



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 10:30 pm GMT

PDB ID : 3V0C
Title : 4.3 angstrom crystal structure of an inactive BoNT/A (E224Q/R363A/Y366F)
Authors : Gu, S.; Rumpel, S.; Zhou, J.; Strotmeier, J.; Bigalke, H.; Perry, K.; Shoemaker, C.B.; Rummel, A.; Jin, R.
Deposited on : 2011-12-07
Resolution : 4.30 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

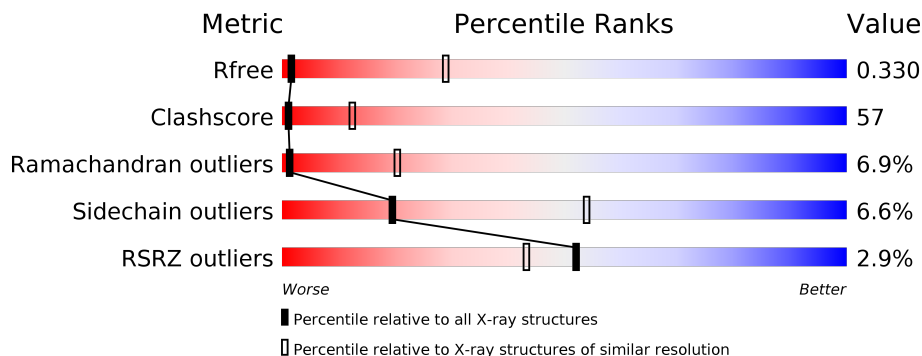
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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))
R_{free}	100719	1002 (4.92-3.62)
Clashscore	112137	1001 (4.92-3.68)
Ramachandran outliers	110173	1012 (4.92-3.64)
Sidechain outliers	110143	1021 (4.92-3.62)
RSRZ outliers	101464	1009 (4.92-3.62)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1312	<div> <div>3%</div> <div>28%</div> <div>59%</div> <div>9%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10390 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	1277	Total	C	N	O	S	0	0	0
			10389	6664	1714	1979	32			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	GLN	GLU	ENGINEERED MUTATION	UNP Q7B8V4
A	363	ALA	ARG	ENGINEERED MUTATION	UNP Q7B8V4
A	366	PHE	TYR	ENGINEERED MUTATION	UNP Q7B8V4
A	1158	ALA	THR	CONFLICT	UNP Q7B8V4
A	1297	VAL	-	EXPRESSION TAG	UNP Q7B8V4
A	1298	PRO	-	EXPRESSION TAG	UNP Q7B8V4
A	1299	PRO	-	EXPRESSION TAG	UNP Q7B8V4
A	1300	THR	-	EXPRESSION TAG	UNP Q7B8V4
A	1301	PRO	-	EXPRESSION TAG	UNP Q7B8V4
A	1302	GLY	-	EXPRESSION TAG	UNP Q7B8V4
A	1303	SER	-	EXPRESSION TAG	UNP Q7B8V4
A	1304	ALA	-	EXPRESSION TAG	UNP Q7B8V4
A	1305	TRP	-	EXPRESSION TAG	UNP Q7B8V4
A	1306	SER	-	EXPRESSION TAG	UNP Q7B8V4
A	1307	HIS	-	EXPRESSION TAG	UNP Q7B8V4
A	1308	PRO	-	EXPRESSION TAG	UNP Q7B8V4
A	1309	GLN	-	EXPRESSION TAG	UNP Q7B8V4
A	1310	PHE	-	EXPRESSION TAG	UNP Q7B8V4
A	1311	GLU	-	EXPRESSION TAG	UNP Q7B8V4
A	1312	LYS	-	EXPRESSION TAG	UNP Q7B8V4

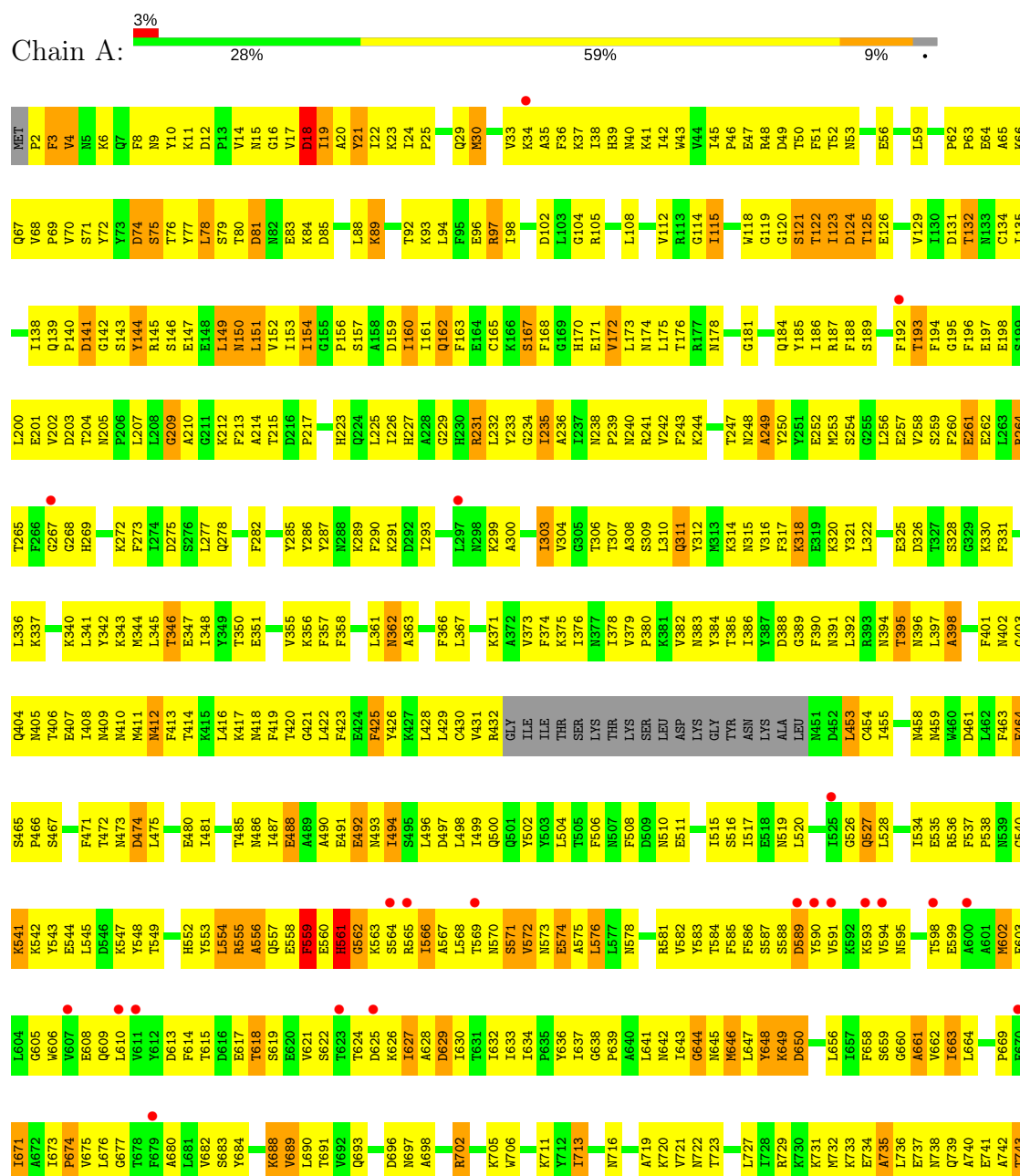
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: BoNT/A





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.52Å 167.52Å 158.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.11 – 4.30 45.11 – 4.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.11-4.30) 99.9 (45.11-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 4.28Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.322 , 0.349 0.312 , 0.330	Depositor DCC
R_{free} test set	912 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	161.8	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 241.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	10390	wwPDB-VP
Average B, all atoms (Å ²)	235.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.16	0/10610	0.66	1/14367 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	151	LEU	CA-CB-CG	6.20	129.55	115.30

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	10389	0	10255	1168	9
2	A	1	0	0	0	0
All	All	10390	0	10255	1168	9

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 57.

The worst 5 of 1168 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:277:LEU:HD22	1:A:474:ASP:HB3	1.24	1.13
1:A:872:ASN:HD21	1:A:874:ILE:HB	1.12	1.11
1:A:948:ARG:HB3	1:A:1068:TRP:HB2	1.28	1.10
1:A:310:LEU:HD11	1:A:314:LYS:HE3	1.38	1.05
1:A:1027:SER:HB2	1:A:1041:ILE:HD11	1.37	1.02

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ASN:OD1	1:A:1273:ARG:NH2[6_555]	1.12	1.08
1:A:63:PRO:O	1:A:309:SER:N[3_564]	1.82	0.38
1:A:486:ASN:CG	1:A:1273:ARG:NH2[6_555]	1.90	0.30
1:A:693:GLN:NE2	1:A:1276:ARG:CB[6_555]	1.96	0.24
1:A:697:ASN:ND2	1:A:1276:ARG:NH2[6_555]	2.00	0.20

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	1273/1312 (97%)	1008 (79%)	177 (14%)	88 (7%)	1	20

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	398	ALA
1	A	488	GLU
1	A	541	LYS
1	A	559	PHE

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	1158/1190 (97%)	1082 (93%)	76 (7%)	19 54

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	554	LEU
1	A	602	MET
1	A	1057	LEU
1	A	555	ARG
1	A	570	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	722	ASN
1	A	880	ASN
1	A	1243	ASN
1	A	765	ASN
1	A	913	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1277/1312 (97%)	0.14	37 (2%)	52 43	119, 222, 356, 750	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	590	TYR	5.5
1	A	569	THR	5.1
1	A	594	VAL	4.6
1	A	625	ASP	4.3
1	A	1044	LEU	4.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	A	1313	1/1	0.92	0.46	-	147,147,147,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.