



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 06:46 pm GMT

PDB ID : 3DDA
Title : Crystal structure of the catalytic domain of Botulinum neurotoxin serotype a with a snap-25 peptide
Authors : Kumaran, D.; Swaminathan, S.
Deposited on : 2008-06-05
Resolution : 1.50 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 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 : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

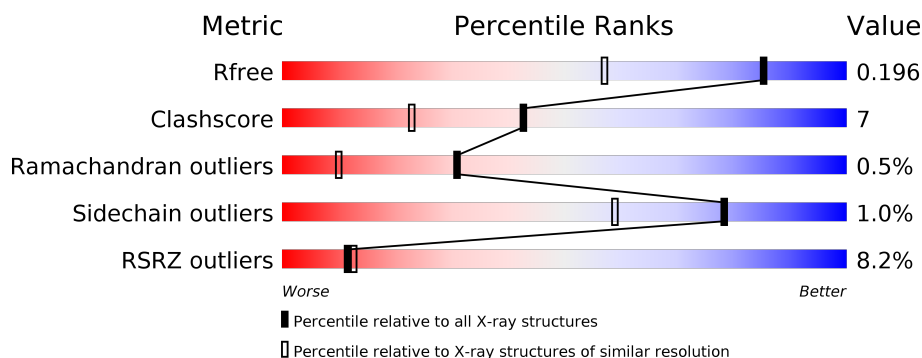
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	111664	2534 (1.50-1.50)
Clashscore	122126	2727 (1.50-1.50)
Ramachandran outliers	120053	2661 (1.50-1.50)
Sidechain outliers	120020	2659 (1.50-1.50)
RSRZ outliers	108989	2481 (1.50-1.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
2	B	7	<div> <div>43%</div> <div> <div>43%</div> <div>29%</div> <div>29%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3854 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
			50	29	12	8	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

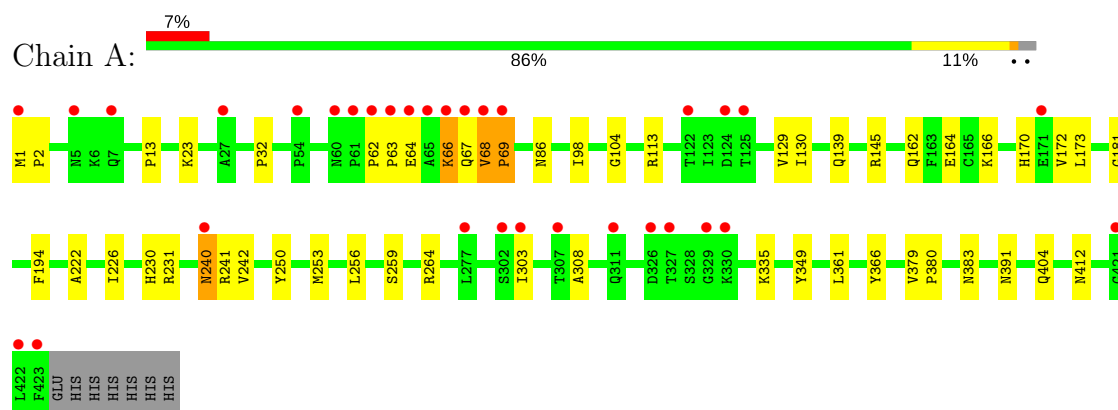
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	371	Total	O	0	0
			371	371		
5	B	4	Total	O	0	0
			4	4		

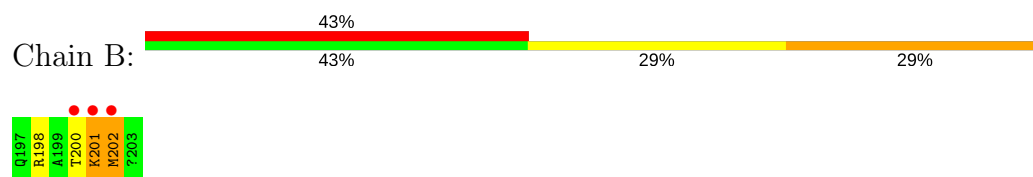
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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	49.14Å 66.19Å 64.82Å 90.00° 99.09° 90.00°	Depositor
Resolution (Å)	39.14 – 1.50 48.53 – 1.49	Depositor EDS
% Data completeness (in resolution range)	95.7 (39.14-1.50) 95.2 (48.53-1.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 1.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.200 0.178 , 0.196	Depositor DCC
R_{free} test set	3193 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3854	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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, SO4, NH2

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	0.31	0/3505	0.58	0/4745
2	B	0.54	0/48	0.76	0/61
All	All	0.32	0/3553	0.58	0/4806

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	A	3423	0	3373	49	0
2	B	50	0	54	5	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	371	0	0	3	0
5	B	4	0	0	0	0
All	All	3854	0	3427	51	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 7.

All (51) 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:226:ILE:HD12	1:A:349:TYR:HB3	1.58	0.85
1:A:66:LYS:HG3	1:A:66:LYS:O	1.75	0.84
1:A:240:ASN:HD22	1:A:241:ARG:N	1.82	0.77
1:A:226:ILE:CD1	1:A:349:TYR:HB3	2.17	0.74
1:A:361:LEU:H	1:A:404:GLN:HE22	1.37	0.71
1:A:139:GLN:NE2	1:A:145:ARG:HD3	2.10	0.67
1:A:68:VAL:HG23	1:A:69:PRO:N	2.08	0.66
1:A:1:MET:N	1:A:2:PRO:HD2	2.12	0.64
2:B:200:THR:O	2:B:201:LYS:HB2	1.99	0.62
1:A:13:PRO:HG2	5:A:770:HOH:O	2.01	0.59
1:A:194:PHE:CE2	2:B:198:ARG:HD2	2.38	0.59
1:A:139:GLN:HE21	1:A:145:ARG:HD3	1.67	0.58
1:A:68:VAL:HB	1:A:69:PRO:HD2	1.86	0.58
1:A:226:ILE:HD12	1:A:349:TYR:CB	2.33	0.57
1:A:63:PRO:HG2	1:A:66:LYS:HB3	1.86	0.56
1:A:62:PRO:HB2	1:A:66:LYS:HG2	1.89	0.55
2:B:200:THR:O	2:B:201:LYS:CB	2.55	0.54
1:A:391:ASN:HD21	1:A:404:GLN:HE21	1.57	0.53
1:A:86:ASN:ND2	1:A:379:VAL:HG21	2.24	0.52
1:A:222:ALA:O	1:A:226:ILE:HG12	2.10	0.51
1:A:240:ASN:ND2	1:A:241:ARG:N	2.57	0.51
1:A:366:TYR:CE2	2:B:200:THR:HG22	2.46	0.50
1:A:230:HIS:CE1	1:A:264:ARG:HD3	2.46	0.50
1:A:256:LEU:HD21	2:B:202:MET:SD	2.52	0.50
1:A:240:ASN:HD22	1:A:241:ARG:H	1.56	0.49
1:A:23:LYS:HE3	1:A:32:PRO:HG3	1.94	0.49
1:A:170:HIS:HD2	1:A:173:LEU:H	1.61	0.49
1:A:68:VAL:CB	1:A:69:PRO:HD2	2.44	0.48
1:A:240:ASN:HD22	1:A:240:ASN:C	2.17	0.48
1:A:1:MET:H3	1:A:2:PRO:HD2	1.77	0.47
1:A:98:ILE:O	1:A:104:GLY:HA3	2.15	0.47
1:A:1:MET:N	1:A:2:PRO:CD	2.77	0.46
1:A:303:ILE:HD13	1:A:308:ALA:O	2.16	0.46
1:A:240:ASN:ND2	1:A:241:ARG:HG2	2.31	0.46
1:A:383:ASN:CG	1:A:412:ASN:HD21	2.18	0.46
1:A:162:GLN:HG2	5:A:615:HOH:O	2.16	0.46
1:A:129:VAL:HG22	1:A:130:ILE:N	2.32	0.45
1:A:64:GLU:HA	1:A:67:GLN:NE2	2.32	0.45
1:A:62:PRO:HB3	1:A:63:PRO:HD2	1.99	0.44
1:A:66:LYS:HE2	1:A:66:LYS:HB2	1.88	0.44
1:A:181:GLY:HA2	1:A:231:ARG:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:TYR:HA	1:A:253:MET:HG2	2.00	0.44
1:A:242:VAL:HG12	1:A:259:SER:HA	2.00	0.43
1:A:164:GLU:OE1	1:A:166:LYS:HE2	2.19	0.43
1:A:240:ASN:C	1:A:240:ASN:ND2	2.72	0.42
1:A:170:HIS:CD2	1:A:173:LEU:H	2.36	0.42
1:A:335:LYS:HD2	5:A:800:HOH:O	2.19	0.42
1:A:113:ARG:HG2	1:A:113:ARG:HH11	1.85	0.41
1:A:170:HIS:CD2	1:A:172:VAL:H	2.38	0.41
1:A:379:VAL:HB	1:A:380:PRO:HD3	2.03	0.40
1:A:68:VAL:HG23	1:A:69:PRO:CD	2.51	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%)	49	24
2	B	5/7 (71%)	4 (80%)	0	1 (20%)	0	0
All	All	426/437 (98%)	413 (97%)	11 (3%)	2 (0%)	31	10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	201	LYS
1	A	69	PRO

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%)	375 (99%)	3 (1%)	83	68
2	B	5/5 (100%)	4 (80%)	1 (20%)	1	0
All	All	383/390 (98%)	379 (99%)	4 (1%)	78	59

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	A	68	VAL
1	A	240	ASN
2	B	202	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	86	ASN
1	A	139	GLN
1	A	170	HIS
1	A	174	ASN
1	A	240	ASN
1	A	269	HIS
1	A	278	GLN
1	A	311	GLN
1	A	362	ASN
1	A	404	GLN
1	A	410	ASN
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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	451	-	4,4,4	0.33	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	451	-	-	0/0/0/0	0/0/0/0

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 [i](#)

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%)	0.29	32 (7%) 14 15	6, 12, 31, 49	0
2	B	6/7 (85%)	3.79	3 (50%) 0 0	21, 26, 40, 43	0
All	All	429/437 (98%)	0.34	35 (8%) 11 13	6, 13, 32, 49	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	ALA	10.4
1	A	63	PRO	10.3
1	A	62	PRO	9.3
2	B	201	LYS	8.3
2	B	202	MET	8.0
1	A	67	GLN	7.6
1	A	68	VAL	7.6
1	A	327	THR	6.9
1	A	27	ALA	6.0
1	A	64	GLU	5.6
1	A	60	ASN	4.9
1	A	69	PRO	4.7
1	A	277	LEU	4.5
1	A	61	PRO	4.3
1	A	66	LYS	4.2
1	A	422	LEU	3.6
1	A	124	ASP	3.1
1	A	7	GLN	3.0
1	A	1	MET	3.0
1	A	5	ASN	3.0
2	B	200	THR	3.0
1	A	171	GLU	2.9
1	A	421	GLY	2.4
1	A	307	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	122	THR	2.3
1	A	329	GLY	2.3
1	A	240	ASN	2.3
1	A	423	PHE	2.2
1	A	311	GLN	2.2
1	A	330	LYS	2.2
1	A	54	PRO	2.1
1	A	303	ILE	2.1
1	A	125	THR	2.0
1	A	326	ASP	2.0
1	A	302	SER	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 carbohydrates 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(\AA^2)	Q<0.9
4	SO4	A	451	5/5	0.93	0.12	40,42,42,42	0
3	ZN	A	450	1/1	1.00	0.04	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.