



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2023 – 10:48 PM EDT

PDB ID : 3N7K
Title : Crystal structure of botulinum neurotoxin serotype C1 binding domain
Authors : Fu, Z.; Kroken, A.; Karalewitz, A.; Baldwin, M.R.; Barbieri, J.T.; Kim, J.-J.P.
Deposited on : 2010-05-27
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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 : 4.02b-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

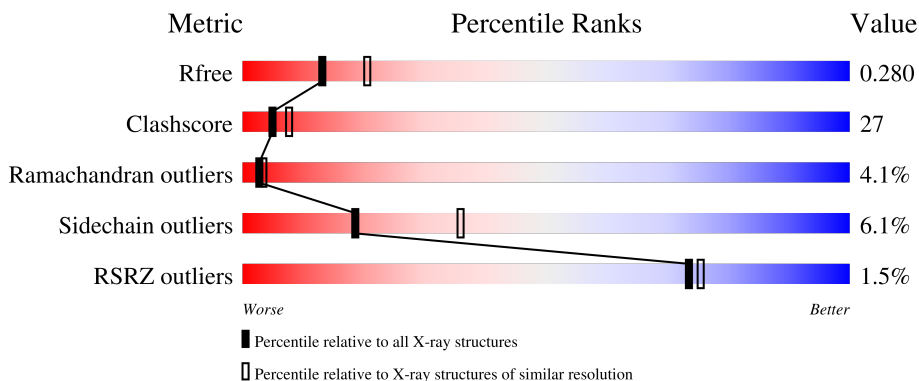
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ≥ 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	426	 2% 51% 42% 5% .
1	B	426	 % 54% 39% 6% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7035 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 C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	422	3466	2207	580	667	12	0	0	0
1	B	421	3459	2203	579	665	12	0	0	0

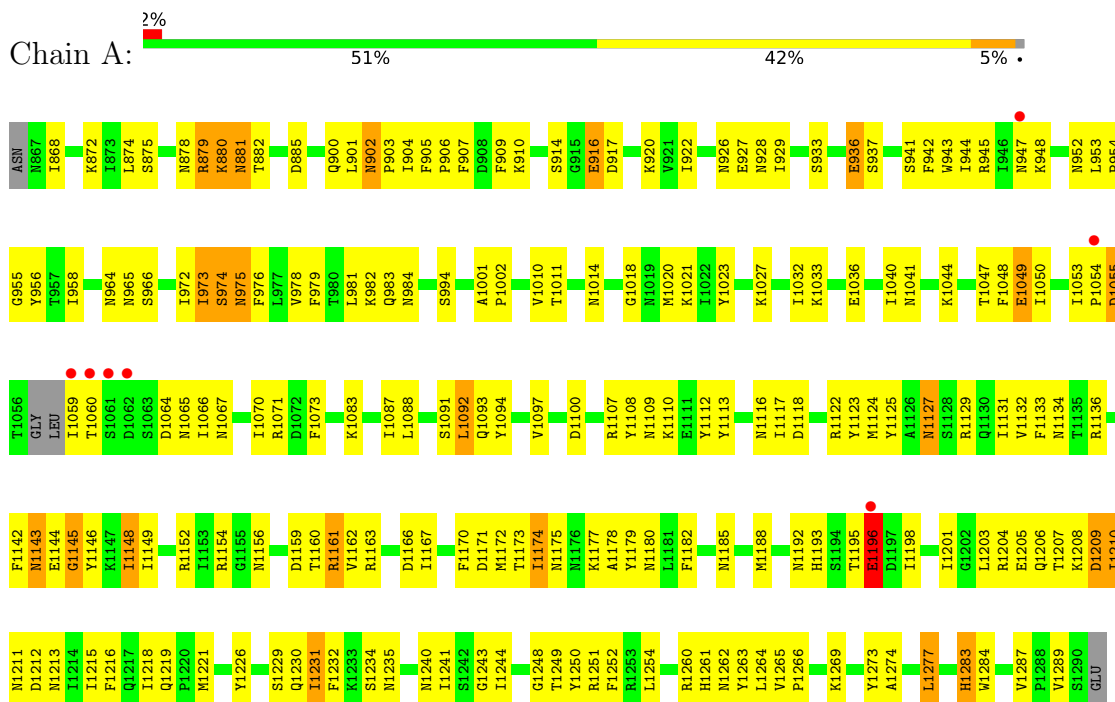
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	51	Total	O	0	0
			51	51		
2	B	59	Total	O	0	0
			59	59		

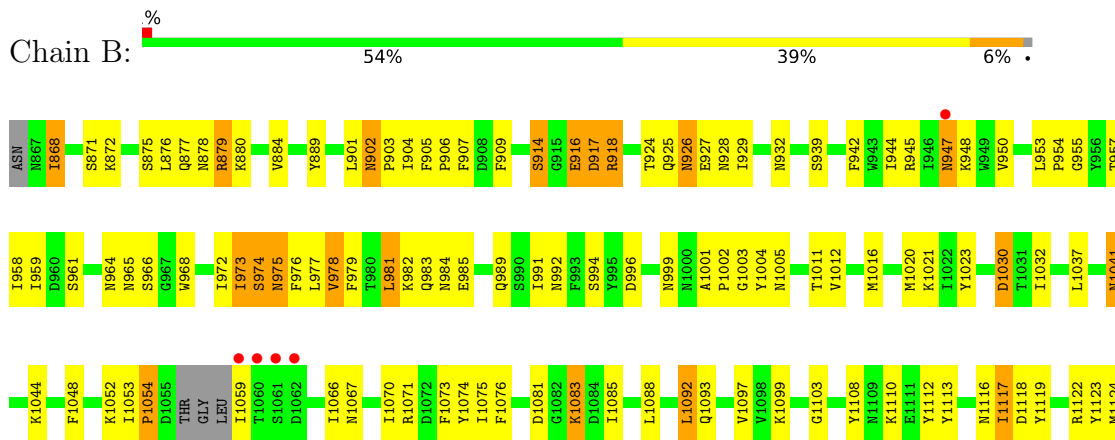
3 Residue-property plots

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 C1



● Molecule 1: Botulinum neurotoxin type C1



V1125	E1196	V1289
A1126	I1201	S1290
M1127	G1202	GLU
S1128	L1203	
R1129	R1204	
F1133	E1205	
M1134	Q1206	
T1135	K1208	
R1136	D1209	
F1142	D1212	
M1143	M1213	
E1144	I1214	
G1145	I1215	
Y1146	Y1226	
K1147	I1231	
I1148	S1234	
I1149	M1237	
I1150	G1238	
K1151	E1239	
R1152	M1240	
I1153	I1241	
R1154	S1242	
G1155	G1243	
M1156	T1249	
D1159	Y1250	
T1160	R1251	
R1161	F1252	
V1162	R1253	
R1163	L1254	
I1167	G1255	
L1168	R1260	
Y1169	H1261	
F1170	M1262	
D1171	Y1263	
M1172	L1264	
T1173	V1265	
I1174	P1266	
M1175	T1267	
M1176	V1268	
K1177	K1269	
A1178	Q1270	
Y1179	Y1273	
M1180	A1274	
L1181	L1277	
F1182	M1284	
M1183	V1287	
K1184	P1288	
M1185		
M1188		
D1191		
M1192		
R1193		
S1194		
T1195		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.18Å 77.35Å 107.39Å 90.00° 116.36° 90.00°	Depositor
Resolution (Å)	29.84 – 2.50 29.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.4 (29.84-2.50) 87.5 (29.84-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.281 0.223 , 0.280	Depositor DCC
R_{free} test set	2085 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 14.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.113 for -H,-K,H+L	Depositor
Outliers	1 of 45891 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7035	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	A	0.43	0/3543	0.69	1/4797 (0.0%)
1	B	0.43	0/3536	0.67	0/4787
All	All	0.43	0/7079	0.68	1/9584 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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	881	ASN	N-CA-C	-5.28	96.73	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1161	ARG	Sidechain

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	3466	0	3339	176	0
1	B	3459	0	3332	197	0
2	A	51	0	0	1	0
2	B	59	0	0	10	0
All	All	7035	0	6671	373	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 27.

The worst 5 of 373 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:B:947:ASN:HB2	1:B:1067:ASN:H	1.12	1.11
1:B:953:LEU:HD12	1:B:954:PRO:HD2	1.42	1.02
1:A:975:ASN:H	1:A:975:ASN:HD22	1.02	0.99
1:A:879:ARG:HE	1:A:879:ARG:HA	1.30	0.97
1:A:880:LYS:HB3	1:A:882:THR:HG22	1.44	0.96

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	418/426 (98%)	352 (84%)	49 (12%)	17 (4%)	3	3
1	B	417/426 (98%)	357 (86%)	43 (10%)	17 (4%)	3	3
All	All	835/852 (98%)	709 (85%)	92 (11%)	34 (4%)	3	3

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	974	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1055	ASP
1	A	1145	GLY
1	A	1193	HIS
1	A	1196	GLU

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	387/390 (99%)	362 (94%)	25 (6%)	17	33
1	B	386/390 (99%)	364 (94%)	22 (6%)	20	39
All	All	773/780 (99%)	726 (94%)	47 (6%)	18	36

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	917	ASP
1	B	1030	ASP
1	B	926	ASN
1	B	978	VAL
1	B	1066	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	928	ASN
1	B	1065	ASN
1	B	1270	GLN
1	B	932	ASN
1	B	992	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 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 [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, 95th 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 ²)	Q<0.9
1	A	422/426 (99%)	-0.27	7 (1%) 70 72	9, 27, 54, 84	0
1	B	421/426 (98%)	-0.25	6 (1%) 75 77	11, 28, 55, 76	0
All	All	843/852 (98%)	-0.26	13 (1%) 73 75	9, 28, 55, 84	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1059	ILE	6.8
1	A	1059	ILE	6.0
1	A	1061	SER	5.1
1	A	1060	THR	4.1
1	B	1060	THR	3.4

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.