wwPDB X-ray Structure Validation Summary Report (i)

Oct 1, 2023 – 10:23 PM EDT

PDB ID	:	6MHJ
Title	:	Structure of BoNT mutant
Authors	:	Lam, K.; Jin, R.
Deposited on	:	2018-09-18
Resolution	:	3.02 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 (i)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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 ⓘ

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

The reported resolution of this entry is 3.02 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 ⓘ

There are 2 unique types of molecules in this entry. The entry contains 2647 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.
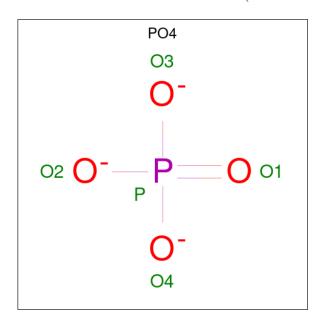
- Molecule 1 is a protein called Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total 2602	C 1670	N 420	O 504	S 8	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	545	GLY	-	expression tag	UNP P0DPI0
A	546	PRO	-	expression tag	UNP P0DPI0
A	658	GLU	PHE	engineered mutation	UNP P0DPI0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	A	1	Total 5	O 4	P 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	A	1	Total 5	O 4	P 1	0	0
2	A	1	Total 5	O 4	P 1	0	0
2	A	1	Total 5	O 4	P 1	0	0
2	A	1	Total 5	O 4	P 1	0	0
2	A	1	Total 5	O 4	P 1	0	0
2	A	1	Total 5	O 4	P 1	0	0

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 63 2 2		Depositor
Cell constants a, b, c, α, β, γ	158.27Å 158.27Å 123.97Å 90.00° 90.00° 120.00°		Depositor
Resolution (Å)	42.87 – 3.02		Depositor
% Data completeness (in resolution range)	99.9 (42.87-3.02)		Depositor
R_{merge}	0.09		Depositor
R_{sym}	(Not available)		Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 3.01Å)		Xtriage
Refinement program	PHENIX 1.9_1692		Depositor
R, R_{free}	0.182 , 0.237		Depositor
Wilson B-factor (Å^2)	75.5		Xtriage
Anisotropy	0.353		Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$		Xtriage
Estimated twinning fraction	No twinning to report.		Xtriage
Total number of atoms	2647		wwPDB-VP
Average B, all atoms (Å^2)	83.0		wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]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 ⓘ

4.1 Standard geometry ⓘ

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

4.2 Too-close contacts ⓘ

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

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

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

4.3.2 Protein sidechains ⓘ

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

4.3.3 RNA ⓘ

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

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

9 ligands are 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	#$|Z| > 2$
2	PO4	A	902	-	4,4,4	0.92	0	6,6,6	0.44	0
2	PO4	A	908	-	4,4,4	2.12	3 (75%)	6,6,6	0.43	0
2	PO4	A	907	-	4,4,4	2.13	3 (75%)	6,6,6	0.42	0
2	PO4	A	903	-	4,4,4	1.71	1 (25%)	6,6,6	0.95	0
2	PO4	A	905	-	4,4,4	2.14	3 (75%)	6,6,6	0.43	0
2	PO4	A	909	-	4,4,4	2.13	3 (75%)	6,6,6	0.44	0
2	PO4	A	901	-	4,4,4	0.92	0	6,6,6	0.44	0
2	PO4	A	904	-	4,4,4	2.14	3 (75%)	6,6,6	0.43	0
2	PO4	A	906	-	4,4,4	2.13	3 (75%)	6,6,6	0.43	0

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	909	PO4	P-O3	-2.36	1.47	1.54
2	A	904	PO4	P-O4	-2.35	1.47	1.54
2	A	905	PO4	P-O2	-2.35	1.47	1.54
2	A	904	PO4	P-O3	-2.34	1.47	1.54
2	A	909	PO4	P-O4	-2.34	1.47	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	909	PO4	0	2
2	A	901	PO4	0	1

4.7 Other polymers ⓘ

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 ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.3 Carbohydrates ⓘ

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

5.4 Ligands ⓘ

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

5.5 Other polymers ⓘ

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