



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 03:25 AM EDT

PDB ID : 5MK6  
Title : Crystal structure of the receptor-binding domain of botulinum neurotoxin A1 (crystal form 1)  
Authors : Davies, J.R.; Acharya, K.R.  
Deposited on : 2016-12-02  
Resolution : 1.45 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	:	2.37.1
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)	:	2.37.1

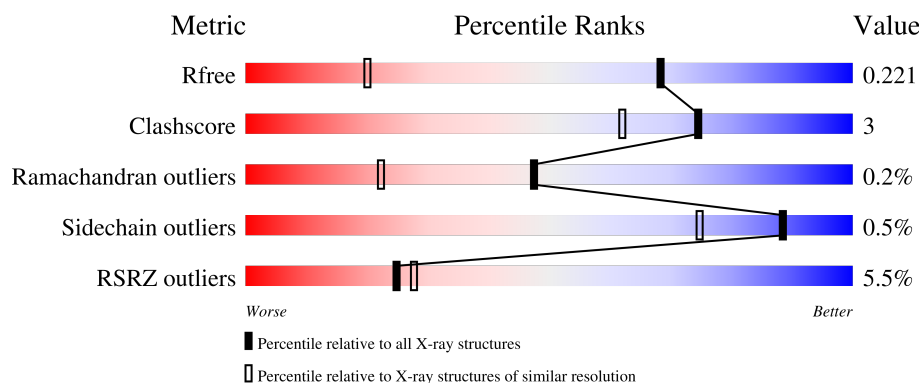
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	A	433	<div> <div>5%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3933 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	421	Total	C	N	O	S	0	12	0
			3511	2240	602	655	14			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	864	MET	-	initiating methionine	UNP P10845
A	865	HIS	-	expression tag	UNP P10845
A	866	HIS	-	expression tag	UNP P10845
A	867	HIS	-	expression tag	UNP P10845
A	868	HIS	-	expression tag	UNP P10845
A	869	HIS	-	expression tag	UNP P10845
A	870	HIS	-	expression tag	UNP P10845

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

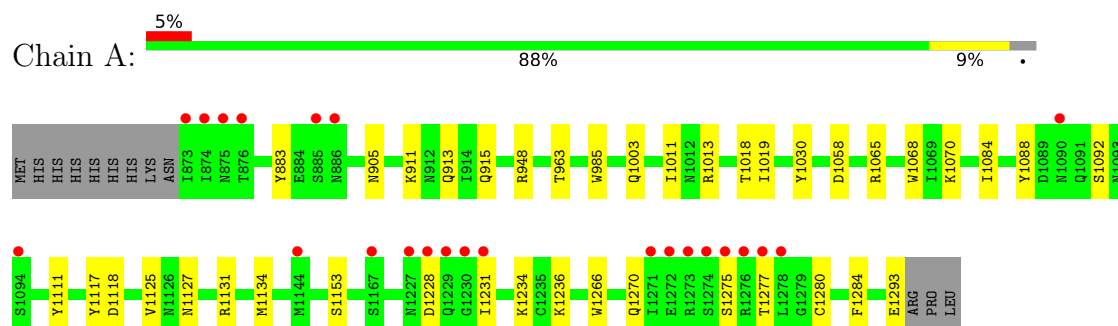
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	421	Total	O	0	0
			421	421		

### 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 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 107.32Å 107.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.05 – 1.45 24.05 – 1.45	Depositor EDS
% Data completeness (in resolution range)	95.3 (24.05-1.45) 95.3 (24.05-1.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 1.45Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.176 , 0.221 0.177 , 0.221	Depositor DCC
$R_{free}$ test set	1985 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.9	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3933	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 5.13% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.24	0/3620	0.46	0/4895

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	3511	0	3482	22	0
2	A	1	0	0	0	0
3	A	421	0	0	0	0
All	All	3933	0	3482	22	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 3.

All (22) 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:1236:LYS:NZ	1:A:1280:CYS:SG	2.67	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1270:GLN:HB2	1:A:1277:THR:HG22	1.78	0.65
1:A:1270:GLN:HB3	1:A:1275:SER:HB2	1.77	0.65
1:A:1266:TRP:O	1:A:1270:GLN:HG2	2.06	0.55
1:A:905[B]:ASN:HB3	1:A:915:GLN:HB3	1.90	0.53
1:A:913:GLN:HG2	1:A:1070:LYS:HD3	1.92	0.52
1:A:1018:THR:HB	1:A:1030:TYR:HB2	1.93	0.50
1:A:1270:GLN:HB2	1:A:1277:THR:CG2	2.40	0.50
1:A:1125[B]:VAL:HG22	1:A:1134[B]:MET:HG2	1.95	0.49
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	1.95	0.48
1:A:1228:ASP:OD2	1:A:1234:LYS:NZ	2.39	0.47
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.49	0.47
1:A:948:ARG:HB3	1:A:1068:TRP:HB2	1.95	0.47
1:A:1088:TYR:O	1:A:1092:SER:OG	2.30	0.46
1:A:1153:SER:OG	1:A:1293:GLU:OE2	2.26	0.45
1:A:883:TYR:CE2	1:A:911:LYS:HD3	2.52	0.44
1:A:1111:TYR:CG	1:A:1284:PHE:HB3	2.53	0.44
1:A:1117:TYR:HD2	1:A:1118:ASP:OD1	2.00	0.43
1:A:963:THR:HB	1:A:1058:ASP:HB3	2.00	0.43
1:A:985:TRP:CE3	1:A:1019:ILE:HD13	2.56	0.41
1:A:1013[A]:ARG:HH12	1:A:1231:ILE:HD11	1.85	0.41
1:A:1018:THR:HG21	1:A:1084:ILE:HG12	2.02	0.40

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	431/433 (100%)	415 (96%)	15 (4%)	1 (0%)	47 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1127	ASN

### 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	396/400 (99%)	393 (99%)	3 (1%)	81 62

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1065	ARG
1	A	1131[A]	ARG
1	A	1131[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 1 ligands modelled in this entry, 1 is 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 [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	421/433 (97%)	0.13	23 (5%)	25 28	13, 19, 40, 90	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1271	ILE	7.2
1	A	1278	LEU	7.1
1	A	1230	GLY	5.8
1	A	1276	ARG	5.2
1	A	1275	SER	4.8
1	A	1227	ASN	4.0
1	A	873	ILE	3.3
1	A	1229	GLN	3.3
1	A	1273	ARG	3.1
1	A	1231	ILE	3.1
1	A	874	ILE	3.0
1	A	876	THR	2.9
1	A	875	ASN	2.8
1	A	1274	SER	2.8
1	A	1277	THR	2.7
1	A	1272	GLU	2.7
1	A	885	SER	2.4
1	A	886	ASN	2.4
1	A	1167	SER	2.3
1	A	1144	MET	2.2
1	A	1094	SER	2.2
1	A	1228	ASP	2.2
1	A	1090	ASN	2.1

## 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](#)

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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NA	A	1301	1/1	1.00	0.12	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.