Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 03:11 AM EDT

PDB ID	:	6MHM
Title	:	Crystal structure of human acid ceramidase in covalent complex with carmofur
Authors	:	Dementiev, A.; Joachimiak, A.; Doan, N.
Deposited on	:	2018-09-18
Resolution	:	2.74 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*
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.

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)
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 2.74 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.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	JRY	B	407	-	X	-	-
7	JRY	D	408	-	X	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6208 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 Acid ceramidase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			910	599	142	163	6			
1	C	114	Total	C	N	O	S	0	0	0
			906	596	141	163	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ASP	-	expression tag	UNP Q13510
A	13	ARG	-	expression tag	UNP Q13510
A	14	HIS	-	expression tag	UNP Q13510
A	15	HIS	-	expression tag	UNP Q13510
A	16	HIS	-	expression tag	UNP Q13510
A	17	HIS	-	expression tag	UNP Q13510
A	18	HIS	-	expression tag	UNP Q13510
A	19	HIS	-	expression tag	UNP Q13510
A	20	LYS	-	expression tag	UNP Q13510
A	21	LEU	-	expression tag	UNP Q13510
A	72	MET	VAL	variant	UNP Q13510
A	93	VAL	ILE	variant	UNP Q13510
C	12	ASP	-	expression tag	UNP Q13510
C	13	ARG	-	expression tag	UNP Q13510
C	14	HIS	-	expression tag	UNP Q13510
C	15	HIS	-	expression tag	UNP Q13510
C	16	HIS	-	expression tag	UNP Q13510
C	17	HIS	-	expression tag	UNP Q13510
C	18	HIS	-	expression tag	UNP Q13510
C	19	HIS	-	expression tag	UNP Q13510
C	20	LYS	-	expression tag	UNP Q13510
C	21	LEU	-	expression tag	UNP Q13510
C	72	MET	VAL	variant	UNP Q13510
C	93	VAL	ILE	variant	UNP Q13510

- Molecule 2 is a protein called Acid ceramidase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	253	Total	C	N	O	S	0	0	0
			2033	1306	341	376	10			
2	D	253	Total	C	N	O	S	0	0	0
			2015	1294	335	376	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	246	ALA	VAL	variant	UNP Q13510
D	246	ALA	VAL	variant	UNP Q13510

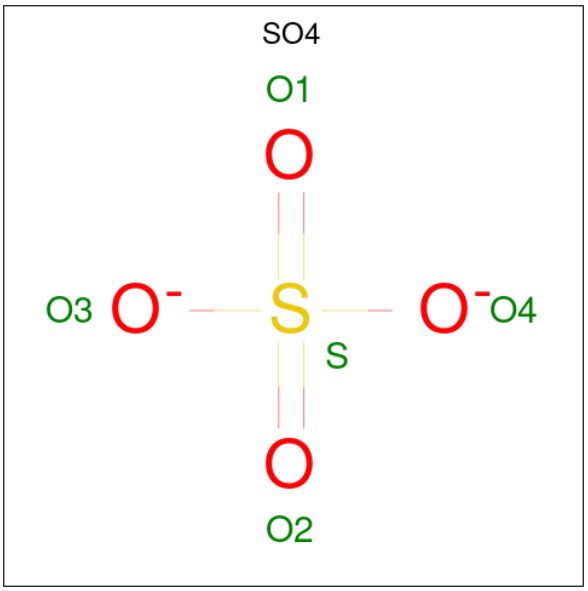
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			42	24	3	15			
3	G	3	Total	C	N	O	0	0	0
			42	24	3	15			

- 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
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

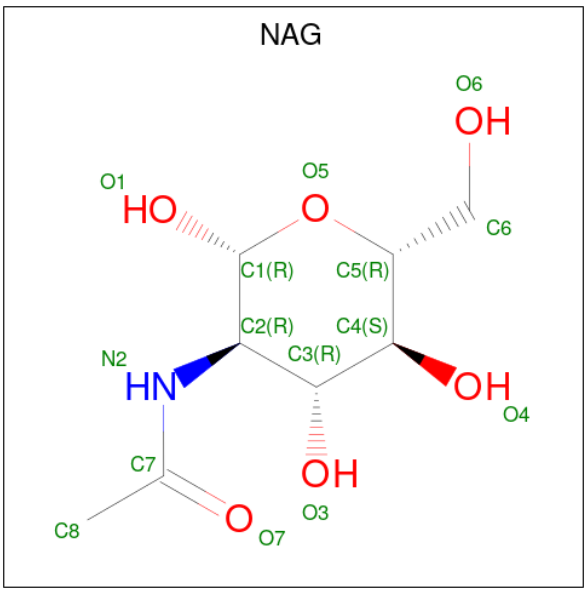
- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

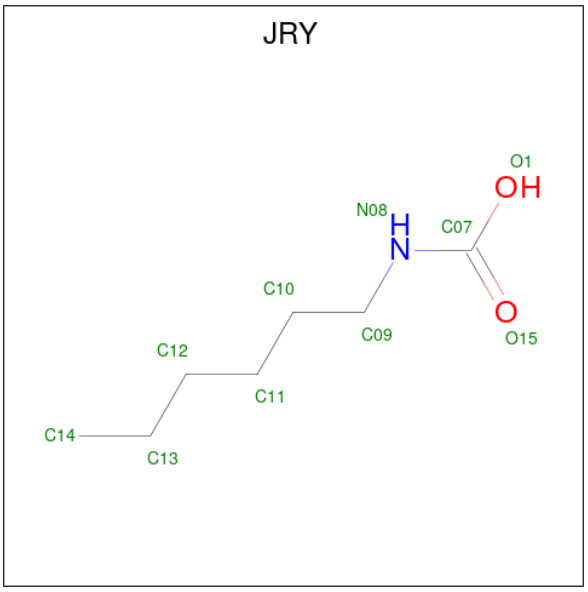
- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is hexylcarbamic acid (three-letter code: JRY) (formula: $C_7H_{15}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 9 7 1 1	0	0
7	D	1	Total C N O 9 7 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	13	Total O 13 13	0	0
8	B	29	Total O 29 29	0	0
8	C	12	Total O 12 12	0	0
8	D	25	Total O 25 25	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	153.72Å 68.65Å 98.39Å 90.00° 120.73° 90.00°	Depositor
Resolution (Å)	48.65 – 2.74	Depositor
% Data completeness (in resolution range)	99.7 (48.65-2.74)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.214 , 0.262	Depositor
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.362	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6208	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.54% 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

10 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	2,3	14,14,15	0.36	0	17,19,21	0.62	0
3	NAG	E	2	3	14,14,15	0.23	0	17,19,21	0.63	0
3	NAG	E	3	3	14,14,15	0.48	0	17,19,21	1.22	2 (11%)
4	NAG	F	1	2,4	14,14,15	0.54	0	17,19,21	0.55	0
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.53	0
3	NAG	G	1	2,3	14,14,15	0.34	0	17,19,21	0.54	0
3	NAG	G	2	3	14,14,15	0.28	0	17,19,21	0.82	1 (5%)
3	NAG	G	3	3	14,14,15	0.70	1 (7%)	17,19,21	0.57	0
4	NAG	H	1	2,4	14,14,15	0.44	0	17,19,21	0.50	0
4	NAG	H	2	4	14,14,15	0.21	0	17,19,21	0.58	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
3	NAG	E	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	3	3	-	3/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
3	NAG	G	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	3	3	-	4/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	NAG	C1-C2	2.32	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	3	NAG	C2-N2-C7	4.02	128.62	122.90
3	E	3	NAG	C1-O5-C5	2.08	115.01	112.19
3	G	2	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

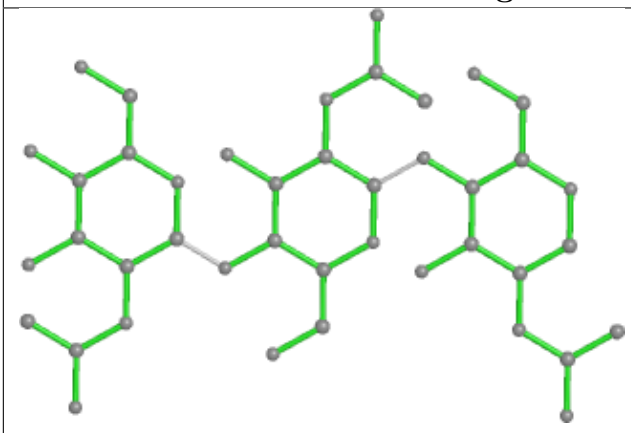
Mol	Chain	Res	Type	Atoms
3	E	3	NAG	C3-C2-N2-C7
4	H	1	NAG	O5-C5-C6-O6
3	G	3	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	E	3	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
3	G	3	NAG	C8-C7-N2-C2
3	G	3	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	G	3	NAG	C4-C5-C6-O6
3	E	3	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6

There are no ring outliers.

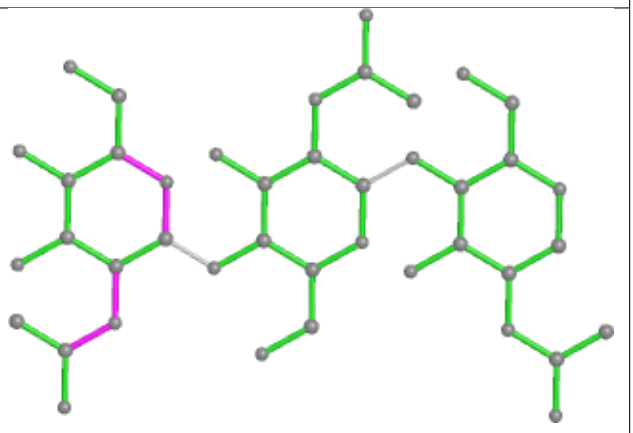
No monomer is involved in short contacts.

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

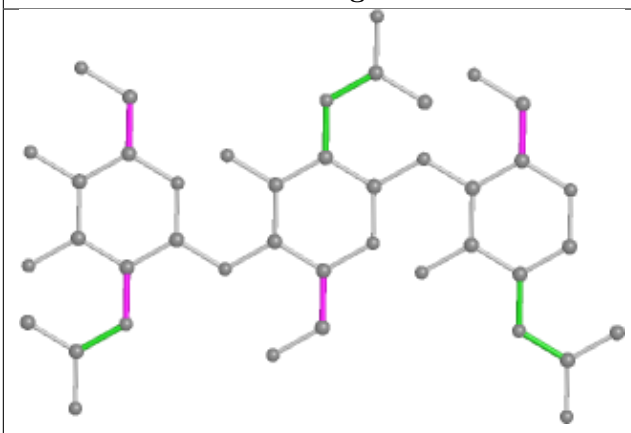
Oligosaccharide Chain E



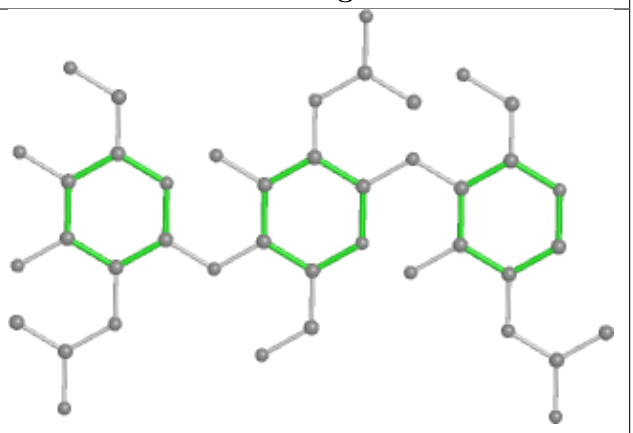
Bond lengths



Bond angles

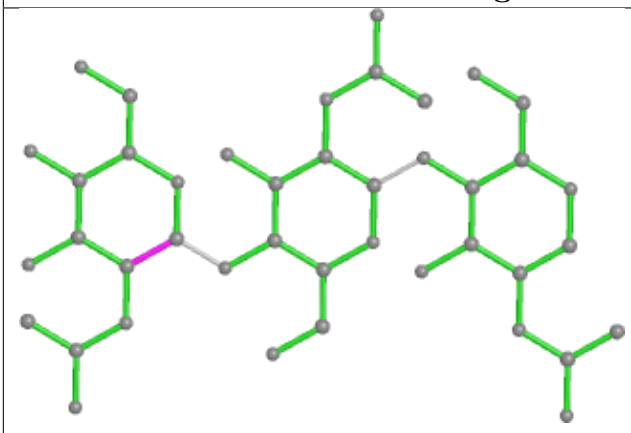


Torsions

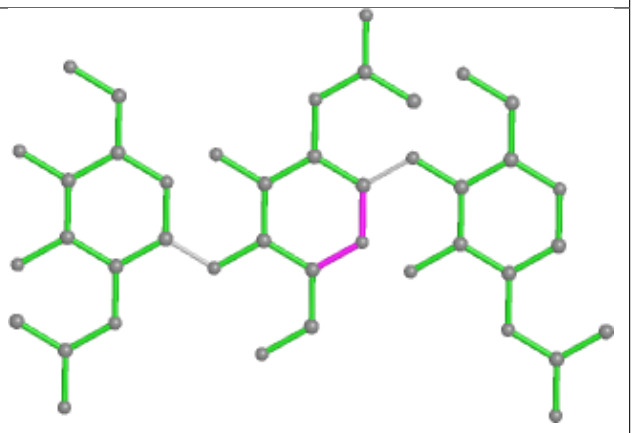


Rings

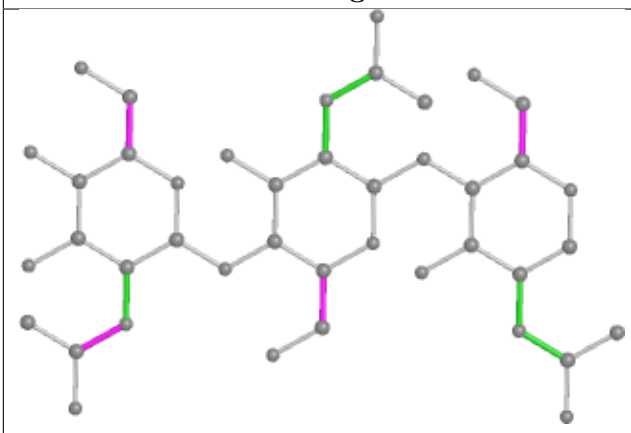
Oligosaccharide Chain G



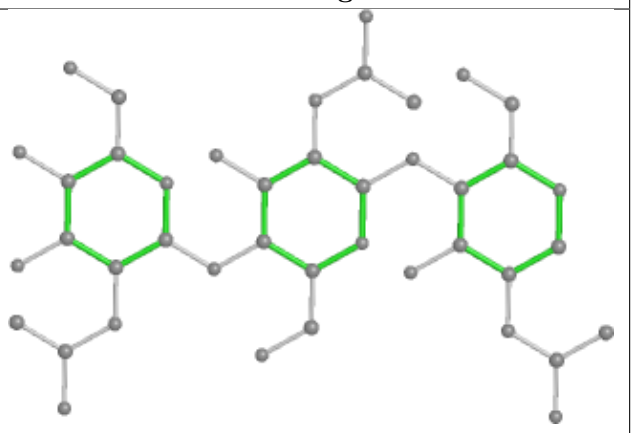
Bond lengths



Bond angles

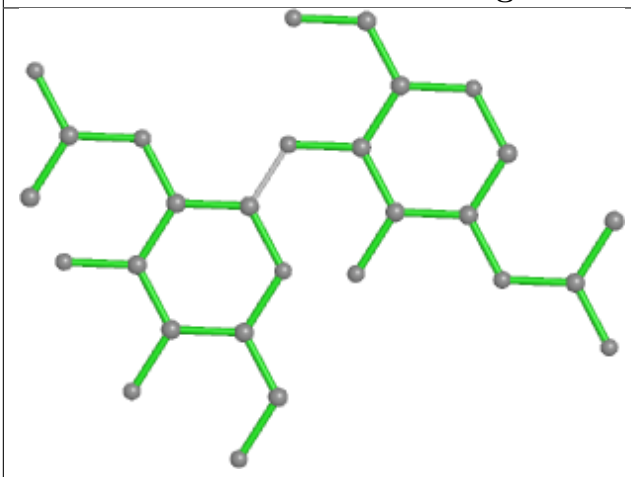


Torsions

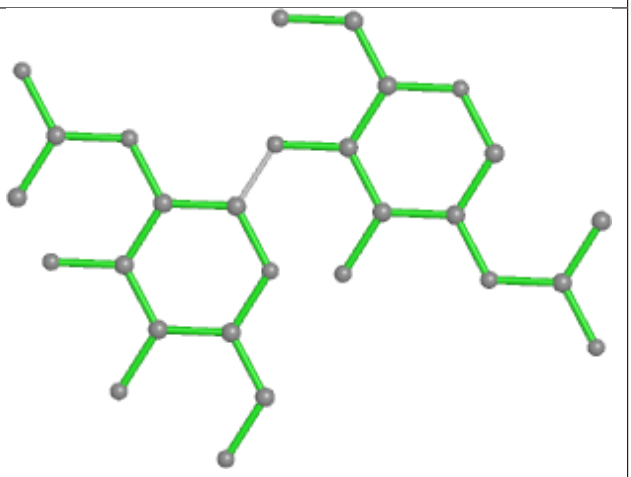


Rings

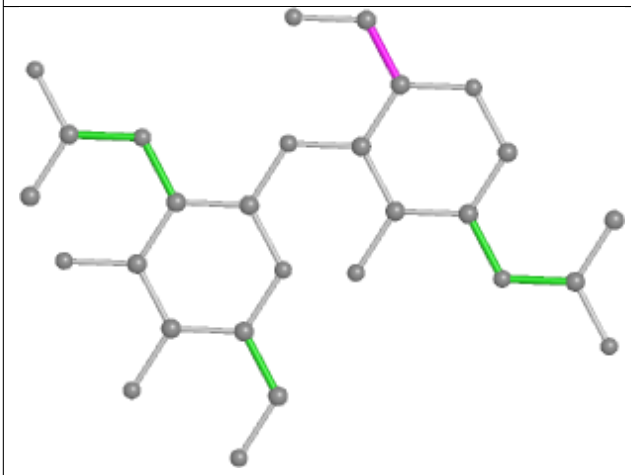
Oligosaccharide Chain F



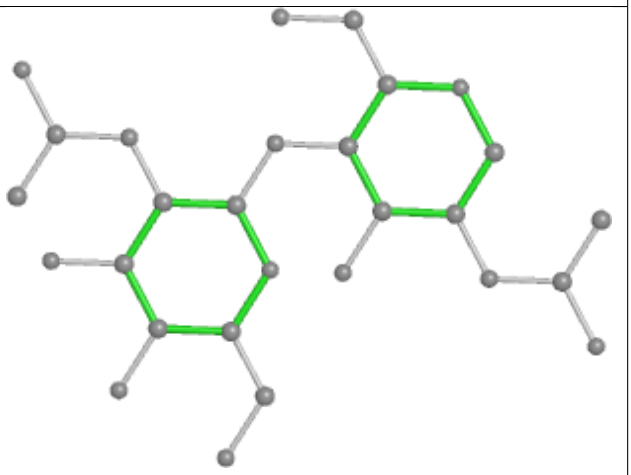
Bond lengths



Bond angles

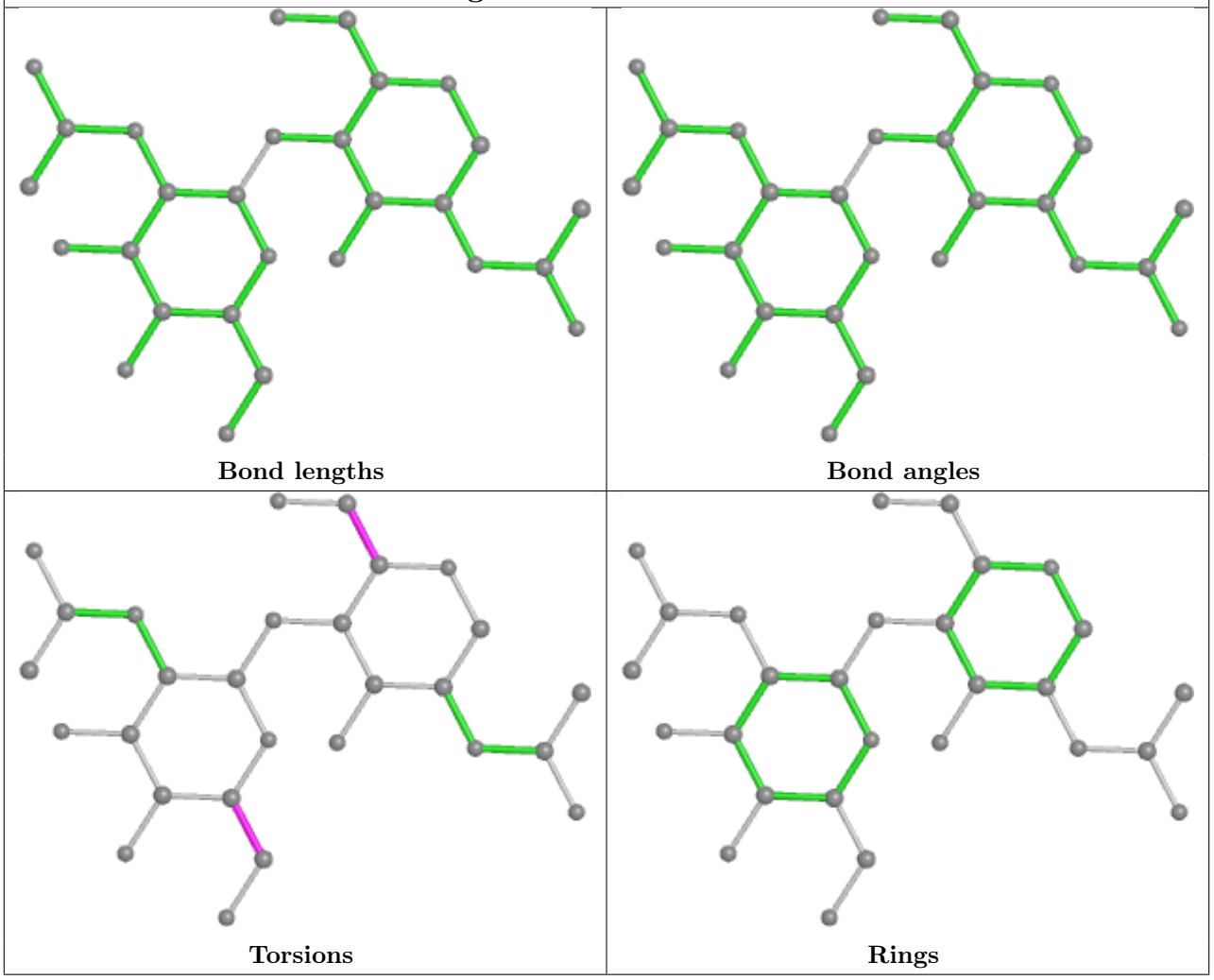


Torsions



Rings

Oligosaccharide Chain H



4.6 Ligand geometry (i)

18 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	SO4	A	202	-	4,4,4	0.14	0	6,6,6	0.16	0
5	SO4	B	409	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	A	201	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	408	-	4,4,4	0.14	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SO4	C	201	-	4,4,4	0.14	0	6,6,6	0.05	0
7	JRY	D	408	2	8,8,9	1.85	1 (12%)	6,7,9	6.12	4 (66%)
5	SO4	D	409	-	4,4,4	0.13	0	6,6,6	0.10	0
5	SO4	D	411	-	4,4,4	0.13	0	6,6,6	0.05	0
6	NAG	D	407	2	14,14,15	1.05	1 (7%)	17,19,21	0.92	1 (5%)
5	SO4	D	410	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	C	202	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	B	410	-	4,4,4	0.13	0	6,6,6	0.09	0
5	SO4	C	203	-	4,4,4	0.17	0	6,6,6	0.09	0
7	JRY	B	407	2	8,8,9	1.99	3 (37%)	6,7,9	7.49	4 (66%)
6	NAG	D	404	2	14,14,15	0.30	0	17,19,21	0.35	0
5	SO4	A	203	-	4,4,4	0.39	0	6,6,6	0.29	0
5	SO4	D	412	-	4,4,4	0.14	0	6,6,6	0.06	0
6	NAG	B	406	2	14,14,15	0.28	0	17,19,21	0.56	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
7	JRY	D	408	2	-	4/6/6/7	-
6	NAG	D	407	2	-	2/6/23/26	0/1/1/1
7	JRY	B	407	2	-	5/6/6/7	-
6	NAG	D	404	2	-	2/6/23/26	0/1/1/1
6	NAG	B	406	2	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	408	JRY	C07-N08	4.43	1.42	1.33
7	B	407	JRY	C07-N08	4.37	1.42	1.33
6	D	407	NAG	C1-C2	3.58	1.57	1.52
7	B	407	JRY	C09-N08	-2.53	1.40	1.46
7	B	407	JRY	O15-C07	-2.43	1.15	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	407	JRY	O15-C07-N08	-16.79	107.93	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	408	JRY	O15-C07-N08	-13.24	111.52	124.89
7	B	407	JRY	C10-C09-N08	6.39	136.17	112.84
7	D	408	JRY	C10-C09-N08	5.40	132.55	112.84
7	D	408	JRY	C11-C10-C09	3.71	131.14	113.56
7	B	407	JRY	C11-C10-C09	2.72	126.44	113.56
6	D	407	NAG	C4-C3-C2	2.54	114.73	111.02
7	B	407	JRY	C12-C11-C10	-2.48	101.86	114.42
7	D	408	JRY	C12-C11-C10	-2.45	101.97	114.42

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	404	NAG	O5-C5-C6-O6
7	D	408	JRY	N08-C09-C10-C11
6	D	407	NAG	O5-C5-C6-O6
7	D	408	JRY	C10-C11-C12-C13
7	B	407	JRY	C10-C09-N08-C07
7	D	408	JRY	C10-C09-N08-C07
6	D	404	NAG	C4-C5-C6-O6
7	B	407	JRY	C09-C10-C11-C12
7	B	407	JRY	O15-C07-N08-C09
7	D	408	JRY	O15-C07-N08-C09
7	B	407	JRY	C10-C11-C12-C13
6	D	407	NAG	C4-C5-C6-O6
6	B	406	NAG	C3-C2-N2-C7
7	B	407	JRY	N08-C09-C10-C11

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.