



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 23, 2018 – 08:44 am GMT

PDB ID : 1E7W
Title : One active site, two modes of reduction correlate the mechanism of leishmania pteridine reductase with pterin metabolism and antifolate drug resistance in trpanosomes
Authors : Gourley, D.G.; Hunter, W.N.
Deposited on : 2000-09-11
Resolution : 1.75 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 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

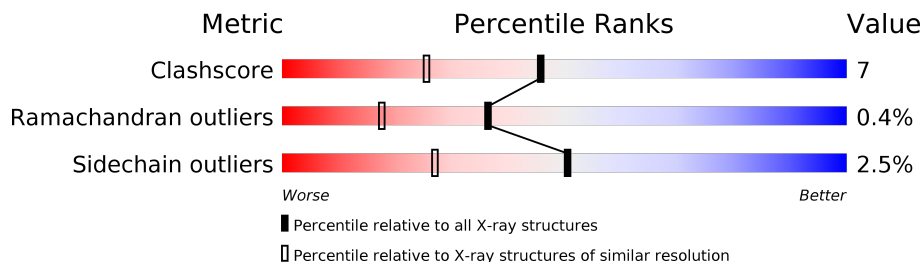
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2073 (1.76-1.76)
Ramachandran outliers	120005	2051 (1.76-1.76)
Sidechain outliers	119972	2051 (1.76-1.76)

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 ≥ 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	291	
1	B	291	

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
3	MTX	B	301	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 4584 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 PTERIDINE REDUCTASE.

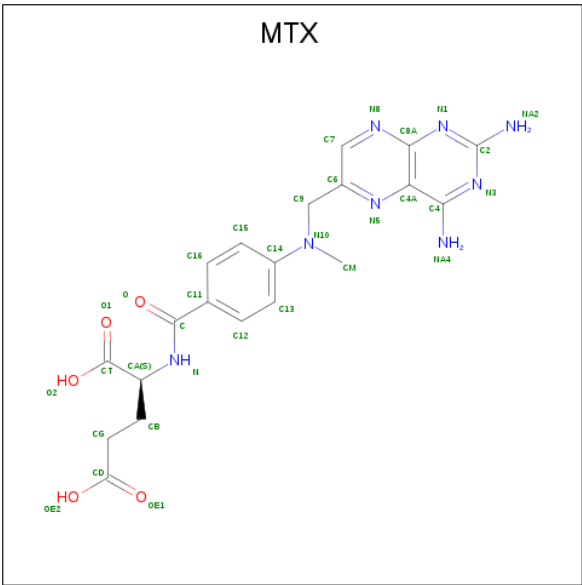
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	12	2	0
			1996	1260	353	372	11			
1	B	258	Total	C	N	O	S	20	1	0
			1938	1220	348	360	10			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



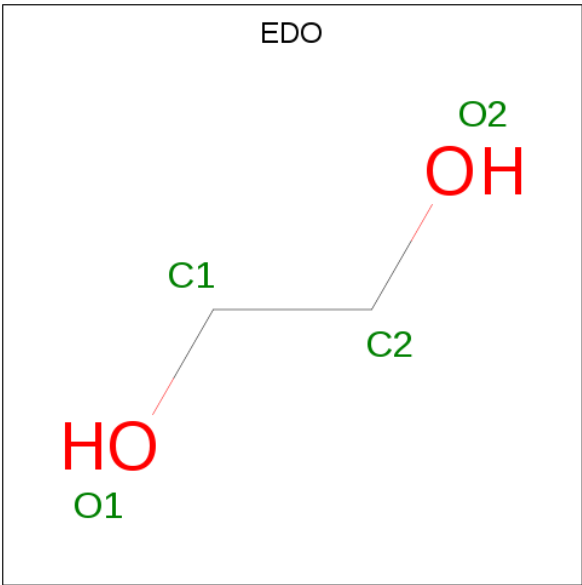
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is METHOTREXATE (three-letter code: MTX) (formula: C₂₀H₂₂N₈O₅).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 5 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	265	Total	O	0	0
			265	265		
5	B	211	Total	O	0	0
			211	211		

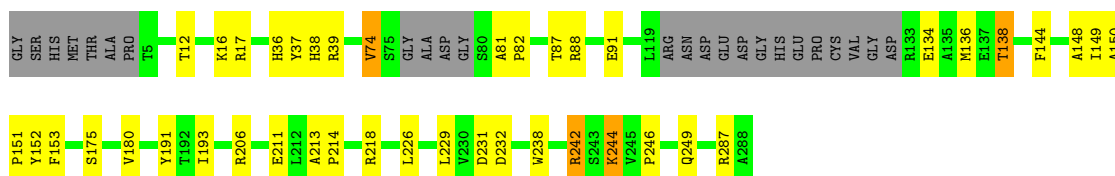
3 Residue-property plots

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

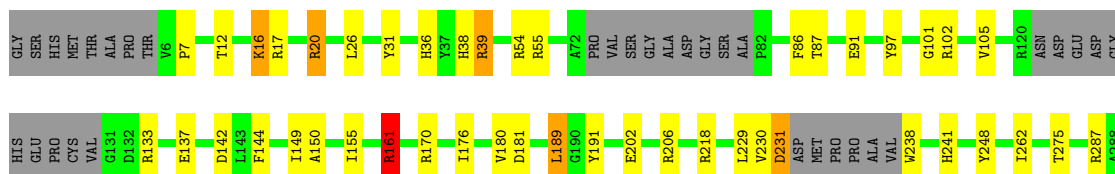
• Molecule 1: PTERIDINE REDUCTASE

Chain A: 



• Molecule 1: PTERIDINE REDUCTASE

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.31 Å 80.80 Å 90.75 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75	Depositor
% Data completeness (in resolution range)	98.2 (30.00-1.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.45	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4584	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: NDP, MTX, EDO

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	0.81	0/2044	1.53	22/2786 (0.8%)
1	B	0.65	0/1976	1.42	21/2684 (0.8%)
All	All	0.74	0/4020	1.48	43/5470 (0.8%)

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	ARG	NE-CZ-NH2	17.29	128.94	120.30
1	A	242	ARG	NE-CZ-NH1	15.02	127.81	120.30
1	A	88	ARG	NE-CZ-NH2	11.67	126.13	120.30
1	B	287	ARG	NE-CZ-NH1	-10.51	115.04	120.30
1	A	287	ARG	NE-CZ-NH2	10.42	125.51	120.30

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	1996	0	2008	25	0
1	B	1938	0	1950	27	0
2	A	48	0	26	0	0
2	B	48	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	33	0	20	7	0
3	B	33	0	18	10	0
4	A	8	0	12	0	0
4	B	4	0	6	0	0
5	A	265	0	0	6	1
5	B	211	0	0	8	2
All	All	4584	0	4065	56	2

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 7.

The worst 5 of 56 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:244:LYS:HA	1:A:244:LYS:HE2	1.33	1.07
1:A:232:ASP:OD2	3:A:301:MTX:H7	1.77	0.84
1:A:244:LYS:HE2	1:A:244:LYS:CA	2.10	0.81
1:B:191:TYR:OH	3:B:301:MTX:O2	2.07	0.72
1:B:39[A]:ARG:HH11	1:B:39[A]:ARG:HG2	1.58	0.69

All (2) 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)
5:A:2133:HOH:O	5:B:2131:HOH:O[2_555]	1.91	0.29
5:B:2148:HOH:O	5:B:2168:HOH:O[2_555]	2.16	0.04

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	263/291 (90%)	248 (94%)	14 (5%)	1 (0%)	36	18
1	B	251/291 (86%)	238 (95%)	12 (5%)	1 (0%)	36	18
All	All	514/582 (88%)	486 (95%)	26 (5%)	2 (0%)	36	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	VAL
1	B	180	VAL

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	210/225 (93%)	207 (99%)	3 (1%)	69	54
1	B	201/225 (89%)	193 (96%)	8 (4%)	34	12
All	All	411/450 (91%)	400 (97%)	11 (3%)	50	24

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	39[A]	ARG
1	B	39[B]	ARG
1	B	229	LEU
1	B	16	LYS
1	B	189	LEU

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

Mol	Chain	Res	Type
1	A	249	GLN
1	B	63	GLN
1	B	38	HIS
1	A	241	HIS

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Mol	Chain	Res	Type
1	B	57	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 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	$\# Z > 2$
4	EDO	A	1289	-	3,3,3	0.66	0	2,2,2	0.35	0
4	EDO	A	1290	-	3,3,3	0.47	0	2,2,2	0.26	0
2	NDP	A	300	-	45,52,52	1.51	8 (17%)	54,80,80	1.75	11 (20%)
3	MTX	A	301	-	28,35,35	1.92	8 (28%)	36,49,49	3.17	17 (47%)
4	EDO	B	1289	-	3,3,3	0.80	0	2,2,2	0.80	0
2	NDP	B	300	-	45,52,52	1.34	7 (15%)	54,80,80	1.77	15 (27%)
3	MTX	B	301	-	28,35,35	2.48	7 (25%)	36,49,49	5.52	12 (33%)

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	EDO	A	1289	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1290	-	-	0/1/1/1	0/0/0/0
2	NDP	A	300	-	-	0/30/77/77	0/5/5/5
3	MTX	A	301	-	-	0/19/25/25	0/3/3/3
4	EDO	B	1289	-	-	0/1/1/1	0/0/0/0
2	NDP	B	300	-	-	0/30/77/77	0/5/5/5
3	MTX	B	301	-	-	1/19/25/25	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	MTX	CA-N	-6.45	1.37	1.46
3	A	301	MTX	C9-N10	-4.25	1.39	1.46
3	B	301	MTX	C9-N10	-4.08	1.40	1.46
2	B	300	NDP	C4N-C5N	-3.62	1.41	1.49
3	A	301	MTX	C11-C	-3.48	1.42	1.50

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	MTX	N1-C2-N3	-6.41	118.00	127.41
2	B	300	NDP	N3A-C2A-N1A	-6.10	123.64	128.86
3	A	301	MTX	N1-C2-N3	-5.67	119.09	127.41
2	A	300	NDP	N3A-C2A-N1A	-5.06	124.53	128.86
3	B	301	MTX	CM-N10-C14	-5.04	110.69	119.60

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	MTX	CB-CA-N-C

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	MTX	7	0
3	B	301	MTX	10	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

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.