



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:06 AM UTC

PDB ID : 3MPP / pdb\_00003mpp  
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>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

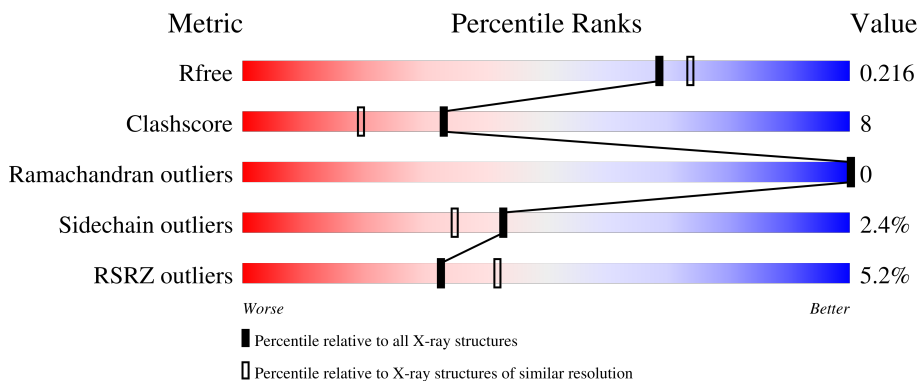
# 1 Overall quality at a glance

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))
$R_{free}$	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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

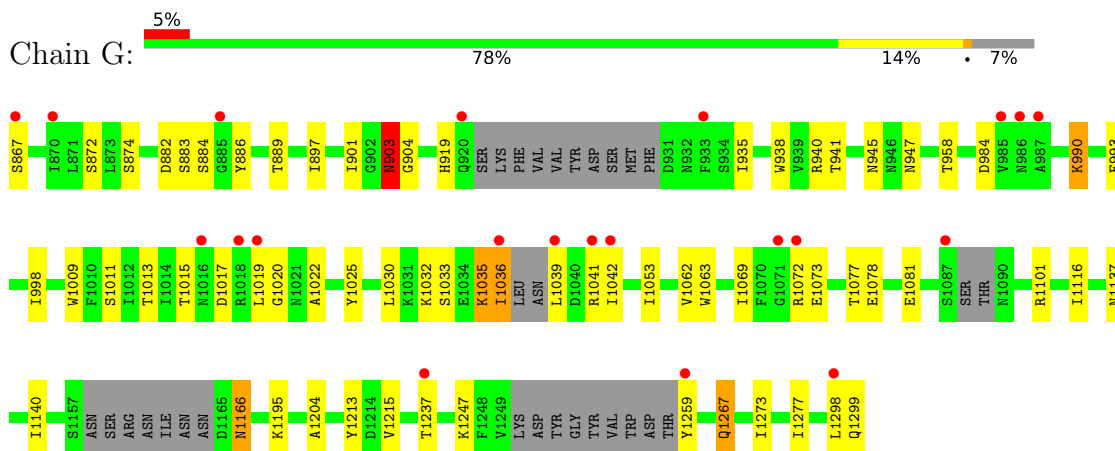
- Molecule 2 is water.

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

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 0.172 , 0.216	Depositor DCC
$R_{free}$ test set	1694 reflections (5.01%)	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 , 64.1	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	0.44	0/3470	0.74	3/4689 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	G	903	ASN	N-CA-C	6.67	120.17	109.83
1	G	1204	ALA	N-CA-C	5.84	115.02	108.25
1	G	1237	THR	N-CA-C	-5.11	107.00	113.18

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	52	0
2	G	332	0	0	2	0
All	All	3712	0	3295	52	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 (52) 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:1247:LYS:HZ2	1:G:1259:TYR:HE1	1.33	0.74
1:G:1035:LYS:HB2	1:G:1036:ILE:HA	1.72	0.69
1:G:941:THR:HG23	2:G:175:HOH:O	1.92	0.69
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:1116:ILE:HD12	1:G:1116:ILE:C	2.37	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: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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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%)	369 (98%)	9 (2%)	43 35

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	903	ASN
1	G	990	LYS
1	G	1030	LEU
1	G	1035	LYS
1	G	1036	ILE
1	G	1041	ARG
1	G	1078	GLU
1	G	1166	ASN
1	G	1267	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	903	ASN
1	G	915	ASN
1	G	920	GLN
1	G	936	ASN
1	G	965	ASN
1	G	1016	ASN
1	G	1021	ASN
1	G	1023	ASN
1	G	1068	ASN
1	G	1115	ASN
1	G	1166	ASN
1	G	1193	ASN
1	G	1267	GLN
1	G	1278	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 oligosaccharides 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	0.17	21 (5%) 33 42	17, 35, 86, 204	9 (2%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1019	LEU	7.0
1	G	1039	LEU	5.4
1	G	870	ILE	5.3
1	G	1036	ILE	5.0
1	G	1259	TYR	4.1
1	G	867	SER	3.8
1	G	1041	ARG	3.6
1	G	1018	ARG	3.3
1	G	1016	ASN	2.8
1	G	987	ALA	2.8
1	G	1298	LEU	2.8
1	G	920	GLN	2.8
1	G	1087	SER	2.7
1	G	1072	ARG	2.5
1	G	885	GLY	2.3
1	G	1237	THR	2.2
1	G	933	PHE	2.1
1	G	985	VAL	2.1
1	G	1071	GLY	2.0
1	G	986	ASN	2.0
1	G	1042	ILE	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 oligosaccharides 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.