



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 10:04 pm GMT

PDB ID : 1S0B
Title : Crystal structure of botulinum neurotoxin type B at pH 4.0
Authors : Eswaramoorthy, S.; Kumaran, D.; Keller, J.; Swaminathan, S.
Deposited on : 2003-12-30
Resolution : 2.00 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

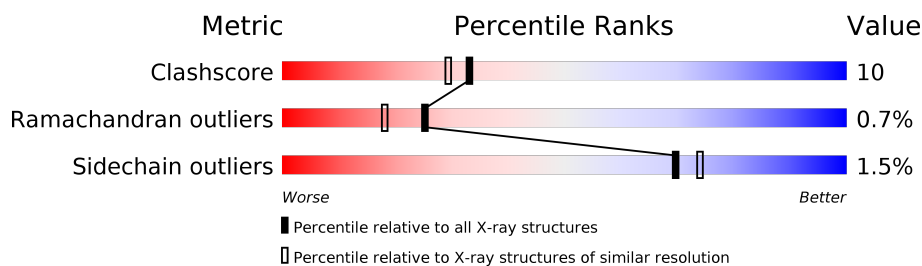
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1290	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11507 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 B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1287	Total	C	N	O	S	0	0	0
			10586	6827	1704	2022	33			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	919	Total	O	0	0
			919	919		

Note EDS was not executed.

- Chain A: 79% 20%

	R1161	K1162	E1163	L1192	A1195	P1196	D1201	I1209	Q1215	C1220	Q1221	I1247	V1248	F1249	I1258	M1272	L1275	M1278	F1281	E1290
T833	L1021	M1024	T1025	D1026	I1027	K1028	D1029	I1030	R1031	E1032	I1039	F1040	F1041	D1046	M1055	E1064	R1065	S1066	M1069	L1083
1834		T845	T846	T847	L848	K849	E850	D851	E858		D871	M872	M873	L874	L877	I908	R909	V910	I917	Q942
D845		T680	L685	T686	K687	E688	M689	E690	F691	M692	E730	N749	I750	N760	N764	N771	N775	M786	L787	K793
T846		S478	Y480	T481	K482	M483	D484	F485	P486	E489	D493	L496	I497	S498	K499	E505	Q523	I529	K578	A590
T847		K367	T368	K369	A370	S371	Y372	L377	P378	F379	V380	Y391	T392	I393	N398	K402	D403	M404	E405	M605
L848		Y479	T480	T481	K482	M483	D484	F485	P486	E489	D493	L496	I497	S498	K499	E505	Q523	I529	K578	A590
K849		K367	T368	K369	A370	S371	Y372	L377	P378	F379	V380	Y391	T392	I393	N398	K402	D403	M404	E405	M605
E850		Y479	T480	T481	K482	M483	D484	F485	P486	E489	D493	L496	I497	S498	K499	E505	Q523	I529	K578	A590
D1029		K367	T368	K369	A370	S371	Y372	L377	P378	F379	V380	Y391	T392	I393	N398	K402	D403	M404	E405	M605
I1030		Y479	T480	T481	K482	M483	D484	F485	P486	E489	D493	L496	I497	S498	K499	E505	Q523	I529	K578	A590
R1031		K367	T368	K369	A370	S371	Y372	L377	P378	F379	V380	Y391	T392	I393	N398	K402	D403	M404	E405	M605
E1032		Y479	T480	T481	K482	M483	D484	F485	P486	E489	D493	L496	I497	S498	K499	E505	Q523	I529	K578	A590
I1039		K367	T368	K369	A370	S371	Y372	L377	P378	F379	V380	Y391	T392	I393	N398	K402	D403	M404	E405	M605
F1040		Y479	T480	T481	K482	M483	D484	F485	P486	E489	D493	L496	I497	S498	K499	E505	Q523	I529	K578	A590
F1041		K367	T368	K369	A370	S371	Y372	L377	P378	F379	V380	Y391	T392	I393	N398	K402	D403	M404	E405	M605
D1046		Y479	T480	T481	K482	M483	D484	F485	P486	E489	D493	L496	I497	S498	K499	E505	Q523	I529	K578	A590
M1055		K367	T368	K369	A370	S371	Y372	L377	P378	F379	V380	Y391	T392	I393	N398	K402	D403	M404	E405	M605
E1064		Y479	T480	T481	K482	M483	D484	F485	P486	E489	D493	L496	I497	S498	K499	E505	Q523	I529	K578	A590
R1065		K367	T368	K369	A370	S371	Y372	L377	P378	F379	V380	Y391	T392	I393	N398	K402	D403			

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.23Å 123.15Å 95.56Å 90.00° 113.18° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00	Depositor
% Data completeness (in resolution range)	86.5 (50.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11507	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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: CA

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	0.35	0/10816	0.58	0/14611

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	10586	0	10419	206	0
2	A	2	0	0	0	0
3	A	919	0	0	12	0
All	All	11507	0	10419	206	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 10.

The worst 5 of 206 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:435:MET:HG2	1:A:529:ILE:HD11	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:LYS:HE2	1:A:1215:GLN:HE22	1.32	0.92
1:A:367:LYS:H	1:A:411:GLN:HE22	1.16	0.89
1:A:814:LEU:HD23	1:A:814:LEU:H	1.35	0.89
1:A:826:LYS:HA	1:A:829:LYS:HE2	1.56	0.87

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	1283/1290 (100%)	1214 (95%)	60 (5%)	9 (1%)	25 18

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1151	ASN
1	A	30	GLY
1	A	31	ARG
1	A	817	ILE
1	A	1128	GLN

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 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1176/1189 (99%)	1158 (98%)	18 (2%)	70 74

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	871	ASP
1	A	873	ASN
1	A	1055	MET
1	A	814	LEU
1	A	858	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	683	ASN
1	A	799	ASN
1	A	1215	GLN
1	A	749	ASN
1	A	764	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.