



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:03 AM UTC

PDB ID : 2CB6 / pdb_00002cb6
Title : Crystal structure of the catalytic domain of the mosquitocidal toxin from *Bacillus sphaericus*, mutant E195Q
Authors : Reinert, D.J.; Carpusca, I.; Aktories, K.; Schulz, G.E.
Deposited on : 2005-12-29
Resolution : 3.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

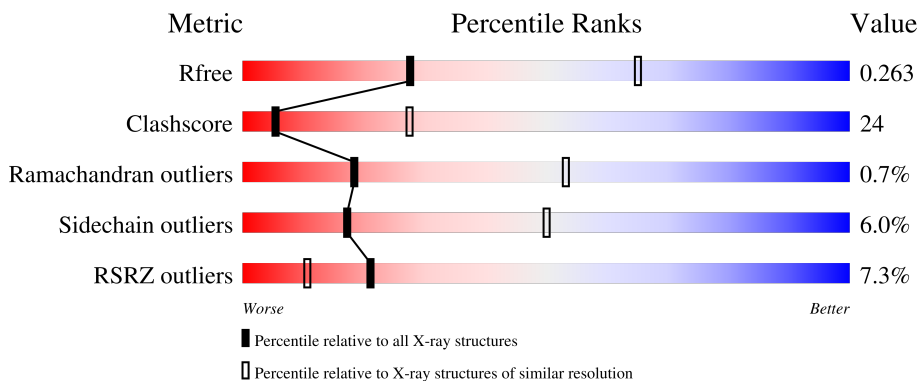
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



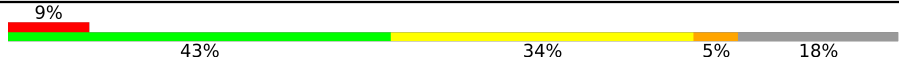
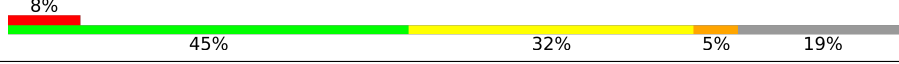
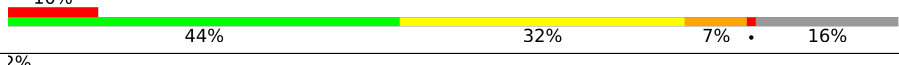
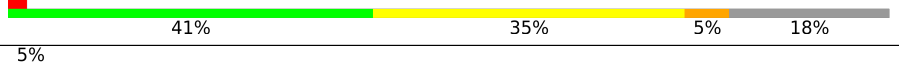
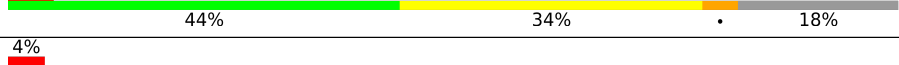

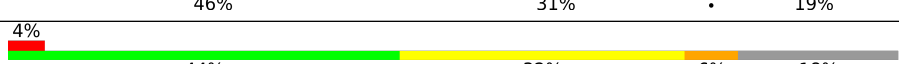
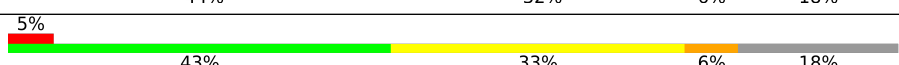



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	291	
1	B	291	
1	C	291	
1	D	291	
1	E	291	

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Mol	Chain	Length	Quality of chain
1	F	291	
1	G	291	
1	H	291	
1	I	291	
1	J	291	
1	K	291	
1	L	291	
1	M	291	
1	N	291	
1	O	291	
1	P	291	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31202 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 MOSQUITOCIDAL TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	B	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	C	244	Total 1986	C 1252	N 353	O 378	S 3	0	0	0
1	D	244	Total 1986	C 1252	N 353	O 378	S 3	0	0	0
1	E	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	F	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	G	236	Total 1918	C 1210	N 338	O 367	S 3	0	0	0
1	H	245	Total 1992	C 1255	N 354	O 380	S 3	0	0	0
1	I	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	J	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	K	244	Total 1986	C 1252	N 353	O 378	S 3	0	0	0
1	L	236	Total 1918	C 1210	N 338	O 367	S 3	0	0	0
1	M	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	N	238	Total 1939	C 1223	N 346	O 367	S 3	0	0	0
1	O	236	Total 1918	C 1210	N 338	O 367	S 3	0	0	0
1	P	244	Total 1986	C 1252	N 353	O 378	S 3	0	0	0

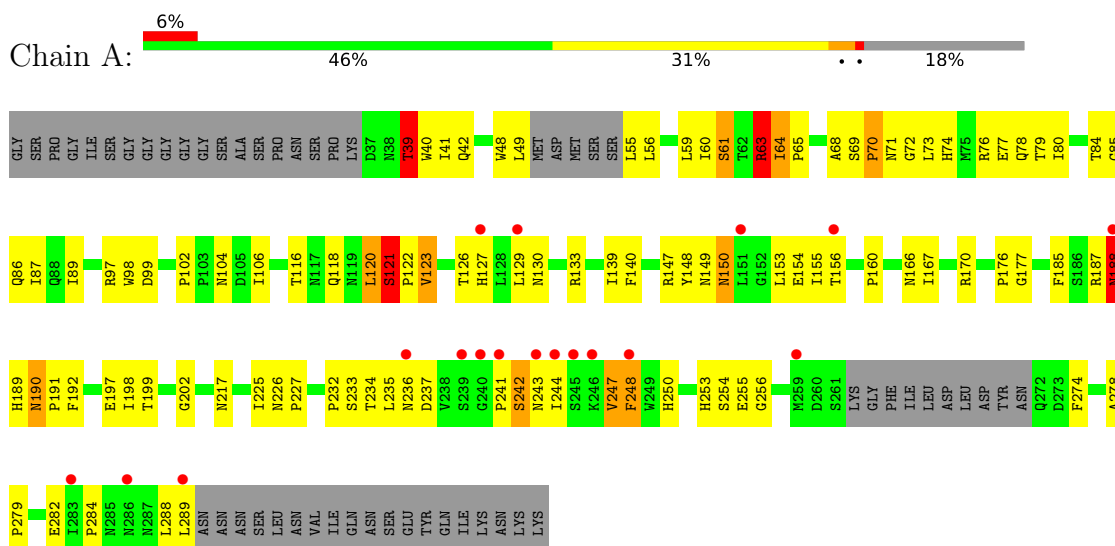
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	GLN	GLU	engineered mutation	UNP Q03988
B	195	GLN	GLU	engineered mutation	UNP Q03988
C	195	GLN	GLU	engineered mutation	UNP Q03988
D	195	GLN	GLU	engineered mutation	UNP Q03988
E	195	GLN	GLU	engineered mutation	UNP Q03988
F	195	GLN	GLU	engineered mutation	UNP Q03988
G	195	GLN	GLU	engineered mutation	UNP Q03988
H	195	GLN	GLU	engineered mutation	UNP Q03988
I	195	GLN	GLU	engineered mutation	UNP Q03988
J	195	GLN	GLU	engineered mutation	UNP Q03988
K	195	GLN	GLU	engineered mutation	UNP Q03988
L	195	GLN	GLU	engineered mutation	UNP Q03988
M	195	GLN	GLU	engineered mutation	UNP Q03988
N	195	GLN	GLU	engineered mutation	UNP Q03988
O	195	GLN	GLU	engineered mutation	UNP Q03988
P	195	GLN	GLU	engineered mutation	UNP Q03988

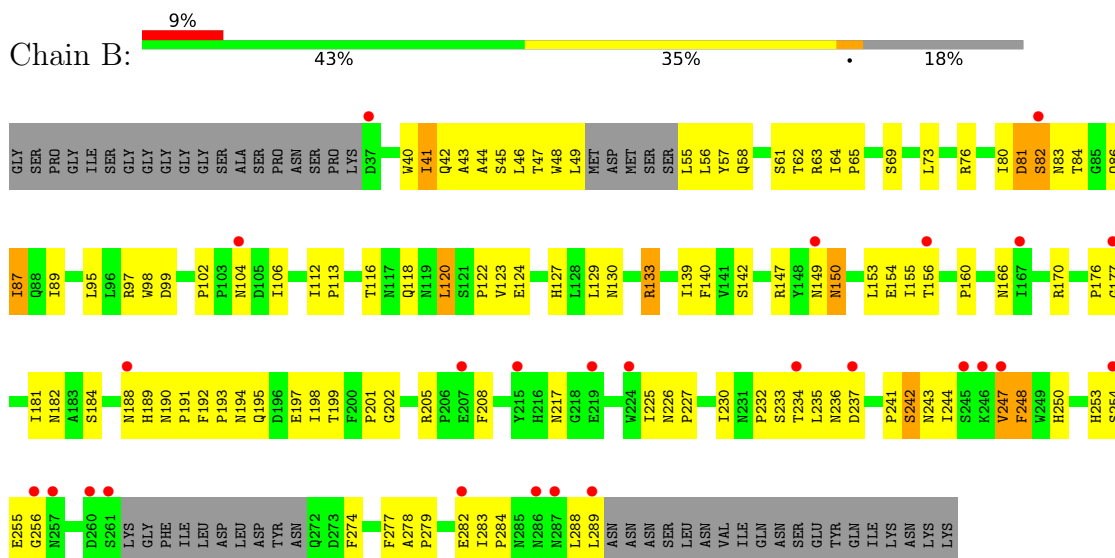
3 Residue-property plots i

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: MOSQUITOCIDAL TOXIN

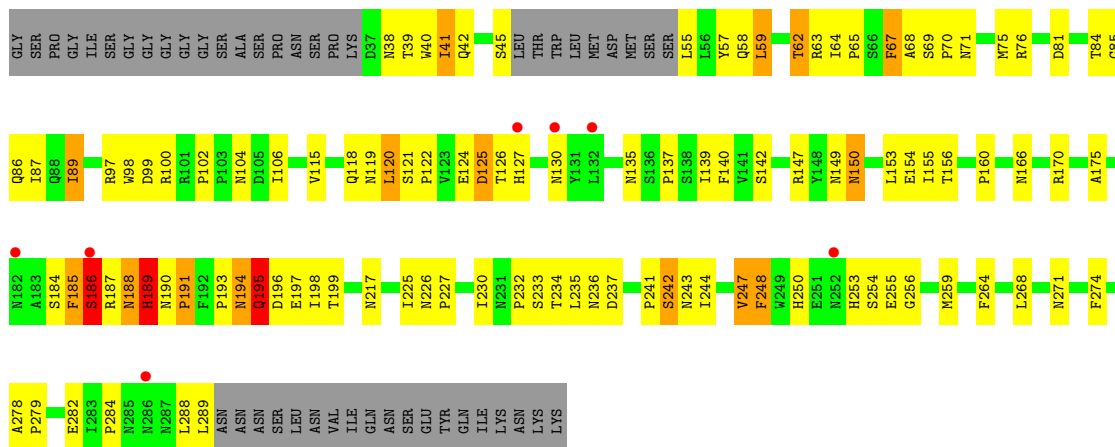


• Molecule 1: MOSQUITOCIDAL TOXIN

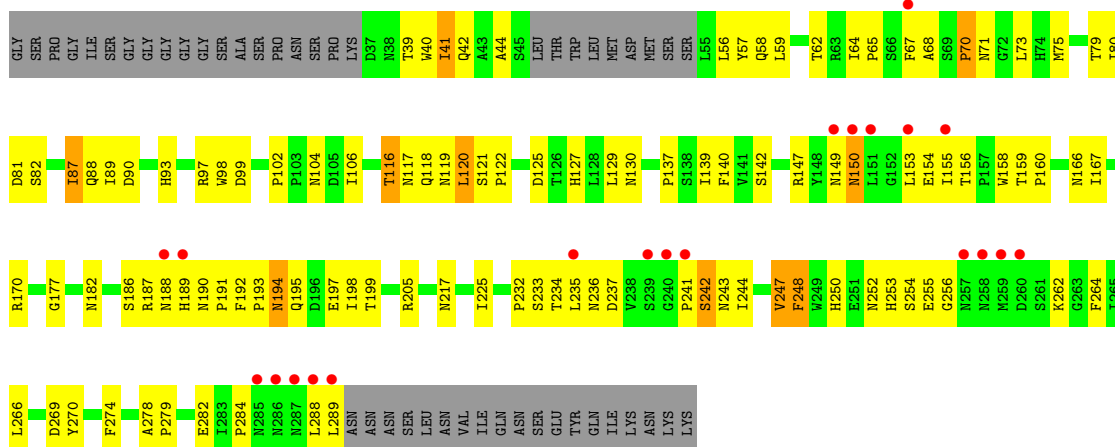


• Molecule 1: MOSQUITOCIDAL TOXIN

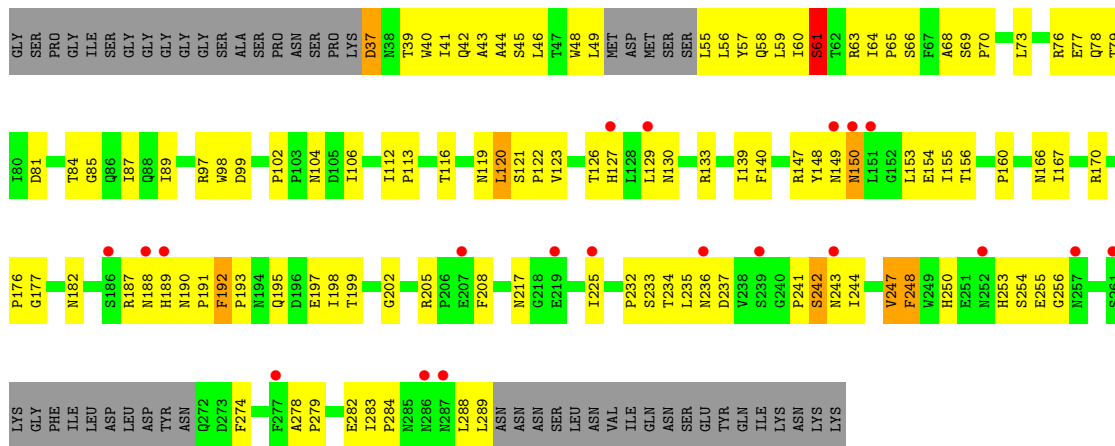
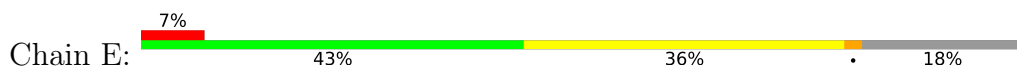




• Molecule 1: MOSQUITOCIDAL TOXIN



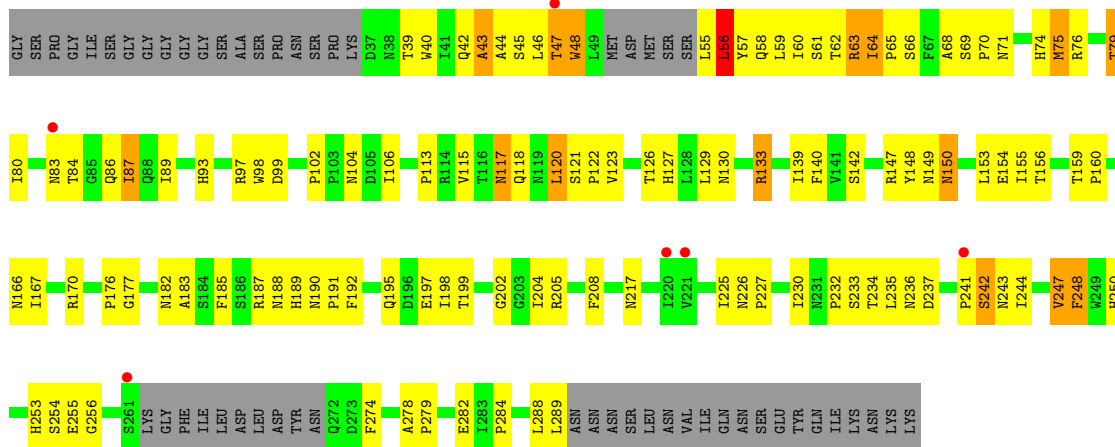
• Molecule 1: MOSQUITOCIDAL TOXIN



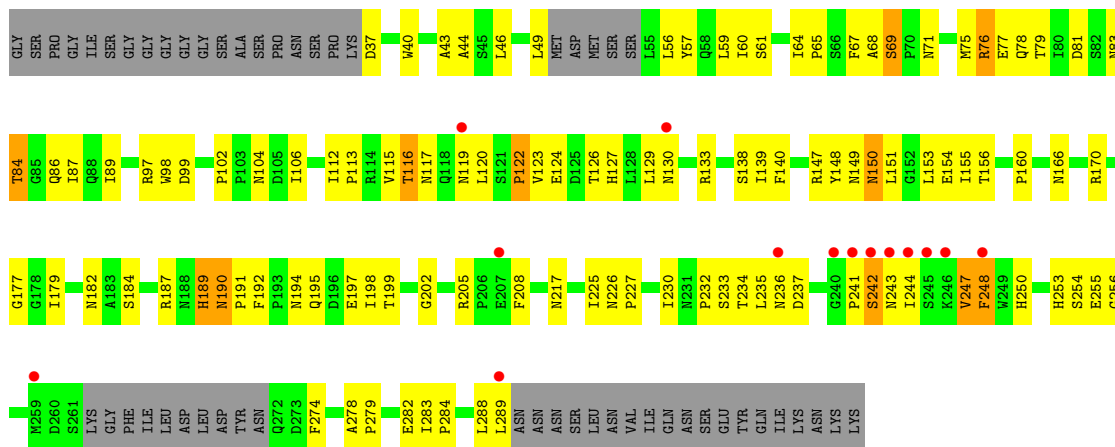
• Molecule 1: MOSQUITOCIDAL TOXIN



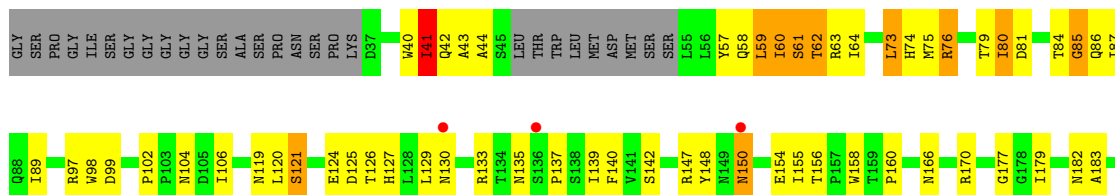
● Molecule 1: MOSQUITOCIDAL TOXIN



● Molecule 1: MOSQUITOCIDAL TOXIN

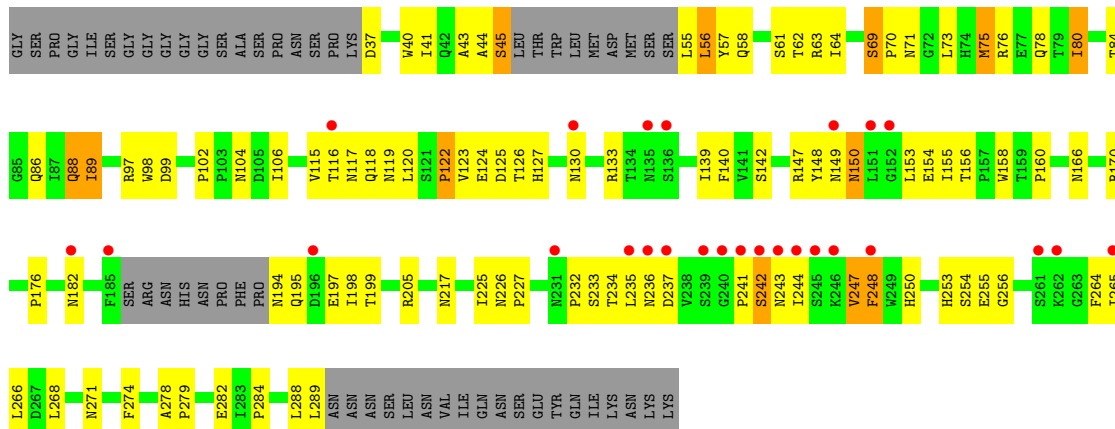


● Molecule 1: MOSQUITOCIDAL TOXIN

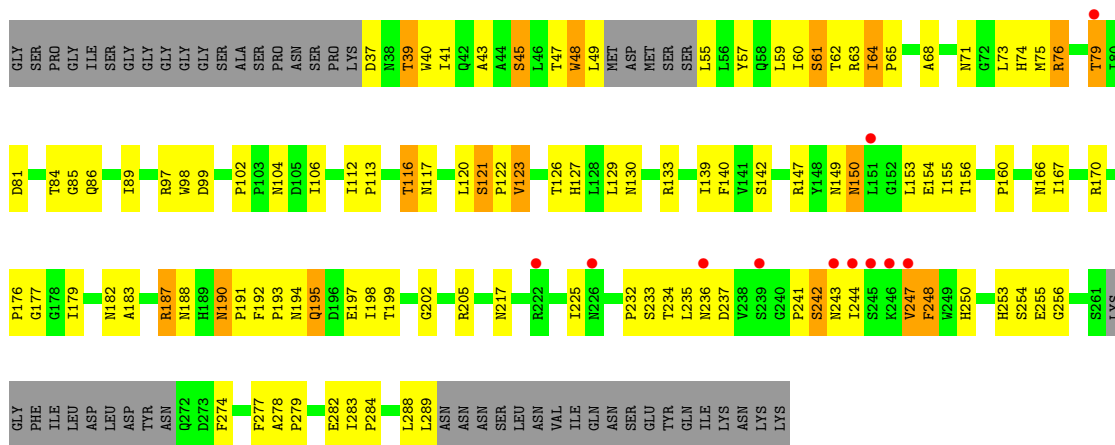
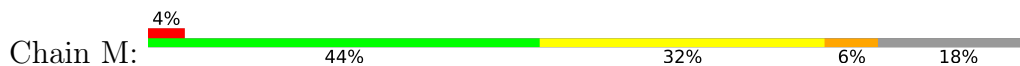




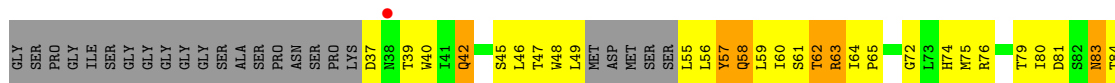
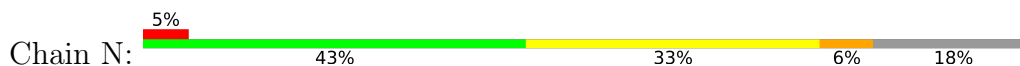
- Molecule 1: MOSQUITOCIDAL TOXIN

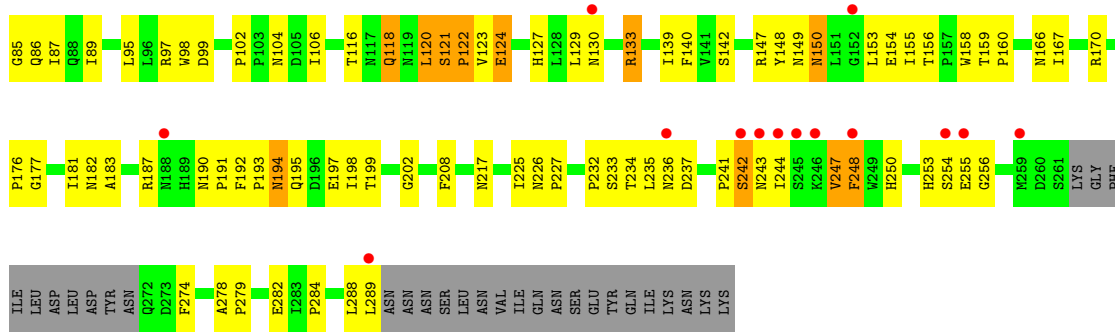


- Molecule 1: MOSQUITOCIDAL TOXIN

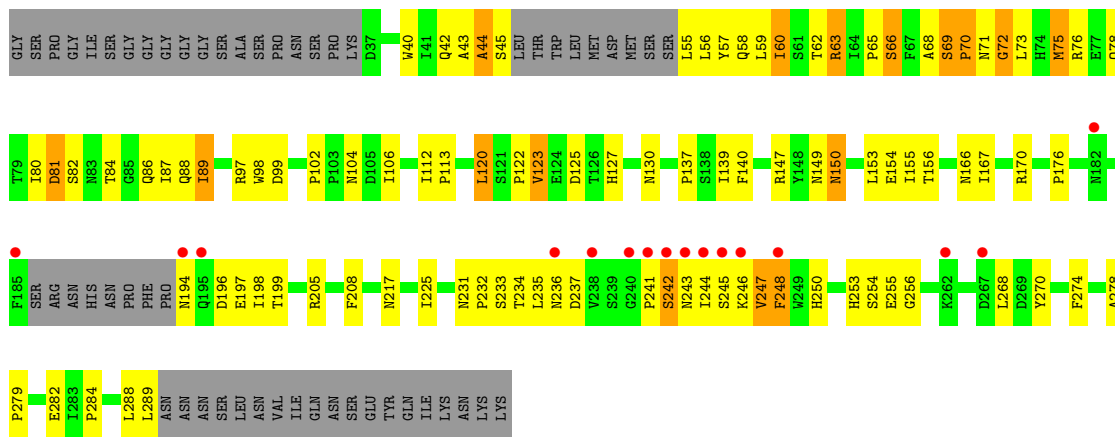


- Molecule 1: MOSQUITOCIDAL TOXIN

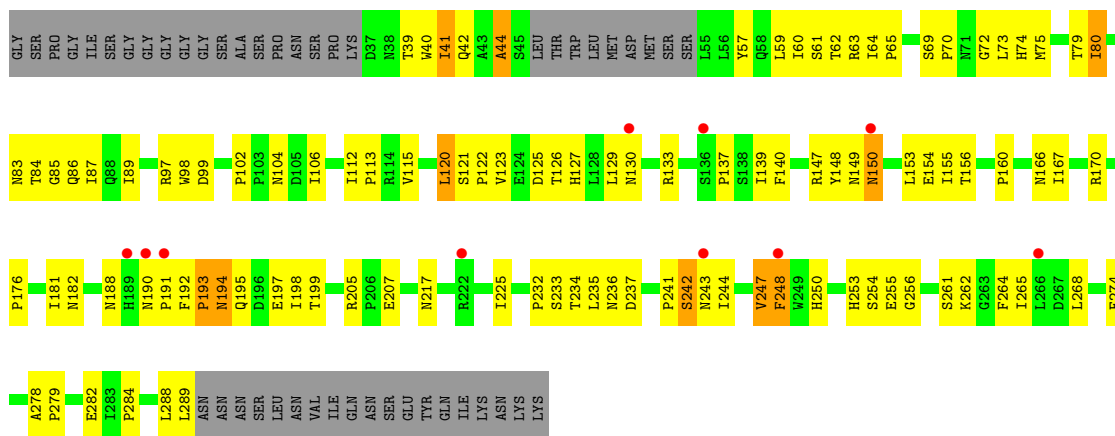




● Molecule 1: MOSQUITOCIDAL TOXIN



● Molecule 1: MOSQUITOCIDAL TOXIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.30Å 175.80Å 335.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 99.6 (50.00-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.01Å)	Xtrriage
Refinement program	TNT 5.6.1	Depositor
R, R_{free}	0.227 , 0.246 (Not available) , 0.263	Depositor DCC
R_{free} test set	6301 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	31202	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.83 % 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 3.5553e-03.*

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 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	0.61	0/1995	1.14	16/2726 (0.6%)
1	B	0.57	0/1995	1.05	9/2726 (0.3%)
1	C	0.62	0/2043	1.13	19/2790 (0.7%)
1	D	0.62	0/2043	1.12	14/2790 (0.5%)
1	E	0.62	1/1995 (0.1%)	1.10	12/2726 (0.4%)
1	F	0.55	0/1995	1.05	9/2726 (0.3%)
1	G	0.58	0/1970	1.08	11/2688 (0.4%)
1	H	0.63	1/2049 (0.0%)	1.19	21/2798 (0.8%)
1	I	0.58	1/1995 (0.1%)	1.09	13/2726 (0.5%)
1	J	0.58	0/1995	1.12	13/2726 (0.5%)
1	K	0.57	0/2043	1.08	12/2790 (0.4%)
1	L	0.61	1/1970 (0.1%)	1.15	13/2688 (0.5%)
1	M	0.54	0/1995	1.12	15/2726 (0.6%)
1	N	0.59	1/1995 (0.1%)	1.10	15/2726 (0.6%)
1	O	0.62	0/1970	1.18	17/2688 (0.6%)
1	P	0.60	0/2043	1.08	10/2790 (0.4%)
All	All	0.59	5/32091 (0.0%)	1.11	219/43830 (0.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	75	MET	SD-CE	6.70	1.96	1.79
1	H	195	GLN	CA-C	-5.76	1.45	1.52
1	I	115	VAL	CA-CB	5.33	1.60	1.53
1	N	123	VAL	CA-CB	-5.09	1.48	1.54
1	E	60	ILE	CA-C	-5.06	1.46	1.52

The worst 5 of 219 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	187	ARG	N-CA-C	13.29	125.76	111.28
1	H	187	ARG	N-CA-C	-11.90	95.09	111.87
1	H	60	ILE	N-CA-C	10.96	120.94	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	83	ASN	N-CA-C	-10.95	98.52	114.39
1	M	85	GLY	N-CA-C	-10.54	98.73	116.01

There are no chirality outliers.

There are no planarity outliers.

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	A	1939	0	1829	103	0
1	B	1939	0	1829	110	0
1	C	1986	0	1872	99	0
1	D	1986	0	1872	93	1
1	E	1939	0	1829	120	0
1	F	1939	0	1829	110	0
1	G	1918	0	1811	95	0
1	H	1992	0	1877	104	1
1	I	1939	0	1829	110	0
1	J	1939	0	1829	90	0
1	K	1986	0	1872	104	0
1	L	1918	0	1811	87	0
1	M	1939	0	1829	88	0
1	N	1939	0	1829	94	0
1	O	1918	0	1811	86	0
1	P	1986	0	1872	89	0
All	All	31202	0	29430	1450	1

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 24.

The worst 5 of 1450 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:J:87:ILE:HD12	1:J:230:ILE:HG21	1.22	1.15
1:I:64:ILE:HG23	1:I:129:LEU:HD11	1.25	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:THR:HB	1:A:86:GLN:HG2	1.11	1.10
1:A:64:ILE:HG23	1:A:129:LEU:HD11	1.17	1.08
1:D:254:SER:HB3	1:O:244:ILE:O	1.53	1.07

All (1) 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:D:150:ASN:O	1:H:148:TYR:N[2_664]	1.96	0.24

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	232/291 (80%)	202 (87%)	29 (12%)	1 (0%)	30	65
1	B	232/291 (80%)	205 (88%)	27 (12%)	0	100	100
1	C	240/291 (82%)	211 (88%)	28 (12%)	1 (0%)	30	65
1	D	240/291 (82%)	216 (90%)	21 (9%)	3 (1%)	9	38
1	E	232/291 (80%)	200 (86%)	30 (13%)	2 (1%)	14	48
1	F	232/291 (80%)	205 (88%)	25 (11%)	2 (1%)	14	48
1	G	230/291 (79%)	208 (90%)	22 (10%)	0	100	100
1	H	241/291 (83%)	211 (88%)	27 (11%)	3 (1%)	10	40
1	I	232/291 (80%)	208 (90%)	21 (9%)	3 (1%)	9	38
1	J	232/291 (80%)	208 (90%)	23 (10%)	1 (0%)	30	65
1	K	240/291 (82%)	211 (88%)	28 (12%)	1 (0%)	30	65
1	L	230/291 (79%)	202 (88%)	26 (11%)	2 (1%)	14	48
1	M	232/291 (80%)	206 (89%)	25 (11%)	1 (0%)	30	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	232/291 (80%)	206 (89%)	23 (10%)	3 (1%)	9	38
1	O	230/291 (79%)	201 (87%)	27 (12%)	2 (1%)	14	48
1	P	240/291 (82%)	212 (88%)	25 (10%)	3 (1%)	9	38
All	All	3747/4656 (80%)	3312 (88%)	407 (11%)	28 (1%)	18	53

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	70	PRO
1	O	70	PRO
1	A	70	PRO
1	N	62	THR
1	P	83	ASN

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	218/262 (83%)	204 (94%)	14 (6%)	16	48
1	B	218/262 (83%)	204 (94%)	14 (6%)	16	48
1	C	223/262 (85%)	210 (94%)	13 (6%)	18	51
1	D	223/262 (85%)	214 (96%)	9 (4%)	28	62
1	E	218/262 (83%)	206 (94%)	12 (6%)	19	53
1	F	218/262 (83%)	203 (93%)	15 (7%)	14	45
1	G	215/262 (82%)	199 (93%)	16 (7%)	13	42
1	H	224/262 (86%)	208 (93%)	16 (7%)	13	43
1	I	218/262 (83%)	204 (94%)	14 (6%)	16	48
1	J	218/262 (83%)	205 (94%)	13 (6%)	17	50
1	K	223/262 (85%)	209 (94%)	14 (6%)	16	48
1	L	215/262 (82%)	202 (94%)	13 (6%)	17	50
1	M	218/262 (83%)	202 (93%)	16 (7%)	13	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	218/262 (83%)	205 (94%)	13 (6%)	17	50
1	O	215/262 (82%)	204 (95%)	11 (5%)	21	55
1	P	223/262 (85%)	214 (96%)	9 (4%)	28	62
All	All	3505/4192 (84%)	3293 (94%)	212 (6%)	17	50

5 of 212 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	120	LEU
1	K	192	PHE
1	O	233	SER
1	I	233	SER
1	J	190	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	190	ASN
1	K	86	GLN
1	P	117	ASN
1	J	78	GLN
1	J	195	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 oligosaccharides 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, 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	238/291 (81%)	0.61	18 (7%) 20 10	15, 35, 66, 84	0
1	B	238/291 (81%)	0.79	26 (10%) 10 6	17, 41, 71, 84	0
1	C	244/291 (83%)	0.34	7 (2%) 53 31	13, 32, 58, 78	0
1	D	244/291 (83%)	0.59	21 (8%) 16 8	14, 36, 65, 92	0
1	E	238/291 (81%)	0.73	20 (8%) 17 9	15, 40, 71, 83	0
1	F	238/291 (81%)	0.85	26 (10%) 10 6	14, 36, 67, 86	0
1	G	236/291 (81%)	0.71	22 (9%) 14 7	18, 37, 66, 77	0
1	H	245/291 (84%)	0.75	29 (11%) 9 5	13, 30, 57, 71	0
1	I	238/291 (81%)	0.63	6 (2%) 58 35	23, 42, 72, 85	0
1	J	238/291 (81%)	0.59	14 (5%) 28 14	16, 39, 68, 81	0
1	K	244/291 (83%)	0.34	12 (4%) 35 18	10, 35, 68, 85	0
1	L	236/291 (81%)	0.78	26 (11%) 10 6	18, 34, 64, 76	0
1	M	238/291 (81%)	0.75	11 (4%) 37 20	17, 40, 71, 87	0
1	N	238/291 (81%)	0.48	15 (6%) 26 13	14, 40, 69, 83	0
1	O	236/291 (81%)	0.50	16 (6%) 23 12	9, 34, 64, 79	0
1	P	244/291 (83%)	0.41	10 (4%) 41 23	12, 35, 67, 87	0
All	All	3833/4656 (82%)	0.61	279 (7%) 21 11	9, 37, 67, 92	0

The worst 5 of 279 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	150	ASN	8.5
1	J	245	SER	7.4
1	G	150	ASN	6.5
1	L	243	ASN	6.1
1	N	243	ASN	5.9

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 oligosaccharides 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.