



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2018 – 05:31 pm GMT

PDB ID : 1DF7  
Title : DIHYDROFOLATE REDUCTASE OF MYCOBACTERIUM TUBERCULOSIS COMPLEXED WITH NADPH AND METHOTREXATE  
Authors : Li, R.; Sirawaraporn, R.; Chitnumsub, P.; Sirawaraporn, W.; Wooden, J.; Athappilly, F.; Turley, S.; Hol, W.G.  
Deposited on : 1999-11-17  
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](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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

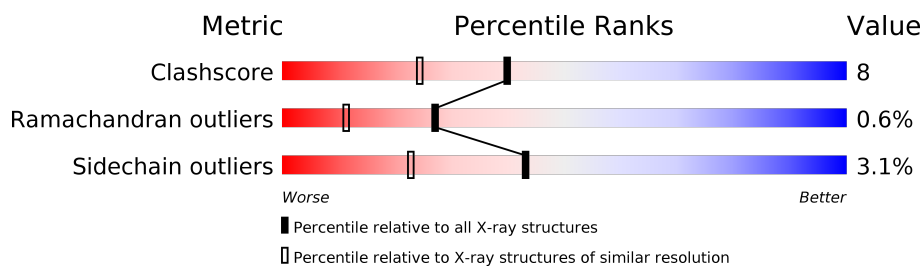
# 1 Overall quality at a glance

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))
Clashscore	122078	4165 (1.70-1.70)
Ramachandran outliers	120005	4098 (1.70-1.70)
Sidechain outliers	119972	4098 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	159	

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	SO4	A	506	-	X	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 1549 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 DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1244	783	228	228	5			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



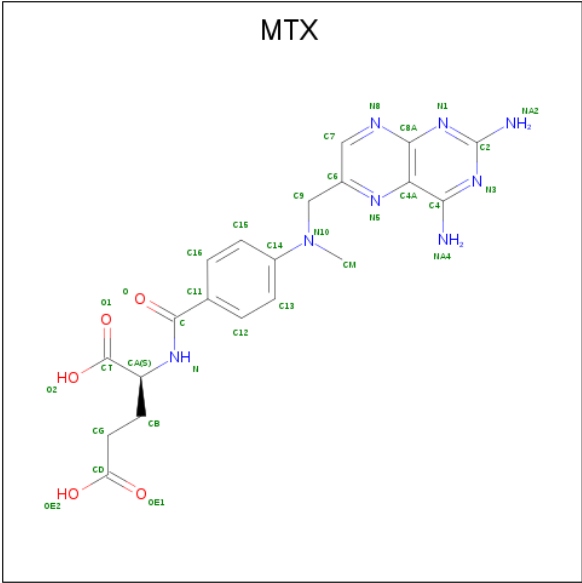
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is METHOTREXATE (three-letter code: MTX) (formula: C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			33	20	8	5		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is water.

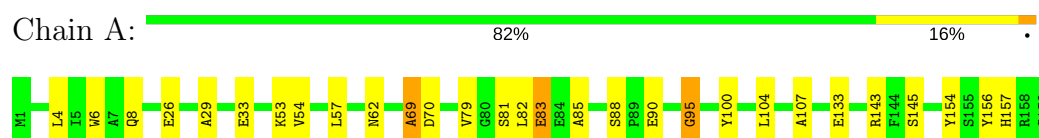
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	195	Total	O	0	0
			195	195		

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

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

#### • Molecule 1: DIHYDROFOLATE REDUCTASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.51Å 60.51Å 58.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70	Depositor
% Data completeness (in resolution range)	90.0 (50.00-1.70)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.187 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1549	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

## 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, MTX, SO4, NDP

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	0.72	2/1275 (0.2%)	0.85	0/1732

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	GLY	N-CA	-8.67	1.33	1.46
1	A	95	GLY	CA-C	6.79	1.62	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	TYR	Sidechain
1	A	156	TYR	Sidechain

### 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	1244	0	1223	19	0
2	A	5	0	0	0	0
3	A	48	0	26	0	0
4	A	33	0	20	1	0
5	A	24	0	32	2	0
6	A	195	0	0	9	0
All	All	1549	0	1301	21	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 8.

All (21) 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:57:LEU:H	1:A:62:ASN:HD21	1.25	0.83
1:A:33:GLU:HB3	6:A:656:HOH:O	1.94	0.66
5:A:504:GOL:H2	6:A:677:HOH:O	2.04	0.57
1:A:81:SER:OG	1:A:83:GLU:HG3	2.07	0.55
1:A:88:SER:HB3	6:A:665:HOH:O	2.06	0.54
1:A:69:ALA:HA	6:A:697:HOH:O	2.09	0.53
1:A:57:LEU:H	1:A:62:ASN:ND2	2.02	0.50
1:A:53:LYS:HG2	6:A:533:HOH:O	2.14	0.48
1:A:26:GLU:OE1	1:A:145:SER:HB2	2.14	0.48
1:A:54:VAL:HB	1:A:57:LEU:HD23	1.95	0.47
1:A:79:VAL:HG21	1:A:85:ALA:HB2	1.97	0.46
1:A:29:ALA:O	1:A:33:GLU:HG3	2.15	0.46
1:A:70:ASP:HB3	6:A:664:HOH:O	2.15	0.46
4:A:501:MTX:H13	4:A:501:MTX:HM1	1.89	0.44
1:A:8:GLN:NE2	5:A:505:GOL:H12	2.33	0.44
1:A:143:ARG:NH2	6:A:526:HOH:O	2.50	0.43
1:A:133:GLU:HB2	6:A:573:HOH:O	2.19	0.43
1:A:6:TRP:HB3	1:A:100:TYR:CZ	2.54	0.42
1:A:95:GLY:HA2	1:A:100:TYR:CZ	2.54	0.42
1:A:157:HIS:HB3	6:A:570:HOH:O	2.18	0.42
1:A:4:LEU:HD13	1:A:107:ALA:HB2	2.02	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	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	27	11

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ALA

### 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	127/127 (100%)	123 (97%)	4 (3%)	43	23

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

Mol	Chain	Res	Type
1	A	82	LEU
1	A	83	GLU
1	A	90	GLU
1	A	104	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	98	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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$
3	NDP	A	500	-	45,52,52	1.55	7 (15%)	54,80,80	1.44	8 (14%)
4	MTX	A	501	-	28,35,35	3.50	10 (35%)	36,49,49	5.70	23 (63%)
5	GOL	A	502	-	5,5,5	0.47	0	5,5,5	0.96	0
5	GOL	A	503	-	5,5,5	0.49	0	5,5,5	1.25	0
5	GOL	A	504	-	5,5,5	0.70	0	5,5,5	1.40	1 (20%)
5	GOL	A	505	-	5,5,5	0.81	0	5,5,5	1.37	1 (20%)
2	SO4	A	506	-	4,4,4	0.18	0	6,6,6	3.69	4 (66%)

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
3	NDP	A	500	-	-	0/30/77/77	0/5/5/5
4	MTX	A	501	-	-	0/19/25/25	0/3/3/3
5	GOL	A	502	-	-	0/4/4/4	0/0/0/0
5	GOL	A	503	-	-	0/4/4/4	0/0/0/0
5	GOL	A	504	-	-	0/4/4/4	0/0/0/0
5	GOL	A	505	-	-	0/4/4/4	0/0/0/0
2	SO4	A	506	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	MTX	CA-N	-9.21	1.34	1.46
4	A	501	MTX	C11-C	-7.76	1.33	1.50
4	A	501	MTX	C7-N8	-4.99	1.23	1.31
4	A	501	MTX	C16-C15	-4.97	1.30	1.38
4	A	501	MTX	C9-N10	-2.87	1.42	1.46
3	A	500	NDP	C4N-C5N	-2.21	1.44	1.49
4	A	501	MTX	C-N	-2.02	1.29	1.34
3	A	500	NDP	P2B-O1X	-2.02	1.43	1.50
3	A	500	NDP	C2A-N1A	2.06	1.37	1.33
3	A	500	NDP	C3B-C2B	2.06	1.57	1.53
3	A	500	NDP	O4B-C1B	2.82	1.45	1.41
4	A	501	MTX	CM-N10	3.25	1.51	1.46
4	A	501	MTX	CB-CA	3.96	1.58	1.53
3	A	500	NDP	C7N-C3N	4.24	1.57	1.48
4	A	501	MTX	C15-C14	5.24	1.49	1.39
3	A	500	NDP	P2B-O2B	5.29	1.69	1.59
4	A	501	MTX	C13-C14	7.81	1.54	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	MTX	O-C-N	-14.26	96.89	122.47
4	A	501	MTX	CB-CA-CT	-9.08	98.62	112.11
4	A	501	MTX	C12-C13-C14	-8.03	109.71	120.34
2	A	506	SO4	O2-S-O1	-6.09	67.67	109.86
4	A	501	MTX	C7-C6-N5	-5.03	117.56	120.85
4	A	501	MTX	N1-C2-N3	-4.33	121.06	127.41
3	A	500	NDP	C3N-C2N-N1N	-4.24	116.99	123.09
3	A	500	NDP	C1D-N1N-C2N	-3.76	114.75	121.10
4	A	501	MTX	C15-C14-N10	-3.34	116.73	121.65
4	A	501	MTX	CM-N10-C14	-2.93	114.41	119.60
4	A	501	MTX	C15-C16-C11	-2.65	117.78	120.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	MTX	C6-C9-N10	-2.37	109.55	113.66
3	A	500	NDP	O7N-C7N-C3N	-2.34	116.50	120.90
2	A	506	SO4	O4-S-O1	-2.28	96.93	109.24
3	A	500	NDP	O2X-P2B-O2B	-2.21	96.07	105.99
5	A	504	GOL	O2-C2-C1	2.02	118.23	109.00
5	A	505	GOL	O2-C2-C1	2.02	118.23	109.00
4	A	501	MTX	C13-C14-N10	2.30	125.03	121.65
3	A	500	NDP	O3X-P2B-O2X	2.38	117.02	107.59
3	A	500	NDP	O3B-C3B-C2B	2.45	118.11	111.17
3	A	500	NDP	C4A-C5A-N7A	2.57	111.90	109.41
4	A	501	MTX	NA4-C4-N3	2.72	125.00	116.59
3	A	500	NDP	PN-O3-PA	2.83	142.13	132.63
4	A	501	MTX	C9-C6-C7	3.49	127.68	121.60
4	A	501	MTX	C2-N3-C4	3.49	127.53	116.73
4	A	501	MTX	NA2-C2-N3	3.70	123.06	117.25
4	A	501	MTX	C16-C15-C14	3.72	125.25	120.34
4	A	501	MTX	CG-CB-CA	3.85	120.88	113.19
2	A	506	SO4	O3-S-O1	3.93	130.50	109.24
2	A	506	SO4	O4-S-O2	4.56	133.88	109.24
4	A	501	MTX	C11-C-N	4.84	125.78	116.98
4	A	501	MTX	C9-N10-C14	6.66	132.67	119.50
4	A	501	MTX	C6-C7-N8	7.15	130.13	123.13
4	A	501	MTX	CB-CA-N	8.57	122.73	110.19
4	A	501	MTX	C13-C12-C11	9.09	131.09	120.78
4	A	501	MTX	O-C-C11	9.32	137.29	120.93
4	A	501	MTX	CA-N-C	16.89	144.81	122.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	MTX	1	0
5	A	504	GOL	1	0
5	A	505	GOL	1	0

## 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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.