



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:18 PM GMT

PDB ID : 1T0B
Title : Structure of ThuA-like protein from Bacillus stearothermophilus
Authors : Borek, D.; Chen, Y.; Collart, F.; Joachimiak, A.; Otwinowski, Z.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2004-04-08
Resolution : 1.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

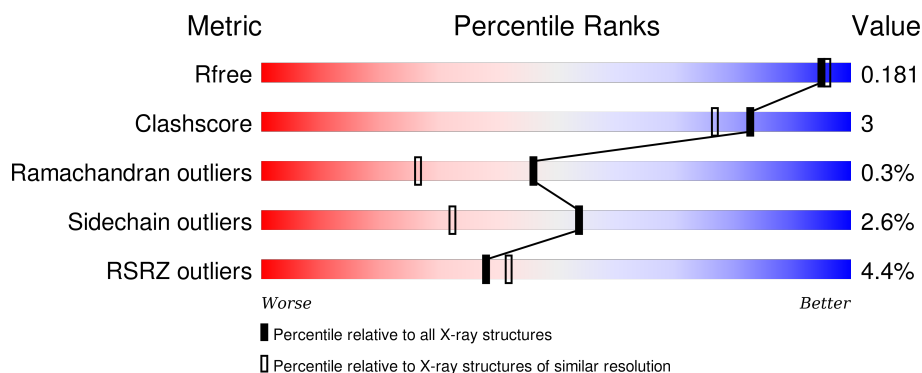
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	252	<div> <div>5%</div> <div>86% 8% • 5%</div> </div>
1	B	252	<div> <div>4%</div> <div>87% 7% 5%</div> </div>
1	C	252	<div> <div>6%</div> <div>86% 9% 5%</div> </div>
1	D	252	<div> <div>4%</div> <div>91% • 5%</div> </div>
1	E	252	<div> <div>3%</div> <div>85% 10% • 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	252	
1	G	252	
1	H	252	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	3001	-	-	-	X
2	ZN	B	3002	-	-	-	X
2	ZN	C	3003	-	-	-	X
2	ZN	D	3008	-	-	-	X
2	ZN	E	3005	-	-	-	X
2	ZN	F	3006	-	-	-	X
2	ZN	G	3007	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17343 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 ThuA-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	2	4	0
			1965	1267	336	355	7			
1	B	240	Total	C	N	O	S	0	2	0
			1953	1260	334	352	7			
1	C	240	Total	C	N	O	S	0	5	0
			1963	1268	333	355	7			
1	D	240	Total	C	N	O	S	0	2	0
			1954	1261	333	353	7			
1	E	240	Total	C	N	O	S	0	5	0
			1962	1267	334	354	7			
1	F	241	Total	C	N	O	S	0	4	0
			1968	1271	335	355	7			
1	G	242	Total	C	N	O	S	0	5	0
			1981	1279	340	355	7			
1	H	241	Total	C	N	O	S	0	2	0
			1965	1271	335	352	7			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

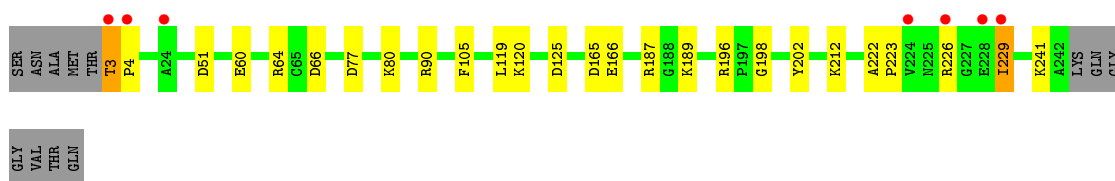
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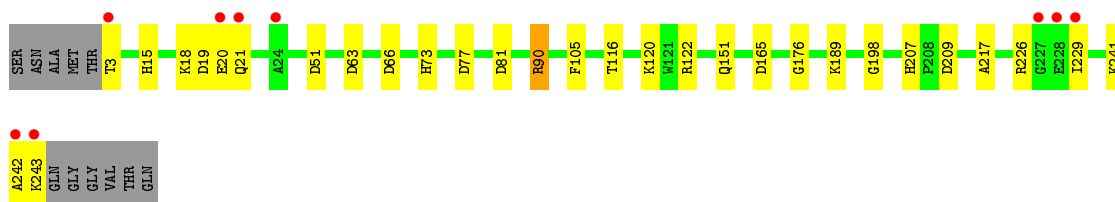
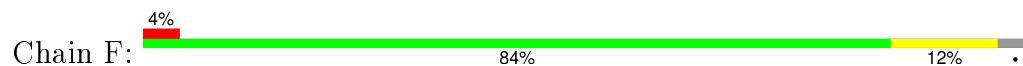
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	F	1	Total 1	Zn 1	0	0

- Molecule 3 is water.

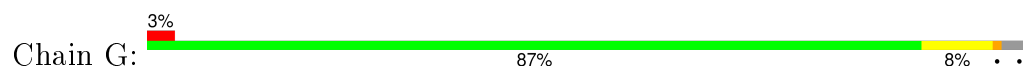
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	197	Total 197	O 197	0	0
3	B	194	Total 194	O 194	0	0
3	C	184	Total 184	O 184	0	0
3	D	209	Total 209	O 209	0	0
3	E	204	Total 204	O 204	0	0
3	F	204	Total 204	O 204	0	0
3	G	198	Total 198	O 198	0	0
3	H	234	Total 234	O 234	0	0



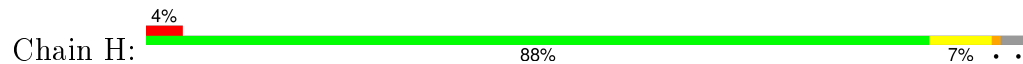
- Molecule 1: ThuA-like protein



- Molecule 1: ThuA-like protein



- Molecule 1: ThuA-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.54Å 74.60Å 123.52Å 90.84° 97.78° 118.69°	Depositor
Resolution (Å)	20.00 – 1.70 19.98 – 1.70	Depositor EDS
% Data completeness (in resolution range)	85.4 (20.00-1.70) 84.0 (19.98-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0001	Depositor
R, R_{free}	0.145 , 0.175 0.165 , 0.181	Depositor DCC
R_{free} test set	1037 reflections (0.50%)	DCC
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 58.5	EDS
Estimated twinning fraction	0.019 for -h-k,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 207543 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17343	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.99	1/2040 (0.0%)	1.00	7/2770 (0.3%)
1	B	1.04	0/2020	0.99	5/2744 (0.2%)
1	C	1.01	0/2045	0.97	5/2778 (0.2%)
1	D	0.99	0/2021	0.94	4/2745 (0.1%)
1	E	1.00	0/2044	0.98	6/2775 (0.2%)
1	F	1.03	1/2044 (0.0%)	1.00	9/2775 (0.3%)
1	G	1.06	0/2065	0.98	4/2801 (0.1%)
1	H	0.99	0/2033	0.96	3/2760 (0.1%)
All	All	1.02	2/16312 (0.0%)	0.98	43/22148 (0.2%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	217	ALA	CA-CB	-5.44	1.41	1.52
1	A	77	ASP	CB-CG	5.36	1.63	1.51

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	ASP	CB-CG-OD2	7.74	125.27	118.30
1	A	90	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	A	77	ASP	CB-CG-OD2	7.43	124.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	122	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	G	165	ASP	CB-CG-OD1	7.13	124.72	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	227	GLY	Peptide

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	1965	0	1892	12	0
1	B	1953	0	1890	15	0
1	C	1963	0	1892	16	0
1	D	1954	0	1887	5	0
1	E	1962	0	1897	17	0
1	F	1968	0	1908	13	0
1	G	1981	0	1926	12	0
1	H	1965	0	1905	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	197	0	0	4	0
3	B	194	0	0	3	0
3	C	184	0	0	2	0
3	D	209	0	0	0	0
3	E	204	0	0	6	0
3	F	204	0	0	2	0
3	G	198	0	0	3	0
3	H	234	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17343	0	15197	97	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 97 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:90:ARG:HH22	1:B:226:ARG:CZ	1.45	1.28
1:G:163:GLU:CD	3:G:1604:HOH:O	1.77	1.23
1:E:90:ARG:HH12	1:E:226:ARG:HE	1.09	0.97
1:B:90:ARG:NH2	1:B:226:ARG:CZ	2.29	0.95
1:G:90:ARG:HH12	1:G:226:ARG:HE	1.14	0.94

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	242/252 (96%)	236 (98%)	5 (2%)	1 (0%)	39	20
1	B	240/252 (95%)	235 (98%)	5 (2%)	0	100	100
1	C	243/252 (96%)	238 (98%)	4 (2%)	1 (0%)	39	20
1	D	240/252 (95%)	232 (97%)	8 (3%)	0	100	100
1	E	243/252 (96%)	236 (97%)	6 (2%)	1 (0%)	39	20
1	F	243/252 (96%)	237 (98%)	5 (2%)	1 (0%)	39	20
1	G	245/252 (97%)	239 (98%)	5 (2%)	1 (0%)	39	20
1	H	241/252 (96%)	237 (98%)	3 (1%)	1 (0%)	39	20
All	All	1937/2016 (96%)	1890 (98%)	41 (2%)	6 (0%)	46	26

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	GLY
1	F	198	GLY
1	G	198	GLY
1	C	198	GLY
1	E	198	GLY

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	209/214 (98%)	205 (98%)	4 (2%)	65	46
1	B	207/214 (97%)	203 (98%)	4 (2%)	65	46
1	C	210/214 (98%)	203 (97%)	7 (3%)	45	22
1	D	207/214 (97%)	203 (98%)	4 (2%)	65	46
1	E	210/214 (98%)	206 (98%)	4 (2%)	65	46
1	F	210/214 (98%)	205 (98%)	5 (2%)	57	36
1	G	212/214 (99%)	203 (96%)	9 (4%)	36	14
1	H	208/214 (97%)	202 (97%)	6 (3%)	50	27
All	All	1673/1712 (98%)	1630 (97%)	43 (3%)	54	32

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

Mol	Chain	Res	Type
1	E	3	THR
1	F	18	LYS
1	H	105[B]	PHE
1	E	105	PHE
1	E	119	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	233	ASN
1	G	244	GLN
1	G	73	HIS
1	F	73	HIS
1	G	21	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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	A	240/252 (95%)	0.25	13 (5%) 29 31	13, 18, 28, 41	22 (9%)
1	B	240/252 (95%)	0.17	11 (4%) 36 40	11, 17, 27, 43	16 (6%)
1	C	240/252 (95%)	0.20	15 (6%) 23 25	12, 17, 29, 40	22 (9%)
1	D	240/252 (95%)	0.18	10 (4%) 40 44	11, 17, 27, 38	15 (6%)
1	E	240/252 (95%)	0.17	7 (2%) 55 59	12, 17, 26, 40	18 (7%)
1	F	241/252 (95%)	0.10	9 (3%) 45 50	11, 17, 27, 40	19 (7%)
1	G	242/252 (96%)	0.12	8 (3%) 50 54	10, 17, 29, 42	20 (8%)
1	H	241/252 (95%)	0.17	11 (4%) 36 40	12, 17, 27, 49	19 (7%)
All	All	1924/2016 (95%)	0.17	84 (4%) 38 42	10, 17, 28, 49	151 (7%)

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	242	ALA	9.5
1	H	242	ALA	8.8
1	D	242	ALA	8.7
1	B	227	GLY	8.1
1	F	3	THR	7.9

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	B	3002	1/1	0.92	0.50	33.09	39,39,39,39	1
2	ZN	E	3005	1/1	0.93	0.24	10.87	37,37,37,37	1
2	ZN	D	3008	1/1	0.95	0.22	8.22	29,29,29,29	1
2	ZN	G	3007	1/1	0.96	0.14	3.89	26,26,26,26	1
2	ZN	A	3001	1/1	0.94	0.13	3.58	38,38,38,38	1
2	ZN	F	3006	1/1	0.99	0.15	3.47	32,32,32,32	1
2	ZN	C	3003	1/1	0.92	0.15	2.48	25,25,25,25	1
2	ZN	H	3004	1/1	0.97	0.06	-3.04	12,12,12,12	1

6.5 Other polymers [i](#)

There are no such residues in this entry.