



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2022 – 01:18 PM EDT

PDB ID : 7UXR  
Title : Crystal structure of the BtTir TIR domain  
Authors : Shi, Y.; Masic, V.; Mosaiab, T.; Vasquez, E.; Ve, T.  
Deposited on : 2022-05-06  
Resolution : 1.42 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

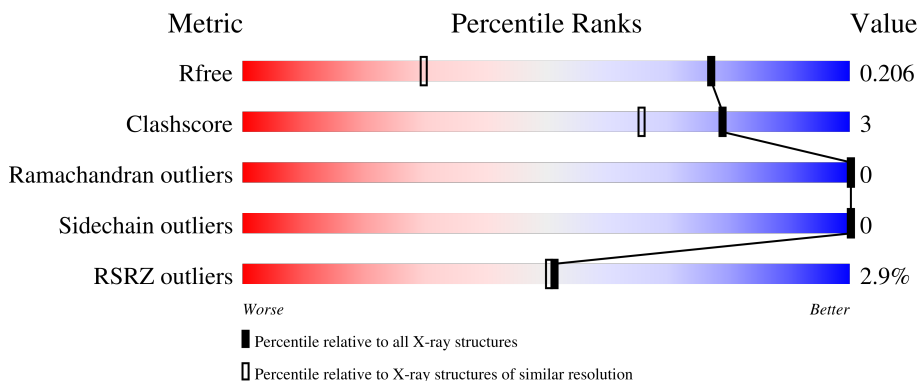
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.42 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))
$R_{free}$	130704	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	177	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>5%</div> <div>21%</div> </div> </div>
1	B	177	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>7%</div> <div>22%</div> </div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4748 atoms, of which 2255 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 TIR domain protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	139	Total	C	H	N	O	S	0	3	0
			2300	745	1131	204	218	2			
1	B	138	Total	C	H	N	O	S	0	3	0
			2283	739	1124	201	217	2			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	MET	-	expression tag	UNP A0A0P0FGV9
A	118	SER	-	expression tag	UNP A0A0P0FGV9
A	119	ALA	-	expression tag	UNP A0A0P0FGV9
A	120	TRP	-	expression tag	UNP A0A0P0FGV9
A	121	HIS	-	expression tag	UNP A0A0P0FGV9
A	122	PRO	-	expression tag	UNP A0A0P0FGV9
A	123	GLN	-	expression tag	UNP A0A0P0FGV9
A	124	PHE	-	expression tag	UNP A0A0P0FGV9
A	125	GLU	-	expression tag	UNP A0A0P0FGV9
A	126	LYS	-	expression tag	UNP A0A0P0FGV9
A	127	GLY	-	expression tag	UNP A0A0P0FGV9
A	128	GLY	-	expression tag	UNP A0A0P0FGV9
A	129	GLY	-	expression tag	UNP A0A0P0FGV9
A	130	SER	-	expression tag	UNP A0A0P0FGV9
A	131	GLY	-	expression tag	UNP A0A0P0FGV9
A	132	GLY	-	expression tag	UNP A0A0P0FGV9
A	133	GLY	-	expression tag	UNP A0A0P0FGV9
A	134	SER	-	expression tag	UNP A0A0P0FGV9
A	135	ALA	-	expression tag	UNP A0A0P0FGV9
A	136	TRP	-	expression tag	UNP A0A0P0FGV9
A	137	SER	-	expression tag	UNP A0A0P0FGV9
A	138	HIS	-	expression tag	UNP A0A0P0FGV9
A	139	PRO	-	expression tag	UNP A0A0P0FGV9
A	140	GLN	-	expression tag	UNP A0A0P0FGV9
A	141	PRO	-	expression tag	UNP A0A0P0FGV9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	142	GLN	-	expression tag	UNP A0A0P0FGV9
A	143	PHE	-	expression tag	UNP A0A0P0FGV9
A	144	GLU	-	expression tag	UNP A0A0P0FGV9
A	145	LYS	-	expression tag	UNP A0A0P0FGV9
A	146	GLY	-	expression tag	UNP A0A0P0FGV9
A	147	GLY	-	expression tag	UNP A0A0P0FGV9
A	148	GLY	-	expression tag	UNP A0A0P0FGV9
A	149	SER	-	expression tag	UNP A0A0P0FGV9
A	150	SER	-	expression tag	UNP A0A0P0FGV9
A	151	GLY	-	expression tag	UNP A0A0P0FGV9
A	152	GLY	-	expression tag	UNP A0A0P0FGV9
A	153	GLY	-	expression tag	UNP A0A0P0FGV9
A	154	ALA	-	expression tag	UNP A0A0P0FGV9
A	155	SER	-	expression tag	UNP A0A0P0FGV9
A	288	HIS	-	expression tag	UNP A0A0P0FGV9
A	289	HIS	-	expression tag	UNP A0A0P0FGV9
A	290	HIS	-	expression tag	UNP A0A0P0FGV9
A	291	HIS	-	expression tag	UNP A0A0P0FGV9
A	292	HIS	-	expression tag	UNP A0A0P0FGV9
A	293	HIS	-	expression tag	UNP A0A0P0FGV9
B	117	MET	-	expression tag	UNP A0A0P0FGV9
B	118	SER	-	expression tag	UNP A0A0P0FGV9
B	119	ALA	-	expression tag	UNP A0A0P0FGV9
B	120	TRP	-	expression tag	UNP A0A0P0FGV9
B	121	HIS	-	expression tag	UNP A0A0P0FGV9
B	122	PRO	-	expression tag	UNP A0A0P0FGV9
B	123	GLN	-	expression tag	UNP A0A0P0FGV9
B	124	PHE	-	expression tag	UNP A0A0P0FGV9
B	125	GLU	-	expression tag	UNP A0A0P0FGV9
B	126	LYS	-	expression tag	UNP A0A0P0FGV9
B	127	GLY	-	expression tag	UNP A0A0P0FGV9
B	128	GLY	-	expression tag	UNP A0A0P0FGV9
B	129	GLY	-	expression tag	UNP A0A0P0FGV9
B	130	SER	-	expression tag	UNP A0A0P0FGV9
B	131	GLY	-	expression tag	UNP A0A0P0FGV9
B	132	GLY	-	expression tag	UNP A0A0P0FGV9
B	133	GLY	-	expression tag	UNP A0A0P0FGV9
B	134	SER	-	expression tag	UNP A0A0P0FGV9
B	135	ALA	-	expression tag	UNP A0A0P0FGV9
B	136	TRP	-	expression tag	UNP A0A0P0FGV9
B	137	SER	-	expression tag	UNP A0A0P0FGV9
B	138	HIS	-	expression tag	UNP A0A0P0FGV9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	139	PRO	-	expression tag	UNP A0A0P0FGV9
B	140	GLN	-	expression tag	UNP A0A0P0FGV9
B	141	PRO	-	expression tag	UNP A0A0P0FGV9
B	142	GLN	-	expression tag	UNP A0A0P0FGV9
B	143	PHE	-	expression tag	UNP A0A0P0FGV9
B	144	GLU	-	expression tag	UNP A0A0P0FGV9
B	145	LYS	-	expression tag	UNP A0A0P0FGV9
B	146	GLY	-	expression tag	UNP A0A0P0FGV9
B	147	GLY	-	expression tag	UNP A0A0P0FGV9
B	148	GLY	-	expression tag	UNP A0A0P0FGV9
B	149	SER	-	expression tag	UNP A0A0P0FGV9
B	150	SER	-	expression tag	UNP A0A0P0FGV9
B	151	GLY	-	expression tag	UNP A0A0P0FGV9
B	152	GLY	-	expression tag	UNP A0A0P0FGV9
B	153	GLY	-	expression tag	UNP A0A0P0FGV9
B	154	ALA	-	expression tag	UNP A0A0P0FGV9
B	155	SER	-	expression tag	UNP A0A0P0FGV9
B	288	HIS	-	expression tag	UNP A0A0P0FGV9
B	289	HIS	-	expression tag	UNP A0A0P0FGV9
B	290	HIS	-	expression tag	UNP A0A0P0FGV9
B	291	HIS	-	expression tag	UNP A0A0P0FGV9
B	292	HIS	-	expression tag	UNP A0A0P0FGV9
B	293	HIS	-	expression tag	UNP A0A0P0FGV9

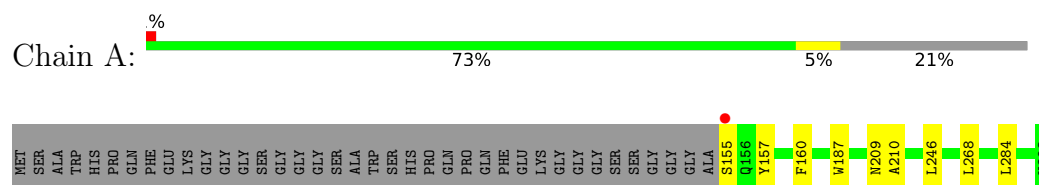
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	107	Total O 107 107	0	0
2	B	58	Total O 58 58	0	0

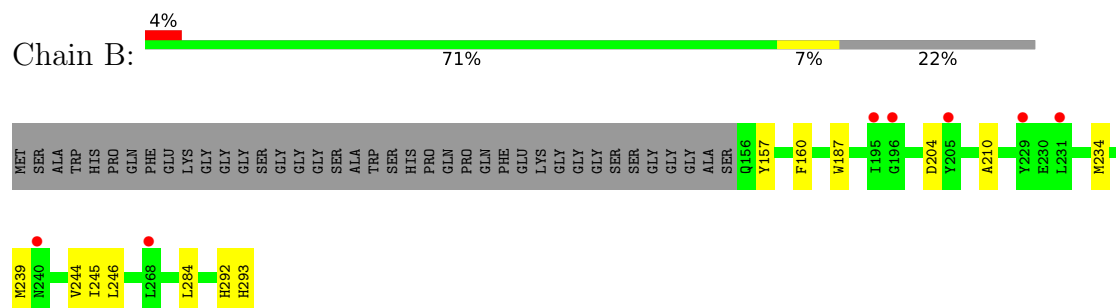
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: TIR domain protein



- Molecule 1: TIR domain protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.69Å 43.13Å 98.76Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	39.52 – 1.42 39.52 – 1.42	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.52-1.42) 98.1 (39.52-1.42)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 1.42Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.189 , 0.208 0.188 , 0.206	Depositor DCC
$R_{free}$ test set	2011 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.2	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4748	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.22% 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

### 5.1 Standard geometry

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	0.54	0/1199	0.75	0/1621
1	B	0.37	0/1188	0.58	0/1607
All	All	0.46	0/2387	0.67	0/3228

There are no bond length outliers.

There are no bond angle outliers.

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	1169	1131	1128	6	0
1	B	1159	1124	1122	7	0
2	A	107	0	0	0	0
2	B	58	0	0	1	0
All	All	2493	2255	2250	13	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 3.

The worst 5 of 13 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:155:SER:O	1:A:209:ASN:ND2	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:HD13	1:B:284:LEU:CD2	2.36	0.56
1:B:239:MET:HB3	1:B:244:VAL:HG11	1.91	0.53
1:A:246:LEU:HD13	1:A:284:LEU:CD2	2.47	0.45
1:B:292:HIS:O	1:B:293:HIS:HB2	2.18	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	140/177 (79%)	136 (97%)	4 (3%)	0	100	100
1	B	139/177 (78%)	134 (96%)	5 (4%)	0	100	100
All	All	279/354 (79%)	270 (97%)	9 (3%)	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	129/149 (87%)	129 (100%)	0	100	100
1	B	128/149 (86%)	128 (100%)	0	100	100
All	All	257/298 (86%)	257 (100%)	0	100	100

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

Sometimes 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 monosaccharides 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	139/177 (78%)	-0.05	1 (0%) 87 86	11, 17, 38, 52	0
1	B	138/177 (77%)	0.24	7 (5%) 28 26	15, 29, 58, 70	0
All	All	277/354 (78%)	0.09	8 (2%) 51 50	11, 22, 52, 70	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	ILE	6.3
1	B	240	ASN	4.3
1	B	229	TYR	4.1
1	B	268	LEU	3.1
1	B	196	GLY	2.7

### 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 monosaccharides 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.