

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID : 6NIV

Title : Racemic Phenol-Soluble Modulin Alpha 3 Peptide

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Deposited on : 2018-12-31

Resolution : 1.45 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 (i) 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 (1)) 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) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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 (i)

There are 2 unique types of molecules in this entry. The entry contains 422 atoms, of which 206 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 Phenol-soluble modulin PSM-alpha-3.

Mol	Chain	Residues		P	Atom	S			ZeroOcc	AltConf	Trace
1	A	23	Total 396	C 132	H 206	N 29	O 28	S 1	0	1	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Α	23	NH2	-	amidation	UNP H9BRQ7

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	26	Total O 26 26	0	0

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



3 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P -1	Depositor	
Cell constants	11.16Å 28.36Å 29.41Å	Depositor	
a, b, c, α , β , γ	111.79° 94.27° 95.12°	Depositor	
Resolution (Å)	16.02 - 1.45	Depositor	
% Data completeness	89.2 (16.02-1.45)	Depositor	
(in resolution range)	,	-	
R_{merge}	0.06	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) >$	-	Xtriage	
Refinement program	PHENIX (1.13_2998)	Depositor	
R, R_{free}	0.179 , 0.216	Depositor	
Wilson B-factor (A^2)	(Not available)	Xtriage	
Anisotropy	(Not available)	Xtriage	
L-test for twinning ¹	$ < L >=$ (Not available), $ =$ (Not available)	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	422	wwPDB-VP	
Average B, all atoms (\mathring{A}^2)	20.0	wwPDB-VP	

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

Theoretical values of $<|L|>, < L^2>$ 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)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

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 (i)

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.

