



wwPDB EM Model Validation Summary Report ⓘ

Mar 9, 2020 – 11:04 AM EDT

PDB ID : 6V1S
EMDB ID : EMD-21016
Title : Structure of the Clostridioides difficile transferase toxin
Authors : Sheedlo, M.J.; Anderson, D.M.; Thomas, A.K.; Lacy, D.B.
Deposited on : 2019-11-21
Resolution : 3.80 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

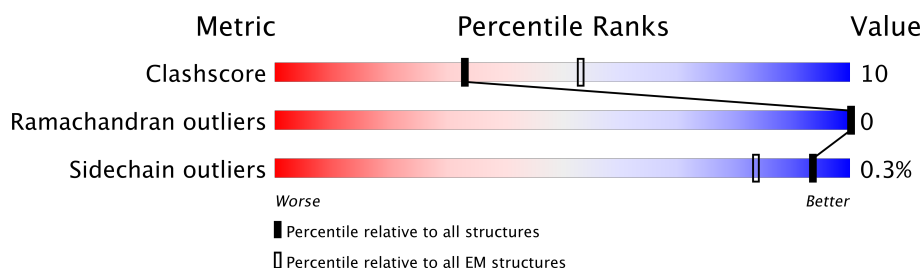
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	876	26% 5% 69%
1	B	876	23% 7% 69%
1	C	876	21% 9% 70%
1	D	876	23% 8% 69%
1	E	876	24% 7% 68%
1	F	876	25% 6% 69%
1	G	876	24% 7% 69%
2	Z	463	63% 22% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17964 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ADP-ribosyltransferase binding component.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	272	Total	C	N	O	S	0	0
			2114	1318	344	449	3		
1	B	268	Total	C	N	O	S	0	0
			2081	1299	340	439	3		
1	C	265	Total	C	N	O	S	0	0
			2058	1287	336	432	3		
1	D	273	Total	C	N	O	S	0	0
			2122	1322	345	452	3		
1	E	276	Total	C	N	O	S	0	0
			2153	1342	349	459	3		
1	F	272	Total	C	N	O	S	0	0
			2114	1318	344	449	3		
1	G	273	Total	C	N	O	S	0	0
			2122	1322	345	452	3		

- Molecule 2 is a protein called ADP-ribosylating binary toxin enzymatic subunit CdtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	394	Total	C	N	O	S	0	0
			3186	2027	532	622	5		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

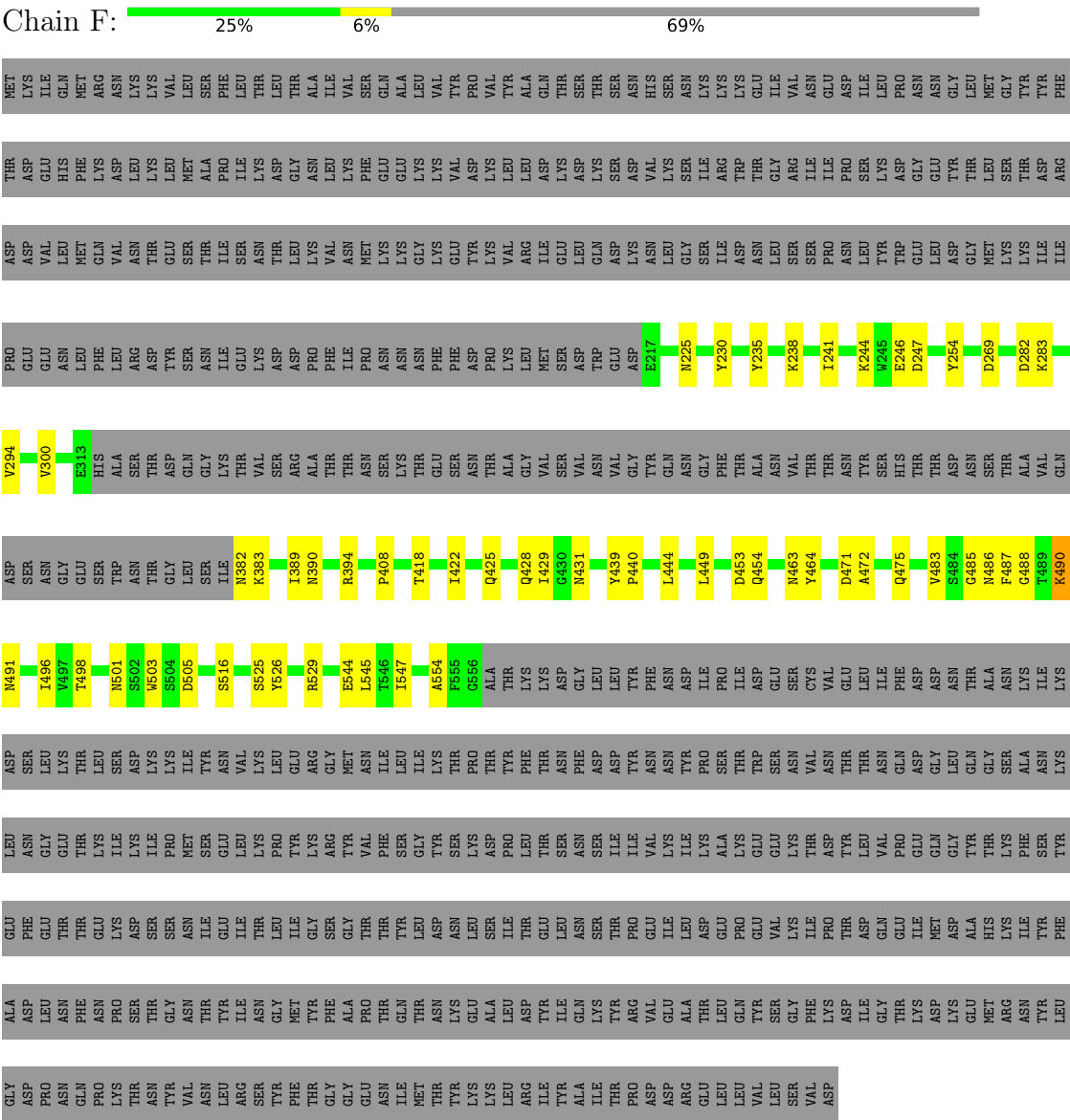
Mol	Chain	Residues	Atoms		AltConf
3	G	2	Total	Ca	0
			2	2	
3	D	2	Total	Ca	0
			2	2	
3	E	2	Total	Ca	0
			2	2	
3	B	2	Total	Ca	0
			2	2	
3	C	2	Total	Ca	0
			2	2	

Continued on next page...

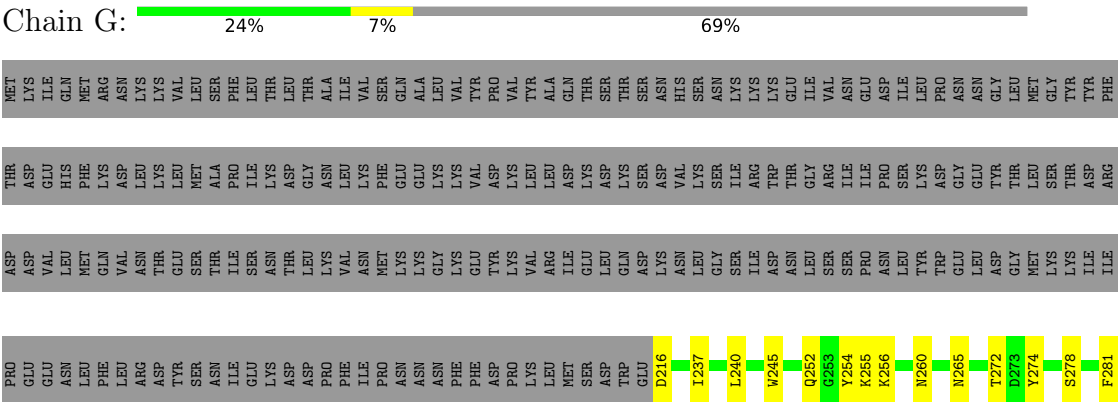
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total 2	Ca 2	0
3	F	2	Total 2	Ca 2	0

- Molecule 1: ADP-ribosyltransferase binding component



- Molecule 1: ADP-ribosyltransferase binding component



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31377	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61.34	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.39	0/2149	0.51	0/2915
1	B	0.40	0/2116	0.53	0/2870
1	C	0.40	0/2093	0.54	0/2838
1	D	0.42	0/2157	0.53	0/2926
1	E	0.43	0/2190	0.53	0/2972
1	F	0.43	0/2149	0.54	0/2915
1	G	0.40	0/2157	0.51	0/2926
2	Z	0.32	0/3253	0.45	0/4391
All	All	0.40	0/18264	0.51	0/24753

There are no bond length outliers.

There are no bond angle outliers.

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	2114	0	2045	30	0
1	B	2081	0	2020	42	0
1	C	2058	0	2003	54	0
1	D	2122	0	2049	45	0
1	E	2153	0	2069	45	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2114	0	2045	43	0
1	G	2122	0	2049	40	0
2	Z	3186	0	3169	67	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
All	All	17964	0	17449	353	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 10.

The worst 5 of 353 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)
2:Z:311:LEU:HD21	2:Z:317:GLU:HB2	1.64	0.77
1:A:283:LYS:HB2	1:G:509:GLN:HG3	1.67	0.76
2:Z:340:TYR:O	2:Z:393:GLY:HA2	1.85	0.75
1:G:490:LYS:HG3	1:G:492:SER:H	1.53	0.74
1:D:304:MET:HG2	1:D:478:LEU:HB3	1.69	0.74

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 PDB entries followed by that with respect to all EM entries.

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	268/876 (31%)	236 (88%)	32 (12%)	0	100	100
1	B	264/876 (30%)	234 (89%)	30 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	261/876 (30%)	227 (87%)	34 (13%)	0	100	100
1	D	269/876 (31%)	230 (86%)	39 (14%)	0	100	100
1	E	272/876 (31%)	236 (87%)	36 (13%)	0	100	100
1	F	268/876 (31%)	233 (87%)	35 (13%)	0	100	100
1	G	269/876 (31%)	238 (88%)	31 (12%)	0	100	100
2	Z	392/463 (85%)	343 (88%)	49 (12%)	0	100	100
All	All	2263/6595 (34%)	1977 (87%)	286 (13%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	235/790 (30%)	234 (100%)	1 (0%)	92	96
1	B	231/790 (29%)	230 (100%)	1 (0%)	92	96
1	C	228/790 (29%)	228 (100%)	0	100	100
1	D	236/790 (30%)	234 (99%)	2 (1%)	83	92
1	E	239/790 (30%)	239 (100%)	0	100	100
1	F	235/790 (30%)	234 (100%)	1 (0%)	92	96
1	G	236/790 (30%)	235 (100%)	1 (0%)	92	96
2	Z	354/418 (85%)	354 (100%)	0	100	100
All	All	1994/5948 (34%)	1988 (100%)	6 (0%)	93	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	281	PHE
1	G	447	LEU
1	D	505	ASP
1	B	471	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	490	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	427	ASN
1	D	466	GLN
1	G	432	ASN
1	C	509	GLN
1	D	252	GLN

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 ⓘ

Of 14 ligands modelled in this entry, 14 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.