



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:46 AM UTC

PDB ID : 8YXK / pdb_00008yxk
Title : X-ray structure of Clostridioides difficile endolysin Ecd09610 glucosaminidase domain.
Authors : Kamitori, S.; Tamai, E.
Deposited on : 2024-04-02
Resolution : 1.87 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

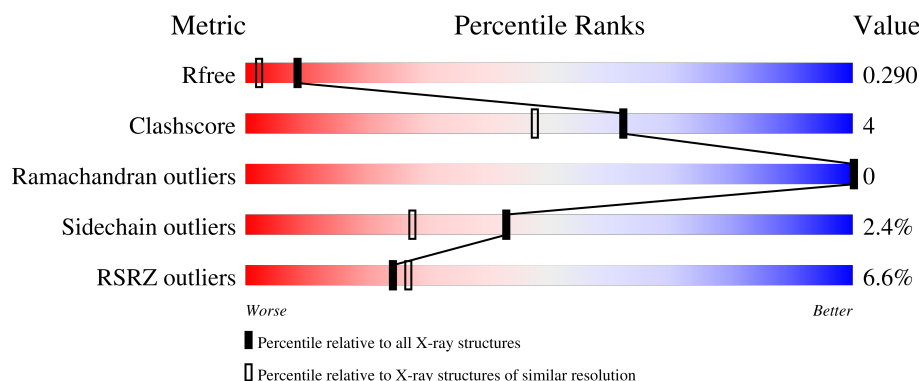
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	201	5% 67% 8% 25%
1	B	201	4% 67% 7% 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2406 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 Phage cell wall hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1163	725	206	227	5			
1	B	151	Total	C	N	O	S	0	0	0
			1163	725	206	227	5			

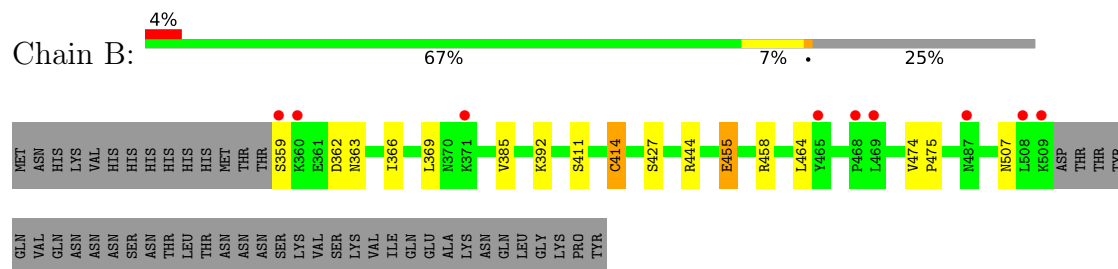
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	345	MET	-	initiating methionine	UNP Q183Y3
A	346	ASN	-	expression tag	UNP Q183Y3
A	347	HIS	-	expression tag	UNP Q183Y3
A	348	LYS	-	expression tag	UNP Q183Y3
A	349	VAL	-	expression tag	UNP Q183Y3
A	350	HIS	-	expression tag	UNP Q183Y3
A	351	HIS	-	expression tag	UNP Q183Y3
A	352	HIS	-	expression tag	UNP Q183Y3
A	353	HIS	-	expression tag	UNP Q183Y3
A	354	HIS	-	expression tag	UNP Q183Y3
A	355	HIS	-	expression tag	UNP Q183Y3
A	356	MET	-	expression tag	UNP Q183Y3
B	345	MET	-	initiating methionine	UNP Q183Y3
B	346	ASN	-	expression tag	UNP Q183Y3
B	347	HIS	-	expression tag	UNP Q183Y3
B	348	LYS	-	expression tag	UNP Q183Y3
B	349	VAL	-	expression tag	UNP Q183Y3
B	350	HIS	-	expression tag	UNP Q183Y3
B	351	HIS	-	expression tag	UNP Q183Y3
B	352	HIS	-	expression tag	UNP Q183Y3
B	353	HIS	-	expression tag	UNP Q183Y3
B	354	HIS	-	expression tag	UNP Q183Y3
B	355	HIS	-	expression tag	UNP Q183Y3
B	356	MET	-	expression tag	UNP Q183Y3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	33	Total 33	O 33	0	0
2	B	47	Total 47	O 47	0	0

- Molecule 1: Phage cell wall hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.43Å 80.47Å 48.77Å 90.00° 104.12° 90.00°	Depositor
Resolution (Å)	19.32 – 1.87 19.32 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.32-1.87) 98.5 (19.32-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.247 , 0.287 0.252 , 0.290	Depositor DCC
R_{free} test set	1501 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2406	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4034e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	1.02	0/1182	1.37	0/1583
1	B	1.00	0/1182	1.39	0/1583
All	All	1.01	0/2364	1.38	0/3166

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	1163	0	1154	8	0
1	B	1163	0	1154	11	0
2	A	33	0	0	0	0
2	B	47	0	0	4	0
All	All	2406	0	2308	19	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.

All (19) 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:444:ARG:HD3	2:B:603:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:SER:OG	1:B:414:CYS:HB3	2.07	0.55
1:A:442:LEU:O	1:A:446:TYR:HB2	2.07	0.54
1:A:366:ILE:HG13	1:A:385:VAL:HG21	1.93	0.51
1:A:421:PHE:CD2	1:A:438:GLY:HA3	2.48	0.48
1:A:392:LYS:HE3	1:A:507:ASN:ND2	2.29	0.48
1:B:392:LYS:HE3	1:B:507:ASN:HD21	1.79	0.47
1:B:455:GLU:CG	2:B:638:HOH:O	2.64	0.46
1:B:458:ARG:HD3	1:B:464:LEU:CD1	2.46	0.45
1:A:376:LYS:HD2	1:A:415:LYS:HA	1.98	0.44
1:A:413:LEU:HD12	1:A:417:LYS:CD	2.47	0.44
1:B:359:SER:HA	1:B:362:ASP:HB2	1.99	0.43
1:A:413:LEU:HD12	1:A:417:LYS:HD3	2.01	0.42
1:B:455:GLU:HG3	2:B:638:HOH:O	2.20	0.42
1:B:359:SER:O	1:B:363:ASN:ND2	2.53	0.41
1:B:366:ILE:HG13	1:B:385:VAL:HG21	2.03	0.41
1:B:474:VAL:N	1:B:475:PRO:CD	2.84	0.41
1:B:444:ARG:CG	2:B:603:HOH:O	2.69	0.40
1:A:474:VAL:N	1:A:475:PRO:HD2	2.36	0.40

There are no symmetry-related clashes.

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	149/201 (74%)	147 (99%)	2 (1%)	0	100	100
1	B	149/201 (74%)	146 (98%)	3 (2%)	0	100	100
All	All	298/402 (74%)	293 (98%)	5 (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	127/175 (73%)	125 (98%)	2 (2%)	55	43
1	B	127/175 (73%)	123 (97%)	4 (3%)	35	18
All	All	254/350 (73%)	248 (98%)	6 (2%)	43	27

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	369	LEU
1	A	455	GLU
1	B	369	LEU
1	B	414	CYS
1	B	427	SER
1	B	455	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	448	HIS
1	B	363	ASN
1	B	501	ASN
1	B	507	ASN

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	151/201 (75%)	0.52	11 (7%) 21 24	14, 20, 38, 66	0
1	B	151/201 (75%)	0.45	9 (5%) 27 30	12, 20, 38, 64	0
All	All	302/402 (75%)	0.48	20 (6%) 24 27	12, 20, 38, 66	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	TYR	5.3
1	B	509	LYS	5.1
1	B	508	LEU	4.3
1	A	509	LYS	4.0
1	A	464	LEU	3.8
1	A	359	SER	3.5
1	B	359	SER	3.4
1	A	360	LYS	3.1
1	A	508	LEU	3.1
1	A	427	SER	2.9
1	A	363	ASN	2.8
1	B	469	LEU	2.5
1	A	361	GLU	2.5
1	A	471	LYS	2.3
1	A	507	ASN	2.2
1	B	360	LYS	2.2
1	B	468	PRO	2.2
1	B	487	ASN	2.1
1	B	371	LYS	2.0
1	A	465	TYR	2.0

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.