wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 04:26 AM EDT

PDB ID	:	6VFT
Title	:	Crystal structure of human delta protocadherin 17 EC1-EC4
Authors	:	Harrison, O.J.; Brasch, J.; Shapiro, L.
Deposited on	:	2020-01-06
Resolution	:	3.71 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 (i)) 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 3.71 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 10 unique types of molecules in this entry. The entry contains 25685 atoms, of which 12355 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-17.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	413	Total	C	H	N	O	S	0	0	0
			6153	1977	2969	558	641	8			
1	B	414	Total	C	H	N	O	S	0	0	0
			6218	1981	3027	559	643	8			
1	C	420	Total	C	H	N	O	S	0	0	0
			6215	2007	2979	569	652	8			
1	D	418	Total	C	H	N	O	S	0	0	0
			6176	1994	2962	563	649	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	448	HIS	-	expression tag	UNP O14917
A	449	HIS	-	expression tag	UNP O14917
A	450	HIS	-	expression tag	UNP O14917
A	451	HIS	-	expression tag	UNP O14917
A	452	HIS	-	expression tag	UNP O14917
A	453	HIS	-	expression tag	UNP O14917
B	448	HIS	-	expression tag	UNP O14917
B	449	HIS	-	expression tag	UNP O14917
B	450	HIS	-	expression tag	UNP O14917
B	451	HIS	-	expression tag	UNP O14917
B	452	HIS	-	expression tag	UNP O14917
B	453	HIS	-	expression tag	UNP O14917
C	448	HIS	-	expression tag	UNP O14917
C	449	HIS	-	expression tag	UNP O14917
C	450	HIS	-	expression tag	UNP O14917
C	451	HIS	-	expression tag	UNP O14917
C	452	HIS	-	expression tag	UNP O14917
C	453	HIS	-	expression tag	UNP O14917
D	448	HIS	-	expression tag	UNP O14917
D	449	HIS	-	expression tag	UNP O14917
D	450	HIS	-	expression tag	UNP O14917

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Chain	Residue	Modelled	Actual	Comment	Reference
D	451	HIS	-	expression tag	UNP O14917
D	452	HIS	-	expression tag	UNP O14917
D	453	HIS	-	expression tag	UNP O14917

- Molecule 2 is an oligosaccharide called 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	E	3	Total	C	H	N	O	0	0	0
			75	22	37	2	14			
2	F	3	Total	C	H	N	O	0	0	0
			74	22	36	2	14			

- Molecule 3 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
3	G	2	Total	C	H	N	O	0	0	0
			54	16	26	2	10			
3	L	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 4 is an oligosaccharide called 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
4	H	4	Total	C	H	N	O	0	0	0
			84	28	35	2	19			
4	K	4	Total	C	H	N	O	0	0	0
			95	28	46	2	19			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			

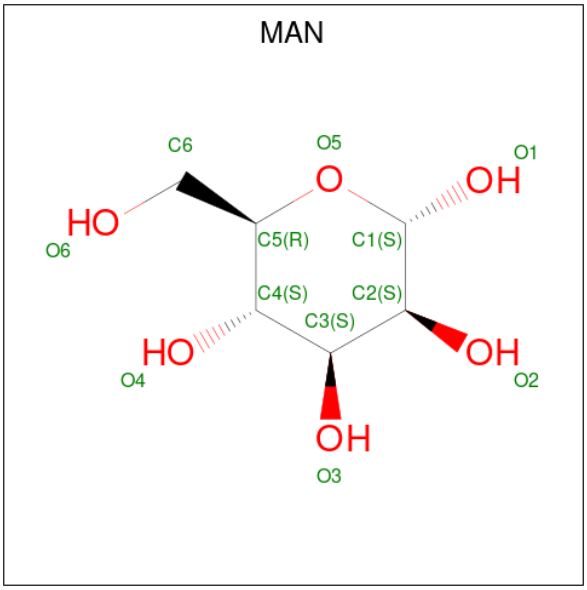
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	5	Total	C	H	N	O	0	0	0
			115	34	55	2	24			

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	10	Total	Ca	0	0
			10	10		
7	B	10	Total	Ca	0	0
			10	10		
7	C	10	Total	Ca	0	0
			10	10		
7	D	10	Total	Ca	0	0
			10	10		

- Molecule 8 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	O		0	0
			21	6	10	5			
8	A	1	Total	C	H	O		0	0
			21	6	10	5			
8	B	1	Total	C	H	O		0	0
			21	6	10	5			
8	B	1	Total	C	H	O		0	0
			21	6	10	5			
8	C	1	Total	C	H	O		0	0
			21	6	10	5			

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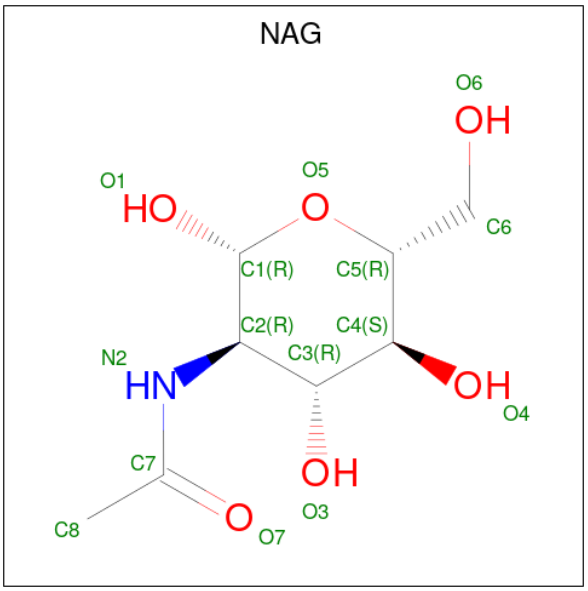
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C H O 21 6 10 5	0	0
8	D	1	Total C H O 21 6 10 5	0	0
8	D	1	Total C H O 21 6 10 5	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C H N O 28 8 14 1 5	0	0
9	C	1	Total C H N O 28 8 14 1 5	0	0
9	C	1	Total C H N O 28 8 14 1 5	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O 1 1	0	0
10	B	3	Total O 3 3	0	0
10	D	2	Total O 2 2	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, α, β, γ	214.55Å 105.84Å 101.40Å 90.00° 101.04° 90.00°	Depositor
Resolution (Å)	19.94 – 3.71	Depositor
% Data completeness (in resolution range)	96.3 (19.94-3.71)	Depositor
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.63 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.253 , 0.300	Depositor
Wilson B-factor (Å^2)	80.4	Xtriage
Anisotropy	0.261	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25685	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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

26 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	E	1	1,2	14,14,15	0.23	0	17,19,21	0.36	0
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	1.04	1 (5%)
2	FUC	E	3	2	10,10,11	0.74	0	14,14,16	0.82	0
2	NAG	F	1	1,2	14,14,15	0.49	0	17,19,21	0.91	1 (5%)
2	NAG	F	2	2	14,14,15	0.37	0	17,19,21	0.40	0
2	FUC	F	3	2	10,10,11	1.20	2 (20%)	14,14,16	1.48	3 (21%)
3	NAG	G	1	3,1	14,14,15	0.84	1 (7%)	17,19,21	0.82	1 (5%)
3	NAG	G	2	3	14,14,15	0.86	1 (7%)	17,19,21	0.61	0
4	NAG	H	1	4,1	14,14,15	0.76	1 (7%)	17,19,21	0.59	0
4	NAG	H	2	4	14,14,15	0.23	0	17,19,21	0.51	0
4	BMA	H	3	4	11,11,12	0.57	0	15,15,17	0.77	0
4	FUC	H	4	4	10,10,11	1.18	1 (10%)	14,14,16	1.10	2 (14%)
5	NAG	I	1	5,1	14,14,15	0.79	1 (7%)	17,19,21	0.60	0
5	NAG	I	2	5	14,14,15	0.84	1 (7%)	17,19,21	1.10	2 (11%)
5	BMA	I	3	5	11,11,12	0.65	0	15,15,17	0.78	0
6	NAG	J	1	6,1	14,14,15	0.82	1 (7%)	17,19,21	0.84	1 (5%)
6	NAG	J	2	6	14,14,15	0.81	1 (7%)	17,19,21	0.72	0
6	BMA	J	3	6	11,11,12	0.63	0	15,15,17	0.78	0
6	MAN	J	4	6	11,11,12	1.06	1 (9%)	15,15,17	1.13	2 (13%)
6	FUC	J	5	6	10,10,11	1.64	2 (20%)	14,14,16	2.04	2 (14%)
4	NAG	K	1	4,1	14,14,15	0.40	0	17,19,21	0.45	0
4	NAG	K	2	4	14,14,15	0.91	1 (7%)	17,19,21	0.68	0
4	BMA	K	3	4	11,11,12	0.64	0	15,15,17	0.72	0
4	FUC	K	4	4	10,10,11	0.73	0	14,14,16	1.23	2 (14%)
3	NAG	L	1	3,1	14,14,15	0.67	0	17,19,21	2.22	3 (17%)
3	NAG	L	2	3	14,14,15	0.45	0	17,19,21	0.42	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	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	5/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	F	3	2	-	-	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
4	FUC	H	4	4	-	-	0/1/1/1
5	NAG	I	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	3/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	2/2/19/22	0/1/1/1
6	FUC	J	5	6	-	-	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	4/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
4	FUC	K	4	4	-	-	0/1/1/1
3	NAG	L	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	5	FUC	C2-C3	3.42	1.57	1.52
6	J	4	MAN	C1-C2	3.08	1.59	1.52
6	J	5	FUC	C1-C2	3.08	1.59	1.52
3	G	1	NAG	O5-C1	-3.03	1.38	1.43
5	I	2	NAG	O5-C1	-2.92	1.39	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	1	NAG	C1-O5-C5	7.99	123.02	112.19
6	J	5	FUC	C1-C2-C3	6.16	117.23	109.67
2	E	2	NAG	C2-N2-C7	3.38	127.72	122.90
5	I	2	NAG	C3-C4-C5	3.25	116.04	110.24
6	J	4	MAN	C1-O5-C5	3.22	116.55	112.19

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

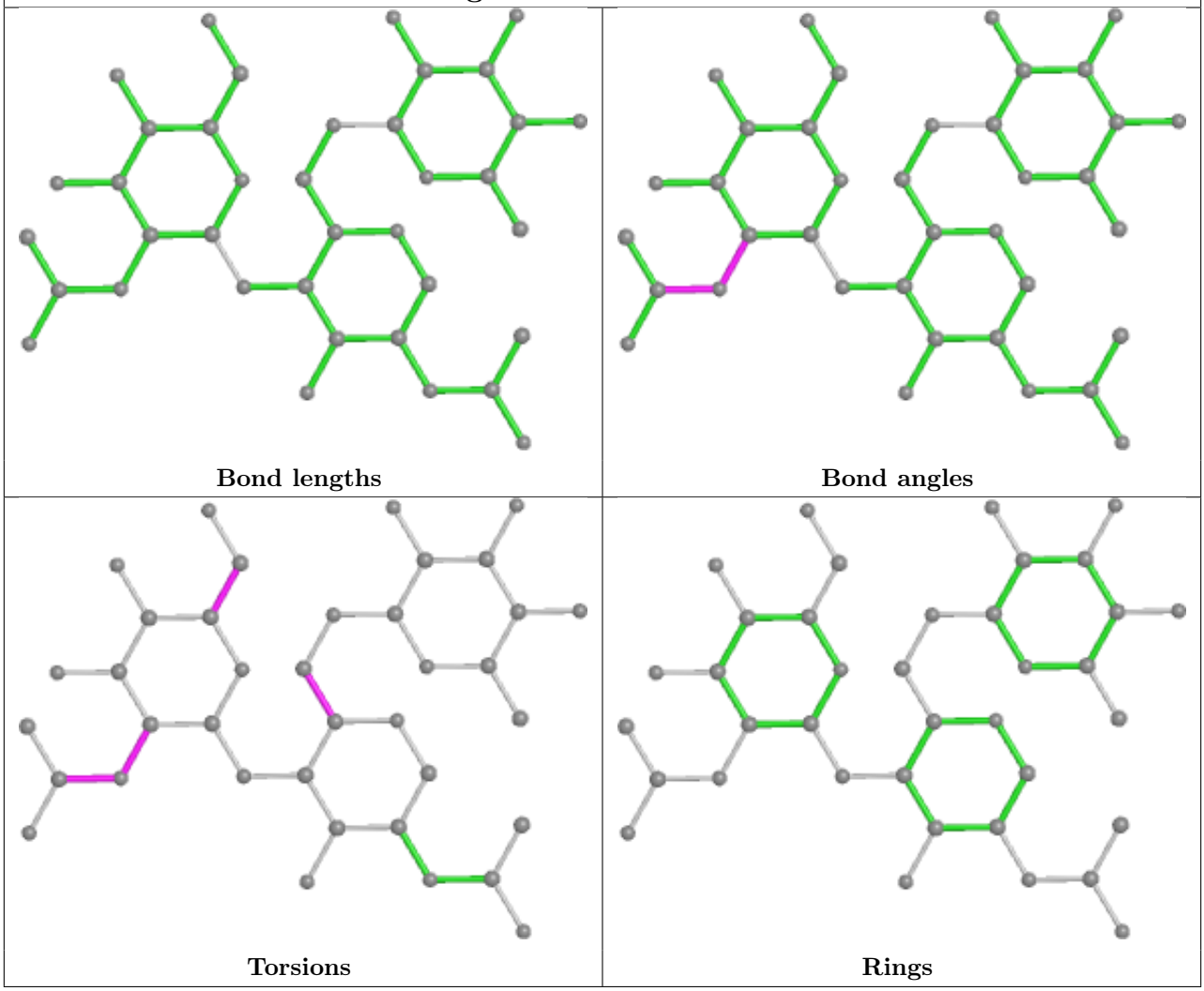
Mol	Chain	Res	Type	Atoms
4	K	2	NAG	C1-C2-N2-C7
6	J	2	NAG	C3-C2-N2-C7
4	K	3	BMA	O5-C5-C6-O6
6	J	4	MAN	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6

There are no ring outliers.

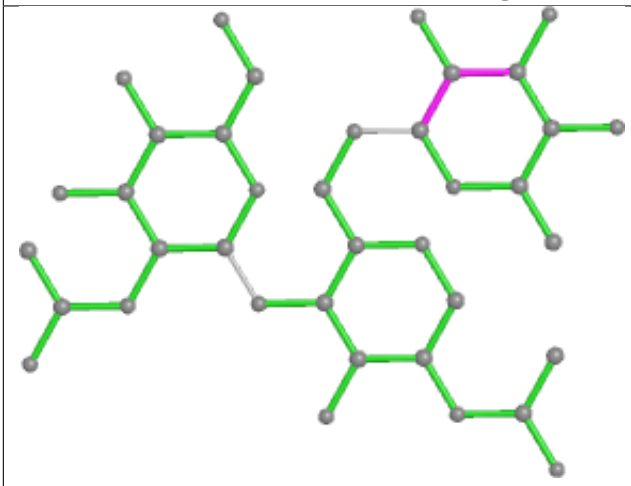
No monomer is involved in short contacts.

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

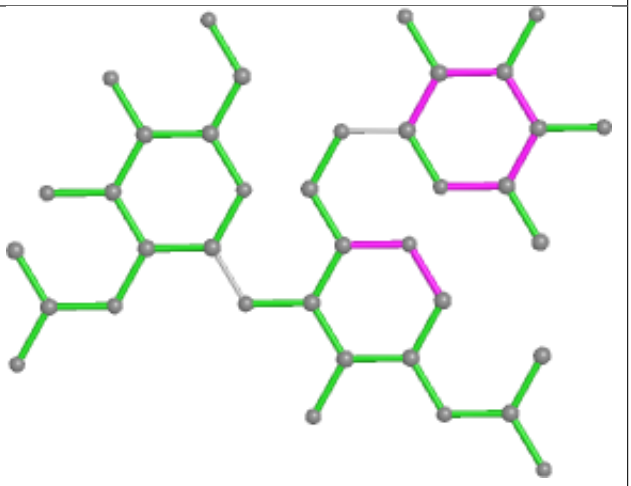
Oligosaccharide Chain E



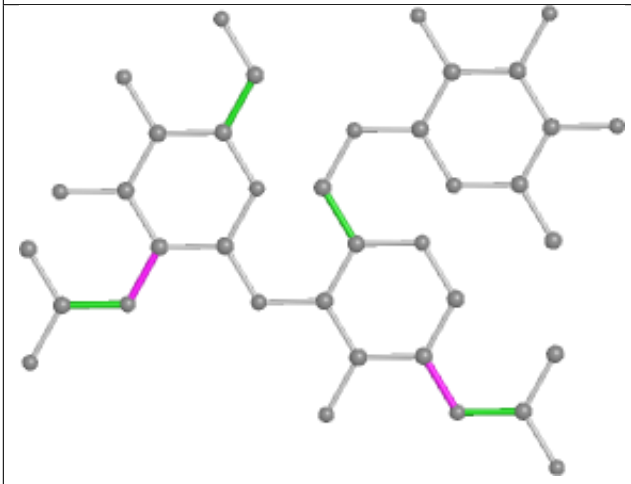
Oligosaccharide Chain F



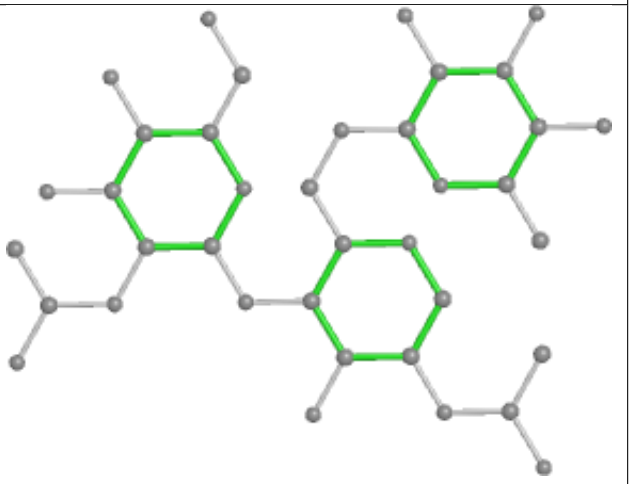
Bond lengths



Bond angles

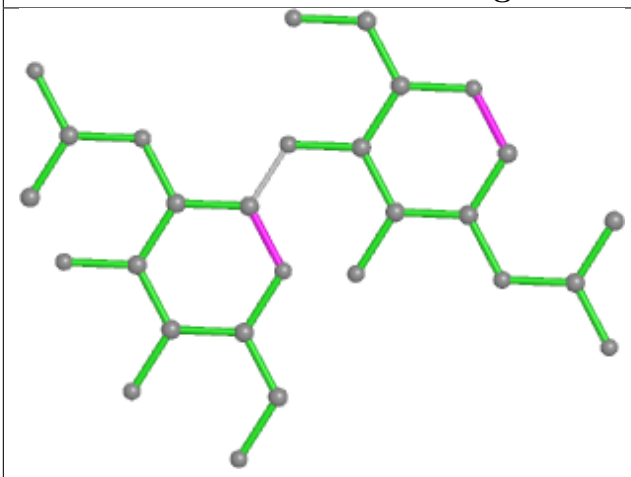


Torsions

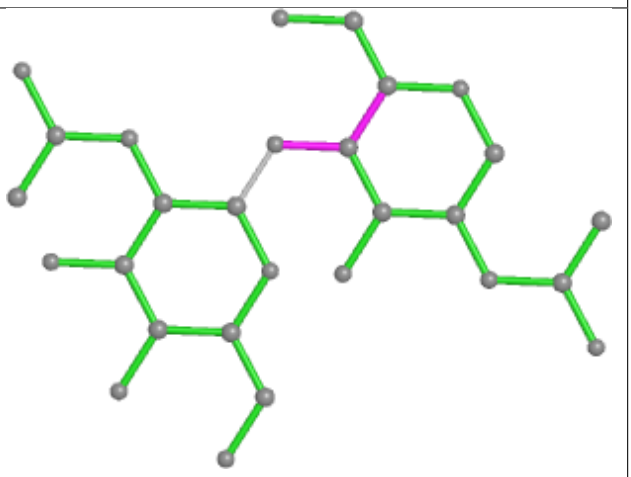


Rings

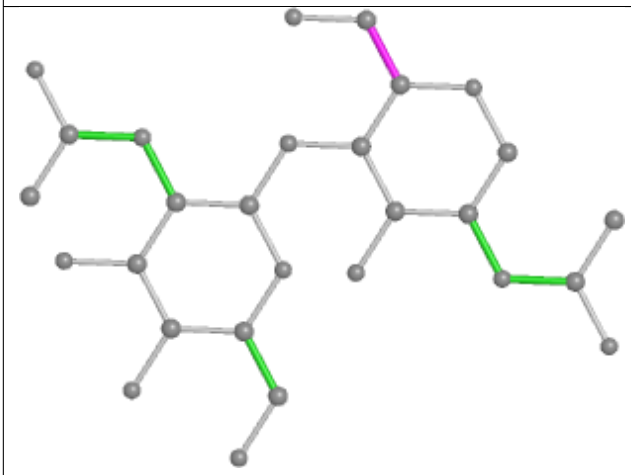
Oligosaccharide Chain G



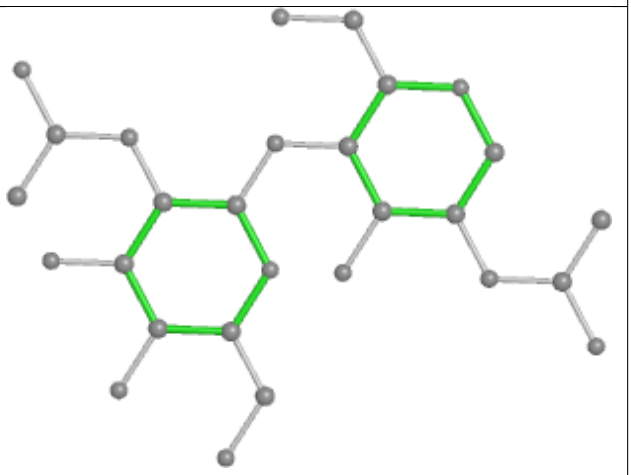
Bond lengths



Bond angles

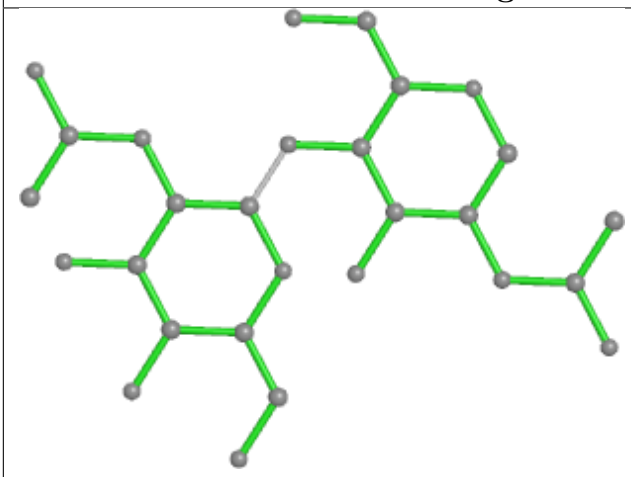


Torsions

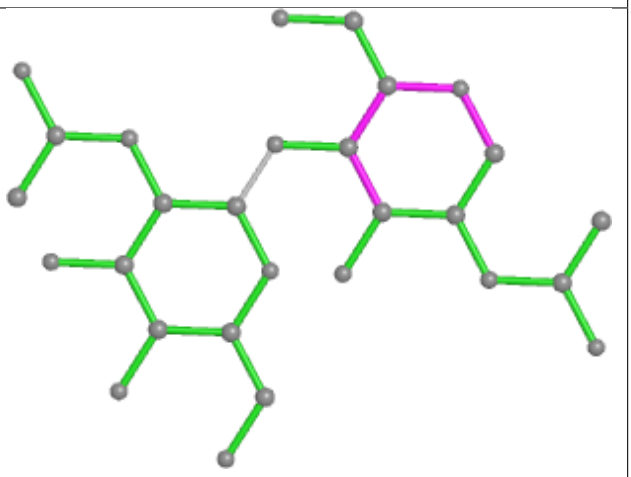


Rings

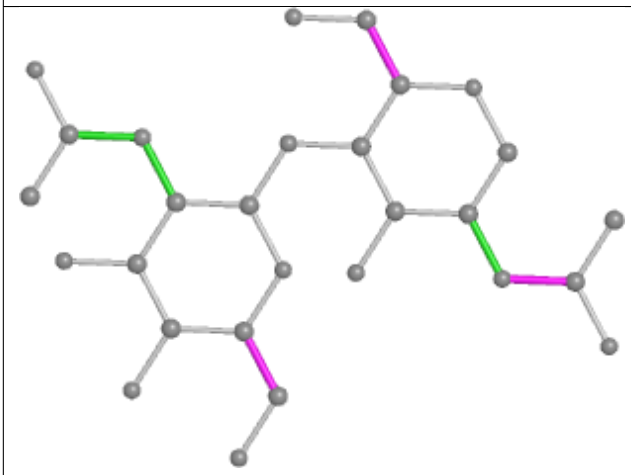
Oligosaccharide Chain L



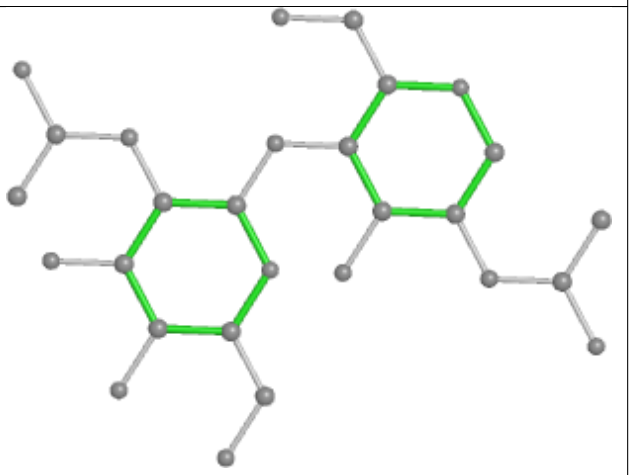
Bond lengths



Bond angles

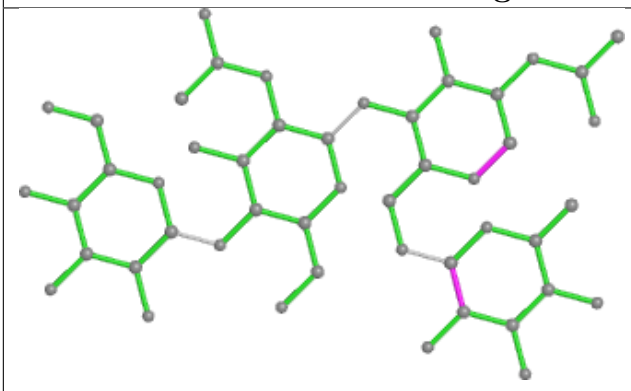


Torsions

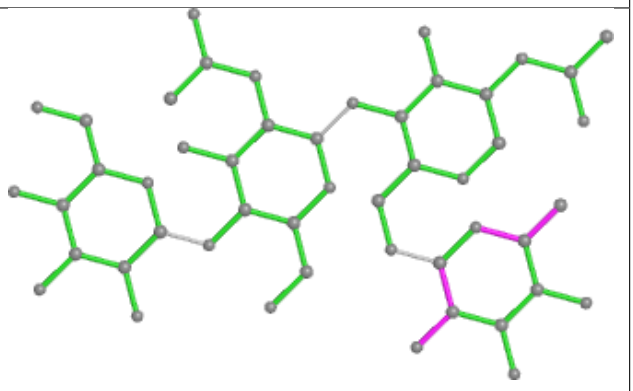


Rings

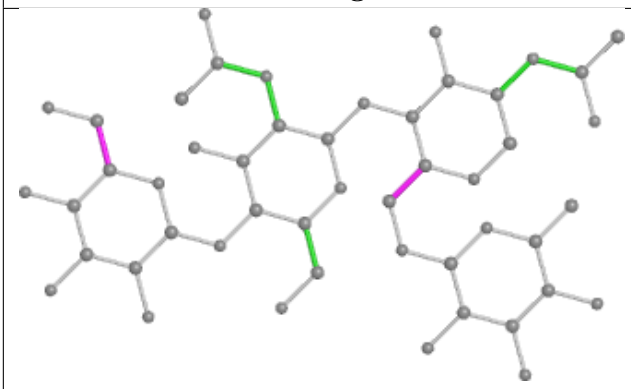
Oligosaccharide Chain H



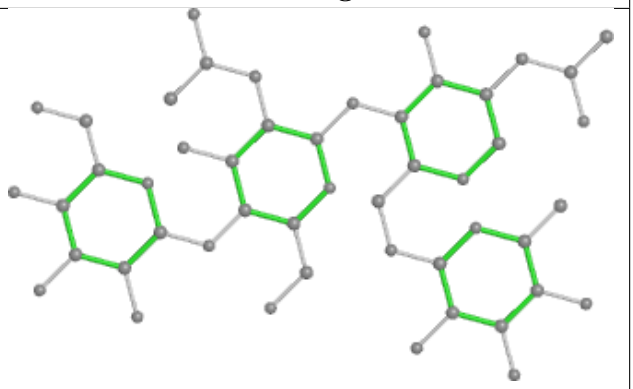
Bond lengths



Bond angles

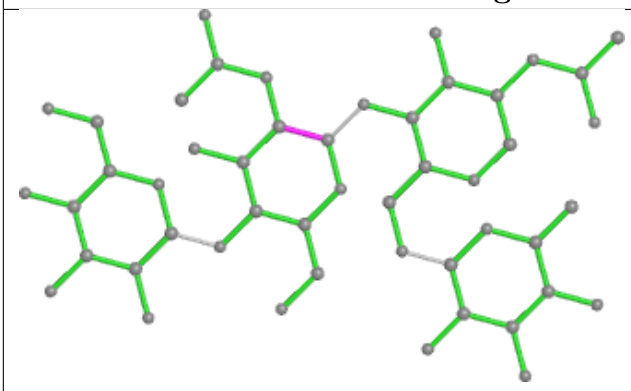


Torsions

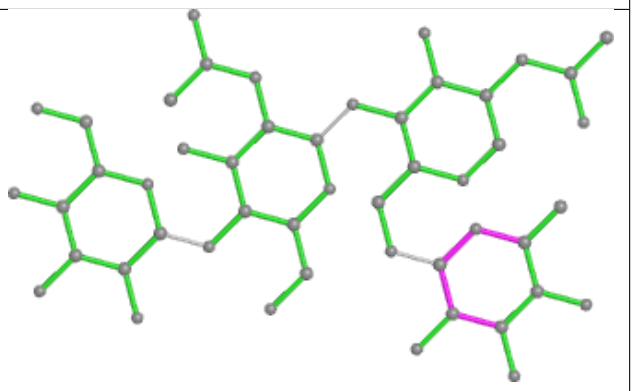


Rings

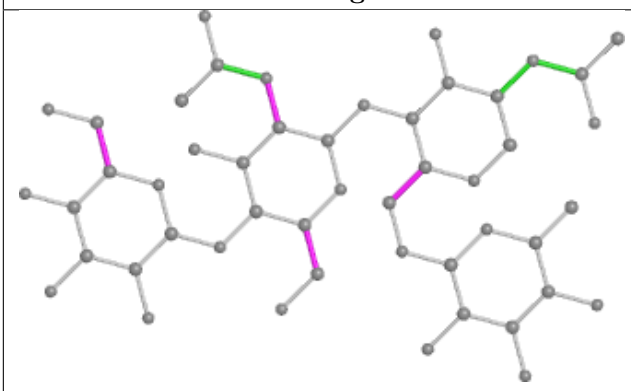
Oligosaccharide Chain K



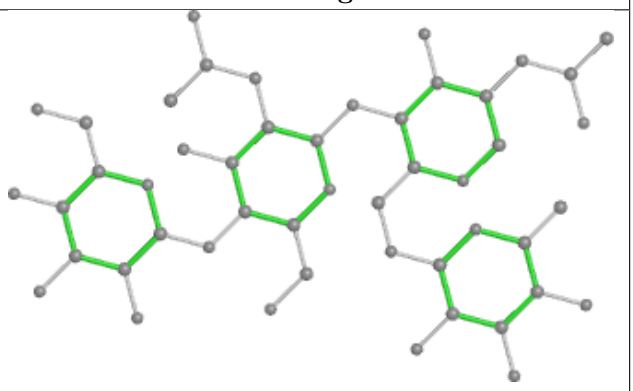
Bond lengths



Bond angles

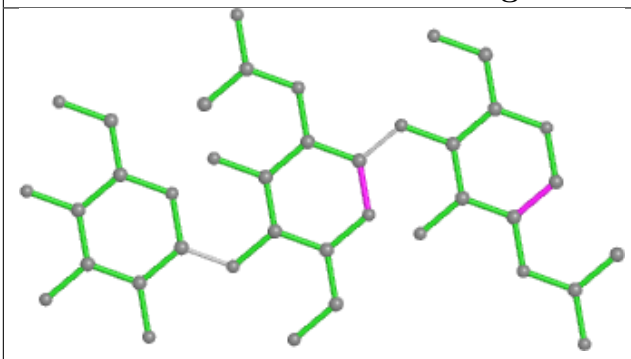


Torsions

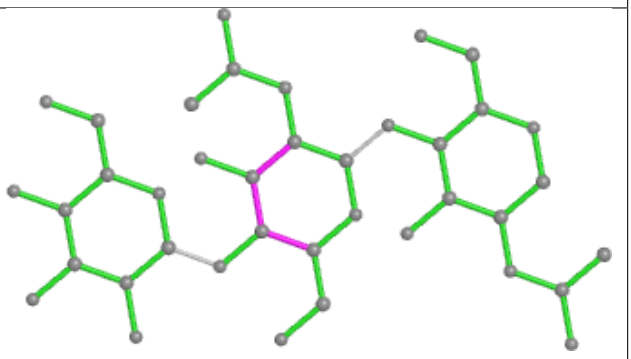


Rings

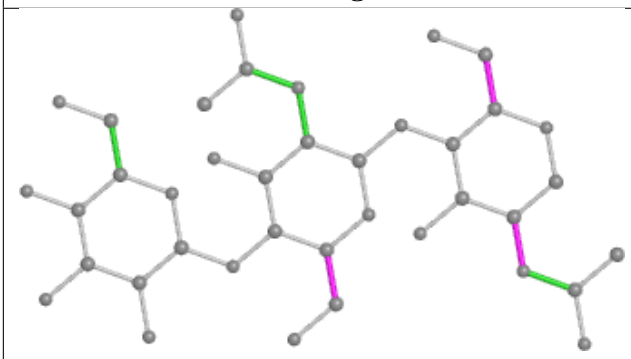
Oligosaccharide Chain I



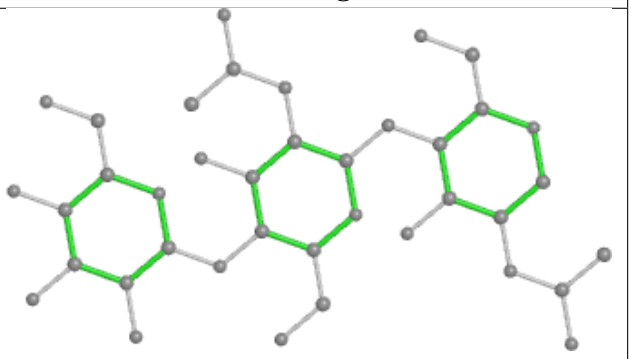
Bond lengths



Bond angles

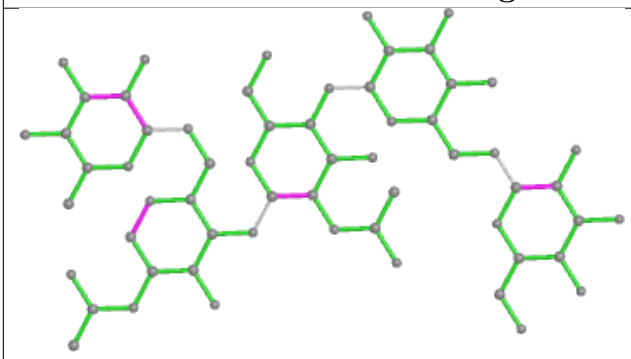


Torsions

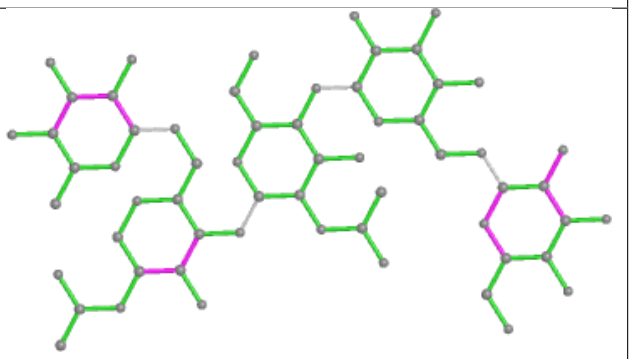


Rings

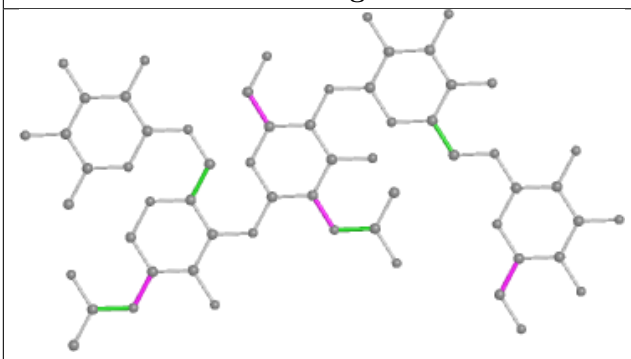
Oligosaccharide Chain J



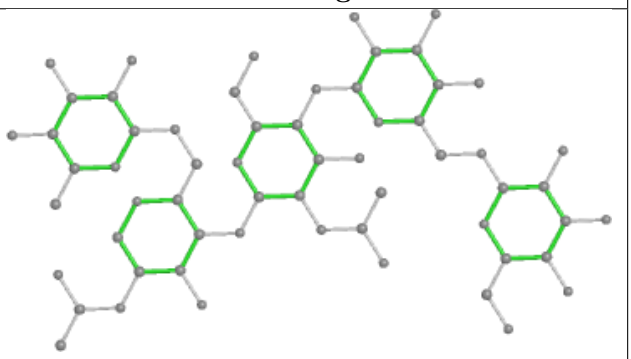
Bond lengths



Bond angles



Torsions



Rings

4.6 Ligand geometry (i)

Of 51 ligands modelled in this entry, 40 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
8	MAN	D	517	1	11,11,12	1.13	1 (9%)	15,15,17	1.23	2 (13%)
8	MAN	A	510	1	11,11,12	1.45	2 (18%)	15,15,17	1.49	3 (20%)
8	MAN	C	511	1	11,11,12	0.61	0	15,15,17	1.09	2 (13%)
8	MAN	A	514	1	11,11,12	0.79	0	15,15,17	1.21	3 (20%)
8	MAN	C	510	1	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
9	NAG	C	513	1	14,14,15	0.21	0	17,19,21	0.43	0
8	MAN	D	516	1	11,11,12	0.66	0	15,15,17	1.43	3 (20%)
9	NAG	B	519	1	14,14,15	0.22	0	17,19,21	0.32	0
8	MAN	B	511	1	11,11,12	0.90	1 (9%)	15,15,17	1.01	2 (13%)
8	MAN	B	510	1	11,11,12	0.75	0	15,15,17	1.29	2 (13%)
9	NAG	C	512	1	14,14,15	0.29	0	17,19,21	0.32	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
8	MAN	D	517	1	-	2/2/19/22	0/1/1/1
8	MAN	A	510	1	-	1/2/19/22	0/1/1/1
8	MAN	C	511	1	-	2/2/19/22	0/1/1/1
8	MAN	A	514	1	-	0/2/19/22	0/1/1/1
8	MAN	C	510	1	-	2/2/19/22	0/1/1/1
9	NAG	C	513	1	-	0/6/23/26	0/1/1/1
8	MAN	D	516	1	-	2/2/19/22	0/1/1/1
9	NAG	B	519	1	-	2/6/23/26	0/1/1/1
8	MAN	B	511	1	-	2/2/19/22	0/1/1/1
8	MAN	B	510	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	C	512	1	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	510	MAN	O5-C1	-3.93	1.37	1.43
8	D	517	MAN	O5-C1	-3.02	1.38	1.43
8	B	511	MAN	O5-C1	-2.59	1.39	1.43
8	A	510	MAN	C4-C5	2.03	1.57	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	510	MAN	C1-O5-C5	3.77	117.31	112.19
8	D	516	MAN	C1-O5-C5	3.24	116.58	112.19
8	A	510	MAN	C3-C4-C5	3.18	115.92	110.24
8	C	511	MAN	C1-O5-C5	2.83	116.03	112.19
8	D	516	MAN	O5-C1-C2	2.81	115.11	110.77

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	511	MAN	O5-C5-C6-O6
8	D	516	MAN	O5-C5-C6-O6
8	C	511	MAN	C4-C5-C6-O6
8	D	516	MAN	C4-C5-C6-O6
9	B	519	NAG	O5-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

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.