



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 09:11 AM GMT

PDB ID : 3K3Q
Title : Crystal Structure of a Llama Antibody complexed with the C. Botulinum Neurotoxin Serotype A Catalytic Domain
Authors : Thompson, A.A.; Dong, J.; Marks, J.D.; Stevens, R.C.
Deposited on : 2009-10-04
Resolution : 2.60 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

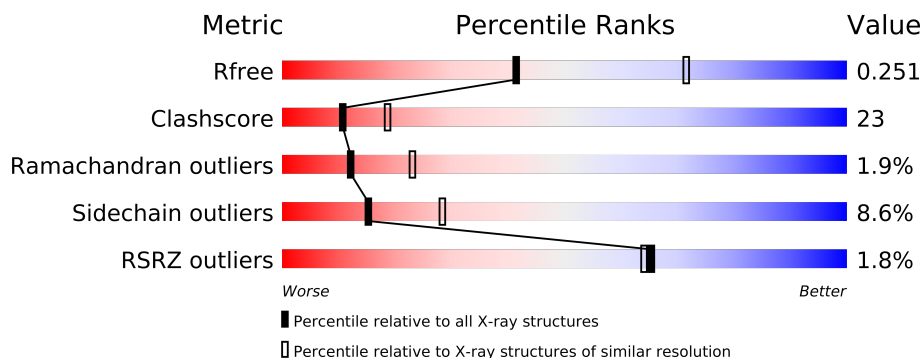
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	151	
2	B	252	
3	C	175	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4358 atoms, of which 0 are hydrogen and 0 are deuterium.

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 llama Aa1 VHH domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1016	628	180	202	6			

- Molecule 2 is a protein called Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1904	1221	317	362	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	EXPRESSION TAG	UNP A5HZZ9
B	0	ALA	-	EXPRESSION TAG	UNP A5HZZ9
B	1	VAL	-	EXPRESSION TAG	UNP A5HZZ9
B	2	GLN	-	EXPRESSION TAG	UNP A5HZZ9
B	27	VAL	ALA	SEE REMARK 999	UNP A5HZZ9

- Molecule 3 is a protein called Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	165	Total	C	N	O	S	0	0	0
			1367	887	221	255	4			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total 12	O 12	0	0
5	B	35	Total 35	O 35	0	0
5	C	23	Total 23	O 23	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.28Å 48.76Å 103.64Å 90.00° 116.75° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 38.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.4 (40.00-2.60) 90.5 (38.99-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.256 0.215 , 0.251	Depositor DCC
R_{free} test set	1029 reflections (4.84%)	DCC
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.763	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 20.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 22641 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4358	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.45	0/1035	0.68	1/1403 (0.1%)
2	B	0.52	0/1952	0.75	3/2652 (0.1%)
3	C	0.46	0/1394	0.61	0/1870
All	All	0.48	0/4381	0.69	4/5925 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	ASN	CB-CA-C	-5.55	99.30	110.40
2	B	248	ASN	N-CA-C	-5.43	96.34	111.00
1	A	78	LEU	N-CA-C	5.38	125.51	111.00
2	B	59	LEU	CA-CB-CG	-5.36	102.98	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1016	0	967	76	0
2	B	1904	0	1858	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1367	0	1366	68	0
4	B	1	0	0	0	0
5	A	12	0	0	4	0
5	B	35	0	0	5	0
5	C	23	0	0	4	0
All	All	4358	0	4191	194	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

The worst 5 of 194 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:66:LYS:H	2:B:66:LYS:HD2	1.14	1.05
1:A:22:ARG:NH1	1:A:96:GLN:HE21	1.59	1.00
1:A:69:THR:HG22	1:A:70:ASP:H	1.30	0.97
3:C:307:THR:HG23	3:C:308:ALA:H	1.33	0.94
3:C:307:THR:HG23	3:C:308:ALA:N	1.83	0.91

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	135/151 (89%)	111 (82%)	20 (15%)	4 (3%)	7	10
2	B	234/252 (93%)	210 (90%)	19 (8%)	5 (2%)	11	19
3	C	163/175 (93%)	145 (89%)	17 (10%)	1 (1%)	33	63
All	All	532/578 (92%)	466 (88%)	56 (10%)	10 (2%)	12	23

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	GLU

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Mol	Chain	Res	Type
3	C	307	THR
1	A	35	GLY
2	B	67	GLN
1	A	90	ALA

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	103/114 (90%)	90 (87%)	13 (13%)	7	12
2	B	211/222 (95%)	195 (92%)	16 (8%)	19	36
3	C	151/160 (94%)	140 (93%)	11 (7%)	20	38
All	All	465/496 (94%)	425 (91%)	40 (9%)	15	28

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	115	ILE
2	B	144	TYR
3	C	313	MET
2	B	124	ASP
2	B	146	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	162	GLN
3	C	278	GLN
3	C	311	GLN
2	B	139	GLN
3	C	288	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

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	137/151 (90%)	0.25	5 (3%) 41 37	31, 55, 85, 90	0
2	B	238/252 (94%)	-0.18	3 (1%) 74 75	13, 34, 73, 86	0
3	C	165/175 (94%)	-0.26	2 (1%) 75 77	15, 37, 56, 71	0
All	All	540/578 (93%)	-0.09	10 (1%) 65 61	13, 39, 77, 90	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	VAL	3.7
2	B	64	GLU	3.3
2	B	198	GLU	2.7
1	A	103	ASP	2.5
2	B	199	SER	2.5

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ZN	B	251	1/1	0.07	-2.97	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.