



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:49 PM UTC

PDB ID : 1T3A / pdb_00001t3a
Title : Crystal structure of Clostridium botulinum neurotoxin type E catalytic domain
Authors : Agarwal, R.; Eswaramoorthy, S.; Kumaran, D.; Binz, T.; Swaminathan, S.
Deposited on : 2004-04-26
Resolution : 2.16 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

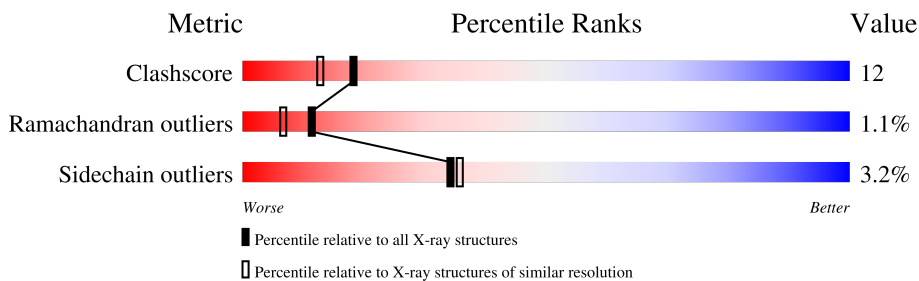
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	421	 76% 18% • 5%
1	B	421	 65% 26% • 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6743 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 neurotoxin type E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3207	2052	533	614	8			
1	B	398	Total	C	N	O	S	0	0	0
			3190	2040	531	612	7			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	211	Total	O	0	0
			211	211		
4	B	132	Total	O	0	0
			132	132		

3 Residue-property plots

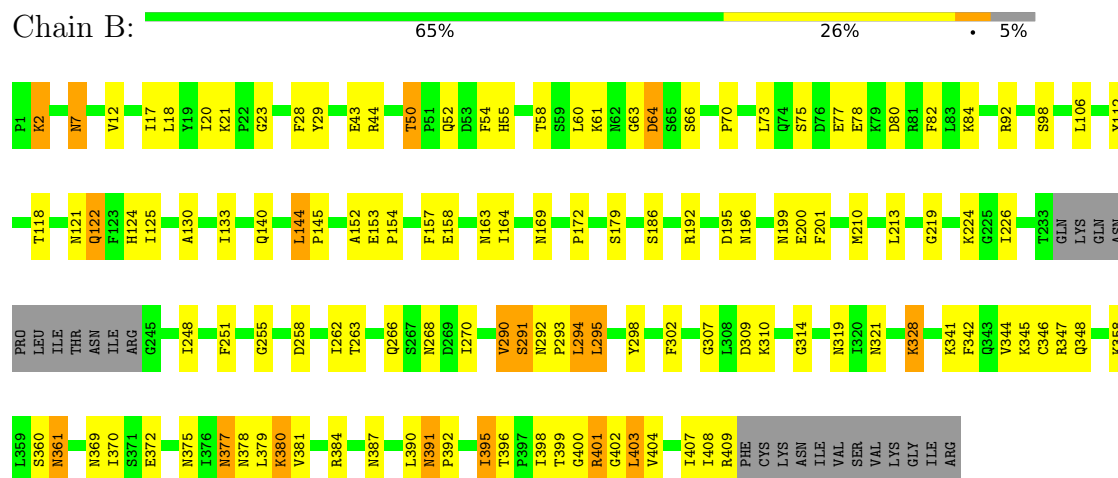
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: neurotoxin type E



• Molecule 1: neurotoxin type E



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.33Å 144.46Å 83.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.69 – 2.16	Depositor
% Data completeness (in resolution range)	97.0 (41.69-2.16)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6743	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ZN

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	0.42	0/3279	0.95	12/4440 (0.3%)
1	B	0.36	0/3261	0.89	13/4416 (0.3%)
All	All	0.39	0/6540	0.92	25/8856 (0.3%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ASN	N-CA-C	-10.66	97.82	111.90
1	B	399	THR	N-CA-C	7.13	121.83	113.20
1	A	408	ILE	N-CA-C	-7.07	94.64	109.34
1	A	370	ILE	N-CA-C	6.90	117.04	110.42
1	B	7	ASN	N-CA-C	-6.87	98.53	109.59

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3207	0	3158	62	0
1	B	3190	0	3144	95	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	211	0	0	4	0
4	B	132	0	0	5	0
All	All	6743	0	6302	153	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 12.

The worst 5 of 153 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:167:ARG:HG3	1:A:167:ARG:HH11	0.97	1.08
1:A:167:ARG:HG3	1:A:167:ARG:NH1	1.75	0.98
1:B:263:THR:H	1:B:266:GLN:HE21	1.22	0.85
1:A:167:ARG:HH11	1:A:167:ARG:CG	1.88	0.84
1:A:332:SER:HB2	4:A:639:HOH:O	1.77	0.83

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 X-ray entries followed by that with respect to entries of similar resolution.

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	396/421 (94%)	377 (95%)	15 (4%)	4 (1%)	12	8
1	B	394/421 (94%)	368 (93%)	21 (5%)	5 (1%)	9	5
All	All	790/842 (94%)	745 (94%)	36 (5%)	9 (1%)	11	7

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	ASP

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Mol	Chain	Res	Type
1	B	290	VAL
1	A	408	ILE
1	A	169	ASN
1	A	361	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	361/381 (95%)	354 (98%)	7 (2%)	50	56
1	B	359/381 (94%)	343 (96%)	16 (4%)	24	22
All	All	720/762 (94%)	697 (97%)	23 (3%)	34	36

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	268	ASN
1	B	298	TYR
1	B	295	LEU
1	B	328	LYS
1	A	411	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	348	GLN
1	B	375	ASN
1	B	382	ASN
1	A	375	ASN
1	A	353	GLN

5.3.3 RNA ⓘ

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.