Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:38 PM GMT

PDB ID	:	1GLH
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

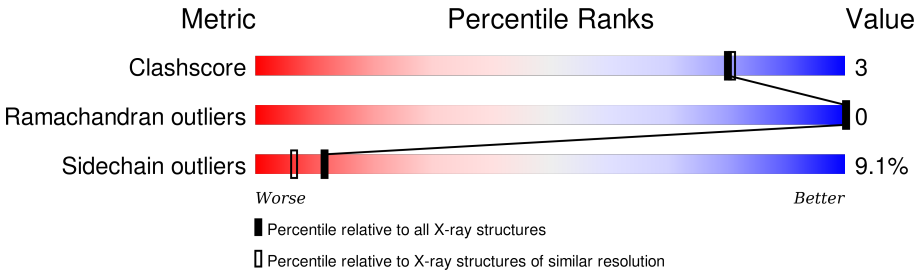
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	214	73% 19% 6% •

2 Entry composition (i)

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 (three-letter code: 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		

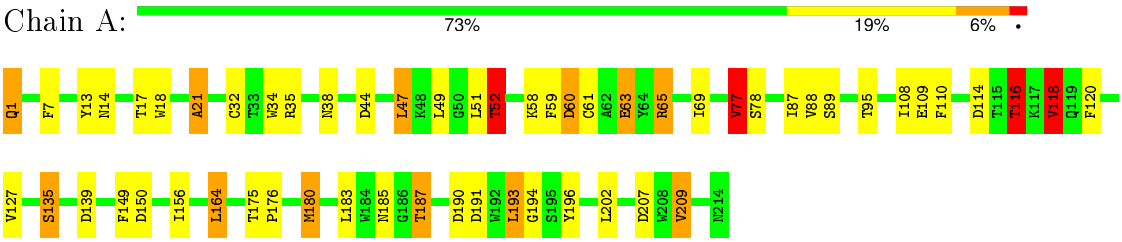
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 1,3-1,4-BETA-GLUCANASE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	0.94	1/1753 (0.1%)	2.14	67/2384 (2.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLU	CD-OE2	5.28	1.31	1.25

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	ARG	NE-CZ-NH1	19.30	129.95	120.30
1	A	65	ARG	NE-CZ-NH2	-19.17	110.71	120.30
1	A	65	ARG	CD-NE-CZ	16.69	146.97	123.60
1	A	35	ARG	NE-CZ-NH1	13.52	127.06	120.30
1	A	187	THR	N-CA-CB	11.68	132.50	110.30
1	A	47	LEU	CA-CB-CG	11.55	141.86	115.30
1	A	52	THR	N-CA-CB	-11.52	88.41	110.30
1	A	35	ARG	NE-CZ-NH2	-11.39	114.61	120.30
1	A	139	ASP	CB-CG-OD1	11.04	128.24	118.30
1	A	21	ALA	CB-CA-C	10.50	125.85	110.10
1	A	190	ASP	CB-CG-OD1	10.47	127.72	118.30
1	A	77	VAL	CB-CA-C	-10.29	91.84	111.40
1	A	34	TRP	CB-CG-CD1	-9.02	115.27	127.00
1	A	207	ASP	CB-CG-OD1	8.95	126.36	118.30
1	A	118	VAL	CB-CA-C	-8.95	94.40	111.40
1	A	44	ASP	CB-CG-OD1	8.90	126.31	118.30
1	A	59	PHE	CB-CG-CD2	-8.83	114.62	120.80
1	A	18	TRP	CG-CD2-CE3	-8.63	126.13	133.90
1	A	34	TRP	CB-CG-CD2	8.51	137.66	126.60
1	A	139	ASP	CB-CG-OD2	-8.38	110.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	PHE	CB-CG-CD2	-7.43	115.60	120.80
1	A	89	SER	N-CA-CB	7.42	121.63	110.50
1	A	190	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	A	164	LEU	CA-CB-CG	7.39	132.30	115.30
1	A	13	TYR	CB-CG-CD2	-7.08	116.75	121.00
1	A	149	PHE	N-CA-CB	6.97	123.14	110.60
1	A	65	ARG	O-C-N	6.87	133.68	122.70
1	A	52	THR	CA-CB-CG2	6.74	121.83	112.40
1	A	49	LEU	CB-CG-CD1	-6.59	99.80	111.00
1	A	51	LEU	C-N-CA	6.52	137.99	121.70
1	A	60	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	118	VAL	O-C-N	6.26	132.72	122.70
1	A	109	GLU	CG-CD-OE2	-6.18	105.93	118.30
1	A	135	SER	N-CA-CB	6.12	119.67	110.50
1	A	47	LEU	N-CA-C	-5.97	94.88	111.00
1	A	187	THR	CB-CA-C	-5.94	95.56	111.60
1	A	207	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	21	ALA	N-CA-CB	-5.82	101.95	110.10
1	A	47	LEU	N-CA-CB	5.76	121.93	110.40
1	A	13	TYR	CB-CG-CD1	5.76	124.46	121.00
1	A	18	TRP	CE2-CD2-CE3	5.76	125.61	118.70
1	A	156	ILE	N-CA-CB	5.76	124.04	110.80
1	A	65	ARG	CA-C-O	-5.75	108.02	120.10
1	A	65	ARG	CB-CA-C	-5.72	98.96	110.40
1	A	1	GLN	CB-CG-CD	5.72	126.47	111.60
1	A	196	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	A	209	VAL	CA-CB-CG2	5.59	119.29	110.90
1	A	18	TRP	CA-CB-CG	5.58	124.30	113.70
1	A	209	VAL	N-CA-CB	5.50	123.61	111.50
1	A	118	VAL	CG1-CB-CG2	5.47	119.65	110.90
1	A	95	THR	N-CA-CB	5.44	120.64	110.30
1	A	193	LEU	N-CA-CB	-5.43	99.54	110.40
1	A	78	SER	N-CA-CB	5.43	118.64	110.50
1	A	194	GLY	N-CA-C	-5.41	99.57	113.10
1	A	77	VAL	CG1-CB-CG2	5.34	119.45	110.90
1	A	18	TRP	NE1-CE2-CZ2	5.33	136.26	130.40
1	A	150	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	44	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	116	THR	CA-CB-CG2	5.28	119.80	112.40
1	A	108	ILE	N-CA-CB	5.28	122.94	110.80
1	A	1	GLN	CA-CB-CG	5.27	124.99	113.40
1	A	63	GLU	CG-CD-OE1	5.26	128.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7	PHE	N-CA-CB	5.23	120.02	110.60
1	A	193	LEU	N-CA-C	5.21	125.06	111.00
1	A	127	VAL	CA-CB-CG2	5.20	118.70	110.90
1	A	180	MET	CG-SD-CE	5.12	108.39	100.20
1	A	88	VAL	CG1-CB-CG2	-5.05	102.83	110.90

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	1556	11	0
2	A	1	0	0	0	0
3	A	115	0	0	0	0
All	All	1813	0	1556	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 (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	212/214 (99%)	201 (95%)	11 (5%)	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	176/176 (100%)	160 (91%)	16 (9%)	12 6

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	14	ASN
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

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Mol	Chain	Res	Type
1	A	135	SER
1	A	164	LEU
1	A	180	MET
1	A	187	THR
1	A	191	ASP
1	A	193	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	38	ASN
1	A	43	ASN
1	A	99	HIS
1	A	102	GLN
1	A	152	GLN
1	A	185	ASN
1	A	214	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.