



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6FWV / pdb_00006fwv
Title : The Bacillus anthracis TIE protein
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Deposited on : 2018-03-07
Resolution : 2.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

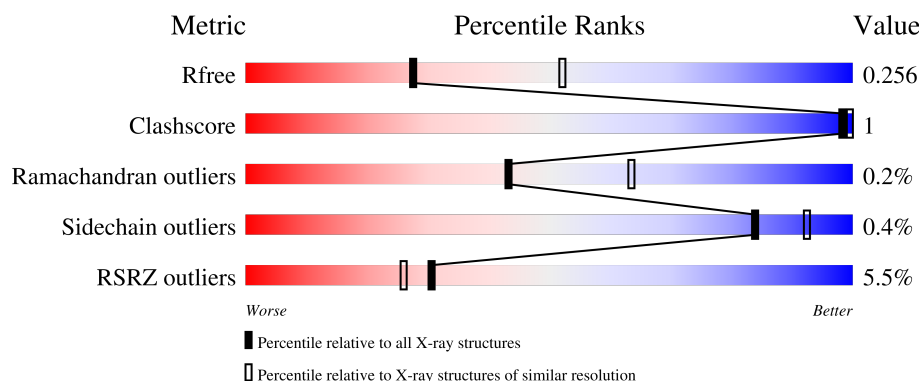
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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 $\leq 5\%$. 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	526	3% 98% ..
1	B	526	8% 97% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8226 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 Collagen Adhesion protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	Se	0	0	0
			4092	2593	675	817	1	6			
1	B	520	Total	C	N	O	S	Se	0	0	0
			4072	2580	671	813	1	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A0F7RA58
A	2	ALA	-	expression tag	UNP A0A0F7RA58
A	3	MSE	-	expression tag	UNP A0A0F7RA58
B	1	GLY	-	expression tag	UNP A0A0F7RA58
B	2	ALA	-	expression tag	UNP A0A0F7RA58
B	3	MSE	-	expression tag	UNP A0A0F7RA58

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Zn	0	0
			4	4		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		
3	B	24	Total	O	0	0
			24	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 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.

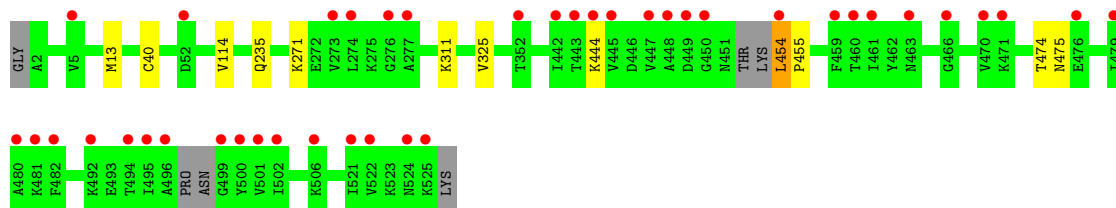
- Molecule 1: Collagen Adhesion protein

Chain A: 3% 98% ..



- Molecule 1: Collagen Adhesion protein

Chain B: 8% 97% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.82Å 66.50Å 106.58Å 90.00° 116.81° 90.00°	Depositor
Resolution (Å)	93.18 – 2.58 93.18 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.8 (93.18-2.58) 98.8 (93.18-2.58)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.221 , 0.256 0.224 , 0.256	Depositor DCC
R_{free} test set	2028 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8226	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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](#)

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	0.60	0/4148	0.73	1/5577 (0.0%)
1	B	0.61	0/4125	0.74	0/5544
All	All	0.61	0/8273	0.74	1/11121 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LYS	N-CA-C	-7.90	103.86	113.97

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	4092	0	4133	3	0
1	B	4072	0	4106	7	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
3	A	31	0	0	0	0
3	B	24	0	0	0	0
All	All	8226	0	8239	10	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 1.

All (10) 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:40:CYS:SG	1:B:235:GLN:CD	2.13	1.32
1:A:40:CYS:SG	1:A:235:GLN:CD	2.13	1.31
1:A:232:GLU:HA	1:A:232:GLU:OE1	1.86	0.76
1:B:13:MSE:HE1	1:B:114:VAL:HG21	1.90	0.53
1:B:13:MSE:CE	1:B:114:VAL:HG21	2.38	0.52
1:B:455:PRO:HA	1:B:474:THR:HG23	1.96	0.47
1:B:40:CYS:SG	1:B:235:GLN:OE1	2.68	0.46
1:B:311:LYS:HD3	1:B:325:VAL:HG12	2.01	0.41
1:B:444:LYS:HG3	1:B:454:LEU:HD11	2.02	0.41
1:A:40:CYS:SG	1:A:235:GLN:OE1	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	518/526 (98%)	507 (98%)	11 (2%)	0	100	100
1	B	514/526 (98%)	503 (98%)	9 (2%)	2 (0%)	30	49
All	All	1032/1052 (98%)	1010 (98%)	20 (2%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	271	LYS
1	B	475	ASN

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	452/447 (101%)	449 (99%)	3 (1%)	76	88
1	B	449/447 (100%)	448 (100%)	1 (0%)	87	95
All	All	901/894 (101%)	897 (100%)	4 (0%)	84	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	52	ASP
1	A	273	VAL
1	B	454	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	161	GLN
1	A	222	ASN
1	A	302	ASN
1	B	139	ASN
1	B	161	GLN
1	B	222	ASN
1	B	288	GLN
1	B	302	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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	516/526 (98%)	0.21	16 (3%)	51 46	40, 64, 153, 211	0
1	B	513/526 (97%)	0.43	41 (7%)	18 15	35, 69, 179, 233	0
All	All	1029/1052 (97%)	0.32	57 (5%)	30 26	35, 66, 168, 233	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	ALA	4.8
1	B	454	LEU	4.6
1	B	448	ALA	4.1
1	A	448	ALA	4.0
1	B	502	ILE	4.0
1	B	494	THR	3.6
1	B	495	ILE	3.5
1	B	499	GLY	3.4
1	B	501	VAL	3.2
1	B	480	ALA	3.0
1	A	499	GLY	3.0
1	B	522	VAL	2.9
1	B	442	ILE	2.9
1	B	273	VAL	2.8
1	B	274	LEU	2.8
1	A	5	VAL	2.8
1	A	501	VAL	2.7
1	A	271	LYS	2.7
1	B	463	ASN	2.7
1	B	444	LYS	2.7
1	B	525	LYS	2.7
1	B	5	VAL	2.6
1	B	459	PHE	2.5
1	B	460	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	466	GLY	2.5
1	B	481	LYS	2.5
1	B	445	VAL	2.5
1	B	479	ILE	2.4
1	B	500	TYR	2.4
1	B	470	VAL	2.4
1	B	471	LYS	2.4
1	B	52	ASP	2.4
1	B	482	PHE	2.4
1	B	443	THR	2.3
1	B	277	ALA	2.3
1	B	461	ILE	2.3
1	B	276	GLY	2.3
1	B	450	GLY	2.3
1	B	524	ASN	2.2
1	A	479	ILE	2.2
1	B	447	VAL	2.2
1	A	233	LYS	2.2
1	A	452	THR	2.2
1	B	352	THR	2.2
1	A	454	LEU	2.2
1	B	449	ASP	2.2
1	B	506	LYS	2.1
1	A	273	VAL	2.1
1	B	476	GLU	2.1
1	A	446	ASP	2.1
1	B	492	LYS	2.1
1	A	443	THR	2.1
1	A	494	THR	2.1
1	B	521	ILE	2.1
1	A	502	ILE	2.0
1	A	447	VAL	2.0
1	A	52	ASP	2.0

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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
2	ZN	A	604	1/1	0.92	0.07	115,115,115,115	0
2	ZN	B	602	1/1	0.94	0.08	104,104,104,104	0
2	ZN	A	603	1/1	0.95	0.05	104,104,104,104	0
2	ZN	A	602	1/1	0.97	0.05	70,70,70,70	0
2	ZN	B	601	1/1	0.98	0.09	72,72,72,72	0
2	ZN	B	603	1/1	0.99	0.03	48,48,48,48	0
2	ZN	A	601	1/1	1.00	0.02	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.