



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 07:55 PM BST

PDB ID : 5XXM
Title : Crystal structure of GH3 beta-glucosidase from *Bacteroides thetaiotaomicron* in complex with gluconolactone
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Deposited on : 2017-07-04
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

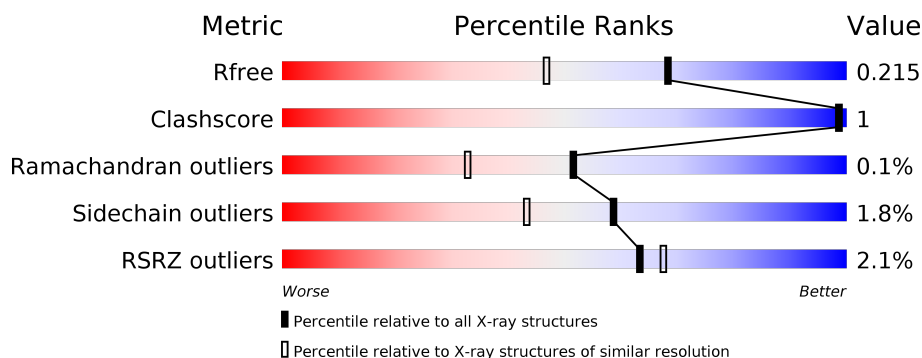
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	760	<div> <div>%</div> <div> <div></div> <div>96%</div> <div>..</div> </div> </div>
1	B	760	<div> <div>3%</div> <div> <div></div> <div>95%</div> <div>..</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12778 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 Periplasmic beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	749	Total	C	N	O	S	0	3	0
			5822	3683	986	1118	35			
1	B	744	Total	C	N	O	S	0	3	0
			5784	3660	981	1108	35			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	expression tag	UNP Q8A1U1
A	772	LEU	-	expression tag	UNP Q8A1U1
A	773	GLU	-	expression tag	UNP Q8A1U1
A	774	HIS	-	expression tag	UNP Q8A1U1
A	775	HIS	-	expression tag	UNP Q8A1U1
A	776	HIS	-	expression tag	UNP Q8A1U1
A	777	HIS	-	expression tag	UNP Q8A1U1
A	778	HIS	-	expression tag	UNP Q8A1U1
A	779	HIS	-	expression tag	UNP Q8A1U1
B	20	MET	-	expression tag	UNP Q8A1U1
B	772	LEU	-	expression tag	UNP Q8A1U1
B	773	GLU	-	expression tag	UNP Q8A1U1
B	774	HIS	-	expression tag	UNP Q8A1U1
B	775	HIS	-	expression tag	UNP Q8A1U1
B	776	HIS	-	expression tag	UNP Q8A1U1
B	777	HIS	-	expression tag	UNP Q8A1U1
B	778	HIS	-	expression tag	UNP Q8A1U1
B	779	HIS	-	expression tag	UNP Q8A1U1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

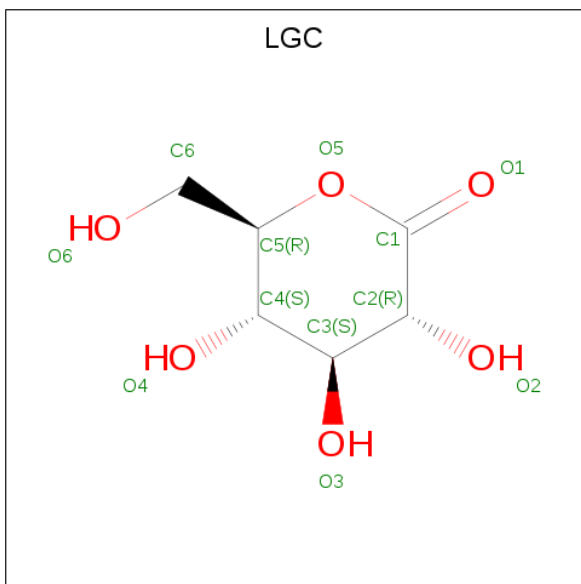
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		

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

- Molecule 3 is D-glucono-1,5-lactone (three-letter code: LGC) (formula: C₆H₁₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		

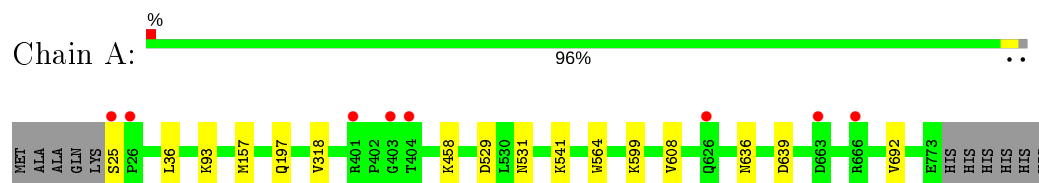
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	623	Total	O	0	0
			623	623		
5	B	510	Total	O	0	0
			510	510		

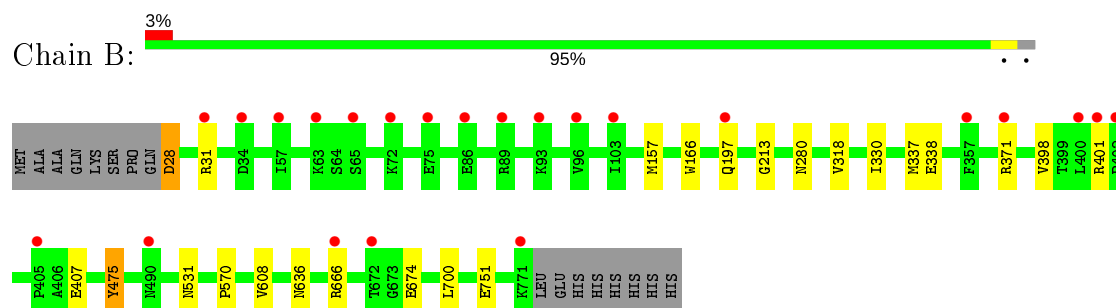
3 Residue-property plots [i](#)

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 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: Periplasmic beta-glucosidase



- Molecule 1: Periplasmic beta-glucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	81.82Å 167.69Å 224.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.70 – 1.70 42.70 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.4 (42.70-1.70) 93.4 (42.70-1.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.181 , 0.208 0.190 , 0.215	Depositor DCC
R_{free} test set	7865 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12778	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LGC, PG4, MG

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	0.39	0/5937	0.65	0/8036
1	B	0.39	0/5898	0.66	0/7982
All	All	0.39	0/11835	0.66	0/16018

There are no bond length outliers.

There are no bond angle outliers.

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	5822	0	5778	7	0
1	B	5784	0	5745	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	10	0	0
3	B	12	0	10	0	0
4	A	13	0	18	1	0
5	A	623	0	0	0	0
5	B	510	0	0	0	0
All	All	12778	0	11561	12	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 1.

All (12) 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:608[B]:VAL:HG23	1:B:608[B]:VAL:HG23	1.59	0.83
1:A:608[B]:VAL:CG2	1:B:608[B]:VAL:HG23	2.29	0.60
1:A:608[B]:VAL:HG23	1:B:608[B]:VAL:CG2	2.29	0.60
1:A:36:LEU:HD13	4:A:803:PG4:H72	1.85	0.58
1:A:639:ASP:HB3	1:B:475:TYR:HE2	1.70	0.55
1:B:28:ASP:OD1	1:B:28:ASP:N	2.41	0.54
1:B:330:ILE:HG21	1:B:337:MET:CE	2.44	0.46
1:B:700:LEU:HD12	1:B:751:GLU:HB3	1.97	0.45
1:B:398:VAL:CG2	1:B:570:PRO:HB3	2.48	0.43
1:A:541:LYS:HG2	1:A:564:TRP:CZ2	2.55	0.42
1:A:599:LYS:HG3	1:A:692:VAL:HB	2.02	0.41
1:B:166:TRP:CZ3	1:B:213:GLY:HA2	2.56	0.41

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	750/760 (99%)	731 (98%)	18 (2%)	1 (0%)	51	33
1	B	745/760 (98%)	730 (98%)	14 (2%)	1 (0%)	51	33
All	All	1495/1520 (98%)	1461 (98%)	32 (2%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	318	VAL
1	A	318	VAL

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	625/631 (99%)	616 (99%)	9 (1%)	67	53
1	B	620/631 (98%)	606 (98%)	14 (2%)	50	33
All	All	1245/1262 (99%)	1222 (98%)	23 (2%)	59	43

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	93	LYS
1	A	157	MET
1	A	197	GLN
1	A	458	LYS
1	A	529[A]	ASP
1	A	529[B]	ASP
1	A	531	ASN
1	A	636	ASN
1	B	28	ASP
1	B	31	ARG
1	B	157	MET
1	B	197	GLN
1	B	280	ASN
1	B	338	GLU
1	B	371	ARG
1	B	401	ARG
1	B	407	GLU
1	B	475	TYR
1	B	531	ASN
1	B	636	ASN
1	B	666	ARG
1	B	674	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	490	ASN
1	A	506	GLN
1	B	197	GLN
1	B	280	ASN
1	B	531	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
4	PG4	A	803	-	12,12,12	0.55	0	11,11,11	0.46	0
3	LGC	A	802	-	12,12,12	2.05	1 (8%)	15,17,17	1.07	1 (6%)
3	LGC	B	802	-	12,12,12	2.20	2 (16%)	15,17,17	1.00	2 (13%)

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	PG4	A	803	-	-	4/10/10/10	-
3	LGC	A	802	-	-	0/2/22/22	0/1/1/1
3	LGC	B	802	-	-	0/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	LGC	O5-C1	7.03	1.45	1.34
3	A	802	LGC	O5-C1	6.71	1.44	1.34
3	B	802	LGC	O5-C5	-2.56	1.42	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	LGC	O5-C1-O1	-2.74	114.48	118.47
3	B	802	LGC	O5-C1-O1	-2.38	115.00	118.47
3	B	802	LGC	O5-C1-C2	2.17	122.44	119.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	PG4	O1-C1-C2-O2
4	A	803	PG4	O4-C7-C8-O5
4	A	803	PG4	C3-C4-O3-C5
4	A	803	PG4	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	PG4	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	749/760 (98%)	-0.08	8 (1%) 80 83	7, 12, 25, 47	0
1	B	744/760 (97%)	0.15	23 (3%) 49 53	7, 16, 34, 52	0
All	All	1493/1520 (98%)	0.03	31 (2%) 63 67	7, 14, 31, 52	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	401	ARG	4.4
1	B	400	LEU	3.8
1	B	405	PRO	3.3
1	B	65	SER	3.2
1	B	34	ASP	3.1
1	B	197	GLN	3.0
1	A	626	GLN	2.9
1	B	72	LYS	2.9
1	B	31	ARG	2.7
1	A	663	ASP	2.7
1	B	666	ARG	2.7
1	B	93	LYS	2.6
1	A	26	PRO	2.5
1	B	86	GLU	2.5
1	B	402	PRO	2.4
1	B	96	VAL	2.4
1	A	404	THR	2.4
1	A	403	GLY	2.3
1	B	357	PHE	2.3
1	A	666	ARG	2.3
1	B	57	ILE	2.3
1	A	401	ARG	2.2
1	B	63	LYS	2.3
1	B	672	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	25	SER	2.2
1	B	771	LYS	2.2
1	B	103	ILE	2.1
1	B	371	ARG	2.1
1	B	75	GLU	2.1
1	B	490	ASN	2.1
1	B	89	ARG	2.0

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 monosaccharides 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, 95th 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	B-factors(\AA^2)	Q<0.9
4	PG4	A	803	13/13	0.86	0.13	27,29,32,32	0
2	MG	A	801	1/1	0.95	0.05	28,28,28,28	0
2	MG	B	801	1/1	0.96	0.10	21,21,21,21	0
3	LGC	B	802	12/12	0.96	0.09	11,11,11,11	0
3	LGC	A	802	12/12	0.98	0.09	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.