



## wwPDB EM Validation Summary Report ⓘ

Mar 3, 2025 – 12:11 pm GMT

PDB ID : 9F25  
EMDB ID : EMD-50138  
Title : Cryo-EM structure of Botulinum neurotoxin A LC-HN domain  
Authors : Khanppnavar, B.; Leka, O.; Korkhov, V.; Kammerer, R.  
Deposited on : 2024-04-22  
Resolution : 3.70 Å (reported)  
Based on initial model : 6UL6

This is a wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

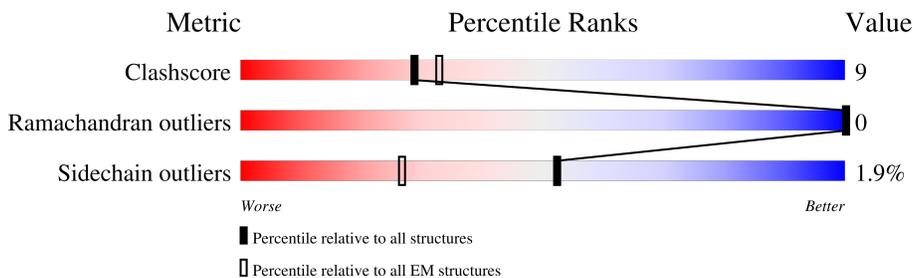
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1329	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6717 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
			Total	C	N	O	S		
1	A	830	6717	4331	1079	1288	19	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP P0DPI0
A	-15	ARG	-	expression tag	UNP P0DPI0
A	-14	GLY	-	expression tag	UNP P0DPI0
A	-13	SER	-	expression tag	UNP P0DPI0
A	-12	HIS	-	expression tag	UNP P0DPI0
A	-11	HIS	-	expression tag	UNP P0DPI0
A	-10	HIS	-	expression tag	UNP P0DPI0
A	-9	HIS	-	expression tag	UNP P0DPI0
A	-8	HIS	-	expression tag	UNP P0DPI0
A	-7	HIS	-	expression tag	UNP P0DPI0
A	-6	GLY	-	expression tag	UNP P0DPI0
A	-5	SER	-	expression tag	UNP P0DPI0
A	-4	LEU	-	expression tag	UNP P0DPI0
A	-3	VAL	-	expression tag	UNP P0DPI0
A	-2	PRO	-	expression tag	UNP P0DPI0
A	-1	ARG	-	expression tag	UNP P0DPI0
A	0	GLY	-	expression tag	UNP P0DPI0
A	1	SER	-	expression tag	UNP P0DPI0
A	27	ALA	VAL	variant	UNP P0DPI0
A	224	GLN	GLU	engineered mutation	UNP P0DPI0
A	363	ALA	ARG	engineered mutation	UNP P0DPI0
A	366	PHE	TYR	engineered mutation	UNP P0DPI0
A	1158	ALA	THR	conflict	UNP P0DPI0
A	1297	VAL	-	expression tag	UNP P0DPI0
A	1298	PRO	-	expression tag	UNP P0DPI0
A	1299	PRO	-	expression tag	UNP P0DPI0
A	1300	THR	-	expression tag	UNP P0DPI0
A	1301	PRO	-	expression tag	UNP P0DPI0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1302	GLY	-	expression tag	UNP P0DPI0
A	1303	SER	-	expression tag	UNP P0DPI0
A	1304	ALA	-	expression tag	UNP P0DPI0
A	1305	TRP	-	expression tag	UNP P0DPI0
A	1306	SER	-	expression tag	UNP P0DPI0
A	1307	HIS	-	expression tag	UNP P0DPI0
A	1308	PRO	-	expression tag	UNP P0DPI0
A	1309	GLN	-	expression tag	UNP P0DPI0
A	1310	PHE	-	expression tag	UNP P0DPI0
A	1311	GLU	-	expression tag	UNP P0DPI0
A	1312	LYS	-	expression tag	UNP P0DPI0



ASP  
ILE  
GLY  
PHE  
ILE  
GLY  
PHE  
HIS  
GLN  
PHE  
ASN  
ASN  
ILE  
ALA  
LYS  
LEU  
VAL  
ALA  
SER  
ASN  
TRP  
TYR  
ASN  
ASN  
ARG  
GLN  
ILE  
GLU  
ARG  
SER  
SER  
THR  
LEU  
GLY  
CYS  
SER  
TRP  
TRP  
GLU  
PHE  
ILE  
PRO  
VAL  
ASP  
ASP  
GLY  
TRP  
GLY  
GLU  
ARG  
ARG  
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LEU  
VAL  
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PRO  
GLY  
SER  
ALA  
TRP

SER  
HIS  
PRO  
GLN  
PHE  
GLU  
LYS

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121176	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor

## 5 Model quality [i](#)

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

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	0.26	0/6862	0.46	0/9294

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 [i](#)

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	6717	0	6618	123	0
All	All	6717	0	6618	123	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 9.

The worst 5 of 123 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:430:CYS:HB3	1:A:454:CYS:HA	1.50	0.93
1:A:633:ILE:HG13	1:A:656:LEU:HD23	1.60	0.83
1:A:107:LEU:HD21	1:A:225:LEU:HB3	1.67	0.77
1:A:726:ASP:OD1	1:A:729:ARG:NH2	2.28	0.67
1:A:605:GLY:O	1:A:609:GLN:HG3	1.95	0.66

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 PDB entries followed by that with respect to all EM entries.

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	822/1329 (62%)	806 (98%)	16 (2%)	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 PDB entries followed by that with respect to all EM entries.

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	747/1204 (62%)	733 (98%)	14 (2%)	52	70

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	592	LYS
1	A	612	TYR
1	A	824	TYR
1	A	696	ASP
1	A	729	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	642	ASN

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Mol	Chain	Res	Type
1	A	693	GLN
1	A	763	ASN
1	A	739	GLN
1	A	400	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 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.