



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 03:03 AM EDT

PDB ID : 6UYM  
Title : Structure of Hepatitis C Virus Envelope Glycoprotein E2mc3-v6 redesigned core from genotype 1a bound to broadly neutralizing antibody AR3C  
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Deposited on : 2019-11-13  
Resolution : 2.85 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](mailto: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>.

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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)  
Xtrriage (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

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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 5 unique types of molecules in this entry. The entry contains 8859 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 Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	145	Total	C	N	O	S	0	0	0
			1143	735	192	203	13			
1	F	137	Total	C	N	O	S	0	0	0
			1075	692	181	190	12			

- Molecule 2 is a protein called Fab AR3C heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	221	Total	C	N	O	S	0	0	0
			1650	1039	279	325	7			
2	A	223	Total	C	N	O	S	0	0	0
			1665	1047	282	329	7			

- Molecule 3 is a protein called Fab AR3C light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	211	Total	C	N	O	S	0	0	0
			1612	1005	277	326	4			
3	B	208	Total	C	N	O	S	0	0	0
			1588	992	271	321	4			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	E	1	14	8	1	5	0	0
5	E	1	14	8	1	5	0	0
5	E	1	14	8	1	5	0	0
5	F	1	14	8	1	5	0	0
5	F	1	14	8	1	5	0	0

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	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.10Å 90.84Å 94.03Å 84.50° 78.11° 77.09°	Depositor
Resolution (Å)	29.47 – 2.85	Depositor
% Data completeness (in resolution range)	87.7 (29.47-2.85)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.85Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.214 , 0.260	Depositor
Wilson B-factor (Å <sup>2</sup> )	61.3	Xtrriage
Anisotropy	0.435	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.006 for -h,-l,-k	Xtrriage
Total number of atoms	8859	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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

### 4.2 Too-close contacts [i](#)

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

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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

#### 4.3.2 Protein sidechains [i](#)

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

#### 4.3.3 RNA [i](#)

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

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 4.5 Carbohydrates [i](#)

4 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
4	NAG	C	1	1,4	14,14,15	1.25	1 (7%)	17,19,21	1.20	1 (5%)
4	NAG	C	2	4	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	D	1	1,4	14,14,15	0.46	0	17,19,21	0.57	0
4	NAG	D	2	4	14,14,15	0.30	0	17,19,21	0.44	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
4	NAG	C	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NAG	O5-C1	-4.59	1.36	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	NAG	C3-C4-C5	3.11	115.79	110.24

There are no chirality outliers.

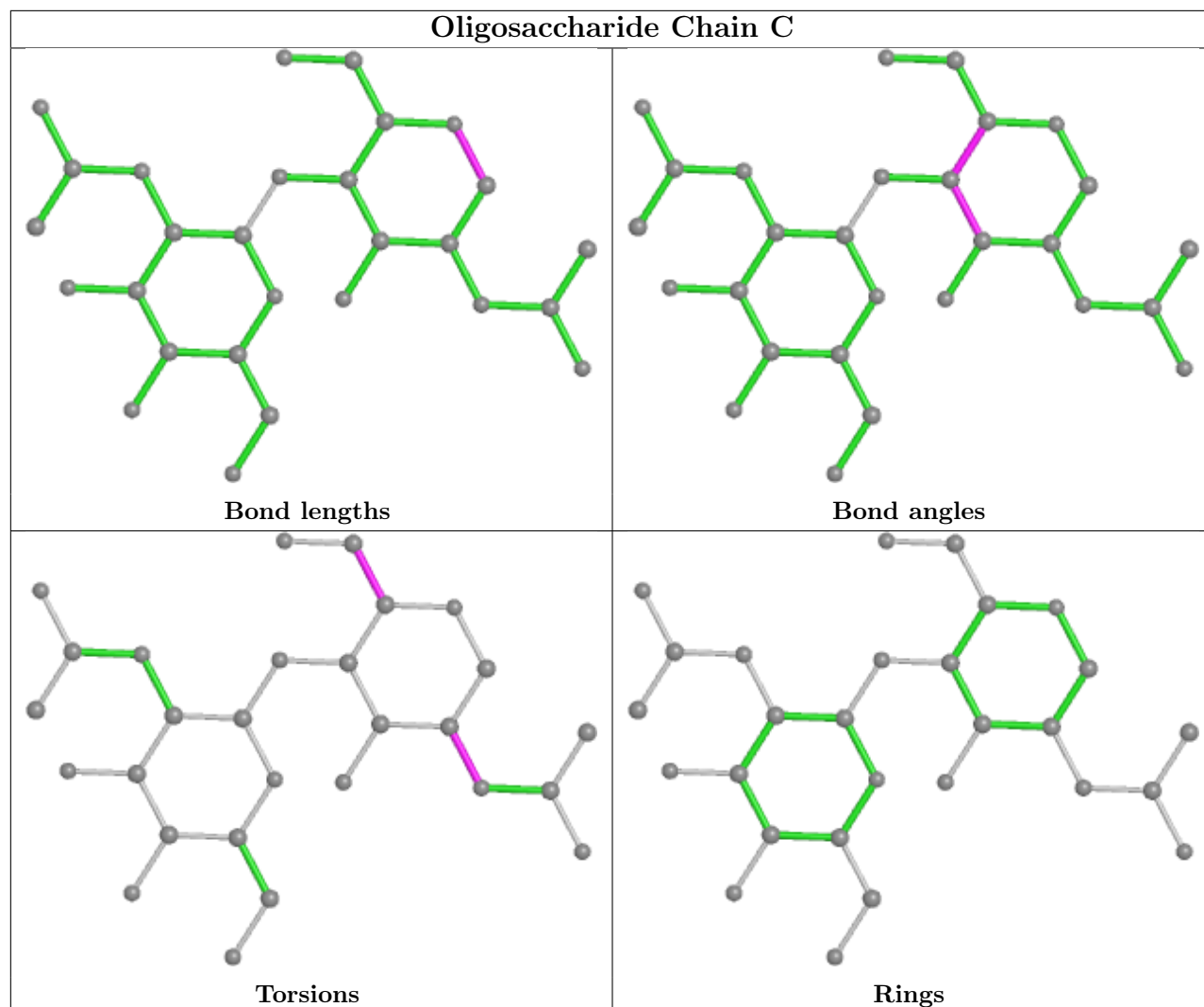
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	NAG	C1-C2-N2-C7
4	C	1	NAG	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
4	C	1	NAG	C3-C2-N2-C7

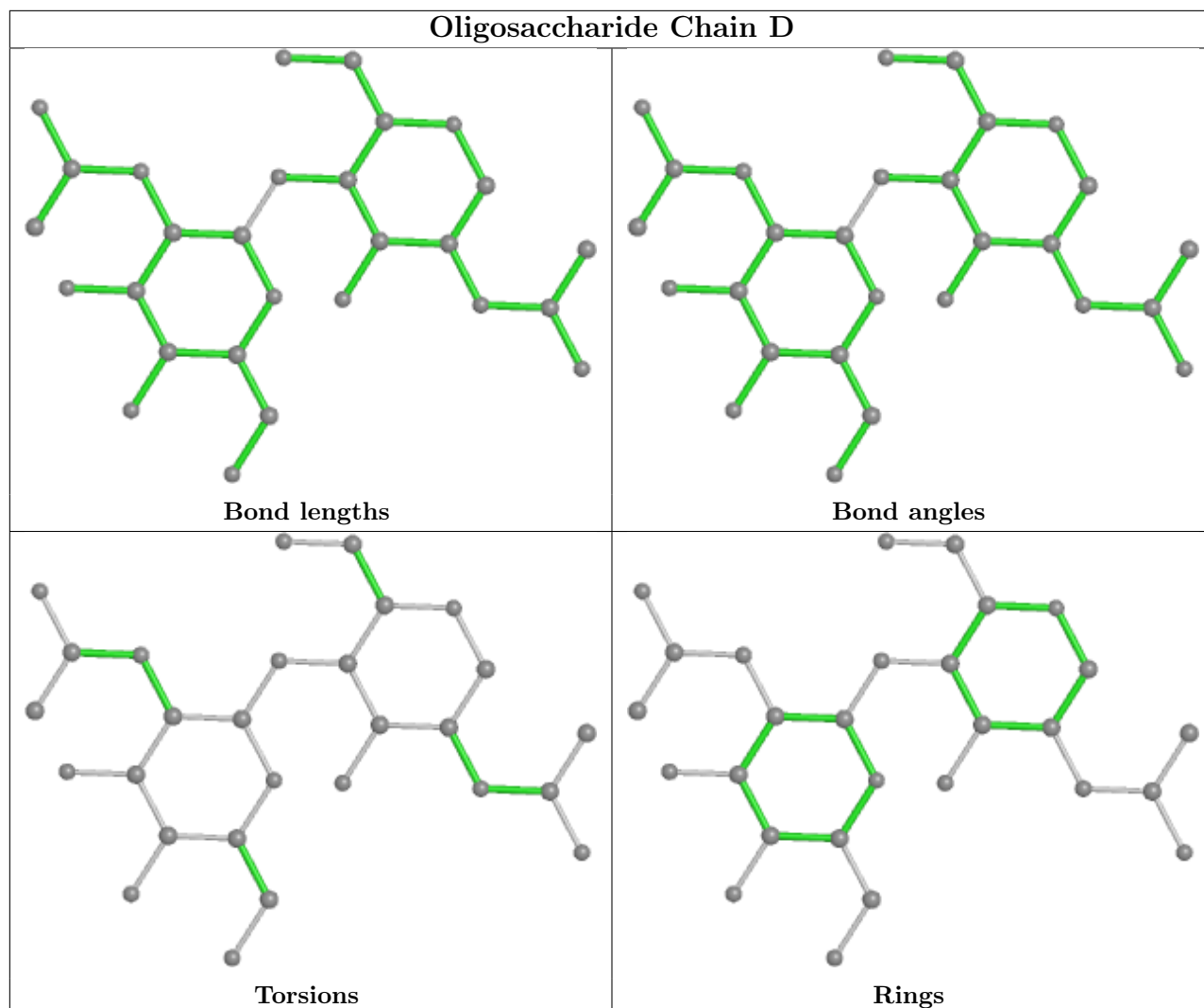
There are no ring outliers.

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.







## 4.6 Ligand geometry [i](#)

5 ligands 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	$\# Z  > 2$
5	NAG	E	703	1	14,14,15	0.48	0	17,19,21	0.57	0
5	NAG	E	702	1	14,14,15	0.46	0	17,19,21	1.30	2 (11%)
5	NAG	F	701	1	14,14,15	0.44	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	F	702	1	14,14,15	0.37	0	17,19,21	0.52	0
5	NAG	E	701	1	14,14,15	0.62	0	17,19,21	0.64	1 (5%)

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
5	NAG	E	703	1	-	4/6/23/26	0/1/1/1
5	NAG	E	702	1	-	5/6/23/26	0/1/1/1
5	NAG	F	701	1	-	4/6/23/26	0/1/1/1
5	NAG	F	702	1	-	4/6/23/26	0/1/1/1
5	NAG	E	701	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	702	NAG	C2-N2-C7	4.27	128.99	122.90
5	E	702	NAG	C1-C2-N2	2.20	114.25	110.49
5	E	701	NAG	C1-O5-C5	2.13	115.07	112.19

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	702	NAG	O5-C5-C6-O6
5	F	701	NAG	O5-C5-C6-O6
5	E	702	NAG	C4-C5-C6-O6
5	E	703	NAG	O5-C5-C6-O6
5	F	702	NAG	O5-C5-C6-O6
5	F	702	NAG	C4-C5-C6-O6
5	E	703	NAG	C4-C5-C6-O6
5	F	701	NAG	C4-C5-C6-O6
5	E	702	NAG	C8-C7-N2-C2
5	E	702	NAG	O7-C7-N2-C2
5	F	702	NAG	C8-C7-N2-C2
5	F	702	NAG	O7-C7-N2-C2
5	F	701	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	E	701	NAG	C1-C2-N2-C7
5	E	703	NAG	C1-C2-N2-C7
5	E	702	NAG	C3-C2-N2-C7
5	E	701	NAG	C3-C2-N2-C7
5	E	703	NAG	C3-C2-N2-C7
5	F	701	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

#### 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.