



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2024 – 03:55 PM EDT

PDB ID : 4TTL  
Title : Racemic structure of cyclic Vc1.1 (cVc1.1-1)  
Authors : Wang, C.K.; King, G.J.; Craik, D.J.  
Deposited on : 2014-06-22  
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](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	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

## 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.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 183 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-conotoxin Vc1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	22	Total	C	N	O	S	0	3	0
			162	94	28	36	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	insertion	UNP P69747
A	19	ALA	-	insertion	UNP P69747
A	20	ALA	-	insertion	UNP P69747
A	21	GLY	-	insertion	UNP P69747
A	22	GLY	-	insertion	UNP P69747

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		

MolProbity and EDS failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P b c a	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	30.26Å 20.71Å 38.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.12 – 1.70	Depositor
% Data completeness (in resolution range)	99.7 (19.12-1.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.189 , 0.226	Depositor
Wilson B-factor (Å <sup>2</sup> )	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
L-test for twinning <sup>1</sup>	$\langle  L  \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

<sup>1</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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

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### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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#### 4.3.2 Protein sidechains [i](#)

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#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.