

wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 01:37 am BST

PDB ID : 2VCC

> Title : Family 89 Glycoside Hydrolase from Clostridium perfringens

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2007-09-19 Deposited on

2.00 Å(reported) Resolution

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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

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) Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

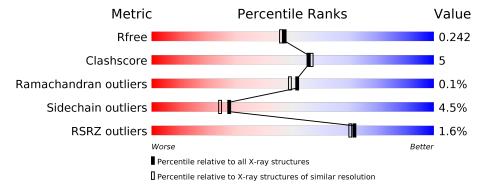
Validation Pipeline (wwPDB-VP) 2.11

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 2.00 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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		
			2%		
1	A	891	85%	13%	•



2 Entry composition (i)

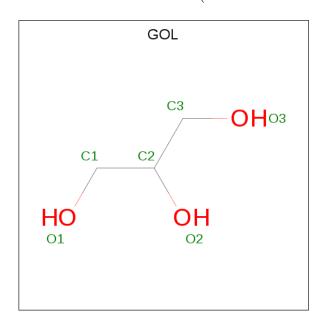
There are 5 unique types of molecules in this entry. The entry contains 7830 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALPHA-N-ACETYLGLUCOSAMINIDASE.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	A	887	Total 7228	C 4582	N 1194	O 1423	S 29	59	7	1

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	A	1	Total 5	O 4	S 1	0	0

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

\mathbf{M}	ol	Chain	Residues	Ator	ns	ZeroOcc	AltConf
4	:	A	1	Total 1	Ca 1	0	0

 \bullet Molecule 5 is water.

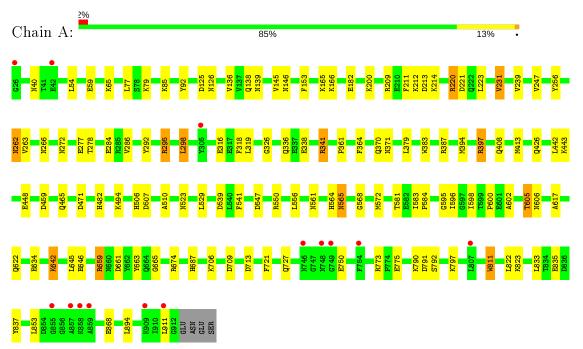
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
5	A	554	Total O 578 578	0	24



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 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: ALPHA-N-ACETYLGLUCOSAMINIDASE





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants	$90.71 \text{\AA} 90.71 \text{Å} 252.66 \text{Å}$	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 - 2.00	Depositor
Resolution (A)	45.36 - 2.00	EDS
% Data completeness	96.5 (20.00-2.00)	Depositor
(in resolution range)	$66.1 \ (45.36 - 2.00)$	EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.38 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
P. P.	0.210 , 0.255	Depositor
R, R_{free}	0.198 , 0.242	DCC
R_{free} test set	2675 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37 , 48.5	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	0.050 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7830	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: GOL, CA, SO4

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).

Mal	Chain	Boı	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.52	$6/7401 \; (0.1\%)$	0.56	0/10015	

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	A	1	0		

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	284	GLU	CD-OE1	-15.69	1.08	1.25
1	A	750	GLU	CG-CD	8.71	1.65	1.51
1	A	448	GLU	CB-CG	-7.92	1.37	1.52
1	A	213	ASP	CG-OD2	-5.72	1.12	1.25
1	A	835	GLU	CG-CD	5.40	1.60	1.51

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	278	THR	СВ

There are no planarity outliers.



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	7228	0	6825	71	0
2	A	18	0	24	0	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	578	0	0	8	0
All	All	7830	0	6849	71	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 5.

The worst 5 of 71 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap} & (ext{Å}) \end{aligned}$
1:A:371:ASN:HD21	1:A:482:HIS:HD2	1.13	0.94
1:A:605:THR:HG21	5:A:2384:HOH:O	1.65	0.94
1:A:790:LYS:CB	5:A:2503:HOH:O	2.22	0.87
1:A:790:LYS:CA	5:A:2503:HOH:O	2.28	0.80
1:A:790:LYS:N	5:A:2503:HOH:O	2.16	0.77

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	nalysed Favoured		Allowed Outliers	
1	A	891/891 (100%)	861 (97%)	29 (3%)	1 (0%)	51 49



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	LEU

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	ysed Rotameric		Percentiles	
1	A	769/767 (100%)	734 (95%)	35 (5%)	27 23	

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	ARG
1	A	541	PHE
1	A	823	LYS
1	A	442	LEU
1	A	471	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	${f Res}$	\mathbf{Type}
1	A	455	GLN
1	A	482	HIS
1	A	847	ASN
1	A	465	GLN
1	A	506	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	ol Type Chain Res L			Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	1914	_	5,5,5	0.42	0	5, 5, 5	0.12	0
3	SO4	A	1916	-	4,4,4	0.13	0	6,6,6	0.11	0
2	GOL	A	1915	-	5,5,5	0.35	0	5, 5, 5	0.45	0
2	GOL	A	1913	-	5,5,5	0.37	0	5,5,5	0.33	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	GOL	A	1914	-	-	4/4/4/4	-
2	GOL	A	1915	-	-	3/4/4/4	-
2	GOL	A	1913	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1914	GOL	O1-C1-C2-C3
2	A	1915	GOL	C1-C2-C3-O3
2	A	1915	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	1914	GOL	C1-C2-C3-O3
2	A	1913	GOL	O1-C1-C2-C3

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q < 0.9
1	A	886/891 (99%)	-0.21	14 (1%)	72 70	20, 31, 44, 57	20 (2%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	857	ALA	5.9
1	A	26	GLY	3.4
1	A	909	LYS	3.3
1	A	855	GLY	3.0
1	A	858	LYS	2.7

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 carbohydrates 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	$oxed{f B-factors({ m \AA}^2)}$	Q<0.9
2	GOL	A	1913	6/6	0.74	0.27	59,61,61,61	0
2	GOL	A	1914	6/6	0.83	0.16	48,50,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q<0.9
3	SO4	A	1916	5/5	0.90	0.24	94,94,94,94	0
2	GOL	A	1915	6/6	0.91	0.27	41,42,43,44	0
4	CA	A	1917	1/1	0.99	0.05	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.

