



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:51 PM UTC

PDB ID : 3HQ1 / pdb_00003hq1
Title : Crystal structure of Mycobacterium tuberculosis LeuA complexed with citrate and Mn²⁺
Authors : Koon, N.; Squire, C.J.; Baker, E.N.
Deposited on : 2009-06-05
Resolution : 1.70 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

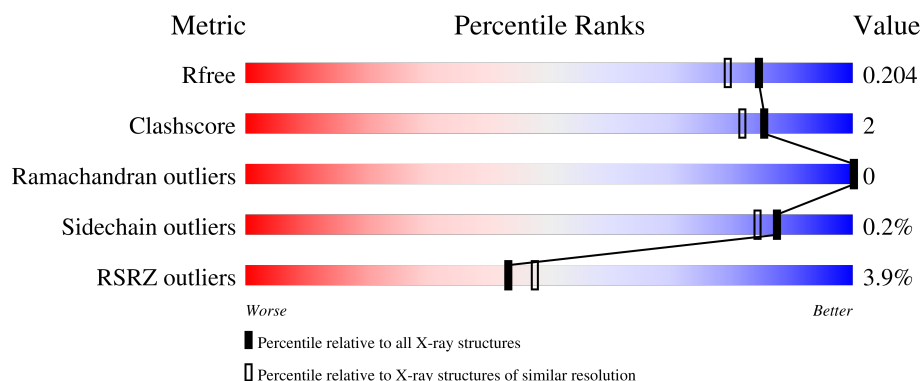
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	644	4% 86% • 11%
1	B	644	3% 84% 5% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9713 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 2-isopropylmalate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	5	0
			4360	2749	748	843	20			
1	B	576	Total	C	N	O	S	0	9	0
			4408	2779	764	843	22			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	1
			2	2		
2	B	1	Total	Mn	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

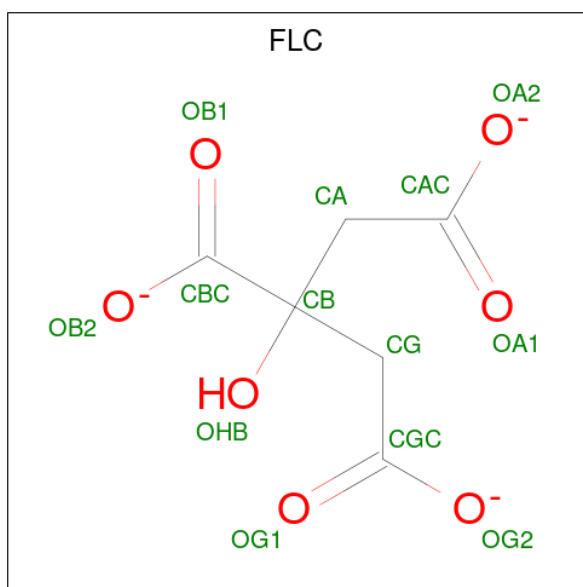
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	1
			26	12	14		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	470	Total 470	O 470	0	0
6	B	426	Total 426	O 426	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.36Å 154.80Å 69.11Å 90.00° 98.04° 90.00°	Depositor
Resolution (Å)	38.69 – 1.70 38.69 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.7 (38.69-1.70) 94.7 (38.69-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.204 0.170 , 0.204	Depositor DCC
R_{free} test set	5974 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9713	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FLC, MN, CL

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	0.71	0/4470	0.83	1/6102 (0.0%)
1	B	0.68	0/4530	0.81	2/6180 (0.0%)
All	All	0.69	0/9000	0.82	3/12282 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	ALA	N-CA-C	5.65	113.31	108.22
1	B	134	ILE	N-CA-C	5.13	112.63	107.55
1	B	163	ARG	CG-CD-NE	-5.01	100.98	112.00

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	4360	0	4163	15	0
1	B	4408	0	4234	23	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	1	0
4	A	6	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	12	0	16	0	0
5	B	26	0	8	1	0
6	A	470	0	0	5	0
6	B	426	0	0	4	0
All	All	9713	0	8429	37	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.

All (37) 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:559:MET:HE1	1:B:623:ILE:HG23	1.30	1.09
1:B:559:MET:HE3	1:B:566:GLN:CB	2.15	0.77
1:B:559:MET:HE3	1:B:566:GLN:HB3	1.65	0.76
1:A:19:ILE:HG12	6:B:776:HOH:O	1.91	0.69
6:A:786:HOH:O	1:B:19:ILE:HG12	1.93	0.68
1:B:559:MET:HE2	1:B:567:ALA:C	2.20	0.67
1:A:423:GLU:HG3	6:A:804:HOH:O	1.96	0.64
1:A:412:PRO:HG2	6:A:988:HOH:O	1.99	0.60
1:A:405:LEU:HD11	1:B:47:ARG:HG3	1.84	0.59
1:A:457:PHE:CE2	1:A:461:ILE:HD11	2.38	0.59
1:B:460:VAL:HG11	1:B:487:GLU:HG3	1.86	0.56
1:B:559:MET:CE	1:B:566:GLN:HB3	2.34	0.56
1:B:500:GLN:HG3	1:B:514:ILE:HD11	1.89	0.55
1:A:47:ARG:HD2	1:A:51:GLU:HG2	1.89	0.54
1:B:559:MET:HE3	1:B:566:GLN:HB2	1.89	0.54
1:B:487:GLU:OE2	1:B:641:ARG:NH1	2.42	0.52
1:B:152:GLU:HG3	1:B:198:LYS:HE3	1.95	0.49
1:A:406:TRP:CE3	1:A:414:ASP:HB2	2.49	0.48
1:B:95:LYS:HE2	6:B:962:HOH:O	2.14	0.48
1:A:375:PHE:CE2	1:A:425:VAL:HB	2.49	0.47
1:B:440:ILE:HG22	1:B:480:MET:HE1	1.96	0.47
1:B:63:TRP:HB3	1:B:303:ALA:HA	1.97	0.46
1:B:75:CYS:HB3	1:B:309:GLU:HG2	1.98	0.46
1:A:475:VAL:HG13	1:A:479:GLU:HB3	1.98	0.45
1:B:123:ASP:OD2	6:B:718:HOH:O	2.20	0.45
1:A:545:VAL:HG13	1:A:545:VAL:O	2.17	0.45
1:B:225:LEU:HD21	1:B:266:SER:HB2	2.00	0.44
1:A:423:GLU:CG	6:A:804:HOH:O	2.60	0.43
1:B:428:VAL:HG11	1:B:440:ILE:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:HD13	1:A:265:ASP:OD2	2.18	0.43
1:B:199:CYS:HB3	1:B:213:PHE:CE2	2.54	0.42
1:B:547:PHE:HD2	1:B:577:ILE:HG12	1.84	0.42
1:B:80:ARG:NH1	5:B:705[B]:FLC:OA2	2.50	0.42
1:A:545:VAL:O	1:A:545:VAL:CG1	2.68	0.41
1:A:150:LEU:HD13	6:A:1046:HOH:O	2.20	0.40
1:B:633:ARG:NE	6:B:751:HOH:O	2.54	0.40
1:A:533:GLY:HA3	3:A:703:CL:CL	2.58	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	570/644 (88%)	559 (98%)	11 (2%)	0	100	100
1	B	577/644 (90%)	565 (98%)	12 (2%)	0	100	100
All	All	1147/1288 (89%)	1124 (98%)	23 (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	447/520 (86%)	446 (100%)	1 (0%)	87	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	453/520 (87%)	452 (100%)	1 (0%)	87	84
All	All	900/1040 (86%)	898 (100%)	2 (0%)	87	84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	545	VAL
1	B	163	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	84	GLN
1	A	156	GLN
1	A	454	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](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	706	-	5,5,5	0.30	0	5,5,5	0.27	0
4	GOL	B	707	-	5,5,5	0.29	0	5,5,5	0.37	0
4	GOL	B	708	-	5,5,5	0.33	0	5,5,5	0.89	0
5	FLC	B	705[B]	2	12,12,12	1.08	0	17,17,17	1.32	1 (5%)
5	FLC	B	705[A]	2	12,12,12	1.09	0	17,17,17	1.27	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	706	-	-	0/4/4/4	-
4	GOL	B	707	-	-	0/4/4/4	-
4	GOL	B	708	-	-	2/4/4/4	-
5	FLC	B	705[B]	2	-	10/16/16/16	-
5	FLC	B	705[A]	2	-	6/16/16/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	705[B]	FLC	OB2-CBC-CB	3.31	119.48	113.14
5	B	705[A]	FLC	OB2-CBC-CB	3.29	119.46	113.14

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	705[A]	FLC	OHB-CB-CBC-OB1
5	B	705[A]	FLC	OHB-CB-CBC-OB2
4	B	708	GOL	O1-C1-C2-C3
5	B	705[A]	FLC	CG-CB-CBC-OB1
5	B	705[A]	FLC	CG-CB-CBC-OB2
4	B	708	GOL	O1-C1-C2-O2
5	B	705[B]	FLC	OHB-CB-CBC-OB1
5	B	705[B]	FLC	CA-CB-CBC-OB2
5	B	705[B]	FLC	CA-CB-CBC-OB1
5	B	705[B]	FLC	CG-CB-CBC-OB1
5	B	705[B]	FLC	CG-CB-CBC-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	705[B]	FLC	OHB-CB-CBC-OB2
5	B	705[A]	FLC	CA-CB-CBC-OB2
5	B	705[B]	FLC	CB-CA-CAC-OA1
5	B	705[A]	FLC	CA-CB-CBC-OB1
5	B	705[B]	FLC	CB-CA-CAC-OA2
5	B	705[B]	FLC	OHB-CB-CG-CGC
5	B	705[B]	FLC	CBC-CB-CG-CGC

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	705[B]	FLC	1	0

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	573/644 (88%)	-0.02	28 (4%) 35 38	7, 17, 35, 56	5 (0%)
1	B	576/644 (89%)	-0.10	17 (2%) 52 56	7, 17, 33, 42	9 (1%)
All	All	1149/1288 (89%)	-0.06	45 (3%) 43 47	7, 17, 34, 56	14 (1%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	464	ILE	4.9
1	A	396	ALA	4.5
1	B	429	ASN	4.4
1	A	565	ALA	4.2
1	A	461	ILE	4.0
1	A	434	LYS	3.9
1	B	57	ARG	3.5
1	A	399	CYS	3.4
1	A	435	GLY	3.4
1	A	577	ILE	3.4
1	A	458	SER	3.2
1	A	460	VAL	3.2
1	A	564	ASP	3.0
1	A	562	GLY	3.0
1	A	56	ILE	2.9
1	A	615	SER	2.9
1	B	614	THR	2.8
1	A	426	ILE	2.8
1	B	561	ALA	2.7
1	A	475	VAL	2.7
1	B	396	ALA	2.7
1	B	398	ASP	2.6
1	A	28	VAL	2.6
1	B	428	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	462	GLN	2.5
1	A	425	VAL	2.5
1	B	434	LYS	2.4
1	A	561	ALA	2.4
1	B	399	CYS	2.4
1	A	455	ILE	2.4
1	B	461	ILE	2.4
1	A	560	SER	2.3
1	B	435	GLY	2.3
1	B	578	ALA	2.2
1	A	397	ALA	2.2
1	A	563	ASP	2.1
1	A	424	ALA	2.1
1	B	520	ILE	2.1
1	A	545	VAL	2.1
1	A	463	LYS	2.1
1	B	18	THR	2.1
1	A	208	GLY	2.0
1	B	524	GLU	2.0
1	B	19	ILE	2.0
1	B	439	TYR	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	704	1/1	0.87	0.14	45,45,45,45	0
4	GOL	B	708	6/6	0.89	0.11	35,36,37,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FLC	B	705[A]	13/13	0.93	0.07	10,15,16,16	13
5	FLC	B	705[B]	13/13	0.93	0.07	11,15,16,16	13
4	GOL	A	706	6/6	0.95	0.07	14,15,17,18	0
3	CL	A	703	1/1	0.96	0.06	27,27,27,27	0
4	GOL	B	707	6/6	0.97	0.05	12,15,16,16	0
2	MN	A	701[B]	1/1	0.99	0.02	12,12,12,12	1
2	MN	A	701[A]	1/1	0.99	0.02	10,10,10,10	1
2	MN	B	702	1/1	1.00	0.02	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.