



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6ECC / pdb\_00006ecc  
Title : Vlm2 thioesterase domain wild type structure 2  
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Deposited on : 2018-08-07  
Resolution : 1.80 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](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  
Xtrriage (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

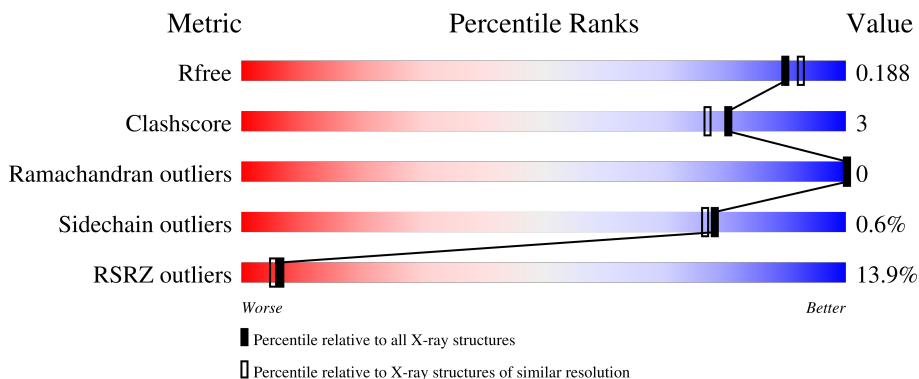
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	303	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3631 atoms, of which 1714 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 Vlm2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	231	3460	1118	1714	309	312	7	0	1	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2353	MET	-	expression tag	UNP Q1PSF3
A	2354	HIS	-	expression tag	UNP Q1PSF3
A	2355	HIS	-	expression tag	UNP Q1PSF3
A	2356	HIS	-	expression tag	UNP Q1PSF3
A	2357	HIS	-	expression tag	UNP Q1PSF3
A	2358	HIS	-	expression tag	UNP Q1PSF3
A	2359	HIS	-	expression tag	UNP Q1PSF3
A	2360	HIS	-	expression tag	UNP Q1PSF3
A	2361	HIS	-	expression tag	UNP Q1PSF3
A	2362	GLU	-	expression tag	UNP Q1PSF3
A	2363	ASN	-	expression tag	UNP Q1PSF3
A	2364	LEU	-	expression tag	UNP Q1PSF3
A	2365	TYR	-	expression tag	UNP Q1PSF3
A	2366	PHE	-	expression tag	UNP Q1PSF3
A	2367	GLN	-	expression tag	UNP Q1PSF3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	171	Total	O	0	0
			171	171		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.20Å 152.20Å 152.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.87 – 1.80 87.87 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (87.87-1.80) 93.6 (87.87-1.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.80 (at 1.80Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.176 , 0.190 0.175 , 0.188	Depositor DCC
$R_{free}$ test set	3093 reflections (5.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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 [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	0.89	0/1793	0.84	0/2439

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 [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	1746	1714	1712	9	0
2	A	171	0	0	2	0
All	All	1917	1714	1712	9	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.

All (9) 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:2470:PHE:O	1:A:2474[B]:THR:HG23	1.91	0.70
1:A:2557:SER:O	1:A:2561:LEU:HD22	2.04	0.58
1:A:2584:LYS:NZ	2:A:2703:HOH:O	2.41	0.53
1:A:2402:THR:OG1	1:A:2404:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2382:ARG:NH2	1:A:2386:ARG:HA	2.29	0.47
1:A:2474[B]:THR:HG21	2:A:2820:HOH:O	2.16	0.44
1:A:2381:VAL:HG11	1:A:2555:PHE:CE2	2.54	0.43
1:A:2474[B]:THR:HG22	1:A:2585:LEU:HD13	2.01	0.42
1:A:2550:PRO:HA	1:A:2553:SER:HB3	2.03	0.41

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	226/303 (75%)	223 (99%)	3 (1%)	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	178/242 (74%)	177 (99%)	1 (1%)	78   77

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

Mol	Chain	Res	Type
1	A	2561	LEU

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

Mol	Chain	Res	Type
1	A	2590	HIS

### 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

### 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, 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	231/303 (76%)	0.44	32 (13%) <b>6</b> <b>5</b>	15, 34, 92, 146	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2556	LEU	10.7
1	A	2375	ASP	9.4
1	A	2548	ASN	9.1
1	A	2499	PRO	7.7
1	A	2542	LEU	6.1
1	A	2541	LEU	6.0
1	A	2498	ILE	5.8
1	A	2647	LEU	5.6
1	A	2386	ARG	5.4
1	A	2555	PHE	5.4
1	A	2387	GLY	5.2
1	A	2554	ALA	5.0
1	A	2546	ALA	4.9
1	A	2551	ARG	4.9
1	A	2543	LEU	4.6
1	A	2497	ASP	4.6
1	A	2547	LYS	4.4
1	A	2385	PRO	4.4
1	A	2545	ARG	4.3
1	A	2544	ASP	4.3
1	A	2428	GLY	4.1
1	A	2550	PRO	4.0
1	A	2558	GLU	3.6
1	A	2552	VAL	3.6
1	A	2549	ASP	3.0
1	A	2553	SER	2.7
1	A	2636	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	2540	GLN	2.4
1	A	2557	SER	2.2
1	A	2569	MET	2.1
1	A	2626	ALA	2.1
1	A	2411	ARG	2.1

## 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.