wwPDB X-ray Structure Validation Summary Report (i)

Mar 13, 2024 – 05:21 PM JST

PDB ID	:	5GQC
Title	:	Crystal structure of lacto-N-biosidase LnbX from Bifidobacterium longum subsp. longum, ligand-free form
Authors	:	Yamada, C.; Arakawa, T.; Katayama, T.; Fushinobu, S.
Deposited on	:	2016-08-07
Resolution	:	2.36 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

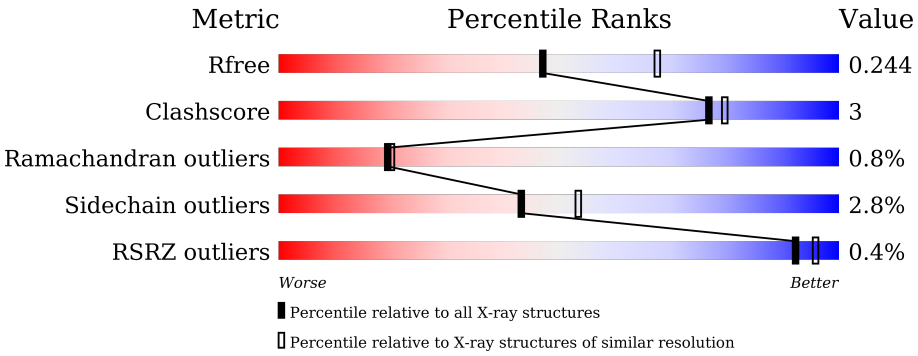
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	606	83% 13% •
1	B	606	87% 9% •
1	C	606	87% 7% • •
1	D	606	% 85% 10% • •
1	E	606	85% 10% • •
1	F	606	87% 8% • •

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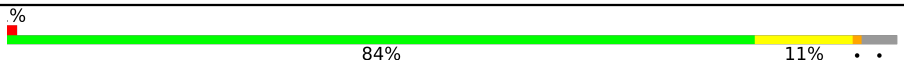
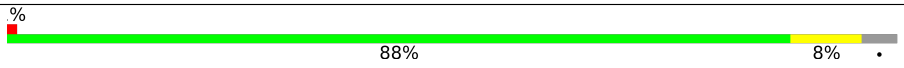
Mol	Chain	Length	Quality of chain
1	G	606	
1	H	606	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 36887 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 Lacto-N-biosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4468	2760	772	924	12			
1	B	582	Total	C	N	O	S	0	0	0
			4468	2760	772	924	12			
1	C	582	Total	C	N	O	S	0	0	0
			4468	2760	772	924	12			
1	D	583	Total	C	N	O	S	0	0	0
			4474	2763	773	926	12			
1	E	583	Total	C	N	O	S	0	0	0
			4474	2763	773	926	12			
1	F	583	Total	C	N	O	S	0	0	0
			4474	2763	773	926	12			
1	G	583	Total	C	N	O	S	0	0	0
			4474	2763	773	926	12			
1	H	583	Total	C	N	O	S	0	0	0
			4474	2763	773	926	12			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP A0A024QYS6
A	626	ALA	-	expression tag	UNP A0A024QYS6
A	627	ALA	-	expression tag	UNP A0A024QYS6
A	628	LEU	-	expression tag	UNP A0A024QYS6
A	629	GLU	-	expression tag	UNP A0A024QYS6
A	630	HIS	-	expression tag	UNP A0A024QYS6
A	631	HIS	-	expression tag	UNP A0A024QYS6
A	632	HIS	-	expression tag	UNP A0A024QYS6
A	633	HIS	-	expression tag	UNP A0A024QYS6
A	634	HIS	-	expression tag	UNP A0A024QYS6
A	635	HIS	-	expression tag	UNP A0A024QYS6
B	30	MET	-	expression tag	UNP A0A024QYS6
B	626	ALA	-	expression tag	UNP A0A024QYS6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	627	ALA	-	expression tag	UNP A0A024QYS6
B	628	LEU	-	expression tag	UNP A0A024QYS6
B	629	GLU	-	expression tag	UNP A0A024QYS6
B	630	HIS	-	expression tag	UNP A0A024QYS6
B	631	HIS	-	expression tag	UNP A0A024QYS6
B	632	HIS	-	expression tag	UNP A0A024QYS6
B	633	HIS	-	expression tag	UNP A0A024QYS6
B	634	HIS	-	expression tag	UNP A0A024QYS6
B	635	HIS	-	expression tag	UNP A0A024QYS6
C	30	MET	-	expression tag	UNP A0A024QYS6
C	626	ALA	-	expression tag	UNP A0A024QYS6
C	627	ALA	-	expression tag	UNP A0A024QYS6
C	628	LEU	-	expression tag	UNP A0A024QYS6
C	629	GLU	-	expression tag	UNP A0A024QYS6
C	630	HIS	-	expression tag	UNP A0A024QYS6
C	631	HIS	-	expression tag	UNP A0A024QYS6
C	632	HIS	-	expression tag	UNP A0A024QYS6
C	633	HIS	-	expression tag	UNP A0A024QYS6
C	634	HIS	-	expression tag	UNP A0A024QYS6
C	635	HIS	-	expression tag	UNP A0A024QYS6
D	30	MET	-	expression tag	UNP A0A024QYS6
D	626	ALA	-	expression tag	UNP A0A024QYS6
D	627	ALA	-	expression tag	UNP A0A024QYS6
D	628	LEU	-	expression tag	UNP A0A024QYS6
D	629	GLU	-	expression tag	UNP A0A024QYS6
D	630	HIS	-	expression tag	UNP A0A024QYS6
D	631	HIS	-	expression tag	UNP A0A024QYS6
D	632	HIS	-	expression tag	UNP A0A024QYS6
D	633	HIS	-	expression tag	UNP A0A024QYS6
D	634	HIS	-	expression tag	UNP A0A024QYS6
D	635	HIS	-	expression tag	UNP A0A024QYS6
E	30	MET	-	expression tag	UNP A0A024QYS6
E	626	ALA	-	expression tag	UNP A0A024QYS6
E	627	ALA	-	expression tag	UNP A0A024QYS6
E	628	LEU	-	expression tag	UNP A0A024QYS6
E	629	GLU	-	expression tag	UNP A0A024QYS6
E	630	HIS	-	expression tag	UNP A0A024QYS6
E	631	HIS	-	expression tag	UNP A0A024QYS6
E	632	HIS	-	expression tag	UNP A0A024QYS6
E	633	HIS	-	expression tag	UNP A0A024QYS6
E	634	HIS	-	expression tag	UNP A0A024QYS6
E	635	HIS	-	expression tag	UNP A0A024QYS6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	30	MET	-	expression tag	UNP A0A024QYS6
F	626	ALA	-	expression tag	UNP A0A024QYS6
F	627	ALA	-	expression tag	UNP A0A024QYS6
F	628	LEU	-	expression tag	UNP A0A024QYS6
F	629	GLU	-	expression tag	UNP A0A024QYS6
F	630	HIS	-	expression tag	UNP A0A024QYS6
F	631	HIS	-	expression tag	UNP A0A024QYS6
F	632	HIS	-	expression tag	UNP A0A024QYS6
F	633	HIS	-	expression tag	UNP A0A024QYS6
F	634	HIS	-	expression tag	UNP A0A024QYS6
F	635	HIS	-	expression tag	UNP A0A024QYS6
G	30	MET	-	expression tag	UNP A0A024QYS6
G	626	ALA	-	expression tag	UNP A0A024QYS6
G	627	ALA	-	expression tag	UNP A0A024QYS6
G	628	LEU	-	expression tag	UNP A0A024QYS6
G	629	GLU	-	expression tag	UNP A0A024QYS6
G	630	HIS	-	expression tag	UNP A0A024QYS6
G	631	HIS	-	expression tag	UNP A0A024QYS6
G	632	HIS	-	expression tag	UNP A0A024QYS6
G	633	HIS	-	expression tag	UNP A0A024QYS6
G	634	HIS	-	expression tag	UNP A0A024QYS6
G	635	HIS	-	expression tag	UNP A0A024QYS6
H	30	MET	-	expression tag	UNP A0A024QYS6
H	626	ALA	-	expression tag	UNP A0A024QYS6
H	627	ALA	-	expression tag	UNP A0A024QYS6
H	628	LEU	-	expression tag	UNP A0A024QYS6
H	629	GLU	-	expression tag	UNP A0A024QYS6
H	630	HIS	-	expression tag	UNP A0A024QYS6
H	631	HIS	-	expression tag	UNP A0A024QYS6
H	632	HIS	-	expression tag	UNP A0A024QYS6
H	633	HIS	-	expression tag	UNP A0A024QYS6
H	634	HIS	-	expression tag	UNP A0A024QYS6
H	635	HIS	-	expression tag	UNP A0A024QYS6

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0
3	D	2	Total Ca 2 2	0	0
3	E	2	Total Ca 2 2	0	0
3	F	2	Total Ca 2 2	0	0
3	G	2	Total Ca 2 2	0	0
3	H	2	Total Ca 2 2	0	0

- Molecule 4 is water.

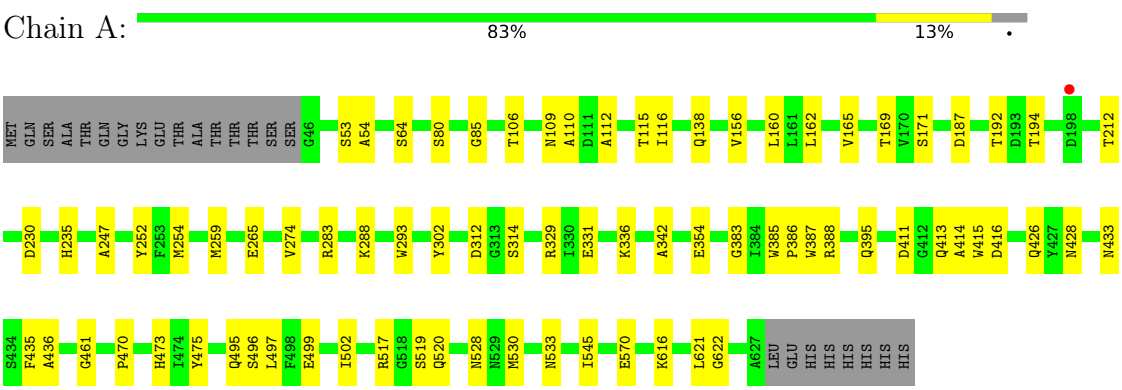
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	118	Total O 118 118	0	0
4	B	138	Total O 138 138	0	0
4	C	126	Total O 126 126	0	0
4	D	144	Total O 144 144	0	0
4	E	159	Total O 159 159	0	0
4	F	150	Total O 150 150	0	0
4	G	121	Total O 121 121	0	0
4	H	142	Total O 142 142	0	0

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.

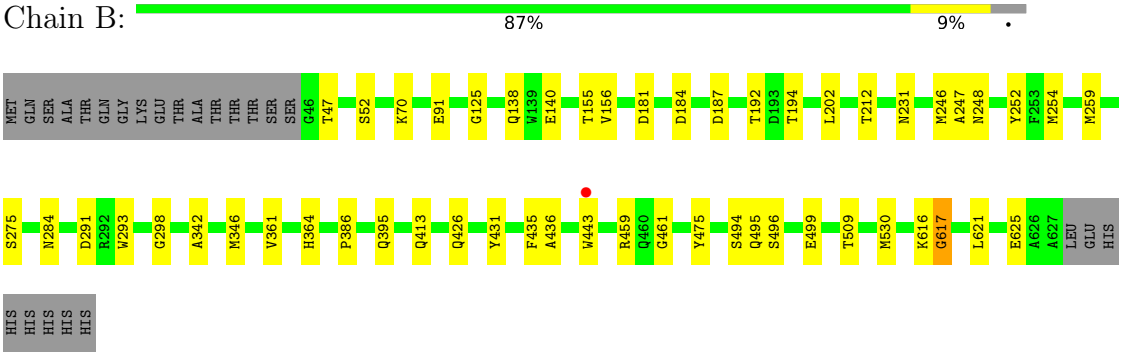
• Molecule 1: Lacto-N-biosidase

Chain A:



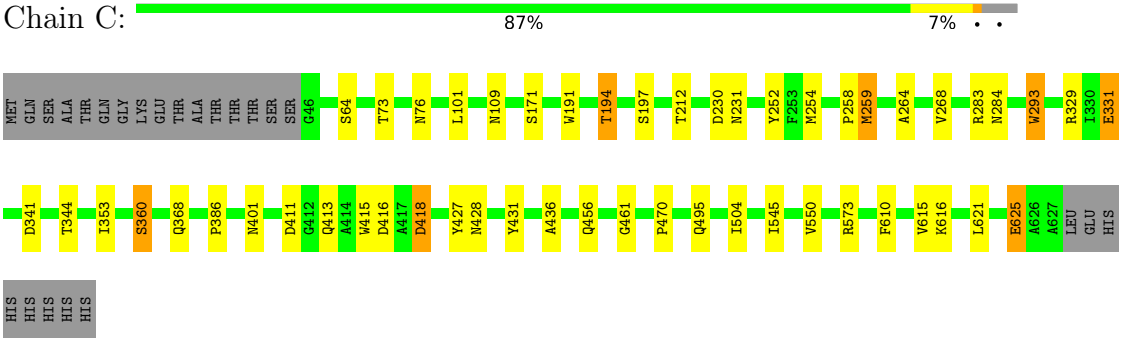
• Molecule 1: Lacto-N-biosidase

Chain B:



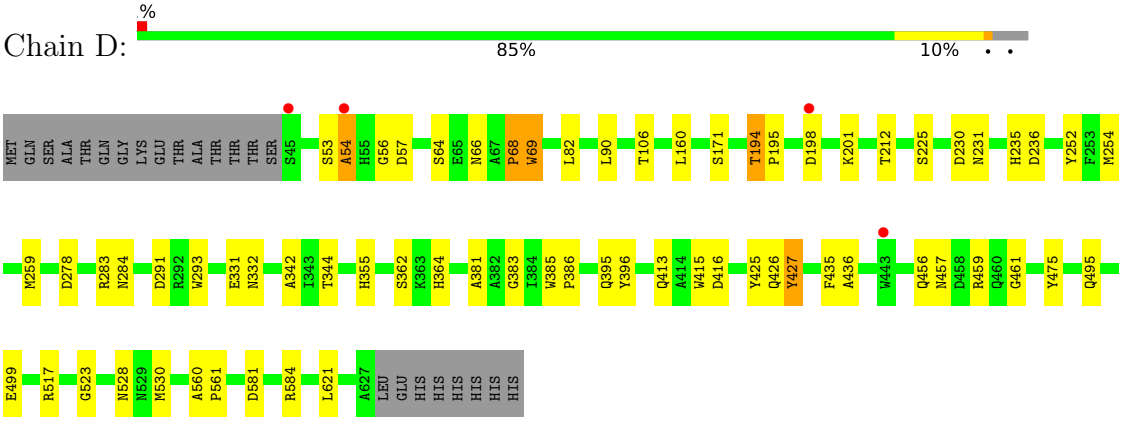
• Molecule 1: Lacto-N-biosidase

Chain C:



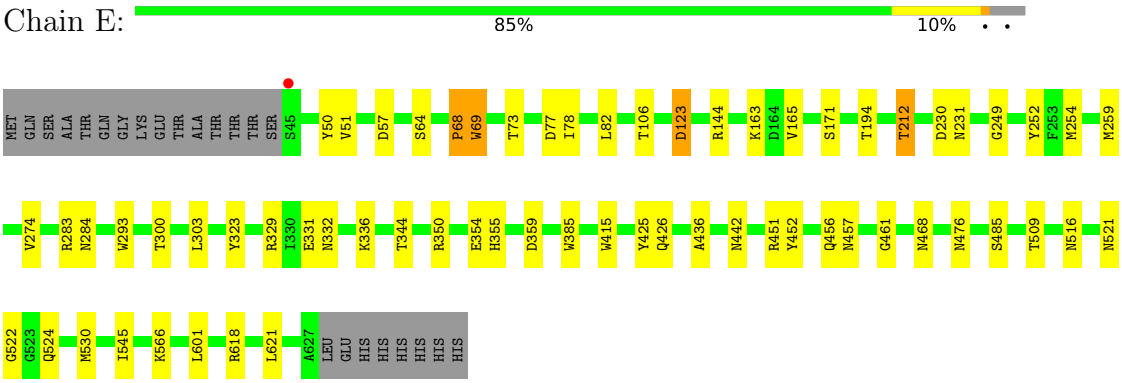
• Molecule 1: Lacto-N-biosidase

Chain D:



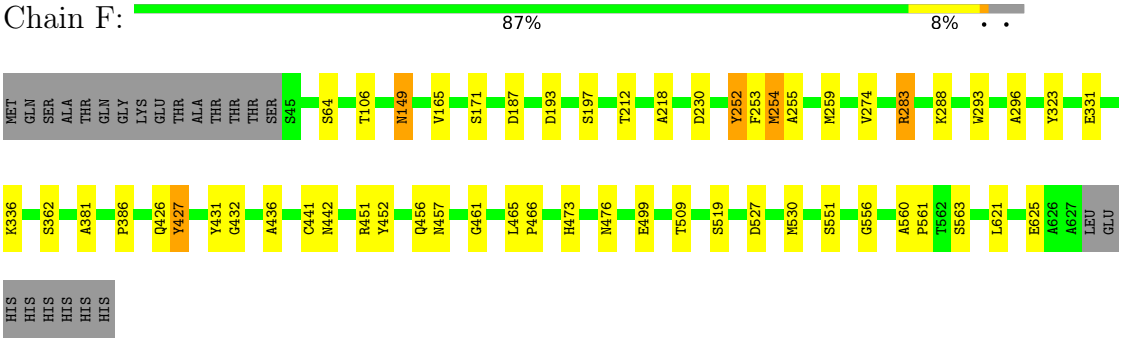
• Molecule 1: Lacto-N-biosidase

Chain E:



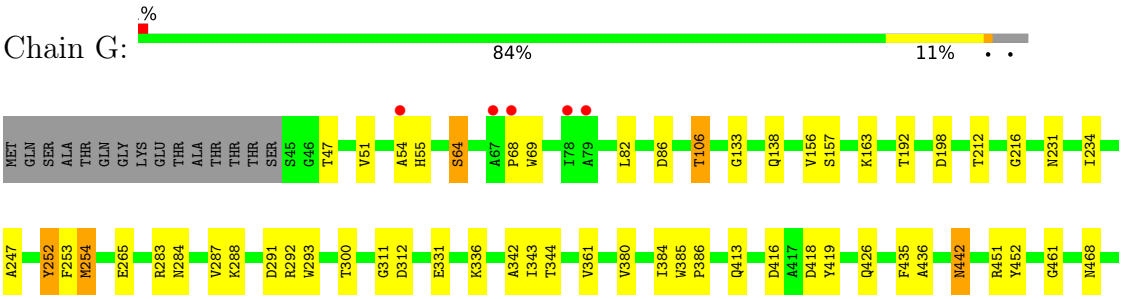
• Molecule 1: Lacto-N-biosidase

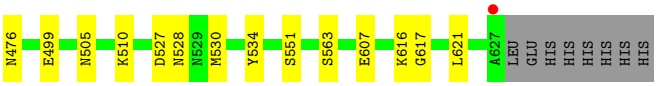
Chain F:



• Molecule 1: Lacto-N-biosidase

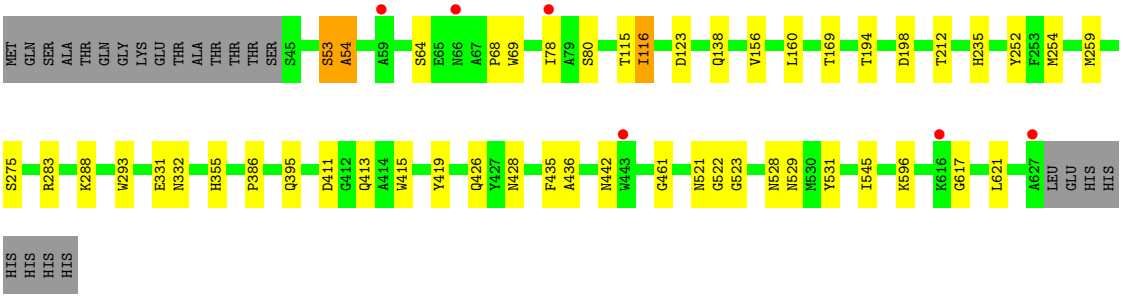
Chain G:





• Molecule 1: Lacto-N-biosidase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	128.32Å 142.72Å 157.01Å 90.00° 114.04° 90.00°	Depositor
Resolution (Å)	143.39 – 2.36 45.15 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.4 (143.39-2.36) 99.4 (45.15-2.36)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.182 , 0.240 0.189 , 0.244	Depositor DCC
R_{free} test set	10451 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 19.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.337 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	36887	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5566e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, 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	0.68	0/4567	0.84	4/6224 (0.1%)
1	B	0.70	0/4567	0.83	2/6224 (0.0%)
1	C	0.76	1/4567 (0.0%)	0.87	0/6224
1	D	0.74	0/4573	0.87	4/6232 (0.1%)
1	E	0.75	0/4573	0.86	5/6232 (0.1%)
1	F	0.72	0/4573	0.84	1/6232 (0.0%)
1	G	0.69	0/4573	0.82	1/6232 (0.0%)
1	H	0.71	0/4573	0.84	2/6232 (0.0%)
All	All	0.72	1/36566 (0.0%)	0.85	19/49832 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	293	TRP	CE3-CZ3	-5.99	1.28	1.38

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	581	ASP	CB-CG-OD1	6.36	124.03	118.30
1	A	329	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	D	517	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	329	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	H	523	GLY	N-CA-C	-5.66	98.94	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	521	ASN	Peptide
1	F	197	SER	Peptide
1	G	442	ASN	Peptide
1	H	521	ASN	Peptide

5.2 Too-close contacts (i)

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	4468	0	4135	32	0
1	B	4468	0	4135	23	0
1	C	4468	0	4135	27	0
1	D	4474	0	4140	29	0
1	E	4474	0	4140	29	1
1	F	4474	0	4140	26	1
1	G	4474	0	4140	26	0
1	H	4474	0	4140	18	0
2	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	118	0	0	1	0
4	B	138	0	0	0	0
4	C	126	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	144	0	0	1	0
4	E	159	0	0	0	0
4	F	150	0	0	1	0
4	G	121	0	0	0	0
4	H	142	0	0	0	0
All	All	36887	0	33105	203	1

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.

The worst 5 of 203 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:115:THR:O	1:A:169:THR:O	2.06	0.73
1:F:253:PHE:C	1:F:254:MET:HG3	2.14	0.68
1:B:291:ASP:OD1	1:B:364:HIS:ND1	2.25	0.66
1:G:54:ALA:O	1:G:55:HIS:ND1	2.29	0.64
1:E:82:LEU:O	1:E:106:THR:OG1	2.11	0.64

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:ASP:OD2	1:F:519:SER:OG[1_655]	1.98	0.22

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	580/606 (96%)	525 (90%)	50 (9%)	5 (1%)	17	17
1	B	580/606 (96%)	533 (92%)	43 (7%)	4 (1%)	22	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	580/606 (96%)	545 (94%)	32 (6%)	3 (0%)	29	32
1	D	581/606 (96%)	535 (92%)	41 (7%)	5 (1%)	17	17
1	E	581/606 (96%)	542 (93%)	35 (6%)	4 (1%)	22	23
1	F	581/606 (96%)	542 (93%)	37 (6%)	2 (0%)	41	47
1	G	581/606 (96%)	520 (90%)	53 (9%)	8 (1%)	11	9
1	H	581/606 (96%)	532 (92%)	41 (7%)	8 (1%)	11	9
All	All	4645/4848 (96%)	4274 (92%)	332 (7%)	39 (1%)	19	20

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	617	GLY
1	D	57	ASP
1	D	68	PRO
1	D	69	TRP
1	E	69	TRP

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	470/491 (96%)	456 (97%)	14 (3%)	41	50
1	B	470/491 (96%)	458 (97%)	12 (3%)	46	56
1	C	470/491 (96%)	459 (98%)	11 (2%)	50	61
1	D	471/491 (96%)	458 (97%)	13 (3%)	43	53
1	E	471/491 (96%)	459 (98%)	12 (2%)	47	58
1	F	471/491 (96%)	458 (97%)	13 (3%)	43	53
1	G	471/491 (96%)	453 (96%)	18 (4%)	33	41
1	H	471/491 (96%)	460 (98%)	11 (2%)	50	61
All	All	3765/3928 (96%)	3661 (97%)	104 (3%)	43	53

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	259	MET
1	F	427	TYR
1	H	252	TYR
1	E	300	THR
1	F	212	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	368	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 15 are 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

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, 95^{th} 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	582/606 (96%)	-0.31	1 (0%) 95 97	26, 40, 66, 95	0
1	B	582/606 (96%)	-0.36	1 (0%) 95 97	26, 39, 65, 94	0
1	C	582/606 (96%)	-0.29	0 100 100	24, 38, 57, 80	0
1	D	583/606 (96%)	-0.38	4 (0%) 87 92	23, 35, 60, 91	0
1	E	583/606 (96%)	-0.36	1 (0%) 95 97	23, 36, 55, 84	0
1	F	583/606 (96%)	-0.43	0 100 100	25, 36, 56, 81	0
1	G	583/606 (96%)	-0.19	6 (1%) 82 88	26, 42, 69, 99	0
1	H	583/606 (96%)	-0.36	6 (1%) 82 88	22, 37, 65, 96	0
All	All	4661/4848 (96%)	-0.34	19 (0%) 92 96	22, 38, 63, 99	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	68	PRO	4.5
1	H	443	TRP	4.4
1	H	627	ALA	3.5
1	B	443	TRP	3.3
1	G	67	ALA	3.0

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

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

6.3 Carbohydrates

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, 95^{th} 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(Å^2)	Q<0.9
3	CA	D	701	1/1	0.85	0.10	78,78,78,78	0
3	CA	C	701	1/1	0.88	0.08	76,76,76,76	0
3	CA	E	701	1/1	0.90	0.06	79,79,79,79	0
3	CA	G	702	1/1	0.90	0.07	72,72,72,72	0
3	CA	C	702	1/1	0.91	0.15	61,61,61,61	0
3	CA	F	701	1/1	0.94	0.17	65,65,65,65	0
2	NA	A	701	1/1	0.94	0.11	38,38,38,38	0
3	CA	H	702	1/1	0.95	0.07	64,64,64,64	0
3	CA	D	702	1/1	0.96	0.04	56,56,56,56	0
3	CA	F	702	1/1	0.97	0.05	61,61,61,61	0
3	CA	H	701	1/1	0.97	0.04	66,66,66,66	0
3	CA	G	701	1/1	0.97	0.05	67,67,67,67	0
3	CA	B	702	1/1	0.98	0.04	68,68,68,68	0
3	CA	B	701	1/1	0.98	0.06	57,57,57,57	0
3	CA	E	702	1/1	0.99	0.04	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.