wwPDB X-ray Structure Validation Summary Report (i)

Jan 20, 2025 – 02:03 PM EST

PDB ID	:	8V13
Title	:	Crystal structure of Black mamba toxin in complex with Centi-SNX-B03 antibody
Authors	:	Pletnev, S.; Glanville, J.; Kwong, P.D.
Deposited on	:	2023-11-19
Resolution	:	1.80 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:

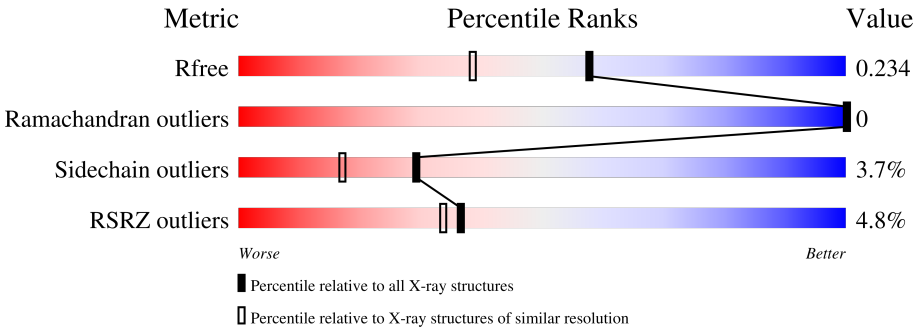
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 1.80 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}	164625	7108 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	H	230	6% 97%
1	h	230	3% 92%
2	L	215	2% 95%
2	l	215	% 96%
3	T	60	23% 85% 15%
3	t	60	10% 95% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8271 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 Centi-SNX-B03 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	229	Total	C	N	O	S	0	0	0
			1692	1061	284	340	7			
1	h	220	Total	C	N	O	S	0	0	0
			1619	1013	273	326	7			

- Molecule 2 is a protein called Centi-SNX-B03 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1571	979	267	321	4			
2	l	211	Total	C	N	O	S	0	0	0
			1571	979	267	321	4			

- Molecule 3 is a protein called Short neurotoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	60	Total	C	N	O	S	0	0	0
			478	289	93	88	8			
3	t	60	Total	C	N	O	S	0	0	0
			478	289	93	88	8			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Na	0	0
			1	1		
4	l	1	Total	Na	0	0
			1	1		

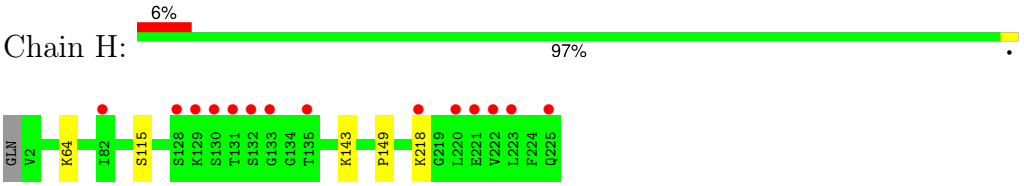
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	200	Total O 200 200	0	0
5	L	212	Total O 212 212	0	0
5	T	35	Total O 35 35	0	0
5	h	170	Total O 170 170	0	0
5	l	211	Total O 211 211	0	0
5	t	32	Total O 32 32	0	0

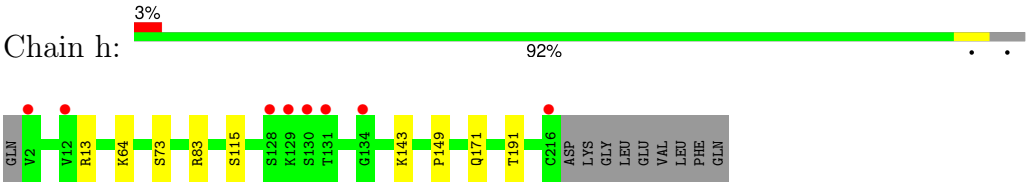
3 Residue-property plots (i)

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.

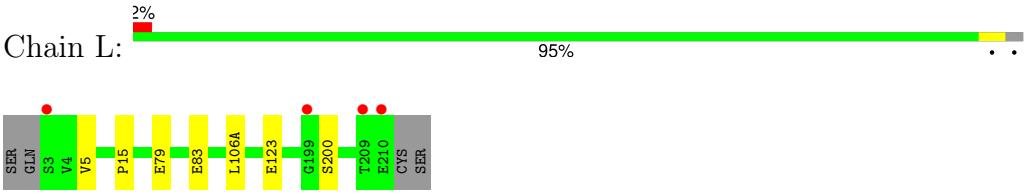
• Molecule 1: Centi-SNX-B03 Fab heavy chain



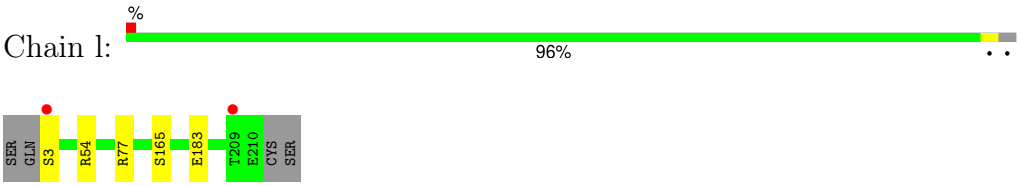
• Molecule 1: Centi-SNX-B03 Fab heavy chain



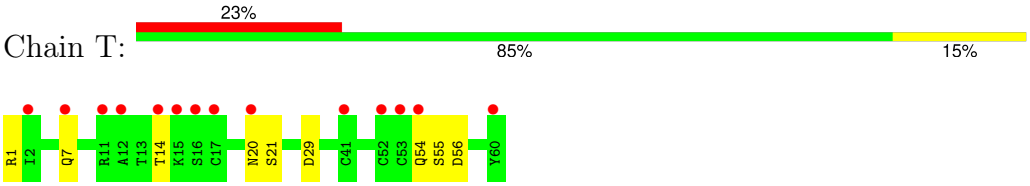
• Molecule 2: Centi-SNX-B03 Fab light chain



• Molecule 2: Centi-SNX-B03 Fab light chain

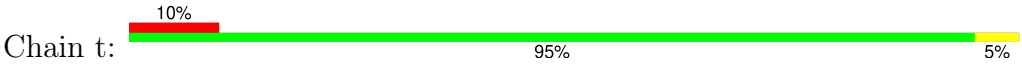


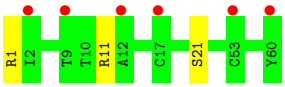
• Molecule 3: Short neurotoxin 1



• Molecule 3: Short neurotoxin 1

Chain t:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.54Å 72.25Å 179.66Å 90.00° 91.99° 90.00°	Depositor
Resolution (Å)	30.01 – 1.80 30.01 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.01-1.80) 98.6 (30.01-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.181 , 0.229 0.190 , 0.234	Depositor DCC
R_{free} test set	1172 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8271	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4733e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] 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.

5 Model quality

5.1 Standard geometry

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

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	H	0.80	0/1729	0.90	0/2350
1	h	0.78	0/1655	0.91	0/2251
2	L	0.83	1/1609 (0.1%)	0.94	1/2201 (0.0%)
2	l	0.77	1/1609 (0.1%)	0.91	4/2201 (0.2%)
3	T	0.66	0/488	0.92	1/654 (0.2%)
3	t	0.69	0/488	0.91	0/654
All	All	0.78	2/7578 (0.0%)	0.92	6/10311 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	165	SER	CB-OG	5.36	1.49	1.42
2	L	83	GLU	CD-OE2	5.26	1.31	1.25

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	l	77	ARG	NE-CZ-NH1	7.27	123.93	120.30
2	l	77	ARG	NE-CZ-NH2	-6.83	116.89	120.30
3	T	29	ASP	CB-CA-C	6.03	122.46	110.40
2	l	54	ARG	NE-CZ-NH2	-5.83	117.39	120.30
2	l	54	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	106(A)	LEU	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	H	227/230 (99%)	224 (99%)	3 (1%)	0	100	100
1	h	218/230 (95%)	212 (97%)	6 (3%)	0	100	100
2	L	209/215 (97%)	206 (99%)	3 (1%)	0	100	100
2	l	209/215 (97%)	204 (98%)	5 (2%)	0	100	100
3	T	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
3	t	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
All	All	979/1010 (97%)	954 (97%)	25 (3%)	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	Percentiles
1	H	190/191 (100%)	185 (97%)	5 (3%)	41 29
1	h	182/191 (95%)	173 (95%)	9 (5%)	21 9
2	L	177/181 (98%)	173 (98%)	4 (2%)	45 34
2	l	177/181 (98%)	175 (99%)	2 (1%)	70 65
3	T	54/54 (100%)	46 (85%)	8 (15%)	2 0
3	t	54/54 (100%)	51 (94%)	3 (6%)	17 7
All	All	834/852 (98%)	803 (96%)	31 (4%)	29 17

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	T	54	GLN
2	l	183	GLU
1	h	13	ARG
3	t	11	ARG
1	h	171	GLN

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

Mol	Chain	Res	Type
2	L	26	ASN
2	L	126	GLN
3	T	54	GLN
1	h	199	ASN
2	l	94	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are 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.

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 (i)

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, 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>2			OWAB(Å^2)	Q<0.9
1	H	229/230 (99%)	0.20	14 (6%)	28	26	22, 33, 65, 117	0
1	h	220/230 (95%)	0.26	8 (3%)	46	44	22, 36, 62, 114	0
2	L	211/215 (98%)	-0.21	4 (1%)	66	64	17, 26, 47, 84	0
2	l	211/215 (98%)	-0.09	2 (0%)	81	80	20, 30, 61, 113	0
3	T	60/60 (100%)	1.01	14 (23%)	2	2	25, 60, 94, 100	0
3	t	60/60 (100%)	0.83	6 (10%)	14	11	23, 57, 79, 99	0
All	All	991/1010 (98%)	0.15	48 (4%)	36	34	17, 32, 75, 117	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	129	LYS	7.0
1	H	131	THR	5.6
1	H	130	SER	4.5
3	T	2	ILE	4.4
3	T	60	TYR	4.4

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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(Å^2)	Q<0.9
4	NA	l	301	1/1	0.97	0.05	27,27,27,27	0
4	NA	L	301	1/1	0.98	0.05	25,25,25,25	0

6.5 Other polymers

There are no such residues in this entry.