



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:19 AM GMT

PDB ID : 3I05  
Title : Tryptophanyl-tRNA synthetase from Trypanosoma brucei  
Authors : Arakaki, T.; Merritt, E.A.  
Deposited on : 2009-06-24  
Resolution : 2.80 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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

**i**

## X-RAY DIFFRACTION

A.



Similar resolution  
(#Entries, resolution range(Å))

## Quality of chain

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5215 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	1	0
			2601	1688	428	466	19			
1	B	331	Total	C	N	O	S	0	1	0
			2614	1694	434	467	19			

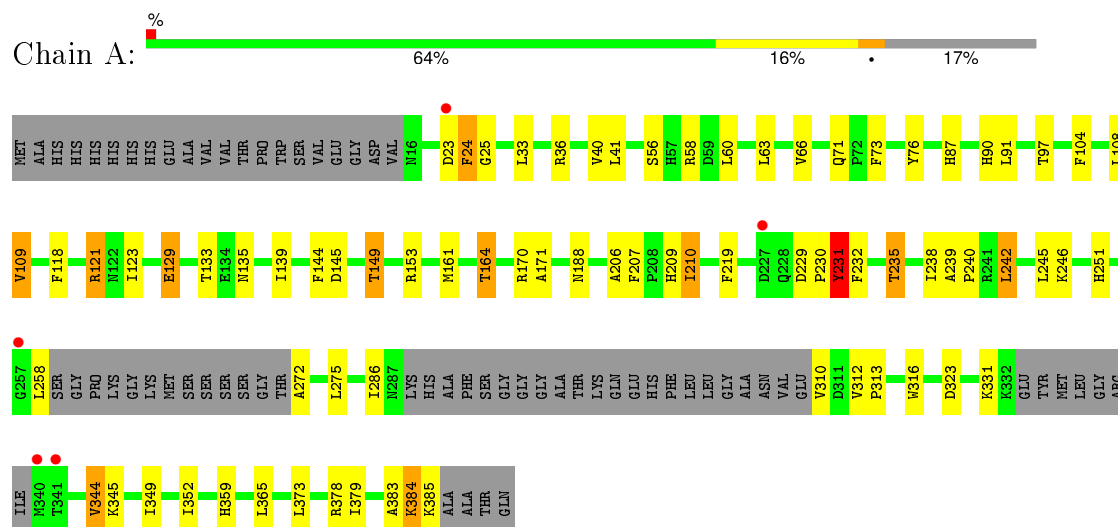
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	UNP Q580R7
A	-7	ALA	-	EXPRESSION TAG	UNP Q580R7
A	-6	HIS	-	EXPRESSION TAG	UNP Q580R7
A	-5	HIS	-	EXPRESSION TAG	UNP Q580R7
A	-4	HIS	-	EXPRESSION TAG	UNP Q580R7
A	-3	HIS	-	EXPRESSION TAG	UNP Q580R7
A	-2	HIS	-	EXPRESSION TAG	UNP Q580R7
A	-1	HIS	-	EXPRESSION TAG	UNP Q580R7
B	-8	MET	-	EXPRESSION TAG	UNP Q580R7
B	-7	ALA	-	EXPRESSION TAG	UNP Q580R7
B	-6	HIS	-	EXPRESSION TAG	UNP Q580R7
B	-5	HIS	-	EXPRESSION TAG	UNP Q580R7
B	-4	HIS	-	EXPRESSION TAG	UNP Q580R7
B	-3	HIS	-	EXPRESSION TAG	UNP Q580R7
B	-2	HIS	-	EXPRESSION TAG	UNP Q580R7
B	-1	HIS	-	EXPRESSION TAG	UNP Q580R7

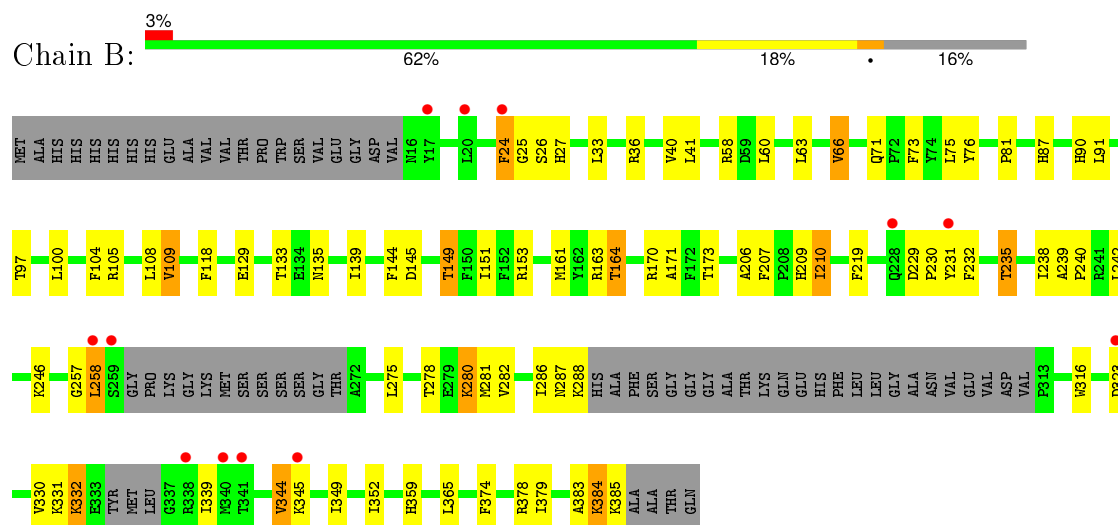
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: Tryptophanyl-tRNA synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.29 Å 51.43 Å 89.97 Å 95.29° 100.14° 106.05°	Depositor
Resolution (Å)	30.76 – 2.80 30.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.76-2.80) 92.0 (30.76-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.5.0096	Depositor
R, $R_{free}$	0.241 , 0.301 0.238 , 0.287	Depositor DCC
$R_{free}$ test set	1065 reflections (5.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 34.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 20556 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	5.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.72% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.49	0/2668	0.63	0/3616
1	B	0.50	0/2680	0.64	0/3627
All	All	0.50	0/5348	0.63	0/7243

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
1	B	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	TYR	Peptide
1	A	24	PHE	Peptide
1	B	231	TYR	Peptide
1	B	24	PHE	Peptide

### 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	2601	0	2503	50	0
1	B	2614	0	2527	52	0
All	All	5215	0	5030	98	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 10.

The worst 5 of 98 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:145:ASP:O	1:B:149:THR:HG22	1.50	1.12
1:A:145:ASP:O	1:A:149:THR:HG22	1.64	0.98
1:A:135:ASN:O	1:A:139:ILE:HD12	1.77	0.84
1:B:135:ASN:O	1:B:139:ILE:HD12	1.87	0.73
1:B:257:GLY:C	1:B:258:LEU:HD22	2.10	0.71

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	321/395 (81%)	309 (96%)	11 (3%)	1 (0%)	46	79
1	B	324/395 (82%)	313 (97%)	9 (3%)	2 (1%)	30	65
All	All	645/790 (82%)	622 (96%)	20 (3%)	3 (0%)	34	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	LYS
1	A	331	LYS
1	B	331	LYS

### 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	273/342 (80%)	252 (92%)	21 (8%)	16	41
1	B	274/342 (80%)	252 (92%)	22 (8%)	15	40
All	All	547/684 (80%)	504 (92%)	43 (8%)	15	40

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	378	ARG
1	B	91	LEU
1	B	344	VAL
1	A	384	LYS
1	B	24	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	HIS
1	A	287	ASN
1	B	209	HIS
1	B	287	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 [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	328/395 (83%)	-0.17	5 (1%) 76 68	2, 5, 11, 35	0
1	B	331/395 (83%)	-0.02	12 (3%) 46 34	2, 5, 10, 30	0
All	All	659/790 (83%)	-0.09	17 (2%) 59 47	2, 5, 11, 35	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	SER	5.0
1	B	338	ARG	3.4
1	B	340	MET	2.9
1	B	24	PHE	2.8
1	A	227	ASP	2.8

### 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.