



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:15 AM UTC

PDB ID : 1G01 / pdb_00001g01
Title : ALKALINE CELLULASE K CATALYTIC DOMAIN
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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

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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

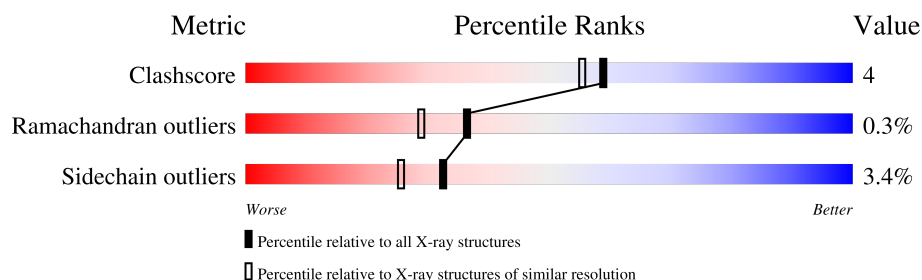
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	364	 78% 17% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3286 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
1	A	357	Total	C	N	O	S	0	0	0
			2791	1758	470	554	9			

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 CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 4 is water.

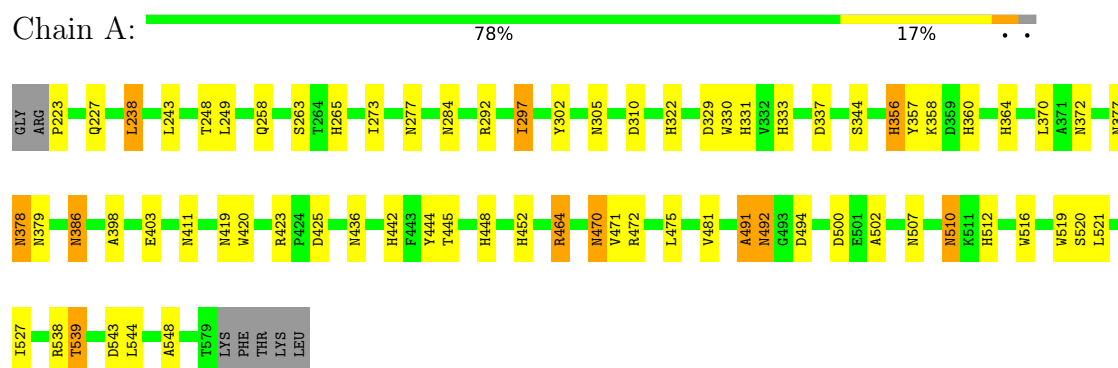
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	465	Total	O	0	0
			465	465		

3 Residue-property plots

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. 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. 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



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, α , β , γ	98.20 Å 98.20 Å 122.00 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.196 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3286	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, 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	0.87	15/2871 (0.5%)	1.58	43/3918 (1.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356	HIS	CD2-NE2	-7.88	1.29	1.37
1	A	442	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	360	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	364	HIS	CD2-NE2	-6.71	1.30	1.37
1	A	322	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	333	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	331	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	265	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	448	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	333	HIS	CG-ND1	-5.96	1.31	1.38
1	A	452	HIS	CG-ND1	-5.94	1.31	1.38
1	A	512	HIS	CD2-NE2	-5.31	1.32	1.37
1	A	452	HIS	CD2-NE2	-5.22	1.32	1.37
1	A	512	HIS	CG-ND1	-5.09	1.32	1.38
1	A	442	HIS	CG-ND1	-5.01	1.32	1.38

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	HIS	CB-CG-CD2	-9.30	119.10	131.20
1	A	510	ASN	OD1-CG-ND2	-8.68	113.92	122.60
1	A	356	HIS	CB-CG-ND1	8.23	135.05	122.70
1	A	360	HIS	CB-CG-CD2	-8.16	120.59	131.20
1	A	329	ASP	CA-CB-CG	7.71	120.31	112.60
1	A	470	ASN	OD1-CG-ND2	-7.28	115.33	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ASN	OD1-CG-ND2	-6.78	115.83	122.60
1	A	360	HIS	CB-CG-ND1	6.67	132.71	122.70
1	A	277	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	A	436	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	A	386	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	A	302	TYR	N-CA-C	5.97	118.56	111.33
1	A	500	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	398	ALA	N-CA-C	5.79	117.68	111.36
1	A	448	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	A	358	LYS	CB-CA-C	-5.70	101.27	110.74
1	A	377	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	A	491	ALA	N-CA-C	5.65	122.83	110.80
1	A	372	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	A	492	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	A	344	SER	N-CA-C	5.57	118.11	111.71
1	A	507	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	A	411	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	A	548	ALA	N-CA-C	5.44	117.97	111.71
1	A	331	HIS	CB-CG-CD2	-5.33	124.28	131.20
1	A	379	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	420	TRP	CG-CD2-CE3	5.31	139.21	133.90
1	A	265	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	A	527	ILE	N-CA-C	5.25	115.98	110.62
1	A	543	ASP	CA-CB-CG	5.25	117.84	112.60
1	A	370	LEU	N-CA-C	5.22	118.80	112.23
1	A	265	HIS	N-CA-C	-5.19	101.70	109.79
1	A	420	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	A	448	HIS	CB-CG-ND1	5.18	130.47	122.70
1	A	310	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	331	HIS	N-CA-C	5.10	117.50	109.39
1	A	297	ILE	N-CA-C	-5.10	107.18	111.56
1	A	403	GLU	CA-CB-CG	-5.08	103.95	114.10
1	A	464	ARG	NE-CZ-NH1	5.04	126.53	121.50
1	A	305	ASN	CA-C-N	5.00	124.66	119.56
1	A	305	ASN	C-N-CA	5.00	124.66	119.56
1	A	337	ASP	CA-CB-CG	5.00	117.60	112.60
1	A	372	ASN	CA-CB-CG	5.00	117.60	112.60

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	2791	0	2579	24	0
2	A	10	0	0	0	0
3	A	20	0	15	2	0
4	A	465	0	0	0	0
All	All	3286	0	2594	24	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 (24) 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:538:ARG:O	1:A:539:THR:HG23	1.63	0.99
1:A:273:ILE:HG12	1:A:521:LEU:HD13	1.55	0.88
1:A:273:ILE:CG1	1:A:521:LEU:HD13	2.28	0.59
1:A:386:ASN:HD21	1:A:423:ARG:HH11	1.54	0.55
1:A:258:GLN:HE22	1:A:510:ASN:HD22	1.60	0.49
1:A:386:ASN:ND2	1:A:423:ARG:HH11	2.10	0.48
1:A:273:ILE:HG12	1:A:521:LEU:CD1	2.35	0.48
1:A:510:ASN:HD21	1:A:516:TRP:HE1	1.64	0.46
1:A:444:TYR:CG	1:A:491:ALA:HA	2.52	0.45
1:A:284:ASN:HD21	3:A:597:ACY:H3	1.82	0.44
1:A:471:VAL:HG13	1:A:481:VAL:HG21	2.00	0.43
1:A:472:ARG:HA	3:A:598:ACY:H2	2.00	0.43
1:A:263:SER:HA	1:A:292:ARG:HB3	2.01	0.42
1:A:238:LEU:HG	1:A:249:LEU:HD11	2.00	0.42
1:A:425:ASP:OD2	1:A:464:ARG:HD2	2.20	0.42
1:A:538:ARG:O	1:A:539:THR:CG2	2.51	0.42
1:A:464:ARG:HB3	1:A:470:ASN:ND2	2.35	0.41
1:A:510:ASN:ND2	1:A:516:TRP:HE1	2.19	0.41
1:A:297:ILE:HG12	1:A:330:TRP:CZ2	2.55	0.41
1:A:475:LEU:HD21	1:A:481:VAL:HG22	2.03	0.41
1:A:519:TRP:CG	1:A:520:SER:HB3	2.56	0.41
1:A:356:HIS:HD2	1:A:357:TYR:CE2	2.39	0.41
1:A:519:TRP:CD2	1:A:520:SER:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:THR:HG21	1:A:502:ALA:HA	2.04	0.40

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	355/364 (98%)	337 (95%)	17 (5%)	1 (0%)	36 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	539	THR

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	291/297 (98%)	281 (97%)	10 (3%)	32 25

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	PRO
1	A	227	GLN

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Mol	Chain	Res	Type
1	A	238	LEU
1	A	243	LEU
1	A	248	THR
1	A	378	ASN
1	A	419	ASN
1	A	492	ASN
1	A	494	ASP
1	A	544	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	ASN
1	A	305	ASN
1	A	322	HIS
1	A	378	ASN
1	A	386	ASN
1	A	411	ASN
1	A	436	ASN
1	A	470	ASN
1	A	510	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](#)

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	$\# Z > 2$
3	ACY	A	599	2	3,3,3	0.91	0	3,3,3	1.41	0
3	ACY	A	595	2	3,3,3	1.00	0	3,3,3	2.00	2 (66%)
3	ACY	A	597	2	3,3,3	0.82	0	3,3,3	2.18	2 (66%)
3	ACY	A	596	2	3,3,3	0.87	0	3,3,3	2.81	2 (66%)
3	ACY	A	598	2	3,3,3	1.27	0	3,3,3	0.91	0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	596	ACY	OXT-C-CH3	3.61	130.18	115.05
3	A	596	ACY	O-C-CH3	-3.24	109.24	122.53
3	A	597	ACY	OXT-C-CH3	2.73	126.49	115.05
3	A	595	ACY	OXT-C-CH3	2.61	126.02	115.05
3	A	597	ACY	O-C-CH3	-2.61	111.81	122.53
3	A	595	ACY	OXT-C-O	-2.17	113.96	122.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	597	ACY	1	0
3	A	598	ACY	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.