



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 30, 2016 – 10:56 AM EST

PDB ID : 5B37  
Title : Crystal structure of L-tryptophan dehydrogenase from *Nostoc punctiforme*  
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Deposited on : 2016-02-11  
Resolution : 3.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

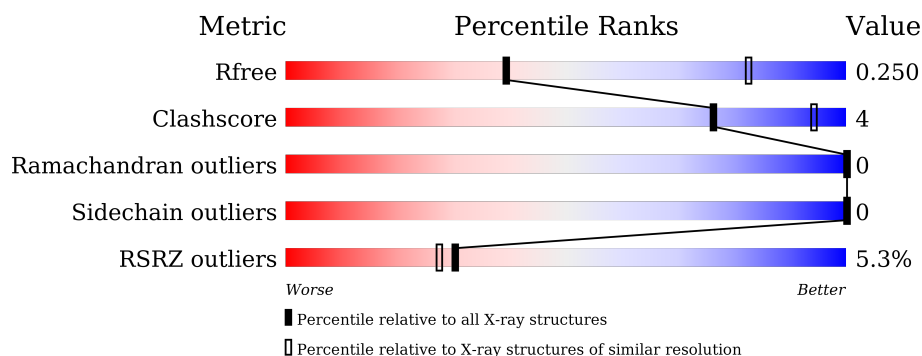
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 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.

Mol	Chain	Length	Quality of chain
1	A	361	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>
1	B	361	<div> <div>7%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>7%</div> </div> </div>
1	C	361	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>8%</div> </div> </div>
1	D	361	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>9%</div> </div> </div>
1	E	361	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>7%</div> </div> </div>
1	F	361	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15403 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 Tryptophan dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2542	1608	443	481	10			
1	B	336	Total	C	N	O	S	0	0	0
			2587	1634	452	491	10			
1	C	333	Total	C	N	O	S	0	0	0
			2571	1626	451	484	10			
1	D	328	Total	C	N	O	S	0	0	0
			2516	1589	442	475	10			
1	E	335	Total	C	N	O	S	0	0	0
			2583	1632	454	487	10			
1	F	334	Total	C	N	O	S	0	0	0
			2576	1626	452	488	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	LEU	-	expression tag	UNP W8CV45
A	355	GLU	-	expression tag	UNP W8CV45
A	356	HIS	-	expression tag	UNP W8CV45
A	357	HIS	-	expression tag	UNP W8CV45
A	358	HIS	-	expression tag	UNP W8CV45
A	359	HIS	-	expression tag	UNP W8CV45
A	360	HIS	-	expression tag	UNP W8CV45
A	361	HIS	-	expression tag	UNP W8CV45
B	354	LEU	-	expression tag	UNP W8CV45
B	355	GLU	-	expression tag	UNP W8CV45
B	356	HIS	-	expression tag	UNP W8CV45
B	357	HIS	-	expression tag	UNP W8CV45
B	358	HIS	-	expression tag	UNP W8CV45
B	359	HIS	-	expression tag	UNP W8CV45
B	360	HIS	-	expression tag	UNP W8CV45
B	361	HIS	-	expression tag	UNP W8CV45
C	354	LEU	-	expression tag	UNP W8CV45

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Chain	Residue	Modelled	Actual	Comment	Reference
C	355	GLU	-	expression tag	UNP W8CV45
C	356	HIS	-	expression tag	UNP W8CV45
C	357	HIS	-	expression tag	UNP W8CV45
C	358	HIS	-	expression tag	UNP W8CV45
C	359	HIS	-	expression tag	UNP W8CV45
C	360	HIS	-	expression tag	UNP W8CV45
C	361	HIS	-	expression tag	UNP W8CV45
D	354	LEU	-	expression tag	UNP W8CV45
D	355	GLU	-	expression tag	UNP W8CV45
D	356	HIS	-	expression tag	UNP W8CV45
D	357	HIS	-	expression tag	UNP W8CV45
D	358	HIS	-	expression tag	UNP W8CV45
D	359	HIS	-	expression tag	UNP W8CV45
D	360	HIS	-	expression tag	UNP W8CV45
D	361	HIS	-	expression tag	UNP W8CV45
E	354	LEU	-	expression tag	UNP W8CV45
E	355	GLU	-	expression tag	UNP W8CV45
E	356	HIS	-	expression tag	UNP W8CV45
E	357	HIS	-	expression tag	UNP W8CV45
E	358	HIS	-	expression tag	UNP W8CV45
E	359	HIS	-	expression tag	UNP W8CV45
E	360	HIS	-	expression tag	UNP W8CV45
E	361	HIS	-	expression tag	UNP W8CV45
F	354	LEU	-	expression tag	UNP W8CV45
F	355	GLU	-	expression tag	UNP W8CV45
F	356	HIS	-	expression tag	UNP W8CV45
F	357	HIS	-	expression tag	UNP W8CV45
F	358	HIS	-	expression tag	UNP W8CV45
F	359	HIS	-	expression tag	UNP W8CV45
F	360	HIS	-	expression tag	UNP W8CV45
F	361	HIS	-	expression tag	UNP W8CV45

- Molecule 2 is water.

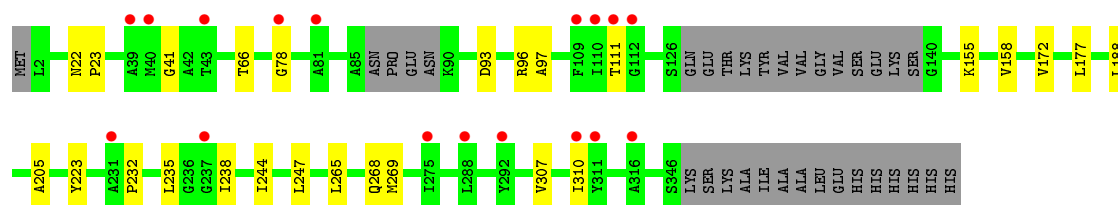
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0
2	B	3	Total O 3 3	0	0
2	C	6	Total O 6 6	0	0
2	D	6	Total O 6 6	0	0

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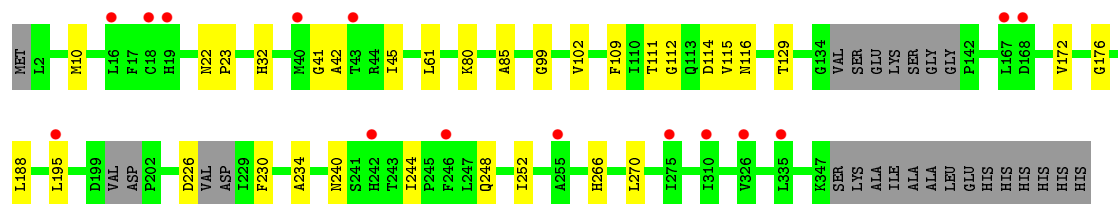
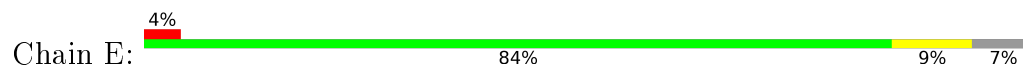
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total	O	0	0
			2	2		
2	F	9	Total	O	0	0
			9	9		

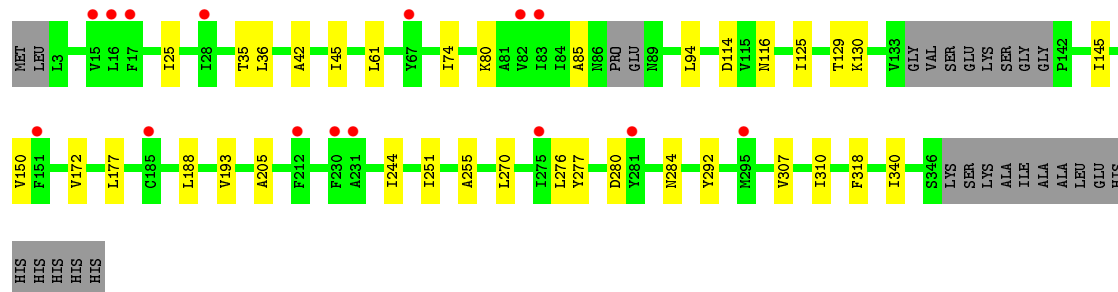
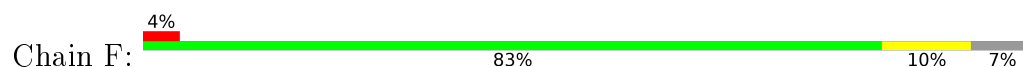




• Molecule 1: Tryptophan dehydrogenase



• Molecule 1: Tryptophan dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.71Å 337.77Å 63.65Å 90.00° 120.03° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 49.53 – 3.39	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-3.40) 98.3 (49.53-3.39)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.203 , 0.254 0.203 , 0.250	Depositor DCC
$R_{free}$ test set	1487 reflections (4.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.8	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.398 for -h-l,k,h 0.398 for l,k,-h-l 0.417 for -h-l,-k,l 0.408 for l,-k,h 0.408 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.180 for H, K, L 0.144 for -H, -K, H+L 0.194 for H+L, -K, -L 0.167 for L, K, -H-L 0.159 for -H-L, K, H 0.157 for L, -K, H	Depositor
Outliers	0 of 31703 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15403	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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](#)

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	0.38	0/2584	0.62	0/3499
1	B	0.38	0/2629	0.61	0/3557
1	C	0.38	0/2613	0.62	0/3534
1	D	0.40	0/2556	0.64	1/3457 (0.0%)
1	E	0.38	0/2624	0.61	0/3545
1	F	0.39	0/2617	0.62	0/3540
All	All	0.39	0/15623	0.62	1/21132 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	22	ASN	C-N-CD	5.26	139.46	128.40

There are no chirality outliers.

There are no planarity outliers.

### 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	2542	0	2558	19	0
1	B	2587	0	2604	14	0
1	C	2571	0	2598	21	0
1	D	2516	0	2538	17	0
1	E	2583	0	2609	20	0
1	F	2576	0	2595	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
2	E	2	0	0	0	0
2	F	9	0	0	0	0
All	All	15403	0	15502	117	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 4.

The worst 5 of 117 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:172:VAL:HG13	1:B:195:LEU:HD23	1.66	0.76
1:F:172:VAL:HG11	1:F:188:LEU:HD13	1.67	0.75
1:A:172:VAL:HG13	1:A:195:LEU:HD23	1.70	0.73
1:E:172:VAL:HG13	1:E:195:LEU:HD23	1.74	0.69
1:D:155:LYS:HA	1:D:158:VAL:HG22	1.76	0.66

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	324/361 (90%)	310 (96%)	14 (4%)	0	100	100
1	B	330/361 (91%)	321 (97%)	9 (3%)	0	100	100
1	C	327/361 (91%)	311 (95%)	16 (5%)	0	100	100
1	D	322/361 (89%)	312 (97%)	10 (3%)	0	100	100
1	E	327/361 (91%)	308 (94%)	19 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	328/361 (91%)	316 (96%)	12 (4%)	0	100	100
All	All	1958/2166 (90%)	1878 (96%)	80 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	271/296 (92%)	271 (100%)	0	100	100
1	B	276/296 (93%)	276 (100%)	0	100	100
1	C	274/296 (93%)	274 (100%)	0	100	100
1	D	267/296 (90%)	267 (100%)	0	100	100
1	E	275/296 (93%)	275 (100%)	0	100	100
1	F	275/296 (93%)	275 (100%)	0	100	100
All	All	1638/1776 (92%)	1638 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	341	ASN
1	E	116	ASN
1	F	191	HIS
1	C	293	ASN
1	E	163	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](#)

There are no ligands in this entry.

## 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 [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, 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	330/361 (91%)	0.37	18 (5%)	29	26	75, 97, 113, 121	0
1	B	336/361 (93%)	0.44	24 (7%)	19	18	77, 98, 114, 124	0
1	C	333/361 (92%)	0.33	17 (5%)	32	28	75, 97, 113, 128	0
1	D	328/361 (90%)	0.39	17 (5%)	31	28	75, 96, 110, 119	0
1	E	335/361 (92%)	0.34	15 (4%)	37	33	79, 97, 114, 124	0
1	F	334/361 (92%)	0.34	15 (4%)	37	33	78, 96, 114, 123	0
All	All	1996/2166 (92%)	0.37	106 (5%)	30	27	75, 97, 113, 128	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	GLY	8.8
1	B	236	GLY	7.7
1	C	331	ALA	4.7
1	D	40	MET	4.5
1	B	238	ILE	4.4

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.