



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 9, 2026 – 09:21 PM UTC

PDB ID : 11TS / pdb\_000011ts  
Title : Crystal structure of apo alpha/beta-hydrolase macrolide esterase EstT from *Sphingobacterium faecium* (S126A mutant)  
Authors : Hemmings, M.Z.; Blanchet, J.; Kelly, E.T.R.; Berghuis, A.M.  
Deposited on : 2026-03-12  
Resolution : 3.19 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	:	4-5-2 with Phenix2.0
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

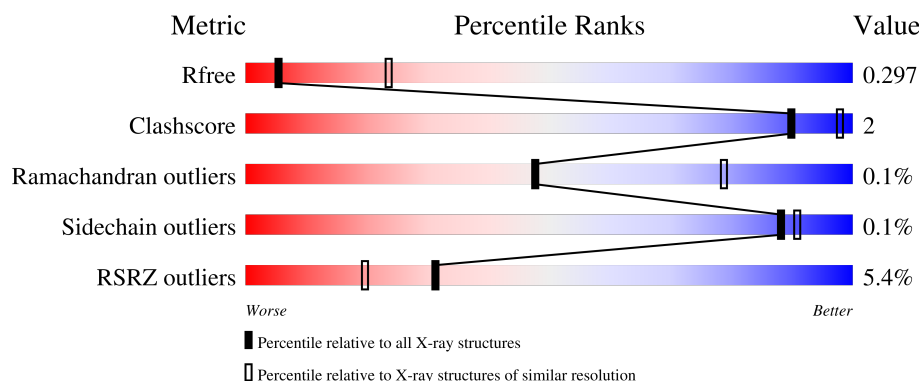
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	311	<div> <div>2%</div> <div>87%</div> <div>11%</div> </div>
1	B	311	<div> <div>2%</div> <div>88%</div> <div>9%</div> </div>
1	C	311	<div> <div>5%</div> <div>86%</div> <div>5%</div> <div>9%</div> </div>
1	D	311	<div> <div>3%</div> <div>74%</div> <div>6%</div> <div>20%</div> </div>
1	E	311	<div> <div>11%</div> <div>69%</div> <div>26%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9644 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 alpha/beta-hydrolase macrolide esterase EstT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2113	1341	354	411	7			
1	B	284	Total	C	N	O	S	0	0	0
			2105	1326	349	422	8			
1	C	283	Total	C	N	O	S	0	0	0
			2094	1323	358	407	6			
1	D	250	Total	C	N	O	S	0	0	0
			1829	1162	310	350	7			
1	E	229	Total	C	N	O	S	0	0	0
			1489	938	261	287	3			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	ALA	SER	engineered mutation	UNP A0ABU1EVH8
A	307	LEU	-	expression tag	UNP A0ABU1EVH8
A	308	GLU	-	expression tag	UNP A0ABU1EVH8
A	309	HIS	-	expression tag	UNP A0ABU1EVH8
A	310	HIS	-	expression tag	UNP A0ABU1EVH8
A	311	HIS	-	expression tag	UNP A0ABU1EVH8
B	126	ALA	SER	engineered mutation	UNP A0ABU1EVH8
B	307	LEU	-	expression tag	UNP A0ABU1EVH8
B	308	GLU	-	expression tag	UNP A0ABU1EVH8
B	309	HIS	-	expression tag	UNP A0ABU1EVH8
B	310	HIS	-	expression tag	UNP A0ABU1EVH8
B	311	HIS	-	expression tag	UNP A0ABU1EVH8
C	126	ALA	SER	engineered mutation	UNP A0ABU1EVH8
C	307	LEU	-	expression tag	UNP A0ABU1EVH8
C	308	GLU	-	expression tag	UNP A0ABU1EVH8
C	309	HIS	-	expression tag	UNP A0ABU1EVH8
C	310	HIS	-	expression tag	UNP A0ABU1EVH8
C	311	HIS	-	expression tag	UNP A0ABU1EVH8
D	126	ALA	SER	engineered mutation	UNP A0ABU1EVH8

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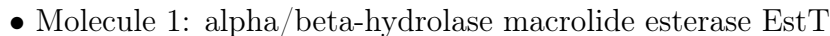
Chain	Residue	Modelled	Actual	Comment	Reference
D	307	LEU	-	expression tag	UNP A0ABU1EVH8
D	308	GLU	-	expression tag	UNP A0ABU1EVH8
D	309	HIS	-	expression tag	UNP A0ABU1EVH8
D	310	HIS	-	expression tag	UNP A0ABU1EVH8
D	311	HIS	-	expression tag	UNP A0ABU1EVH8
E	126	ALA	SER	engineered mutation	UNP A0ABU1EVH8
E	307	LEU	-	expression tag	UNP A0ABU1EVH8
E	308	GLU	-	expression tag	UNP A0ABU1EVH8
E	309	HIS	-	expression tag	UNP A0ABU1EVH8
E	310	HIS	-	expression tag	UNP A0ABU1EVH8
E	311	HIS	-	expression tag	UNP A0ABU1EVH8

- Molecule 2 is water.

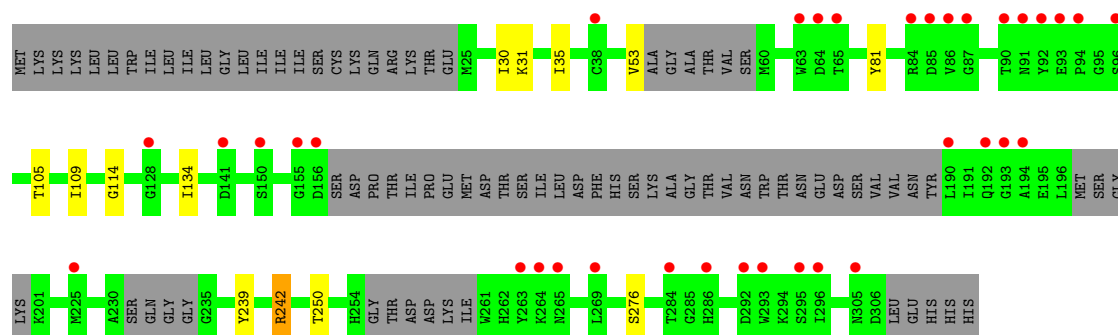
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	2	Total O 2 2	0	0
2	C	5	Total O 5 5	0	0
2	D	3	Total O 3 3	0	0



- Molecule 1: alpha/beta-hydrolase macrolide esterase EstT



- Chain E: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.92Å 82.32Å 392.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.44 – 3.19 29.44 – 3.19	Depositor EDS
% Data completeness (in resolution range)	83.6 (29.44-3.19) 83.4 (29.44-3.19)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.74 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.265 , 0.296 0.265 , 0.297	Depositor DCC
$R_{free}$ test set	1180 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	9644	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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	0.34	0/2156	0.73	2/2927 (0.1%)
1	B	0.33	0/2148	0.74	0/2928
1	C	0.37	1/2139 (0.0%)	0.74	0/2913
1	D	0.33	0/1865	0.64	0/2541
1	E	0.30	0/1508	0.68	0/2064
All	All	0.34	1/9816 (0.0%)	0.71	2/13373 (0.0%)

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	A	0	1
1	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	161	ILE	C-N	8.14	1.44	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ALA	CA-C-N	5.38	131.83	121.54
1	A	56	ALA	C-N-CA	5.38	131.83	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	242	ARG	Sidechain
1	E	242	ARG	Sidechain

## 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	2113	0	1993	3	0
1	B	2105	0	1902	5	0
1	C	2094	0	1890	8	0
1	D	1829	0	1633	9	0
1	E	1489	0	1171	7	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	5	0	0	0	0
2	D	3	0	0	0	0
All	All	9644	0	8589	32	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 32 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:153:PRO:HB3	1:A:243:LEU:HD11	1.80	0.62
1:C:149:MET:HG2	1:C:253:ILE:HB	1.82	0.61
1:D:149:MET:HG2	1:D:253:ILE:HB	1.82	0.61
1:E:250:THR:O	1:E:276:SER:HA	2.09	0.53
1:E:31:LYS:HA	1:E:35:ILE:O	2.11	0.51

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	274/311 (88%)	263 (96%)	11 (4%)	0	100	100
1	B	282/311 (91%)	271 (96%)	10 (4%)	1 (0%)	30	62
1	C	279/311 (90%)	268 (96%)	11 (4%)	0	100	100
1	D	244/311 (78%)	237 (97%)	7 (3%)	0	100	100
1	E	217/311 (70%)	206 (95%)	11 (5%)	0	100	100
All	All	1296/1555 (83%)	1245 (96%)	50 (4%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	157	SER

### 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	218/270 (81%)	218 (100%)	0	100	100
1	B	210/270 (78%)	210 (100%)	0	100	100
1	C	204/270 (76%)	204 (100%)	0	100	100
1	D	170/270 (63%)	169 (99%)	1 (1%)	78	84
1	E	104/270 (38%)	104 (100%)	0	100	100
All	All	906/1350 (67%)	905 (100%)	1 (0%)	88	91

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

Mol	Chain	Res	Type
1	D	144	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	221	ASN
1	D	69	GLN
1	B	188	ASN
1	C	262	HIS
1	B	106	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](#)

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	278/311 (89%)	0.23	7 (2%) 58 39	24, 44, 62, 73	0
1	B	284/311 (91%)	0.27	5 (1%) 67 48	25, 45, 74, 84	0
1	C	283/311 (90%)	0.50	14 (4%) 35 22	26, 50, 90, 101	0
1	D	250/311 (80%)	0.57	10 (4%) 42 26	34, 62, 97, 108	0
1	E	229/311 (73%)	1.13	35 (15%) 5 4	44, 77, 104, 109	0
All	All	1324/1555 (85%)	0.52	71 (5%) 31 20	24, 53, 96, 109	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	GLY	5.7
1	E	85	ASP	4.5
1	E	96	SER	4.5
1	E	155	GLY	4.2
1	C	308	GLU	3.9

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.