Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 02:36 AM EDT

PDB ID	:	6VHO
Title	:	Glycoside hydrolase family 16 endo-glucanase from Bacteroides ovatus in complex with G4G4G3G-NHCOCH2Br
Authors	:	Tamura, K.; Brumer, H.; van Petegem, F.
Deposited on	:	2020-01-10
Resolution	:	2.15 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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.15 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7688 atoms, of which 3658 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 Glycosyl hydrolase family 16.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	237	Total	C	H	N	O	S	111	1	0
			3705	1210	1808	315	365	7			
1	BBB	237	Total	C	H	N	O	S	111	1	0
			3712	1211	1815	316	363	7			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	MET	-	initiating methionine	UNP A7LY25
AAA	1	GLY	-	expression tag	UNP A7LY25
AAA	2	SER	-	expression tag	UNP A7LY25
AAA	3	SER	-	expression tag	UNP A7LY25
AAA	4	HIS	-	expression tag	UNP A7LY25
AAA	5	HIS	-	expression tag	UNP A7LY25
AAA	6	HIS	-	expression tag	UNP A7LY25
AAA	7	HIS	-	expression tag	UNP A7LY25
AAA	8	HIS	-	expression tag	UNP A7LY25
AAA	9	HIS	-	expression tag	UNP A7LY25
AAA	10	SER	-	expression tag	UNP A7LY25
AAA	11	SER	-	expression tag	UNP A7LY25
AAA	12	GLY	-	expression tag	UNP A7LY25
AAA	13	LEU	-	expression tag	UNP A7LY25
AAA	14	VAL	-	expression tag	UNP A7LY25
AAA	15	PRO	-	expression tag	UNP A7LY25
AAA	16	ARG	-	expression tag	UNP A7LY25
AAA	17	GLY	-	expression tag	UNP A7LY25
AAA	18	SER	-	expression tag	UNP A7LY25
AAA	19	HIS	-	expression tag	UNP A7LY25
AAA	20	MET	-	expression tag	UNP A7LY25
BBB	0	MET	-	initiating methionine	UNP A7LY25
BBB	1	GLY	-	expression tag	UNP A7LY25
BBB	2	SER	-	expression tag	UNP A7LY25
BBB	3	SER	-	expression tag	UNP A7LY25

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	4	HIS	-	expression tag	UNP A7LY25
BBB	5	HIS	-	expression tag	UNP A7LY25
BBB	6	HIS	-	expression tag	UNP A7LY25
BBB	7	HIS	-	expression tag	UNP A7LY25
BBB	8	HIS	-	expression tag	UNP A7LY25
BBB	9	HIS	-	expression tag	UNP A7LY25
BBB	10	SER	-	expression tag	UNP A7LY25
BBB	11	SER	-	expression tag	UNP A7LY25
BBB	12	GLY	-	expression tag	UNP A7LY25
BBB	13	LEU	-	expression tag	UNP A7LY25
BBB	14	VAL	-	expression tag	UNP A7LY25
BBB	15	PRO	-	expression tag	UNP A7LY25
BBB	16	ARG	-	expression tag	UNP A7LY25
BBB	17	GLY	-	expression tag	UNP A7LY25
BBB	18	SER	-	expression tag	UNP A7LY25
BBB	19	HIS	-	expression tag	UNP A7LY25
BBB	20	MET	-	expression tag	UNP A7LY25

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-N-acetyl-beta-D-glucopyranosylamine.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	3	Total	C	H	N	O	7	0	0
			72	20	35	1	16			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	106	Total	O	0	0
			106	106		
3	BBB	93	Total	O	0	0
			93	93		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.58Å 61.15Å 49.41Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	84.12 – 2.15	Depositor
% Data completeness (in resolution range)	99.5 (84.12-2.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.186 , 0.207	Depositor
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.389	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7688	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

3 monosaccharides are modelled in this entry.

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	$\#\|Z\|>2$
2	NBG	A	1	2	15,15,15	0.94	2 (13%)	21,21,21	2.99	7 (33%)
2	BGC	A	2	2	11,11,12	1.06	1 (9%)	15,15,17	1.46	3 (20%)
2	BGC	A	3	2	11,11,12	0.53	0	15,15,17	0.93	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
2	NBG	A	1	2	-	2/6/26/26	0/1/1/1
2	BGC	A	2	2	-	0/2/19/22	0/1/1/1
2	BGC	A	3	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	BGC	O4-C4	-3.30	1.35	1.43
2	A	1	NBG	C1-N1	2.23	1.46	1.43
2	A	1	NBG	C2-C1	2.03	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	NBG	O5-C1-C2	7.69	117.55	109.83
2	A	1	NBG	C5-O5-C1	6.88	121.85	112.52
2	A	1	NBG	C2-C1-N1	-5.21	105.20	111.30
2	A	1	NBG	C3-C2-C1	3.87	115.57	109.94
2	A	2	BGC	C1-O5-C5	3.32	116.69	112.19
2	A	1	NBG	C1-N1-C7	3.29	126.56	122.57
2	A	1	NBG	C8-C7-N1	2.69	120.66	116.10
2	A	1	NBG	C3-C4-C5	-2.51	105.76	110.24
2	A	2	BGC	C1-C2-C3	2.49	112.72	109.67
2	A	2	BGC	O4-C4-C5	-2.44	103.24	109.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

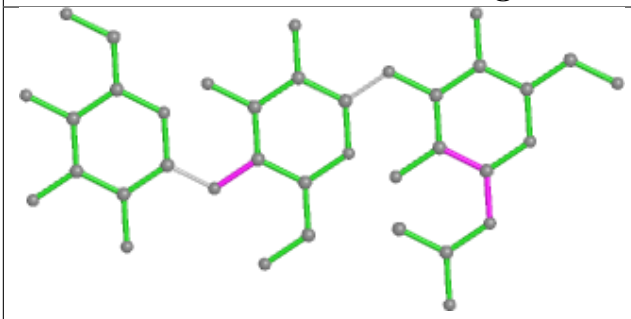
Mol	Chain	Res	Type	Atoms
2	A	1	NBG	C8-C7-N1-C1
2	A	1	NBG	O7-C7-N1-C1

There are no ring outliers.

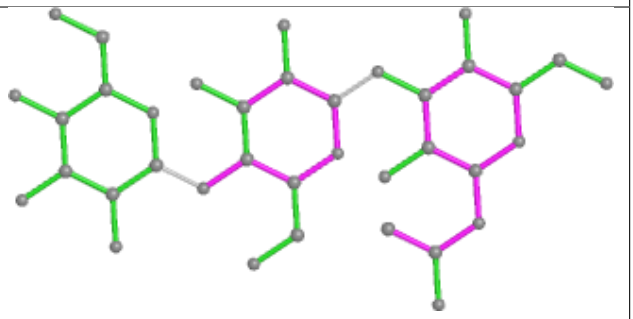
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

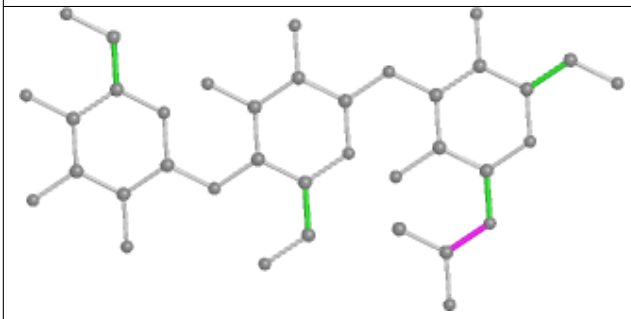
Oligosaccharide Chain A



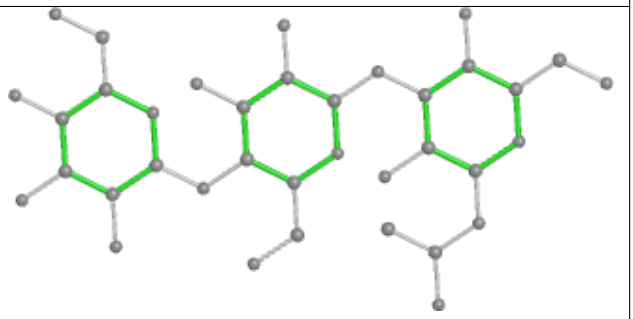
Bond lengths



Bond angles



Torsions



Rings

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.