



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2018 – 09:47 pm GMT

PDB ID : 1G0C  
Title : ALKALINE CELLULASE K CATALYTIC DOMAIN-CELLOBIOSE COM-  
PLEX  
Authors : Shirai, T.; Ishida, H.; Noda, J.; Yamane, T.; Ozaki, K.; Hakamada, Y.; Ito, S.  
Deposited on : 2000-10-05  
Resolution : 1.90 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

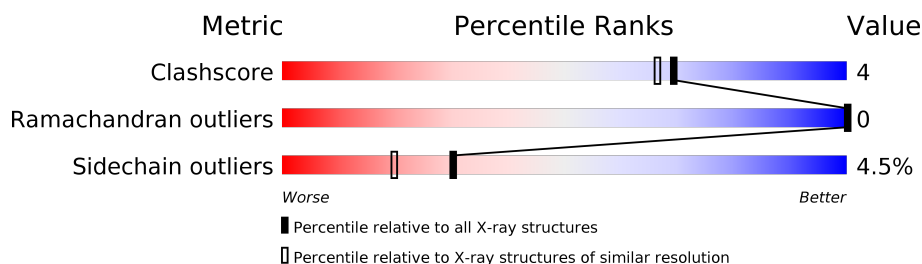
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	122078	6112 (1.90-1.90)
Ramachandran outliers	120005	6045 (1.90-1.90)
Sidechain outliers	119972	6045 (1.90-1.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	364	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CBI	A	585	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3319 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.

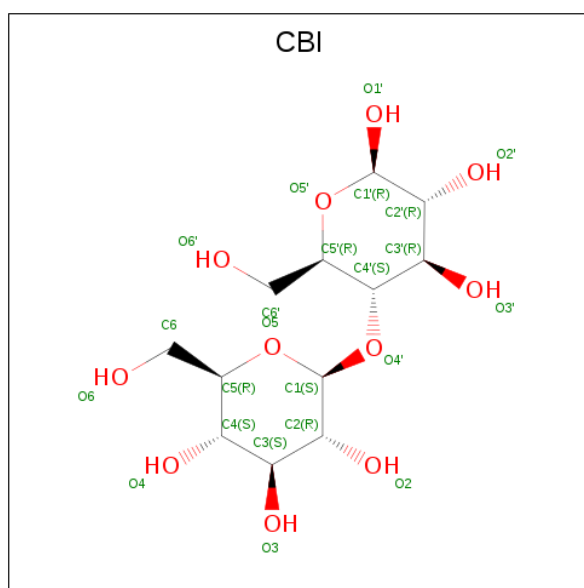
- Molecule 1 is a protein called ENDOGLUCANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	2796	1761	471	555	9	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	GLY	-	CLONING ARTIFACT	UNP P19424
A	222	ARG	-	CLONING ARTIFACT	UNP P19424
A	223	PRO	-	CLONING ARTIFACT	UNP P19424
A	224	ALA	-	CLONING ARTIFACT	UNP P19424
A	225	GLY	-	CLONING ARTIFACT	UNP P19424
A	226	MET	-	CLONING ARTIFACT	UNP P19424
A	227	GLN	-	CLONING ARTIFACT	UNP P19424

- Molecule 2 is CELLOBIOSE (three-letter code: CBI) (formula:  $C_{12}H_{22}O_{11}$ ).

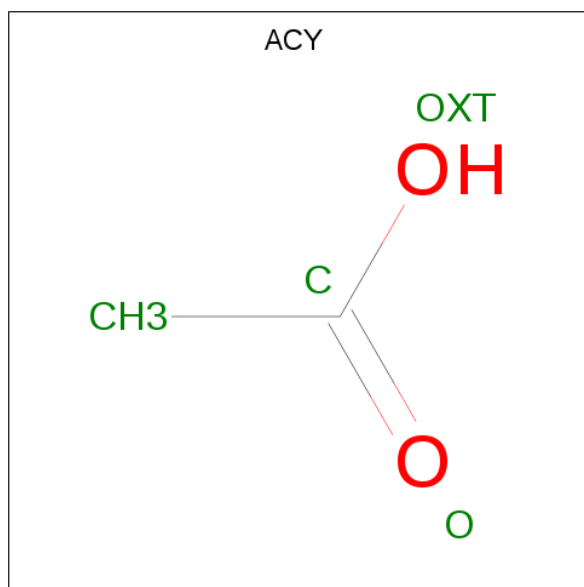


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	Cd	0	0
			10	10		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

- Molecule 5 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	474	Total	O	0	0
			474	474		

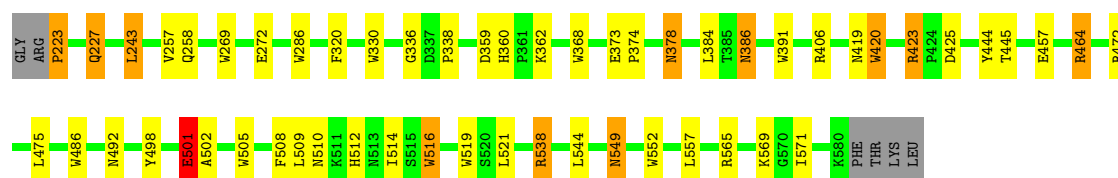
### 3 Residue-property plots [i](#)

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.

Note EDS was not executed.

#### • Molecule 1: ENDOGLUCANASE

Chain A:  83% 12% . .



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.90Å 97.90Å 121.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 1.90	Depositor
% Data completeness (in resolution range)	87.2 (8.00-1.90)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.181 , 0.204	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

## 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: ACY, CBI, CD

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	0.83	0/2876	1.50	46/3925 (1.2%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	ARG	NE-CZ-NH1	16.25	128.43	120.30
1	A	423	ARG	NE-CZ-NH1	-15.76	112.42	120.30
1	A	406	ARG	NE-CZ-NH2	-14.98	112.81	120.30
1	A	464	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	A	423	ARG	NE-CZ-NH2	12.88	126.74	120.30
1	A	464	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	A	391	TRP	CD1-CG-CD2	9.09	113.58	106.30
1	A	420	TRP	CD1-CG-CD2	9.09	113.58	106.30
1	A	486	TRP	CD1-CG-CD2	8.57	113.16	106.30
1	A	391	TRP	CE2-CD2-CG	-8.12	100.80	107.30
1	A	420	TRP	CE2-CD2-CG	-7.96	100.93	107.30
1	A	516	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	A	330	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	A	505	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	A	552	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	A	330	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	A	286	TRP	CD1-CG-CD2	7.45	112.26	106.30
1	A	519	TRP	CD1-CG-CD2	7.42	112.23	106.30
1	A	516	TRP	CE2-CD2-CG	-7.42	101.37	107.30
1	A	486	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	A	505	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	A	552	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	A	519	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	A	368	TRP	CD1-CG-CD2	6.99	111.89	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	TRP	CE2-CD2-CG	-6.93	101.76	107.30
1	A	330	TRP	CG-CD2-CE3	6.80	140.02	133.90
1	A	269	TRP	CD1-CG-CD2	6.43	111.44	106.30
1	A	269	TRP	CE2-CD2-CG	-6.26	102.29	107.30
1	A	368	TRP	CE2-CD2-CG	-6.17	102.36	107.30
1	A	391	TRP	CG-CD2-CE3	6.08	139.37	133.90
1	A	257	VAL	CG1-CB-CG2	-5.91	101.44	110.90
1	A	391	TRP	CG-CD1-NE1	-5.91	104.19	110.10
1	A	472	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	A	519	TRP	CG-CD2-CE3	5.77	139.09	133.90
1	A	444	TYR	CB-CG-CD1	-5.68	117.59	121.00
1	A	359	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	538	ARG	NE-CZ-NH2	5.53	123.07	120.30
1	A	486	TRP	CG-CD1-NE1	-5.51	104.59	110.10
1	A	501	GLU	CA-CB-CG	5.47	125.43	113.40
1	A	565	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	391	TRP	CB-CG-CD1	-5.29	120.12	127.00
1	A	420	TRP	CB-CG-CD1	-5.20	120.24	127.00
1	A	320	PHE	CB-CG-CD1	-5.09	117.24	120.80
1	A	519	TRP	CB-CG-CD1	-5.07	120.41	127.00
1	A	420	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	A	549	ASN	CB-CG-ND2	5.04	128.80	116.70

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	2796	0	2581	22	0
2	A	23	0	22	0	0
3	A	10	0	0	0	0
4	A	16	0	12	0	0
5	A	474	0	0	5	0
All	All	3319	0	2615	22	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 (22) 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:258:GLN:HE22	1:A:510:ASN:HD22	1.23	0.84
1:A:508:PHE:O	1:A:512:HIS:HD2	1.77	0.67
1:A:386:ASN:HD21	1:A:423:ARG:HE	1.43	0.67
1:A:258:GLN:HE22	1:A:510:ASN:ND2	1.93	0.67
1:A:360:HIS:HD2	1:A:362:LYS:H	1.46	0.63
1:A:272:GLU:HG2	1:A:544:LEU:HD12	1.85	0.59
1:A:510:ASN:HD21	1:A:516:TRP:HE1	1.49	0.59
1:A:227:GLN:HB3	5:A:934:HOH:O	2.05	0.56
1:A:457:GLU:HG3	5:A:919:HOH:O	2.07	0.55
1:A:475:LEU:HD11	1:A:514:ILE:HD11	1.90	0.52
1:A:378:ASN:H	1:A:378:ASN:HD22	1.59	0.49
1:A:498:TYR:HB3	1:A:501:GLU:HG2	1.96	0.47
1:A:223:PRO:HG2	1:A:571:ILE:HG22	1.98	0.46
1:A:243:LEU:HB3	5:A:619:HOH:O	2.16	0.45
1:A:223:PRO:N	5:A:937:HOH:O	2.50	0.44
1:A:360:HIS:HE1	5:A:818:HOH:O	2.00	0.43
1:A:425:ASP:OD2	1:A:464:ARG:HD2	2.19	0.42
1:A:336:GLY:O	1:A:374:PRO:HA	2.21	0.41
1:A:338:PRO:HD2	1:A:384:LEU:HD11	2.01	0.41
1:A:445:THR:HG21	1:A:502:ALA:HA	2.03	0.41
1:A:373:GLU:HB3	1:A:420:TRP:HA	2.03	0.40
1:A:223:PRO:HD2	1:A:569:LYS:O	2.22	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	356/364 (98%)	344 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	291/297 (98%)	278 (96%)	13 (4%)	30	20

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	PRO
1	A	227	GLN
1	A	243	LEU
1	A	378	ASN
1	A	386	ASN
1	A	419	ASN
1	A	492	ASN
1	A	501	GLU
1	A	509	LEU
1	A	521	LEU
1	A	538	ARG
1	A	549	ASN
1	A	557	LEU

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

Mol	Chain	Res	Type
1	A	239	GLN
1	A	284	ASN
1	A	360	HIS
1	A	378	ASN
1	A	386	ASN

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Mol	Chain	Res	Type
1	A	411	ASN
1	A	436	ASN
1	A	470	ASN
1	A	507	ASN
1	A	510	ASN
1	A	512	HIS
1	A	513	ASN
1	A	550	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 10 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CBI	A	585	-	24,24,24	0.47	0	35,35,35	0.84	3 (8%)
4	ACY	A	596	3	1,3,3	1.61	0	0,3,3	0.00	-
4	ACY	A	597	3	1,3,3	3.11	1 (100%)	0,3,3	0.00	-
4	ACY	A	598	3	1,3,3	3.70	1 (100%)	0,3,3	0.00	-
4	ACY	A	599	3	1,3,3	2.00	1 (100%)	0,3,3	0.00	-

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
2	CBI	A	585	-	1/1/10/10	0/8/48/48	0/2/2/2
4	ACY	A	596	3	-	0/0/0/0	0/0/0/0
4	ACY	A	597	3	-	0/0/0/0	0/0/0/0
4	ACY	A	598	3	-	0/0/0/0	0/0/0/0
4	ACY	A	599	3	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	599	ACY	CH3-C	2.00	1.51	1.48
4	A	597	ACY	CH3-C	3.11	1.52	1.48
4	A	598	ACY	CH3-C	3.70	1.53	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	585	CBI	C3'-C4'-C5'	-2.19	105.84	110.93
2	A	585	CBI	O1'-C1'-O5'	-2.02	104.37	110.44
2	A	585	CBI	C1'-C2'-C3'	2.26	114.88	110.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	585	CBI	C1'

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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.