



# Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 01:37 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 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

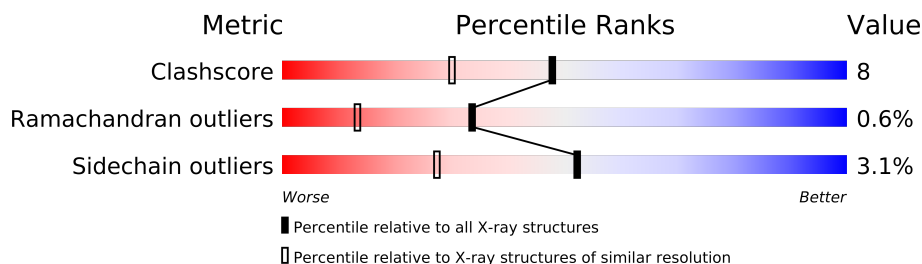
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	159	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 1549 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

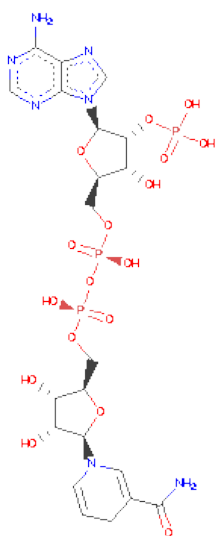
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1244	783	228	228	5			

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



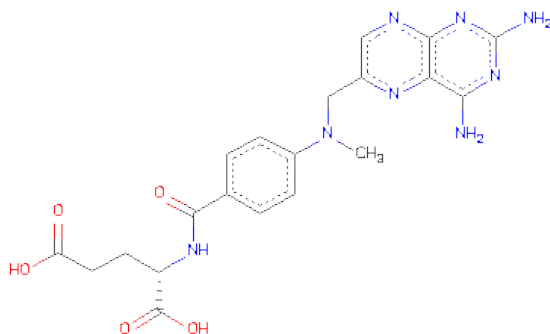
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (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
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0

- Molecule 4 is METHOTREXATE (three-letter code: MTX) (formula:  $C_{20}H_{22}N_8O_5$ ).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

### 5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,



and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (21) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

### 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	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	33 13

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ALA

### 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	127/127 (100%)	123 (97%)	4 (3%)	52 27

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
1	A	98	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	-	52,52,52	1.59	9 (17%)	80,80,80	1.45	14 (17%)
4	MTX	A	501	-	35,35,35	3.08	14 (40%)	49,49,49	4.86	32 (65%)
5	GOL	A	502	-	5,5,5	0.41	0	5,5,5	1.02	0
5	GOL	A	503	-	5,5,5	0.41	0	5,5,5	1.32	0
5	GOL	A	504	-	5,5,5	0.62	0	5,5,5	1.44	1 (20%)
5	GOL	A	505	-	5,5,5	0.75	0	5,5,5	1.41	1 (20%)
2	SO4	A	506	-	4,4,4	0.34	0	6,6,6	5.41	3 (50%)

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	-	-	0/35/77/77	0/3/5/5
4	MTX	A	501	-	-	0/25/25/25	0/1/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	MTX	C11-C	-7.83	1.33	1.50
4	A	501	MTX	C13-C14	7.58	1.54	1.39
4	A	501	MTX	CG-CD	6.53	1.67	1.50
4	A	501	MTX	CA-N	-5.31	1.34	1.45
4	A	501	MTX	C15-C14	5.08	1.49	1.39
3	A	500	NDP	C7N-C3N	4.59	1.57	1.47
4	A	501	MTX	C7-N8	-4.59	1.23	1.31
4	A	501	MTX	C16-C15	-4.52	1.30	1.38
4	A	501	MTX	OE1-CD	4.17	1.37	1.22
3	A	500	NDP	PA-O3	-4.04	1.52	1.59
4	A	501	MTX	CM-N10	3.74	1.51	1.46
3	A	500	NDP	P2B-O2B	3.06	1.69	1.59
3	A	500	NDP	C2N-N1N	2.91	1.42	1.36
3	A	500	NDP	C4N-C3N	-2.84	1.44	1.50
4	A	501	MTX	C9-N10	-2.79	1.42	1.46
3	A	500	NDP	O4B-C1B	2.49	1.45	1.41
3	A	500	NDP	C1D-N1N	2.44	1.51	1.46
4	A	501	MTX	O2-CT	2.30	1.38	1.30
4	A	501	MTX	CB-CA	2.23	1.58	1.53
3	A	500	NDP	C4N-C5N	-2.19	1.44	1.49
3	A	500	NDP	P2B-O1X	-2.18	1.43	1.51
4	A	501	MTX	C-N	-2.07	1.29	1.34
4	A	501	MTX	C16-C11	2.01	1.42	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	MTX	O-C-N	-14.15	96.89	122.44
2	A	506	SO4	O2-S-O1	-12.65	67.67	109.53
4	A	501	MTX	CA-N-C	10.31	144.81	121.80
4	A	501	MTX	OE2-CD-OE1	9.46	147.37	123.30
4	A	501	MTX	O-C-C11	9.28	137.29	121.01
4	A	501	MTX	CB-CG-CD	8.88	134.43	112.88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	MTX	C13-C12-C11	8.65	131.09	120.76
4	A	501	MTX	C12-C13-C14	-7.98	109.71	120.44
4	A	501	MTX	OE2-CD-CG	-7.65	87.17	114.22
4	A	501	MTX	C6-C7-N8	6.62	130.13	123.16
4	A	501	MTX	C9-N10-C14	6.40	132.67	119.36
4	A	501	MTX	CB-CA-N	6.25	122.73	110.83
4	A	501	MTX	CB-CA-CT	-5.62	98.62	110.71
4	A	501	MTX	C11-C-N	5.33	125.78	116.89
4	A	501	MTX	C7-C6-N5	-4.57	117.56	120.75
3	A	500	NDP	C3N-C2N-N1N	-4.27	116.99	123.05
4	A	501	MTX	N1-C2-N3	-4.10	121.06	127.54
4	A	501	MTX	CG-CB-CA	4.02	120.88	112.99
3	A	500	NDP	O2X-P2B-O2B	-3.83	96.07	107.09
4	A	501	MTX	C4-C4A-C8A	3.73	119.98	116.87
3	A	500	NDP	C1D-N1N-C2N	-3.68	114.75	121.02
4	A	501	MTX	C7-N8-C8A	-3.68	112.71	116.85
4	A	501	MTX	C16-C15-C14	3.58	125.25	120.44
3	A	500	NDP	PN-O3-PA	3.56	142.13	131.68
4	A	501	MTX	C15-C14-N10	-3.54	116.73	121.61
4	A	501	MTX	C9-C6-C7	3.47	127.68	121.49
4	A	501	MTX	NA2-C2-N3	3.40	123.06	117.19
4	A	501	MTX	O1-CT-CA	3.22	133.65	121.86
4	A	501	MTX	C2-N3-C4	3.10	127.53	116.50
4	A	501	MTX	O2-CT-O1	-3.00	117.30	124.07
3	A	500	NDP	C5N-C6N-N1N	-2.88	117.15	123.03
4	A	501	MTX	CM-N10-C14	-2.78	114.41	119.58
3	A	500	NDP	C4A-C5A-N7A	2.77	111.90	109.52
3	A	500	NDP	C4N-C3N-C2N	2.65	124.91	121.68
4	A	501	MTX	C8A-C4A-N5	-2.62	119.44	122.66
2	A	506	SO4	O4-S-O2	2.62	133.88	110.12
4	A	501	MTX	NA4-C4-N3	2.50	125.00	116.23
4	A	501	MTX	C15-C16-C11	-2.49	117.78	120.76
4	A	501	MTX	C13-C14-N10	2.48	125.03	121.61
4	A	501	MTX	C6-C9-N10	-2.43	109.55	113.79
3	A	500	NDP	O3X-P2B-O2X	2.42	117.02	107.61
3	A	500	NDP	O3B-C3B-C2B	2.35	118.11	111.20
3	A	500	NDP	C6N-N1N-C2N	2.34	122.50	119.44
3	A	500	NDP	O4B-C1B-N9A	2.27	110.55	108.44
2	A	506	SO4	O3-S-O1	2.24	130.50	110.12
3	A	500	NDP	C4N-C5N-C6N	2.23	126.69	122.61
5	A	504	GOL	O2-C2-C1	2.20	118.23	108.22
5	A	505	GOL	O2-C2-C1	2.20	118.23	108.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	NDP	O7N-C7N-C3N	-2.14	116.50	120.51
4	A	501	MTX	C4A-C4-N3	-2.05	112.39	119.27
3	A	500	NDP	O3X-P2B-O2B	-2.01	101.29	107.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.