



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:19 PM UTC

PDB ID : 6ZVN / pdb_00006zvn
Title : Botulinum neurotoxin B2 binding domain in complex with human synaptotagmin I
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Deposited on : 2020-07-25
Resolution : 2.50 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

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

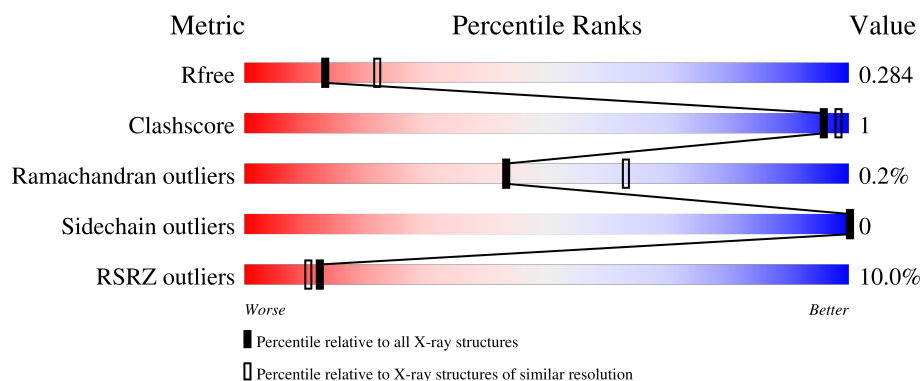
1 Overall quality at a glance

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	AAA	438	9% 89% 8%
2	BBB	21	5% 57% 10% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3603 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 Neurotoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	404	Total	C	N	O	S	0	0	0
			3444	2224	566	647	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	854	SER	-	expression tag	UNP Q8GR96
AAA	855	HIS	-	expression tag	UNP Q8GR96
AAA	856	MET	-	expression tag	UNP Q8GR96

- Molecule 2 is a protein called Synaptotagmin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	14	Total	C	N	O	S	0	0	0
			120	79	20	20	1			

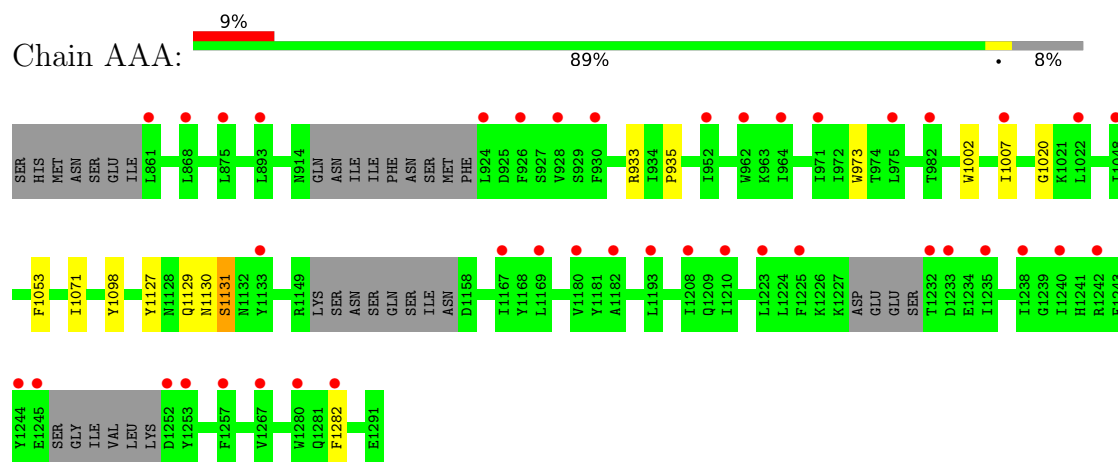
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	39	Total	O	0	0
			39	39		

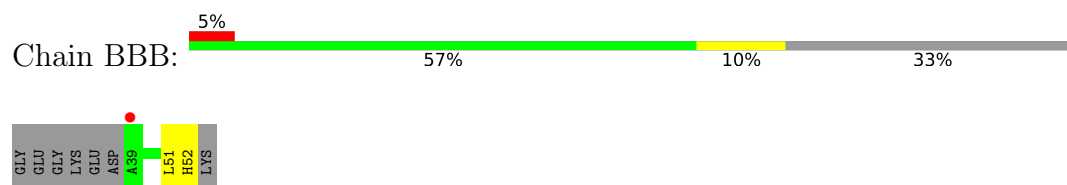
3 Residue-property plots

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: Neurotoxin



• Molecule 2: Synaptotagmin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.68Å 82.53Å 106.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.79 – 2.50 50.79 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.79-2.50) 99.5 (50.79-2.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.259 , 0.283 0.264 , 0.284	Depositor DCC
R_{free} test set	1106 reflections (6.07%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3603	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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	AAA	0.98	0/3524	1.24	0/4748
2	BBB	0.94	0/122	1.67	0/159
All	All	0.98	0/3646	1.25	0/4907

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

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	AAA	3444	0	3344	7	0
2	BBB	120	0	122	1	0
3	AAA	39	0	0	0	0
All	All	3603	0	3466	8	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 1.

All (8) 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:AAA:933:ARG:HD3	1:AAA:1002:TRP:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:1098:TYR:CG	1:AAA:1282:PHE:HB3	2.46	0.50
2:BBB:51:LEU:O	2:BBB:52:HIS:C	2.55	0.50
1:AAA:935:PRO:HG3	1:AAA:1053:PHE:CE2	2.52	0.45
1:AAA:1020:GLY:HA2	1:AAA:1071:ILE:HG22	1.99	0.45
1:AAA:1127:TYR:CZ	1:AAA:1129:GLN:HB2	2.55	0.42
1:AAA:973:TRP:CD2	1:AAA:1007:ILE:HG21	2.56	0.41
1:AAA:1130:ASN:O	1:AAA:1131:SER:C	2.64	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	AAA	394/438 (90%)	376 (95%)	17 (4%)	1 (0%)	36	55
2	BBB	12/21 (57%)	12 (100%)	0	0	100	100
All	All	406/459 (88%)	388 (96%)	17 (4%)	1 (0%)	43	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	1131	SER

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	AAA	379/412 (92%)	379 (100%)	0	100	100
2	BBB	13/18 (72%)	13 (100%)	0	100	100
All	All	392/430 (91%)	392 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	AAA	404/438 (92%)	0.78	41 (10%) 12 10	42, 57, 77, 99	0
2	BBB	14/21 (66%)	0.97	1 (7%) 22 19	64, 73, 78, 81	0
All	All	418/459 (91%)	0.79	42 (10%) 12 10	42, 57, 78, 99	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	1225	PHE	7.4
1	AAA	1223	LEU	6.7
1	AAA	1257	PHE	6.4
1	AAA	861	LEU	5.3
1	AAA	1238	ILE	5.0
1	AAA	1208	ILE	4.7
1	AAA	1210	ILE	4.6
1	AAA	1232	THR	4.3
1	AAA	952	ILE	4.3
1	AAA	924	LEU	4.1
1	AAA	964	ILE	3.9
1	AAA	1235	ILE	3.9
1	AAA	1133	TYR	3.8
1	AAA	1169	LEU	3.7
1	AAA	1182	ALA	3.5
1	AAA	1007	ILE	3.3
1	AAA	962	TRP	3.1
1	AAA	1282	PHE	3.1
1	AAA	1167	ILE	3.0
1	AAA	971	ILE	2.9
1	AAA	1180	VAL	2.9
1	AAA	1244	TYR	2.7
1	AAA	1280	TRP	2.6
1	AAA	1253	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	AAA	975	LEU	2.5
1	AAA	1193	LEU	2.5
1	AAA	875	LEU	2.5
1	AAA	1252	ASP	2.5
1	AAA	1022	LEU	2.5
1	AAA	930	PHE	2.5
1	AAA	1267	VAL	2.4
1	AAA	982	THR	2.4
1	AAA	1048	ILE	2.4
2	BBB	39	ALA	2.2
1	AAA	928	VAL	2.2
1	AAA	893	LEU	2.2
1	AAA	1233	ASP	2.2
1	AAA	1242	ARG	2.2
1	AAA	1240	ILE	2.1
1	AAA	868	LEU	2.1
1	AAA	1245	GLU	2.1
1	AAA	926	PHE	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.