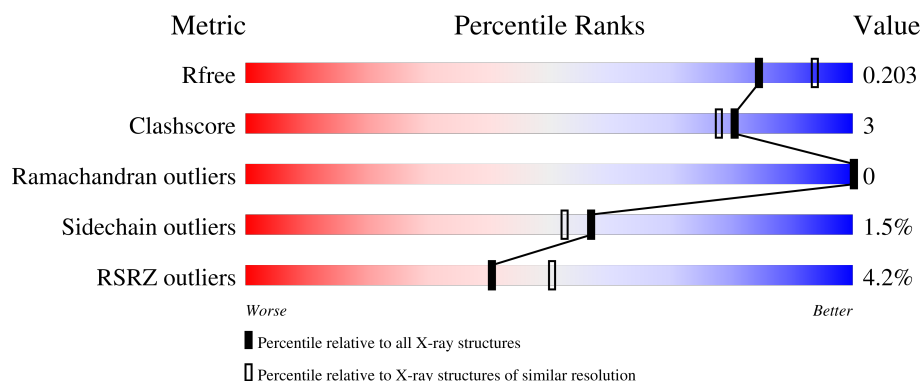
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	269	3% 78% 11% 10%
1	B	269	6% 79% 9% 11%
1	C	269	3% 74% 11% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5621 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 Enoyl-CoA hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1731	1085	319	316	11			
1	B	239	Total	C	N	O	S	0	0	0
			1702	1069	314	308	11			
1	C	230	Total	C	N	O	S	0	0	0
			1640	1037	298	294	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	HIS	-	expression tag	UNP I6Y4E8
A	265	HIS	-	expression tag	UNP I6Y4E8
A	266	HIS	-	expression tag	UNP I6Y4E8
A	267	HIS	-	expression tag	UNP I6Y4E8
A	268	HIS	-	expression tag	UNP I6Y4E8
A	269	HIS	-	expression tag	UNP I6Y4E8
B	264	HIS	-	expression tag	UNP I6Y4E8
B	265	HIS	-	expression tag	UNP I6Y4E8
B	266	HIS	-	expression tag	UNP I6Y4E8
B	267	HIS	-	expression tag	UNP I6Y4E8
B	268	HIS	-	expression tag	UNP I6Y4E8
B	269	HIS	-	expression tag	UNP I6Y4E8
C	264	HIS	-	expression tag	UNP I6Y4E8
C	265	HIS	-	expression tag	UNP I6Y4E8
C	266	HIS	-	expression tag	UNP I6Y4E8
C	267	HIS	-	expression tag	UNP I6Y4E8
C	268	HIS	-	expression tag	UNP I6Y4E8
C	269	HIS	-	expression tag	UNP I6Y4E8

- Molecule 2 is water.

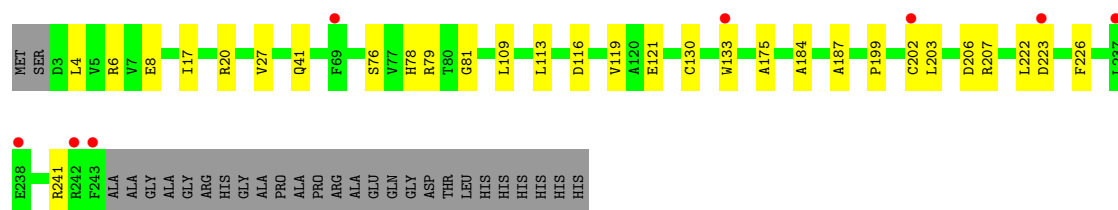
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	195	Total 195	O 195	0	0
2	B	202	Total 202	O 202	0	0
2	C	151	Total 151	O 151	0	0

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.

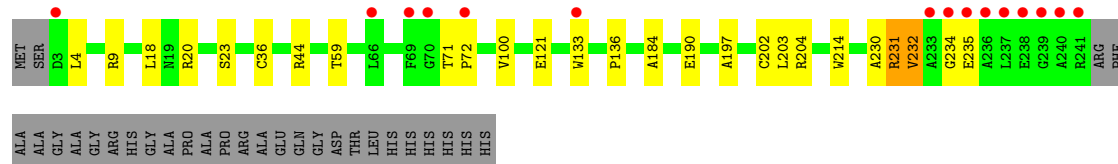
• Molecule 1: Enoyl-CoA hydratase

Chain A: 



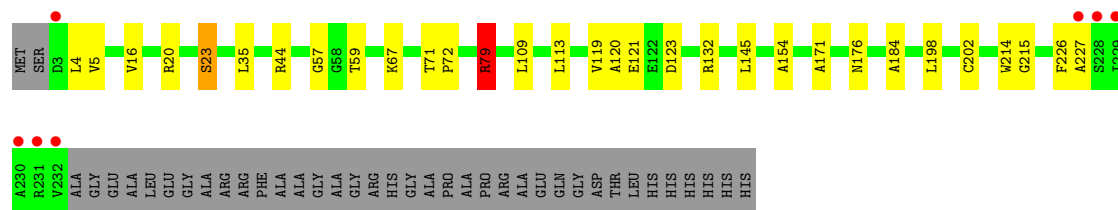
• Molecule 1: Enoyl-CoA hydratase

Chain B: 



• Molecule 1: Enoyl-CoA hydratase

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.71Å 136.71Å 125.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.53 – 1.97 39.53 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.53-1.97) 99.3 (39.53-1.97)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.168 , 0.195 0.177 , 0.203	Depositor DCC
R_{free} test set	4831 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5621	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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

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	1.64	14/1761 (0.8%)	1.21	2/2390 (0.1%)
1	B	1.64	11/1732 (0.6%)	1.29	4/2351 (0.2%)
1	C	1.65	15/1671 (0.9%)	1.27	9/2269 (0.4%)
All	All	1.64	40/5164 (0.8%)	1.26	15/7010 (0.2%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	215	GLY	N-CA	8.63	1.57	1.45
1	A	78	HIS	CA-C	-7.40	1.43	1.52
1	B	9	ARG	CA-C	-6.91	1.44	1.52
1	A	119	VAL	C-O	-6.82	1.16	1.24
1	C	198	LEU	N-CA	6.79	1.53	1.46
1	A	199	PRO	CA-C	6.64	1.59	1.52
1	B	231	ARG	CD-NE	-6.15	1.37	1.46
1	C	119	VAL	C-O	-6.05	1.17	1.24
1	A	27	VAL	N-CA	-6.03	1.38	1.46
1	A	226	PHE	C-O	-5.93	1.16	1.24
1	C	176	ASN	N-CA	-5.90	1.38	1.46
1	C	23	SER	N-CA	5.84	1.52	1.46
1	B	214	TRP	CA-C	5.82	1.60	1.52
1	C	171	ALA	C-O	-5.81	1.16	1.24
1	C	154	ALA	N-CA	-5.81	1.39	1.46
1	A	187	ALA	CA-C	5.72	1.60	1.52
1	B	231	ARG	C-O	-5.68	1.17	1.24
1	A	206	ASP	CB-CG	5.67	1.66	1.52
1	B	197	ALA	C-O	-5.66	1.16	1.24
1	C	120	ALA	N-CA	-5.59	1.39	1.45
1	B	44	ARG	C-O	-5.57	1.16	1.24
1	A	175	ALA	CA-C	-5.55	1.45	1.52
1	C	67	LYS	C-O	-5.52	1.17	1.24
1	A	79	ARG	N-CA	-5.46	1.39	1.46
1	B	36	CYS	CA-C	-5.42	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	PRO	N-CA	5.41	1.54	1.47
1	A	17	ILE	CA-CB	-5.40	1.47	1.54
1	C	16	VAL	C-O	-5.38	1.18	1.24
1	B	230	ALA	C-O	-5.33	1.17	1.24
1	B	204	ARG	N-CA	-5.31	1.40	1.46
1	B	100	VAL	N-CA	-5.31	1.39	1.46
1	C	215	GLY	CA-C	5.30	1.59	1.51
1	C	226	PHE	C-O	-5.30	1.17	1.24
1	A	27	VAL	C-O	-5.29	1.18	1.24
1	C	35	LEU	CA-C	-5.19	1.46	1.52
1	C	57	GLY	C-O	-5.14	1.17	1.24
1	A	81	GLY	CA-C	5.12	1.59	1.51
1	C	5	VAL	C-O	-5.08	1.19	1.24
1	B	234	GLY	N-CA	5.06	1.52	1.45
1	A	222	LEU	N-CA	5.06	1.52	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ARG	NE-CZ-NH1	-9.94	111.56	121.50
1	B	231	ARG	NE-CZ-NH2	9.58	127.82	119.20
1	C	215	GLY	N-CA-C	6.71	129.08	113.18
1	C	227	ALA	N-CA-C	6.21	120.41	112.34
1	C	214	TRP	CA-C-N	-6.06	109.53	121.41
1	C	214	TRP	C-N-CA	-6.06	109.53	121.41
1	C	79	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	C	214	TRP	N-CA-C	-5.65	102.53	110.50
1	C	123	ASP	N-CA-CB	-5.62	100.97	110.41
1	B	231	ARG	CD-NE-CZ	5.43	132.00	124.40
1	A	202	CYS	N-CA-CB	5.42	118.08	110.12
1	B	202	CYS	N-CA-CB	-5.33	102.28	110.16
1	A	241	ARG	N-CA-C	5.06	118.55	112.38
1	C	145	LEU	CA-C-N	-5.01	113.77	119.28
1	C	145	LEU	C-N-CA	-5.01	113.77	119.28

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	1731	0	1713	10	0
1	B	1702	0	1688	11	0
1	C	1640	0	1616	7	1
2	A	195	0	0	3	0
2	B	202	0	0	4	1
2	C	151	0	0	1	0
All	All	5621	0	5017	26	1

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 (26) 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:B:4:LEU:HD22	1:B:20:ARG:HD3	1.75	0.68
1:A:4:LEU:HD22	1:A:20:ARG:HD3	1.79	0.64
1:C:4:LEU:HD22	1:C:20:ARG:HD3	1.80	0.63
1:C:121:GLU:HG3	1:C:184:ALA:HB2	1.82	0.62
1:A:41:GLN:HG2	2:A:395:HOH:O	1.98	0.62
1:A:203:LEU:C	1:A:203:LEU:HD23	2.25	0.62
1:C:44:ARG:CG	2:C:427:HOH:O	2.50	0.60
1:A:20:ARG:HD2	2:A:447:HOH:O	2.04	0.58
1:B:231:ARG:HD3	2:B:448:HOH:O	2.05	0.57
1:B:59:THR:HG22	2:B:314:HOH:O	2.05	0.56
1:B:133:TRP:HZ3	2:B:482:HOH:O	1.89	0.56
1:B:232:VAL:HG23	1:B:232:VAL:O	2.06	0.55
1:A:130:CYS:HA	1:A:133:TRP:CE3	2.49	0.48
1:B:190:GLU:HG3	2:B:384:HOH:O	2.12	0.48
1:B:136:PRO:HA	1:C:202:CYS:SG	2.54	0.48
1:A:223:ASP:OD1	1:C:79:ARG:HD2	2.15	0.47
1:A:6:ARG:NH1	1:A:8:GLU:OE2	2.48	0.46
2:A:429:HOH:O	1:B:235:GLU:CA	2.65	0.45
1:B:203:LEU:HD23	1:B:203:LEU:C	2.41	0.45
1:C:71:THR:HB	1:C:72:PRO:HD2	2.01	0.43
1:A:116:ASP:CG	1:A:207:ARG:HE	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLU:HG3	1:B:184:ALA:HB2	2.02	0.42
1:C:109:LEU:O	1:C:113:LEU:HG	2.19	0.41
1:A:109:LEU:O	1:A:113:LEU:HG	2.20	0.41
1:A:121:GLU:HG3	1:A:184:ALA:HB2	2.02	0.41
1:B:71:THR:HB	1:B:72:PRO:HD2	2.02	0.41

All (1) 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)
1:C:132:ARG:CG	2:B:483:HOH:O[2_565]	2.18	0.02

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	239/269 (89%)	232 (97%)	7 (3%)	0	100	100
1	B	237/269 (88%)	230 (97%)	7 (3%)	0	100	100
1	C	228/269 (85%)	222 (97%)	6 (3%)	0	100	100
All	All	704/807 (87%)	684 (97%)	20 (3%)	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	163/192 (85%)	162 (99%)	1 (1%)	78	76
1	B	159/192 (83%)	156 (98%)	3 (2%)	50	44
1	C	151/192 (79%)	148 (98%)	3 (2%)	48	42
All	All	473/576 (82%)	466 (98%)	7 (2%)	57	52

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	SER
1	B	18	LEU
1	B	23	SER
1	B	232	VAL
1	C	23	SER
1	C	59	THR
1	C	79	ARG

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	75	ASN
1	B	78	HIS
1	C	75	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 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	241/269 (89%)	-0.03	8 (3%) 49 59	18, 27, 49, 67	0
1	B	239/269 (88%)	0.17	15 (6%) 26 34	20, 29, 57, 82	0
1	C	230/269 (85%)	0.34	7 (3%) 52 62	19, 33, 53, 85	0
All	All	710/807 (87%)	0.16	30 (4%) 40 50	18, 30, 54, 85	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	232	VAL	6.5
1	B	240	ALA	5.6
1	B	133	TRP	5.4
1	B	237	LEU	4.7
1	B	234	GLY	4.5
1	C	229	ILE	4.4
1	C	228	SER	3.8
1	B	241	ARG	3.8
1	B	236	ALA	3.7
1	A	133	TRP	3.5
1	C	231	ARG	3.5
1	B	233	ALA	3.3
1	B	235	GLU	3.2
1	A	243	PHE	3.0
1	A	69	PHE	2.9
1	B	3	ASP	2.9
1	C	3	ASP	2.9
1	A	242	ARG	2.7
1	B	238	GLU	2.7
1	C	227	ALA	2.6
1	A	237	LEU	2.5
1	A	238	GLU	2.4
1	B	69	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	230	ALA	2.3
1	B	72	PRO	2.3
1	B	66	LEU	2.1
1	B	70	GLY	2.1
1	B	239	GLY	2.1
1	A	202	CYS	2.1
1	A	223	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 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.