



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 07:04 PM GMT

PDB ID : 3D3X  
Title : Crystal structure of botulinum neurotoxin serotype E catalytic domain in complex with SNAP-25 substrate peptide  
Authors : Agarwal, R.; Swaminathan, S.  
Deposited on : 2008-05-13  
Resolution : 2.25 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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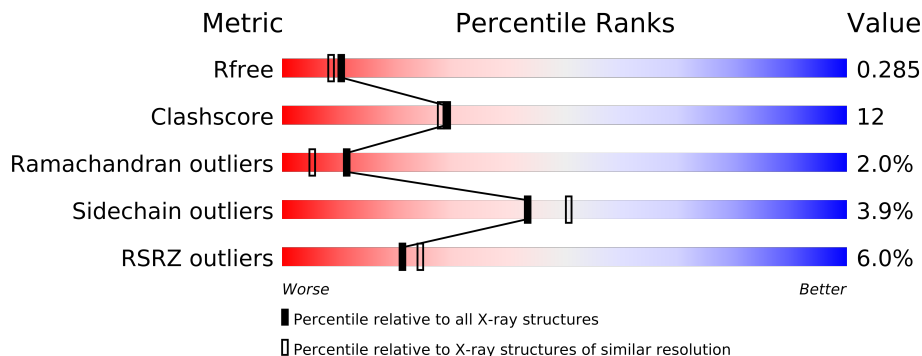
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.25 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	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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  $\geq 3$ , 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	427	
1	B	427	
2	C	5	
2	D	5	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	A	892	-	X
4	SO4	B	895	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6883 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 Type E botulinum toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3263	2086	545	624	8			
1	B	407	Total	C	N	O	S	0	0	0
			3265	2085	548	625	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	HIS	-	EXPRESSION TAG	UNP Q9K395
A	423	HIS	-	EXPRESSION TAG	UNP Q9K395
A	424	HIS	-	EXPRESSION TAG	UNP Q9K395
A	425	HIS	-	EXPRESSION TAG	UNP Q9K395
A	426	HIS	-	EXPRESSION TAG	UNP Q9K395
A	427	HIS	-	EXPRESSION TAG	UNP Q9K395
B	422	HIS	-	EXPRESSION TAG	UNP Q9K395
B	423	HIS	-	EXPRESSION TAG	UNP Q9K395
B	424	HIS	-	EXPRESSION TAG	UNP Q9K395
B	425	HIS	-	EXPRESSION TAG	UNP Q9K395
B	426	HIS	-	EXPRESSION TAG	UNP Q9K395
B	427	HIS	-	EXPRESSION TAG	UNP Q9K395

- Molecule 2 is a protein called SNAP-25 substrate peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	S	0	0	0
			21	14	3	3	1			
2	D	5	Total	C	N	O	S	0	1	1
			41	24	8	8	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	148	Total 148	O 148	0	0
5	B	102	Total 102	O 102	0	0
5	D	1	Total 1	O 1	0	0



- Molecule 2: SNAP-25 substrate peptide

Chain D: 

E180
I181
M182
E183
I184

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.41Å 144.74Å 83.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.48 – 2.25 33.47 – 2.25	Depositor EDS
% Data completeness (in resolution range)	91.6 (33.48-2.25) 91.7 (33.47-2.25)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.66 (at 2.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.235 , 0.288 0.235 , 0.285	Depositor DCC
$R_{free}$ test set	1426 reflections (3.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 27.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 49175 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6883	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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, SO4, NH2

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	0.44	0/3335	0.70	2/4516 (0.0%)
1	B	0.45	0/3337	0.66	0/4519
2	C	0.60	0/20	0.73	0/25
2	D	0.54	0/43	0.61	0/53
All	All	0.45	0/6735	0.68	2/9113 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	ARG	N-CA-C	5.93	127.01	111.00
1	A	378	ASN	N-CA-C	-5.50	96.15	111.00

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	3263	0	3216	83	0
1	B	3265	0	3220	81	0
2	C	21	0	21	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	41	0	40	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	30	0	0	1	0
4	B	10	0	0	0	0
5	A	148	0	0	5	0
5	B	102	0	0	4	0
5	D	1	0	0	0	0
All	All	6883	0	6497	162	0

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 12.

The worst 5 of 162 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:237:ASN:H	1:B:238:PRO:HD2	1.31	0.95
1:A:409:ARG:HG2	1:A:409:ARG:HH11	1.36	0.90
1:B:2:LYS:HD3	1:B:2:LYS:H	1.37	0.90
1:B:56:PRO:HG3	1:B:68:TYR:HB2	1.57	0.85
1:A:58:THR:HG23	1:A:59:SER:H	1.44	0.82

There are no symmetry-related clashes.

## 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	403/427 (94%)	374 (93%)	22 (6%)	7 (2%)	14	7
1	B	403/427 (94%)	363 (90%)	31 (8%)	9 (2%)	10	4
2	C	1/5 (20%)	1 (100%)	0	0	100	100
2	D	4/5 (80%)	4 (100%)	0	0	100	100
All	All	811/864 (94%)	742 (92%)	53 (6%)	16 (2%)	11	5

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	243	ILE
1	A	244	ARG
1	A	378	ASN
1	B	57	PRO

### 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	367/387 (95%)	357 (97%)	10 (3%)	57	67
1	B	367/387 (95%)	349 (95%)	18 (5%)	35	38
2	C	2/4 (50%)	2 (100%)	0	100	100
2	D	5/4 (125%)	3 (60%)	2 (40%)	0	0
All	All	741/782 (95%)	711 (96%)	30 (4%)	43	49

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	77	GLU
1	B	237	ASN
1	B	409	ARG
1	B	199	ASN
1	B	239	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	ASN
1	B	168	ASN
1	B	377	ASN
1	B	124	HIS
1	B	163	ASN

### 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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	A	891	-	4,4,4	0.45	0	6,6,6	0.10	0
4	SO4	A	892	-	4,4,4	0.66	0	6,6,6	0.09	0
4	SO4	A	893	-	4,4,4	0.50	0	6,6,6	0.12	0
4	SO4	A	894	-	4,4,4	0.52	0	6,6,6	0.19	0
4	SO4	A	896	-	4,4,4	0.60	0	6,6,6	0.14	0
4	SO4	A	897	-	4,4,4	0.43	0	6,6,6	0.09	0
4	SO4	B	890	-	4,4,4	0.47	0	6,6,6	0.12	0
4	SO4	B	895	-	4,4,4	0.61	0	6,6,6	0.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	891	-	-	0/0/0/0	0/0/0/0
4	SO4	A	892	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	893	-	-	0/0/0/0	0/0/0/0
4	SO4	A	894	-	-	0/0/0/0	0/0/0/0
4	SO4	A	896	-	-	0/0/0/0	0/0/0/0
4	SO4	A	897	-	-	0/0/0/0	0/0/0/0
4	SO4	B	890	-	-	0/0/0/0	0/0/0/0
4	SO4	B	895	-	-	0/0/0/0	0/0/0/0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	407/427 (95%)	0.13	20 (4%) 28 32	21, 35, 46, 58	0
1	B	407/427 (95%)	0.35	29 (7%) 16 19	26, 39, 51, 56	0
2	C	3/5 (60%)	1.30	1 (33%) 1 0	46, 46, 49, 54	0
2	D	5/5 (100%)	0.56	0 100 100	43, 43, 48, 49	0
All	All	822/864 (95%)	0.24	50 (6%) 21 23	21, 37, 49, 58	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	THR	5.7
1	B	237	ASN	5.1
1	B	233	THR	4.9
1	B	61	LYS	4.6
1	B	239	LEU	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	892	5/5	0.16	7.48	51,51,52,53	5
4	SO4	B	895	5/5	0.27	2.67	60,61,61,62	5
4	SO4	A	897	5/5	0.15	0.98	50,50,51,51	5
4	SO4	A	896	5/5	0.15	0.75	54,54,55,55	5
4	SO4	A	893	5/5	0.14	0.45	52,53,53,54	5
4	SO4	A	894	5/5	0.15	0.31	50,52,52,53	5
4	SO4	A	891	5/5	0.11	-0.57	40,44,44,45	5
4	SO4	B	890	5/5	0.11	-0.86	46,46,48,49	4
3	ZN	A	428	1/1	0.08	-2.10	50,50,50,50	0
3	ZN	B	822	1/1	0.04	-2.64	43,43,43,43	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.