



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:13 PM UTC

PDB ID : 8DCN / pdb_00008dcn
Title : Crystal structure of Clostridioides difficile binary toxin CDTb D4 fragment in complex with BINTOXB/9 Fab
Authors : Goldsmith, J.A.; McLellan, J.S.
Deposited on : 2022-06-16
Resolution : 2.60 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

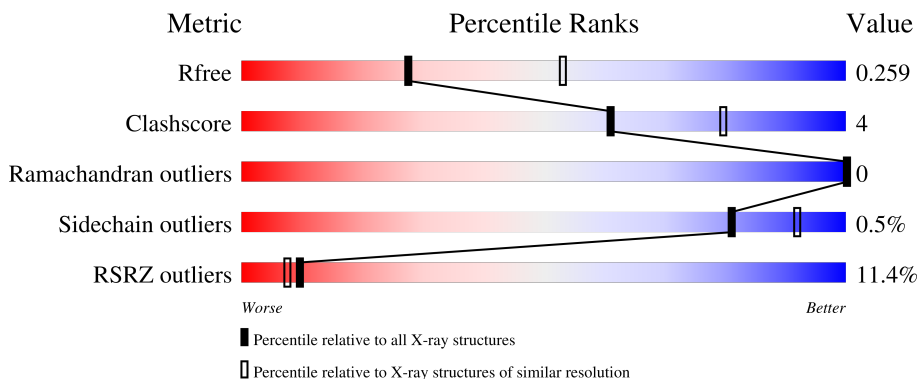
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	231	 2% 86% 6% 7%
1	D	231	 6% 86% 6% 7%
2	B	219	 8% 91% 8%
2	E	219	 18% 90% 9%
3	C	130	 8% 75% 18% 7%

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Mol	Chain	Length	Quality of chain
3	F	130	 <p>A horizontal bar chart showing the quality of chain for Mol 3, Chain F, Length 130. The bar is divided into four segments: 29% red, 76% green, 17% yellow, and 7% grey. The percentages are labeled above and below the segments.</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8723 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 BINTOXB/9 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	Total 1643	C 1043	N 265	O 326	S 9	0	0	0
1	D	214	Total 1639	C 1041	N 264	O 325	S 9	0	0	0

- Molecule 2 is a protein called BINTOXB/9 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	218	Total 1692	C 1055	N 286	O 344	S 7	0	0	0
2	E	218	Total 1692	C 1055	N 286	O 344	S 7	0	0	0

- Molecule 3 is a protein called ADP-ribosylating binary toxin binding subunit CdtB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	121	Total 989	C 631	N 162	O 192	S 4	0	0	0
3	F	121	Total 989	C 631	N 162	O 192	S 4	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	753	MET	-	initiating methionine	UNP A8DS70
C	877	HIS	-	expression tag	UNP A8DS70
C	878	HIS	-	expression tag	UNP A8DS70
C	879	HIS	-	expression tag	UNP A8DS70
C	880	HIS	-	expression tag	UNP A8DS70
C	881	HIS	-	expression tag	UNP A8DS70
C	882	HIS	-	expression tag	UNP A8DS70
F	753	MET	-	initiating methionine	UNP A8DS70

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Chain	Residue	Modelled	Actual	Comment	Reference
F	877	HIS	-	expression tag	UNP A8DS70
F	878	HIS	-	expression tag	UNP A8DS70
F	879	HIS	-	expression tag	UNP A8DS70
F	880	HIS	-	expression tag	UNP A8DS70
F	881	HIS	-	expression tag	UNP A8DS70
F	882	HIS	-	expression tag	UNP A8DS70

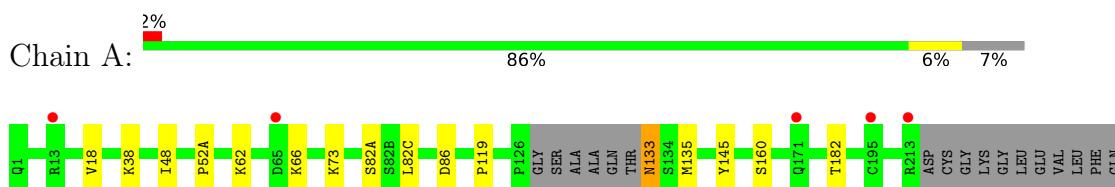
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	20	Total O 20 20	0	0
4	B	21	Total O 21 21	0	0
4	C	4	Total O 4 4	0	0
4	D	19	Total O 19 19	0	0
4	E	13	Total O 13 13	0	0
4	F	2	Total O 2 2	0	0

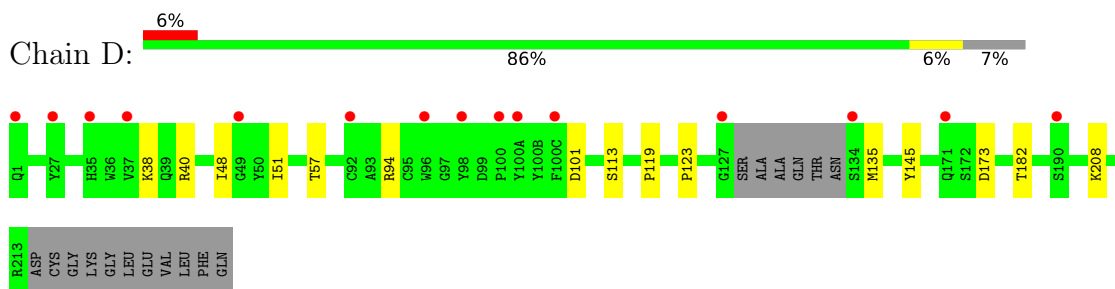
3 Residue-property plots [i](#)

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.

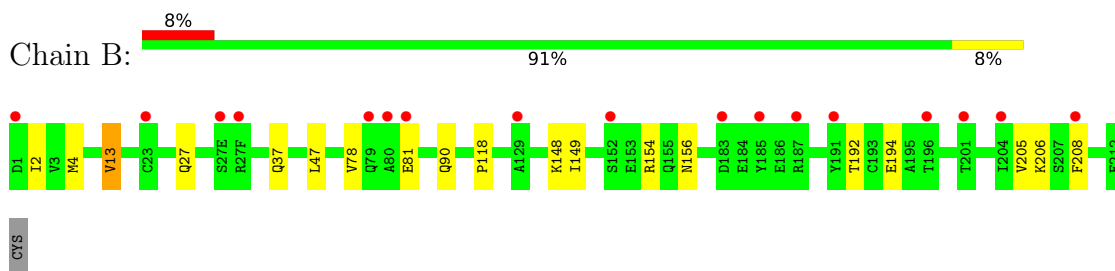
- Molecule 1: BINTOXB/9 Fab heavy chain



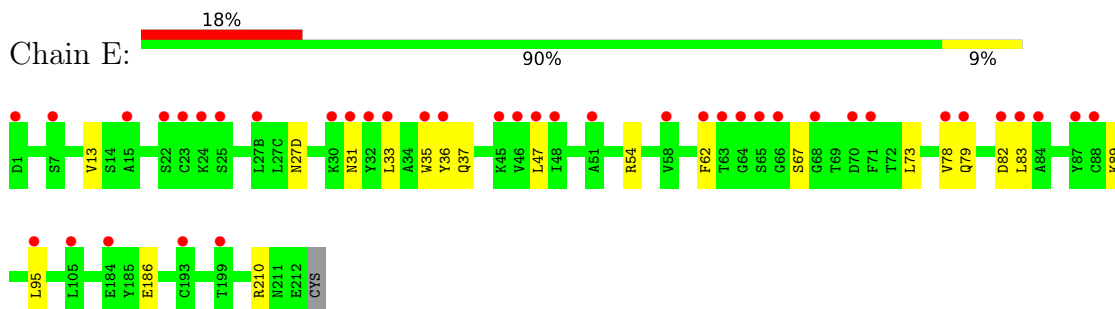
- Molecule 1: BINTOXB/9 Fab heavy chain



- Molecule 2: BINTOXB/9 Fab light chain



- Molecule 2: BINTOXB/9 Fab light chain



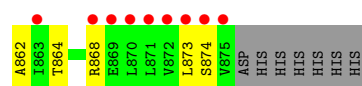
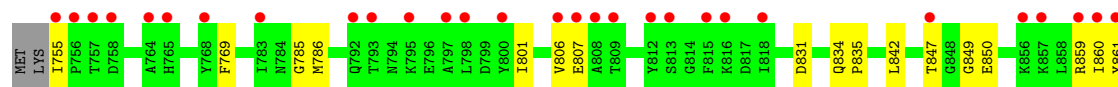
- Molecule 3: ADP-ribosylating binary toxin binding subunit CdtB

Chain C:



- Molecule 3: ADP-ribosylating binary toxin binding subunit CdtB

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.21Å 111.76Å 148.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.88 – 2.60 55.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (55.88-2.60) 99.2 (55.88-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.227 , 0.260 0.227 , 0.259	Depositor DCC
R_{free} test set	2483 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtrriage
Anisotropy	0.353	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8723	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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](#)

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	0.09	0/1691	0.29	0/2314
1	D	0.10	0/1687	0.29	0/2308
2	B	0.20	0/1727	0.33	0/2342
2	E	0.21	0/1727	0.33	0/2342
3	C	0.09	0/1011	0.27	0/1369
3	F	0.09	0/1011	0.29	0/1369
All	All	0.15	0/8854	0.31	0/12044

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	1643	0	1576	9	0
1	D	1639	0	1573	10	0
2	B	1692	0	1646	13	0
2	E	1692	0	1646	12	0
3	C	989	0	964	15	0
3	F	989	0	964	14	0
4	A	20	0	0	0	0
4	B	21	0	0	0	0
4	C	4	0	0	0	0
4	D	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	13	0	0	0	0
4	F	2	0	0	0	0
All	All	8723	0	8369	72	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 4.

The worst 5 of 72 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)
3:C:783:ILE:HD11	3:C:854:THR:HA	1.66	0.77
2:E:13:VAL:HG11	2:E:78:VAL:HG21	1.67	0.76
2:B:13:VAL:HG21	2:B:78:VAL:HG21	1.67	0.76
1:A:52(A):PRO:O	1:A:73:LYS:NZ	2.19	0.75
3:F:801:ILE:HD12	3:F:862:ALA:HB1	1.71	0.70

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	210/231 (91%)	209 (100%)	1 (0%)	0	100	100
1	D	210/231 (91%)	209 (100%)	1 (0%)	0	100	100
2	B	216/219 (99%)	208 (96%)	8 (4%)	0	100	100
2	E	216/219 (99%)	206 (95%)	10 (5%)	0	100	100
3	C	119/130 (92%)	119 (100%)	0	0	100	100
3	F	119/130 (92%)	117 (98%)	2 (2%)	0	100	100
All	All	1090/1160 (94%)	1068 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	187/199 (94%)	185 (99%)	2 (1%)	65	84
1	D	186/199 (94%)	186 (100%)	0	100	100
2	B	194/195 (100%)	193 (100%)	1 (0%)	81	92
2	E	194/195 (100%)	193 (100%)	1 (0%)	81	92
3	C	108/117 (92%)	108 (100%)	0	100	100
3	F	108/117 (92%)	107 (99%)	1 (1%)	70	87
All	All	977/1022 (96%)	972 (100%)	5 (0%)	81	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	160	SER
2	B	13	VAL
2	E	33	LEU
3	F	755	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	27(D)	ASN
2	E	31	ASN
3	F	833	ASN
3	F	784	ASN
3	F	802	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	214/231 (92%)	0.39	5 (2%) 61 55	36, 54, 76, 92	0
1	D	214/231 (92%)	0.54	15 (7%) 22 18	37, 59, 77, 89	0
2	B	218/219 (99%)	0.74	17 (7%) 19 15	42, 58, 91, 108	0
2	E	218/219 (99%)	1.21	40 (18%) 3 3	42, 71, 100, 128	0
3	C	121/130 (93%)	0.87	11 (9%) 15 11	49, 64, 96, 101	0
3	F	121/130 (93%)	1.49	38 (31%) 1 1	53, 72, 121, 141	0
All	All	1106/1160 (95%)	0.82	126 (11%) 10 7	36, 61, 96, 141	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	875	VAL	6.4
2	B	79	GLN	4.6
3	F	871	LEU	4.4
3	F	873	LEU	4.1
2	E	68	GLY	4.0

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.