



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3DDB / pdb_00003ddb
Title : Crystal structure of the catalytic domain of Botulinum neurotoxin serotype a with a substrate analog peptide
Authors : Kumaran, D.; Swaminathan, S.
Deposited on : 2008-06-05
Resolution : 1.60 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

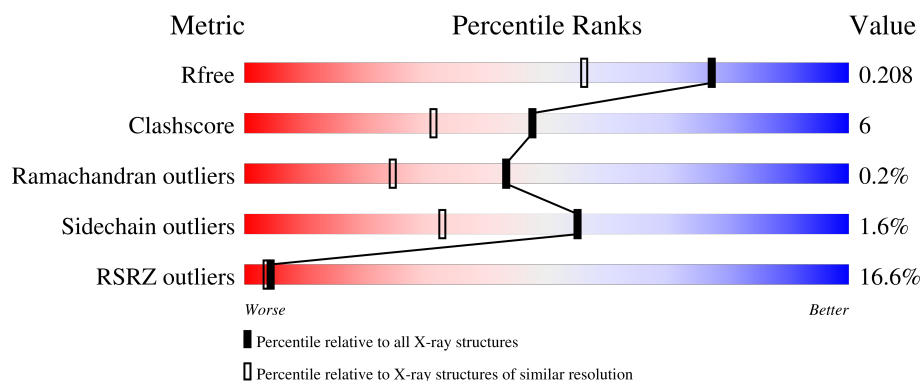
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	430	17% 87% 10% ••
2	B	7	57% 29% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3861 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 A light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3423	2209	559	646	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	425	HIS	-	expression tag	UNP A5HZZ9
A	426	HIS	-	expression tag	UNP A5HZZ9
A	427	HIS	-	expression tag	UNP A5HZZ9
A	428	HIS	-	expression tag	UNP A5HZZ9
A	429	HIS	-	expression tag	UNP A5HZZ9
A	430	HIS	-	expression tag	UNP A5HZZ9

- Molecule 2 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	S	0	0	1
			52	30	14	7	1			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

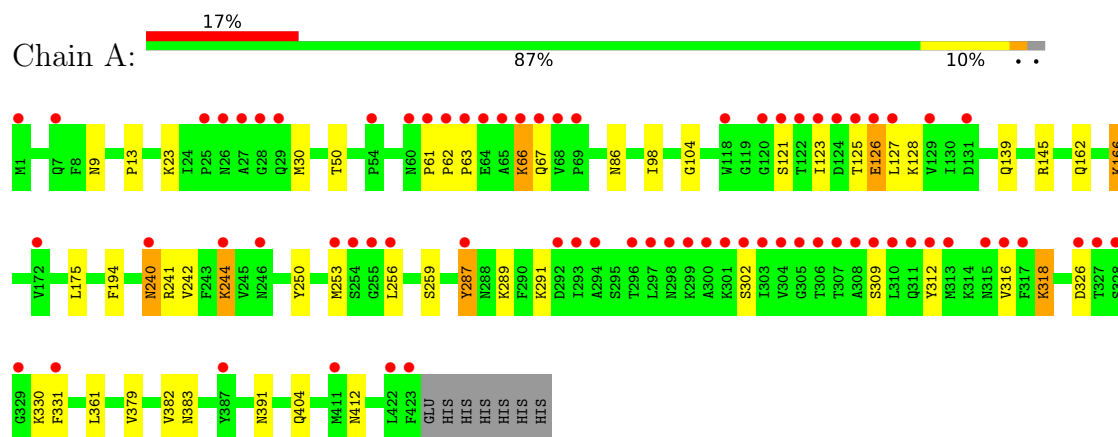
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	372	Total	O	0	0
			372	372		
5	B	3	Total	O	0	0
			3	3		

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 A light chain



- Molecule 2: Synaptosomal-associated protein 25



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.87Å 66.58Å 65.06Å 90.00° 98.34° 90.00°	Depositor
Resolution (Å)	32.42 – 1.60 32.42 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.7 (32.42-1.60) 92.8 (32.42-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.27 (at 1.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.218 0.192 , 0.208	Depositor DCC
R_{free} test set	2672 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å ²)	10.9	Xtriage
Anisotropy	1.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3861	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NH2, SO4

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	0.36	0/3505	0.83	5/4745 (0.1%)
2	B	0.46	0/50	0.95	0/63
All	All	0.36	0/3555	0.83	5/4808 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ASN	N-CA-C	-5.52	100.40	109.40
1	A	175	LEU	N-CA-C	5.42	118.69	111.75
1	A	287	TYR	N-CA-C	-5.30	105.58	111.36
1	A	318	LYS	N-CA-C	-5.17	105.83	111.82
1	A	50	THR	N-CA-C	-5.16	106.30	112.59

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	A	3423	0	3373	37	0
2	B	52	0	59	3	0
3	A	1	0	0	0	0
4	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	372	0	0	7	0
5	B	3	0	0	0	0
All	All	3861	0	3432	39	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 6.

All (39) 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:244:LYS:HE2	1:A:244:LYS:H	1.37	0.90
1:A:139:GLN:NE2	1:A:145:ARG:HD3	1.99	0.77
1:A:312:TYR:O	1:A:316:VAL:HG23	1.87	0.75
1:A:240:ASN:HD22	1:A:241:ARG:N	1.89	0.70
1:A:309:SER:HB2	5:A:661:HOH:O	1.90	0.70
1:A:67:GLN:HA	5:A:622:HOH:O	1.93	0.69
1:A:244:LYS:H	1:A:244:LYS:CE	2.07	0.65
1:A:361:LEU:H	1:A:404:GLN:HE22	1.45	0.63
1:A:13:PRO:HG2	5:A:673:HOH:O	1.99	0.61
1:A:139:GLN:HE21	1:A:145:ARG:HD3	1.65	0.59
1:A:166:LYS:HE3	5:A:800:HOH:O	2.03	0.59
1:A:256:LEU:HD12	2:B:202:MET:HE2	1.86	0.56
1:A:240:ASN:HD22	1:A:240:ASN:C	2.16	0.53
1:A:98:ILE:O	1:A:104:GLY:HA3	2.09	0.53
1:A:123:ILE:HG22	1:A:125:THR:H	1.73	0.51
1:A:23:LYS:HE2	1:A:30:MET:O	2.12	0.50
1:A:121:SER:HA	1:A:128:LYS:HE2	1.93	0.50
1:A:62:PRO:HB3	1:A:63:PRO:HD2	1.95	0.49
1:A:242:VAL:HG12	1:A:259:SER:HA	1.93	0.49
1:A:244:LYS:HE2	1:A:244:LYS:N	2.16	0.47
1:A:383:ASN:CG	1:A:412:ASN:HD21	2.22	0.47
1:A:244:LYS:H	1:A:244:LYS:CD	2.28	0.47
1:A:250:TYR:HA	1:A:253:MET:HE3	1.98	0.46
1:A:326:ASP:OD2	1:A:330:LYS:HB3	2.16	0.46
1:A:86:ASN:ND2	1:A:379:VAL:HG21	2.30	0.46
1:A:287:TYR:CE2	1:A:291:LYS:HD2	2.51	0.46
1:A:240:ASN:C	1:A:240:ASN:ND2	2.74	0.46
1:A:391:ASN:HD21	1:A:404:GLN:HE21	1.65	0.45
2:B:201:LYS:HD2	2:B:201:LYS:HA	1.68	0.43
1:A:63:PRO:HG2	1:A:66:LYS:HB2	2.00	0.43
1:A:382:VAL:HG13	5:A:560:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HA	5:A:582:HOH:O	2.19	0.42
1:A:289:LYS:HE2	5:A:618:HOH:O	2.19	0.42
1:A:62:PRO:CB	1:A:63:PRO:HD2	2.50	0.41
1:A:194:PHE:CD2	1:A:194:PHE:N	2.89	0.41
2:B:197:ARG:HH11	2:B:197:ARG:HG3	1.85	0.41
1:A:126:GLU:HB3	1:A:302:SER:OG	2.21	0.40
1:A:318:LYS:HD2	1:A:331:PHE:HE1	1.85	0.40
1:A:61:PRO:HA	1:A:62:PRO:HD3	1.92	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	A	421/430 (98%)	409 (97%)	11 (3%)	1 (0%)	43	24
2	B	5/7 (71%)	5 (100%)	0	0	100	100
All	All	426/437 (98%)	414 (97%)	11 (3%)	1 (0%)	43	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	LYS

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	378/385 (98%)	373 (99%)	5 (1%)	61	40
2	B	5/5 (100%)	4 (80%)	1 (20%)	1	0
All	All	383/390 (98%)	377 (98%)	6 (2%)	55	33

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	GLU
1	A	162	GLN
1	A	166	LYS
1	A	240	ASN
1	A	244	LYS
2	B	201	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	9	ASN
1	A	60	ASN
1	A	67	GLN
1	A	136	ASN
1	A	139	GLN
1	A	240	ASN
1	A	362	ASN
1	A	404	GLN
1	A	412	ASN

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

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	452	-	4,4,4	0.39	0	6,6,6	0.09	0
4	SO4	A	451	-	4,4,4	0.38	0	6,6,6	0.07	0

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

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	A	423/430 (98%)	0.54	71 (16%) 4 3	10, 18, 45, 53	0
2	B	6/7 (85%)	0.99	0 100 100	20, 29, 33, 35	0
All	All	429/437 (98%)	0.54	71 (16%) 4 4	10, 18, 45, 53	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	VAL	6.8
1	A	27	ALA	5.7
1	A	123	ILE	5.6
1	A	63	PRO	5.5
1	A	125	THR	5.2
1	A	307	THR	5.0
1	A	62	PRO	4.6
1	A	316	VAL	4.5
1	A	124	ASP	4.2
1	A	65	ALA	4.2
1	A	304	VAL	4.2
1	A	122	THR	4.1
1	A	303	ILE	3.9
1	A	301	LYS	3.8
1	A	61	PRO	3.8
1	A	26	ASN	3.6
1	A	244	LYS	3.5
1	A	300	ALA	3.5
1	A	310	LEU	3.5
1	A	302	SER	3.5
1	A	327	THR	3.3
1	A	126	GLU	3.2
1	A	328	SER	3.2
1	A	329	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	312	TYR	3.1
1	A	67	GLN	3.1
1	A	66	LYS	3.0
1	A	308	ALA	3.0
1	A	422	LEU	3.0
1	A	28	GLY	3.0
1	A	315	ASN	2.9
1	A	69	PRO	2.9
1	A	7	GLN	2.9
1	A	298	ASN	2.9
1	A	311	GLN	2.9
1	A	309	SER	2.8
1	A	1	MET	2.7
1	A	294	ALA	2.7
1	A	129	VAL	2.7
1	A	423	PHE	2.7
1	A	127	LEU	2.7
1	A	411	MET	2.7
1	A	387	TYR	2.6
1	A	246	ASN	2.6
1	A	306	THR	2.5
1	A	172	VAL	2.5
1	A	121	SER	2.5
1	A	240	ASN	2.5
1	A	296	THR	2.4
1	A	299	LYS	2.4
1	A	118	TRP	2.4
1	A	120	GLY	2.4
1	A	297	LEU	2.4
1	A	326	ASP	2.4
1	A	256	LEU	2.4
1	A	313	MET	2.4
1	A	60	ASN	2.3
1	A	292	ASP	2.3
1	A	331	PHE	2.3
1	A	64	GLU	2.3
1	A	317	PHE	2.2
1	A	287	TYR	2.2
1	A	29	GLN	2.2
1	A	253	MET	2.1
1	A	25	PRO	2.1
1	A	293	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	305	GLY	2.0
1	A	254	SER	2.0
1	A	54	PRO	2.0
1	A	255	GLY	2.0
1	A	131	ASP	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](#)

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, 95th 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
4	SO4	A	452	5/5	0.67	0.20	39,43,46,47	0
4	SO4	A	451	5/5	0.87	0.11	43,43,44,45	0
3	ZN	A	450	1/1	1.00	0.07	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.