



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:51 PM GMT

PDB ID : 1CTX
Title : THREE-DIMENSIONAL STRUCTURE OF THE-LONG-NEUROTOXIN
FROM COBRA VENOM
Authors : Saenger, W.; Walkinshaw, M.D.
Deposited on : 1982-04-08
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

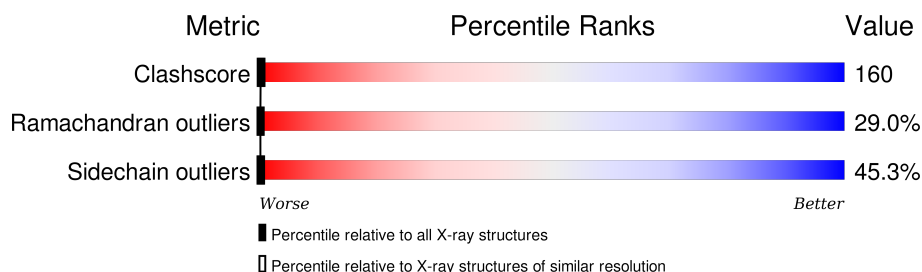
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	71	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 541 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 ALPHA-COBRATOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	71	541	332	98	101	10	0	0	0

Note EDS was not executed.

- Molecule 1: ALPHA-COBRATOXIN

M61	I1
C62	R2
N63	C3
P64	F4
F65	I5
P66	T6
T67	P7
R68	D8
K69	I9
R70	T10
P71	S11
	K12
	D13
	C14
	P15
	N16
	G17
	H18
	V19
	C20
	Y21
	T22
	K23
	T24
	W25
	C26
	D27
	A28
	F29
	C30
	S31
	I32
	R33
	G34
	K35
	R36
	V37
	D38
	L39
	G40
	C41
	A42
	A43
	T44
	C45
	P46
	T47
	V48
	R49
	T50
	B51
	V52
	D53
	I54
	P55
	C56
	C57
	S58
	T59
	R60

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	74.60 Å 74.60 Å 42.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	541	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

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	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	3.45	20/553 (3.6%)	2.20	27/750 (3.6%)

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
1	A	1	1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	PRO	C-OXT	46.91	2.12	1.23
1	A	14	CYS	CB-SG	34.48	2.40	1.82
1	A	14	CYS	CA-CB	-22.04	1.05	1.53
1	A	3	CYS	N-CA	16.55	1.79	1.46
1	A	51	GLY	N-CA	9.13	1.59	1.46

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	CYS	CB-CA-C	18.34	147.07	110.40
1	A	14	CYS	N-CA-CB	-11.74	89.47	110.60
1	A	49	LYS	O-C-N	10.84	140.04	122.70
1	A	33	ARG	NE-CZ-NH2	9.50	125.05	120.30
1	A	60	ASP	CB-CG-OD2	8.41	125.87	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	14	CYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	CYS	Mainchain

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	541	0	524	170	10
All	All	541	0	524	170	10

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 160.

The worst 5 of 170 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:1:ILE:CD1	1:A:19:VAL:N	1.69	1.52
1:A:3:CYS:CA	1:A:3:CYS:N	1.79	1.46
1:A:50:THR:CG2	1:A:51:GLY:H	1.54	1.19
1:A:4:PHE:HB2	1:A:63:ASN:HB3	1.27	1.15
1:A:63:ASN:H	1:A:64:PRO:HD3	1.02	1.14

The worst 5 of 10 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:THR:CG2	1:A:28:ALA:N[5_565]	0.54	1.66
1:A:53:ASP:OD1	1:A:55:GLN:OE1[7_555]	1.30	0.90
1:A:71:PRO:O	1:A:71:PRO:O[7_555]	1.43	0.77
1:A:10:THR:CG2	1:A:27:ASP:C[5_565]	1.46	0.74
1:A:54:ILE:O	1:A:55:GLN:CG[7_555]	1.51	0.69

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	69/71 (97%)	33 (48%)	16 (23%)	20 (29%)	0 0

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	8	ASP
1	A	12	LYS
1	A	13	ASP
1	A	28	ALA

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	64/64 (100%)	35 (55%)	29 (45%)	0 0

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	41	CYS
1	A	61	ASN
1	A	37	VAL
1	A	44	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	55	GLN

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 carbohydrates 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](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.