



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:25 AM UTC

PDB ID : 3N7K / pdb_00003n7k
Title : Crystal structure of botulinum neurotoxin serotype C1 binding domain
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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	:	4-5-2 with Phenix2.0
Xtriage (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

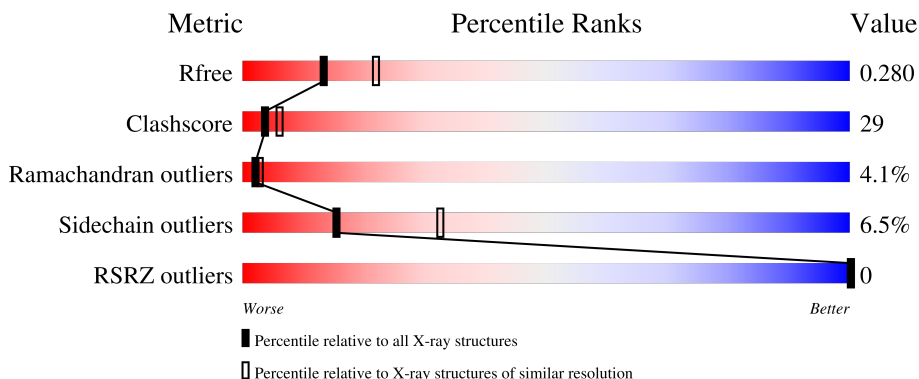
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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	 49% 41% 9% .
1	B	426	 49% 41% 8% ..

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
1	A	422	Total	C	N	O	S	0	0	0
			3466	2207	580	667	12			
1	B	421	Total	C	N	O	S	0	0	0
			3459	2203	579	665	12			

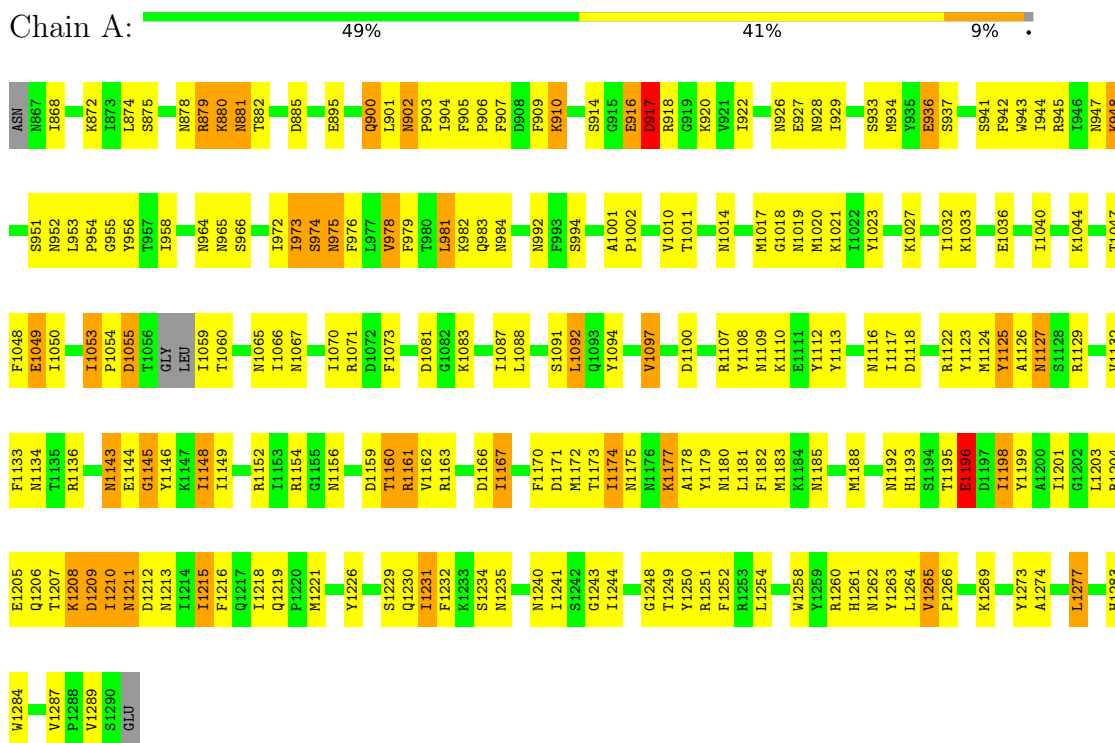
- Molecule 2 is water.

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

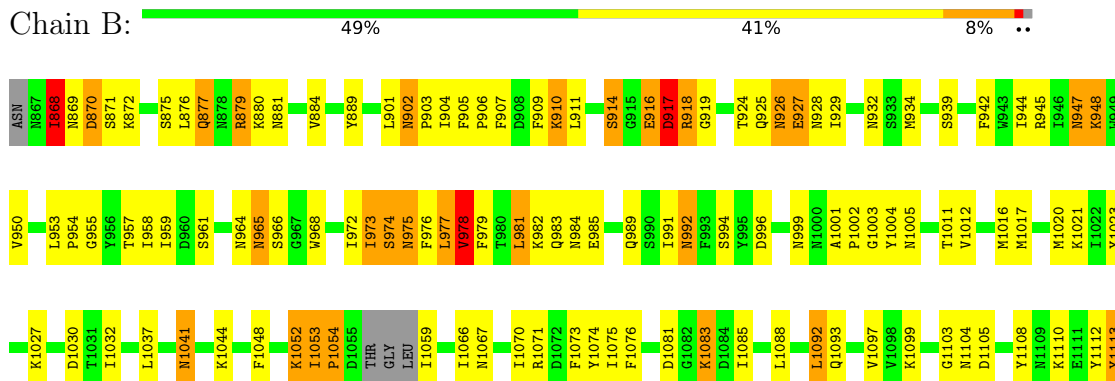
3 Residue-property plots

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



L1264	K1184	M1114
V1265	M1185	V1115
P1266		M1116
V1268	M1188	I1117
K1269		D1118
Q1270	D1191	Y1119
	M1192	
	H1193	
A1273	S1194	M1122
A1274	L1195	M1124
	E1196	Y1125
L1277		A1126
	Y1199	M1127
W1284	A1200	S1128
	I1201	R1129
V1287	G1202	
P1288	L1203	F1133
V1289	R1204	M1134
S1290	E1205	T1135
GLU	Q1206	R1136
	T1207	
	K1208	F1142
	D1209	M1143
		E1144
	D1212	G1145
	M1213	
	I1214	Y1146
	I1215	K1147
		I1148
	Q1219	T1149
		I1150
	Y1226	K1151
		R1152
	I1231	I1153
		R1154
	S1234	G1155
	M1235	M1156
	F1236	
	M1237	D1159
	G1238	T1160
	E1239	R1161
	M1240	V1162
	I1241	R1163
	S1242	
	G1243	I1167
		L1168
	T1249	Y1169
	Y1250	F1170
	R1251	D1171
	F1252	M1172
	R1253	T1173
	L1254	I1174
	G1255	M1175
		M1176
		K1177
	W1258	A1178
	Y1259	Y1179
	R1260	M1180
	H1261	L1181
	M1262	F1182
	Y1263	M1183

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) 87.7 (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)	0.32 , 12.0	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	0.93	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

5.1 Standard geometry

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	0.48	0/3543	1.01	20/4797 (0.4%)
1	B	0.48	0/3536	1.00	25/4787 (0.5%)
All	All	0.48	0/7079	1.00	45/9584 (0.5%)

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.

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	ASN	N-CA-C	-10.74	96.73	111.56
1	A	934	MET	N-CA-C	8.79	122.02	111.82
1	B	1160	THR	N-CA-C	-8.55	100.28	113.02
1	A	1160	THR	N-CA-C	-8.46	99.77	112.54
1	B	868	ILE	N-CA-C	-7.67	105.06	113.43

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

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	183	0
1	B	3459	0	3332	211	0
2	A	51	0	0	1	0
2	B	59	0	0	10	0
All	All	7035	0	6671	394	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 29.

The worst 5 of 394 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

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	418/426 (98%)	352 (84%)	49 (12%)	17 (4%)	2	3
1	B	417/426 (98%)	357 (86%)	43 (10%)	17 (4%)	2	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	835/852 (98%)	709 (85%)	92 (11%)	34 (4%)	2 3

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	974	SER
1	A	1055	ASP
1	A	1145	GLY
1	A	1193	HIS
1	A	1196	GLU

5.3.2 Protein sidechains ⓘ

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%)	360 (93%)	27 (7%)	14 29
1	B	386/390 (99%)	363 (94%)	23 (6%)	17 36
All	All	773/780 (99%)	723 (94%)	50 (6%)	15 32

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	870	ASP
1	B	981	LEU
1	B	1290	SER
1	B	917	ASP
1	B	948	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	902	ASN
1	B	1014	ASN
1	B	1230	GLN

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Mol	Chain	Res	Type
1	B	926	ASN
1	B	975	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, 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%)	-1.63	0 100 100	9, 27, 54, 84	0
1	B	421/426 (98%)	-1.64	0 100 100	11, 28, 55, 76	0
All	All	843/852 (98%)	-1.63	0 100 100	9, 28, 55, 84	0

There are no RSRZ outliers to report.

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.