

wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 01:14 am BST

PDB ID : 5NCD

Title : Crystal structure of the polysaccharide deacetylase Bc1974 from Bacillus cereus

in complex with (2S)-2-amino-5-(diaminomethylideneamino)-N-hydroxypenta

namide

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Deposited on : 2017-03-03

Resolution : 2.45 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

Mol Probity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

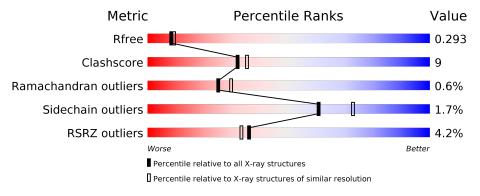
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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 on 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 <=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	247	68%	14%	 17%
1	В	247	67%	15%	17%
1	С	247	65%	18%	17%
1	D	247	67%	16%	17%



2 Entry composition (i)

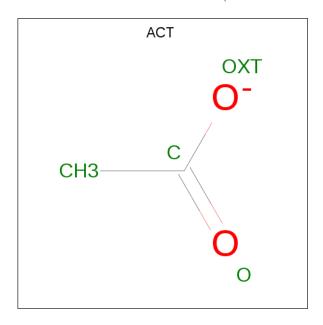
There are 6 unique types of molecules in this entry. The entry contains 6798 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peptidoglycan N-acetylglucosamine deacetylase.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace	
1	Λ	206	Total	С	N	О	S	0	0	0	
1	1 A	200	1651	1057	284	303	7	0	U		
1	В	206	Total	С	N	О	S	0	0	0	
1	Б	200	1651	1057	284	303	7	U			
1	С	206	Total	С	N	О	S	0	0	0	
1		200	1645	1054	281	303	7	U			
1	1 D	D	D 2006	Total	С	N	О	S	0	0	0
1		206	1664	1066	286	305	7	0	2		

• Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	С	1	Total C O 4 2 2	0	0

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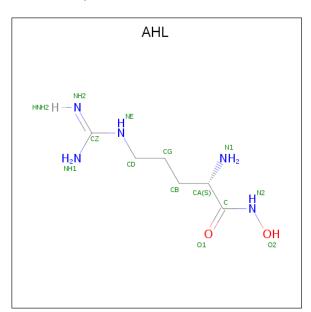
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Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf
2	D	1	Total 4	C 2	O 2	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	С	1	Total Zn 1 1	0	0

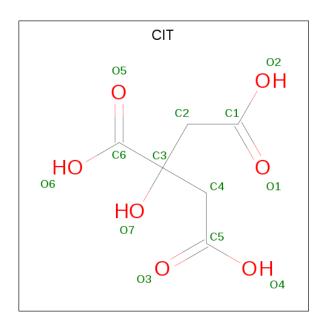
• Molecule 4 is N-HYDROXY-L-ARGININAMIDE (three-letter code: AHL) (formula: $C_6H_{15}N_5O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	В	1	Total 13	C 6	N 5	O 2	0	0

 \bullet Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $\mathrm{C_6H_8O_7}).$





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	В	1	Total 13	C 6	O 7	0	0

• Molecule 6 is water.

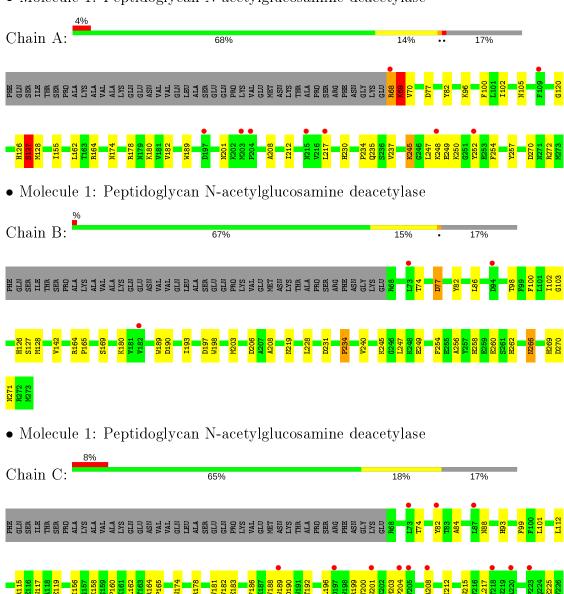
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	39	Total O 39 39	0	0
6	В	45	Total O 45 45	0	0
6	С	30	Total O 30 30	0	0
6	D	31	Total O 31 31	0	0



3 Residue-property plots (i)

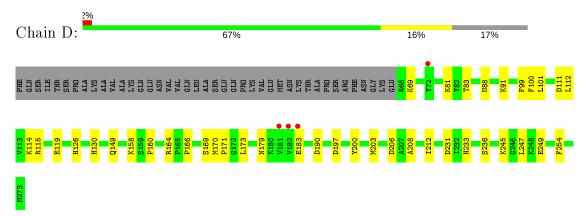
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Peptidoglycan N-acetylglucosamine deacetylase





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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	$50.65 \text{\AA} 117.44 \text{Å} 99.49 \text{Å}$	Danagitan
a, b, c, α , β , γ	90.00° 102.92° 90.00°	Depositor
Resolution (Å)	48.48 - 2.45	Depositor
Resolution (A)	48.48 - 2.45	EDS
% Data completeness	98.0 (48.48-2.45)	Depositor
(in resolution range)	98.4 (48.48-2.45)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.42 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
D D.	0.226 , 0.292	Depositor
R, R_{free}	0.228 , 0.293	DCC
R_{free} test set	2051 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 46.0	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6798	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 19.13% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: ZN, ACT, AHL, CIT

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.45	0/1696	0.62	0/2295	
1	В	0.45	0/1696	0.60	$1/2295 \ (0.0\%)$	
1	С	0.44	0/1690	0.58	0/2288	
1	D	0.43	0/1716	0.56	0/2322	
All	All	0.44	0/6798	0.59	$1/9200 \ (0.0\%)$	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
1	В	77	ASP	CB-CG-OD1	5.05	122.84	118.30

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	1651	0	1611	30	0
1	В	1651	0	1611	31	0
1	С	1645	0	1600	27	0
1	D	1664	0	1624	29	0
2	A	4	0	3	0	0
2	С	4	0	3	1	0

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-	110111	picolous	payc

Mol	Chain	Non-H	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
2	D	4	0	3	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	В	13	0	14	4	0
5	В	13	0	5	2	0
6	A	39	0	0	2	0
6	В	45	0	0	6	0
6	С	30	0	0	0	0
6	D	31	0	0	2	0
All	All	6798	0	6474	117	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 9.

The worst 5 of 117 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:B:128:MET:SD	6:B:408:HOH:O	2.14	1.05
1:C:117:ASN:HD22	1:C:156:ILE:HB	1.32	0.91
1:A:69:LYS:HB2	1:A:252:TYR:HA	1.66	0.76
1:B:228:LEU:HD21	4:B:301:AHL:N1	2.02	0.74
1:C:88:ASN:OD1	1:C:115:ARG:NH2	2.20	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 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	204/247 (83%)	193 (95%)	9 (4%)	2 (1%)	15 16		

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	В	204/247 (83%)	194 (95%)	10 (5%)	0	100	100
1	С	204/247 (83%)	193 (95%)	8 (4%)	3 (2%)	10	9
1	D	206/247 (83%)	194 (94%)	12 (6%)	0	100	100
All	All	818/988 (83%)	774 (95%)	39 (5%)	5 (1%)	25	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	127	SER
1	С	190	ASP
1	С	241	PRO
1	С	204	PRO

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	Chain Analysed Rotameric Outliers		Percentiles	
1	A	173/208~(83%)	167 (96%)	6 (4%)	36 47
1	В	173/208 (83%)	170 (98%)	3 (2%)	60 73
1	С	172/208 (83%)	170 (99%)	2 (1%)	71 81
1	D	175/208~(84%)	174 (99%)	1 (1%)	86 91
All	All	693/832 (83%)	681 (98%)	12 (2%)	60 73

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	${f Res}$	Type
1	A	249	GLU
1	В	189	TRP
1	С	189	TRP
1	A	245	LYS
1	В	266	ASN



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	${f Res}$	Type
1	В	266	ASN
1	С	117	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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	Т	Chain	Res	Link	В	Bond lengths			Bond angles		
Mol Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
4	AHL	В	301	3	12,12,12	0.99	2 (16%)	12,14,14	0.68	0	
2	ACT	С	301	3	1,3,3	1.76	0	0,3,3	0.00	=	
5	CIT	В	303	-	3,12,12	1.34	0	3,17,17	2.16	2 (66%)	
2	ACT	A	301	3	1,3,3	2.25	1 (100%)	0,3,3	0.00	-	
2	ACT	D	301	3	1,3,3	2.29	1 (100%)	0,3,3	0.00	1	

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
4	AHL	В	301	3	-	4/13/13/13	-
5	CIT	В	303	_	-	4/6/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
4	В	301		CZ-NH2		1.42	1.32
2	D	301	ACT	СН3-С	2.29	1.51	1.48
2	A	301	ACT	СН3-С	2.25	1.51	1.48
4	В	301	AHL	CZ-NH1	-2.07	1.26	1.34

All (2) bond angle outliers are listed below:

	Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
	5	В	303	CIT	C3-C4-C5	-2.99	110.20	114.98
Ī	5	В	303	CIT	C3-C2-C1	2.22	118.54	114.98

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	301	AHL	NH1-CZ-NE-CD
4	В	301	AHL	NH2-CZ-NE-CD
5	В	303	CIT	C2-C3-C4-C5
5	В	303	CIT	O7-C3-C4-C5
5	В	303	CIT	C1-C2-C3-C6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	301	AHL	4	0
2	С	301	ACT	1	0
5	В	303	CIT	2	0

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, 95^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	206/247~(83%)	0.60	9 (4%) 34 32	37, 58, 93, 140	0
1	В	206/247~(83%)	0.48	3 (1%) 73 71	34, 55, 74, 112	0
1	С	206/247~(83%)	0.75	19 (9%) 9 6	39, 60, 96, 113	0
1	D	206/247~(83%)	0.55	4 (1%) 66 63	32, 54, 72, 104	0
All	All	824/988 (83%)	0.60	35 (4%) 36 33	32, 57, 92, 140	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	ARG	4.2
1	С	204	PRO	3.5
1	С	245	LYS	3.4
1	A	197	ASP	3.2
1	С	252	TYR	3.1

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 carbohydrates 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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
5	CIT	В	303	13/13	0.78	0.28	74,85,93,96	0
2	ACT	D	301	4/4	0.83	0.21	52,54,60,63	0
2	ACT	A	301	4/4	0.89	0.20	50,56,63,65	0
2	ACT	С	301	4/4	0.90	0.17	44,55,59,60	0
4	AHL	В	301	13/13	0.90	0.23	53,65,80,82	0
3	ZN	A	302	1/1	0.94	0.12	49,49,49,49	0
3	ZN	С	302	1/1	0.95	0.24	79,79,79,79	0
3	ZN	D	302	1/1	0.98	0.17	76,76,76,76	0
3	ZN	В	302	1/1	0.98	0.23	79,79,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.

