

# wwPDB X-ray Structure Validation Summary Report (i)

#### Mar 11, 2024 – 08:07 PM EDT

PDB ID : 8SXP

Title : Crystal structure of long neurotoxin from the venom of the king cobra (3FTx-

L15) in complex with Fab of broadly neutralizing antibody 95Mat5

Authors : Nguyen, T.K.Y.

Deposited on : 2023-05-23

Resolution : 2.90 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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467 Xtriage (Phenix): 1.13

EDS: 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

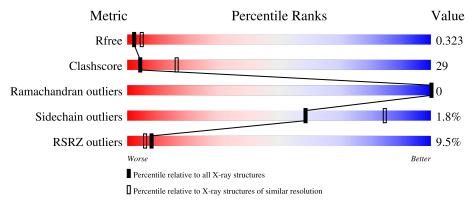
Validation Pipeline (wwPDB-VP) : 2.36

### 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.90 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 $(\# \mathrm{Entries})$	Similar resolution $(\#\text{Entries, resolution range}(\mathring{\mathbf{A}}))$
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	T.	212	6% 65%	33%				
1	L	212			•			
2	С	68	49%	46%	6%			
		220	14%					
3	Н	228	72%	27%				



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3830 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 95Mat5 Fab light chain.

$\mathbf{Mol}$	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	L	212	Total 1629	C 1018	N 271	O 335	S 5	0	0	0

• Molecule 2 is a protein called Long neurotoxin 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	С	68	Total	С	N	О	S	0	0	0
2		00	503	307	85	101	10	U	0	

• Molecule 3 is a protein called 95Mat5 Fab heavy chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	Н	227	Total 1695	C 1076	N 278	O 335	S 6	0	0	0

• Molecule 4 is water.

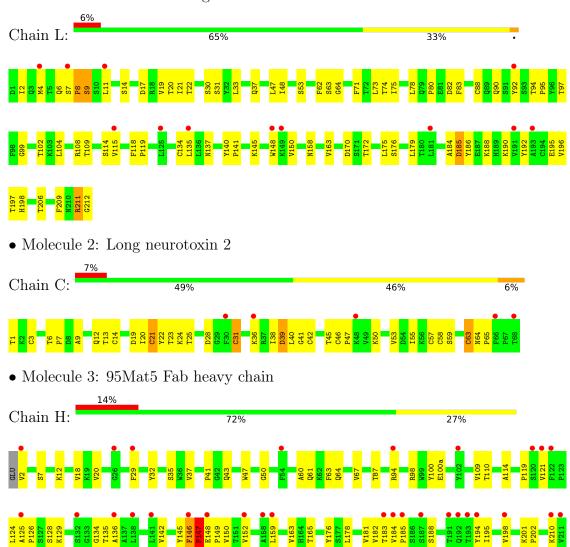
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	Total O 1 1	0	0
4	Н	2	Total O 2 2	0	0



## 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: 95Mat5 Fab light chain





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	135.86Å 42.44Å 103.36Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 103.70° 90.00°	Depositor
Resolution (Å)	45.49 - 2.90	Depositor
Resolution (A)	45.49 - 2.90	EDS
% Data completeness	82.1 (45.49-2.90)	Depositor
(in resolution range)	82.2 (45.49-2.90)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.73 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
P. P.	0.261 , 0.320	Depositor
$R, R_{free}$	0.289 , $0.323$	DCC
$R_{free}$ test set	534 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.1	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.29, 52.7	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	3830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	L	0.61	0/1664	0.84	$2/2259 \ (0.1\%)$	
2	С	0.61	0/514	1.34	5/699~(0.7%)	
3	Н	0.68	1/1739 (0.1%)	0.82	3/2371 (0.1%)	
All	All	0.64	1/3917 (0.0%)	0.91	$10/5329 \ (0.2\%)$	

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	Н	0	1

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
3	Н	147	PRO	N-CD	9.95	1.61	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	С	21	CYS	CB-CA-C	-19.29	71.81	110.40
1	L	9	SER	N-CA-CB	-13.12	90.81	110.50
2	С	31	CYS	N-CA-C	-11.00	81.30	111.00
1	L	8	PRO	CB-CA-C	-10.65	85.38	112.00
2	С	31	CYS	N-CA-CB	7.49	124.09	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	ol Chain R		Type	Group	
3	Н	98	ARG	Sidechain	



### 5.2 Too-close contacts (i)

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	L	1629	0	1580	72	0
2	С	503	0	478	61	0
3	Н	1695	0	1657	76	0
4	С	1	0	0	1	0
4	Н	2	0	0	2	0
All	All	3830	0	3715	203	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 203 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
2:C:25:THR:CB	2:C:36:LYS:HD2	1.62	1.27
3:H:184:VAL:HG12	3:H:185:PRO:CD	1.66	1.25
2:C:6:THR:CG2	2:C:40:LEU:H	1.51	1.23
3:H:184:VAL:CG1	3:H:185:PRO:CD	2.22	1.17
3:H:184:VAL:CG1	3:H:185:PRO:HD2	1.75	1.15

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	L	210/212 (99%)	196 (93%)	14 (7%)	0	100 100

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	$_{ m ntiles}$
2	С	$66/68 \; (97\%)$	59 (89%)	7 (11%)	0	100	100
3	Н	$225/228 \ (99\%)$	207 (92%)	18 (8%)	0	100	100
All	All	501/508 (99%)	462 (92%)	39 (8%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	Perce	$_{ m ntiles}$
1	L	188/188 (100%)	186 (99%)	2 (1%)	73	92
2	С	60/60 (100%)	57 (95%)	3 (5%)	24	57
3	Н	189/190 (100%)	186 (98%)	3 (2%)	62	86
All	All	437/438 (100%)	429 (98%)	8 (2%)	59	85

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Н	147	PRO
3	Н	100(a)	GLU
2	С	63	CYS
2	С	39	ASP
3	Н	29	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	124	GLN
1	L	137	ASN
2	С	64	ASN
3	Н	58	ASN
3	Н	164	HIS



#### 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 monosaccharides 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,  $95^{th}$  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>	$\# \mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	L	$212/212 \ (100\%)$	0.63	12 (5%) 23 19	30, 81, 129, 164	0
2	С	68/68 (100%)	0.34	5 (7%) 14 11	30, 119, 144, 147	0
3	Н	227/228 (99%)	0.78	31 (13%) 3 2	30, 82, 155, 220	0
All	All	507/508 (99%)	0.66	48 (9%) 8 6	30, 86, 143, 220	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Н	29	PHE	6.1
3	Н	125	ALA	5.9
1	L	149	LYS	5.3
1	L	148	TRP	4.8
3	Н	184	VAL	4.7

### 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 monosaccharides 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.

