



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 02:13 PM EDT

PDB ID : 3MPP  
Title : Botulinum Neurotoxin Type G Receptor Binding Domain  
Authors : Schmitt, J.M.; Lacy, D.B.  
Deposited on : 2010-04-27  
Resolution : 1.98 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

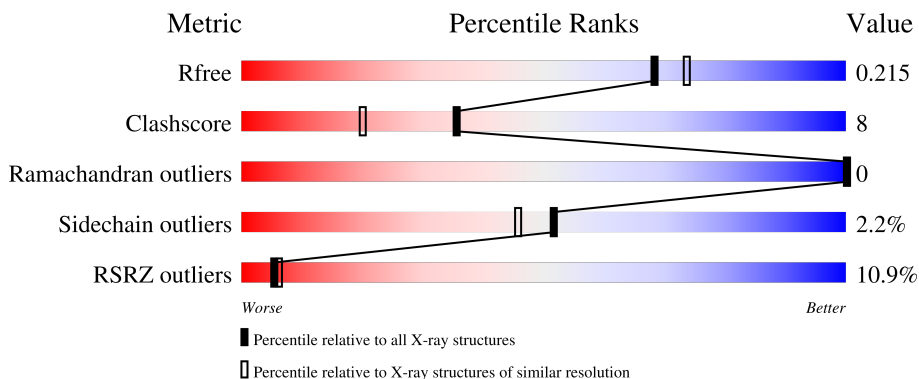
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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))
$R_{free}$	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	G	433	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3712 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 G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	403	3380	2163	563	645	9	0	9	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1080	GLU	SER	engineered mutation	UNP Q60393
G	1081	GLU	SER	engineered mutation	UNP Q60393
G	1082	ARG	LEU	engineered mutation	UNP Q60393
G	1084	LYS	TRP	engineered mutation	UNP Q60393
G	1298	LEU	-	expression tag	UNP Q60393
G	1299	GLN	-	expression tag	UNP Q60393

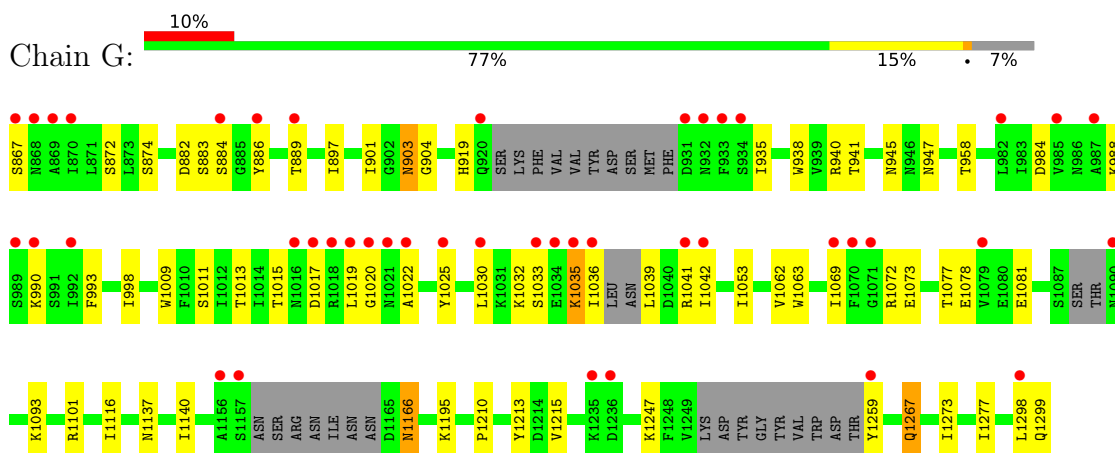
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	332	Total	O	0	0
			332	332		

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Botulinum neurotoxin type G



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.63Å 90.16Å 91.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.94 – 1.98 40.94 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.94-1.98) 99.1 (40.94-1.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 1.98Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 2009_02_15_2320_3)	Depositor
R, $R_{free}$	0.175 , 0.221 0.171 , 0.215	Depositor DCC
$R_{free}$ test set	1694 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtrriage
Anisotropy	0.219	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 63.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.026 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3712	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	G	0.39	0/3470	0.56	0/4689

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	G	3380	0	3295	54	0
2	G	332	0	0	3	0
All	All	3712	0	3295	54	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 8.

All (54) 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:G:1019:LEU:N	1:G:1020:GLY:HA2	1.92	0.85
1:G:940:ARG:HG3	1:G:1009:TRP:CD2	2.19	0.77
1:G:1101:ARG:HH11	1:G:1166:ASN:HD21	1.30	0.76
1:G:1035:LYS:HB2	1:G:1036:ILE:HA	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:941:THR:HG23	2:G:175:HOH:O	1.92	0.69
1:G:1247:LYS:HZ2	1:G:1259:TYR:HE1	1.41	0.68
1:G:889:THR:OG1	1:G:919:HIS:HB2	1.94	0.68
1:G:940:ARG:HB2	1:G:1063:TRP:HB2	1.82	0.62
1:G:1062:VAL:HG22	2:G:251:HOH:O	2.02	0.60
1:G:903:ASN:HD22	1:G:903:ASN:N	1.99	0.60
1:G:1036:ILE:HB	1:G:1039:LEU:HD22	1.83	0.59
1:G:1036:ILE:HD13	1:G:1039:LEU:HB3	1.85	0.58
1:G:867:SER:HB3	1:G:1072:ARG:NH1	2.19	0.57
1:G:940:ARG:HD2	1:G:1009:TRP:CD1	2.39	0.57
1:G:1019:LEU:N	1:G:1020:GLY:CA	2.68	0.57
1:G:1101:ARG:NH1	1:G:1166:ASN:HD21	2.02	0.56
1:G:884:SER:HG	1:G:886:TYR:HD1	1.54	0.55
1:G:1166:ASN:HD22	1:G:1166:ASN:H	1.54	0.53
1:G:935:ILE:CD1	1:G:1069:ILE:HD13	2.39	0.53
1:G:940:ARG:HD2	1:G:1009:TRP:NE1	2.25	0.52
1:G:903:ASN:HD22	1:G:903:ASN:H	1.56	0.52
1:G:901:ILE:O	1:G:904:GLY:HA2	2.11	0.50
1:G:993:PHE:O	1:G:1032:LYS:HD2	2.12	0.50
1:G:1013:THR:HB	1:G:1025:TYR:HB2	1.94	0.49
1:G:935:ILE:HD12	1:G:1069:ILE:HD13	1.94	0.49
1:G:903:ASN:N	1:G:904:GLY:HA2	2.28	0.49
1:G:945[A]:ASN:OD1	1:G:947[A]:ASN:OD1	2.30	0.49
1:G:1195:LYS:O	1:G:1195:LYS:HG3	2.13	0.48
1:G:938:TRP:CE2	1:G:1011:SER:HB2	2.48	0.48
1:G:1022:ALA:O	1:G:1033:SER:HA	2.13	0.47
1:G:1101:ARG:HH11	1:G:1166:ASN:ND2	2.06	0.47
1:G:1273:ILE:HD12	1:G:1277:ILE:HG12	1.96	0.47
1:G:867:SER:HB2	1:G:1072:ARG:HD2	1.96	0.47
1:G:1137:ASN:OD1	1:G:1140:ILE:HG13	2.16	0.46
1:G:940:ARG:HG3	1:G:1009:TRP:CG	2.51	0.45
1:G:1116:ILE:HD12	1:G:1116:ILE:C	2.37	0.45
1:G:988:LYS:HZ3	1:G:1039:LEU:N	2.15	0.45
1:G:1015:THR:HB	1:G:1073:GLU:HG3	1.97	0.45
1:G:984:ASP:HA	1:G:1042:ILE:HD13	1.99	0.44
1:G:1298:LEU:O	1:G:1299:GLN:HB3	2.17	0.44
1:G:897:ILE:HD12	1:G:897:ILE:N	2.32	0.44
1:G:1267:GLN:HE21	1:G:1267:GLN:HA	1.82	0.44
1:G:872:SER:OG	1:G:883:SER:HB2	2.19	0.43
1:G:958:THR:HB	1:G:1053:ILE:HB	2.01	0.43
1:G:1213:TYR:CZ	1:G:1215:VAL:HB	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:998:ILE:HD12	1:G:1140:ILE:HG22	2.01	0.42
1:G:874:SER:HA	1:G:903:ASN:O	2.19	0.42
1:G:1017:ASP:OD1	1:G:1020:GLY:HA2	2.18	0.42
1:G:1077:THR:O	1:G:1081:GLU:HG2	2.19	0.42
1:G:1093:LYS:NZ	2:G:261:HOH:O	2.52	0.41
1:G:990:LYS:NZ	1:G:990:LYS:HB2	2.35	0.41
1:G:882:ASP:OD1	1:G:884:SER:CB	2.68	0.41
1:G:867:SER:HB3	1:G:1072:ARG:HH11	1.86	0.41
1:G:1017:ASP:HB3	1:G:1073:GLU:OE1	2.21	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	G	400/433 (92%)	391 (98%)	9 (2%)	0	100 100

There are no Ramachandran outliers to report.

#### 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	G	378/398 (95%)	370 (98%)	8 (2%)	53 47



All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	903	ASN
1	G	1030	LEU
1	G	1035	LYS
1	G	1041	ARG
1	G	1078	GLU
1	G	1166	ASN
1	G	1210	PRO
1	G	1267	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	903	ASN
1	G	920	GLN
1	G	936	ASN
1	G	965	ASN
1	G	1023	ASN
1	G	1068	ASN
1	G	1144	ASN
1	G	1166	ASN
1	G	1193	ASN
1	G	1267	GLN

### 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 monosaccharides 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	G	403/433 (93%)	0.38	44 (10%) <b>5</b> <b>6</b>	18, 36, 86, 204	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1019	LEU	13.0
1	G	870	ILE	7.4
1	G	1041	ARG	5.6
1	G	1042	ILE	5.2
1	G	990	LYS	4.0
1	G	1071	GLY	4.0
1	G	1035	LYS	3.9
1	G	982	LEU	3.8
1	G	987	ALA	3.8
1	G	1259	TYR	3.5
1	G	1017	ASP	3.5
1	G	1070	PHE	3.4
1	G	1022	ALA	3.2
1	G	884	SER	3.2
1	G	869	ALA	3.0
1	G	1034	GLU	3.0
1	G	1036	ILE	2.8
1	G	1020	GLY	2.8
1	G	1016	ASN	2.8
1	G	1018	ARG	2.7
1	G	886	TYR	2.7
1	G	1033	SER	2.7
1	G	1236	ASP	2.6
1	G	992	ILE	2.5
1	G	1157	SER	2.5
1	G	1090	ASN	2.5
1	G	1030	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	933	PHE	2.4
1	G	920	GLN	2.4
1	G	868	ASN	2.4
1	G	889	THR	2.4
1	G	985	VAL	2.4
1	G	1021	ASN	2.4
1	G	1156	ALA	2.3
1	G	1298	LEU	2.3
1	G	1235	LYS	2.3
1	G	1025	TYR	2.2
1	G	934	SER	2.2
1	G	1079	VAL	2.2
1	G	931	ASP	2.1
1	G	1069	ILE	2.1
1	G	932	ASN	2.1
1	G	989	SER	2.0
1	G	867	SER	2.0

## 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 monosaccharides 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.