



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 04:23 AM EDT

PDB ID : 6VFW  
Title : Crystal structure of human delta protocadherin 10 EC1-EC4  
Authors : Harrison, O.J.; Brasch, J.; Shapiro, L.  
Deposited on : 2020-01-06  
Resolution : 3.60 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](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 3.60 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 32989 atoms, of which 16057 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 Protocadherin-10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	423	6412	2048	3135	550	675	4	0	0	0
1	B	423	6408	2047	3132	550	675	4	0	0	0
1	C	429	6456	2064	3152	556	680	4	0	0	0
1	D	423	6365	2043	3095	548	675	4	0	0	0
1	E	422	6400	2045	3128	549	674	4	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	439	HIS	-	expression tag	UNP Q9P2E7
A	440	HIS	-	expression tag	UNP Q9P2E7
A	441	HIS	-	expression tag	UNP Q9P2E7
A	442	HIS	-	expression tag	UNP Q9P2E7
A	443	HIS	-	expression tag	UNP Q9P2E7
A	444	HIS	-	expression tag	UNP Q9P2E7
B	439	HIS	-	expression tag	UNP Q9P2E7
B	440	HIS	-	expression tag	UNP Q9P2E7
B	441	HIS	-	expression tag	UNP Q9P2E7
B	442	HIS	-	expression tag	UNP Q9P2E7
B	443	HIS	-	expression tag	UNP Q9P2E7
B	444	HIS	-	expression tag	UNP Q9P2E7
C	439	HIS	-	expression tag	UNP Q9P2E7
C	440	HIS	-	expression tag	UNP Q9P2E7
C	441	HIS	-	expression tag	UNP Q9P2E7
C	442	HIS	-	expression tag	UNP Q9P2E7
C	443	HIS	-	expression tag	UNP Q9P2E7
C	444	HIS	-	expression tag	UNP Q9P2E7
D	439	HIS	-	expression tag	UNP Q9P2E7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	440	HIS	-	expression tag	UNP Q9P2E7
D	441	HIS	-	expression tag	UNP Q9P2E7
D	442	HIS	-	expression tag	UNP Q9P2E7
D	443	HIS	-	expression tag	UNP Q9P2E7
D	444	HIS	-	expression tag	UNP Q9P2E7
E	439	HIS	-	expression tag	UNP Q9P2E7
E	440	HIS	-	expression tag	UNP Q9P2E7
E	441	HIS	-	expression tag	UNP Q9P2E7
E	442	HIS	-	expression tag	UNP Q9P2E7
E	443	HIS	-	expression tag	UNP Q9P2E7
E	444	HIS	-	expression tag	UNP Q9P2E7

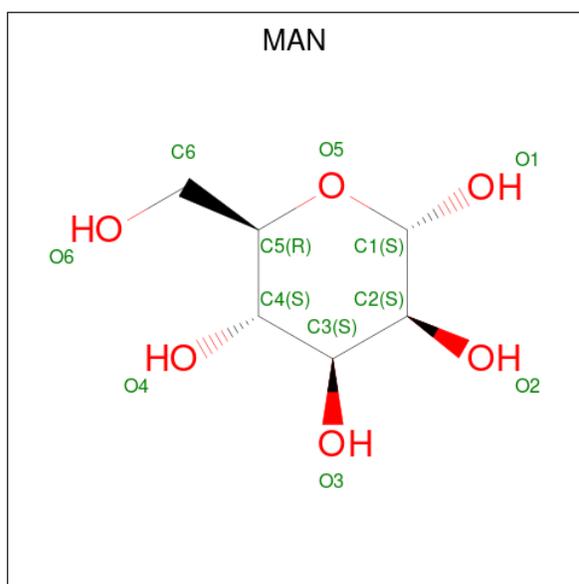
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	F	6	Total	C	H	N	O	0	0	0
			130	40	59	2	29			
2	G	6	Total	C	H	N	O	0	0	0
			134	40	63	2	29			
2	H	6	Total	C	H	N	O	0	0	0
			134	40	63	2	29			
2	I	6	Total	C	H	N	O	0	0	0
			131	40	60	2	29			
2	J	6	Total	C	H	N	O	0	0	0
			131	40	60	2	29			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	Ca	0	0
			9	9		
3	B	9	Total	Ca	0	0
			9	9		
3	C	9	Total	Ca	0	0
			9	9		
3	D	9	Total	Ca	0	0
			9	9		
3	E	9	Total	Ca	0	0
			9	9		

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	H			O
4	A	1	22	6	11	5	0	0
4	A	1	22	6	11	5	0	0
4	B	1	22	6	11	5	0	0
4	B	1	22	6	11	5	0	0
4	C	1	22	6	11	5	0	0
4	C	1	22	6	11	5	0	0
4	D	1	22	6	11	5	0	0
4	D	1	22	6	11	5	0	0
4	E	1	22	6	11	5	0	0
4	E	1	22	6	11	5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	B	5	Total 5	O 5	0	0
5	C	4	Total 4	O 4	0	0
5	D	4	Total 4	O 4	0	0
5	E	5	Total 5	O 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	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	346.55Å 73.19Å 246.33Å 90.00° 132.06° 90.00°	Depositor
Resolution (Å)	19.99 – 3.60	Depositor
% Data completeness (in resolution range)	93.4 (19.99-3.60)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.33 (at 3.57Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.277 , 0.295	Depositor
Wilson B-factor (Å <sup>2</sup> )	120.2	Xtrriage
Anisotropy	0.669	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtrriage
Total number of atoms	32989	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	270.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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](#)

30 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	NAG	F	1	2,1	14,14,15	0.70	1 (7%)	17,19,21	1.00	1 (5%)
2	NAG	F	2	2	14,14,15	1.28	1 (7%)	17,19,21	1.17	2 (11%)
2	BMA	F	3	2	11,11,12	1.14	1 (9%)	15,15,17	1.31	3 (20%)
2	MAN	F	4	2	11,11,12	1.12	1 (9%)	15,15,17	1.57	2 (13%)
2	MAN	F	5	2	11,11,12	1.33	2 (18%)	15,15,17	2.18	4 (26%)
2	FUC	F	6	2	10,10,11	1.17	1 (10%)	14,14,16	1.65	3 (21%)
2	NAG	G	1	2,1	14,14,15	0.97	1 (7%)	17,19,21	0.80	0
2	NAG	G	2	2	14,14,15	0.79	1 (7%)	17,19,21	0.87	1 (5%)
2	BMA	G	3	2	11,11,12	1.34	2 (18%)	15,15,17	0.85	0
2	MAN	G	4	2	11,11,12	0.96	1 (9%)	15,15,17	1.15	2 (13%)
2	MAN	G	5	2	11,11,12	0.86	1 (9%)	15,15,17	1.05	2 (13%)
2	FUC	G	6	2	10,10,11	0.71	0	14,14,16	1.82	4 (28%)
2	NAG	H	1	2,1	14,14,15	0.88	1 (7%)	17,19,21	0.53	0
2	NAG	H	2	2	14,14,15	0.34	0	17,19,21	0.77	1 (5%)
2	BMA	H	3	2	11,11,12	1.50	2 (18%)	15,15,17	1.03	0
2	MAN	H	4	2	11,11,12	1.20	2 (18%)	15,15,17	1.58	3 (20%)
2	MAN	H	5	2	11,11,12	0.90	1 (9%)	15,15,17	1.20	2 (13%)
2	FUC	H	6	2	10,10,11	1.07	1 (10%)	14,14,16	1.10	2 (14%)
2	NAG	I	1	2,1	14,14,15	0.57	1 (7%)	17,19,21	0.82	0
2	NAG	I	2	2	14,14,15	0.87	1 (7%)	17,19,21	0.87	1 (5%)
2	BMA	I	3	2	11,11,12	1.24	2 (18%)	15,15,17	1.41	3 (20%)
2	MAN	I	4	2	11,11,12	0.86	1 (9%)	15,15,17	1.22	2 (13%)
2	MAN	I	5	2	11,11,12	0.92	1 (9%)	15,15,17	1.49	2 (13%)
2	FUC	I	6	2	10,10,11	0.94	0	14,14,16	1.44	3 (21%)
2	NAG	J	1	2,1	14,14,15	0.39	0	17,19,21	0.64	0
2	NAG	J	2	2	14,14,15	0.28	0	17,19,21	0.94	1 (5%)
2	BMA	J	3	2	11,11,12	1.12	1 (9%)	15,15,17	1.17	1 (6%)
2	MAN	J	4	2	11,11,12	0.92	0	15,15,17	1.14	2 (13%)
2	MAN	J	5	2	11,11,12	0.97	1 (9%)	15,15,17	1.29	2 (13%)
2	FUC	J	6	2	10,10,11	0.75	0	14,14,16	0.99	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	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	BMA	F	3	2	-	1/2/19/22	0/1/1/1
2	MAN	F	4	2	-	2/2/19/22	0/1/1/1
2	MAN	F	5	2	-	2/2/19/22	0/1/1/1
2	FUC	F	6	2	-	-	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
2	MAN	G	5	2	-	1/2/19/22	0/1/1/1
2	FUC	G	6	2	-	-	0/1/1/1
2	NAG	H	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	MAN	H	4	2	-	1/2/19/22	0/1/1/1
2	MAN	H	5	2	-	2/2/19/22	0/1/1/1
2	FUC	H	6	2	-	-	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
2	MAN	I	4	2	-	2/2/19/22	0/1/1/1
2	MAN	I	5	2	-	1/2/19/22	1/1/1/1
2	FUC	I	6	2	-	-	0/1/1/1
2	NAG	J	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
2	BMA	J	3	2	-	2/2/19/22	0/1/1/1
2	MAN	J	4	2	-	0/2/19/22	0/1/1/1
2	MAN	J	5	2	-	2/2/19/22	0/1/1/1
2	FUC	J	6	2	-	-	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	C1-C2	4.54	1.59	1.52
2	F	5	MAN	C1-C2	3.63	1.60	1.52
2	G	1	NAG	O5-C1	-3.49	1.38	1.43
2	H	4	MAN	C1-C2	3.17	1.59	1.52
2	F	4	MAN	C1-C2	3.14	1.59	1.52
2	H	1	NAG	O5-C1	-3.12	1.38	1.43
2	J	5	MAN	C1-C2	3.08	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	6	FUC	C1-C2	2.91	1.58	1.52
2	I	3	BMA	O5-C1	-2.80	1.39	1.43
2	I	2	NAG	O5-C1	-2.64	1.39	1.43
2	H	3	BMA	C1-C2	2.63	1.58	1.52
2	G	4	MAN	C1-C2	2.62	1.58	1.52
2	G	3	BMA	C1-C2	2.52	1.58	1.52
2	F	1	NAG	O5-C1	-2.37	1.39	1.43
2	H	3	BMA	C4-C3	2.34	1.58	1.52
2	H	5	MAN	C1-C2	2.32	1.57	1.52
2	I	3	BMA	C4-C5	2.28	1.57	1.53
2	H	6	FUC	C1-C2	2.23	1.57	1.52
2	F	5	MAN	O5-C1	2.20	1.47	1.43
2	G	3	BMA	C4-C5	2.15	1.57	1.53
2	F	3	BMA	C4-C5	2.15	1.57	1.53
2	G	2	NAG	C1-C2	2.14	1.55	1.52
2	I	4	MAN	C1-C2	2.12	1.57	1.52
2	H	4	MAN	O5-C5	2.10	1.47	1.43
2	G	5	MAN	C1-C2	2.07	1.56	1.52
2	I	1	NAG	O5-C1	-2.07	1.40	1.43
2	I	5	MAN	C1-C2	2.06	1.56	1.52
2	J	3	BMA	O3-C3	2.04	1.47	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5	MAN	C1-O5-C5	6.00	120.33	112.19
2	F	4	MAN	C1-O5-C5	4.62	118.45	112.19
2	H	4	MAN	C1-O5-C5	4.41	118.16	112.19
2	I	5	MAN	C1-O5-C5	4.37	118.11	112.19
2	G	6	FUC	O5-C1-C2	4.13	117.14	110.77
2	F	5	MAN	C1-C2-C3	3.88	114.44	109.67
2	F	6	FUC	C1-C2-C3	3.88	114.44	109.67
2	G	6	FUC	C1-O5-C5	3.67	121.09	112.78
2	I	4	MAN	C1-O5-C5	3.42	116.83	112.19
2	F	6	FUC	C1-O5-C5	3.30	120.25	112.78
2	F	2	NAG	C1-O5-C5	-3.12	107.96	112.19
2	I	3	BMA	C1-O5-C5	3.11	116.41	112.19
2	H	5	MAN	C1-O5-C5	3.08	116.37	112.19
2	H	4	MAN	O2-C2-C3	-3.00	104.12	110.14
2	F	5	MAN	O5-C1-C2	2.97	115.35	110.77
2	J	5	MAN	C1-C2-C3	2.86	113.18	109.67
2	I	6	FUC	C1-C2-C3	2.84	113.16	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	3	BMA	O3-C3-C2	2.79	115.34	109.99
2	J	5	MAN	C1-O5-C5	2.77	115.95	112.19
2	F	3	BMA	O5-C5-C6	2.76	111.53	107.20
2	J	4	MAN	O2-C2-C3	-2.75	104.63	110.14
2	F	4	MAN	O2-C2-C3	-2.74	104.64	110.14
2	F	1	NAG	O4-C4-C5	-2.73	102.52	109.30
2	G	4	MAN	O2-C2-C3	-2.71	104.71	110.14
2	F	5	MAN	O2-C2-C3	-2.70	104.73	110.14
2	I	6	FUC	O5-C5-C4	2.68	114.34	109.52
2	G	4	MAN	C1-O5-C5	2.58	115.68	112.19
2	G	6	FUC	O5-C5-C4	2.53	114.06	109.52
2	G	5	MAN	O2-C2-C3	-2.49	105.15	110.14
2	I	4	MAN	O2-C2-C3	-2.47	105.18	110.14
2	H	2	NAG	C2-N2-C7	2.41	126.33	122.90
2	I	6	FUC	C1-O5-C5	2.40	118.22	112.78
2	F	6	FUC	O5-C1-C2	2.39	114.46	110.77
2	J	4	MAN	C1-O5-C5	2.36	115.39	112.19
2	H	5	MAN	O2-C2-C3	-2.34	105.46	110.14
2	G	6	FUC	C1-C2-C3	2.32	112.52	109.67
2	H	4	MAN	C1-C2-C3	2.32	112.51	109.67
2	F	3	BMA	O5-C1-C2	-2.31	107.20	110.77
2	I	3	BMA	C3-C4-C5	2.30	114.34	110.24
2	H	6	FUC	O5-C5-C4	2.25	113.56	109.52
2	I	5	MAN	O2-C2-C3	-2.23	105.67	110.14
2	G	5	MAN	C1-O5-C5	2.21	115.18	112.19
2	H	6	FUC	C1-O5-C5	2.16	117.67	112.78
2	F	2	NAG	O4-C4-C3	2.15	115.32	110.35
2	G	2	NAG	C2-N2-C7	2.12	125.92	122.90
2	I	3	BMA	O5-C5-C6	-2.08	103.94	107.20
2	J	2	NAG	C1-O5-C5	2.06	114.98	112.19
2	I	2	NAG	C1-O5-C5	-2.04	109.43	112.19
2	F	3	BMA	O6-C6-C5	-2.02	104.37	111.29

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C3-C2-N2-C7
2	J	5	MAN	C4-C5-C6-O6
2	G	4	MAN	C4-C5-C6-O6
2	I	4	MAN	C4-C5-C6-O6
2	I	4	MAN	O5-C5-C6-O6

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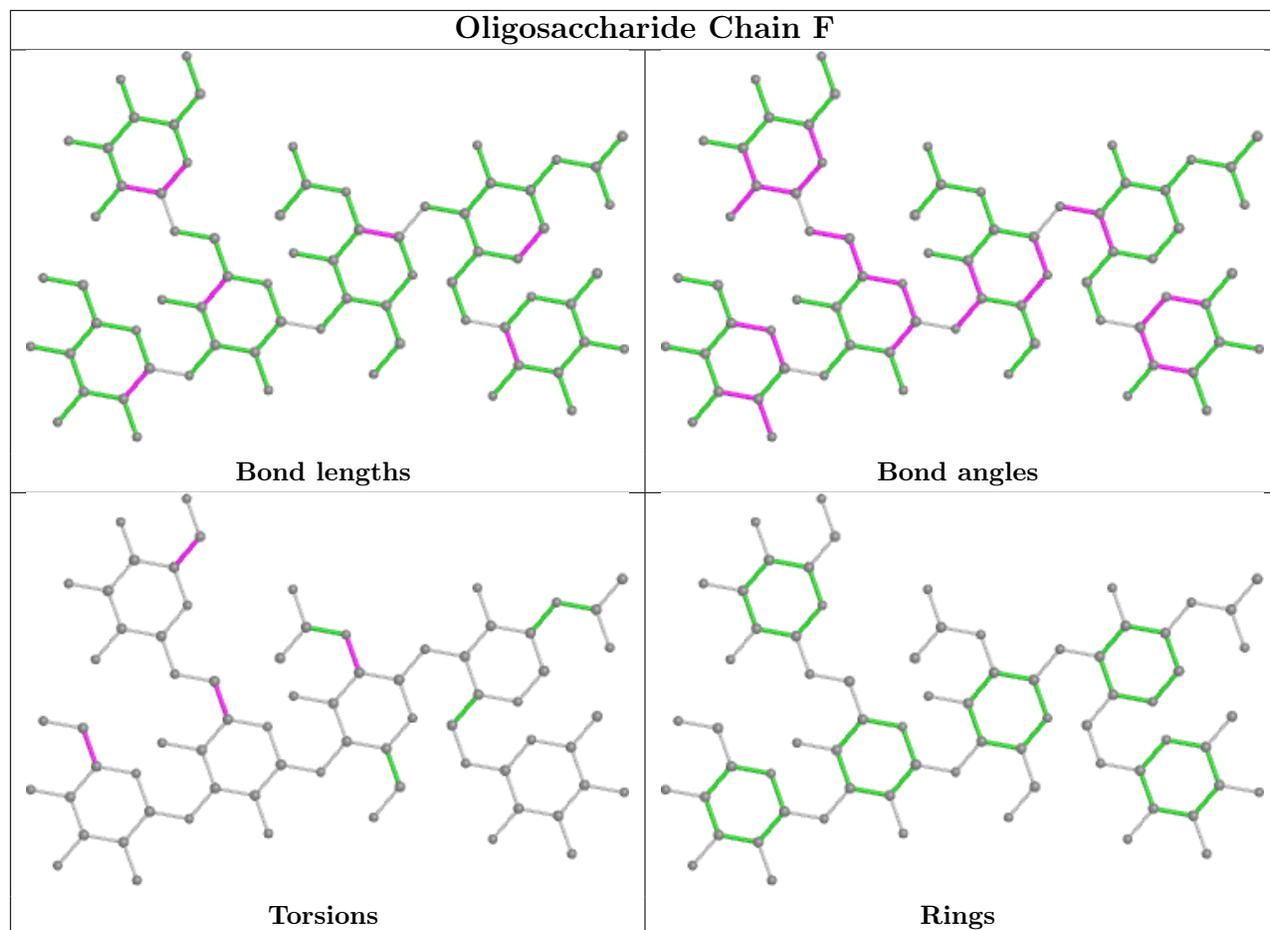
Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C4-C5-C6-O6
2	J	1	NAG	C1-C2-N2-C7
2	F	4	MAN	O5-C5-C6-O6
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
2	H	5	MAN	O5-C5-C6-O6
2	J	5	MAN	O5-C5-C6-O6
2	G	4	MAN	O5-C5-C6-O6
2	H	5	MAN	C4-C5-C6-O6
2	G	5	MAN	O5-C5-C6-O6
2	F	2	NAG	C1-C2-N2-C7
2	H	4	MAN	O5-C5-C6-O6
2	J	3	BMA	C4-C5-C6-O6
2	F	5	MAN	C4-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
2	I	5	MAN	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	F	5	MAN	O5-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	F	4	MAN	C4-C5-C6-O6
2	J	1	NAG	C3-C2-N2-C7
2	J	2	NAG	C3-C2-N2-C7
2	I	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6

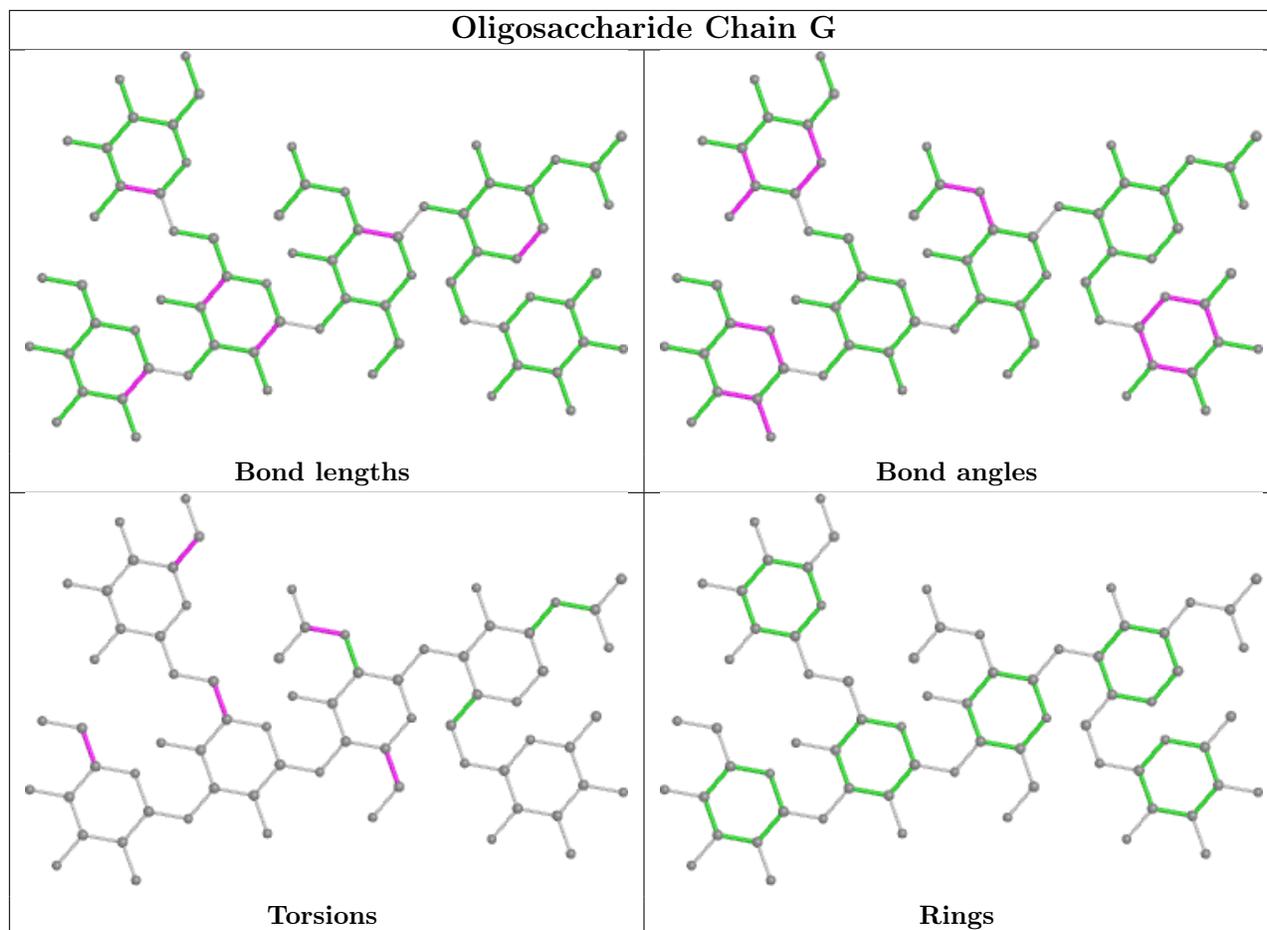
All (1) ring outliers are listed below:

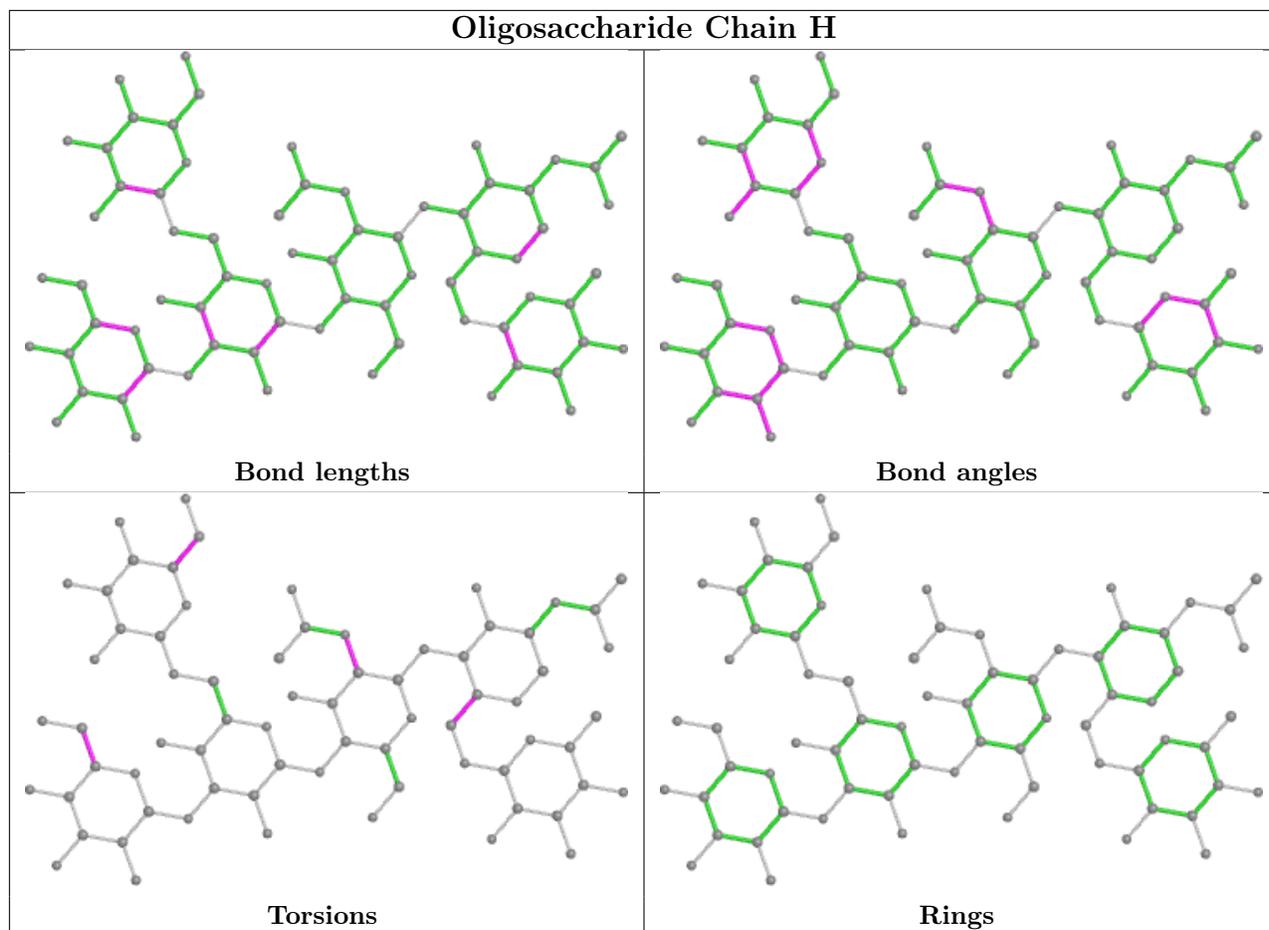
Mol	Chain	Res	Type	Atoms
2	I	5	MAN	C1-C2-C3-C4-C5-O5

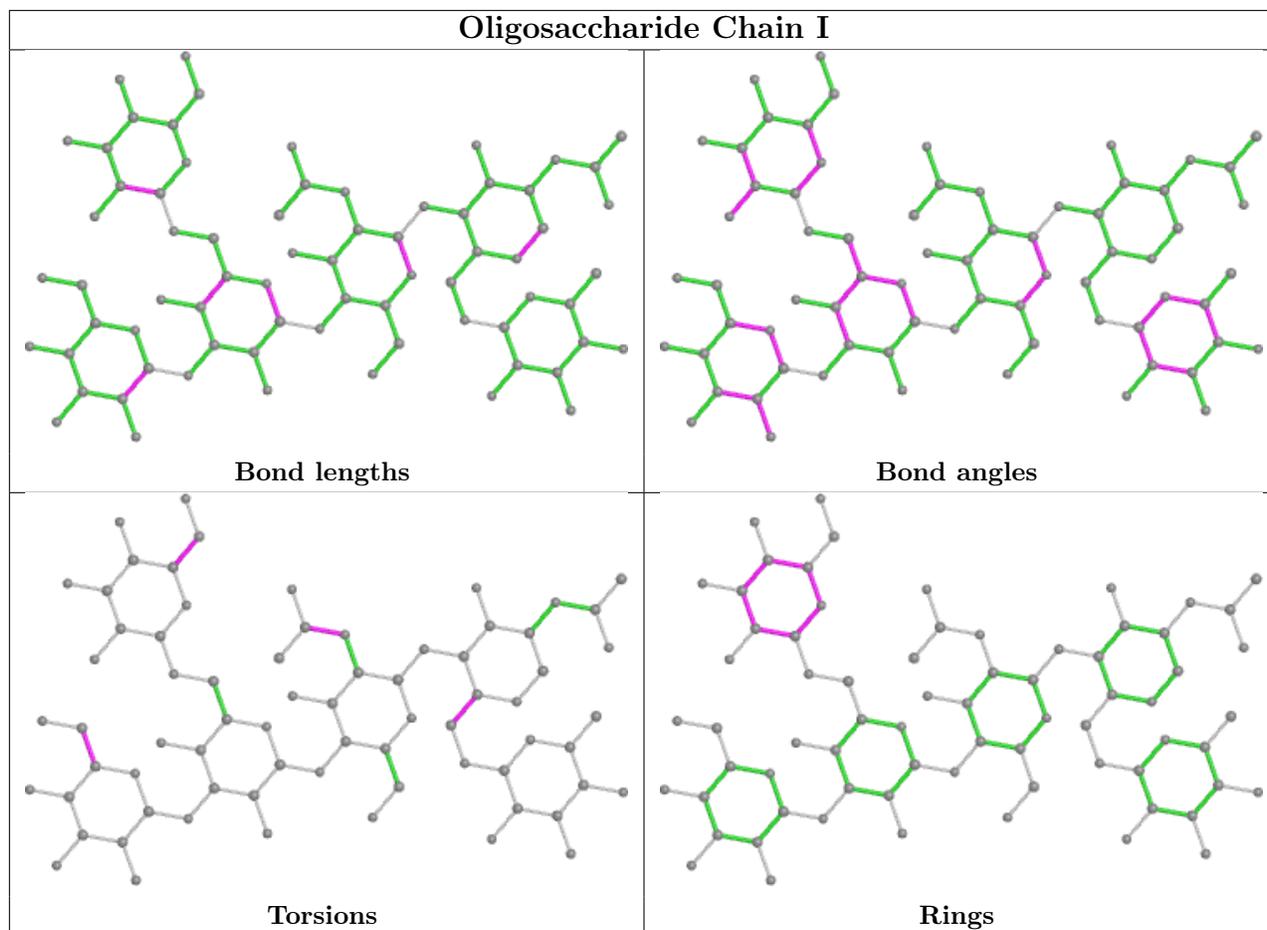
No monomer is involved in short contacts.

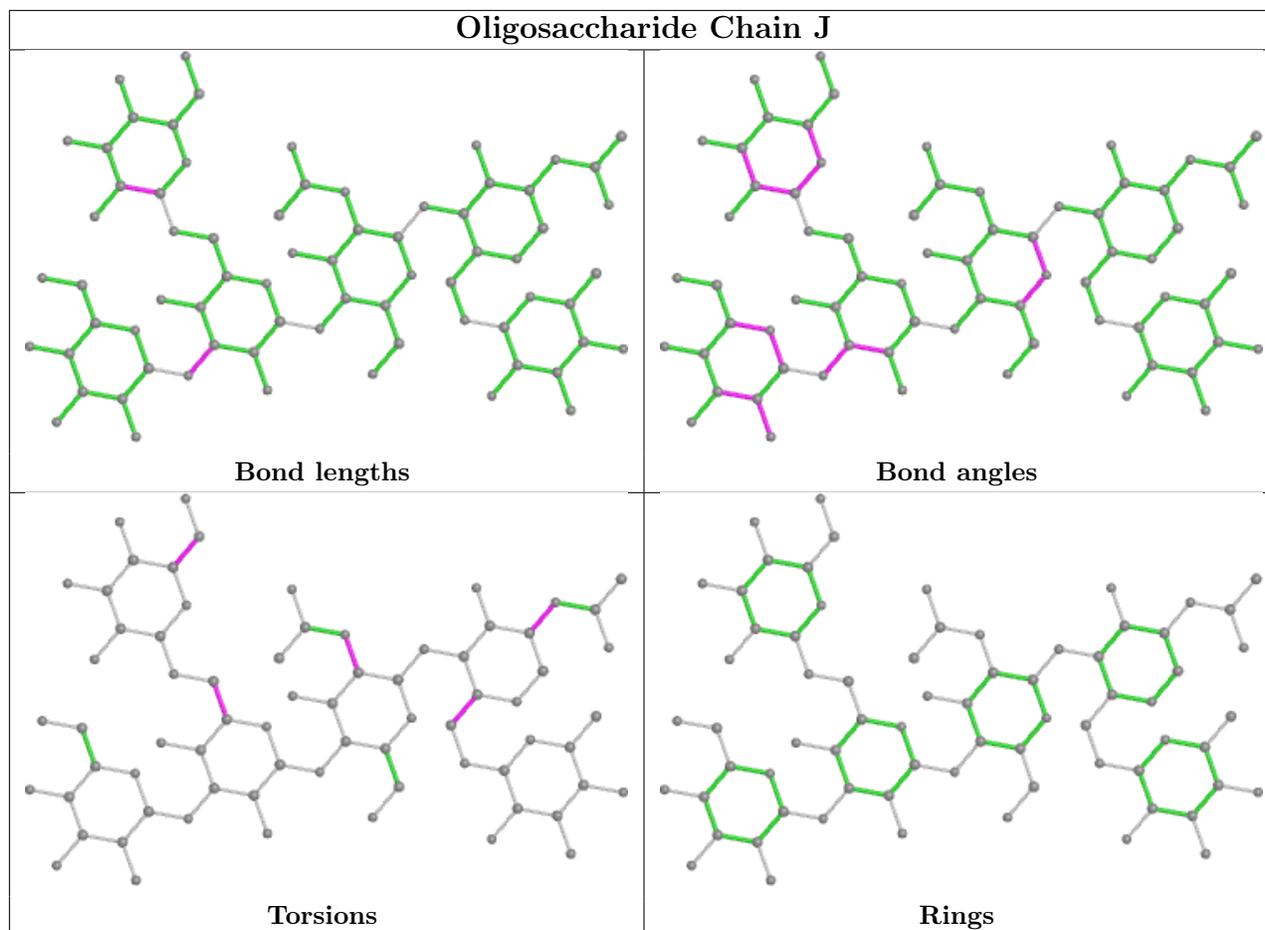
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 4.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 45 are monoatomic - leaving 10 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
4	MAN	D	510	1	11,11,12	0.68	0	15,15,17	1.09	2 (13%)
4	MAN	B	510	1	11,11,12	0.65	0	15,15,17	1.08	2 (13%)
4	MAN	C	510	1	11,11,12	0.77	0	15,15,17	1.12	2 (13%)
4	MAN	E	511	1	11,11,12	0.80	0	15,15,17	1.00	2 (13%)
4	MAN	E	510	1	11,11,12	0.79	0	15,15,17	1.13	2 (13%)
4	MAN	C	511	1	11,11,12	0.91	1 (9%)	15,15,17	0.97	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	A	511	1	11,11,12	0.72	0	15,15,17	1.03	2 (13%)
4	MAN	A	510	1	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
4	MAN	B	511	1	11,11,12	0.80	1 (9%)	15,15,17	0.97	2 (13%)
4	MAN	D	511	1	11,11,12	0.81	1 (9%)	15,15,17	0.98	2 (13%)

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	MAN	D	510	1	-	0/2/19/22	0/1/1/1
4	MAN	B	510	1	-	0/2/19/22	0/1/1/1
4	MAN	C	510	1	-	0/2/19/22	0/1/1/1
4	MAN	E	511	1	-	2/2/19/22	0/1/1/1
4	MAN	E	510	1	-	0/2/19/22	0/1/1/1
4	MAN	C	511	1	-	2/2/19/22	0/1/1/1
4	MAN	A	511	1	-	2/2/19/22	0/1/1/1
4	MAN	A	510	1	-	0/2/19/22	0/1/1/1
4	MAN	B	511	1	-	2/2/19/22	0/1/1/1
4	MAN	D	511	1	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	511	MAN	O5-C1	-2.41	1.39	1.43
4	B	511	MAN	O5-C1	-2.21	1.40	1.43
4	D	511	MAN	O5-C1	-2.13	1.40	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	510	MAN	C1-O5-C5	2.92	116.16	112.19
4	C	510	MAN	C1-O5-C5	2.86	116.06	112.19
4	E	510	MAN	C1-O5-C5	2.76	115.93	112.19
4	D	510	MAN	C1-O5-C5	2.74	115.90	112.19
4	B	510	MAN	C1-O5-C5	2.59	115.70	112.19
4	A	511	MAN	C1-O5-C5	2.59	115.70	112.19
4	E	511	MAN	C1-O5-C5	2.42	115.47	112.19
4	C	510	MAN	O2-C2-C3	-2.39	105.34	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	510	MAN	O2-C2-C3	-2.35	105.44	110.14
4	C	511	MAN	O2-C2-C3	-2.33	105.47	110.14
4	D	510	MAN	O2-C2-C3	-2.32	105.48	110.14
4	D	511	MAN	O2-C2-C3	-2.32	105.48	110.14
4	A	510	MAN	O2-C2-C3	-2.29	105.55	110.14
4	A	511	MAN	O2-C2-C3	-2.29	105.56	110.14
4	B	510	MAN	O2-C2-C3	-2.28	105.56	110.14
4	D	511	MAN	C1-O5-C5	2.28	115.28	112.19
4	E	511	MAN	O2-C2-C3	-2.27	105.60	110.14
4	B	511	MAN	O2-C2-C3	-2.24	105.64	110.14
4	B	511	MAN	C1-O5-C5	2.23	115.21	112.19
4	C	511	MAN	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	511	MAN	O5-C5-C6-O6
4	B	511	MAN	O5-C5-C6-O6
4	C	511	MAN	O5-C5-C6-O6
4	D	511	MAN	O5-C5-C6-O6
4	E	511	MAN	O5-C5-C6-O6
4	B	511	MAN	C4-C5-C6-O6
4	A	511	MAN	C4-C5-C6-O6
4	C	511	MAN	C4-C5-C6-O6
4	D	511	MAN	C4-C5-C6-O6
4	E	511	MAN	C4-C5-C6-O6

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.