



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 01:55 AM 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 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/ValidationPDFNotes.html>

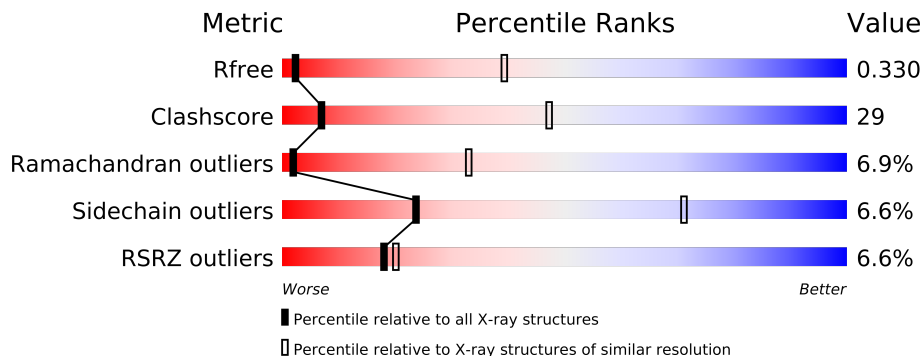
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


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}	66092	1016 (5.08-3.50)
Clashscore	79885	1280 (5.08-3.50)
Ramachandran outliers	78287	1210 (5.08-3.50)
Sidechain outliers	78261	1192 (5.08-3.50)
RSRZ outliers	66119	1016 (5.08-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1312	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ZN	A	1313	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10390 atoms, of which 0 are hydrogen and 0 are deuterium.

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

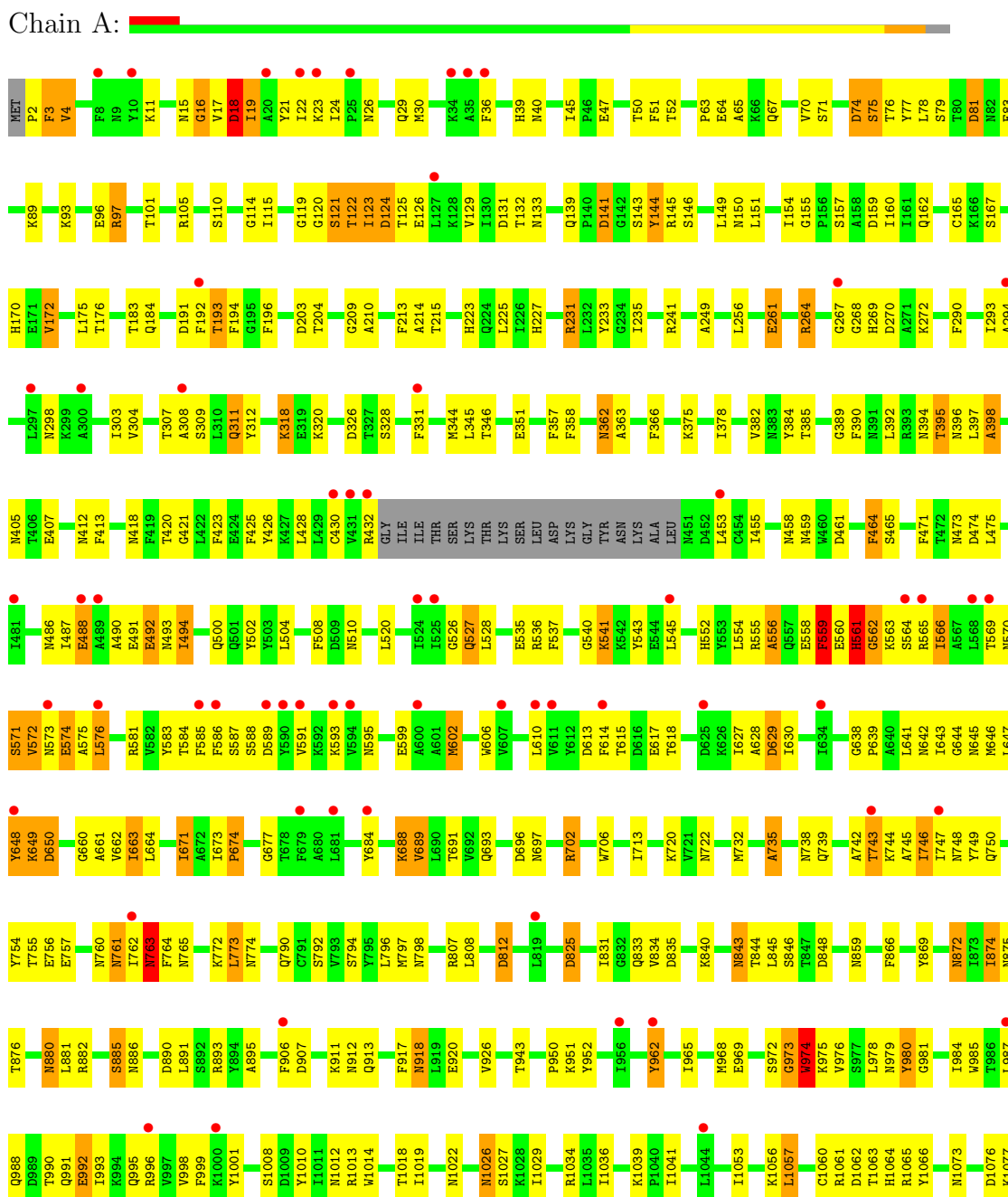
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

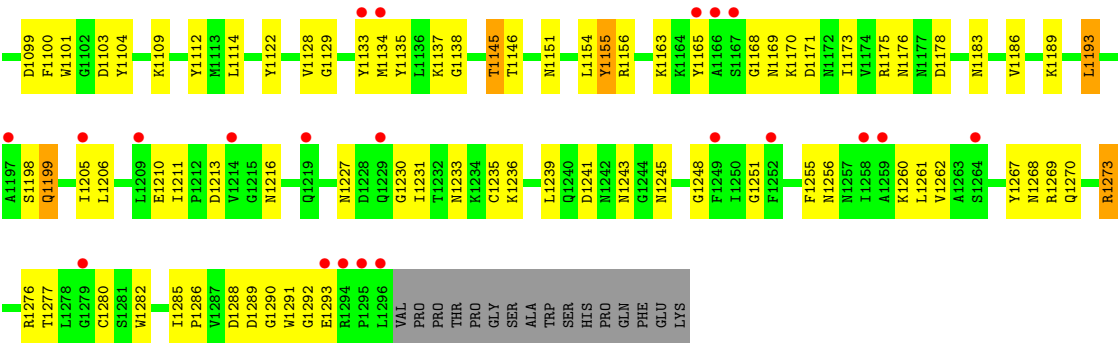
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

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 errors 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)	0.33 , 206.0	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 17872 reflections	Xtriage
F_o, F_c correlation	0.88	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.

5 Model quality

5.1 Standard geometry

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10389	0	0	298	9
2	A	1	0	0	0	0
All	All	10390	0	0	298	9

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 29.

The worst 5 of 298 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:HIS:ND1	1:A:40:ASN:N	2.35	0.74
1:A:210:ALA:N	1:A:405:ASN:ND2	2.40	0.70
1:A:1227:ASN:O	1:A:1230:GLY:N	2.27	0.68
1:A:1101:TRP:CZ3	1:A:1286:PRO:O	2.49	0.65
1:A:643:ILE:O	1:A:645:ASN:N	2.28	0.65

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	Distance(Å)	Clash(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

5.3.1 Protein backbone ⓘ

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%)	2	33

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%)	24 71

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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	0.64	83 (6%)	18 20	119, 222, 356, 750	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	590	TYR	6.5
1	A	569	THR	5.0
1	A	1044	LEU	4.5
1	A	34	LYS	4.5
1	A	594	VAL	4.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	A	1313	1/1	0.51	2.84	147,147,147,147	0

6.5 Other polymers ⓘ

There are no such residues in this entry.