

wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 04:10 AM EDT

PDB ID : 6UL6

Title: Crystal Structure of BoNT/A-LCHn domain in complex with VNA ciA-

D12/11/ciA-B5 and VHH ciA-H7

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Resolution : 2.02 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*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 2.02 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 4 unique types of molecules in this entry. The entry contains 10407 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 BoNT/A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	855	Total 6918	C 4451	N 1115	O 1332	S 20	0	7	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q7B8V4
A	0	PRO	-	expression tag	UNP Q7B8V4
A	224	GLN	GLU	conflict	UNP Q7B8V4
A	363	ALA	ARG	$\operatorname{conflict}$	UNP Q7B8V4
A	366	PHE	TYR	conflict	UNP Q7B8V4

• Molecule 2 is a protein called ciA-D12/11/ciA-B5.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	239	Total 1826	C 1149	N 318	O 349	S 10	0	0	0

• Molecule 3 is a protein called ciA-H7.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	С	114	Total 864	C 537	N 152	O 170	S 5	0	1	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	619	Total O 619 619	0	0
4	В	98	Total O 98 98	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	82	Total O 82 82	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	C 1 2 1	Depositor
Cell constants	141.29Å 90.25Å 144.77Å	Depositor
a, b, c, α , β , γ	90.00° 119.04° 90.00°	Depositor
Resolution (Å)	47.21 - 2.02	Depositor
% Data completeness	99.7 (47.21-2.02)	Depositor
(in resolution range)	, ,	-
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.00 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.183 , 0.194	Depositor
Wilson B-factor (A^2)	26.9	Xtriage
Anisotropy	0.095	Xtriage
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
Total number of atoms	10407	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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.

