

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 5, 2023 – 08:07 AM EDT

PDB ID	:	6VFU
Title	:	Crystal structure of human protocadherin 19 EC1-EC4
Authors	:	Harrison, O.J.; Brasch, J.; Shapiro, L.
Deposited on	:	2020-01-06
Resolution	:	3.50  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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.35.1
EDS Percentile statistics Ideal geometry (proteins)	: : :	FAILED 20191225.v01 (using entries in the PDB archive December 25th 2019) Engh & Huber (2001) Parkinson et al. (1996)

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\hbox{-}RAY\,DIFFRACTION$ 

The reported resolution of this entry is 3.50 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.



#### 6 VFU

# 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 19193 atoms, of which 9270 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	С	428	Total	С	Η	Ν	0	S	0	0	0
L	U	420	6365	2049	3073	569	666	8	0		
1	А	428	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
	Л	420	6402	2049	3110	569	666	8	0		
1	В	411	Total	С	Η	Ν	0	S	0	1	0
1	D	411	6173	1969	3017	539	640	8	0		0

• Molecule 1 is a protein called Protocadherin-19.

There are 18	discrepancies	between	the modelled	and	reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	425	HIS	-	expression tag	UNP Q8TAB3
С	426	HIS	-	expression tag	UNP Q8TAB3
С	427	HIS	-	expression tag	UNP Q8TAB3
С	428	HIS	-	expression tag	UNP Q8TAB3
С	429	HIS	-	expression tag	UNP Q8TAB3
С	430	HIS	-	expression tag	UNP Q8TAB3
А	425	HIS	-	expression tag	UNP Q8TAB3
A	426	HIS	-	expression tag	UNP Q8TAB3
А	427	HIS	-	expression tag	UNP Q8TAB3
А	428	HIS	-	expression tag	UNP Q8TAB3
А	429	HIS	-	expression tag	UNP Q8TAB3
А	430	HIS	-	expression tag	UNP Q8TAB3
В	425	HIS	-	expression tag	UNP Q8TAB3
В	426	HIS	-	expression tag	UNP Q8TAB3
В	427	HIS	-	expression tag	UNP Q8TAB3
В	428	HIS	-	expression tag	UNP Q8TAB3
В	429	HIS	-	expression tag	UNP Q8TAB3
В	430	HIS	-	expression tag	UNP Q8TAB3

• Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopy ranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	D	4	Total	С	Η	Ν	0	0	0	0
_	-	-	84	28	35	2	19	Ŭ	, i i i i i i i i i i i i i i i i i i i	Ŭ

• Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-bet a-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	Е	2	Total 46	C 14	H 22	N 1	O q	0	0	0

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

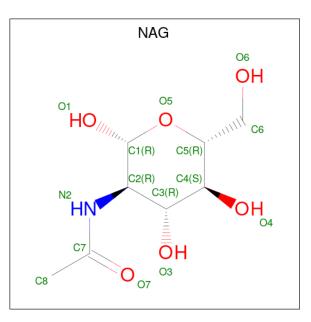
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	F	2	Total C N O   28 16 2 10	0	0	0

• Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	9	Total Ca 9 9	0	0
5	А	9	Total Ca 9 9	0	0
5	В	9	Total Ca 9 9	0	0

• Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	С	1	Total C N O 14 8 1 5	0	0
6	А	1	Total C N O   14 8 1 5	0	0
6	В	1	Total C H N O   27 8 13 1 5	0	0

• Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	С	1	Total Ni 1 1	0	0
7	А	1	Total Ni 1 1	0	0

• Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	С	2	Total Cl 2 2	0	0
8	А	2	Total Cl 2 2	0	0

• Molecule 9 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	С	4	Total O 4 4	0	0
9	А	2	Total O 2 2	0	0
9	В	1	Total O 1 1	0	0

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



# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	108.97Å $108.97$ Å $309.66$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	19.99 - 3.50	Depositor
% Data completeness	99.8 (19.99-3.50)	Depositor
(in resolution range)	· · · ·	-
R <sub>merge</sub>	0.14	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.87 (at 3.48 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
$R, R_{free}$	0.265 , $0.291$	Depositor
Wilson B-factor ( $Å^2$ )	123.0	Xtriage
Anisotropy	0.400	Xtriage
L-test for twinning <sup>2</sup>	$<  L  > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
Total number of atoms	19193	wwPDB-VP
Average B, all atoms $(Å^2)$	193.0	wwPDB-VP

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

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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)

8 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	Turne	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
10101	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	NAG	D	1	1,2	14,14,15	0.39	0	17,19,21	0.90	1 (5%)
2	NAG	D	2	2	$14,\!14,\!15$	0.55	0	$17,\!19,\!21$	0.69	1 (5%)
2	BMA	D	3	2	11,11,12	0.56	0	$15,\!15,\!17$	0.70	0
2	FUC	D	4	2	10,10,11	1.45	2 (20%)	14,14,16	1.47	2 (14%)
3	NAG	Е	1	3,1	14,14,15	0.33	0	17,19,21	0.48	0
3	FUC	Е	2	3	10,10,11	0.74	0	$14,\!14,\!16$	0.76	0
4	NAG	F	1	4,1	14,14,15	0.37	0	17,19,21	0.78	1 (5%)
4	NAG	F	2	4	14,14,15	0.38	0	17,19,21	0.38	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	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	FUC	D	4	2	-	-	0/1/1/1
3	NAG	Е	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	Е	2	3	-	-	0/1/1/1
4	NAG	F	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	FUC	C4-C3	2.42	1.58	1.52
2	D	4	FUC	O5-C1	-2.20	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	D	4	FUC	O5-C5-C6	-3.71	99.34	107.33
2	D	1	NAG	C1-O5-C5	2.60	115.72	112.19
4	F	1	NAG	C1-O5-C5	2.36	115.39	112.19
2	D	4	FUC	O2-C2-C1	2.26	113.78	109.15
2	D	2	NAG	C1-O5-C5	2.14	115.08	112.19

There are no chirality outliers.



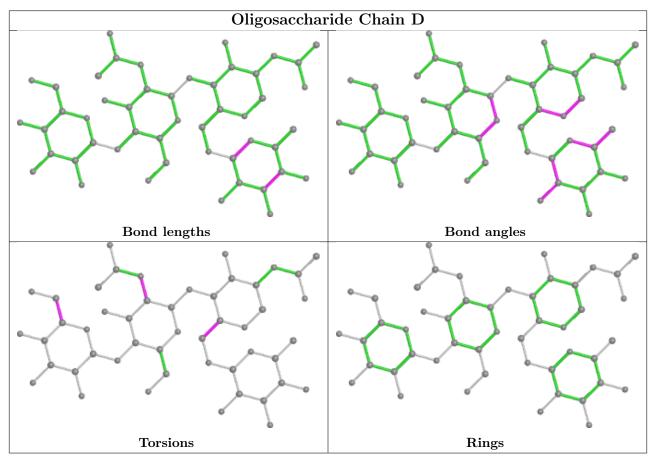
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
2	D	3	BMA	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

5 of 8 torsion outliers are listed below:

There are no ring outliers.

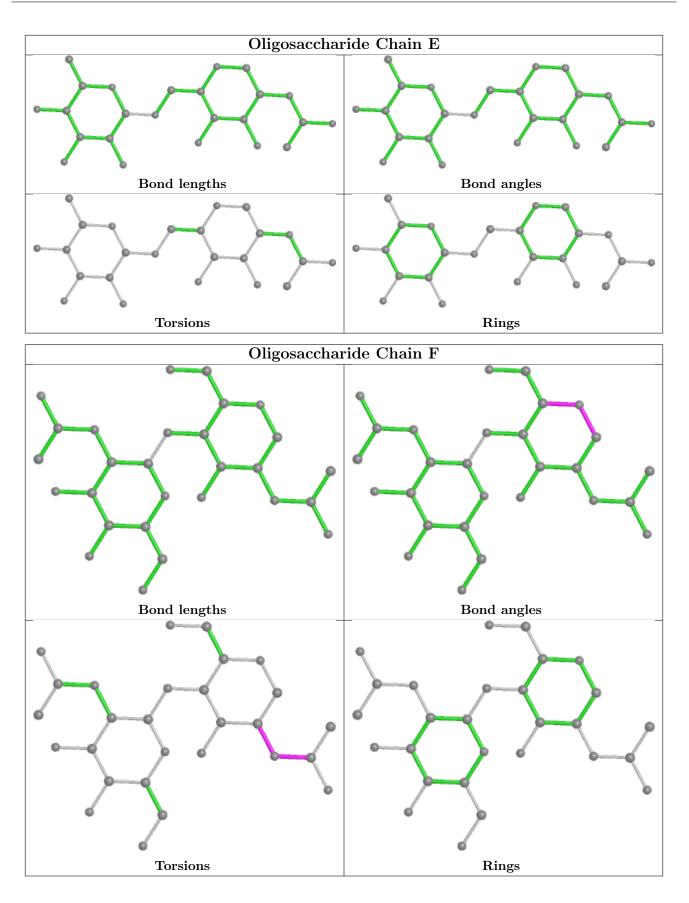
No monomer is involved in short contacts.

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)

Of 36 ligands modelled in this entry, 33 are monoatomic - leaving 3 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	Dec	Link	Bo	ond leng	$\mathbf{ths}$	В	ond ang	les
	туре	Ullaili	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
6	NAG	А	512	1	14,14,15	0.39	0	17,19,21	0.44	0
6	NAG	В	510	1	14,14,15	0.43	0	17,19,21	0.39	0
6	NAG	С	514	1	14,14,15	0.37	0	17,19,21	0.53	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
6	NAG	А	512	1	-	0/6/23/26	0/1/1/1
6	NAG	В	510	1	-	2/6/23/26	0/1/1/1
6	NAG	С	514	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	В	510	NAG	C1-C2-N2-C7
6	В	510	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 (i)

## 5.1 Protein, DNA and RNA chains (i)

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

## 5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

### 5.3 Carbohydrates (i)

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

## 5.4 Ligands (i)

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

### 5.5 Other polymers (i)

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

