



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:45 am BST

PDB ID : 3GZA
Title : Crystal structure of putative alpha-L-fucosidase (NP_812709.1) from BACTEROIDES THETA IOTAOMICRON VPI-5482 at 1.60 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2009-04-06
Resolution : 1.60 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	:	2.11
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)	:	2.11

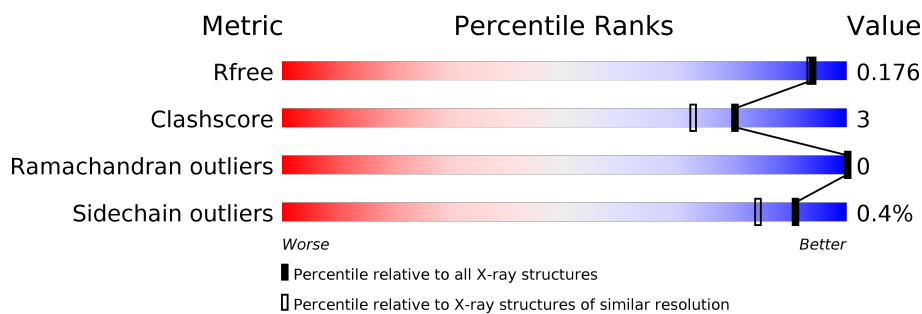
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

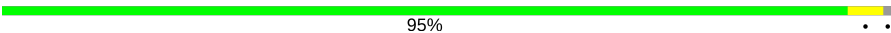

The reported resolution of this entry is 1.60 Å.

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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	443	 95%
1	B	443	 91% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	UNL	B	461	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8405 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.

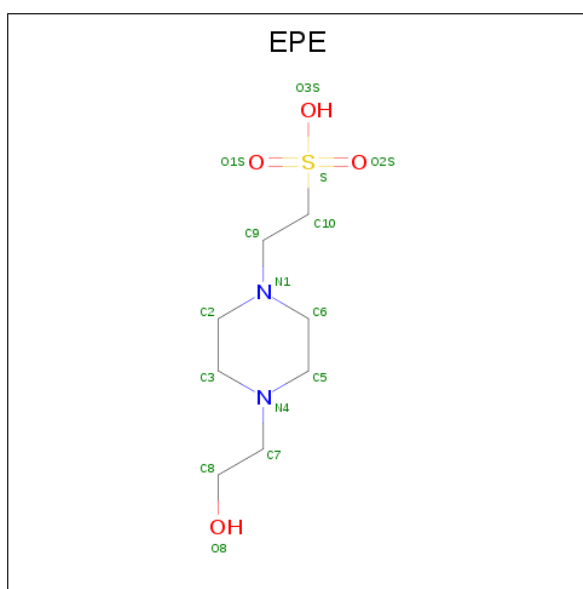
- Molecule 1 is a protein called putative alpha-L-fucosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	Se	0	15	0
			3576	2279	628	652	11	6			
1	B	431	Total	C	N	O	S	Se	0	18	0
			3519	2244	614	643	11	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP Q8A169
B	0	GLY	-	leader sequence	UNP Q8A169

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			15	8	2	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O 9 9	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	667	Total O 677 677	0	11
6	B	567	Total O 575 575	0	14

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 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.

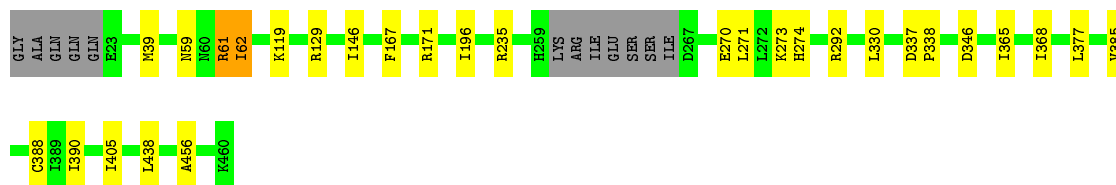
- Molecule 1: putative alpha-L-fucosidase

Chain A:  95%



- Molecule 1: putative alpha-L-fucosidase

Chain B:  91% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.05Å 81.53Å 111.57Å 90.00° 103.55° 90.00°	Depositor
Resolution (Å)	28.07 – 1.60 28.07 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.07-1.60) 99.7 (28.07-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.139 , 0.168 0.149 , 0.176	Depositor DCC
R_{free} test set	6726 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8405	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, EPE, UNL, EDO

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	0.74	1/3710 (0.0%)	0.87	4/5024 (0.1%)
1	B	0.71	1/3656 (0.0%)	0.90	9/4950 (0.2%)
All	All	0.73	2/7366 (0.0%)	0.89	13/9974 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	CYS	CB-SG	-6.38	1.71	1.82
1	B	62	ILE	N-CA	-5.39	1.35	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206[A]	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	A	206[B]	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	B	61[A]	ARG	C-N-CA	9.19	144.68	121.70
1	B	61[B]	ARG	C-N-CA	9.19	144.68	121.70
1	B	171[A]	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	B	171[B]	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	A	288	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	129	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	167	PHE	CB-CG-CD1	5.30	124.51	120.80
1	B	292	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	B	129	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	426	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	235	ARG	NE-CZ-NH2	-5.13	117.73	120.30

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	3576	0	3469	9	0
1	B	3519	0	3412	24	0
2	A	15	0	18	0	0
3	A	12	0	18	0	0
3	B	20	0	30	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	9	0	0	5	0
6	A	677	0	0	3	1
6	B	575	0	0	3	1
All	All	8405	0	6947	38	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.

All (38) 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)
5:B:461:UNL:O4	5:B:461:UNL:O5	1.71	1.09
5:B:461:UNL:O7	5:B:461:UNL:O8	1.74	1.04
5:B:461:UNL:O2	5:B:461:UNL:O3	1.73	1.03
5:B:461:UNL:O6	5:B:461:UNL:O5	1.79	1.00
1:B:388[B]:CYS:SG	1:B:405:ILE:HD13	2.06	0.96
1:B:146:ILE:HD12	1:B:196[B]:ILE:HD11	1.53	0.90
5:B:461:UNL:O2	5:B:461:UNL:O1	1.90	0.88
1:B:388[B]:CYS:SG	1:B:405:ILE:CD1	2.68	0.82
1:A:388[B]:CYS:SG	1:A:405:ILE:HD13	2.24	0.78
1:B:270:GLU:O	1:B:273[A]:LYS:HG2	1.85	0.76
1:A:146:ILE:HD12	1:A:196[B]:ILE:HD11	1.69	0.74
1:A:388[B]:CYS:SG	1:A:405:ILE:CD1	2.81	0.69
6:A:541:HOH:O	1:B:119[B]:LYS:CD	2.41	0.68
1:B:61[B]:ARG:HA	6:B:1033[B]:HOH:O	1.95	0.65
1:B:273[A]:LYS:HA	6:B:509:HOH:O	1.97	0.64
1:B:388[A]:CYS:SG	1:B:438:LEU:HD13	2.39	0.63
1:B:273[B]:LYS:HA	6:B:509:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:LEU:HD12	1:B:456:ALA:HB2	1.84	0.59
1:B:146:ILE:CD1	1:B:196[B]:ILE:HD11	2.27	0.59
1:A:388[A]:CYS:SG	1:A:438:LEU:HD13	2.43	0.59
1:B:270:GLU:CD	1:B:270:GLU:C	2.61	0.58
1:B:273[A]:LYS:HG3	1:B:274:HIS:CD2	2.40	0.56
1:B:270:GLU:HA	1:B:273[A]:LYS:HE3	1.87	0.55
1:B:59:ASN:C	1:B:61[B]:ARG:O	2.45	0.55
1:A:390:ILE:HD11	1:A:405:ILE:HD11	1.91	0.53
1:A:314:ASN:CB	6:A:611:HOH:O	2.58	0.52
1:B:368:ILE:HG22	1:B:377:LEU:HD13	1.93	0.51
1:A:388[A]:CYS:SG	1:A:438:LEU:CD1	2.99	0.50
1:B:365:ILE:CD1	1:B:385[B]:VAL:HG12	2.41	0.50
1:A:162:GLU:HG2	6:A:699:HOH:O	2.12	0.49
1:B:39[A]:MSE:HE3	1:B:330:LEU:HD23	1.95	0.48
1:B:390:ILE:HD11	1:B:405:ILE:HD11	1.97	0.47
1:B:270:GLU:OE1	1:B:271:LEU:N	2.48	0.46
1:B:337:ASP:HB2	1:B:338:PRO:CD	2.47	0.44
1:A:379:LEU:HD11	1:A:385[A]:VAL:HG21	1.99	0.44
1:B:62:ILE:N	1:B:62:ILE:HD13	2.33	0.44
1:B:59:ASN:O	1:B:61[B]:ARG:O	2.36	0.43
1:B:270:GLU:CD	1:B:271:LEU:N	2.72	0.42

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)
6:A:977:HOH:O	6:B:925:HOH:O[4_656]	2.14	0.06

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	452/443 (102%)	433 (96%)	19 (4%)	0	100	100
1	B	445/443 (100%)	427 (96%)	18 (4%)	0	100	100
All	All	897/886 (101%)	860 (96%)	37 (4%)	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	375/370 (101%)	373 (100%)	2 (0%)	88	80
1	B	369/370 (100%)	368 (100%)	1 (0%)	92	87
All	All	744/740 (100%)	741 (100%)	3 (0%)	91	84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	TYR
1	A	346	ASP
1	B	346	ASP

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

Mol	Chain	Res	Type
1	B	59	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 12 ligands modelled in this entry, 1 is unknown and 2 are monoatomic - leaving 9 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	EDO	B	464	-	3,3,3	0.35	0	2,2,2	1.12	0
3	EDO	B	465	-	3,3,3	0.51	0	2,2,2	0.22	0
3	EDO	A	468	-	3,3,3	0.56	0	2,2,2	0.16	0
3	EDO	B	469	-	3,3,3	0.56	0	2,2,2	0.06	0
2	EPE	A	462[A]	-	15,15,15	1.12	1 (6%)	18,20,20	2.28	5 (27%)
3	EDO	B	466	-	3,3,3	1.01	0	2,2,2	0.85	0
3	EDO	A	463	-	3,3,3	0.23	0	2,2,2	0.79	0
3	EDO	A	470	-	3,3,3	0.47	0	2,2,2	0.21	0
3	EDO	B	467	-	3,3,3	0.76	0	2,2,2	0.62	0

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
3	EDO	B	464	-	-	0/1/1/1	-
3	EDO	B	465	-	-	0/1/1/1	-
3	EDO	A	468	-	-	1/1/1/1	-
3	EDO	B	469	-	-	0/1/1/1	-
2	EPE	A	462[A]	-	-	0/9/19/19	0/1/1/1
3	EDO	B	466	-	-	1/1/1/1	-
3	EDO	A	463	-	-	0/1/1/1	-
3	EDO	A	470	-	-	0/1/1/1	-
3	EDO	B	467	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	462[A]	EPE	C10-S	3.53	1.82	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	462[A]	EPE	O1S-S-C10	-6.62	98.94	106.92
2	A	462[A]	EPE	C3-C2-N1	-3.44	103.58	110.64
2	A	462[A]	EPE	C9-N1-C6	3.19	119.39	111.23
2	A	462[A]	EPE	O3S-S-C10	2.60	109.97	105.77
2	A	462[A]	EPE	C7-N4-C5	2.39	117.33	111.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	468	EDO	O1-C1-C2-O2
3	B	466	EDO	O1-C1-C2-O2

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.