



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:34 AM UTC

PDB ID : 6ECD / pdb_00006ecd
Title : Vlm2 thioesterase domain with genetically encoded 2,3-diaminopropionic acid bound with a tetradepsipeptide
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Deposited on : 2018-08-07
Resolution : 1.90 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

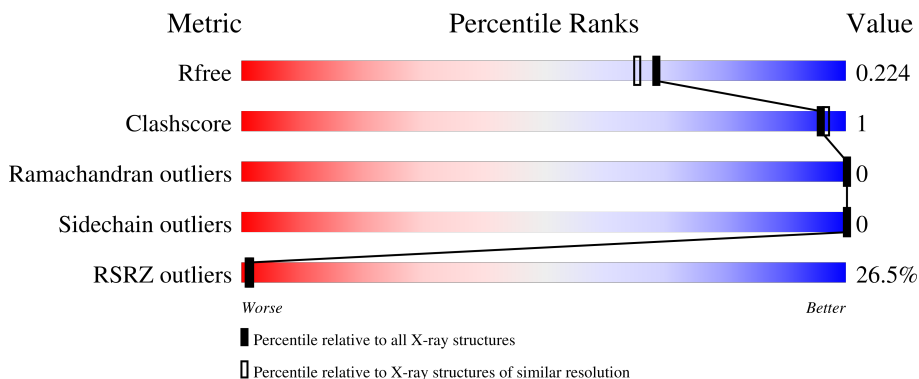
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	303	
2	B	4	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3641 atoms, of which 1723 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	245	3510	1149	1710	320	323	8	0	3	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 a protein called tetradepsipeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	B	2	25	8	13	1	3	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total 106	O 106	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	152.30Å 152.30Å 152.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.69 – 1.90 107.69 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (107.69-1.90) 91.8 (107.69-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.13_2998, PHENIX 1.13_2998	Depositor
R, R_{free}	0.188 , 0.214 0.201 , 0.224	Depositor DCC
R_{free} test set	2658 reflections (5.53%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3641	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2OP, DPP

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	0.79	0/1846	0.80	0/2510
2	B	0.70	0/6	0.56	0/7
All	All	0.79	0/1852	0.80	0/2517

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	1800	1710	1693	4	0
2	B	12	13	14	0	0
3	A	106	0	0	0	0
All	All	1918	1723	1707	4	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 (4) 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:THR:HG23	1.95	0.67
1:A:2375:ASP:N	1:A:2376:PRO:HD2	2.31	0.45
1:A:2474:THR:HG22	1:A:2585:LEU:HD13	2.01	0.41
1:A:2441:MET:HE3	1:A:2445:CYS:SG	2.61	0.40

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	237/303 (78%)	234 (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	173/241 (72%)	173 (100%)	0	100 100
2	B	1/1 (100%)	1 (100%)	0	100 100
All	All	174/242 (72%)	174 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2462	HIS
1	A	2582	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](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	DPP	A	2463	1,2	4,5,6	1.28	1 (25%)	1,5,7	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DPP	A	2463	1,2	-	0/2/4/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2463	DPP	CB-CA	2.33	1.58	1.53

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.

5.5 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, 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	244/303 (80%)	1.19	64 (26%) 1 1	24, 51, 115, 170	2 (0%)
2	B	1/4 (25%)	5.19	1 (100%) 0 0	114, 114, 114, 114	0
All	All	245/307 (79%)	1.20	65 (26%) 1 1	24, 51, 115, 170	2 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2548	ASN	12.5
1	A	2514	ILE	8.2
1	A	2513	PHE	7.5
1	A	2512	VAL	7.5
1	A	2524	ASP	7.5
1	A	2525	GLN	7.4
1	A	2375	ASP	7.1
1	A	2516	ALA	6.6
1	A	2648	PRO	6.6
1	A	2519	ILE	6.5
1	A	2543	LEU	6.5
1	A	2544	ASP	6.5
1	A	2495	LEU	6.5
1	A	2523	LEU	6.5
1	A	2537	GLU	5.9
1	A	2518	GLY	5.6
1	A	2536	GLU	5.3
1	A	2385	PRO	5.2
1	A	2511	LYS	5.2
2	B	3012	VAL	5.2
1	A	2542	LEU	5.1
1	A	2562	ASP	4.8
1	A	2541	LEU	4.8
1	A	2538	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	2554	ALA	4.4
1	A	2515	LEU	4.3
1	A	2428	GLY	4.3
1	A	2624	ASP	4.2
1	A	2540	GLN	3.9
1	A	2556	LEU	3.9
1	A	2382	ARG	3.8
1	A	2553	SER	3.8
1	A	2517	MET	3.7
1	A	2522	MET	3.7
1	A	2550	PRO	3.7
1	A	2539	LYS	3.7
1	A	2551	ARG	3.7
1	A	2546	ALA	3.7
1	A	2647	LEU	3.6
1	A	2630	ARG	3.6
1	A	2545	ARG	3.5
1	A	2583	ARG	3.3
1	A	2559	ASP	3.1
1	A	2547	LYS	3.1
1	A	2639	GLN	3.1
1	A	2521	GLY	3.0
1	A	2626	ALA	3.0
1	A	2569	MET	2.9
1	A	2431	GLU	2.9
1	A	2411	ARG	2.8
1	A	2439	GLU	2.8
1	A	2552	VAL	2.8
1	A	2555	PHE	2.7
1	A	2404	LEU	2.7
1	A	2643	ARG	2.7
1	A	2625	HIS	2.6
1	A	2520	GLY	2.5
1	A	2636	GLU	2.5
1	A	2388	GLY	2.4
1	A	2379	LYS	2.4
1	A	2414	LYS	2.4
1	A	2479	ARG	2.2
1	A	2389	ASP	2.2
1	A	2577	ASP	2.1
1	A	2566[A]	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	DPP	A	2463	6/7	0.96	0.09	31,37,59,71	0

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.