



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:04 PM UTC

PDB ID : 2WE8 / pdb_00002we8
Title : Crystal structure of Mycobacterium tuberculosis Rv0376c homologue from Mycobacterium smegmatis
Authors : Cho, H.J.; Kang, B.S.
Deposited on : 2009-03-29
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

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

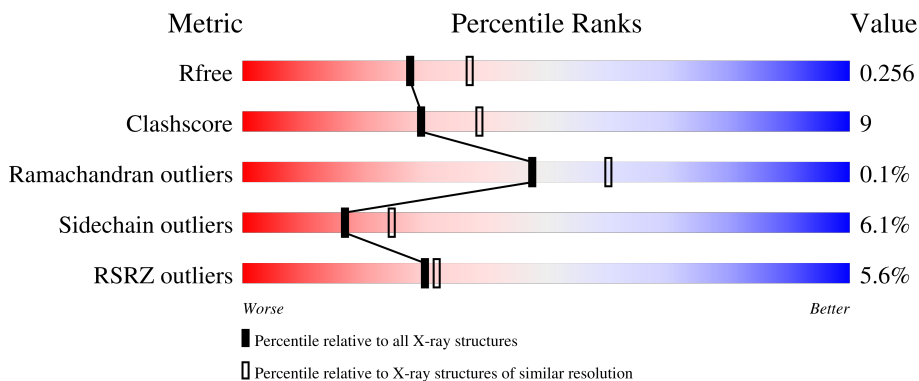
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 ≥ 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	386	 3% 75% 13% • 11%
1	B	386	 7% 68% 18% • 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	1361	-	-	X	-
2	GOL	A	1366	-	-	X	-

2 Entry composition [i](#)

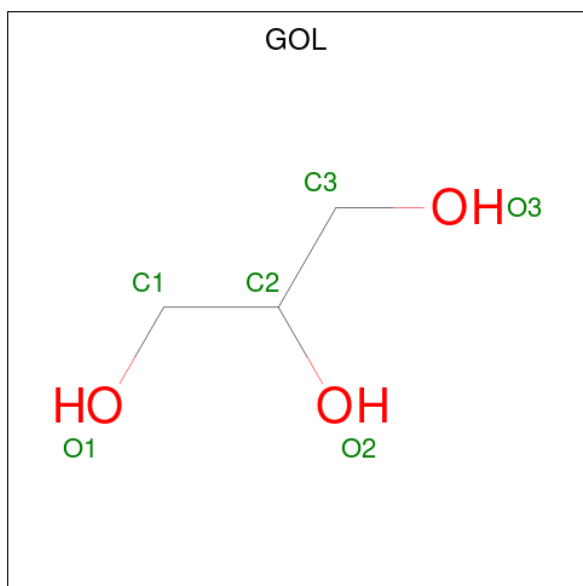
There are 4 unique types of molecules in this entry. The entry contains 5288 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	345	Total 2572	C 1611	N 464	O 490	S 7	0	4	0
1	B	335	Total 2463	C 1544	N 436	O 476	S 7	0	0	0

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



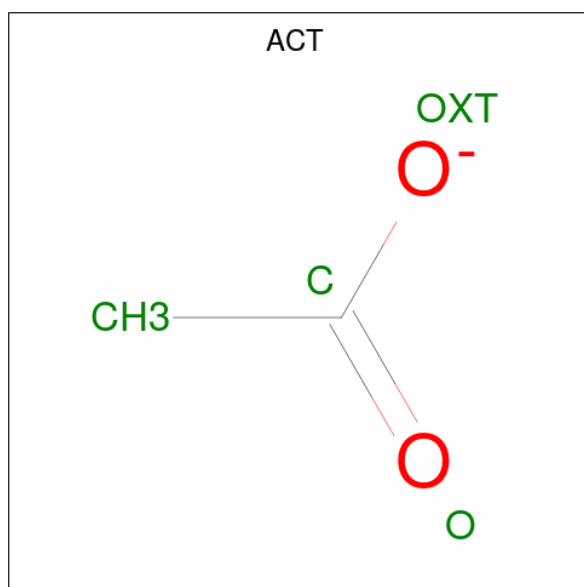
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	182	Total O 182 182	0	0
4	B	17	Total O 17 17	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.21Å 101.21Å 316.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.73 – 2.30 33.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.73-2.30) 99.7 (33.73-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.251 0.204 , 0.256	Depositor DCC
R_{free} test set	2223 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtrriage
Anisotropy	0.014	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5288	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: ACT, GOL

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	0.94	1/2631 (0.0%)	0.98	3/3587 (0.1%)
1	B	0.65	0/2507	0.96	3/3421 (0.1%)
All	All	0.81	1/5138 (0.0%)	0.97	6/7008 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	ILE	C-O	-6.78	1.17	1.24

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	GLY	N-CA-C	-7.17	101.31	112.85
1	B	190	ARG	N-CA-C	-6.55	104.45	113.56
1	A	297	ASP	N-CA-C	5.65	118.21	110.24
1	A	58	CYS	N-CA-C	5.30	117.47	111.11
1	B	39	GLY	N-CA-C	-5.18	108.03	113.58

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	PRO	Peptide

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	2572	0	2574	33	0
1	B	2463	0	2432	48	0
2	A	42	0	56	7	0
3	A	12	0	9	1	0
4	A	182	0	0	2	0
4	B	17	0	0	0	0
All	All	5288	0	5071	87	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 9.

The worst 5 of 87 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:27:VAL:HG23	1:B:38:ALA:HA	1.56	0.87
1:A:241:THR:HG22	1:A:244:ARG:H	1.45	0.81
1:B:162:ASP:O	1:B:166:THR:HG22	1.89	0.72
2:A:1361:GOL:H31	2:A:1366:GOL:H12	1.73	0.71
2:A:1361:GOL:H11	2:A:1366:GOL:H11	1.72	0.70

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	345/386 (89%)	339 (98%)	6 (2%)	0	100	100
1	B	329/386 (85%)	321 (98%)	7 (2%)	1 (0%)	36	46
All	All	674/772 (87%)	660 (98%)	13 (2%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	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	264/290 (91%)	247 (94%)	17 (6%)	16	23
1	B	250/290 (86%)	235 (94%)	15 (6%)	17	25
All	All	514/580 (89%)	482 (94%)	32 (6%)	17	24

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	206	ARG
1	B	308	ARG
1	A	307	ARG
1	A	272	ARG
1	B	310	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	222	GLN
1	B	257	HIS
1	B	280	HIS

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Mol	Chain	Res	Type
1	A	221	GLN
1	A	108	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](#)

10 ligands are modelled in this entry.

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	$\# Z > 2$
2	GOL	A	1361	-	5,5,5	0.48	0	5,5,5	1.03	0
3	ACT	A	1370	-	3,3,3	0.86	0	3,3,3	1.44	0
2	GOL	A	1367	-	5,5,5	0.55	0	5,5,5	0.73	0
2	GOL	A	1363	-	5,5,5	0.50	0	5,5,5	0.60	0
3	ACT	A	1369	-	3,3,3	0.83	0	3,3,3	1.42	0
2	GOL	A	1362	-	5,5,5	0.36	0	5,5,5	0.68	0
2	GOL	A	1365	-	5,5,5	0.35	0	5,5,5	0.33	0
2	GOL	A	1366	-	5,5,5	0.34	0	5,5,5	0.51	0
3	ACT	A	1368	-	3,3,3	0.74	0	3,3,3	1.53	0
2	GOL	A	1364	-	5,5,5	0.38	0	5,5,5	0.28	0

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
2	GOL	A	1361	-	-	4/4/4/4	-
2	GOL	A	1367	-	-	3/4/4/4	-
2	GOL	A	1363	-	-	2/4/4/4	-
2	GOL	A	1362	-	-	2/4/4/4	-
2	GOL	A	1365	-	-	2/4/4/4	-
2	GOL	A	1366	-	-	2/4/4/4	-
2	GOL	A	1364	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1361	GOL	O1-C1-C2-C3
2	A	1361	GOL	C1-C2-C3-O3
2	A	1362	GOL	O1-C1-C2-C3
2	A	1363	GOL	C1-C2-C3-O3
2	A	1367	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1361	GOL	5	0
3	A	1370	ACT	1	0
2	A	1363	GOL	2	0
2	A	1366	GOL	5	0

5.7 Other polymers [i](#)

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 [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, 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	345/386 (89%)	-0.28	12 (3%) 47 49	17, 32, 57, 85	4 (1%)
1	B	335/386 (86%)	0.87	26 (7%) 19 21	42, 76, 99, 110	0
All	All	680/772 (88%)	0.29	38 (5%) 30 32	17, 55, 96, 110	4 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	PRO	6.5
1	B	98	ILE	5.0
1	A	4	GLY	4.6
1	B	96	GLY	4.4
1	A	83	VAL	4.2

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(\AA^2)	Q<0.9
2	GOL	A	1363	6/6	0.73	0.20	70,79,80,81	0
2	GOL	A	1367	6/6	0.77	0.21	57,62,65,65	0
2	GOL	A	1364	6/6	0.82	0.17	56,77,79,80	0
3	ACT	A	1370	4/4	0.82	0.27	57,59,60,60	0
3	ACT	A	1369	4/4	0.83	0.17	83,83,83,83	0
2	GOL	A	1365	6/6	0.83	0.20	76,88,92,93	0
2	GOL	A	1362	6/6	0.85	0.14	50,56,59,60	0
3	ACT	A	1368	4/4	0.86	0.23	68,68,68,68	0
2	GOL	A	1366	6/6	0.90	0.26	46,58,64,69	0
2	GOL	A	1361	6/6	0.95	0.16	46,52,55,59	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.