



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 10:49 PM GMT

PDB ID : 2VPS  
Title : STRUCTURE OF THE BIFUNCTIONAL LEISHMANIA MAJOR TRY-  
PANOTHIONE SYNTHETASE-AMIDASE  
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Deposited on : 2008-03-04  
Resolution : 2.75 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>

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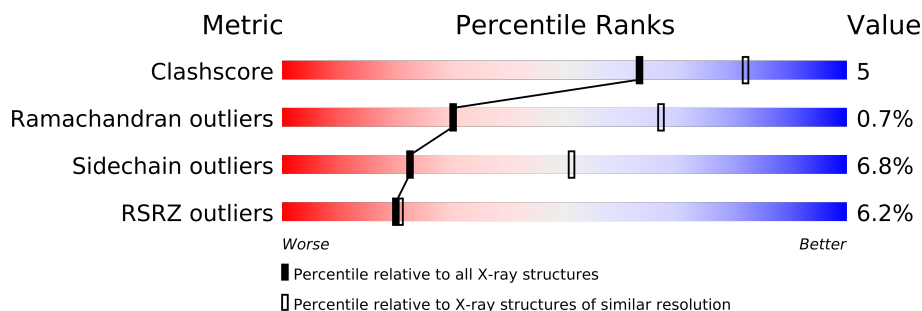
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 2.75 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	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)

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.

Mol	Chain	Length	Quality of chain
1	A	652	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4939 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 TRYPANOTHIONE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	0	0	0
			4887	3126	831	909	21			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Cl	0	0
			5	5		

- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

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

- Molecule 4 is water.

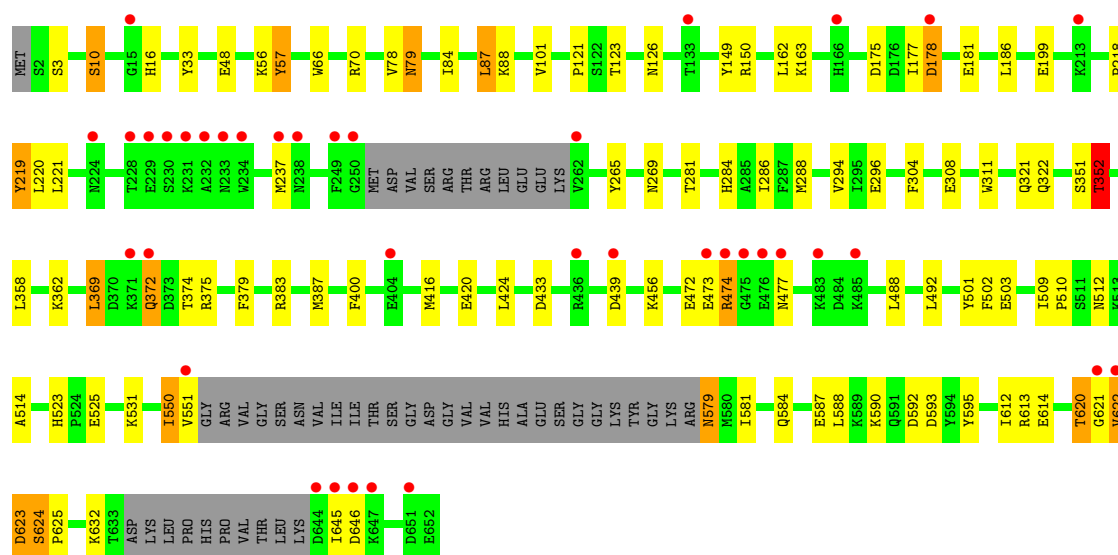
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total	O	0	0
			45	45		

### 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.

#### • Molecule 1: TRYPTANOTHIONE SYNTHETASE

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.05Å 85.60Å 168.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.33 – 2.75 20.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.33-2.75) 99.5 (20.00-2.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.204 , 0.250 0.213 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	53.3	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 27197 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4939	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BR, 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	0.67	0/5024	0.73	3/6814 (0.0%)

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	1	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	57	TYR	N-CA-C	5.46	125.76	111.00
1	A	3	SER	N-CA-C	5.19	125.01	111.00
1	A	503	GLU	N-CA-C	-5.15	97.10	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	281	THR	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	502	PHE	Peptide
1	A	56	LYS	Peptide
1	A	621	GLY	Peptide

## 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	4887	0	4674	52	0
2	A	5	0	0	0	0
3	A	2	0	0	0	0
4	A	45	0	0	4	0
All	All	4939	0	4674	52	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 5.

All (52) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:351:SER:O	1:A:352:THR:HB	1.77	0.84
1:A:79:ASN:H	1:A:79:ASN:ND2	1.91	0.68
1:A:514:ALA:HB2	1:A:550:ILE:HD13	1.76	0.67
1:A:579:ASN:C	1:A:579:ASN:HD22	2.01	0.64
1:A:590:LYS:HE3	1:A:595:TYR:CZ	2.34	0.63
1:A:265:TYR:CE1	1:A:369:LEU:HD11	2.34	0.62
1:A:121:PRO:HB3	1:A:186:LEU:HD21	1.84	0.59
1:A:620:THR:O	1:A:624:SER:HB2	2.06	0.55
1:A:623:ASP:OD1	1:A:623:ASP:N	2.39	0.55
1:A:178:ASP:N	1:A:178:ASP:OD1	2.39	0.54
1:A:308:GLU:HA	1:A:311:TRP:CE2	2.43	0.53
1:A:400:PHE:CE2	1:A:416:MET:HG3	2.45	0.52
1:A:374:THR:HG22	1:A:632:LYS:HA	1.93	0.51
1:A:178:ASP:HB3	4:A:2022:HOH:O	2.10	0.51
1:A:281:THR:CG2	4:A:2008:HOH:O	2.58	0.50
1:A:284:HIS:O	1:A:288:MET:HG2	2.12	0.50
1:A:472:GLU:O	1:A:474:ARG:N	2.46	0.49
1:A:150:ARG:NH2	1:A:177:ILE:HD12	2.28	0.48
1:A:281:THR:HG21	4:A:2008:HOH:O	2.14	0.48
1:A:220:LEU:HD21	1:A:612:ILE:HD11	1.96	0.47
1:A:79:ASN:N	1:A:79:ASN:ND2	2.60	0.47
1:A:550:ILE:HG22	1:A:551:VAL:H	1.80	0.47
1:A:512:ASN:OD1	1:A:550:ILE:HG21	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:162:LEU:HD22	1:A:175:ASP:HA	1.97	0.45
1:A:219:TYR:CD2	1:A:219:TYR:C	2.89	0.45
1:A:612:ILE:CG2	1:A:613:ARG:N	2.80	0.44
1:A:218:PRO:HA	1:A:269:ASN:HD21	1.82	0.44
1:A:10:SER:HB2	1:A:322:GLN:HB2	1.99	0.44
1:A:123:THR:OG1	1:A:126:ASN:N	2.51	0.43
1:A:645:ILE:O	1:A:645:ILE:HG22	2.19	0.43
1:A:420:GLU:HA	1:A:424:LEU:O	2.19	0.43
1:A:372:GLN:HE21	1:A:372:GLN:HB2	1.64	0.43
1:A:79:ASN:HD22	1:A:79:ASN:H	1.63	0.43
1:A:614:GLU:O	1:A:625:PRO:HD2	2.18	0.43
1:A:531:LYS:HG3	1:A:584:GLN:NE2	2.33	0.43
1:A:66:TRP:CZ2	1:A:70:ARG:HG2	2.55	0.42
1:A:588:LEU:N	1:A:588:LEU:CD1	2.82	0.42
1:A:321:GLN:HE22	1:A:501:TYR:H	1.68	0.42
1:A:592:ASP:O	1:A:593:ASP:HB2	2.19	0.42
1:A:488:LEU:HD12	1:A:492:LEU:HD13	2.02	0.42
1:A:472:GLU:N	1:A:472:GLU:OE1	2.53	0.41
1:A:79:ASN:HD22	1:A:79:ASN:N	2.18	0.41
1:A:620:THR:O	1:A:624:SER:CB	2.68	0.41
1:A:178:ASP:CB	4:A:2022:HOH:O	2.68	0.41
1:A:286:ILE:HG12	1:A:523:HIS:CD2	2.56	0.41
1:A:509:ILE:HB	1:A:510:PRO:HD3	2.01	0.41
1:A:294:VAL:HG21	1:A:304:PHE:CZ	2.56	0.41
1:A:375:ARG:NH2	1:A:379:PHE:CD2	2.89	0.41
1:A:84:ILE:HA	1:A:87:LEU:HD22	2.02	0.40
1:A:88:LYS:O	1:A:101:VAL:HG22	2.22	0.40
1:A:622:VAL:HB	1:A:623:ASP:OD1	2.21	0.40
1:A:33:TYR:HB2	1:A:57:TYR:CG	2.56	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	595/652 (91%)	559 (94%)	32 (5%)	4 (1%)	30 67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	352	THR
1	A	473	GLU
1	A	439	ASP
1	A	622	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	515/556 (93%)	480 (93%)	35 (7%)	22 51

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	16	HIS
1	A	48	GLU
1	A	78	VAL
1	A	79	ASN
1	A	87	LEU
1	A	149	TYR
1	A	163	LYS
1	A	178	ASP
1	A	181	GLU
1	A	199	GLU
1	A	219	TYR
1	A	221	LEU
1	A	237	MET
1	A	296	GLU
1	A	352	THR
1	A	358	LEU
1	A	362	LYS
1	A	369	LEU

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Mol	Chain	Res	Type
1	A	372	GLN
1	A	383	ARG
1	A	387	MET
1	A	433	ASP
1	A	456	LYS
1	A	474	ARG
1	A	477	ASN
1	A	525	GLU
1	A	550	ILE
1	A	579	ASN
1	A	581	ILE
1	A	587	GLU
1	A	620	THR
1	A	623	ASP
1	A	624	SER
1	A	646	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	79	ASN
1	A	86	GLN
1	A	152	HIS
1	A	233	ASN
1	A	270	HIS
1	A	293	GLN
1	A	321	GLN
1	A	346	ASN
1	A	372	GLN
1	A	384	ASN
1	A	579	ASN
1	A	583	GLN
1	A	584	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 ⓘ

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	603/652 (92%)	0.29	38 (6%) 19 20	47, 61, 75, 88	12 (1%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	GLU	5.4
1	A	551	VAL	5.3
1	A	228	THR	5.3
1	A	232	ALA	5.1
1	A	233	ASN	4.7
1	A	646	ASP	4.6
1	A	372	GLN	4.5
1	A	645	ILE	4.4
1	A	483	LYS	4.2
1	A	477	ASN	4.1
1	A	230	SER	4.0
1	A	473	GLU	3.7
1	A	647	LYS	3.7
1	A	238	ASN	3.5
1	A	644	ASP	3.3
1	A	436	ARG	3.1
1	A	262	VAL	3.1
1	A	229	GLU	3.0
1	A	485	LYS	2.9
1	A	231	LYS	2.8
1	A	213	LYS	2.6
1	A	474	ARG	2.5
1	A	15	GLY	2.5
1	A	250	GLY	2.5
1	A	475	GLY	2.4
1	A	234	TRP	2.4
1	A	178	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	622	VAL	2.4
1	A	404	GLU	2.2
1	A	166	HIS	2.2
1	A	439	ASP	2.2
1	A	237	MET	2.1
1	A	224	ASN	2.1
1	A	249	PHE	2.1
1	A	371	LYS	2.0
1	A	621	GLY	2.0
1	A	133	THR	2.0
1	A	651	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	A	1653	1/1	0.23	1.78	52,52,52,52	0
2	CL	A	1659	1/1	0.17	0.93	37,37,37,37	0
3	BR	A	1657	1/1	0.06	-2.43	71,71,71,71	0
2	CL	A	1654	1/1	0.08	-2.48	80,80,80,80	0
2	CL	A	1655	1/1	0.13	-2.55	47,47,47,47	0
2	CL	A	1656	1/1	0.10	-2.64	52,52,52,52	0
3	BR	A	1658	1/1	0.07	-5.75	101,101,101,101	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.