



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 27, 2017 – 01:23 AM EDT

PDB ID : 1DM0
Title : SHIGA TOXIN
Authors : Fraser, M.E.; Chernaiia, M.M.; Kozlov, Y.V.; James, M.N.
Deposited on : unknown
Resolution : 2.50 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

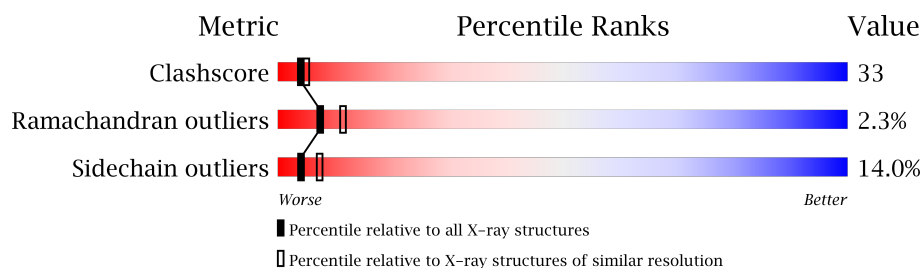
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)


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	287	
1	L	287	
2	B	69	
2	C	69	
2	D	69	
2	E	69	
2	F	69	

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Mol	Chain	Length	Quality of chain
2	G	69	 54% 41% 6%
2	H	69	 33% 51% 14% .
2	I	69	 48% 46% 6%
2	J	69	 38% 39% 22% .
2	K	69	 58% 36% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9538 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 SHIGA TOXIN A SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2046	1284	363	390	9			
1	L	262	Total	C	N	O	S	0	0	0
			2030	1276	361	384	9			

- Molecule 2 is a protein called SHIGA TOXIN B SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	C	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	D	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	E	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	F	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	G	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	H	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	I	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	J	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	K	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			

- Molecule 3 is water.

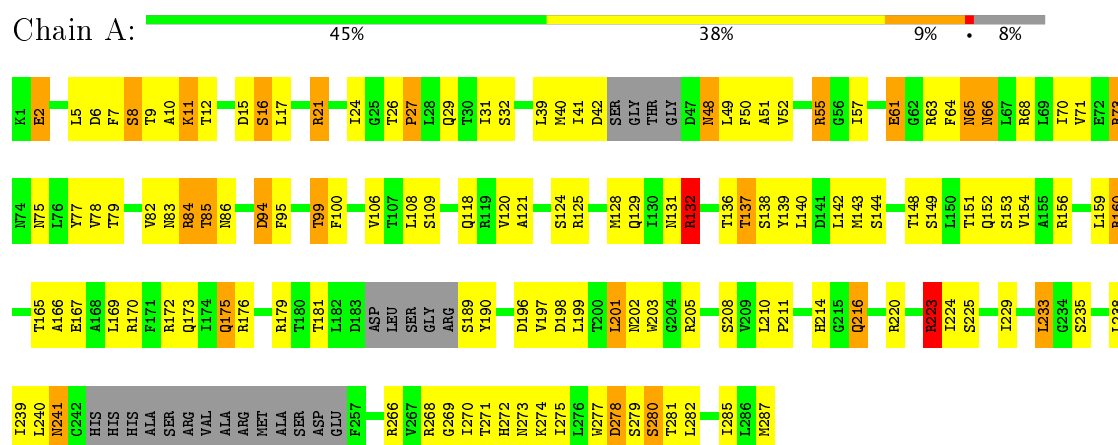
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	L	11	Total 11	O 11	0	0
3	B	1	Total 1	O 1	0	0
3	C	4	Total 4	O 4	0	0
3	D	4	Total 4	O 4	0	0
3	E	5	Total 5	O 5	0	0
3	F	3	Total 3	O 3	0	0
3	G	4	Total 4	O 4	0	0
3	H	1	Total 1	O 1	0	0
3	I	2	Total 2	O 2	0	0
3	J	5	Total 5	O 5	0	0
3	K	10	Total 10	O 10	0	0

3 Residue-property plots

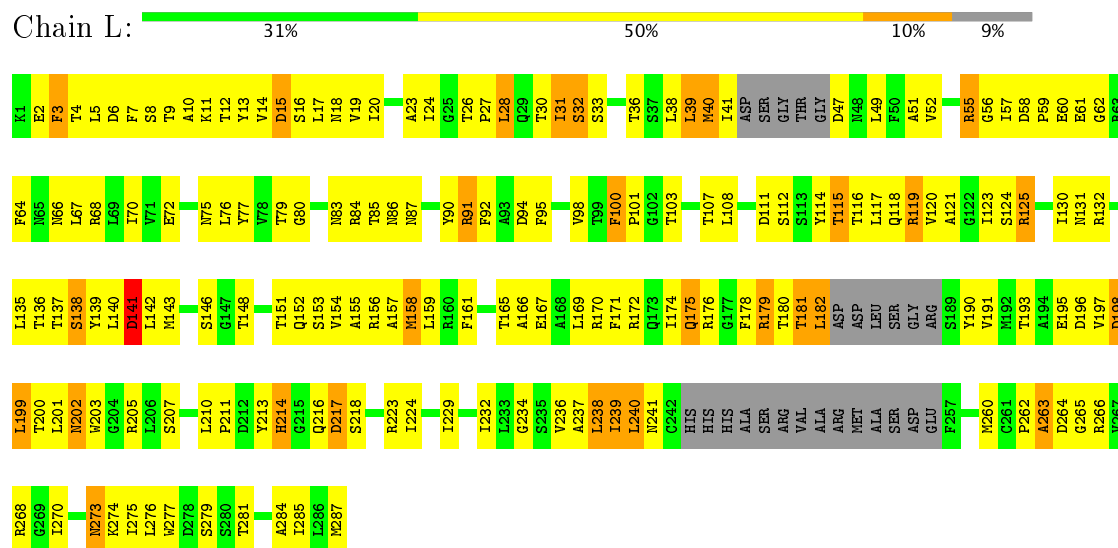
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: SHIGA TOXIN A SUBUNIT



• Molecule 1: SHIGA TOXIN A SUBUNIT



• Molecule 2: SHIGA TOXIN B SUBUNIT





• Molecule 2: SHIGA TOXIN B SUBUNIT



• Molecule 2: SHIGA TOXIN B SUBUNIT



• Molecule 2: SHIGA TOXIN B SUBUNIT



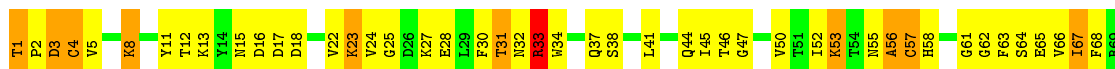
• Molecule 2: SHIGA TOXIN B SUBUNIT



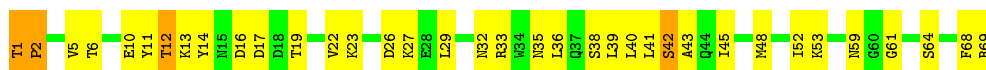
• Molecule 2: SHIGA TOXIN B SUBUNIT



• Molecule 2: SHIGA TOXIN B SUBUNIT



• Molecule 2: SHIGA TOXIN B SUBUNIT



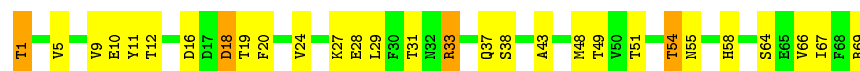
• Molecule 2: SHIGA TOXIN B SUBUNIT

Chain J:  38% 39% 22%



- Molecule 2: SHIGA TOXIN B SUBUNIT

Chain K:  58% 36% 6%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.05Å 147.46Å 83.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	83.1 (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR, TNT	Depositor
R, R_{free}	0.206 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9538	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.07	1/2078 (0.0%)	1.22	7/2815 (0.2%)
1	L	0.91	0/2062	1.14	4/2793 (0.1%)
2	B	1.09	0/549	1.17	1/742 (0.1%)
2	C	1.10	0/549	1.18	2/742 (0.3%)
2	D	1.11	1/549 (0.2%)	1.19	3/742 (0.4%)
2	E	1.29	2/549 (0.4%)	1.35	2/742 (0.3%)
2	F	1.15	2/549 (0.4%)	1.32	3/742 (0.4%)
2	G	1.23	1/549 (0.2%)	1.16	1/742 (0.1%)
2	H	1.04	1/549 (0.2%)	1.07	2/742 (0.3%)
2	I	1.05	0/549	1.13	1/742 (0.1%)
2	J	1.18	0/549	1.31	5/742 (0.7%)
2	K	1.33	3/549 (0.5%)	1.32	4/742 (0.5%)
All	All	1.09	11/9630 (0.1%)	1.21	35/13028 (0.3%)

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	F	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	10	GLU	CG-CD	7.29	1.62	1.51
2	G	22	VAL	CB-CG1	-6.42	1.39	1.52
2	K	10	GLU	CD-OE2	6.20	1.32	1.25
2	K	10	GLU	CD-OE1	6.06	1.32	1.25
2	H	67	ILE	CA-CB	-5.95	1.41	1.54

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	J	1	THR	C-N-CD	-10.21	98.13	120.60
2	E	69	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	A	132	ARG	NE-CZ-NH2	-7.71	116.45	120.30
2	J	33	ARG	NE-CZ-NH1	-7.23	116.69	120.30
2	D	36	LEU	CB-CG-CD2	-6.75	99.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	14	TYR	Sidechain

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	2046	0	2040	126	0
1	L	2030	0	2032	202	0
2	B	540	0	527	35	0
2	C	540	0	527	27	0
2	D	540	0	527	27	0
2	E	540	0	527	20	0
2	F	540	0	527	43	0
2	G	540	0	527	29	0
2	H	540	0	527	53	0
2	I	540	0	527	32	0
2	J	540	0	527	50	0
2	K	540	0	527	18	0
3	A	12	0	0	1	0
3	B	1	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	1	0
3	E	5	0	0	1	0
3	F	3	0	0	0	0
3	G	4	0	0	0	0
3	H	1	0	0	0	0
3	I	2	0	0	0	0
3	J	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	10	0	0	0	0
3	L	11	0	0	1	0
All	All	9538	0	9342	620	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 33.

The worst 5 of 620 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:40:MET:SD	1:A:40:MET:CE	2.04	1.45
1:L:60:GLU:HG2	1:L:61:GLU:HG2	1.31	1.13
2:J:33:ARG:HH12	2:J:64:SER:HB3	1.07	1.06
1:A:151:THR:HG22	1:A:154:VAL:HG23	1.41	1.02
1:A:121:ALA:HB1	1:A:156:ARG:HG2	1.39	1.02

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	A	256/287 (89%)	232 (91%)	20 (8%)	4 (2%)	11	19
1	L	254/287 (88%)	211 (83%)	34 (13%)	9 (4%)	4	5
2	B	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
2	C	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
2	D	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
2	E	67/69 (97%)	63 (94%)	3 (4%)	1 (2%)	12	21
2	F	67/69 (97%)	61 (91%)	5 (8%)	1 (2%)	12	21
2	G	67/69 (97%)	65 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	67/69 (97%)	55 (82%)	7 (10%)	5 (8%)	1	1
2	I	67/69 (97%)	59 (88%)	7 (10%)	1 (2%)	12	21
2	J	67/69 (97%)	57 (85%)	4 (6%)	6 (9%)	1	1
2	K	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
All	All	1180/1264 (93%)	1053 (89%)	100 (8%)	27 (2%)	7	11

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	L	141	ASP
1	L	181	THR
1	L	263	ALA
2	F	17	ASP

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	229/246 (93%)	200 (87%)	29 (13%)	5	9
1	L	227/246 (92%)	194 (86%)	33 (14%)	4	7
2	B	61/61 (100%)	49 (80%)	12 (20%)	1	2
2	C	61/61 (100%)	51 (84%)	10 (16%)	2	5
2	D	61/61 (100%)	56 (92%)	5 (8%)	13	25
2	E	61/61 (100%)	53 (87%)	8 (13%)	5	9
2	F	61/61 (100%)	52 (85%)	9 (15%)	3	6
2	G	61/61 (100%)	55 (90%)	6 (10%)	9	18
2	H	61/61 (100%)	52 (85%)	9 (15%)	3	6
2	I	61/61 (100%)	52 (85%)	9 (15%)	3	6
2	J	61/61 (100%)	48 (79%)	13 (21%)	1	2
2	K	61/61 (100%)	55 (90%)	6 (10%)	9	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1066/1102 (97%)	917 (86%)	149 (14%)	4 7

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	29	LEU
2	C	69	ARG
2	J	30	PHE
2	B	35	ASN
2	C	13	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	35	ASN
2	D	55	ASN
2	J	32	ASN
2	C	32	ASN
2	F	15	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.