



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:50 PM UTC

PDB ID : 1GLH / pdb_00001glh
Title : CATION BINDING TO A BACILLUS (1,3-1,4)-BETA-GLUCANASE.
GEOMETRY, AFFINITY AND EFFECT ON PROTEIN STABILITY
Authors : Keitel, T.; Heinemann, U.
Deposited on : 1994-11-25
Resolution : 2.00 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) : **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

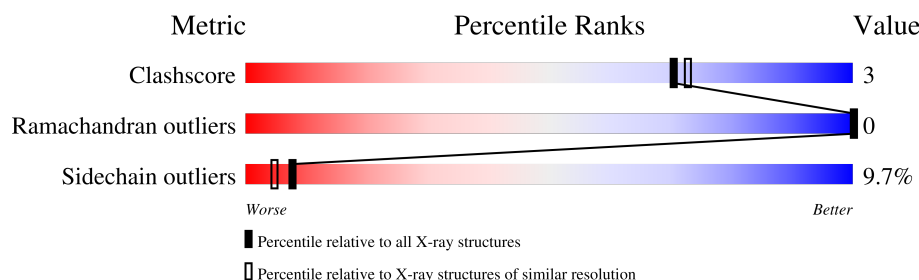
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	214	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1813 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 1,3-1,4-BETA-GLUCANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1697	1090	273	329	5			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		

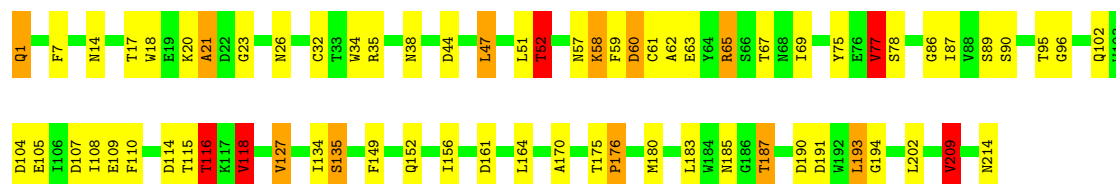
3 Residue-property plots

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: 1,3-1,4-BETA-GLUCANASE

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.22Å 72.56Å 49.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.198 , 0.225	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1813	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: NA

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	1.19	2/1753 (0.1%)	2.40	105/2384 (4.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	ALA	N-CA	5.82	1.53	1.46
1	A	47	LEU	CA-C	5.37	1.59	1.52

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	CD-NE-CZ	16.12	146.97	124.40
1	A	52	THR	N-CA-CB	-14.07	88.41	111.20
1	A	65	ARG	CA-C-O	-12.33	108.02	121.33
1	A	187	THR	N-CA-CB	11.94	132.50	111.13
1	A	77	VAL	CB-CA-C	-10.91	91.84	110.71
1	A	21	ALA	CB-CA-C	9.71	125.85	109.72
1	A	59	PHE	CA-CB-CG	-9.54	104.26	113.80
1	A	193	LEU	N-CA-C	9.50	125.06	113.38
1	A	65	ARG	NE-CZ-NH2	-9.43	110.71	119.20
1	A	65	ARG	O-C-N	9.15	133.68	123.25
1	A	118	VAL	CB-CA-C	-9.11	94.40	110.71
1	A	51	LEU	CA-C-N	9.04	137.99	122.81
1	A	51	LEU	C-N-CA	9.04	137.99	122.81
1	A	194	GLY	N-CA-C	-8.95	99.57	112.81
1	A	44	ASP	CA-CB-CG	8.91	121.51	112.60
1	A	47	LEU	N-CA-C	-8.78	94.88	109.46
1	A	118	VAL	O-C-N	8.53	132.72	123.00
1	A	108	ILE	N-CA-CB	8.47	122.94	112.10
1	A	65	ARG	NE-CZ-NH1	8.45	129.95	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ASP	N-CA-C	8.24	122.53	109.50
1	A	1	GLN	CB-CG-CD	8.16	126.47	112.60
1	A	156	ILE	N-CA-CB	8.14	124.04	111.99
1	A	102	GLN	OE1-CD-NE2	-7.87	114.73	122.60
1	A	18	TRP	CG-CD2-CE3	-7.77	126.13	133.90
1	A	34	TRP	CB-CG-CD2	7.76	137.66	126.80
1	A	34	TRP	CB-CG-CD1	-7.75	115.27	126.90
1	A	20	LYS	CA-C-O	-7.72	112.10	120.36
1	A	51	LEU	CA-C-O	7.68	128.46	120.40
1	A	209	VAL	CA-C-O	7.68	129.20	120.76
1	A	134	ILE	CA-C-O	-7.43	112.59	120.39
1	A	209	VAL	N-CA-CB	7.42	123.61	111.45
1	A	193	LEU	N-CA-CB	-7.38	99.54	110.53
1	A	47	LEU	CA-CB-CG	7.30	141.86	116.30
1	A	47	LEU	N-CA-CB	7.13	121.93	110.16
1	A	58	LYS	CA-C-N	6.95	133.01	122.65
1	A	58	LYS	C-N-CA	6.95	133.01	122.65
1	A	52	THR	N-CA-C	6.89	120.74	109.85
1	A	18	TRP	CE2-CD2-CE3	6.81	125.61	118.80
1	A	187	THR	CB-CA-C	-6.81	95.56	109.38
1	A	149	PHE	N-CA-CB	6.71	123.14	111.13
1	A	65	ARG	N-CA-C	6.67	119.21	109.07
1	A	52	THR	CA-CB-CG2	6.67	121.83	110.50
1	A	176	PRO	CA-C-O	-6.65	114.11	121.23
1	A	105	GLU	CB-CG-CD	6.62	123.85	112.60
1	A	47	LEU	CA-C-O	6.50	127.89	120.54
1	A	75	TYR	CA-C-O	-6.45	113.23	120.32
1	A	107	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	26	ASN	N-CA-C	-6.29	105.57	113.18
1	A	89	SER	N-CA-CB	6.26	121.63	110.80
1	A	57	ASN	CA-C-N	6.06	131.71	123.11
1	A	57	ASN	C-N-CA	6.06	131.71	123.11
1	A	67	THR	CA-CB-OG1	-6.03	100.55	109.60
1	A	118	VAL	CA-C-O	-6.03	114.89	121.28
1	A	135	SER	N-CA-CB	6.01	119.67	109.87
1	A	170	ALA	N-CA-C	5.95	119.33	109.46
1	A	26	ASN	CA-CB-CG	5.91	118.51	112.60
1	A	77	VAL	N-CA-CB	5.90	121.13	111.45
1	A	62	ALA	N-CA-C	5.83	118.14	108.99
1	A	190	ASP	CA-C-N	5.80	127.98	120.44
1	A	190	ASP	C-N-CA	5.80	127.98	120.44
1	A	21	ALA	N-CA-C	-5.77	101.87	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ALA	CA-C-O	5.74	127.03	120.54
1	A	57	ASN	CB-CG-ND2	-5.73	107.81	116.40
1	A	95	THR	CA-CB-OG1	-5.71	101.03	109.60
1	A	18	TRP	CA-CB-CG	5.63	124.30	113.60
1	A	60	ASP	CA-CB-CG	-5.63	106.97	112.60
1	A	118	VAL	N-CA-CB	5.62	122.43	111.92
1	A	67	THR	N-CA-C	-5.62	106.27	113.23
1	A	35	ARG	NE-CZ-NH1	5.56	127.06	121.50
1	A	115	THR	CA-C-N	5.55	132.39	122.06
1	A	115	THR	C-N-CA	5.55	132.39	122.06
1	A	116	THR	CA-C-O	5.53	125.76	119.18
1	A	116	THR	CA-CB-CG2	5.47	119.80	110.50
1	A	127	VAL	N-CA-CB	5.45	118.22	111.41
1	A	214	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	1	GLN	CA-CB-CG	5.45	124.99	114.10
1	A	109	GLU	CG-CD-OE2	-5.42	105.93	118.40
1	A	78	SER	N-CA-C	-5.40	99.71	108.52
1	A	161	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	65	ARG	CB-CA-C	-5.34	98.96	110.45
1	A	7	PHE	N-CA-CB	5.33	120.02	110.80
1	A	14	ASN	CB-CG-ND2	5.29	124.33	116.40
1	A	104	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	96	GLY	O-C-N	5.27	127.04	121.77
1	A	90	SER	O-C-N	5.25	129.06	122.92
1	A	23	GLY	N-CA-C	5.24	122.97	114.90
1	A	149	PHE	CA-CB-CG	5.23	119.03	113.80
1	A	209	VAL	CA-CB-CG2	5.23	119.29	110.40
1	A	21	ALA	N-CA-CB	-5.22	101.95	109.83
1	A	115	THR	CA-CB-OG1	-5.20	101.81	109.60
1	A	116	THR	CA-C-N	5.19	130.74	122.59
1	A	116	THR	C-N-CA	5.19	130.74	122.59
1	A	86	GLY	N-CA-C	5.17	122.49	115.30
1	A	194	GLY	CA-C-N	-5.17	113.22	122.07
1	A	194	GLY	C-N-CA	-5.17	113.22	122.07
1	A	78	SER	N-CA-CB	5.15	118.64	110.55
1	A	89	SER	N-CA-C	-5.13	100.09	108.76
1	A	35	ARG	NE-CZ-NH2	-5.11	114.61	119.20
1	A	90	SER	N-CA-C	5.10	115.78	108.74
1	A	77	VAL	O-C-N	5.10	128.71	123.05
1	A	102	GLN	N-CA-C	-5.06	103.72	110.55
1	A	108	ILE	N-CA-C	-5.06	98.73	107.24
1	A	115	THR	O-C-N	-5.06	115.90	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ALA	O-C-N	-5.05	116.66	122.87
1	A	152	GLN	CB-CG-CD	5.02	121.14	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	1697	0	1557	11	0
2	A	1	0	0	0	0
3	A	115	0	0	0	0
All	All	1813	0	1557	11	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 3.

All (11) 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:52:THR:HG22	1:A:60:ASP:HB2	1.73	0.71
1:A:32:CYS:HB3	1:A:185:ASN:HD21	1.70	0.56
1:A:77:VAL:HG13	1:A:209:VAL:HG12	1.91	0.52
1:A:114:ASP:OD1	1:A:116:THR:HB	2.10	0.52
1:A:38:ASN:HD21	1:A:52:THR:HB	1.76	0.50
1:A:69:ILE:HD12	1:A:176:PRO:HB2	1.97	0.47
1:A:87:ILE:HD13	1:A:202:LEU:HD13	1.99	0.45
1:A:175:THR:HA	1:A:176:PRO:HD3	1.81	0.44
1:A:110:PHE:CE2	1:A:118:VAL:HG13	2.54	0.42
1:A:21:ALA:HB3	1:A:63:GLU:HB3	2.03	0.41
1:A:61:CYS:HB2	1:A:183:LEU:O	2.21	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	212/214 (99%)	201 (95%)	11 (5%)	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	176/176 (100%)	159 (90%)	17 (10%)	8	5

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	17	THR
1	A	47	LEU
1	A	52	THR
1	A	58	LYS
1	A	65	ARG
1	A	77	VAL
1	A	116	THR
1	A	118	VAL
1	A	127	VAL
1	A	135	SER
1	A	164	LEU
1	A	180	MET

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Mol	Chain	Res	Type
1	A	187	THR
1	A	191	ASP
1	A	193	LEU
1	A	209	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	38	ASN
1	A	43	ASN
1	A	84	ASN
1	A	99	HIS
1	A	171	ASN
1	A	185	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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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.