



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:44 AM GMT

PDB ID : 3FUO  
Title : The Crystal structure of receptor binding domain of botulinum neurotoxin serotype A  
Authors : Fu, Z.; Chen, C.; Barbieri, J.T.; Kim, J.-J.P.; Baldwin, M.R.  
Deposited on : 2009-01-14  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

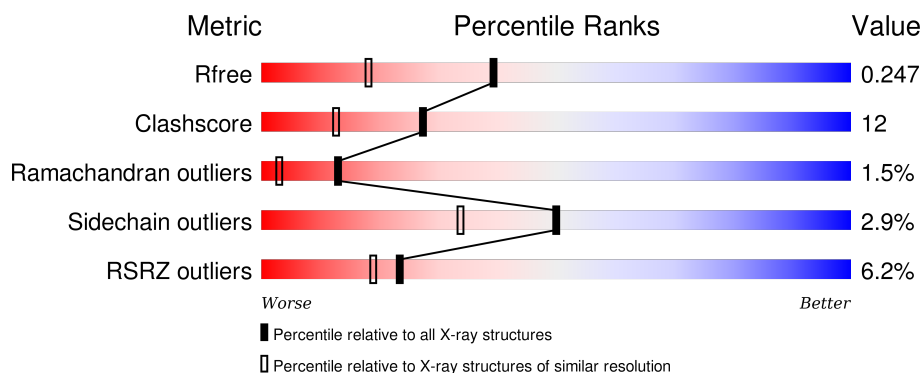
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. 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	426	<div> <div>6%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3635 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 A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3427	2187	588	639	13			

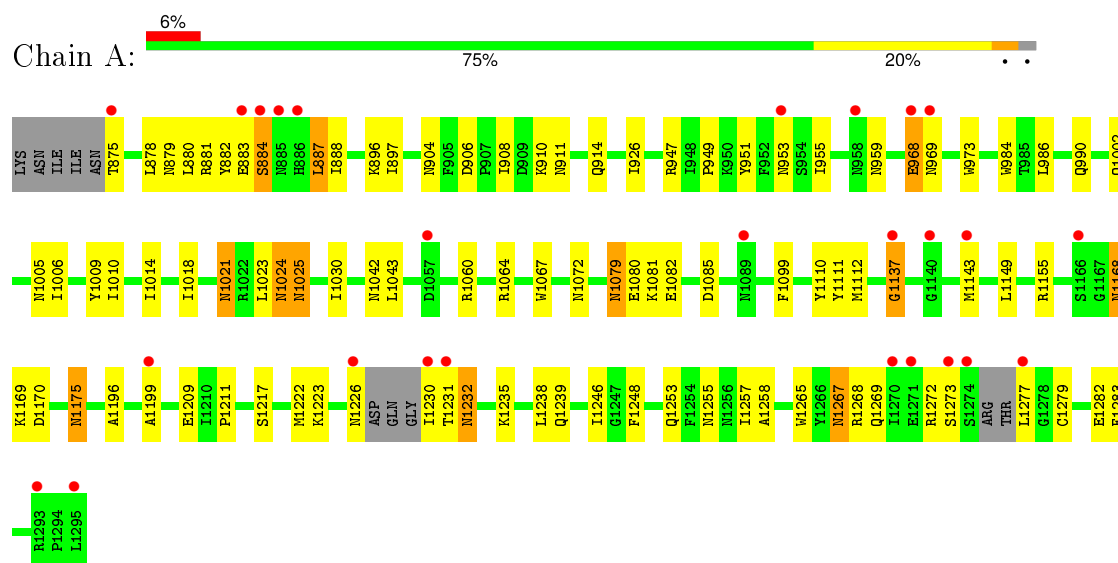
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	208	Total	O	0	0
			208	208		

### 3 Residue-property plots [i](#)

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: Botulinum neurotoxin type A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.77Å 105.14Å 112.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.92 – 1.80 18.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.1 (18.92-1.80) 91.1 (18.92-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.221 , 0.248 0.220 , 0.247	Depositor DCC
$R_{free}$ test set	4080 reflections (10.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 40603 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3635	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.33	0/3498	0.64	1/4726 (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	1137	GLY	N-CA-C	5.18	126.04	113.10

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	3427	0	3389	81	0
2	A	208	0	0	3	0
All	All	3635	0	3389	81	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.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ( $\text{\AA}$ )	Clash overlap ( $\text{\AA}$ )
1:A:1099:PHE:HD1	1:A:1282:GLU:HG2	1.20	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:ARG:HH12	1:A:1072:ASN:HD21	1.07	0.94
1:A:1099:PHE:CD1	1:A:1282:GLU:HG2	2.09	0.87
1:A:951:TYR:H	1:A:1002:GLN:HE22	1.24	0.86
1:A:1024:ASN:HD22	1:A:1025:ASN:H	1.21	0.85
1:A:1079:ASN:ND2	1:A:1082:GLU:H	1.78	0.81
1:A:1267:ASN:HD22	1:A:1267:ASN:H	1.30	0.78
1:A:906:ASP:OD1	1:A:908:ILE:HG22	1.86	0.76
1:A:896:LYS:HD2	1:A:926:ILE:HG13	1.71	0.72
1:A:1238:LEU:HD13	1:A:1239:GLN:N	2.05	0.72
1:A:1005:ASN:C	1:A:1006:ILE:HD12	2.09	0.72
1:A:959:ASN:HD21	1:A:1060:ARG:H	1.41	0.69
1:A:1248:PHE:H	1:A:1267:ASN:HD21	1.37	0.69
1:A:1217:SER:HB3	1:A:1238:LEU:HD11	1.77	0.65
1:A:1099:PHE:HD1	1:A:1282:GLU:CG	2.06	0.65
1:A:881:ARG:HH12	1:A:1072:ASN:ND2	1.89	0.65
1:A:1079:ASN:HD21	1:A:1082:GLU:H	1.42	0.65
1:A:949:PRO:O	1:A:1064:ARG:NH2	2.29	0.65
1:A:1168:ASN:HD22	1:A:1169:LYS:N	1.97	0.63
1:A:1232:ASN:HD22	1:A:1232:ASN:C	2.01	0.62
1:A:1021:ASN:HD22	1:A:1023:LEU:H	1.46	0.62
1:A:1079:ASN:C	1:A:1079:ASN:HD22	2.05	0.58
1:A:1226:ASN:OD1	1:A:1230:ILE:HG13	2.04	0.58
1:A:1238:LEU:CD1	1:A:1246:ILE:HD12	2.33	0.57
1:A:881:ARG:NH1	1:A:1072:ASN:HD21	1.91	0.57
1:A:1021:ASN:C	1:A:1021:ASN:HD22	2.07	0.57
1:A:1253:GLN:NE2	1:A:1258:ALA:HB2	2.19	0.57
1:A:1272:ARG:O	1:A:1273:SER:HB3	2.04	0.57
1:A:1238:LEU:HD12	1:A:1246:ILE:HD12	1.87	0.56
1:A:882:TYR:H	1:A:911:ASN:ND2	2.04	0.56
1:A:878:LEU:C	1:A:878:LEU:HD23	2.26	0.56
1:A:1155:ARG:HA	1:A:1155:ARG:HH11	1.70	0.56
1:A:1002:GLN:HA	1:A:1010:ILE:HD11	1.87	0.56
1:A:1021:ASN:ND2	1:A:1023:LEU:H	2.04	0.56
1:A:1175:ASN:O	1:A:1222:MET:O	2.24	0.55
1:A:1267:ASN:ND2	1:A:1267:ASN:H	2.04	0.55
1:A:953:ASN:HB2	1:A:955:ILE:HG22	1.89	0.55
1:A:1005:ASN:HB3	1:A:1006:ILE:HD12	1.89	0.54
1:A:1196:ALA:HB2	1:A:1246:ILE:HD13	1.89	0.53
1:A:1265:TRP:O	1:A:1269:GLN:HG2	2.08	0.53
1:A:883:GLU:O	1:A:884:SER:C	2.48	0.52
1:A:1112:MET:HE2	1:A:1283:PHE:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1238:LEU:HD12	1:A:1246:ILE:HB	1.92	0.52
1:A:882:TYR:CE2	1:A:910:LYS:HD3	2.44	0.52
1:A:1024:ASN:ND2	1:A:1025:ASN:H	2.00	0.52
1:A:1110:TYR:CB	1:A:1112:MET:HE1	2.41	0.51
1:A:1009:TYR:HB3	1:A:1014:ILE:HD11	1.91	0.51
1:A:1168:ASN:ND2	1:A:1170:ASP:OD1	2.44	0.50
1:A:1014:ILE:CG2	1:A:1030:ILE:HG23	2.41	0.50
1:A:1209:GLU:HG3	1:A:1211:PRO:HD2	1.93	0.50
1:A:1006:ILE:N	1:A:1006:ILE:HD12	2.26	0.50
1:A:984:TRP:CD2	1:A:1018:ILE:HG21	2.49	0.48
1:A:1267:ASN:HD22	1:A:1267:ASN:N	2.04	0.47
1:A:1235:LYS:NZ	1:A:1279:CYS:SG	2.88	0.47
1:A:897:ILE:N	1:A:897:ILE:HD12	2.30	0.47
1:A:1080:GLU:HG3	2:A:651:HOH:O	2.15	0.46
1:A:1110:TYR:HB2	1:A:1112:MET:HE1	1.97	0.46
1:A:1168:ASN:HD22	1:A:1168:ASN:C	2.17	0.46
1:A:888:ILE:HA	1:A:897:ILE:HD13	1.99	0.45
1:A:882:TYR:H	1:A:911:ASN:HD21	1.62	0.45
1:A:1081:LYS:HE3	1:A:1085:ASP:OD2	2.17	0.45
1:A:1255:ASN:O	1:A:1257:ILE:HD12	2.17	0.45
1:A:968:GLU:HB3	2:A:611:HOH:O	2.17	0.44
1:A:1079:ASN:ND2	1:A:1082:GLU:HG3	2.33	0.44
1:A:1231:THR:HG22	1:A:1232:ASN:N	2.33	0.43
1:A:1277:LEU:HD23	2:A:697:HOH:O	2.17	0.43
1:A:959:ASN:ND2	1:A:1060:ARG:H	2.11	0.43
1:A:1079:ASN:C	1:A:1079:ASN:ND2	2.71	0.42
1:A:973:TRP:HB3	1:A:986:LEU:HD23	2.00	0.42
1:A:880:LEU:HD22	1:A:887:LEU:HD22	2.00	0.42
1:A:1111:TYR:C	1:A:1112:MET:HE3	2.40	0.42
1:A:947:ARG:HB3	1:A:1067:TRP:HB2	2.02	0.42
1:A:1238:LEU:HD13	1:A:1238:LEU:C	2.40	0.42
1:A:904:ASN:HD22	1:A:914:GLN:HE21	1.67	0.42
1:A:1110:TYR:HB3	1:A:1112:MET:HE1	2.02	0.42
1:A:896:LYS:HB3	1:A:926:ILE:HB	2.00	0.41
1:A:1143:MET:HB3	1:A:1149:LEU:CD1	2.49	0.41
1:A:1042:ASN:OD1	1:A:1043:LEU:HD12	2.20	0.41
1:A:1223:LYS:HB2	1:A:1235:LYS:HB2	2.01	0.41
1:A:875:THR:HG22	1:A:875:THR:O	2.20	0.40
1:A:1079:ASN:HD22	1:A:1081:LYS:N	2.20	0.40

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	410/426 (96%)	384 (94%)	20 (5%)	6 (2%)	13 3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1137	GLY
1	A	884	SER
1	A	969	ASN
1	A	968	GLU
1	A	1175	ASN
1	A	1199	ALA

### 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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	384/393 (98%)	373 (97%)	11 (3%)	50 34

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	879	ASN
1	A	887	LEU
1	A	990	GLN
1	A	1021	ASN
1	A	1024	ASN

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Mol	Chain	Res	Type
1	A	1025	ASN
1	A	1079	ASN
1	A	1168	ASN
1	A	1232	ASN
1	A	1267	ASN
1	A	1268	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	879	ASN
1	A	911	ASN
1	A	912	GLN
1	A	914	GLN
1	A	959	ASN
1	A	987	GLN
1	A	990	GLN
1	A	1002	GLN
1	A	1011	ASN
1	A	1021	ASN
1	A	1024	ASN
1	A	1025	ASN
1	A	1072	ASN
1	A	1079	ASN
1	A	1168	ASN
1	A	1232	ASN
1	A	1242	ASN
1	A	1253	GLN
1	A	1264	ASN
1	A	1267	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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

### 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	416/426 (97%)	0.37	26 (6%) 23 19	12, 21, 35, 61	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1137	GLY	8.9
1	A	1274	SER	8.2
1	A	1273	SER	6.6
1	A	1277	LEU	6.4
1	A	1295	LEU	5.8
1	A	1271	GLU	5.6
1	A	968	GLU	4.7
1	A	884	SER	4.5
1	A	969	ASN	4.2
1	A	1293	ARG	4.0
1	A	1270	ILE	3.8
1	A	883	GLU	3.7
1	A	885	ASN	3.3
1	A	1140	GLY	3.2
1	A	1166	SER	2.9
1	A	886	HIS	2.9
1	A	1057	ASP	2.7
1	A	1230	ILE	2.7
1	A	953	ASN	2.7
1	A	875	THR	2.6
1	A	1226	ASN	2.5
1	A	1199	ALA	2.4
1	A	1231	THR	2.4
1	A	958	ASN	2.3
1	A	1143	MET	2.3
1	A	1089	ASN	2.2

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.