



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:39 PM UTC

PDB ID : 3SS1 / pdb_00003ss1
Title : Clostridium difficile toxin A (TcdA) glucosyltransferase domain
Authors : Pruitt, R.N.; Chumbler, N.M.; Farrow, M.A.; Seebach, S.A.; Friedman, D.B.;
Spiller, B.W.; Lacy, D.B.
Deposited on : 2011-07-07
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Xtriage (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

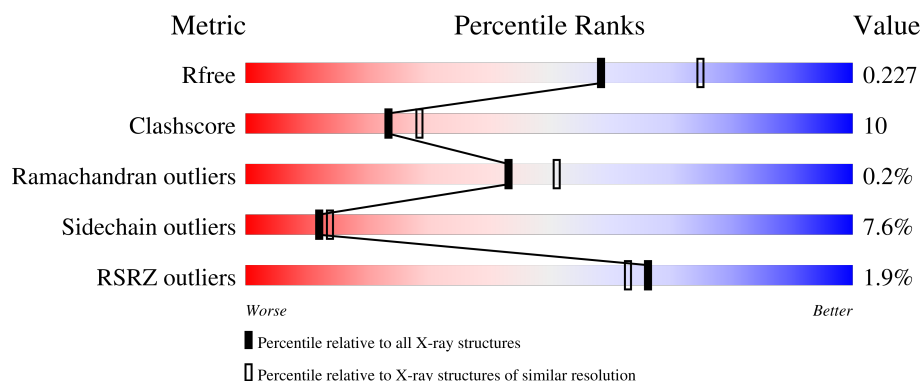
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

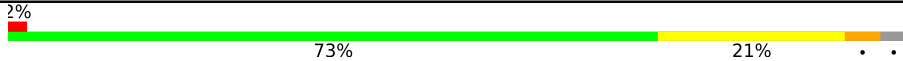
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	555	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4637 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 Toxin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4403	2811	728	856	8			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	543	HIS	-	expression tag	UNP Q189K5
A	544	ALA	-	expression tag	UNP Q189K5
A	545	GLY	-	expression tag	UNP Q189K5
A	546	LEU	-	expression tag	UNP Q189K5
A	547	ARG	-	expression tag	UNP Q189K5
A	548	GLY	-	expression tag	UNP Q189K5
A	549	SER	-	expression tag	UNP Q189K5
A	550	HIS	-	expression tag	UNP Q189K5
A	551	HIS	-	expression tag	UNP Q189K5
A	552	HIS	-	expression tag	UNP Q189K5
A	553	HIS	-	expression tag	UNP Q189K5
A	554	HIS	-	expression tag	UNP Q189K5
A	555	HIS	-	expression tag	UNP Q189K5

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	233	Total	O	0	0
			233	233		

- Molecule 1: Toxin A



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	141.91Å 141.91Å 65.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.30 – 2.20 48.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.30-2.20) 96.3 (48.30-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.182 , 0.227 (Not available) , 0.227	Depositor DCC
R_{free} test set	2014 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4637	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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](#)

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

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	0.47	0/4483	0.76	1/6053 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	VAL	CB-CA-C	-6.80	102.49	111.13

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	4403	0	4401	90	1
2	A	1	0	0	0	0
3	A	233	0	0	8	1
All	All	4637	0	4401	90	2

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.

All (90) 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:18:PRO:O	3:A:720:HOH:O	1.92	0.86
1:A:109:ILE:H	1:A:109:ILE:HD12	1.40	0.84
1:A:384:GLN:HE21	1:A:509:GLN:HE21	1.35	0.74
1:A:250:LEU:HD13	1:A:274:LEU:HD21	1.67	0.73
1:A:90:THR:HG23	1:A:366:ASN:HB3	1.71	0.73
1:A:384:GLN:NE2	1:A:509:GLN:HE21	1.89	0.71
1:A:361:LYS:HB2	1:A:361:LYS:NZ	2.06	0.70
1:A:302:ARG:HH11	1:A:302:ARG:HB2	1.56	0.69
1:A:519:TRP:NE1	1:A:525:SER:OG	2.25	0.68
1:A:55:ILE:HD11	1:A:74:LEU:HD13	1.76	0.66
1:A:362:LEU:HD22	1:A:365:LEU:HD11	1.78	0.66
1:A:91:SER:HB2	1:A:92:PRO:HD2	1.78	0.65
1:A:292:ILE:O	3:A:751:HOH:O	2.13	0.65
1:A:195:LYS:O	3:A:756:HOH:O	2.13	0.64
1:A:336:LYS:HE3	1:A:337:LEU:HA	1.82	0.62
1:A:167:ASN:C	1:A:167:ASN:HD22	2.08	0.61
1:A:5:SER:OG	1:A:8:GLU:HG3	2.01	0.61
1:A:295:ASP:HA	1:A:298:LYS:HB2	1.83	0.60
1:A:478:TYR:HA	1:A:492:LEU:HD22	1.85	0.59
1:A:115:LYS:HE2	1:A:119:ASP:OD2	2.03	0.59
1:A:478:TYR:HD2	1:A:492:LEU:HD13	1.66	0.59
1:A:487:THR:OG1	3:A:729:HOH:O	2.17	0.59
1:A:296:LEU:HD12	1:A:297:PHE:CZ	2.39	0.58
1:A:352:LYS:HG3	1:A:357:GLU:HB3	1.85	0.58
1:A:519:TRP:HE1	1:A:525:SER:HG	1.53	0.57
1:A:32:GLU:O	1:A:36:LEU:HD22	2.04	0.57
1:A:261:ARG:HD2	3:A:644:HOH:O	2.03	0.57
1:A:109:ILE:H	1:A:109:ILE:CD1	2.13	0.56
1:A:374:ILE:HG13	1:A:386:LEU:HD23	1.88	0.56
1:A:77:ASP:OD2	3:A:746:HOH:O	2.17	0.55
1:A:31:ASP:OD2	1:A:35:LYS:HE2	2.06	0.55
1:A:302:ARG:HB2	1:A:302:ARG:NH1	2.20	0.54
1:A:311:TRP:HA	1:A:314:ILE:HD11	1.89	0.54
1:A:120:ILE:HD11	1:A:355:LYS:HG2	1.90	0.54
1:A:40:ASN:OD1	1:A:43:ASN:HB2	2.08	0.54
1:A:208:HIS:HE1	3:A:742:HOH:O	1.90	0.54
1:A:532:LYS:NZ	1:A:536:ASP:OD2	2.39	0.54
1:A:38:THR:O	1:A:44:LYS:NZ	2.41	0.53
1:A:201:ILE:HD13	1:A:259:LEU:HD21	1.90	0.53
1:A:39:ASN:ND2	1:A:89:ASN:HD21	2.06	0.53
1:A:237:ILE:HD11	1:A:242:ASN:HD21	1.73	0.53
1:A:361:LYS:HB2	1:A:361:LYS:HZ2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HD12	1:A:38:THR:HG23	1.91	0.52
1:A:310:ARG:HB2	1:A:310:ARG:NH1	2.24	0.52
1:A:509:GLN:O	1:A:514:GLU:HG2	2.09	0.52
1:A:276:LEU:HG	1:A:388:SER:HB3	1.90	0.52
1:A:216:ASP:OD2	1:A:219:VAL:HG23	2.10	0.51
1:A:189:TYR:CZ	1:A:193:ILE:HG13	2.46	0.50
1:A:193:ILE:HD13	1:A:193:ILE:O	2.11	0.50
1:A:115:LYS:HE3	1:A:115:LYS:HA	1.92	0.50
1:A:444:MET:HE3	1:A:444:MET:HA	1.93	0.49
1:A:167:ASN:C	1:A:167:ASN:ND2	2.70	0.49
1:A:40:ASN:ND2	1:A:43:ASN:H	2.11	0.48
1:A:311:TRP:HE3	1:A:314:ILE:HD11	1.77	0.48
1:A:294:SER:OG	1:A:505:ASN:OD1	2.32	0.48
1:A:97:LEU:HD23	1:A:282:VAL:HB	1.96	0.47
1:A:237:ILE:HD11	1:A:242:ASN:ND2	2.30	0.47
1:A:306:ILE:O	1:A:306:ILE:HD12	2.15	0.47
1:A:86:LYS:O	1:A:368:SER:HB3	2.15	0.46
1:A:229:ARG:HG3	1:A:230:LYS:N	2.29	0.46
1:A:413:LEU:HG	1:A:417:ILE:HG12	1.99	0.45
1:A:369:ASP:HB2	3:A:738:HOH:O	2.16	0.45
1:A:450:ALA:N	1:A:451:PRO:CD	2.79	0.45
1:A:293:HIS:HE1	1:A:356:SER:O	2.00	0.45
1:A:164:GLN:HE21	1:A:164:GLN:HA	1.81	0.45
1:A:12:LEU:HD12	1:A:12:LEU:HA	1.88	0.44
1:A:313:MET:HG2	1:A:510:LEU:HB3	2.00	0.43
1:A:336:LYS:HE3	1:A:337:LEU:HG	1.99	0.43
1:A:336:LYS:HA	1:A:337:LEU:HA	1.76	0.43
1:A:361:LYS:HB2	1:A:361:LYS:HZ3	1.80	0.43
1:A:244:LEU:HA	1:A:244:LEU:HD12	1.73	0.43
1:A:503:PRO:HB2	1:A:506:ASN:ND2	2.32	0.43
1:A:309:ASP:O	1:A:313:MET:HG3	2.19	0.42
1:A:186:ILE:HD13	1:A:186:ILE:HA	1.83	0.42
1:A:339:GLN:HA	1:A:342:LYS:HD3	2.00	0.42
1:A:374:ILE:HD13	1:A:381:VAL:HB	2.01	0.42
1:A:527:LYS:HE2	1:A:531:GLU:OE1	2.19	0.42
1:A:323:LYS:HE2	1:A:349:ILE:HG22	2.01	0.42
1:A:517:SER:C	1:A:519:TRP:H	2.27	0.42
1:A:103:GLY:HA2	1:A:134:ALA:O	2.21	0.41
1:A:341:LEU:H	1:A:341:LEU:HG	1.61	0.41
1:A:49:LYS:HA	1:A:483:LEU:HD22	2.03	0.41
1:A:296:LEU:HD22	1:A:296:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ILE:HG13	1:A:386:LEU:CD2	2.50	0.41
1:A:316:LEU:O	1:A:320:MET:HG2	2.20	0.41
1:A:518:LEU:HD23	1:A:518:LEU:HA	1.93	0.41
1:A:519:TRP:HZ2	1:A:529:GLN:OE1	2.04	0.41
1:A:336:LYS:HB3	1:A:337:LEU:HB2	2.03	0.40
1:A:338:ASP:HB3	1:A:341:LEU:HD11	2.03	0.40
1:A:33:TYR:HA	1:A:36:LEU:CD2	2.51	0.40

All (2) 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)
3:A:777:HOH:O	3:A:781:HOH:O[4_564]	1.93	0.27
1:A:69:ARG:NH2	1:A:157:GLU:OE1[4_564]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

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	457/555 (82%)	440 (96%)	16 (4%)	1 (0%)	43 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	GLU

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	472/509 (93%)	436 (92%)	36 (8%)	12	14

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	7	GLU
1	A	9	LEU
1	A	36	LEU
1	A	38	THR
1	A	39	ASN
1	A	40	ASN
1	A	43	ASN
1	A	74	LEU
1	A	79	LEU
1	A	90	THR
1	A	93	VAL
1	A	128	LEU
1	A	156	LEU
1	A	161	GLN
1	A	167	ASN
1	A	186	ILE
1	A	190	LYS
1	A	193	ILE
1	A	220	LEU
1	A	244	LEU
1	A	247	GLU
1	A	276	LEU
1	A	296	LEU
1	A	302	ARG
1	A	306	ILE
1	A	314	ILE
1	A	340	GLN
1	A	341	LEU
1	A	347	LEU
1	A	361	LYS
1	A	394	LEU
1	A	436	ASN
1	A	446	LEU
1	A	467	LEU

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Mol	Chain	Res	Type
1	A	492	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	96	ASN
1	A	125	ASN
1	A	161	GLN
1	A	164	GLN
1	A	167	ASN
1	A	208	HIS
1	A	226	ASN
1	A	242	ASN
1	A	293	HIS
1	A	366	ASN
1	A	384	GLN
1	A	411	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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 [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	537/555 (96%)	-0.32	10 (1%) 66 63	18, 40, 95, 140	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	LEU	4.1
1	A	306	ILE	3.6
1	A	519	TRP	3.3
1	A	518	LEU	3.1
1	A	324	LYS	2.6
1	A	538	THR	2.6
1	A	161	GLN	2.6
1	A	516	ASN	2.4
1	A	37	THR	2.3
1	A	347	LEU	2.3

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](#)

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	MN	A	1542	1/1	0.94	0.10	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.