wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 05:59 AM EDT

PDB ID	:	6U7G
Title	:	HCoV-229E RBD Class V in complex with human APN
Authors	:	Tomlinson, A.; Li, Z.; Rini, J.M.
Deposited on	:	2019-09-02
Resolution	:	2.35 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 2.35 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 6 unique types of molecules in this entry. The entry contains 33302 atoms, of which 15945 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	898	14262	4623	7012	1223	1380	24	0	0	0
1	B	899	14297	4634	7030	1225	1384	24	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	GLY	-	cloning artifact	UNP P15144
A	63	GLY	-	cloning artifact	UNP P15144
A	64	ARG	-	cloning artifact	UNP P15144
A	65	PRO	-	cloning artifact	UNP P15144
B	62	GLY	-	cloning artifact	UNP P15144
B	63	GLY	-	cloning artifact	UNP P15144
B	64	ARG	-	cloning artifact	UNP P15144
B	65	PRO	-	cloning artifact	UNP P15144

- Molecule 2 is a protein called Spike protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	C	119	1759	579	857	155	159	9	0	0	0
2	D	111	1650	537	809	146	150	8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	289	GLY	-	cloning artifact	UNP H1AG31
C	290	GLY	-	cloning artifact	UNP H1AG31
C	291	ARG	-	cloning artifact	UNP H1AG31
C	292	PRO	-	cloning artifact	UNP H1AG31

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Chain	Residue	Modelled	Actual	Comment	Reference
C	300	MET	THR	conflict	UNP H1AG31
C	412	THR	SER	conflict	UNP H1AG31
C	422	GLY	VAL	conflict	UNP H1AG31
C	428	GLN	LYS	conflict	UNP H1AG31
D	289	GLY	-	cloning artifact	UNP H1AG31
D	290	GLY	-	cloning artifact	UNP H1AG31
D	291	ARG	-	cloning artifact	UNP H1AG31
D	292	PRO	-	cloning artifact	UNP H1AG31
D	300	MET	THR	conflict	UNP H1AG31
D	412	THR	SER	conflict	UNP H1AG31
D	422	GLY	VAL	conflict	UNP H1AG31
D	428	GLN	LYS	conflict	UNP H1AG31

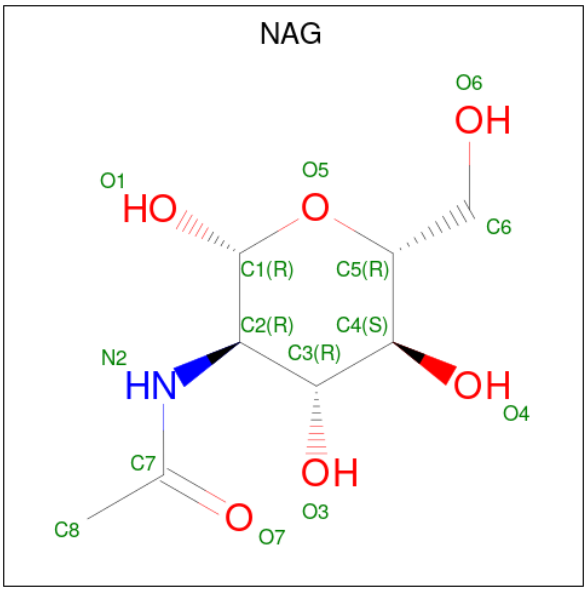
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	2	Total C H N O 56 16 28 2 10	0	0	0
3	F	2	Total C H N O 56 16 28 2 10	0	0	0
3	G	2	Total C H N O 56 16 28 2 10	0	0	0
3	H	2	Total C N O 28 16 2 10	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H N O 28 8 14 1 5	0	0
5	A	1	Total C H N O 28 8 14 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C H N O 28 8 14 1 5	0	0
5	A	1	Total C H N O 27 8 13 1 5	0	0
5	B	1	Total C H N O 28 8 14 1 5	0	0
5	B	1	Total C H N O 28 8 14 1 5	0	0
5	B	1	Total C H N O 28 8 14 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C H N O 28 8 14 1 5	0	0
5	C	1	Total C H N O 28 8 14 1 5	0	0
5	D	1	Total C H N O 28 8 14 1 5	0	0
5	D	1	Total C H N O 28 8 14 1 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	403	403	403	0	0
			Total	O		
6	B	350	350	350	0	0
			Total	O		
6	C	36	36	36	0	0
			Total	O		
6	D	12	12	12	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 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.56Å 98.68Å 147.53Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	45.61 – 2.35	Depositor
% Data completeness (in resolution range)	96.0 (45.61-2.35)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.16rc1_3535	Depositor
R, R_{free}	0.179 , 0.218	Depositor
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.109	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	33302	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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 (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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	E	2	3	14,14,15	0.19	0	17,19,21	0.44	0
3	NAG	F	1	3,1	14,14,15	0.17	0	17,19,21	0.47	0
3	NAG	F	2	3	14,14,15	0.22	0	17,19,21	0.39	0
3	NAG	G	1	3,1	14,14,15	0.24	0	17,19,21	0.38	0
3	NAG	G	2	3	14,14,15	0.24	0	17,19,21	0.37	0
3	NAG	H	1	3,1	14,14,15	2.21	4 (28%)	17,19,21	2.03	7 (41%)
3	NAG	H	2	3	14,14,15	1.24	1 (7%)	17,19,21	1.73	6 (35%)

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
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	-4.74	1.36	1.43
3	H	1	NAG	C1-C2	3.58	1.57	1.52
3	H	2	NAG	O5-C1	-3.34	1.38	1.43
3	H	1	NAG	O5-C5	-3.22	1.36	1.43
3	H	1	NAG	O7-C7	-2.19	1.18	1.23

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	NAG	O3-C3-C4	-4.15	100.76	110.35
3	H	1	NAG	O4-C4-C3	-3.40	102.50	110.35
3	H	2	NAG	C2-N2-C7	-3.21	118.33	122.90
3	H	2	NAG	O5-C1-C2	-3.07	106.44	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	2	NAG	C4-C3-C2	-2.95	106.70	111.02

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

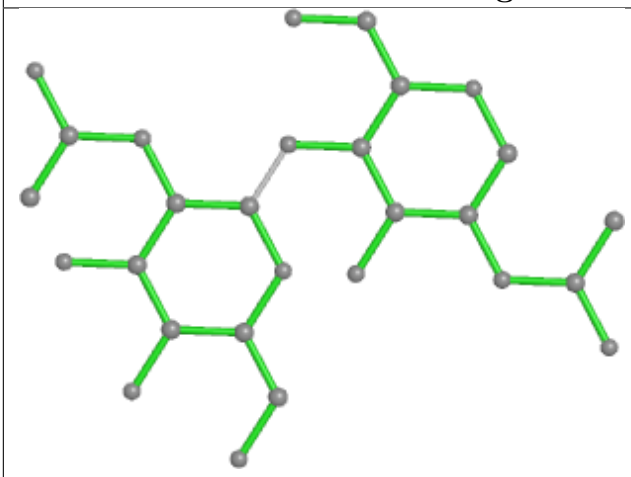
Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6

There are no ring outliers.

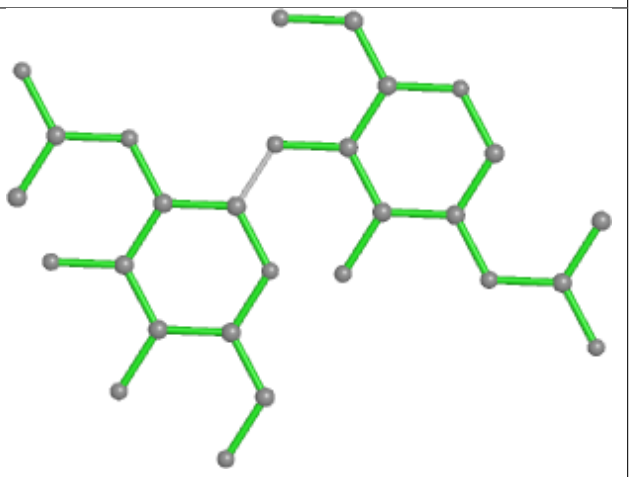
No monomer is involved in short contacts.

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

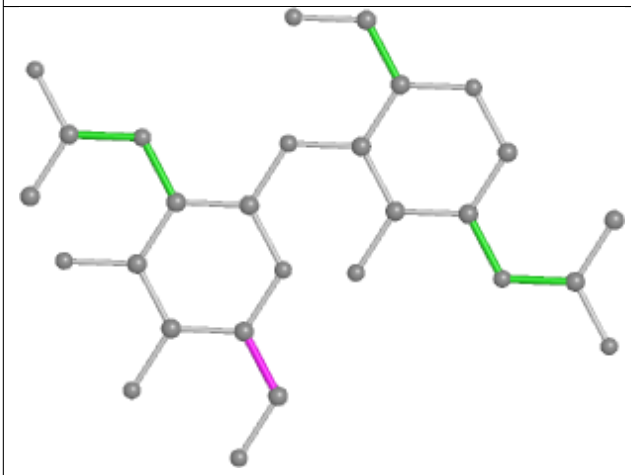
Oligosaccharide Chain E



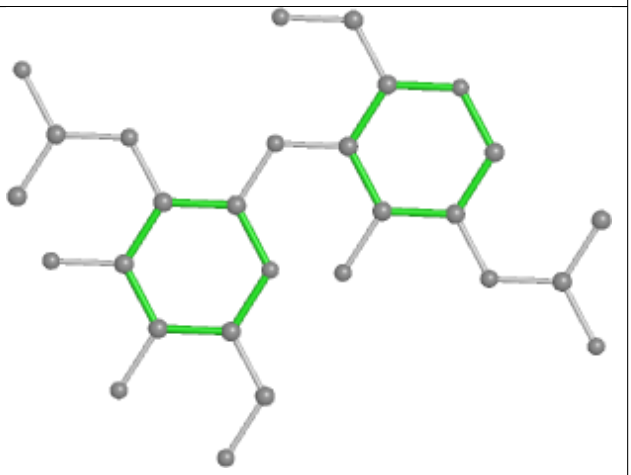
Bond lengths



Bond angles

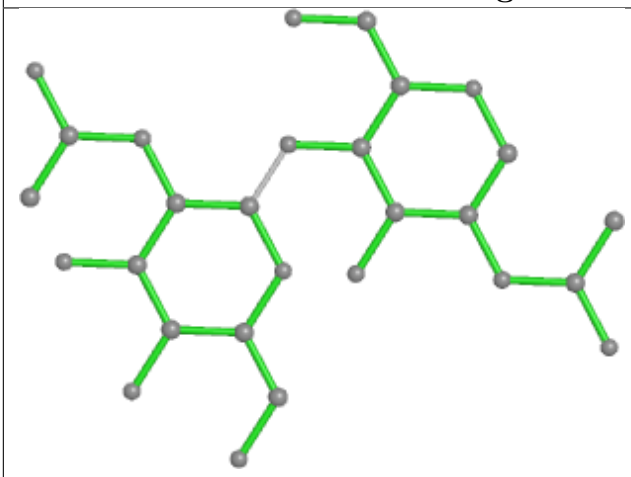


Torsions

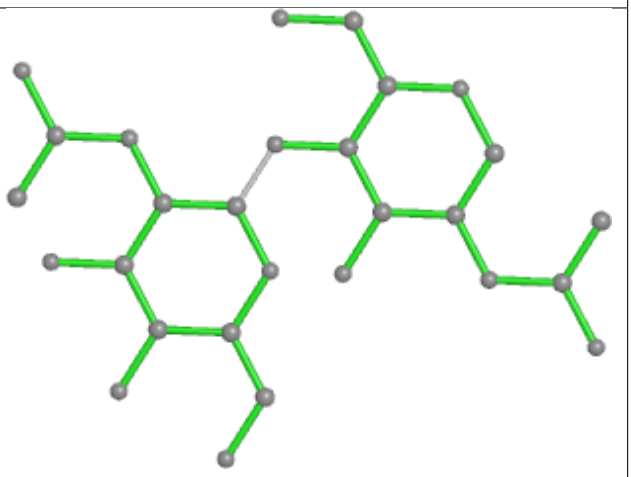


Rings

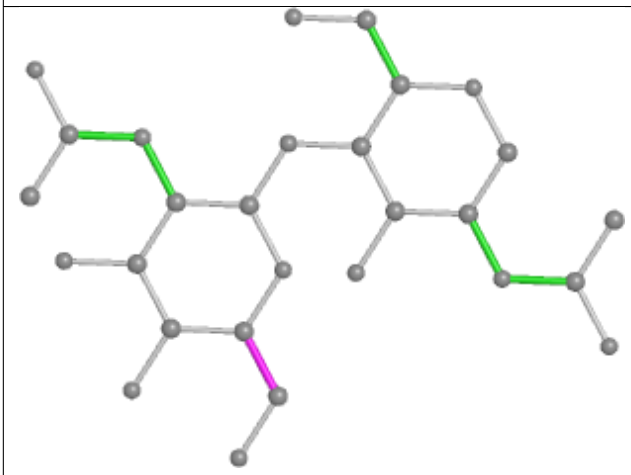
Oligosaccharide Chain F



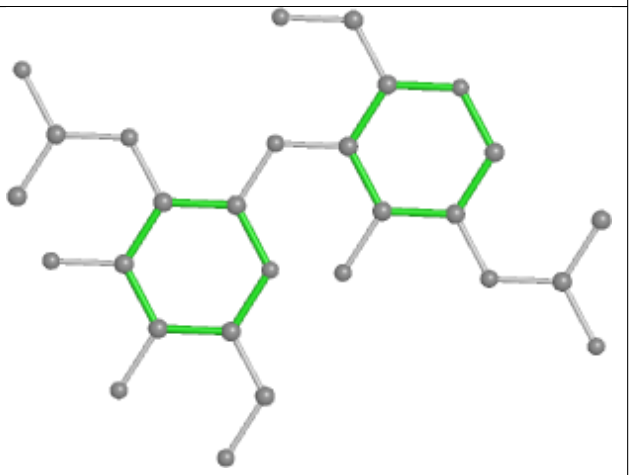
Bond lengths



Bond angles

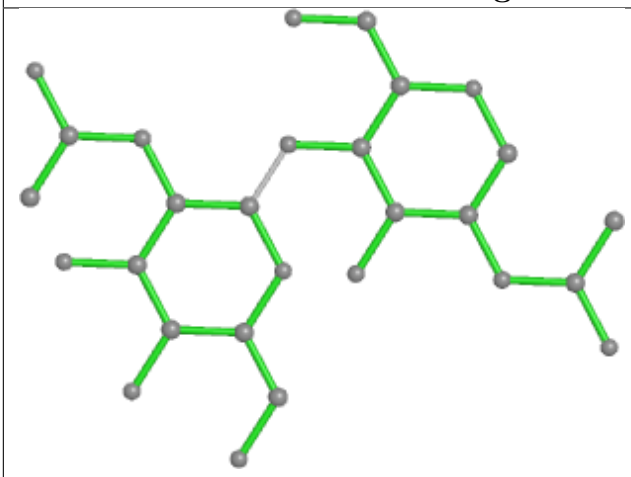


Torsions

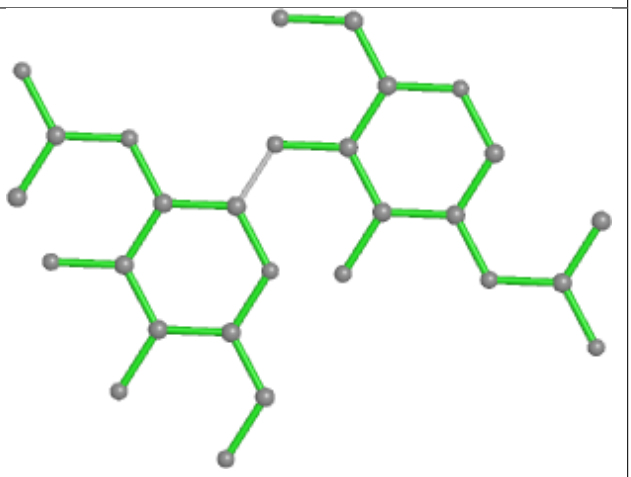


Rings

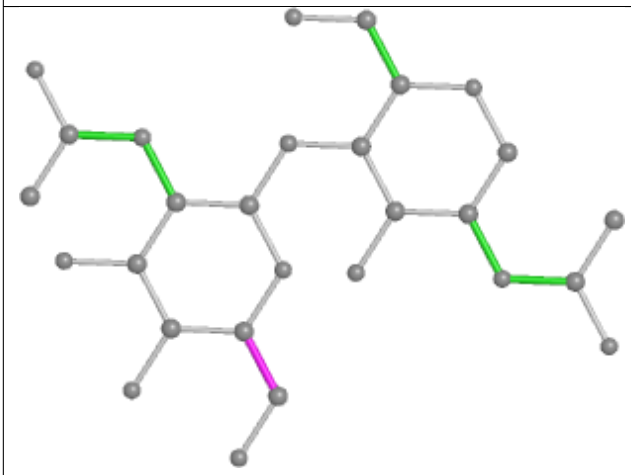
Oligosaccharide Chain G



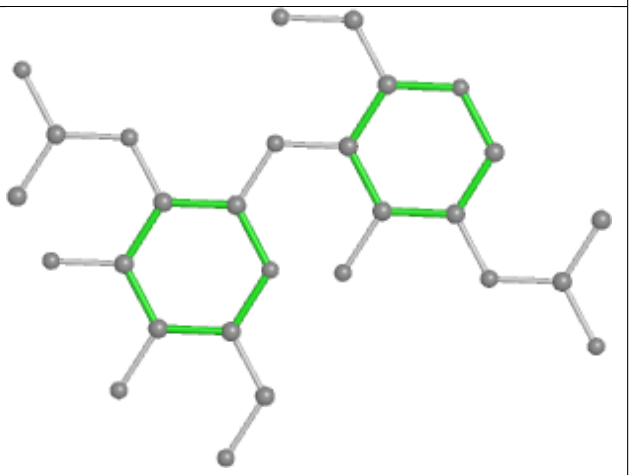
Bond lengths



Bond angles

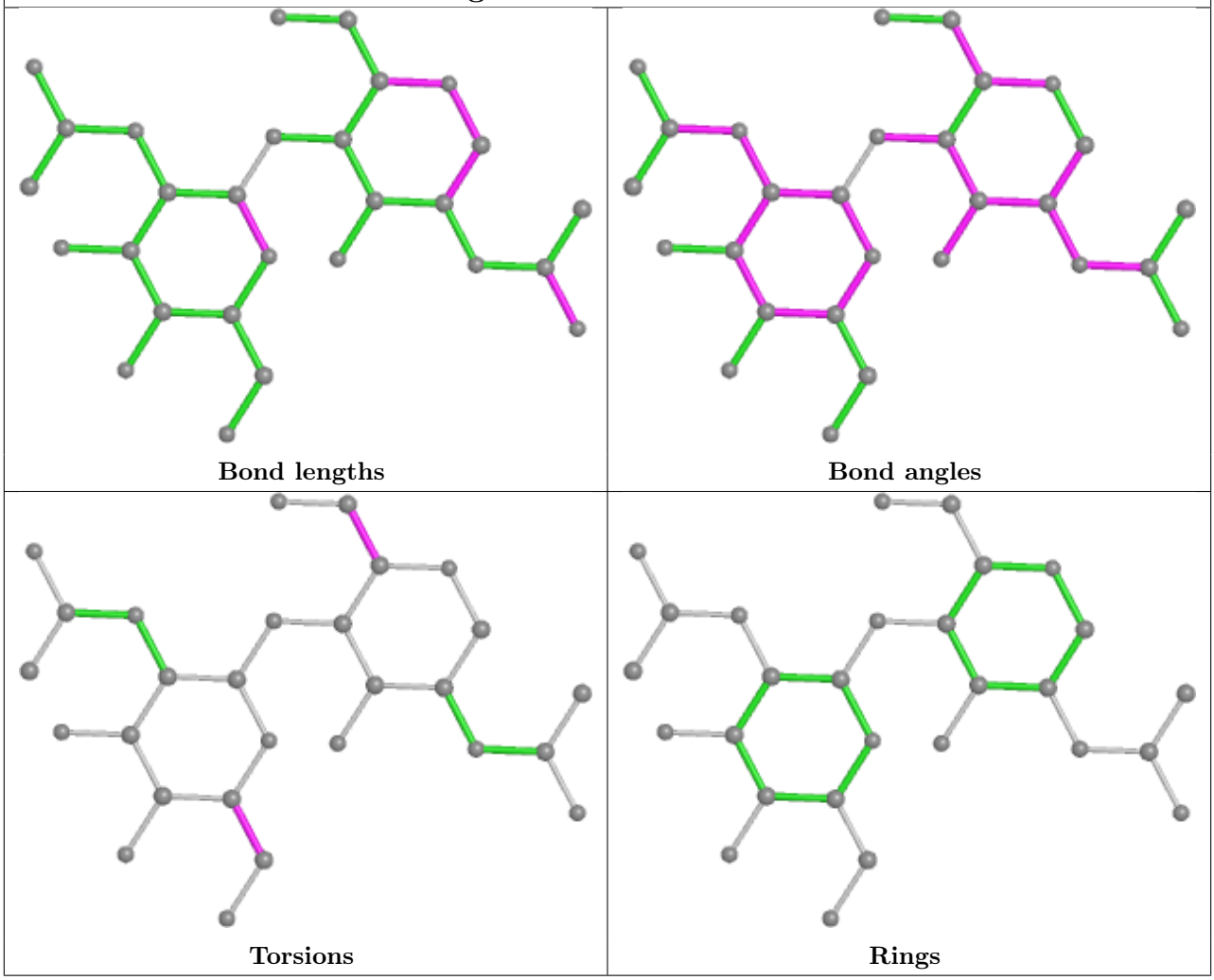


Torsions



Rings

Oligosaccharide Chain H



4.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
5	NAG	B	5006	1	14,14,15	0.17	0	17,19,21	0.45	0
5	NAG	B	5002	1	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	B	5009	1	14,14,15	1.44	2 (14%)	17,19,21	2.03	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	5005	1	14,14,15	0.29	0	17,19,21	0.38	0
5	NAG	B	5005	1	14,14,15	0.25	0	17,19,21	0.38	0
5	NAG	C	2002	2	14,14,15	0.34	0	17,19,21	0.52	0
5	NAG	A	5010	1	14,14,15	0.28	0	17,19,21	0.58	0
5	NAG	A	5007	1	14,14,15	0.21	0	17,19,21	0.40	0
5	NAG	A	5006	1	14,14,15	1.74	5 (35%)	17,19,21	1.72	4 (23%)
5	NAG	A	5002	1	14,14,15	0.27	0	17,19,21	0.38	0
5	NAG	D	501	2	14,14,15	0.28	0	17,19,21	0.52	0
5	NAG	D	502	2	14,14,15	0.59	0	17,19,21	1.47	1 (5%)
5	NAG	C	2001	2	14,14,15	0.32	0	17,19,21	0.47	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
5	NAG	B	5006	1	-	0/6/23/26	0/1/1/1
5	NAG	B	5002	1	-	2/6/23/26	0/1/1/1
5	NAG	B	5009	1	-	0/6/23/26	0/1/1/1
5	NAG	A	5005	1	-	0/6/23/26	0/1/1/1
5	NAG	B	5005	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2002	2	-	0/6/23/26	0/1/1/1
5	NAG	A	5010	1	-	2/6/23/26	0/1/1/1
5	NAG	A	5007	1	-	0/6/23/26	0/1/1/1
5	NAG	A	5006	1	-	0/6/23/26	0/1/1/1
5	NAG	A	5002	1	-	2/6/23/26	0/1/1/1
5	NAG	D	501	2	-	2/6/23/26	0/1/1/1
5	NAG	D	502	2	-	2/6/23/26	0/1/1/1
5	NAG	C	2001	2	-	0/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5006	NAG	O5-C5	-2.97	1.37	1.43
5	A	5006	NAG	O7-C7	-2.83	1.16	1.23
5	B	5009	NAG	O5-C1	-2.55	1.39	1.43
5	B	5009	NAG	O5-C5	-2.23	1.38	1.43
5	A	5006	NAG	C2-N2	-2.18	1.42	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	502	NAG	C1-O5-C5	5.63	119.82	112.19
5	B	5009	NAG	O5-C1-C2	-5.42	102.73	111.29
5	B	5009	NAG	C1-C2-N2	3.27	116.08	110.49
5	A	5006	NAG	C3-C4-C5	-3.20	104.54	110.24
5	B	5009	NAG	C2-N2-C7	-3.07	118.53	122.90

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	502	NAG	O5-C5-C6-O6
5	A	5010	NAG	C8-C7-N2-C2
5	A	5010	NAG	O7-C7-N2-C2
5	D	502	NAG	C4-C5-C6-O6
5	A	5002	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 (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.