

# wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2020 – 08:45 am BST

PDB ID : 6ENN

Title: Tryptophan Repressor TrpR from E.coli variant T44L T81M N87G S88Y with

Indole-3-acetic acid as ligand

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Deposited on : 2017-10-05

Resolution : 1.17 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

 $\begin{array}{cccc} & CCP4 & : & 7.0.044 \; (Gargrove) \\ Ideal \; geometry \; (proteins) & : & Engh \; \& \; Huber \; (2001) \end{array}$ 

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

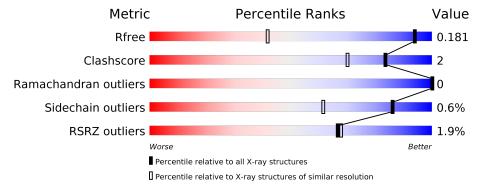
Validation Pipeline (wwPDB-VP) : 2.11

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.17 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$egin{aligned}  ext{Similar resolution} \ (\# ext{Entries},  ext{resolution range}( ext{Å})) \end{aligned}$
$R_{free}$	130704	1123 (1.20-1.16)
Clashscore	141614	1182 (1.20-1.16)
Ramachandran outliers	138981	1134 (1.20-1.16)
Sidechain outliers	138945	1134 (1.20-1.16)
RSRZ outliers	127900	1102 (1.20-1.16)

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 respectively. 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 <=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		
			2%		
1	A	116	84%	6%	10%
	_		2%		
1	В	116	85%	6%	9%



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4113 atoms, of which 1905 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 Trp operon repressor.

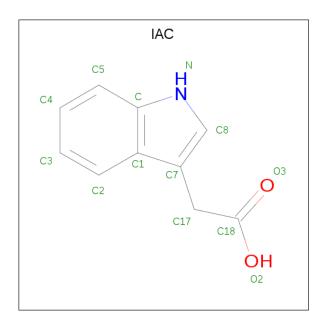
Mol	Chain	Residues	$\mathbf{Atoms}$				ZeroOcc	AltConf	Trace		
1	A	104	Total 1857			N 164	O 164	S 7	0	13	0
1	В	106	Total 1869	C 581	H 945	N 169	O 170	S 4	0	12	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	LEU	THR	engineered mutation	UNP P0A881
A	81	MET	THR	engineered mutation	UNP P0A881
A	87	GLY	ASN	engineered mutation	UNP P0A881
A	88	TYR	SER	engineered mutation	UNP P0A881
A	109	LEU	_	expression tag	UNP P0A881
A	110	GLU	-	expression tag	UNP P0A881
A	111	HIS	-	expression tag	UNP P0A881
A	112	HIS	_	expression tag	UNP P0A881
A	113	HIS	-	expression tag	UNP P0A881
A	114	HIS	=	expression tag	UNP P0A881
A	115	HIS	-	expression tag	UNP P0A881
A	116	HIS	-	expression tag	UNP P0A881
В	44	LEU	THR	engineered mutation	UNP P0A881
В	81	MET	THR	engineered mutation	UNP P0A881
В	87	GLY	ASN	engineered mutation	UNP P0A881
В	88	TYR	SER	engineered mutation	UNP P0A881
В	109	LEU	-	expression tag	UNP P0A881
В	110	GLU	-	expression tag	UNP P0A881
В	111	HIS	-	expression tag	UNP P0A881
В	112	HIS	-	expression tag	UNP P0A881
В	113	HIS	-	expression tag	UNP P0A881
В	114	HIS	-	expression tag	UNP P0A881
В	115	HIS	=	expression tag	UNP P0A881
В	116	HIS	-	expression tag	UNP P0A881



 $\bullet \ \, \text{Molecule 2 is 1H-INDOL-3-YLACETIC ACID (three-letter code: IAC) (formula: $C_{10}H_9NO_2$)}. \\$ 



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	Λ	1	Total	С	Η	N	О	0	0	
	$\begin{array}{ c c c c c c } Z & A & A & \end{array}$		21	10	8	1	2	0		
9	D	1	Total	С	Н	N	О	0	0	
2	2   B	1	21	10	8	1	2	U	U	

• Molecule 3 is water.

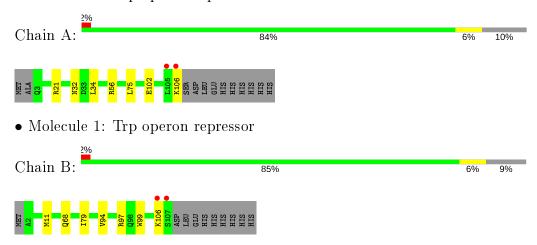
$\mathbf{Mol}$	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
3	A	164	Total O 171 171	0	6
3	В	168	Total O 174 174	0	6



# 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 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.

• Molecule 1: Trp operon repressor





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	54.58Å 63.19Å 64.90Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	41.77 - 1.17	Depositor
rtesolution (A)	41.77 - 1.17	EDS
% Data completeness	98.0 (41.77-1.17)	Depositor
(in resolution range)	98.0 (41.77-1.17)	EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.08 (at 1.17Å)	Xtriage
Refinement program	PHENIX	Depositor
$R, R_{free}$	0.148 , $0.180$	Depositor
It, It free	0.149 , $0.181$	DCC
$R_{free}$ test set	3740  reflections  (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.4	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	$0.37\;,43.0$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 19.56% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: IAC

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		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.50	0/958	0.67	0/1289	
1	В	0.50	0/970	0.72	1/1307 (0.1%)	
All	All	0.50	0/1928	0.70	$1/2596 \ (0.0\%)$	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	11	MET	CG-SD-CE	5.44	108.90	100.20

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	913	944	936	6	0
1	В	924	945	913	4	0
2	A	13	8	8	0	0
2	В	13	8	8	0	0
3	A	171	0	0	1	0
3	В	174	0	0	0	0
All	All	2208	1905	1865	9	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 2.

The worst 5 of 9 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	Clash overlap (Å)
1:B:94[B]:VAL:HG12	1:B:97[B]:ARG:NH1	2.24	0.53
1:A:32[B]:ASN:ND2	1:B:99:TRP:NE1	2.60	0.49
1:A:32[B]:ASN:HD21	1:A:34:LEU:HD12	1.80	0.46
1:B:94[B]:VAL:HG12	1:B:97[B]:ARG:HH12	1.81	0.45
1:A:21:ARG:HD3	3:A:369:HOH:O	2.17	0.44

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	115/116 (99%)	115 (100%)	0	0	100	100	
1	В	116/116 (100%)	116 (100%)	0	0	100	100	
All	All	$231/232 \ (100\%)$	231 (100%)	0	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	Rotameric Outliers		Percentiles		
1	A	100/100 (100%)	100 (100%)	0	100	100		
1	В	101/100 (101%)	100 (99%)	1 (1%)	76	46		
All	All	201/200 (100%)	200 (100%)	1 (0%)	86	66		

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	106	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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)

2 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	T	Chain	Res	Link	Bo	nd leng	${ m ths}$	В	ond ang	les
		Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
	2	IAC	В	201	-	10,14,14	0.93	0	11,19,19	1.34	1 (9%)
	2	IAC	A	201	-	10,14,14	0.72	0	11,19,19	0.97	1 (9%)



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
2	IAC	В	201	-	-	0/2/4/4	0/2/2/2
2	IAC	A	201	-	-	0/2/4/4	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

M	<b>Iol</b>	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
	2	В	201	IAC	C17-C7-C1	3.54	133.44	126.50
	2	A	201	IAC	C17-C7-C1	2.38	131.16	126.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	104/116 (89%)	0.23	2 (1%) 66 68	10, 15, 26, 41	0
1	В	106/116 (91%)	0.15	2 (1%) 66 68	9, 14, 22, 44	0
All	All	$210/232 \ (90\%)$	0.19	4 (1%) 66 68	9, 14, 23, 44	0

#### All (4) RSRZ outliers are listed below:

Mol	Chain	${f Res}$	Type	RSRZ
1	В	107	SER	5.5
1	A	106	LYS	5.2
1	В	106	LYS	4.5
1	A	105	LEU	3.2

## 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)

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. The B-factors column lists the minimum, median,  $95^{th}$  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	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	IAC	В	201	13/13	0.98	0.06	11,14,16,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
2	IAC	A	201	13/13	0.98	0.06	10,12,14,16	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

