



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2025 – 02:14 PM JST

PDB ID : 9UBF / pdb_00009ubf
Title : X-ray structure of Clostridioides difficile autolysin Acd33800 catalytic domain
Authors : Kamitori, S.; Nonaka, Y.; Sekiya, H.; Tamai, E.
Deposited on : 2025-04-03
Resolution : 1.45 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

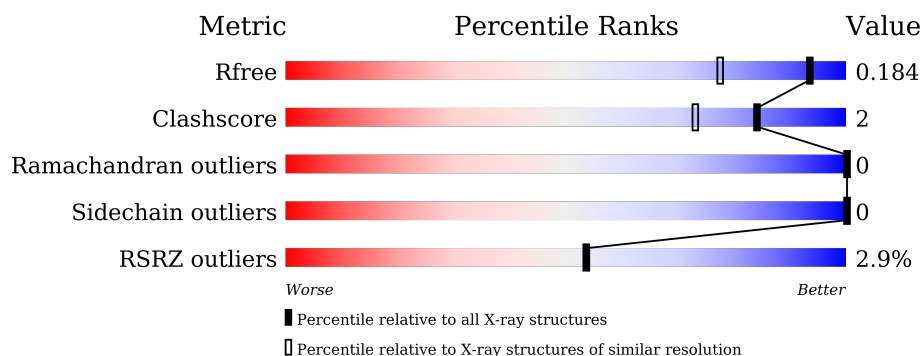
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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}	164625	1556 (1.46-1.46)
Clashscore	180529	1653 (1.46-1.46)
Ramachandran outliers	177936	1635 (1.46-1.46)
Sidechain outliers	177891	1635 (1.46-1.46)
RSRZ outliers	164620	1556 (1.46-1.46)

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	139	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>• • 12%</div> </div> </div>
1	B	139	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>• 13%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2173 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 Cell wall hydrolase Tn916-like,CTn7-Orf16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	2	0
			970	614	164	187	5			
1	B	121	Total	C	N	O	S	0	2	0
			950	603	161	181	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	MET	-	initiating methionine	UNP Q180M8
A	198	ASN	-	expression tag	UNP Q180M8
A	199	HIS	-	expression tag	UNP Q180M8
A	200	LYS	-	expression tag	UNP Q180M8
A	201	VAL	-	expression tag	UNP Q180M8
A	202	HIS	-	expression tag	UNP Q180M8
A	203	HIS	-	expression tag	UNP Q180M8
A	204	HIS	-	expression tag	UNP Q180M8
A	205	HIS	-	expression tag	UNP Q180M8
A	206	HIS	-	expression tag	UNP Q180M8
A	207	HIS	-	expression tag	UNP Q180M8
A	208	MET	-	expression tag	UNP Q180M8
B	197	MET	-	initiating methionine	UNP Q180M8
B	198	ASN	-	expression tag	UNP Q180M8
B	199	HIS	-	expression tag	UNP Q180M8
B	200	LYS	-	expression tag	UNP Q180M8
B	201	VAL	-	expression tag	UNP Q180M8
B	202	HIS	-	expression tag	UNP Q180M8
B	203	HIS	-	expression tag	UNP Q180M8
B	204	HIS	-	expression tag	UNP Q180M8
B	205	HIS	-	expression tag	UNP Q180M8
B	206	HIS	-	expression tag	UNP Q180M8
B	207	HIS	-	expression tag	UNP Q180M8
B	208	MET	-	expression tag	UNP Q180M8

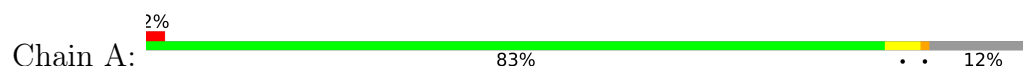
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total 132	O 132	0	0
2	B	121	Total 121	O 121	0	0

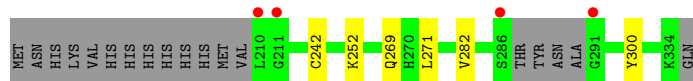
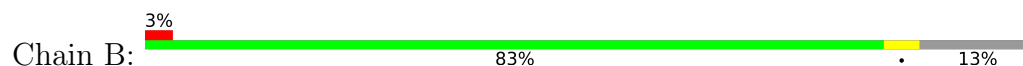
3 Residue-property plots [i](#)

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: Cell wall hydrolase Tn916-like,CTn7-Orf16



- Molecule 1: Cell wall hydrolase Tn916-like,CTn7-Orf16



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	105.26Å 105.26Å 63.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.39 – 1.45 30.39 – 1.45	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.39-1.45) 96.8 (30.39-1.45)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.41 (at 1.45Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.163 , 0.185 0.163 , 0.184	Depositor DCC
R_{free} test set	2106 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.008 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.007 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.008 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.016 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.007 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.017 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2173	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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

5.1 Standard geometry

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

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	0.34	0/984	0.69	0/1335
1	B	0.36	0/962	0.66	0/1302
All	All	0.35	0/1946	0.68	0/2637

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

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	970	0	905	4	0
1	B	950	0	896	4	0
2	A	132	0	0	1	0
2	B	121	0	0	2	0
All	All	2173	0	1801	8	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 2.

The worst 5 of 8 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:B:271:LEU:HD23	1:B:271:LEU:N	2.26	0.51
1:B:252:LYS:HE3	2:B:472:HOH:O	2.14	0.46
1:A:258:PRO:HB2	1:A:263:MHO:HE3	1.97	0.45
1:A:277:LYS:HD3	1:A:332:ARG:NH2	2.32	0.45
1:A:242:OCS:OD1	1:A:296:HIS:HA	2.18	0.43

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	121/139 (87%)	119 (98%)	2 (2%)	0	100	100
1	B	117/139 (84%)	115 (98%)	2 (2%)	0	100	100
All	All	238/278 (86%)	234 (98%)	4 (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	98/112 (88%)	98 (100%)	0	100	100
1	B	96/112 (86%)	96 (100%)	0	100	100
All	All	194/224 (87%)	194 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OCS	B	242	1	7,8,9	0.83	0	6,11,13	3.15	3 (50%)
1	MHO	B	263	1	7,8,9	0.78	0	4,9,11	0.51	0
1	OCS	A	242	1	7,8,9	0.99	0	6,11,13	2.46	3 (50%)
1	MHO	A	263	1	7,8,9	0.73	0	4,9,11	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	B	242	1	-	3/4/7/9	-
1	MHO	B	263	1	-	1/6/7/9	-
1	OCS	A	242	1	-	3/4/7/9	-
1	MHO	A	263	1	-	0/6/7/9	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	OCS	OD3-SG-CB	5.86	113.91	106.94
1	A	242	OCS	OD3-SG-CB	4.62	112.43	106.94
1	B	242	OCS	OD2-SG-CB	3.99	112.10	105.74
1	A	242	OCS	OD1-SG-CB	2.89	110.38	106.94
1	A	242	OCS	OD2-SG-OD3	-2.40	105.42	111.27

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	242	OCS	CA-CB-SG-OD1
1	A	242	OCS	CA-CB-SG-OD2
1	A	242	OCS	CA-CB-SG-OD3
1	B	242	OCS	CA-CB-SG-OD1
1	B	242	OCS	CA-CB-SG-OD2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	242	OCS	1	0
1	A	263	MHO	1	0

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	121/139 (87%)	0.07	3 (2%) 58 58	12, 19, 32, 53	2 (1%)
1	B	119/139 (85%)	0.03	4 (3%) 48 49	9, 20, 41, 56	2 (1%)
All	All	240/278 (86%)	0.05	7 (2%) 54 53	9, 20, 38, 56	4 (1%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	210	LEU	3.6
1	A	231	TYR	3.4
1	A	334	LYS	2.7
1	A	321	SER	2.6
1	B	291	GLY	2.5

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	OCS	A	242	9/10	0.97	0.09	14,17,36,39	0
1	MHO	A	263	9/10	0.98	0.06	16,18,31,33	0
1	OCS	B	242	9/10	0.98	0.06	11,13,20,24	0
1	MHO	B	263	9/10	0.98	0.06	16,16,22,29	0

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.