



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 18, 2023 – 02:31 am GMT

PDB ID : 4ASO
Title : TubR bound to 24 bp of tubC from *Bacillus thuringiensis* serovar israelensis pBtoxis
Authors : Aylett, C.H.S.; Lowe, J.
Deposited on : 2012-05-02
Resolution : 7.00 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

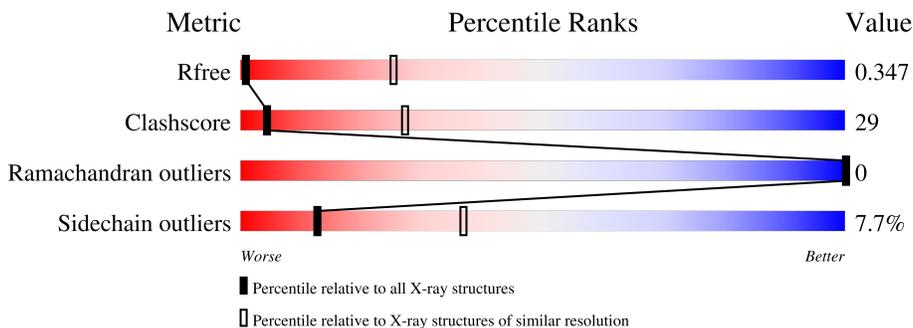
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 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	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)

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 ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	104	62% 24% 11%
1	B	104	65% 20% 11%
1	C	104	66% 21% 11%
1	D	104	65% 20% 11%
1	E	104	61% 26% 11%
1	F	104	62% 23% 11%
1	G	104	65% 21% 11%

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Mol	Chain	Length	Quality of chain	
1	H	104	64%	21% • 11%
1	I	104	63%	24% • 11%
1	J	104	62%	24% • 11%
1	K	104	62%	26% • 11%
1	L	104	62%	23% • 11%
1	M	104	62%	26% • 11%
1	N	104	62%	24% • 11%
1	O	104	62%	26% • 11%
1	P	104	63%	22% • 11%
2	S	24	71%	29%
2	U	24	54%	46%
2	W	24	54%	46%
2	Y	24	46%	54%
3	T	24	63%	38%
3	V	24	42%	58%
3	X	24	50%	50%
3	Z	24	46%	54%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15568 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 TUBR FROM BACILLUS THURINGIENSIS PBTOXIS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	93	727	462	117	142	3	3	0	0	0
1	B	93	727	462	117	142	3	3	0	0	0
1	C	93	727	462	117	142	3	3	0	0	0
1	D	93	727	462	117	142	3	3	0	0	0
1	E	93	727	462	117	142	3	3	0	0	0
1	F	93	727	462	117	142	3	3	0	0	0
1	G	93	727	462	117	142	3	3	0	0	0
1	H	93	727	462	117	142	3	3	0	0	0
1	I	93	727	462	117	142	3	3	0	0	0
1	J	93	727	462	117	142	3	3	0	0	0
1	K	93	727	462	117	142	3	3	0	0	0
1	L	93	727	462	117	142	3	3	0	0	0
1	M	93	727	462	117	142	3	3	0	0	0
1	N	93	727	462	117	142	3	3	0	0	0
1	O	93	727	462	117	142	3	3	0	0	0
1	P	93	727	462	117	142	3	3	0	0	0

- Molecule 2 is a DNA chain called TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	24	Total	C	N	O	P	0	0	0
			488	237	78	149	24			
2	U	24	Total	C	N	O	P	0	0	0
			488	237	78	149	24			
2	W	24	Total	C	N	O	P	0	0	0
			488	237	78	149	24			
2	Y	24	Total	C	N	O	P	0	0	0
			488	237	78	149	24			

- Molecule 3 is a DNA chain called TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	24	Total	C	N	O	P	0	0	0
			496	238	95	139	24			
3	V	24	Total	C	N	O	P	0	0	0
			496	238	95	139	24			
3	X	24	Total	C	N	O	P	0	0	0
			496	238	95	139	24			
3	Z	24	Total	C	N	O	P	0	0	0
			496	238	95	139	24			

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. 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. 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: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS

Chain A: 



- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS

Chain B: 



- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS

Chain C: 



- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS

Chain D: 



- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS

Chain E: 



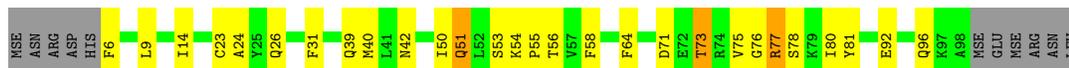
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- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS

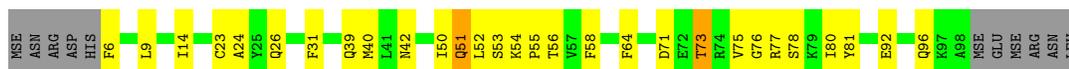
Chain F: 



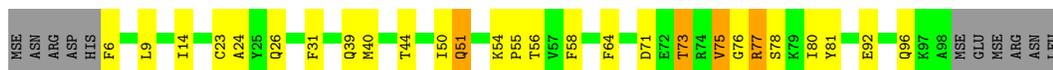
- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS



- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS



- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS



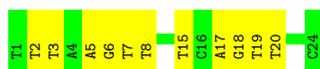
- Molecule 2: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



- Molecule 2: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP

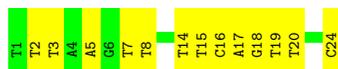


- Molecule 2: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



- Molecule 2: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP

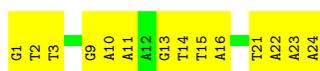




- Molecule 3: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



- Molecule 3: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



- Molecule 3: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



- Molecule 3: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	519.25Å 63.66Å 167.26Å 90.00° 96.66° 90.00°	Depositor
Resolution (Å)	64.47 – 7.00 257.87 – 7.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (64.47-7.00) 96.3 (257.87-7.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 6.74Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.344 , 0.371 0.348 , 0.347	Depositor DCC
R_{free} test set	413 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	473.6	Xtrriage
Anisotropy	0.429	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 26.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	15568	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.58	0/734	0.65	0/986
1	B	0.59	0/734	0.65	0/986
1	C	0.58	0/734	0.65	0/986
1	D	0.58	0/734	0.65	0/986
1	E	0.58	0/734	0.65	0/986
1	F	0.58	0/734	0.65	0/986
1	G	0.58	0/734	0.65	0/986
1	H	0.59	0/734	0.65	0/986
1	I	0.58	0/734	0.65	0/986
1	J	0.58	0/734	0.65	0/986
1	K	0.59	0/734	0.65	0/986
1	L	0.58	0/734	0.65	0/986
1	M	0.58	0/734	0.65	0/986
1	N	0.58	0/734	0.65	0/986
1	O	0.59	0/734	0.65	0/986
1	P	0.59	0/734	0.65	0/986
2	S	0.75	0/542	1.55	0/829
2	U	0.75	0/542	1.55	0/829
2	W	0.75	0/542	1.55	0/829
2	Y	0.75	0/542	1.55	0/829
3	T	0.81	0/556	1.43	0/851
3	V	0.82	0/556	1.43	0/851
3	X	0.82	0/556	1.42	0/851
3	Z	0.82	0/556	1.42	0/851
All	All	0.64	0/16136	0.98	0/22496

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	727	0	717	28	4
1	B	727	0	716	41	0
1	C	727	0	718	34	0
1	D	727	0	717	33	0
1	E	727	0	717	49	0
1	F	727	0	718	101	0
1	G	727	0	717	51	0
1	H	727	0	716	56	0
1	I	727	0	717	43	2
1	J	727	0	718	47	1
1	K	727	0	716	43	0
1	L	727	0	715	70	0
1	M	727	0	716	48	0
1	N	727	0	716	48	0
1	O	727	0	717	52	0
1	P	727	0	718	37	4
2	S	488	0	278	41	1
2	U	488	0	277	98	0
2	W	488	0	278	63	0
2	Y	488	0	279	66	1
3	T	496	0	274	65	1
3	V	496	0	272	113	0
3	X	496	0	273	101	0
3	Z	496	0	271	67	1
All	All	15568	0	13671	848	8

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 29.

The worst 5 of 848 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:H:75:VAL:HG21	1:I:40:MSE:SE	1.44	1.61
2:U:3:DT:C4	3:V:23:DA:H1'	1.09	1.60
1:F:55:PRO:HG3	3:V:15:DT:C7	1.30	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:14:DT:C4	2:U:15:DT:C7	1.83	1.60
1:J:77:ARG:HH12	1:K:44:THR:CG2	1.16	1.58

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:THR:OG1	1:I:8:THR:OG1[2_554]	1.04	1.16
1:A:44:THR:CG2	1:P:77:ARG:NH1[3_434]	1.24	0.96
2:S:1:DT:P	2:Y:24:DC:O3'[3_434]	1.60	0.60
3:T:24:DA:O3'	3:Z:1:DG:P[3_434]	1.60	0.60
1:A:40:MSE:SE	1:P:75:VAL:CG2[3_434]	1.64	0.56

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	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	B	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	C	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	D	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	E	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	F	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	G	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	H	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	I	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	J	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	K	91/104 (88%)	89 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	M	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	N	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	O	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	P	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
All	All	1456/1664 (88%)	1424 (98%)	32 (2%)	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	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	B	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	C	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	D	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	E	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	F	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	G	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	H	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	I	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	J	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	K	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	L	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	M	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	N	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	O	78/83 (94%)	72 (92%)	6 (8%)	13	37
1	P	78/83 (94%)	72 (92%)	6 (8%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1248/1328 (94%)	1152 (92%)	96 (8%)	13 37

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	75	VAL
1	L	78	SER
1	J	78	SER
1	K	78	SER
1	M	75	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	42	ASN

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	V	2
3	Z	2
3	T	2
3	X	2
2	U	2
2	S	2
2	Y	2
2	W	2

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	22:DA	O3'	23:DA	P	11.44
1	Z	10:DA	O3'	11:DA	P	7.83
1	T	10:DA	O3'	11:DA	P	6.96
1	X	22:DA	O3'	23:DA	P	6.47
1	U	2:DT	O3'	3:DT	P	5.85

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.