wwPDB X-ray Structure Validation Summary Report (i)

Nov 10, 2024 – 01:46 AM EST

PDB ID	:	3W9T
Title	:	pore-forming CEL-III
Authors	:	Unno, H.; Goda, S.; Hatakeyama, T.
Deposited on	:	2013-04-16
Resolution	:	2.90 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:

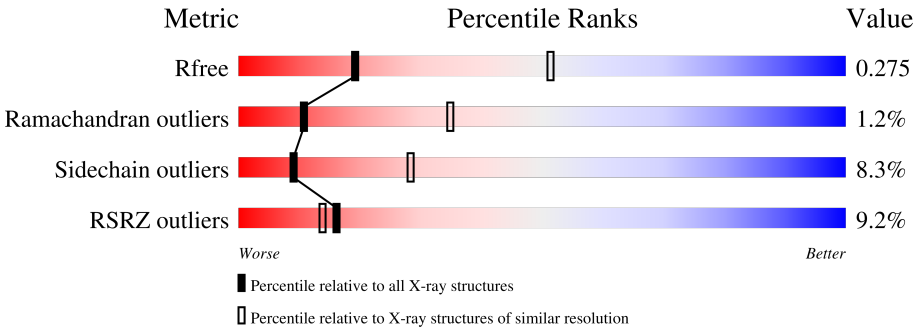
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2335 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	432	9% 92% 7%
1	B	432	6% 90% 9%
1	C	432	7% 91% 7%
1	D	432	8% 91% 9%
1	E	432	7% 91% 8%
1	F	432	13% 91% 8%

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Mol	Chain	Length	Quality of chain
1	G	432	15% 91% 9%
2	H	2	50% 50%
2	I	2	50% 50%
2	J	2	50% 50%
2	K	2	50% 50%
2	L	2	100%
2	M	2	50% 50%
2	N	2	50% 50%
2	O	2	50% 50%
2	P	2	50% 50%
2	Q	2	50% 50%
2	R	2	100%
2	S	2	50% 50%
2	T	2	50% 50%
2	U	2	100%
2	V	2	50% 50%
2	W	2	50% 50%
2	X	2	50% 50%
2	Y	2	100%
2	Z	2	50% 50%
2	a	2	50% 50%
2	b	2	100%
2	c	2	50% 50%
2	d	2	100%
2	e	2	100%

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Mol	Chain	Length	Quality of chain
2	f	2	50% 50%
2	g	2	100%
2	h	2	50% 50%
2	i	2	50% 50%
2	j	2	100%
2	k	2	50% 50%
2	l	2	50% 50%
2	m	2	50% 50%
2	n	2	50% 50%
2	o	2	100%
2	p	2	100%
2	q	2	50% 50%
2	r	2	50% 50%

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
3	CA	C	1014	-	-	X	-

2 Entry composition (i)

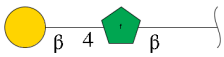
There are 5 unique types of molecules in this entry. The entry contains 24175 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hemolytic lectin CEL-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	C	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	G	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	B	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	F	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	E	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	D	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	2	Total	C	O		0	0	0
			23	12	11				
2	I	2	Total	C	O		0	0	0
			23	12	11				
2	J	2	Total	C	O		0	0	0
			23	12	11				
2	K	2	Total	C	O		0	0	0
			23	12	11				
2	L	2	Total	C	O		0	0	0
			23	12	11				

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	M	2	Total C O 23 12 11	0	0	0
2	N	2	Total C O 23 12 11	0	0	0
2	O	2	Total C O 23 12 11	0	0	0
2	P	2	Total C O 23 12 11	0	0	0
2	Q	2	Total C O 23 12 11	0	0	0
2	R	2	Total C O 23 12 11	0	0	0
2	S	2	Total C O 23 12 11	0	0	0
2	T	2	Total C O 23 12 11	0	0	0
2	U	2	Total C O 23 12 11	0	0	0
2	V	2	Total C O 23 12 11	0	0	0
2	W	2	Total C O 23 12 11	0	0	0
2	X	2	Total C O 23 12 11	0	0	0
2	Y	2	Total C O 23 12 11	0	0	0
2	Z	2	Total C O 23 12 11	0	0	0
2	a	2	Total C O 23 12 11	0	0	0
2	b	2	Total C O 23 12 11	0	0	0
2	c	2	Total C O 23 12 11	0	0	0
2	d	2	Total C O 23 12 11	0	0	0
2	e	2	Total C O 23 12 11	0	0	0
2	f	2	Total C O 23 12 11	0	0	0
2	g	2	Total C O 23 12 11	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	h	2	Total C O 23 12 11	0	0	0
2	i	2	Total C O 23 12 11	0	0	0
2	j	2	Total C O 23 12 11	0	0	0
2	k	2	Total C O 23 12 11	0	0	0
2	l	2	Total C O 23 12 11	0	0	0
2	m	2	Total C O 23 12 11	0	0	0
2	n	2	Total C O 23 12 11	0	0	0
2	o	2	Total C O 23 12 11	0	0	0
2	p	2	Total C O 23 12 11	0	0	0
2	q	2	Total C O 23 12 11	0	0	0
2	r	2	Total C O 23 12 11	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total Ca 6 6	0	0
3	C	7	Total Ca 7 7	0	0
3	G	6	Total Ca 6 6	0	0
3	B	6	Total Ca 6 6	0	0
3	F	6	Total Ca 6 6	0	0
3	E	7	Total Ca 7 7	0	0
3	D	6	Total Ca 6 6	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	C	2	Total Mg 2 2	0	0
4	G	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0
4	F	2	Total Mg 2 2	0	0
4	E	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0

- Molecule 5 is water.

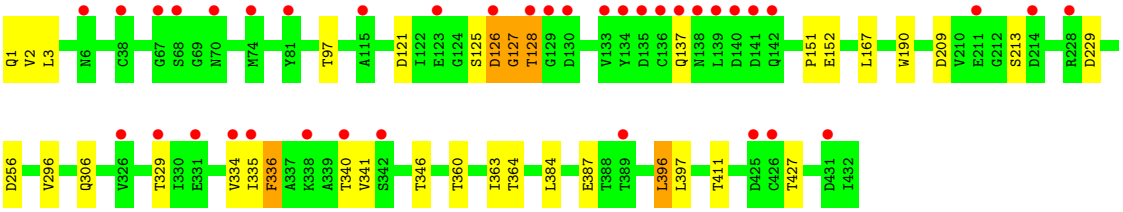
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0
5	C	9	Total O 9 9	0	0
5	G	5	Total O 5 5	0	0
5	B	14	Total O 14 14	0	0
5	F	13	Total O 13 13	0	0
5	E	10	Total O 10 10	0	0
5	D	14	Total O 14 14	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

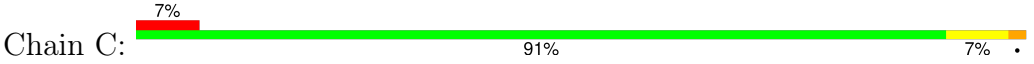
• Molecule 1: Hemolytic lectin CEL-III

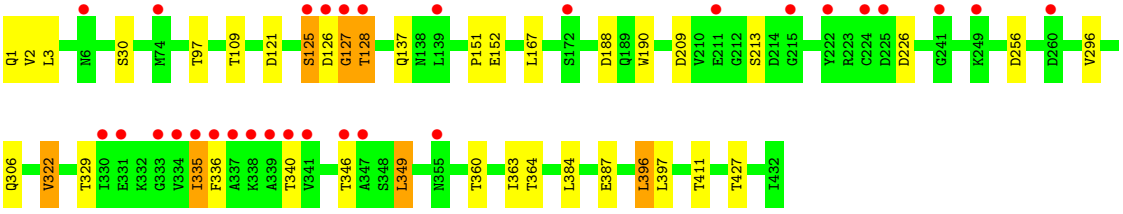
Chain A:



• Molecule 1: Hemolytic lectin CEL-III

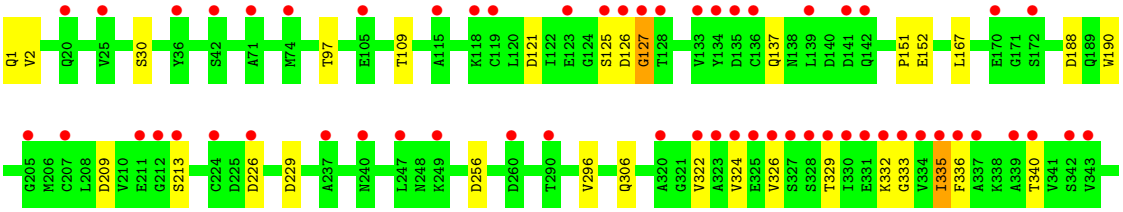
Chain C:





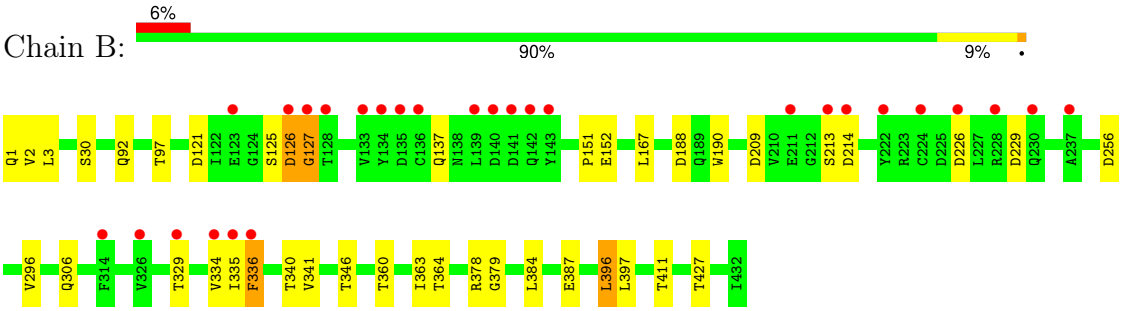
• Molecule 1: Hemolytic lectin CEL-III

Chain G:



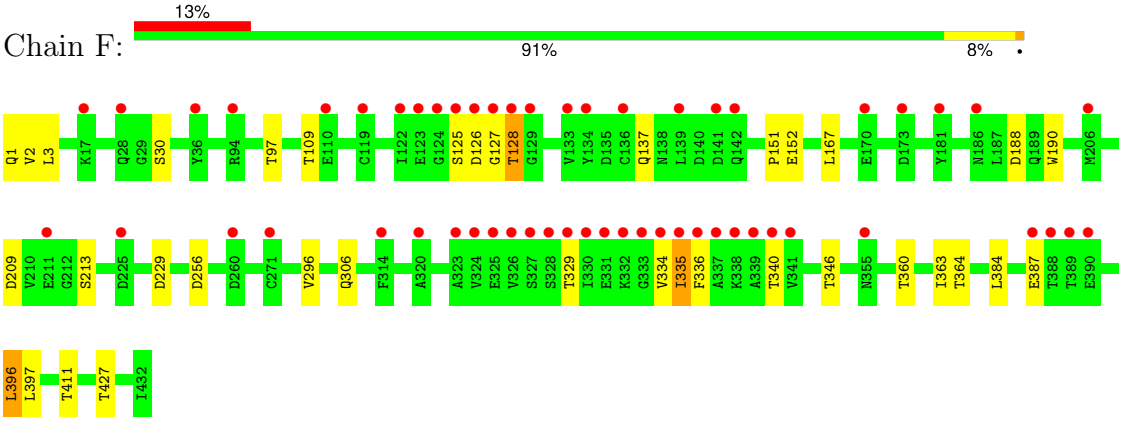
• Molecule 1: Hemolytic lectin CEL-III

Chain B:



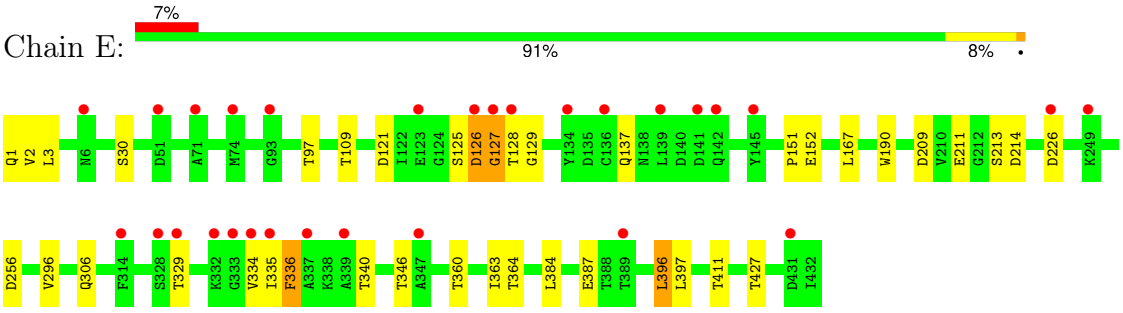
• Molecule 1: Hemolytic lectin CEL-III

Chain F:



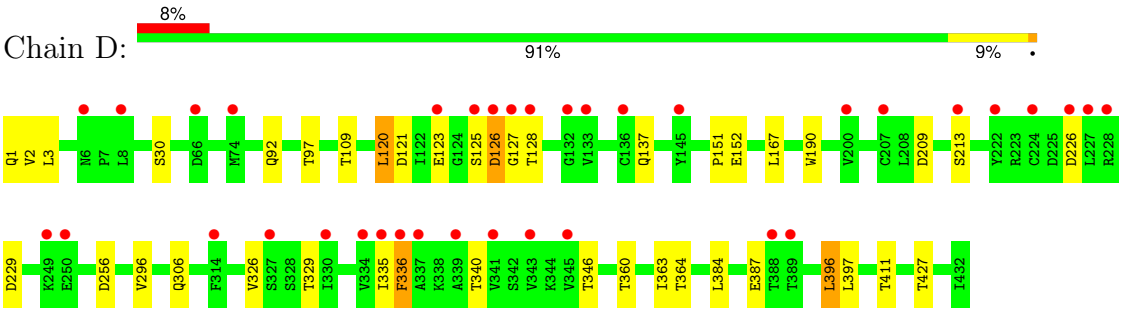
• Molecule 1: Hemolytic lectin CEL-III

Chain E:



• Molecule 1: Hemolytic lectin CEL-III

Chain D:



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain H:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain I:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

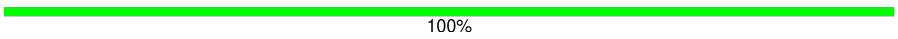
Chain J:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain K:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain L:



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain M:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain N:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain O:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

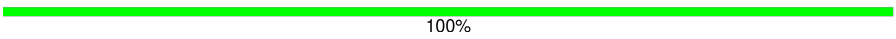
Chain P:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain Q:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain R:



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

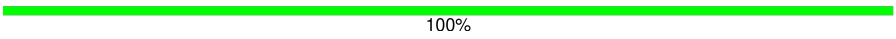
Chain S:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain T:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain U:



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain V:

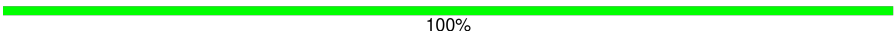
• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain W:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain X: 

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain Y: 

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain Z: 

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain a: 

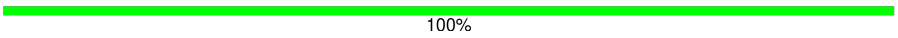
• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain b:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

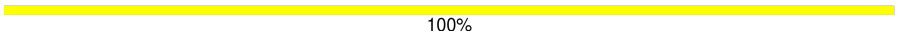
Chain c: 

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain d: 

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain e:

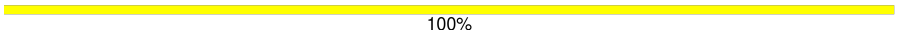


• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain f:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain g:



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

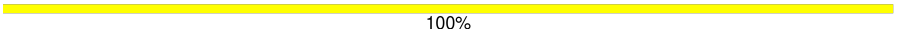
Chain h:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain i:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain j:



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain k:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain l:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

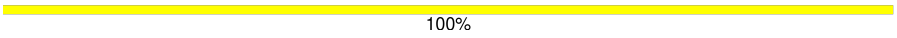
Chain m:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain n:

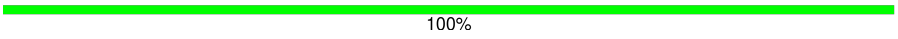
• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain o:



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain p:



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain q:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain r:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	219.80Å 228.65Å 133.02Å 90.00° 127.13° 90.00°	Depositor
Resolution (Å)	48.20 – 2.90 48.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.20-2.90) 98.4 (48.20-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.239 , 0.273 0.239 , 0.275	Depositor DCC
R_{free} test set	5793 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	69.4	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	24175	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.30% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, CA, MG, PCA, FRU

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.47	1/3366 (0.0%)	0.70	3/4566 (0.1%)
1	B	0.47	1/3366 (0.0%)	0.72	4/4566 (0.1%)
1	C	0.46	0/3366	0.71	5/4566 (0.1%)
1	D	0.45	0/3366	0.68	2/4566 (0.0%)
1	E	0.47	0/3366	0.69	2/4566 (0.0%)
1	F	0.49	0/3366	0.70	2/4566 (0.0%)
1	G	0.45	0/3366	0.71	1/4566 (0.0%)
All	All	0.47	2/23562 (0.0%)	0.70	19/31962 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	3
1	G	0	4
All	All	0	25

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ASP	CG-OD2	-7.12	1.08	1.25
1	B	379	GLY	N-CA	-5.95	1.37	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	126	ASP	CB-CG-OD1	13.30	130.27	118.30
1	C	128	THR	N-CA-C	-10.58	82.44	111.00
1	B	378	ARG	C-N-CA	9.70	142.68	122.30
1	A	126	ASP	OD1-CG-OD2	-8.37	107.39	123.30
1	B	378	ARG	CA-C-N	7.94	132.07	116.20

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	PRO	Peptide
1	A	335	ILE	Peptide
1	C	125	SER	Peptide
1	C	127	GLY	Peptide
1	C	151	PRO	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	430/432 (100%)	407 (95%)	18 (4%)	5 (1%)	11 35
1	B	430/432 (100%)	410 (95%)	16 (4%)	4 (1%)	14 43
1	C	430/432 (100%)	410 (95%)	13 (3%)	7 (2%)	8 28
1	D	430/432 (100%)	411 (96%)	15 (4%)	4 (1%)	14 43
1	E	430/432 (100%)	408 (95%)	17 (4%)	5 (1%)	11 35
1	F	430/432 (100%)	410 (95%)	15 (4%)	5 (1%)	11 35
1	G	430/432 (100%)	411 (96%)	12 (3%)	7 (2%)	8 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3010/3024 (100%)	2867 (95%)	106 (4%)	37 (1%)	11 35

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	ASP
1	C	128	THR
1	C	336	PHE
1	G	126	ASP
1	G	336	PHE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	370/370 (100%)	340 (92%)	30 (8%)	9 29
1	B	370/370 (100%)	337 (91%)	33 (9%)	8 26
1	C	370/370 (100%)	340 (92%)	30 (8%)	9 29
1	D	370/370 (100%)	337 (91%)	33 (9%)	8 26
1	E	370/370 (100%)	339 (92%)	31 (8%)	9 28
1	F	370/370 (100%)	341 (92%)	29 (8%)	10 31
1	G	370/370 (100%)	340 (92%)	30 (8%)	9 29
All	All	2590/2590 (100%)	2374 (92%)	216 (8%)	9 28

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	363	ILE
1	F	360	THR
1	D	256	ASP
1	B	396	LEU
1	F	167	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	32	ASN
1	D	306	GLN
1	F	301	ASN
1	D	32	ASN
1	F	270	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PCA	F	1	1	7,8,9	0.53	0	9,10,12	2.25	4 (44%)
1	PCA	B	1	1	7,8,9	0.51	0	9,10,12	2.14	2 (22%)
1	PCA	E	1	1	7,8,9	0.48	0	9,10,12	2.37	3 (33%)
1	PCA	A	1	1	7,8,9	0.58	0	9,10,12	2.31	3 (33%)
1	PCA	D	1	1	7,8,9	0.65	0	9,10,12	2.24	2 (22%)
1	PCA	G	1	1	7,8,9	0.65	0	9,10,12	2.19	3 (33%)
1	PCA	C	1	1	7,8,9	0.52	0	9,10,12	2.30	4 (44%)

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
1	PCA	F	1	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	E	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1
1	PCA	G	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1	PCA	CB-CA-C	5.05	119.59	112.66
1	E	1	PCA	CB-CA-C	4.95	119.45	112.66
1	C	1	PCA	CB-CA-C	4.53	118.87	112.66
1	A	1	PCA	CB-CA-C	4.41	118.70	112.66
1	F	1	PCA	CA-N-CD	-4.32	98.79	113.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

74 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	FRU	H	1	2	11,12,12	0.64	0	10,18,18	0.88	0
2	GAL	H	2	2,3	11,11,12	0.32	0	15,15,17	1.28	1 (6%)
2	FRU	I	1	2	11,12,12	0.64	0	10,18,18	0.86	0
2	GAL	I	2	2,3	11,11,12	0.73	0	15,15,17	2.01	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FRU	J	1	2	11,12,12	0.70	1 (9%)	10,18,18	1.02	0
2	GAL	J	2	2,3	11,11,12	0.39	0	15,15,17	0.87	0
2	FRU	K	1	2	11,12,12	0.59	0	10,18,18	0.71	0
2	GAL	K	2	2,3	11,11,12	0.28	0	15,15,17	0.93	1 (6%)
2	FRU	L	1	2	11,12,12	0.55	0	10,18,18	0.83	0
2	GAL	L	2	2,3	11,11,12	0.33	0	15,15,17	0.79	0
2	FRU	M	1	2	11,12,12	0.72	0	10,18,18	1.04	0
2	GAL	M	2	2,3	11,11,12	0.75	0	15,15,17	1.82	3 (20%)
2	FRU	N	1	2	11,12,12	0.67	0	10,18,18	0.70	0
2	GAL	N	2	2,3	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	FRU	O	1	2	11,12,12	0.62	0	10,18,18	0.81	0
2	GAL	O	2	2,3	11,11,12	0.34	0	15,15,17	1.52	4 (26%)
2	FRU	P	1	2	11,12,12	0.69	0	10,18,18	0.62	0
2	GAL	P	2	2,3	11,11,12	0.55	0	15,15,17	1.25	1 (6%)
2	FRU	Q	1	2	11,12,12	0.70	0	10,18,18	1.07	1 (10%)
2	GAL	Q	2	2,3	11,11,12	0.37	0	15,15,17	0.97	0
2	FRU	R	1	2	11,12,12	0.61	0	10,18,18	0.97	0
2	GAL	R	2	2,3	11,11,12	0.36	0	15,15,17	0.46	0
2	FRU	S	1	2	11,12,12	0.67	0	10,18,18	0.66	0
2	GAL	S	2	2,3	11,11,12	0.31	0	15,15,17	1.07	1 (6%)
2	FRU	T	1	2	11,12,12	0.65	0	10,18,18	0.88	0
2	GAL	T	2	2,3	11,11,12	0.40	0	15,15,17	2.09	2 (13%)
2	FRU	U	1	2	11,12,12	0.59	0	10,18,18	0.84	0
2	GAL	U	2	2,3	11,11,12	0.33	0	15,15,17	0.87	0
2	FRU	V	1	2	11,12,12	0.62	0	10,18,18	0.90	0
2	GAL	V	2	2,3	11,11,12	0.44	0	15,15,17	1.91	2 (13%)
2	FRU	W	1	2	11,12,12	0.72	0	10,18,18	1.45	1 (10%)
2	GAL	W	2	2,3	11,11,12	0.33	0	15,15,17	0.81	0
2	FRU	X	1	2	11,12,12	0.72	0	10,18,18	0.91	0
2	GAL	X	2	2,3	11,11,12	0.72	0	15,15,17	2.03	4 (26%)
2	FRU	Y	1	2	11,12,12	0.64	0	10,18,18	0.74	0
2	GAL	Y	2	2,3	11,11,12	0.28	0	15,15,17	0.74	0
2	FRU	Z	1	2	11,12,12	0.69	0	10,18,18	0.81	0
2	GAL	Z	2	2,3	11,11,12	0.36	0	15,15,17	2.57	4 (26%)
2	FRU	a	1	2	11,12,12	0.56	0	10,18,18	1.08	0
2	GAL	a	2	2,3	11,11,12	0.44	0	15,15,17	1.82	1 (6%)
2	FRU	b	1	2	11,12,12	0.98	1 (9%)	10,18,18	1.19	0
2	GAL	b	2	2	11,11,12	0.56	0	15,15,17	2.99	5 (33%)
2	FRU	c	1	2	11,12,12	0.77	0	10,18,18	1.05	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GAL	c	2	2,3	11,11,12	0.38	0	15,15,17	0.77	0
2	FRU	d	1	2	11,12,12	0.73	0	10,18,18	0.54	0
2	GAL	d	2	2,3	11,11,12	0.30	0	15,15,17	0.78	0
2	FRU	e	1	2	11,12,12	0.88	1 (9%)	10,18,18	0.93	0
2	GAL	e	2	2,3	11,11,12	0.70	0	15,15,17	1.94	2 (13%)
2	FRU	f	1	2	11,12,12	0.60	0	10,18,18	0.58	0
2	GAL	f	2	2,3	11,11,12	0.42	0	15,15,17	1.11	1 (6%)
2	FRU	g	1	2	11,12,12	1.03	1 (9%)	10,18,18	1.13	1 (10%)
2	GAL	g	2	2	11,11,12	0.68	0	15,15,17	2.04	7 (46%)
2	FRU	h	1	2	11,12,12	0.59	0	10,18,18	0.95	0
2	GAL	h	2	2,3	11,11,12	0.58	0	15,15,17	1.29	1 (6%)
2	FRU	i	1	2	11,12,12	0.60	0	10,18,18	0.86	0
2	GAL	i	2	2,3	11,11,12	0.40	0	15,15,17	1.21	1 (6%)
2	FRU	j	1	2	11,12,12	0.74	1 (9%)	10,18,18	0.84	0
2	GAL	j	2	2,3	11,11,12	0.51	0	15,15,17	1.14	2 (13%)
2	FRU	k	1	2	11,12,12	0.65	0	10,18,18	0.84	0
2	GAL	k	2	2,3	11,11,12	0.53	0	15,15,17	1.11	1 (6%)
2	FRU	l	1	2	11,12,12	0.61	0	10,18,18	0.81	0
2	GAL	l	2	2,3	11,11,12	0.65	0	15,15,17	1.78	2 (13%)
2	FRU	m	1	2	11,12,12	0.78	0	10,18,18	1.07	0
2	GAL	m	2	2	11,11,12	0.46	0	15,15,17	2.00	4 (26%)
2	FRU	n	1	2	11,12,12	0.70	1 (9%)	10,18,18	1.11	0
2	GAL	n	2	2,3	11,11,12	0.41	0	15,15,17	0.75	0
2	FRU	o	1	2	11,12,12	0.64	0	10,18,18	0.96	1 (10%)
2	GAL	o	2	2,3	11,11,12	0.46	0	15,15,17	1.57	1 (6%)
2	FRU	p	1	2	11,12,12	0.67	0	10,18,18	0.78	0
2	GAL	p	2	2,3	11,11,12	0.58	0	15,15,17	1.11	0
2	FRU	q	1	2	11,12,12	0.64	0	10,18,18	0.84	0
2	GAL	q	2	2,3	11,11,12	0.40	0	15,15,17	2.18	1 (6%)
2	FRU	r	1	2	11,12,12	0.51	0	10,18,18	0.95	0
2	GAL	r	2	2,3	11,11,12	0.33	0	15,15,17	1.58	4 (26%)

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	FRU	H	1	2	-	5/5/24/24	0/1/1/1
2	GAL	H	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	I	1	2	-	2/5/24/24	0/1/1/1
2	GAL	I	2	2,3	-	1/2/19/22	0/1/1/1
2	FRU	J	1	2	-	4/5/24/24	0/1/1/1
2	GAL	J	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	K	1	2	-	2/5/24/24	0/1/1/1
2	GAL	K	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	L	1	2	-	3/5/24/24	0/1/1/1
2	GAL	L	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	M	1	2	-	0/5/24/24	0/1/1/1
2	GAL	M	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	N	1	2	-	3/5/24/24	0/1/1/1
2	GAL	N	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	O	1	2	-	3/5/24/24	0/1/1/1
2	GAL	O	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	P	1	2	-	3/5/24/24	0/1/1/1
2	GAL	P	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	Q	1	2	-	3/5/24/24	0/1/1/1
2	GAL	Q	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	R	1	2	-	3/5/24/24	0/1/1/1
2	GAL	R	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	S	1	2	-	0/5/24/24	0/1/1/1
2	GAL	S	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	T	1	2	-	4/5/24/24	0/1/1/1
2	GAL	T	2	2,3	-	1/2/19/22	0/1/1/1
2	FRU	U	1	2	-	3/5/24/24	0/1/1/1
2	GAL	U	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	V	1	2	-	4/5/24/24	0/1/1/1
2	GAL	V	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	W	1	2	-	3/5/24/24	0/1/1/1
2	GAL	W	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	X	1	2	-	5/5/24/24	0/1/1/1
2	GAL	X	2	2,3	-	1/2/19/22	0/1/1/1
2	FRU	Y	1	2	-	2/5/24/24	0/1/1/1
2	GAL	Y	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	Z	1	2	-	2/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	Z	2	2,3	-	1/2/19/22	0/1/1/1
2	FRU	a	1	2	-	2/5/24/24	0/1/1/1
2	GAL	a	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	b	1	2	-	3/5/24/24	0/1/1/1
2	GAL	b	2	2	-	2/2/19/22	0/1/1/1
2	FRU	c	1	2	-	0/5/24/24	0/1/1/1
2	GAL	c	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	d	1	2	-	1/5/24/24	0/1/1/1
2	GAL	d	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	e	1	2	-	2/5/24/24	0/1/1/1
2	GAL	e	2	2,3	-	1/2/19/22	0/1/1/1
2	FRU	f	1	2	-	3/5/24/24	0/1/1/1
2	GAL	f	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	g	1	2	-	3/5/24/24	0/1/1/1
2	GAL	g	2	2	-	0/2/19/22	0/1/1/1
2	FRU	h	1	2	-	2/5/24/24	0/1/1/1
2	GAL	h	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	i	1	2	-	3/5/24/24	0/1/1/1
2	GAL	i	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	j	1	2	-	3/5/24/24	0/1/1/1
2	GAL	j	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	k	1	2	-	2/5/24/24	0/1/1/1
2	GAL	k	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	l	1	2	-	3/5/24/24	0/1/1/1
2	GAL	l	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	m	1	2	-	2/5/24/24	0/1/1/1
2	GAL	m	2	2	-	0/2/19/22	0/1/1/1
2	FRU	n	1	2	-	2/5/24/24	0/1/1/1
2	GAL	n	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	o	1	2	-	5/5/24/24	0/1/1/1
2	GAL	o	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	p	1	2	-	3/5/24/24	0/1/1/1
2	GAL	p	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	q	1	2	-	5/5/24/24	0/1/1/1
2	GAL	q	2	2,3	-	1/2/19/22	0/1/1/1
2	FRU	r	1	2	-	4/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	r	2	2,3	-	2/2/19/22	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	1	FRU	O2-C2	2.12	1.44	1.40
2	j	1	FRU	O2-C2	2.11	1.44	1.40
2	J	1	FRU	O2-C2	2.09	1.44	1.40
2	g	1	FRU	O5-C2	-2.08	1.40	1.43
2	b	1	FRU	O2-C2	2.08	1.44	1.40

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	2	GAL	C1-O5-C5	-9.71	99.17	112.19
2	q	2	GAL	C1-O5-C5	7.69	122.50	112.19
2	T	2	GAL	C1-O5-C5	6.62	121.06	112.19
2	I	2	GAL	C1-O5-C5	6.46	120.85	112.19
2	a	2	GAL	C1-O5-C5	6.15	120.43	112.19

There are no chirality outliers.

5 of 148 torsion outliers are listed below:

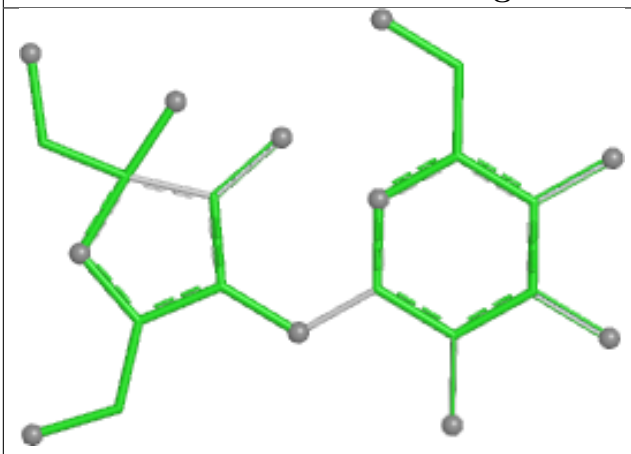
Mol	Chain	Res	Type	Atoms
2	H	1	FRU	O1-C1-C2-C3
2	H	1	FRU	O1-C1-C2-O2
2	H	1	FRU	O1-C1-C2-O5
2	I	1	FRU	O1-C1-C2-O2
2	J	1	FRU	O1-C1-C2-C3

There are no ring outliers.

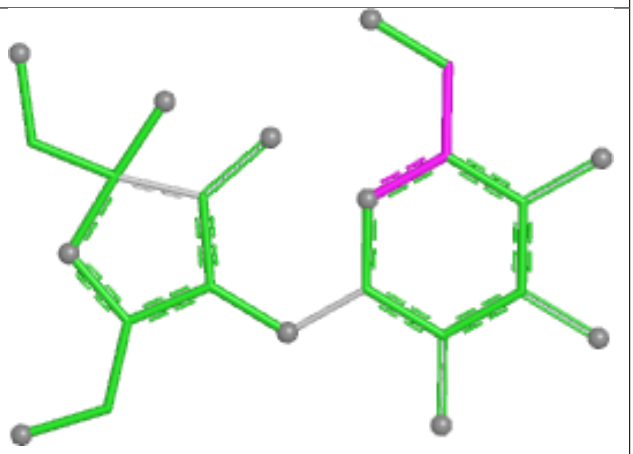
No monomer is involved in short contacts.

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

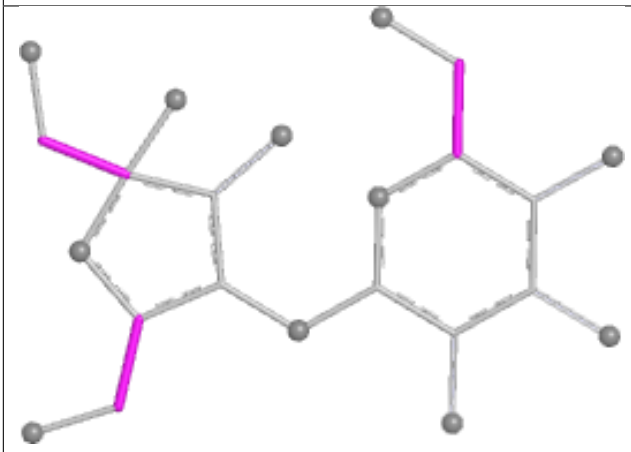
Oligosaccharide Chain H



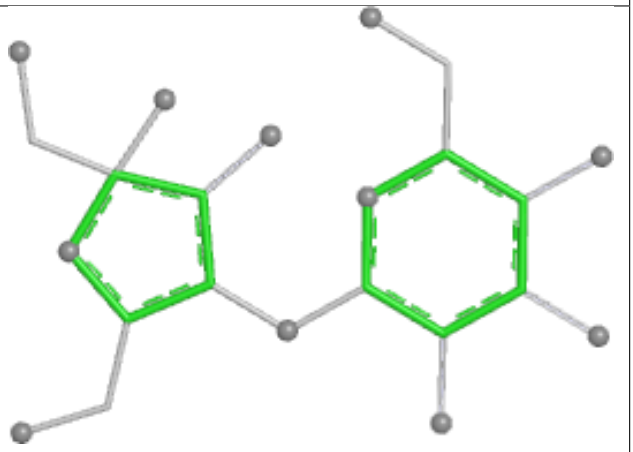
Bond lengths



Bond angles

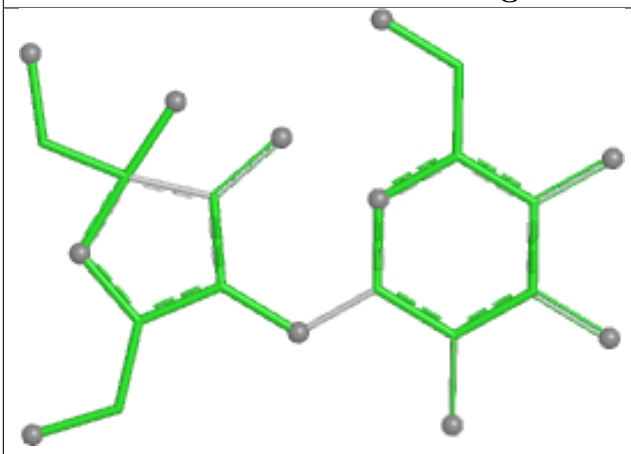


Torsions

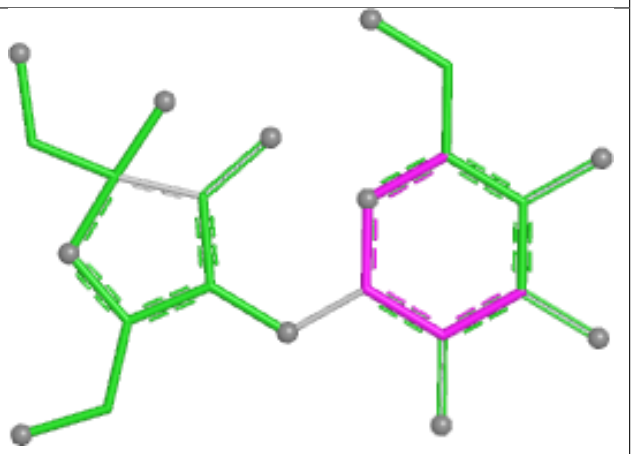


Rings

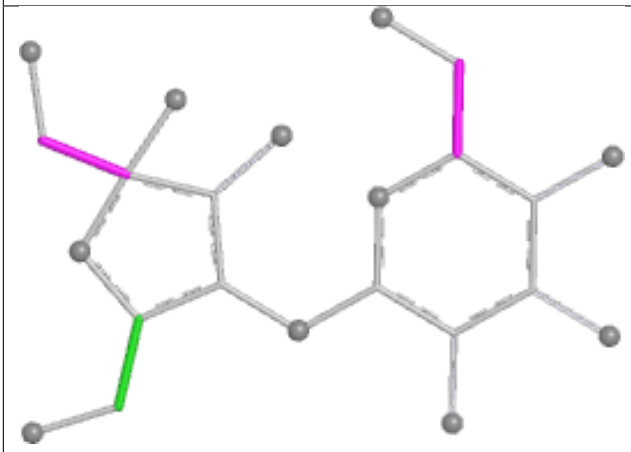
Oligosaccharide Chain I



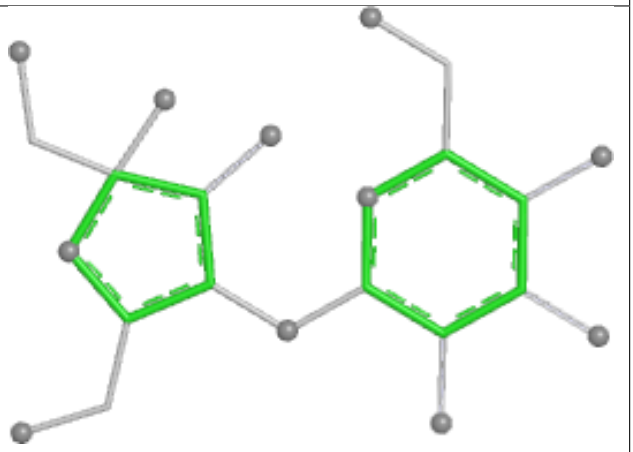
Bond lengths



Bond angles

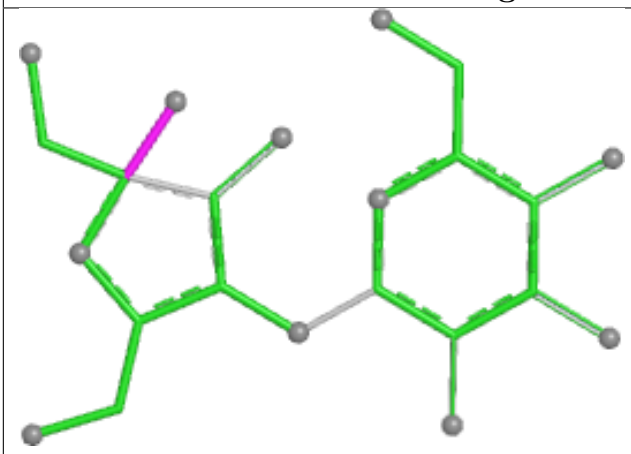


Torsions

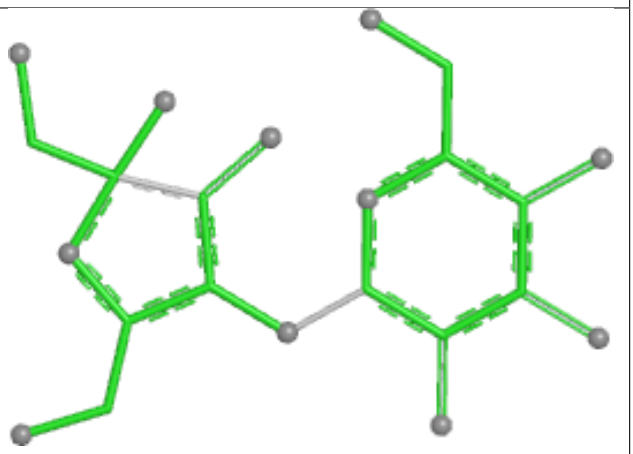


Rings

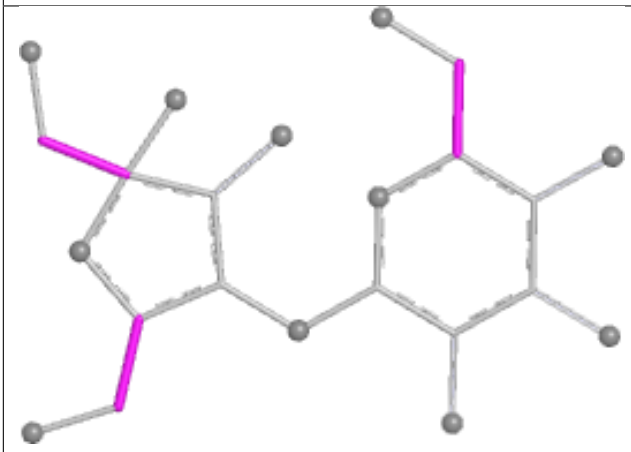
Oligosaccharide Chain J



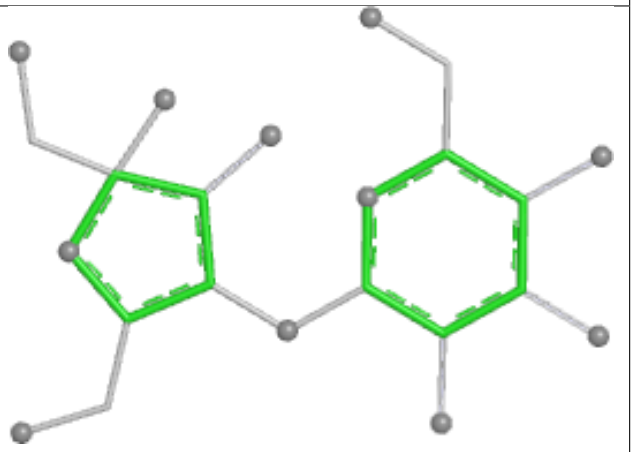
Bond lengths



Bond angles

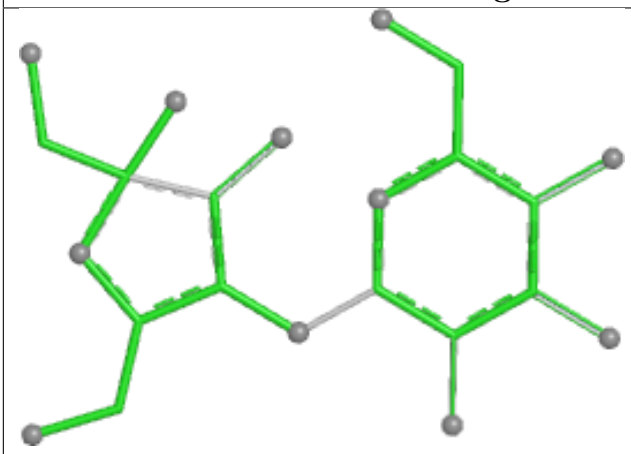


Torsions

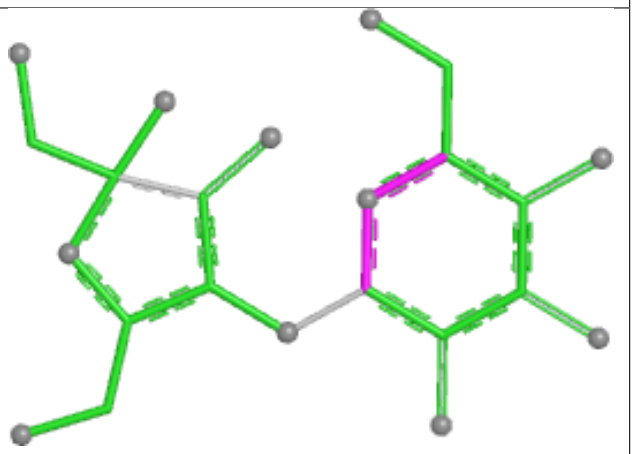


Rings

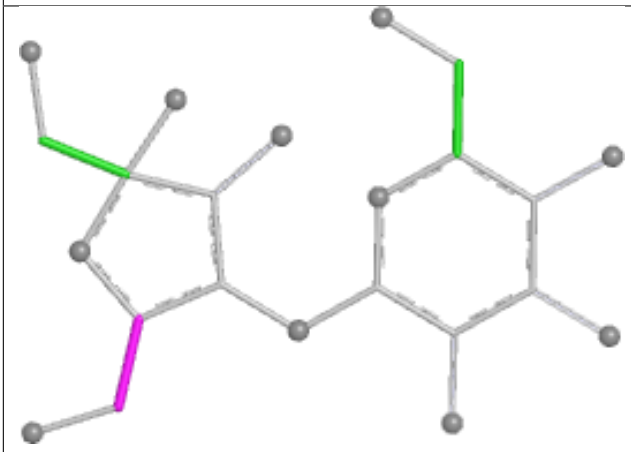
Oligosaccharide Chain K



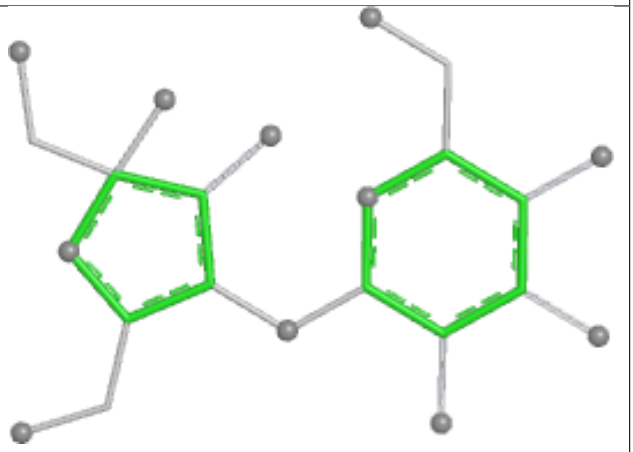
Bond lengths



Bond angles

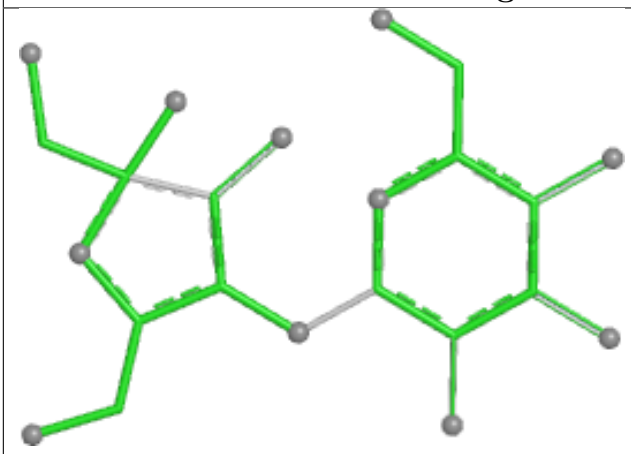


Torsions

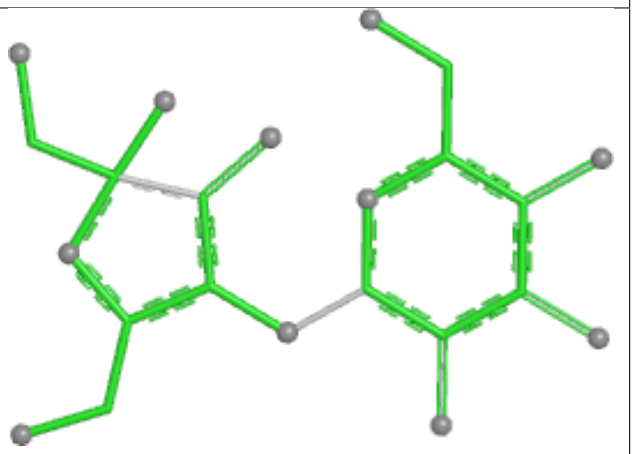


Rings

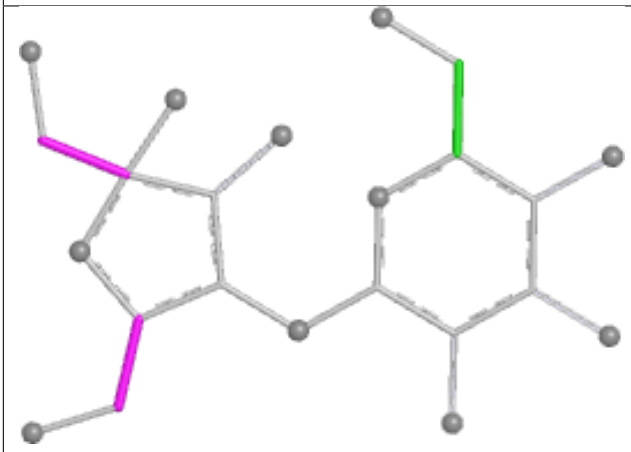
Oligosaccharide Chain L



Bond lengths



Bond angles



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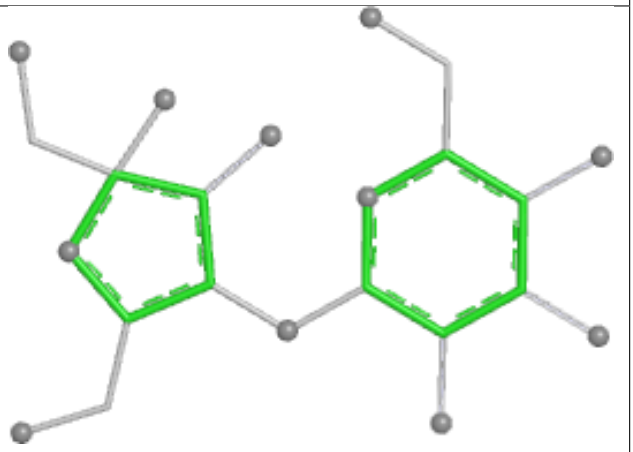
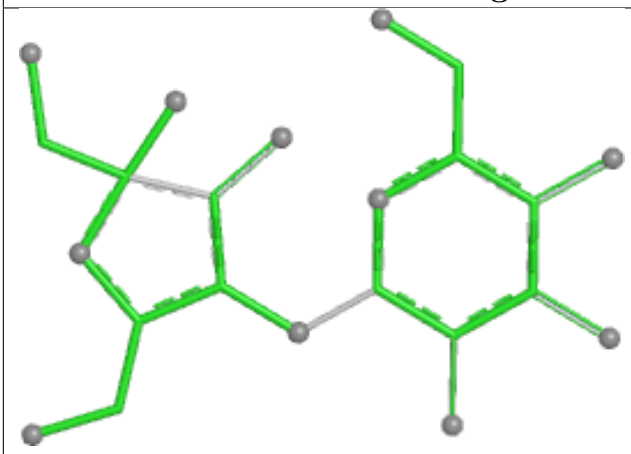


Rings

Oligosaccharide Chain M



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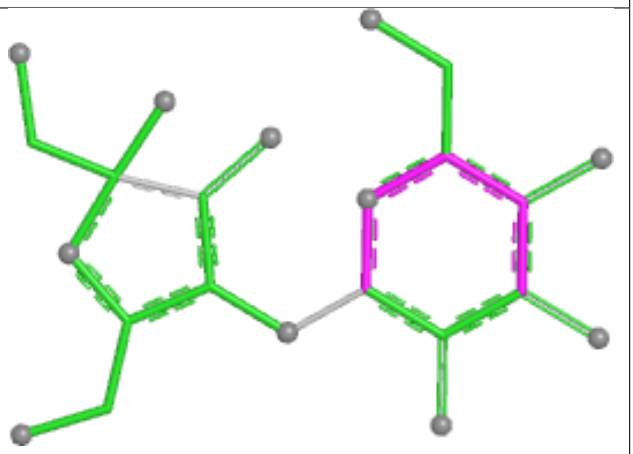

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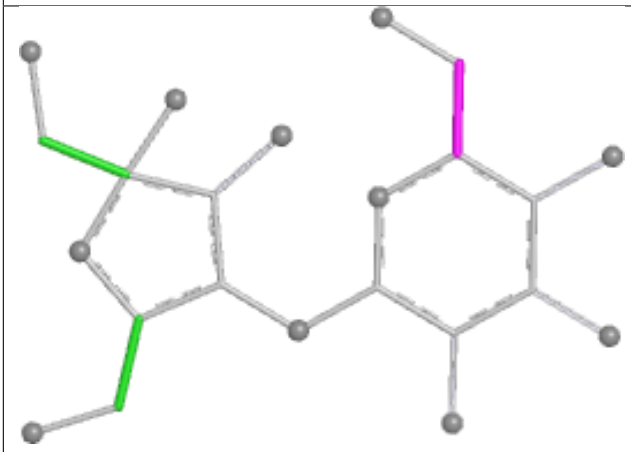

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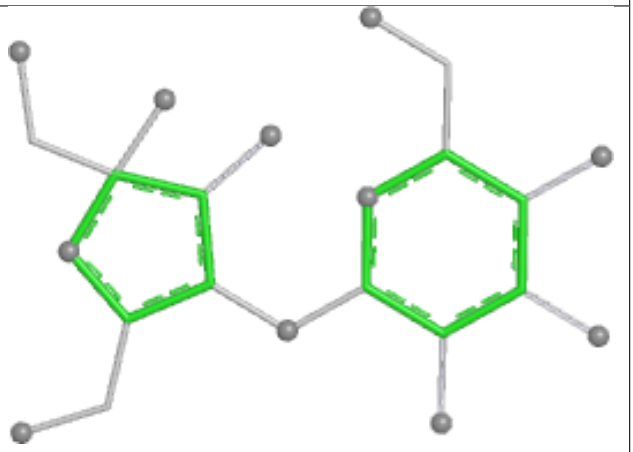
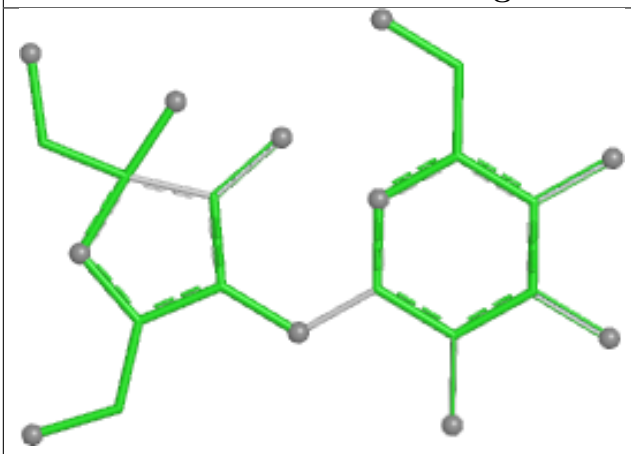
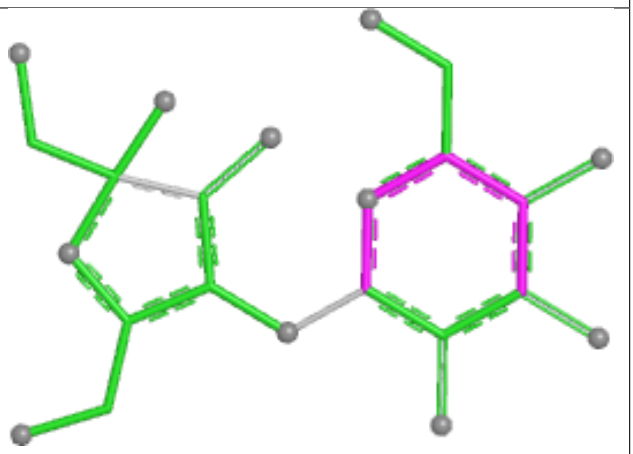


Rings

Oligosaccharide Chain N



Bond lengths



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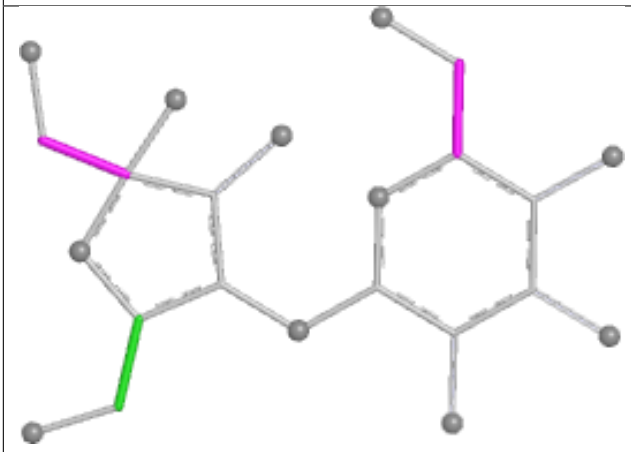

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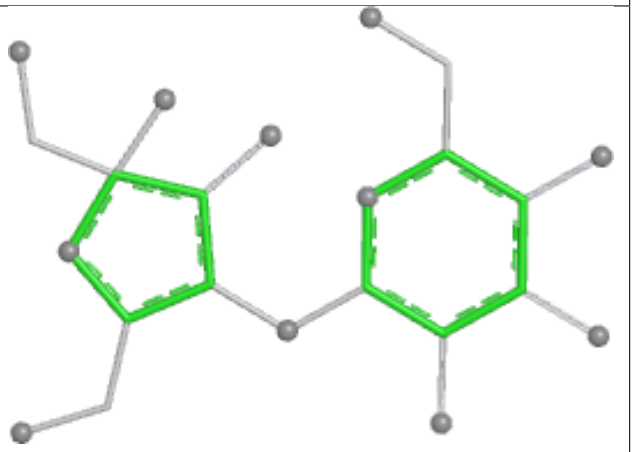
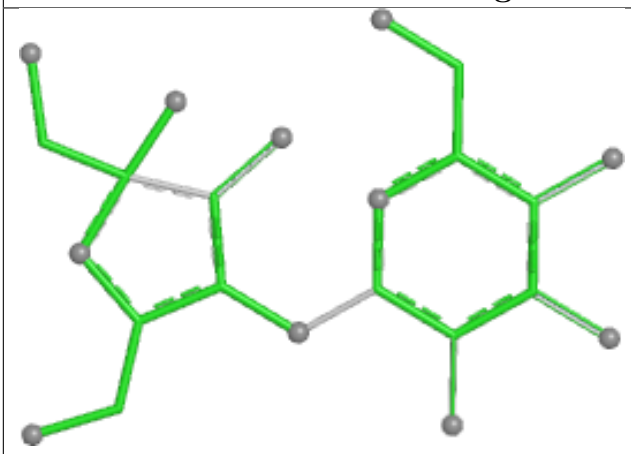


Rings

Oligosaccharide Chain O



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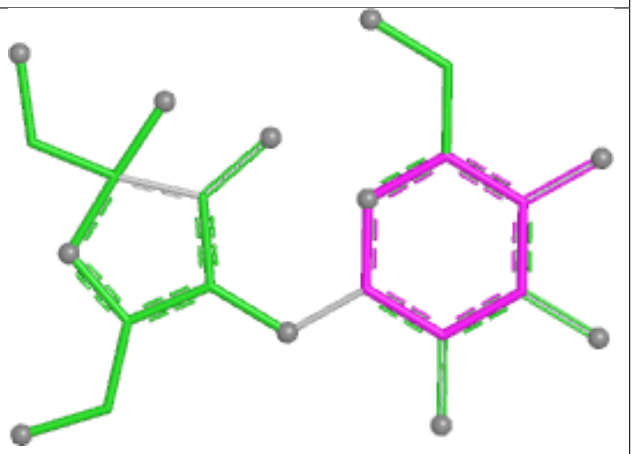
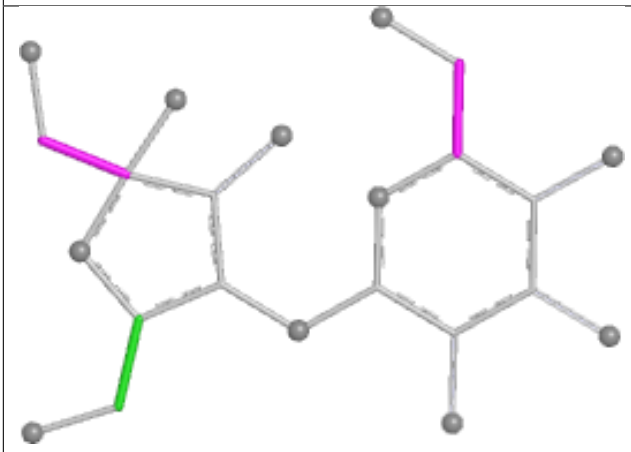


Bond angles



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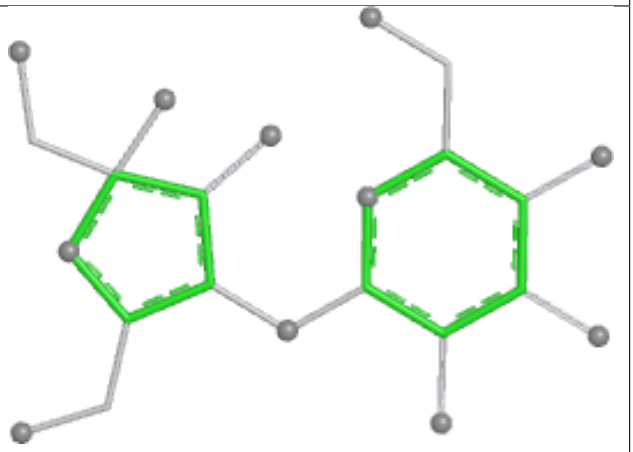
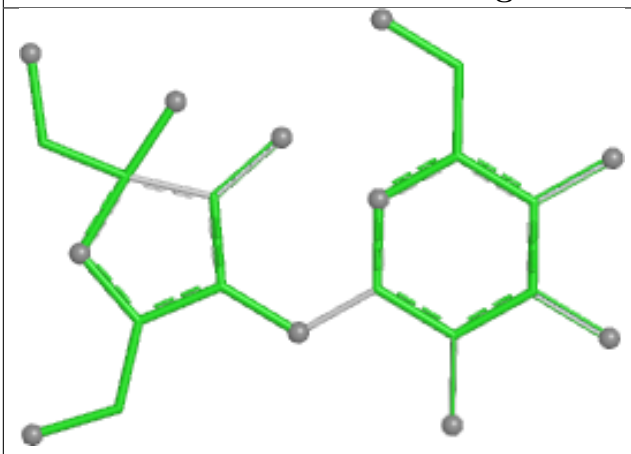
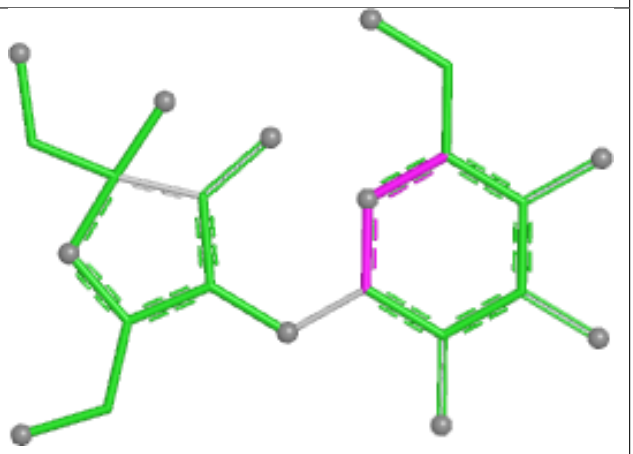


Rings

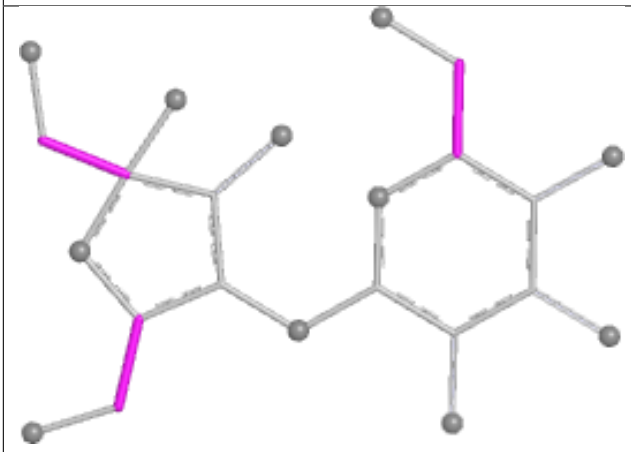
Oligosaccharide Chain P



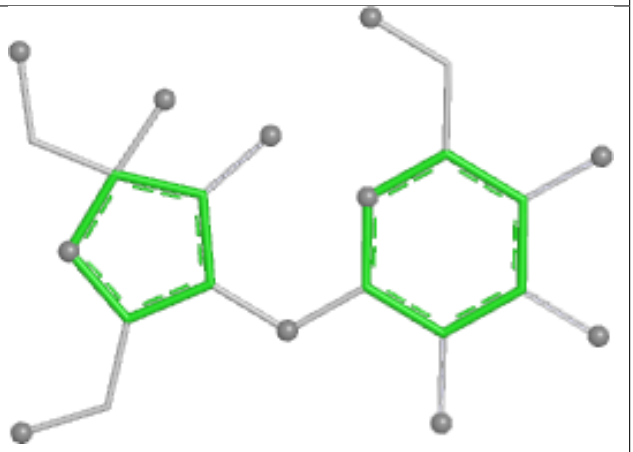
Bond lengths



Bond angles

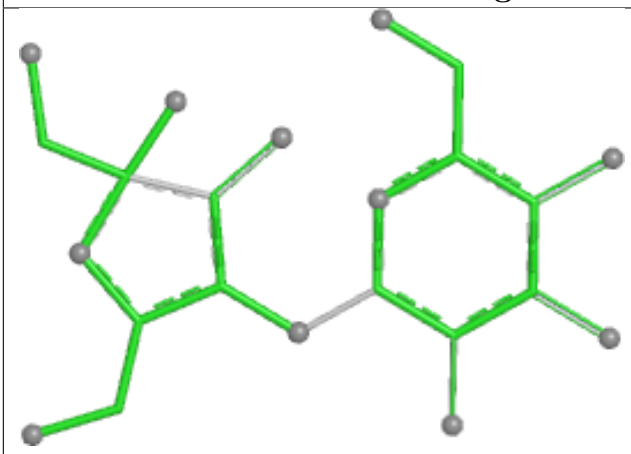


Torsions

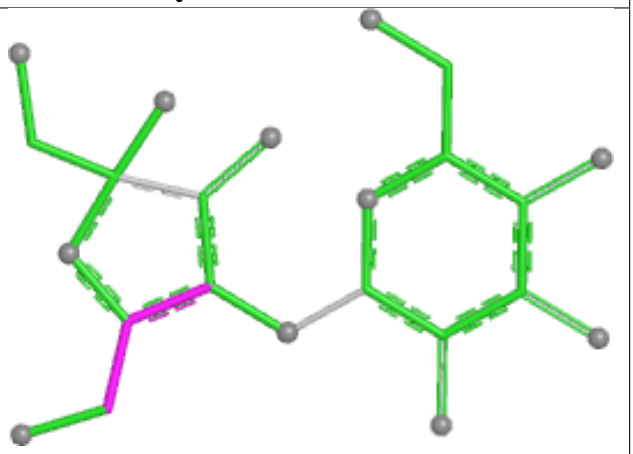


Rings

Oligosaccharide Chain Q



Bond lengths



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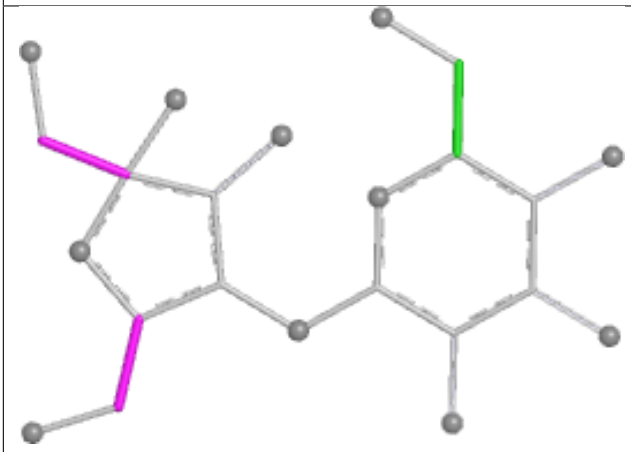
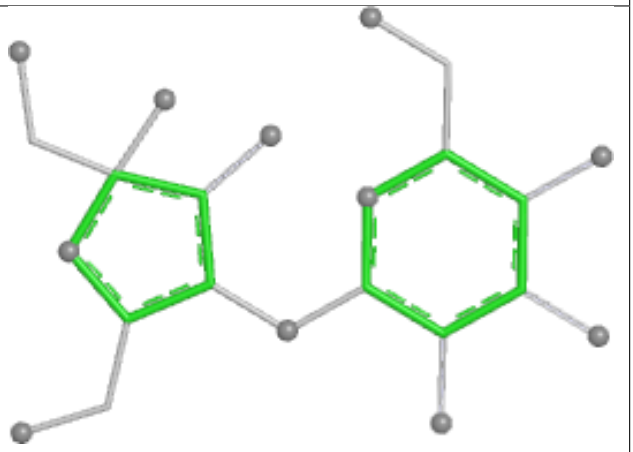
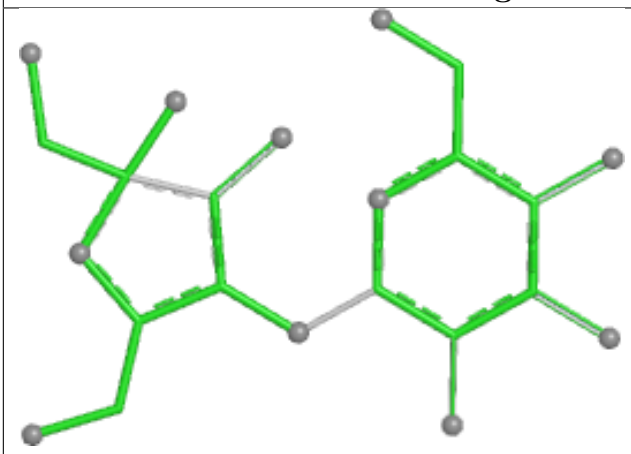


Torsions

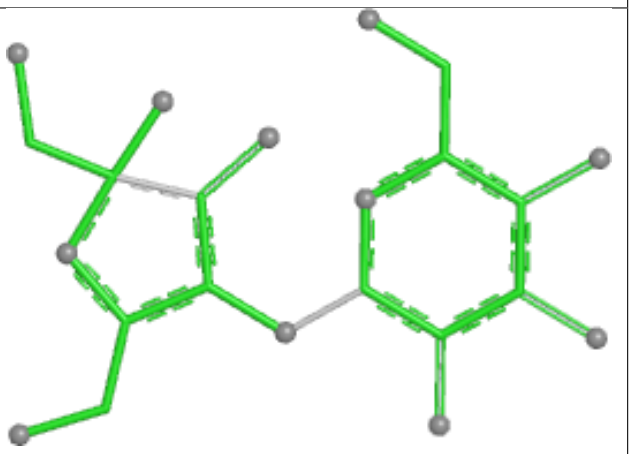


Rings

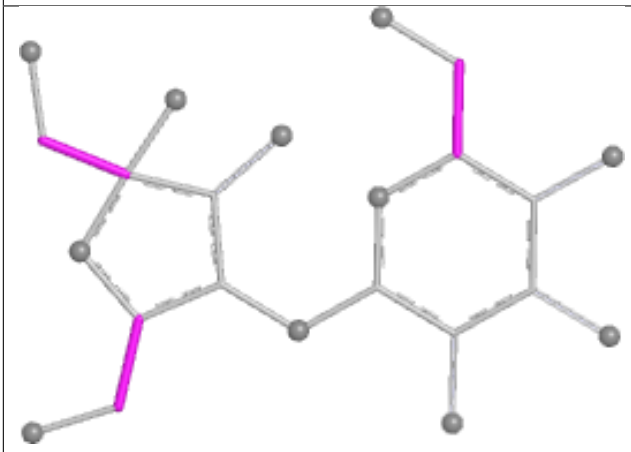
Oligosaccharide Chain R



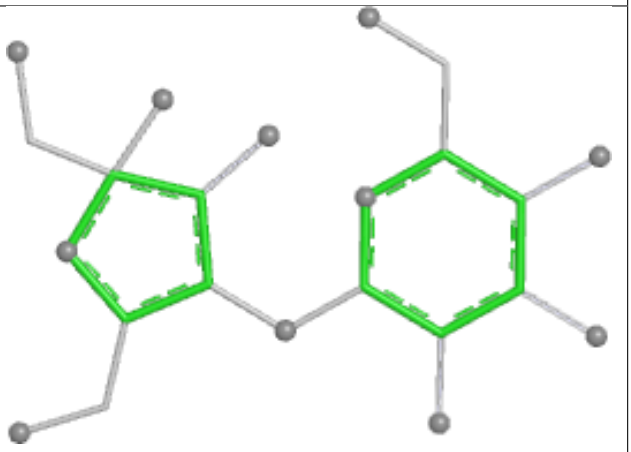
Bond lengths



Bond angles

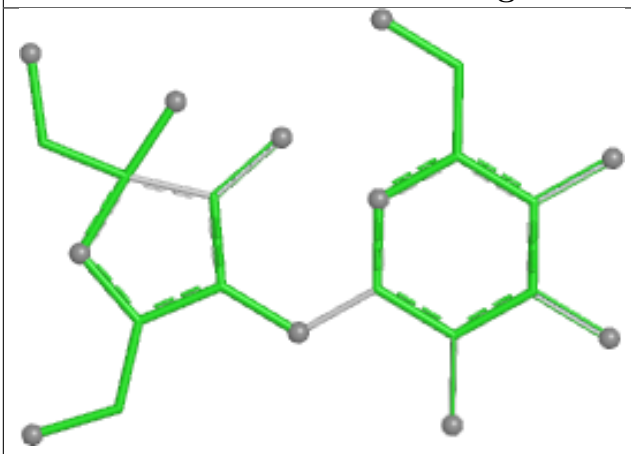


Torsions

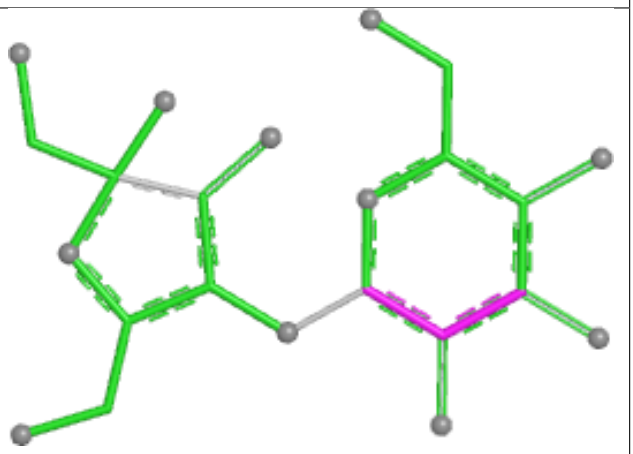


Rings

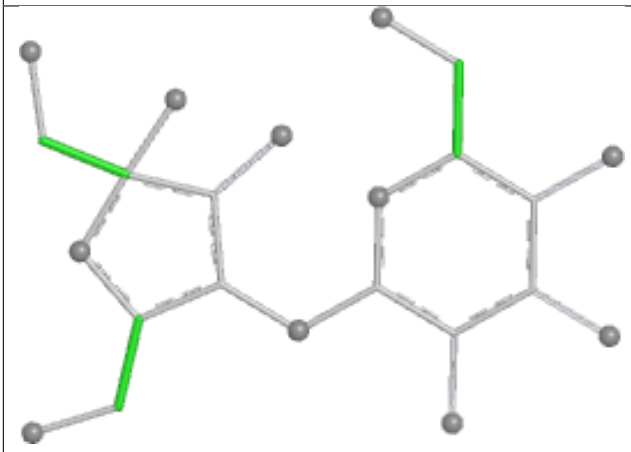
Oligosaccharide Chain S



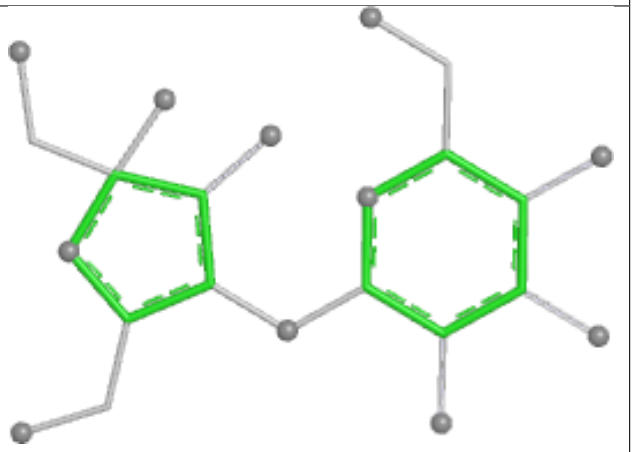
Bond lengths



Bond angles

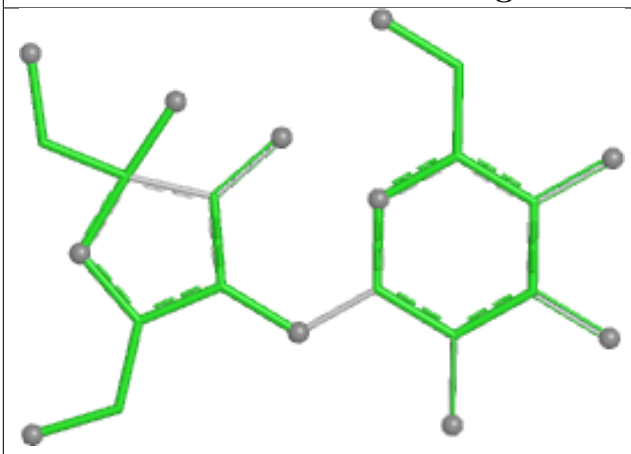


Torsions

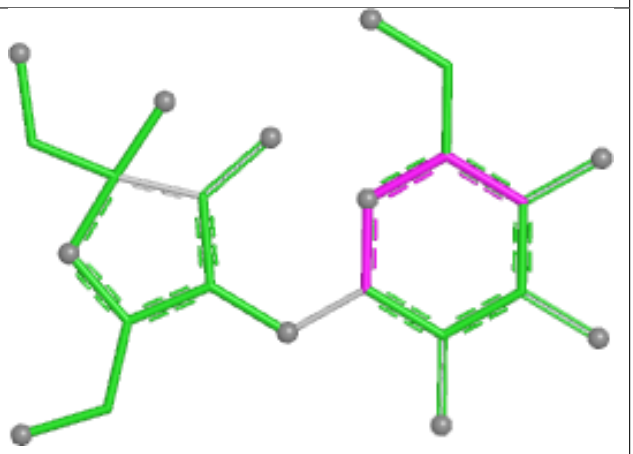


Rings

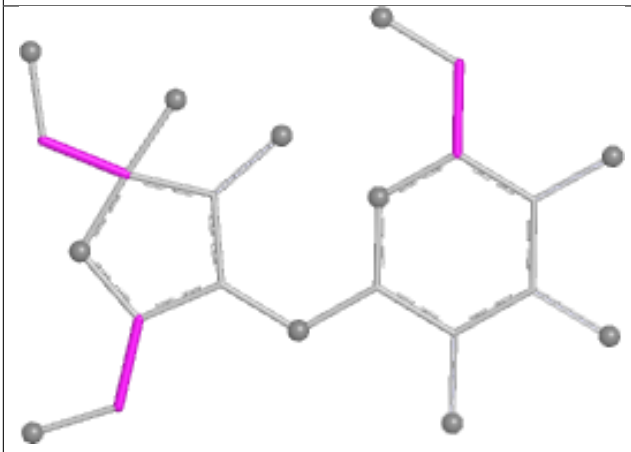
Oligosaccharide Chain T



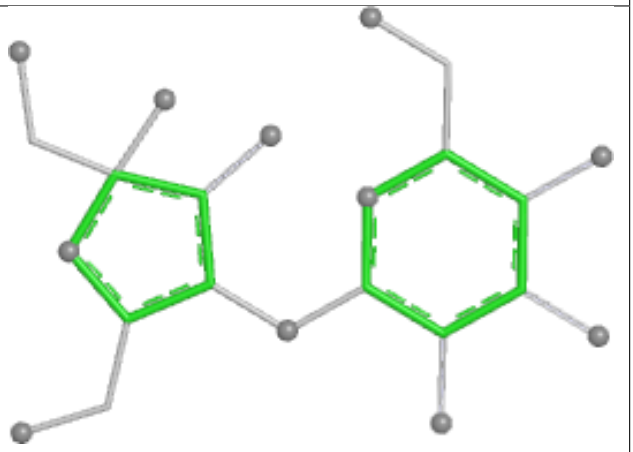
Bond lengths



Bond angles

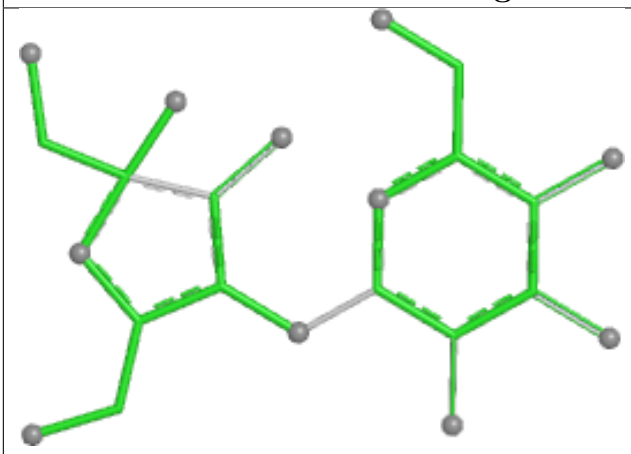


Torsions

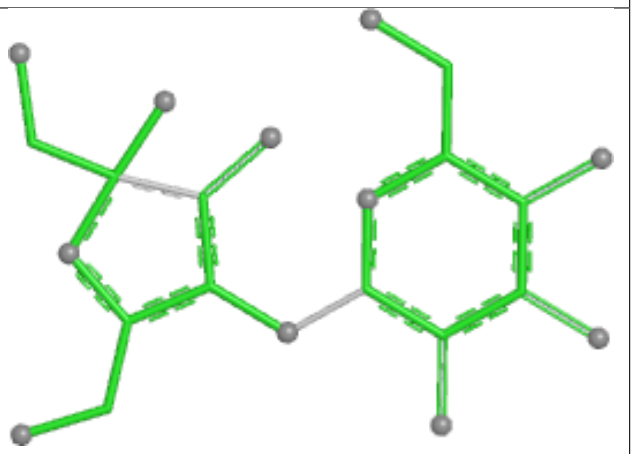


Rings

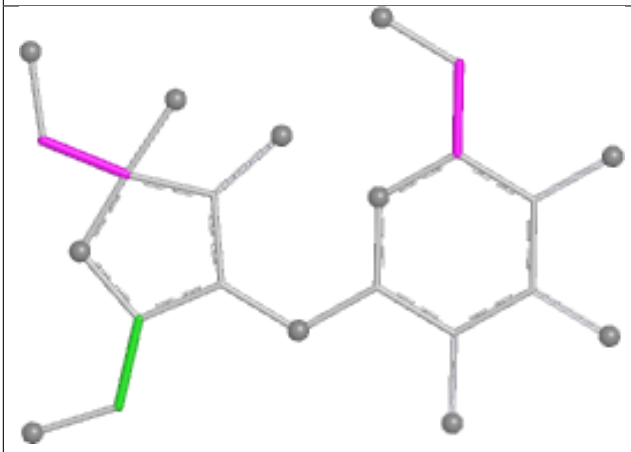
Oligosaccharide Chain U



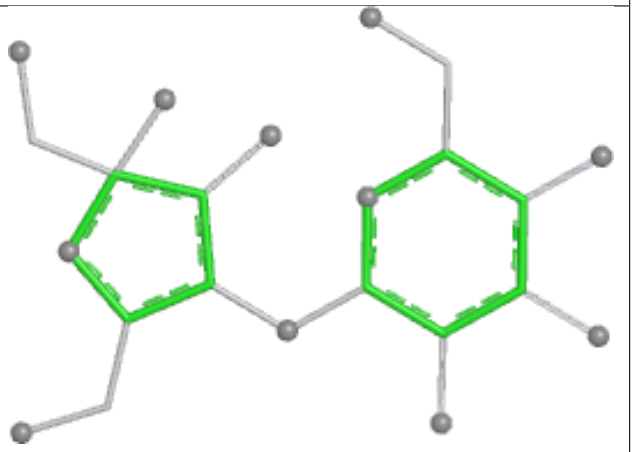
Bond lengths



Bond angles

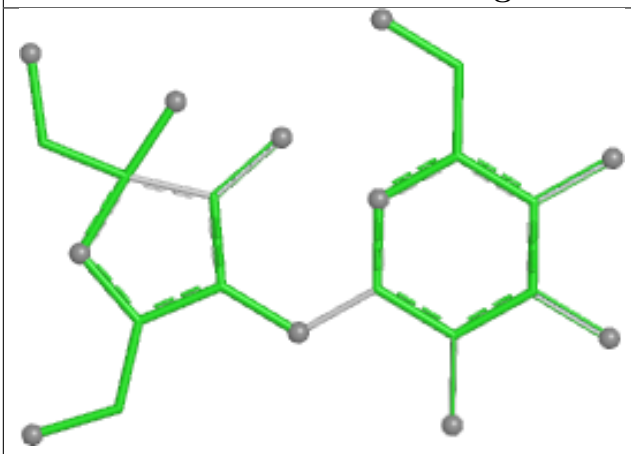


Torsions



Rings

Oligosaccharide Chain V



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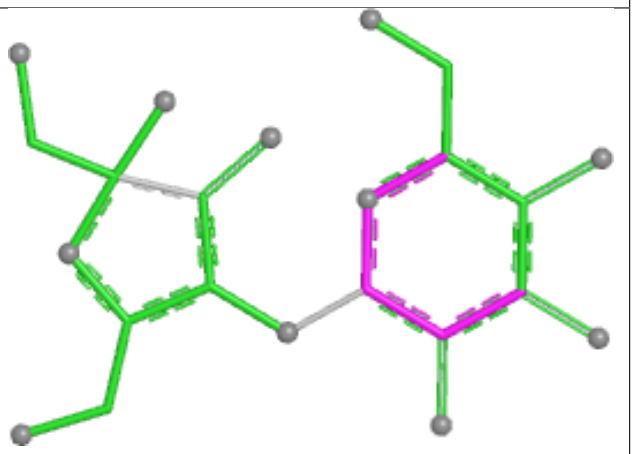

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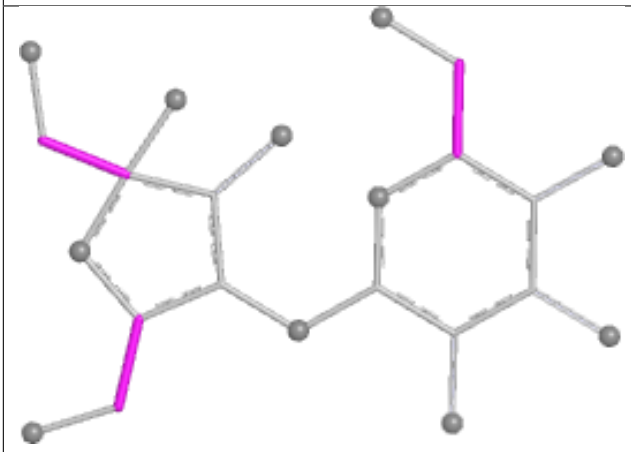

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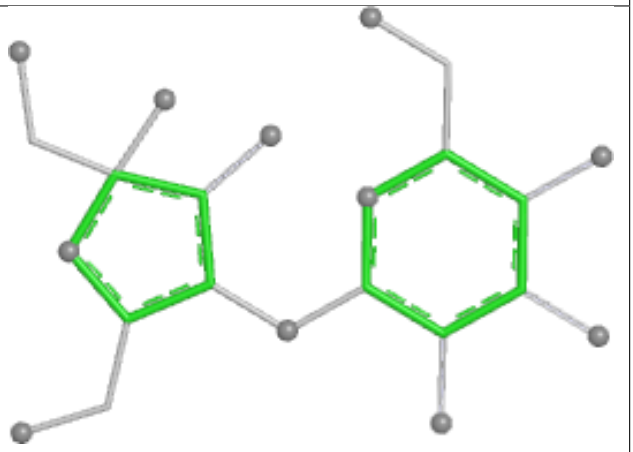
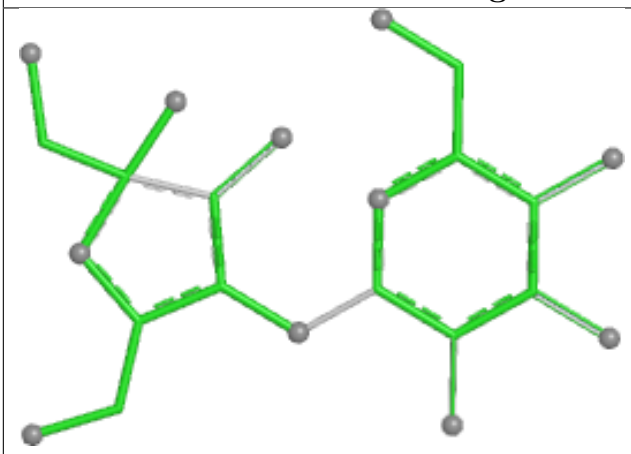


Rings

Oligosaccharide Chain W



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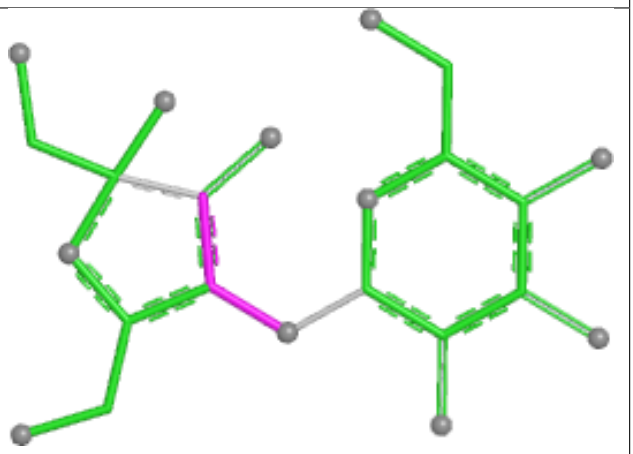
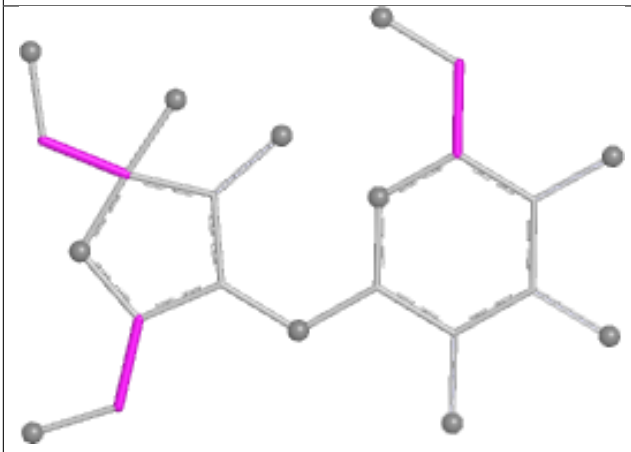


Bond angles



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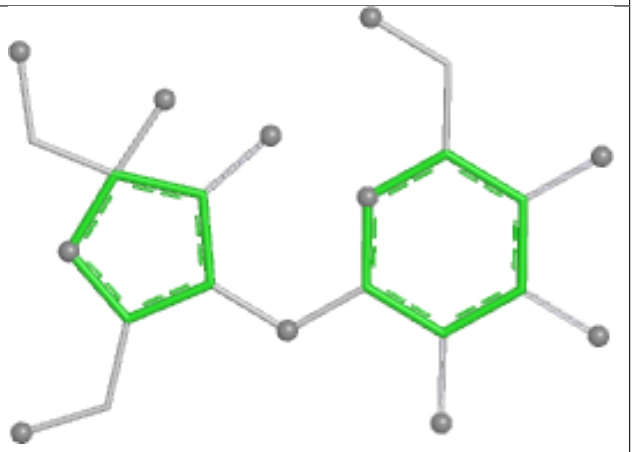
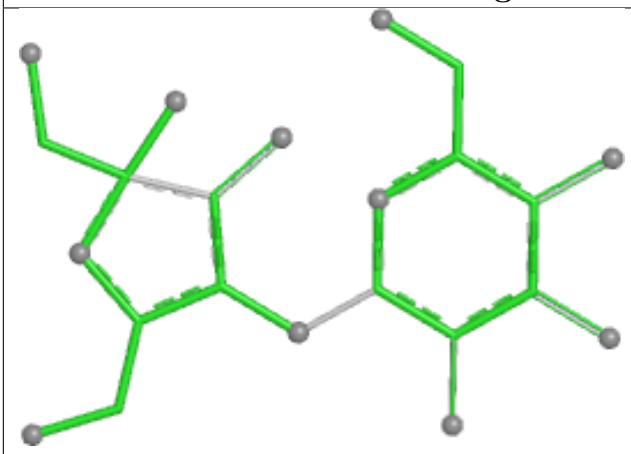


Rings

Oligosaccharide Chain X



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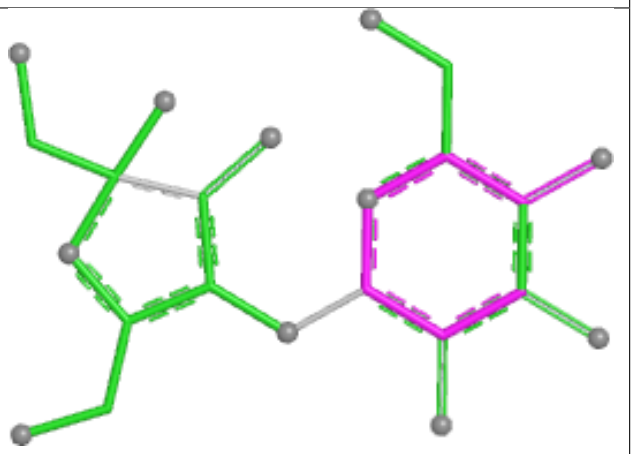
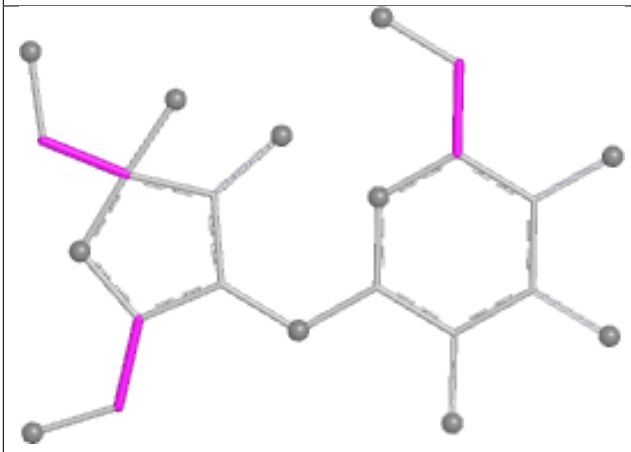


Bond angles



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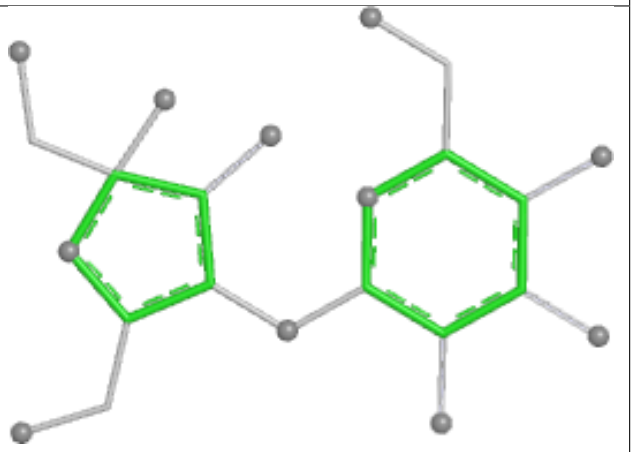
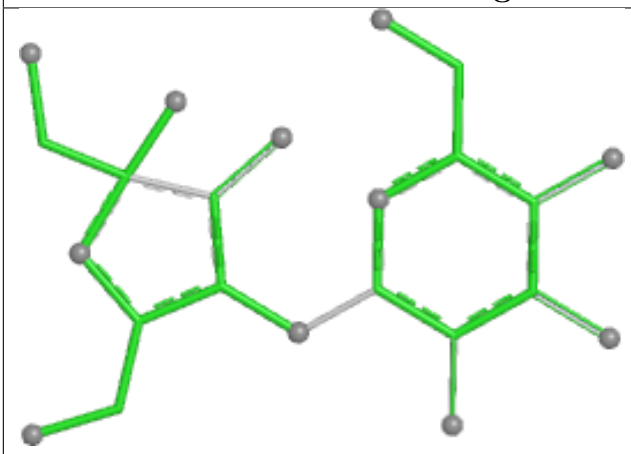


Rings

Oligosaccharide Chain Y



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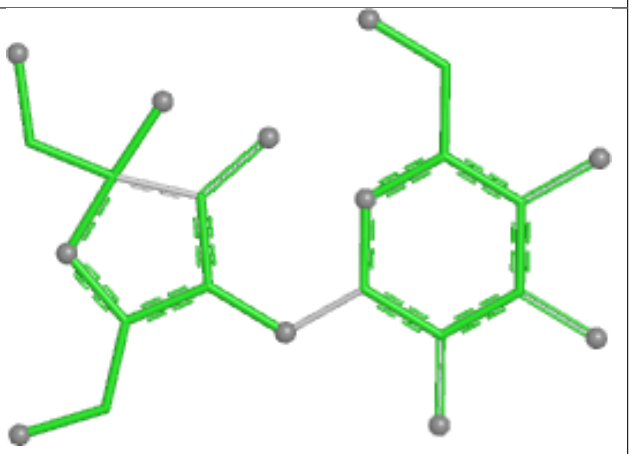
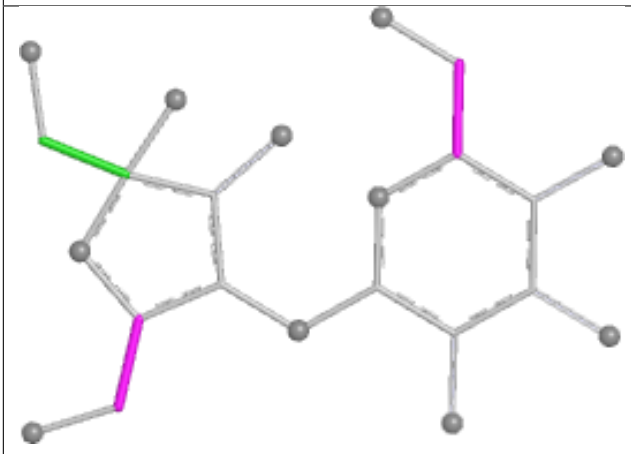


Bond angles



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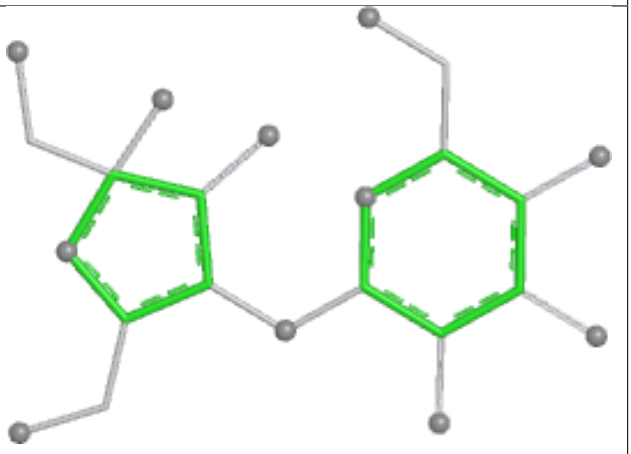
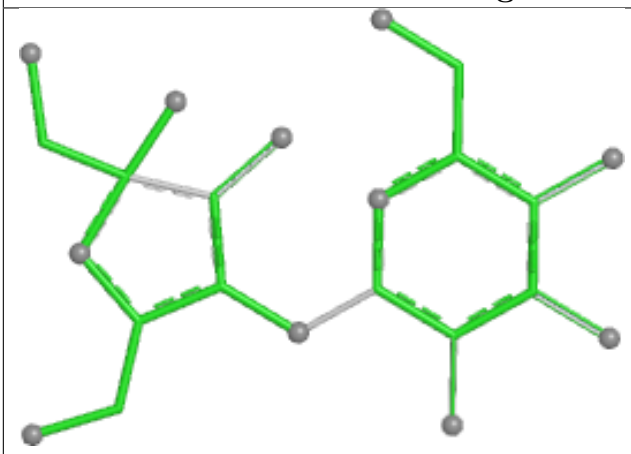


Rings

Oligosaccharide Chain Z



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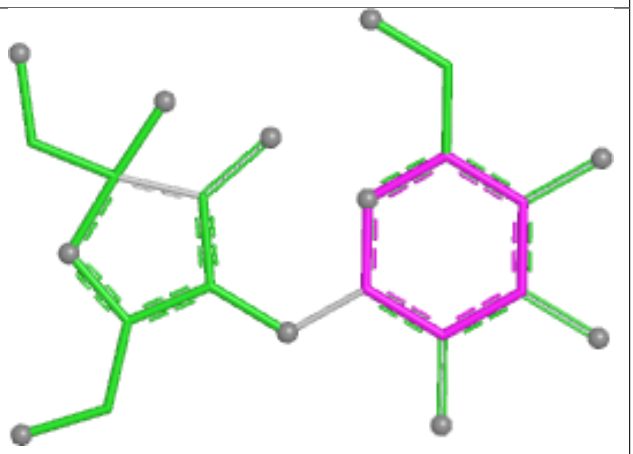
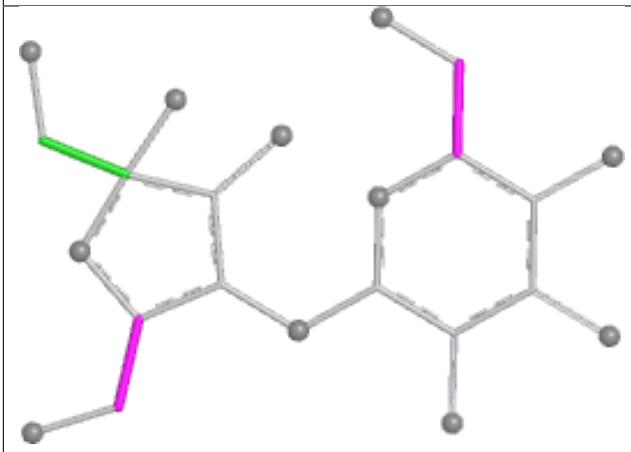


Bond angles



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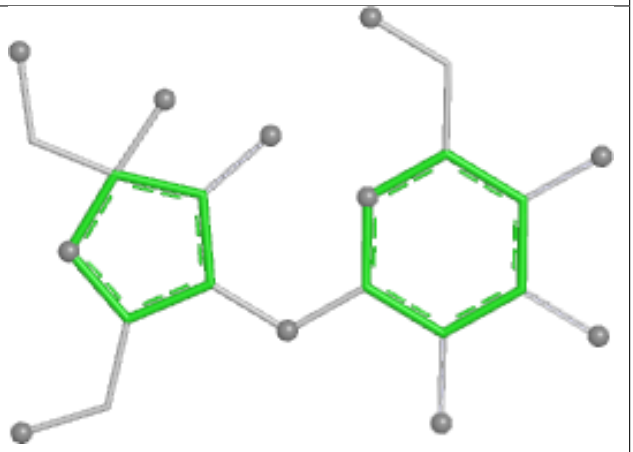
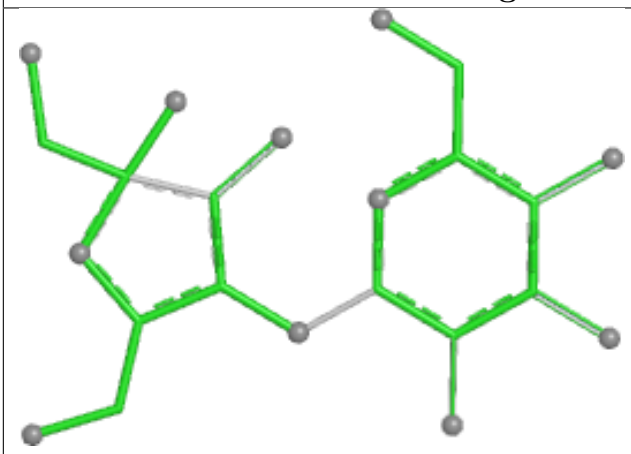


Rings

Oligosaccharide Chain a



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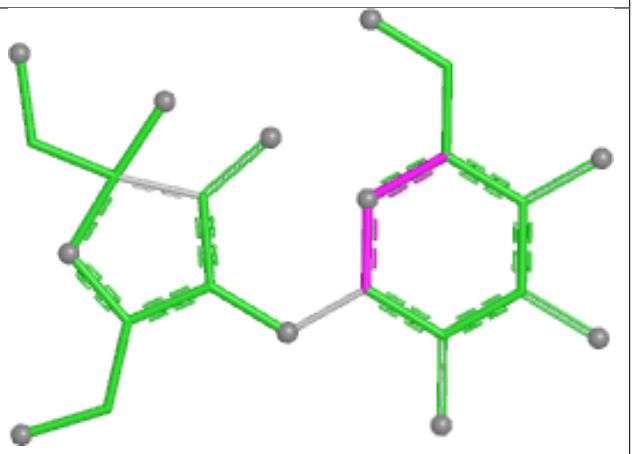
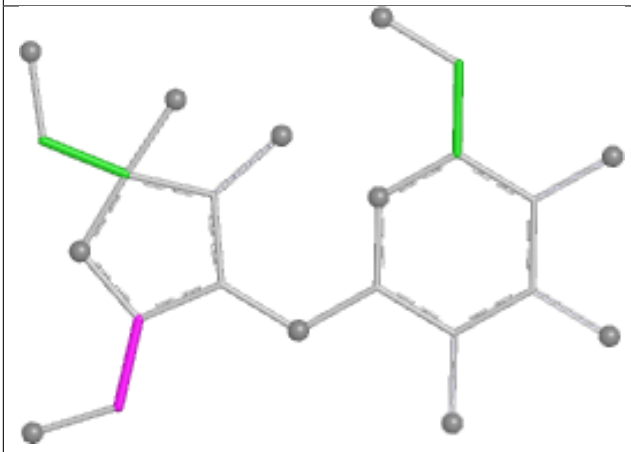


Bond angles



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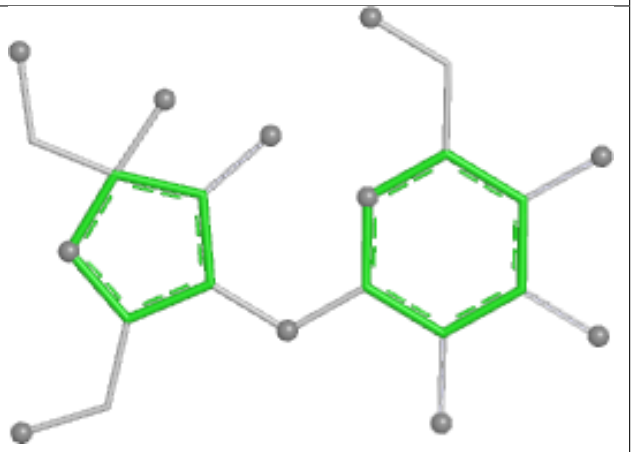
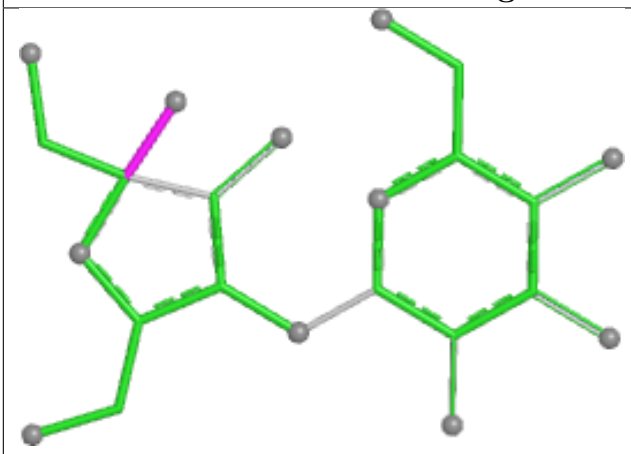


Rings

Oligosaccharide Chain b



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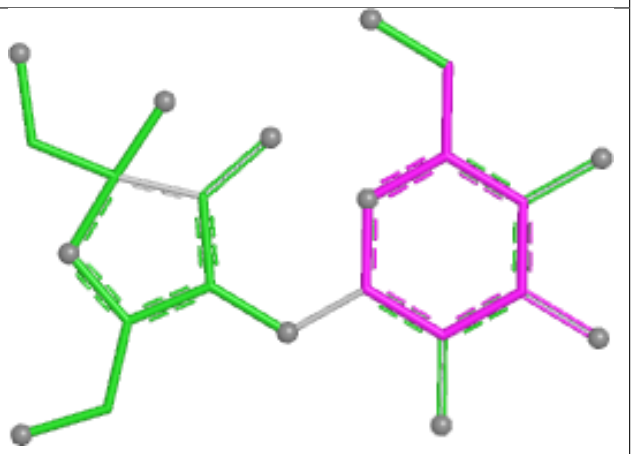
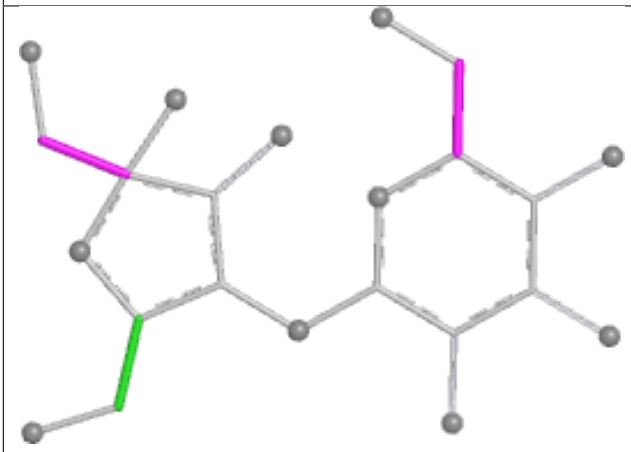
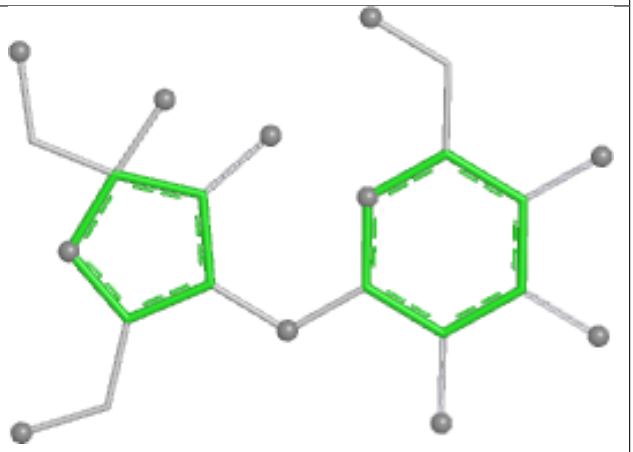


Bond angles

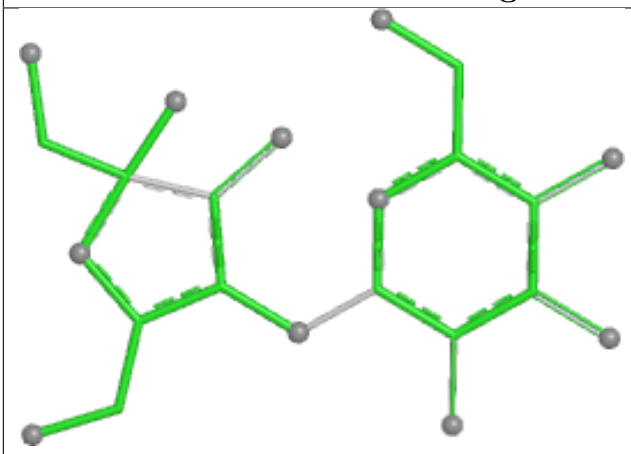


Torsions



Rings

Oligosaccharide Chain c



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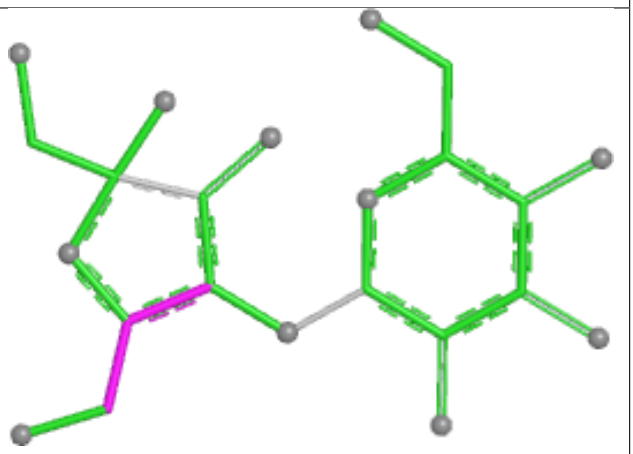
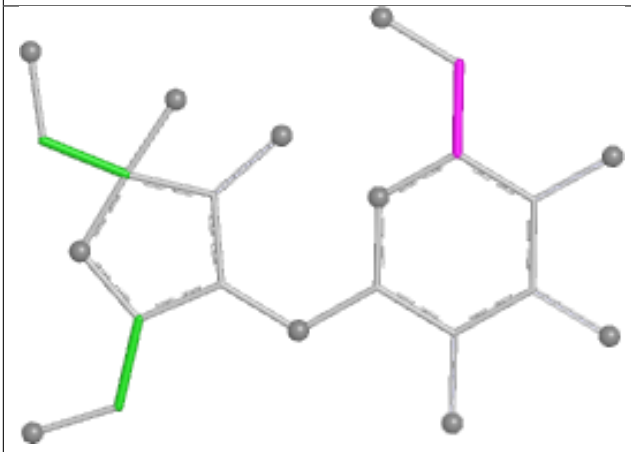
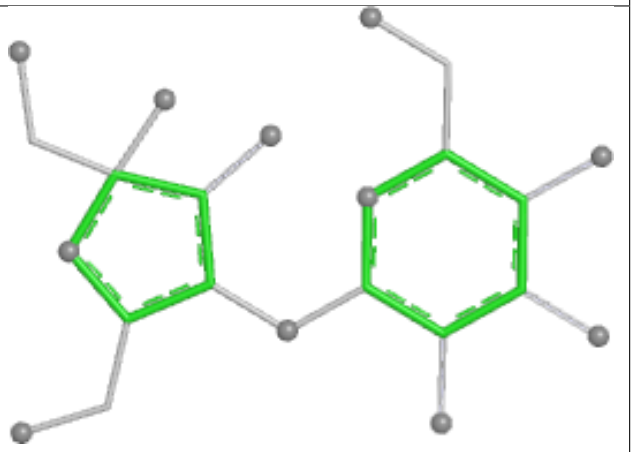


Bond angles

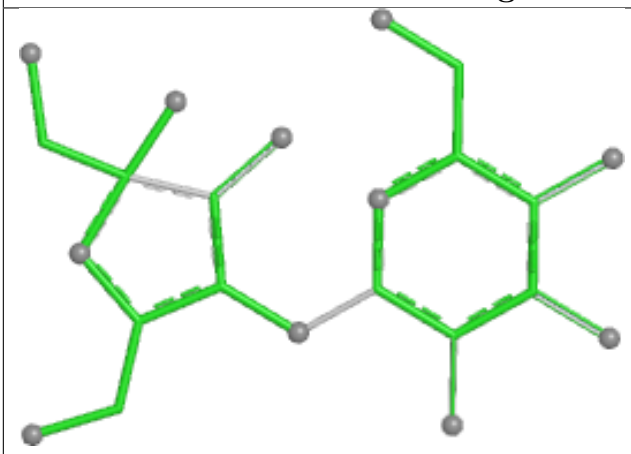


Torsions



Rings

Oligosaccharide Chain d



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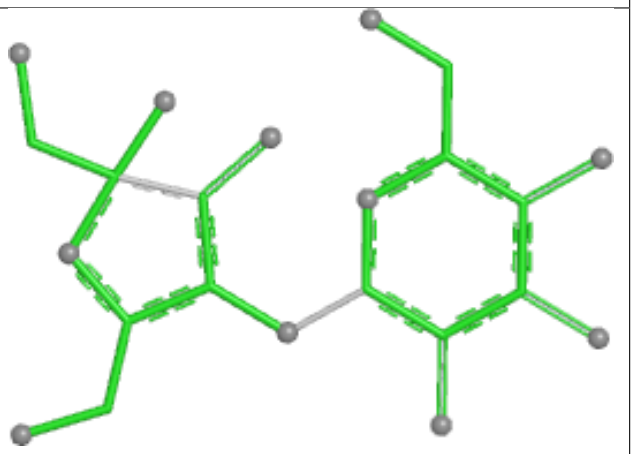

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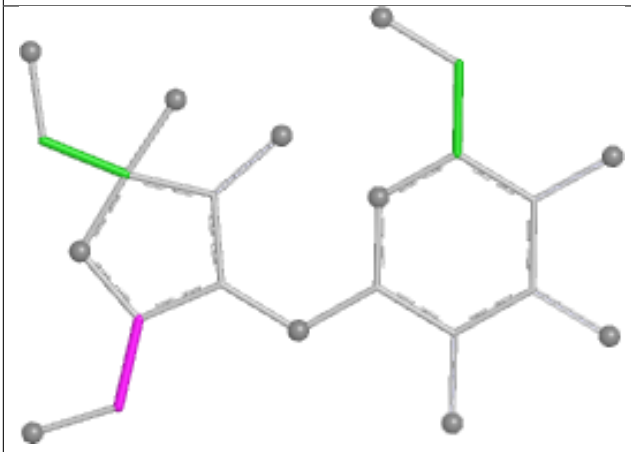
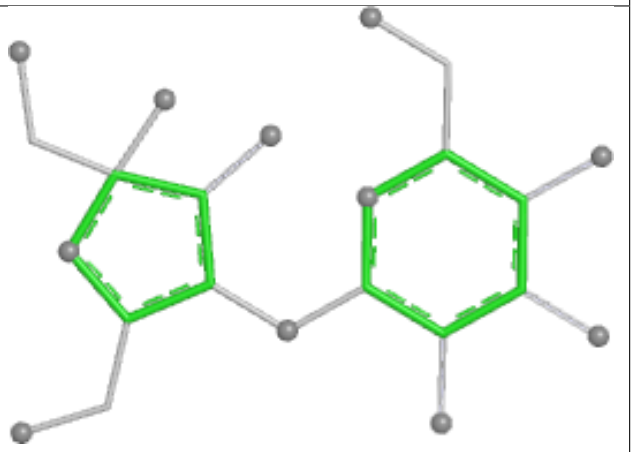
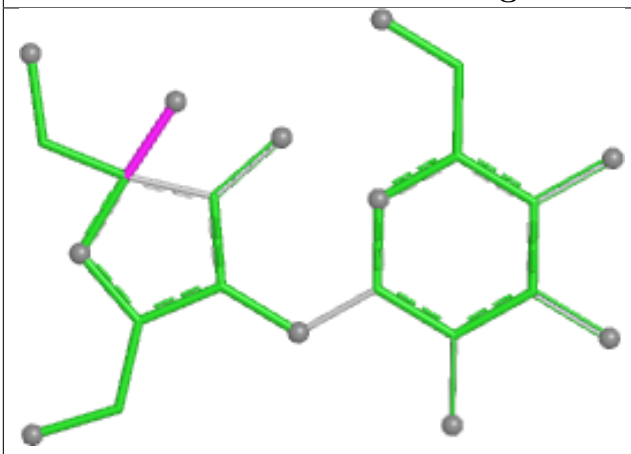


Torsions



Rings

Oligosaccharide Chain e



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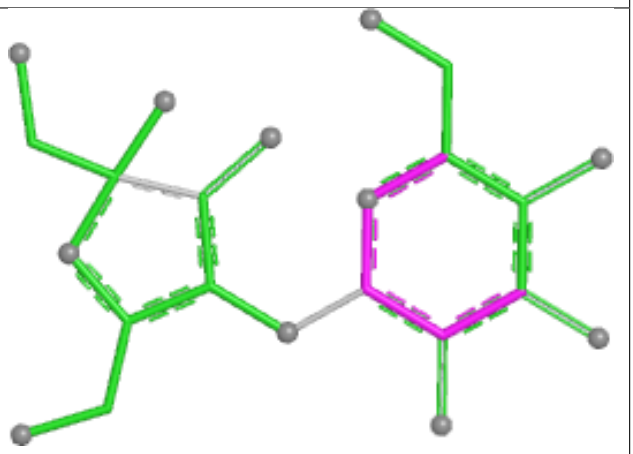
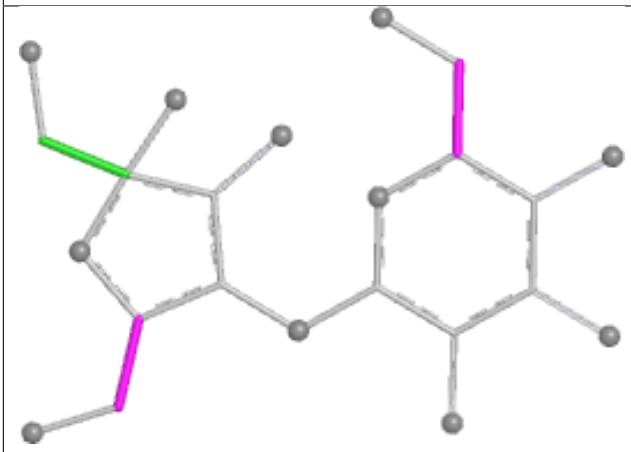
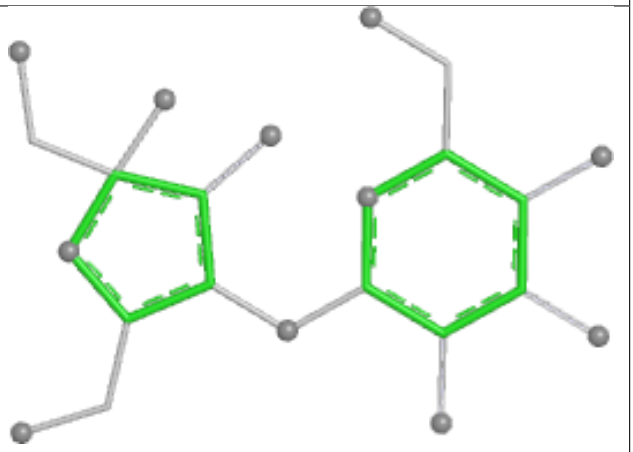


Bond angles

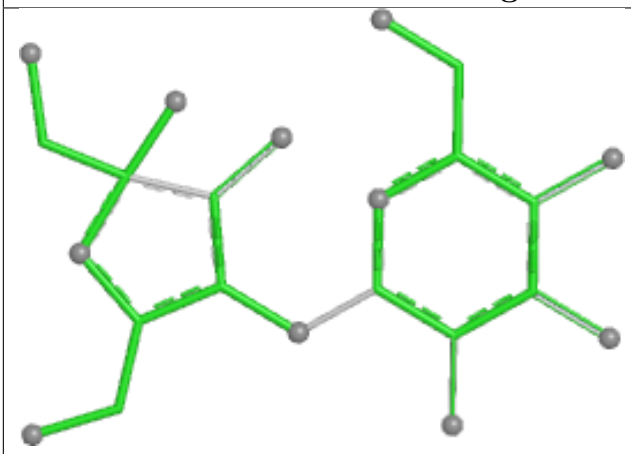


Torsions



Rings

Oligosaccharide Chain f



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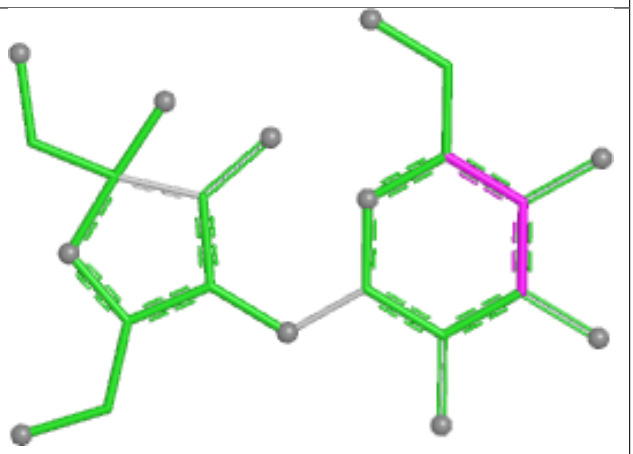
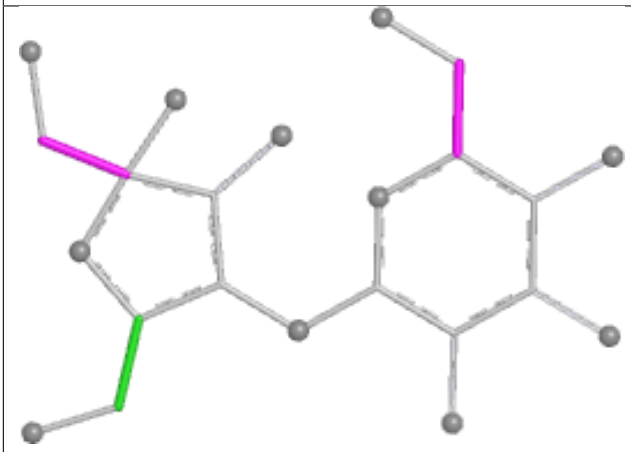
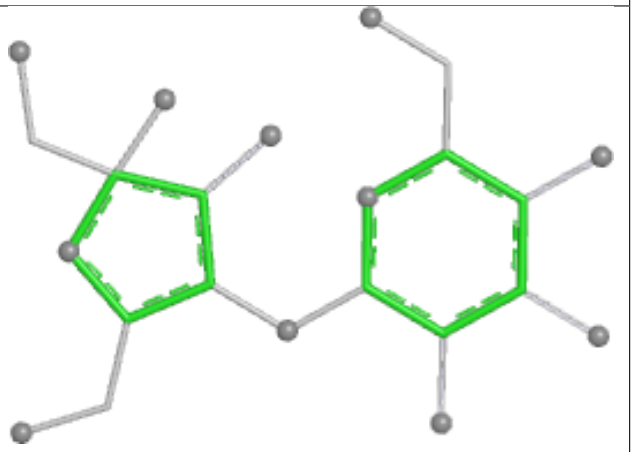


Bond angles

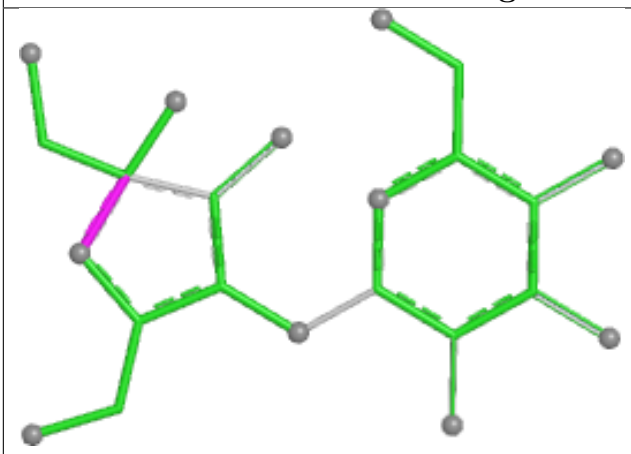


Torsions



Rings

Oligosaccharide Chain g



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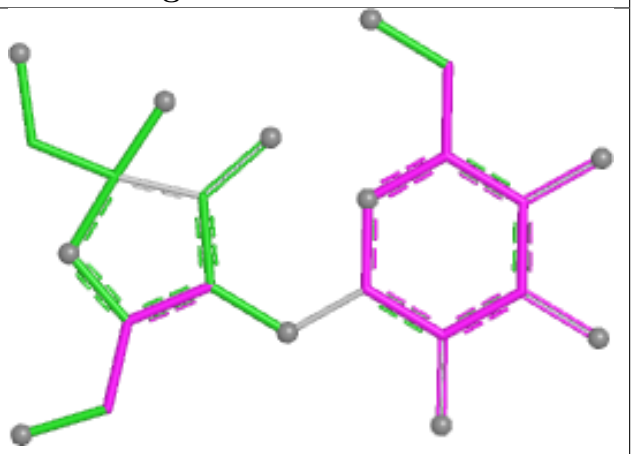
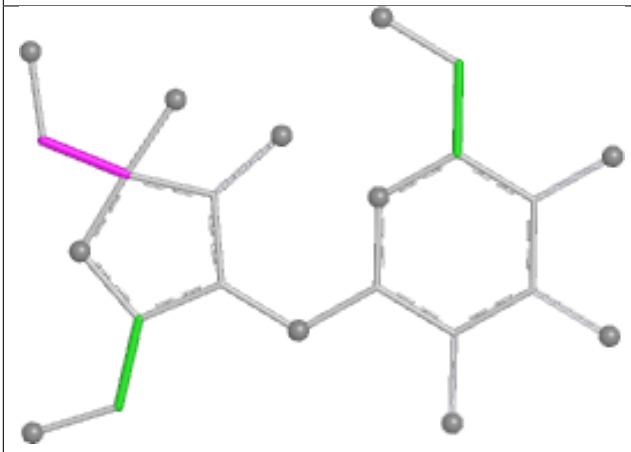
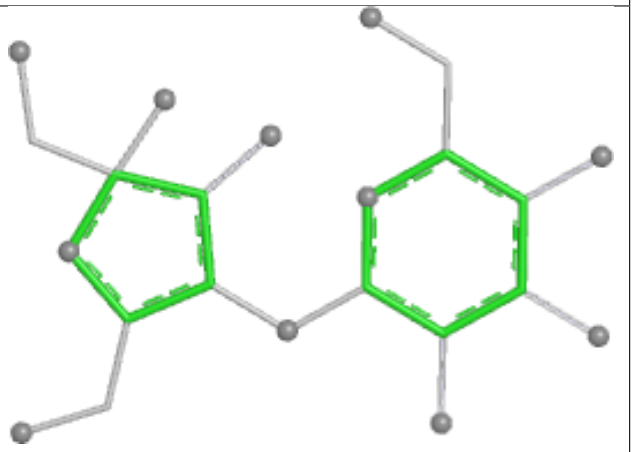


Bond angles

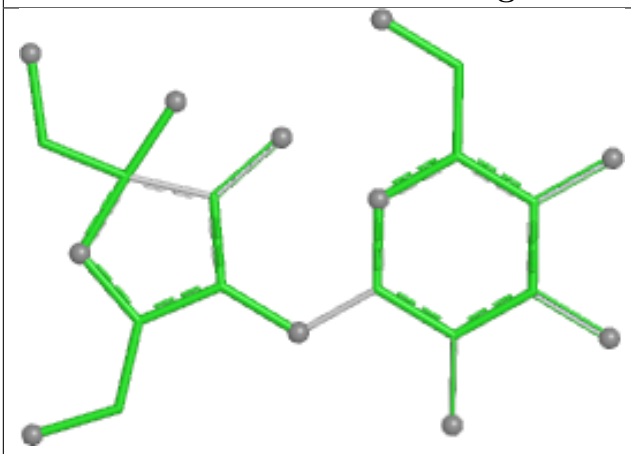


Torsions



Rings

Oligosaccharide Chain h



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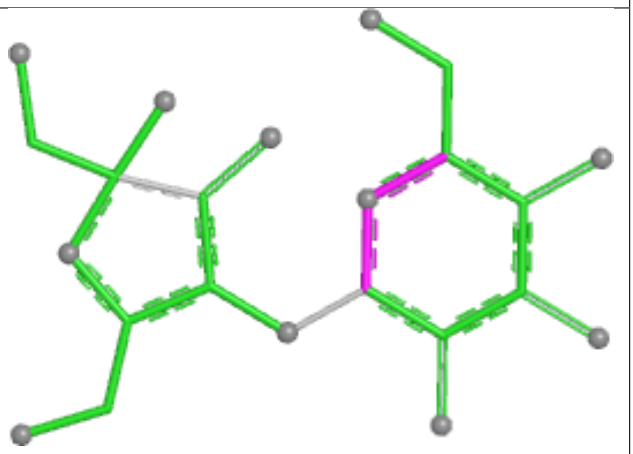
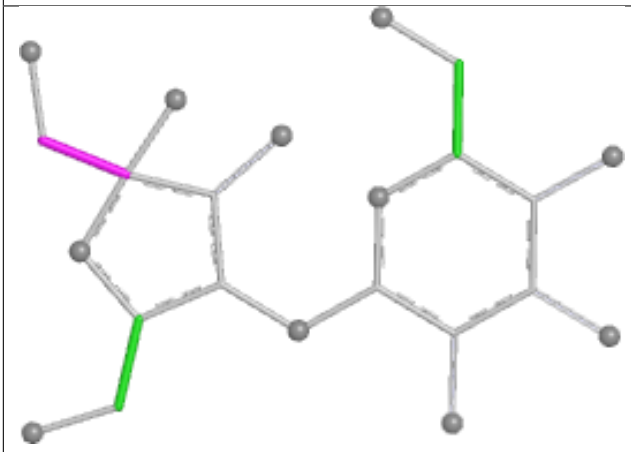
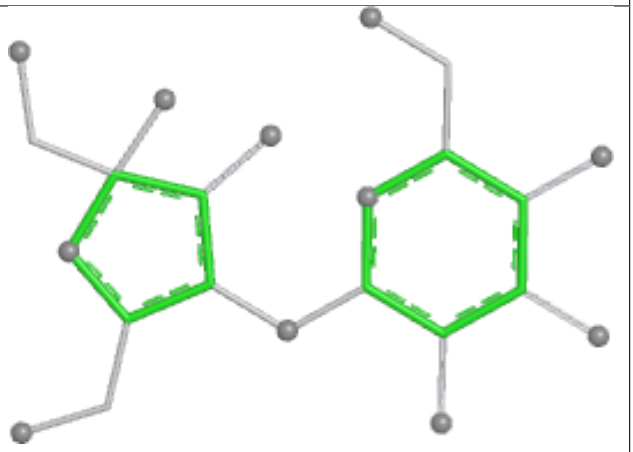


Bond angles

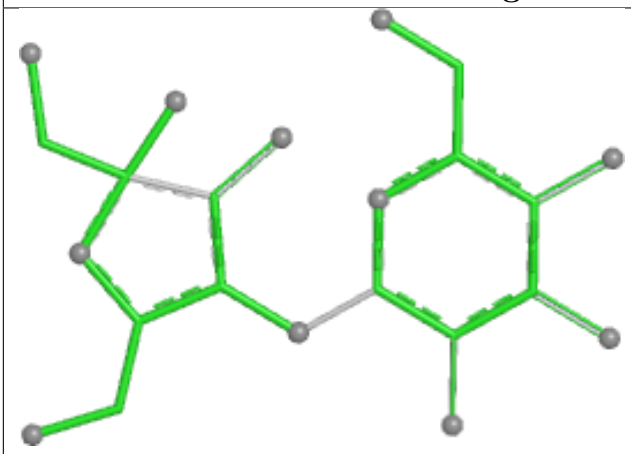


Torsions

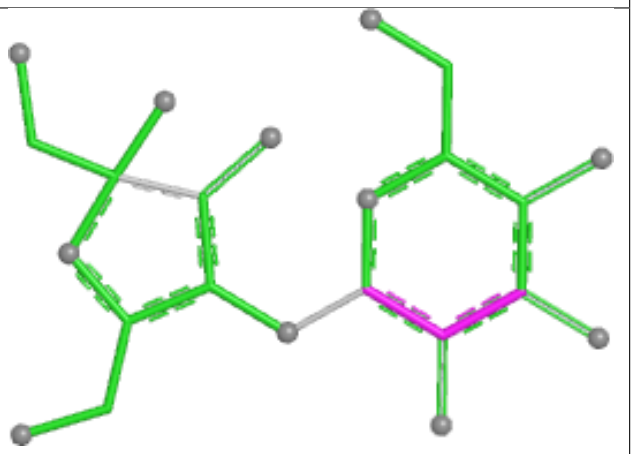


Rings

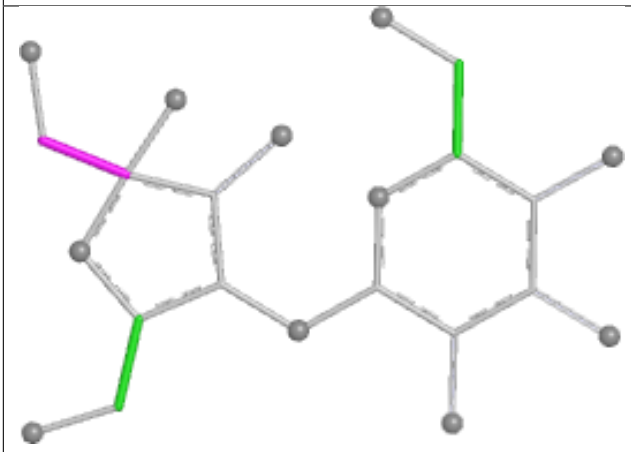
Oligosaccharide Chain i



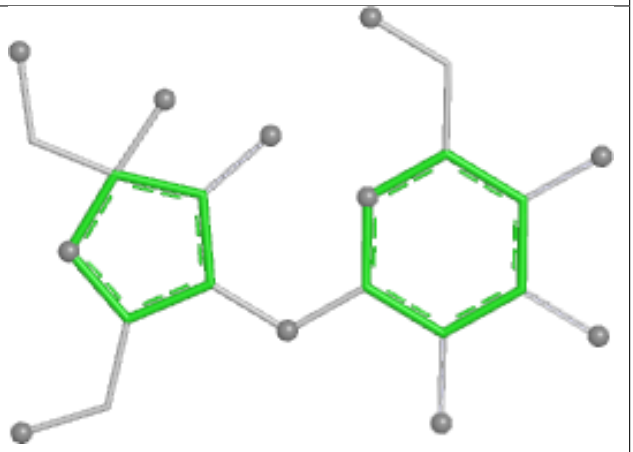
Bond lengths



Bond angles

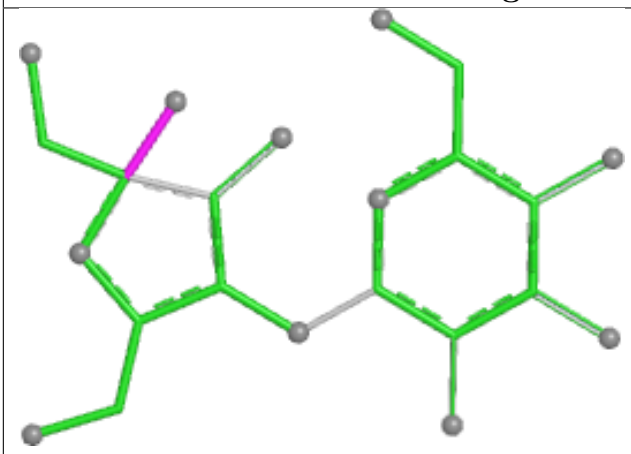


Torsions

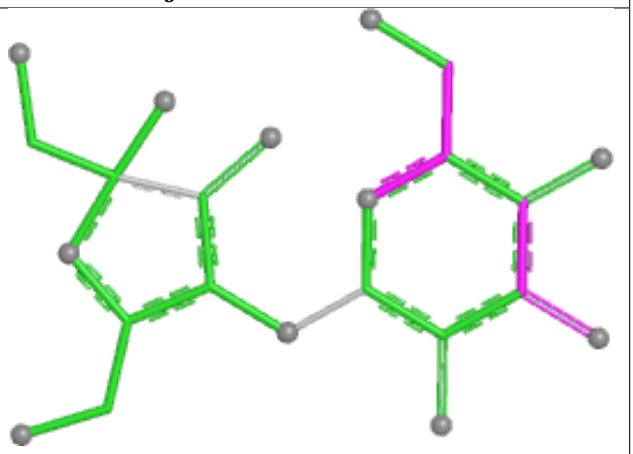


Rings

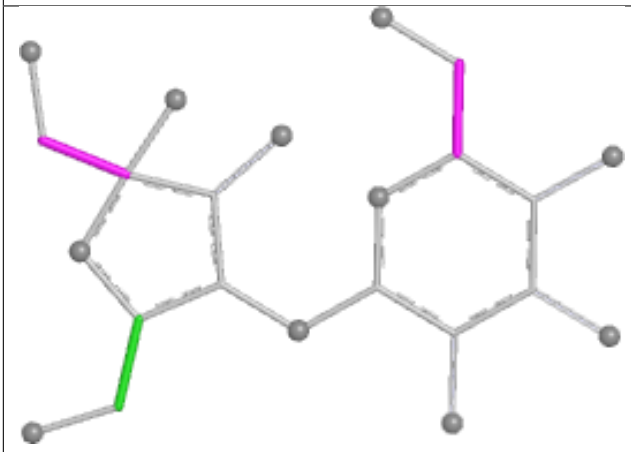
Oligosaccharide Chain j



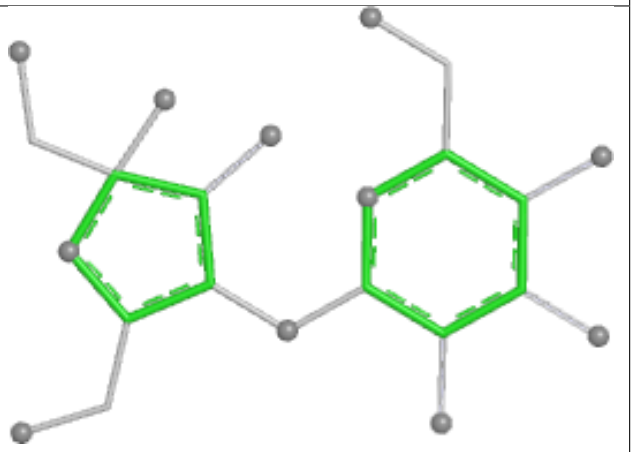
Bond lengths



Bond angles

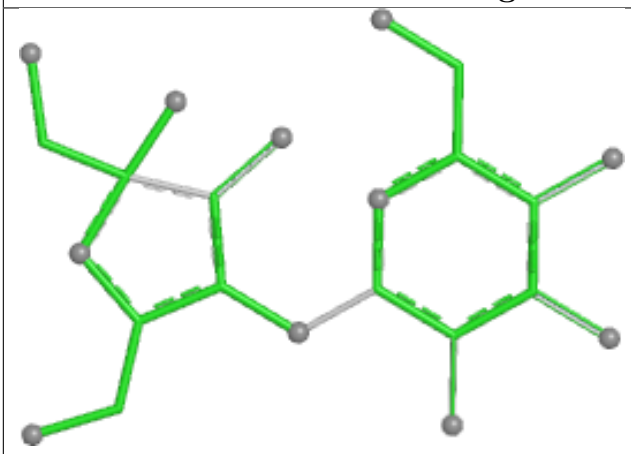


Torsions

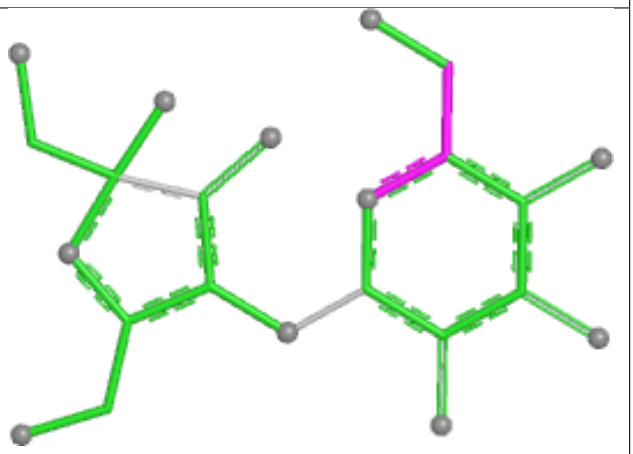


Rings

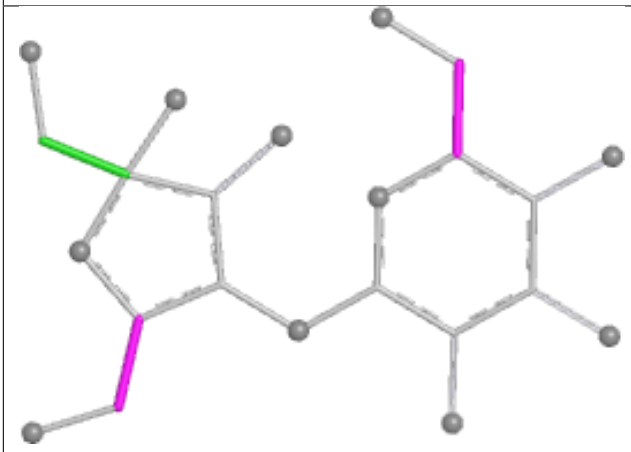
Oligosaccharide Chain k



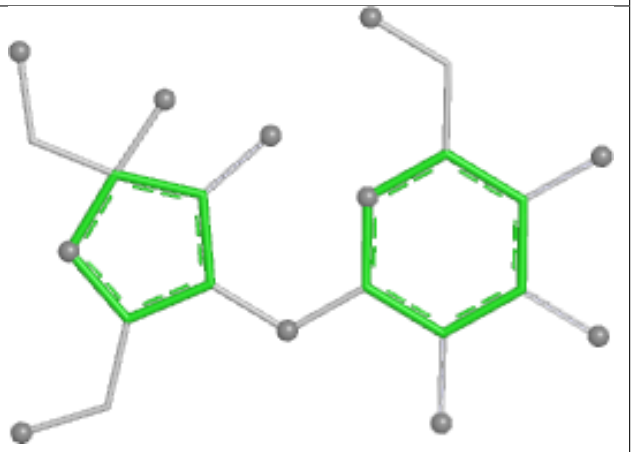
Bond lengths



Bond angles

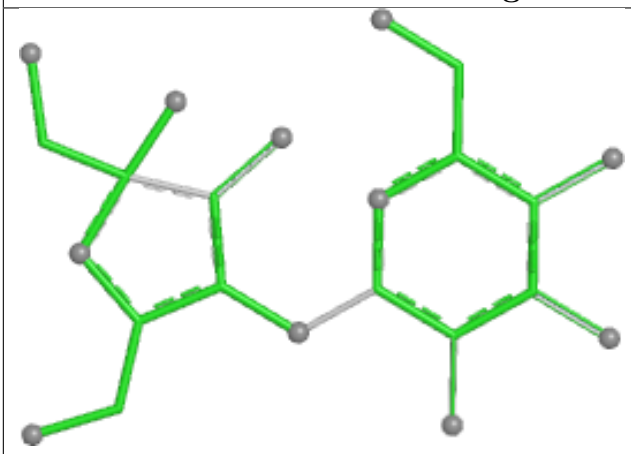


Torsions

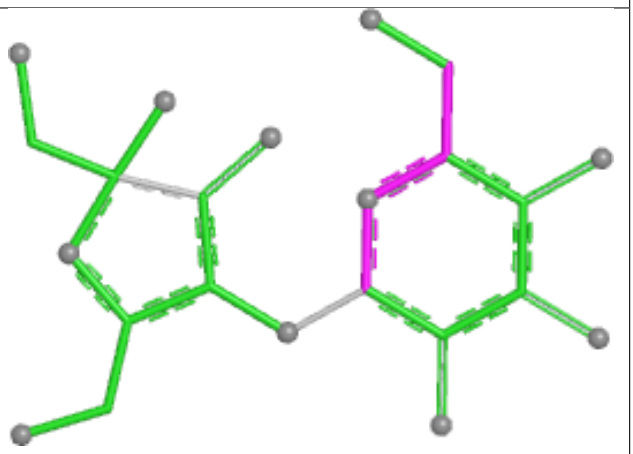


Rings

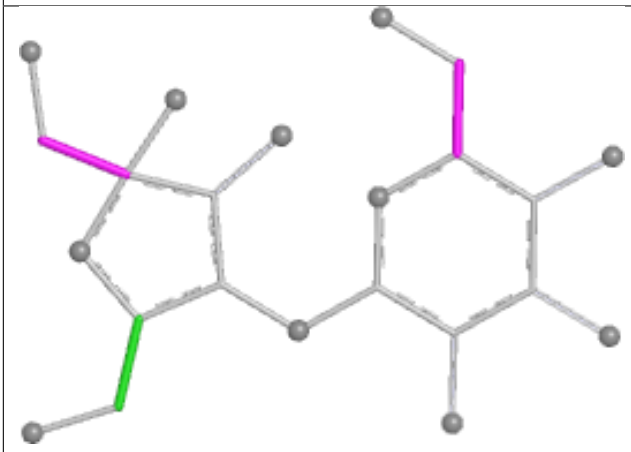
Oligosaccharide Chain l



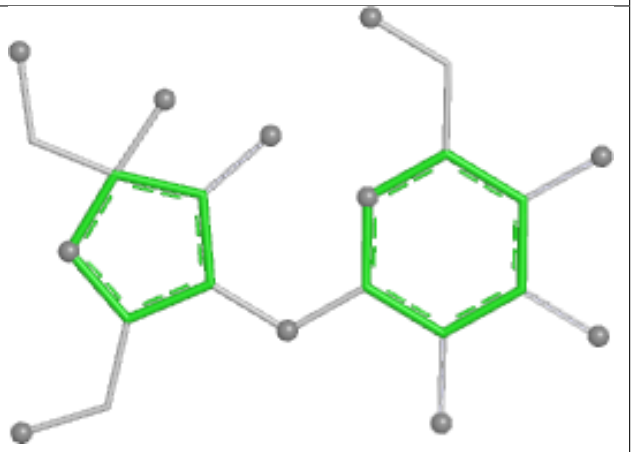
Bond lengths



Bond angles

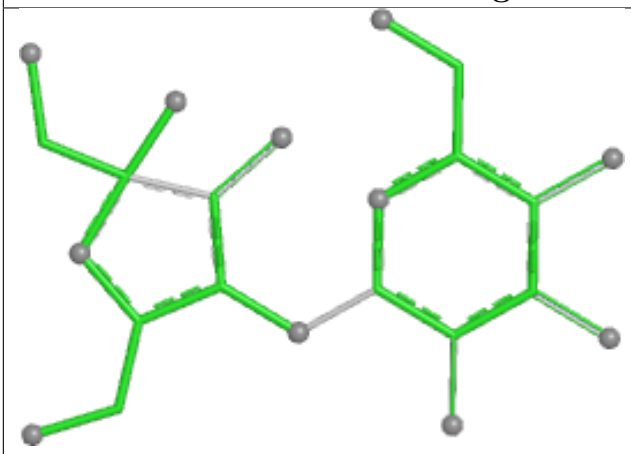


Torsions

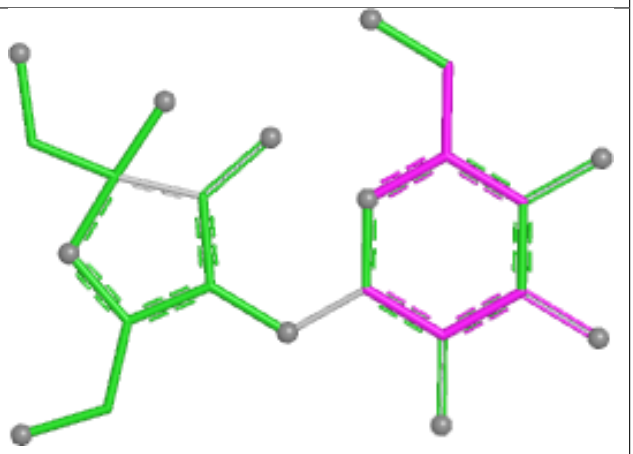


Rings

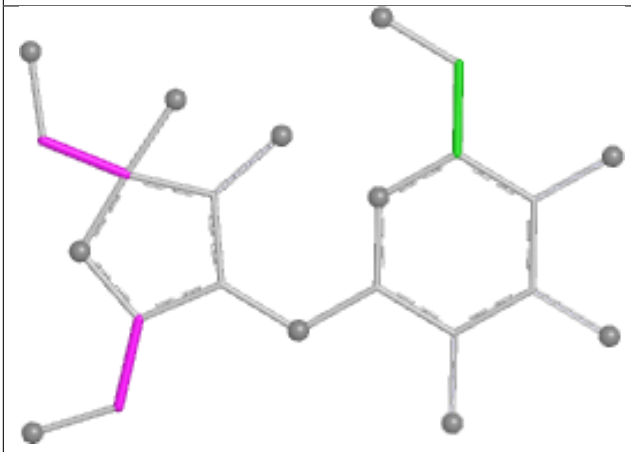
Oligosaccharide Chain m



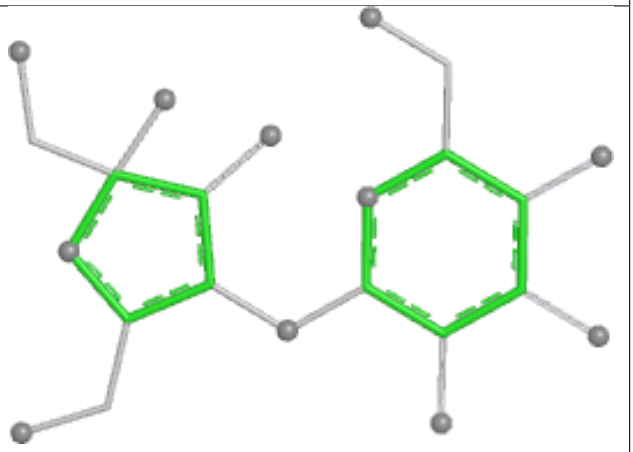
Bond lengths



Bond angles

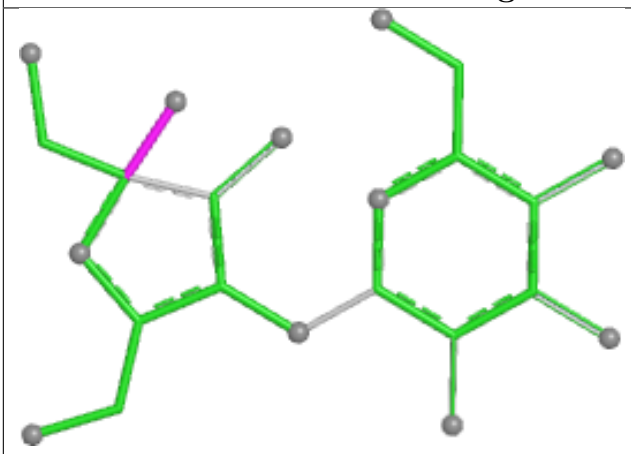


Torsions

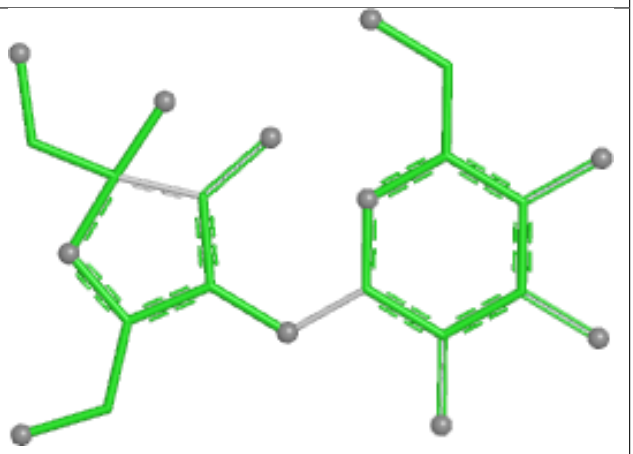


Rings

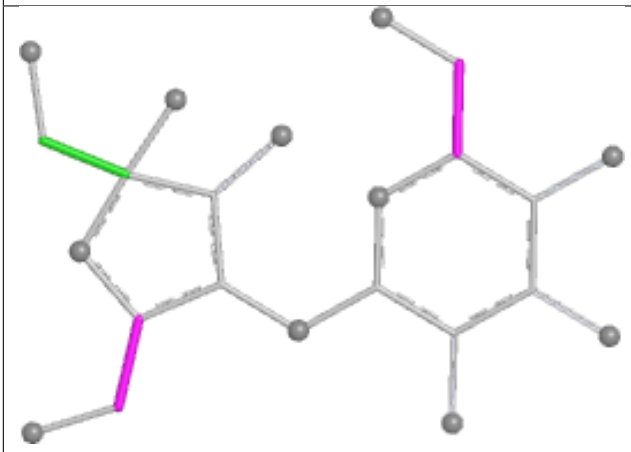
Oligosaccharide Chain n



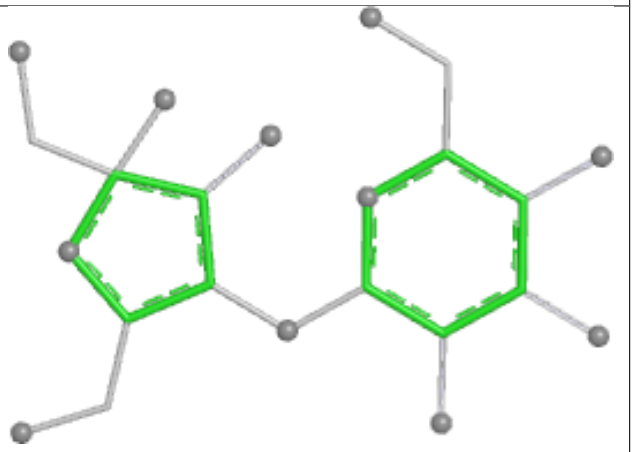
Bond lengths



Bond angles

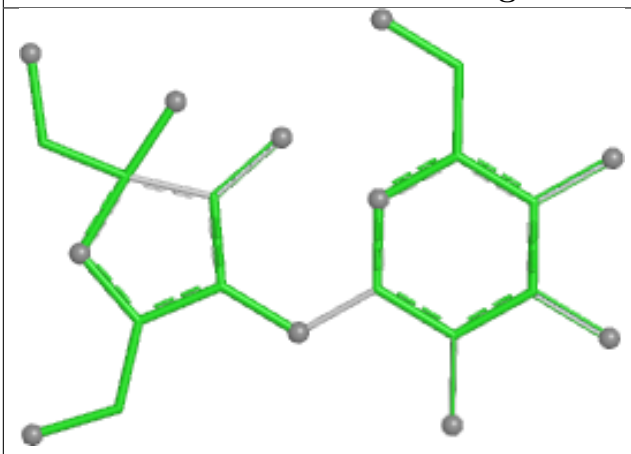


Torsions

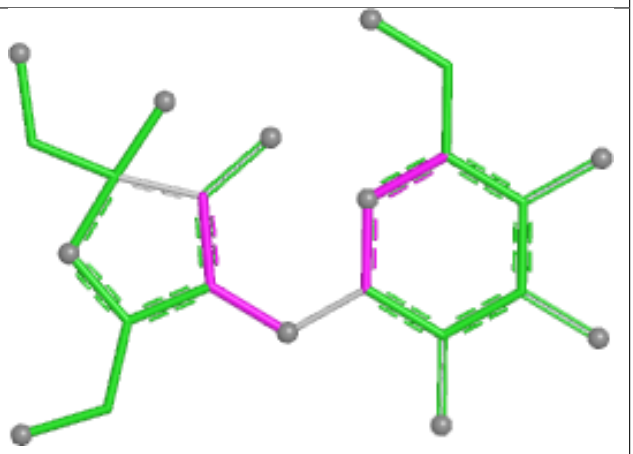


Rings

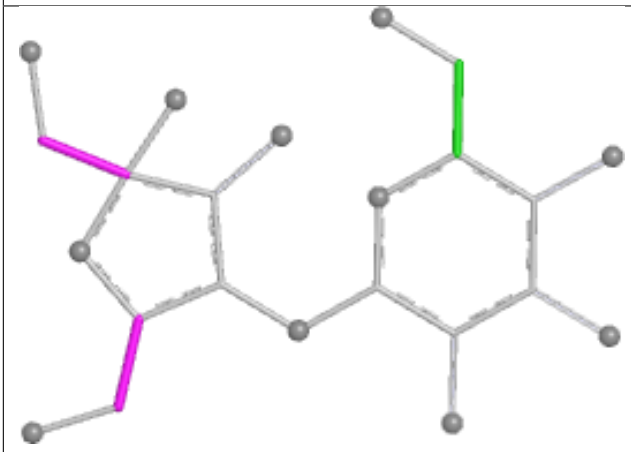
Oligosaccharide Chain o



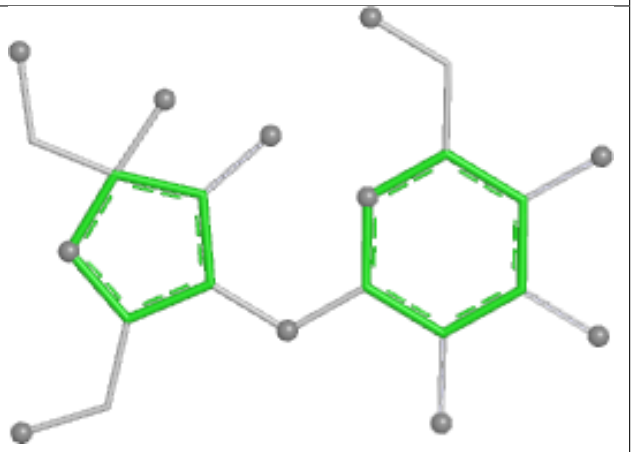
Bond lengths



Bond angles

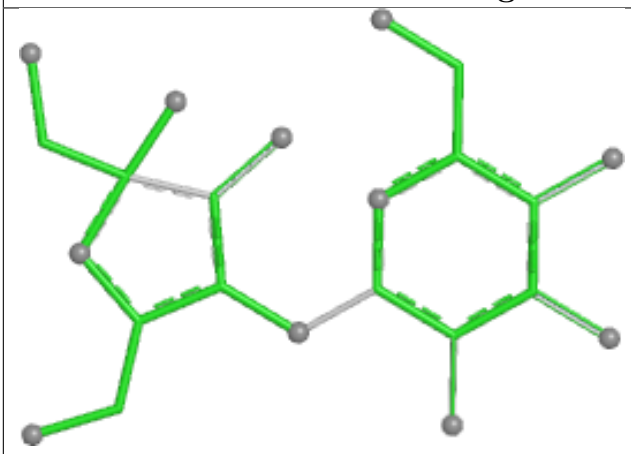


Torsions

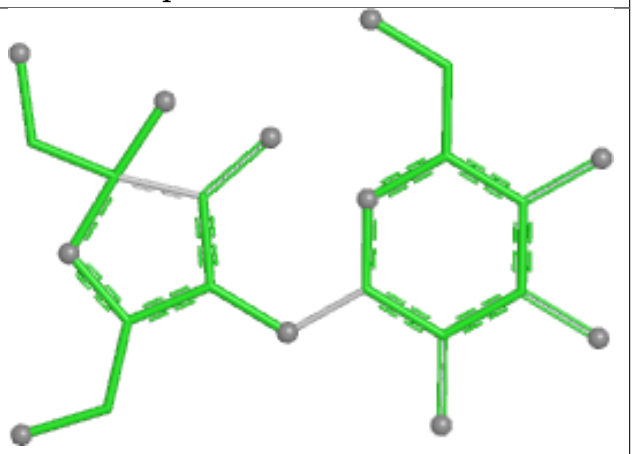


Rings

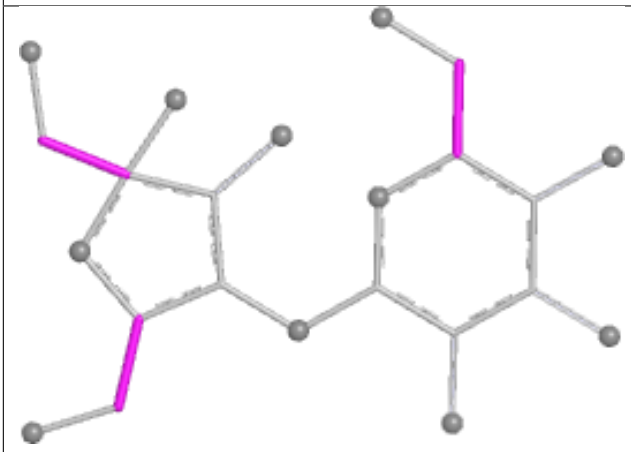
Oligosaccharide Chain p



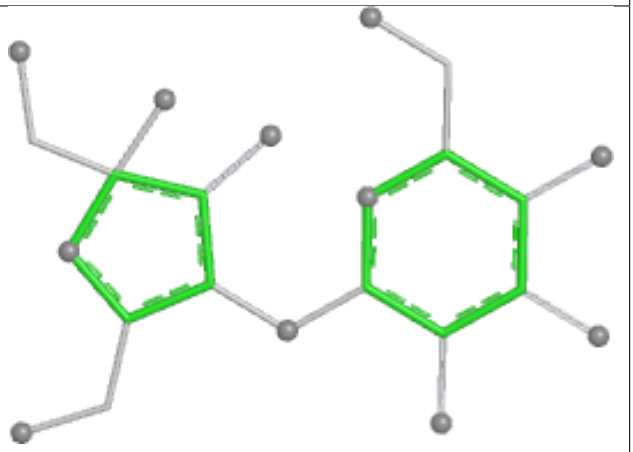
Bond lengths



Bond angles

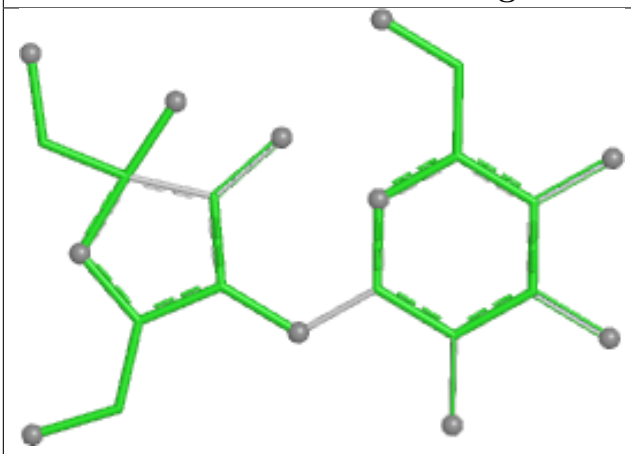


Torsions

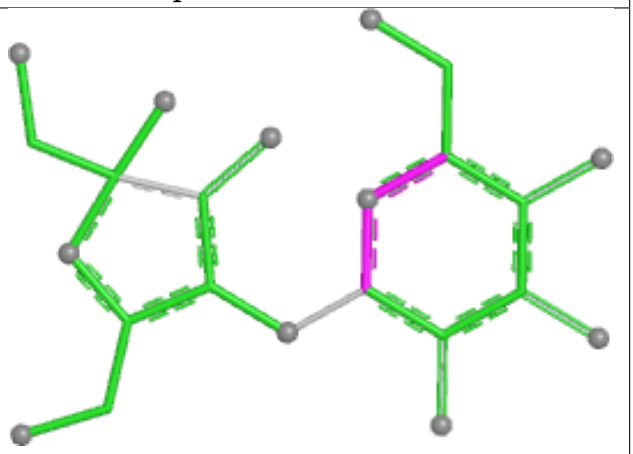


Rings

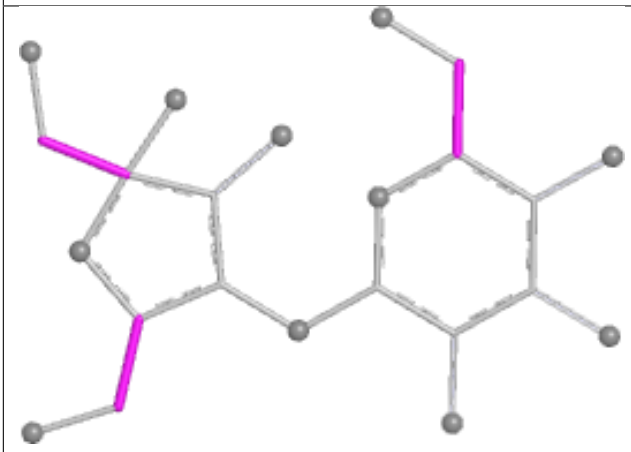
Oligosaccharide Chain q



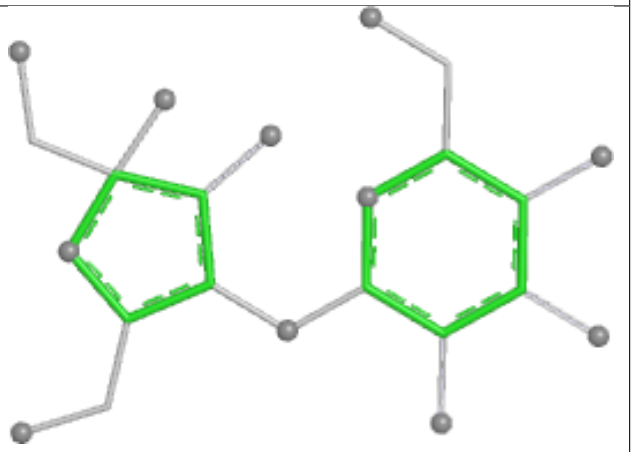
Bond lengths



Bond angles

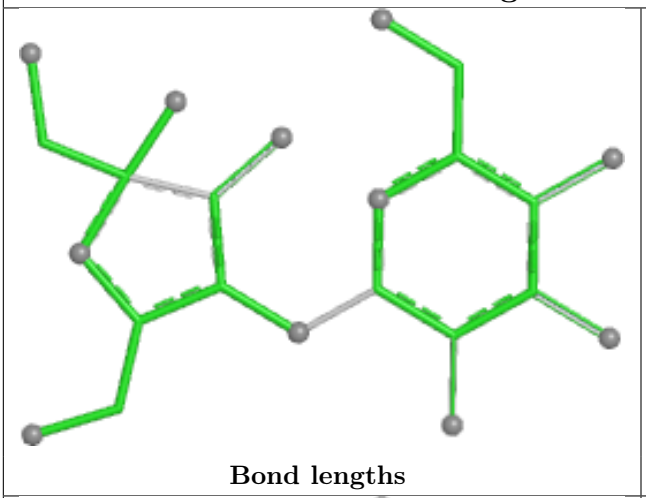


Torsions

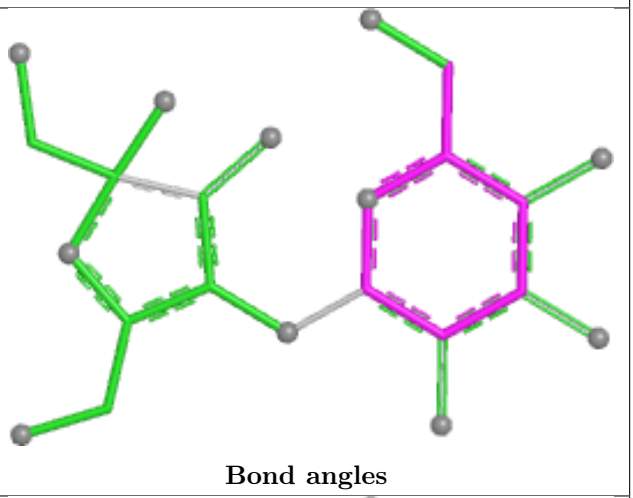


Rings

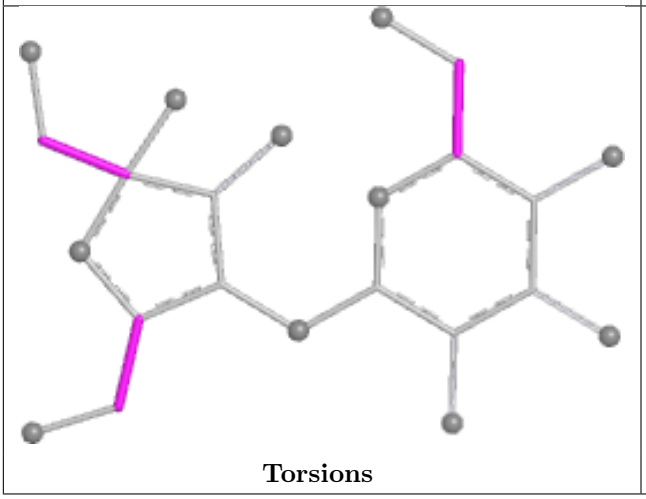
Oligosaccharide Chain r



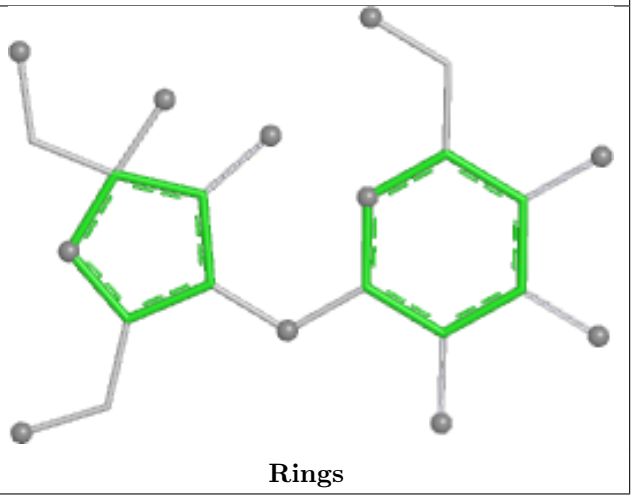
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 58 ligands modelled in this entry, 58 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	431/432 (99%)	0.60	38 (8%) 17 15	42, 73, 121, 211	0
1	B	431/432 (99%)	0.52	28 (6%) 26 22	44, 73, 111, 196	0
1	C	431/432 (99%)	0.50	30 (6%) 24 20	47, 75, 114, 165	0
1	D	431/432 (99%)	0.49	36 (8%) 18 16	43, 77, 119, 218	0
1	E	431/432 (99%)	0.47	29 (6%) 25 21	45, 73, 123, 193	0
1	F	431/432 (99%)	0.88	55 (12%) 9 7	46, 74, 137, 209	0
1	G	431/432 (99%)	0.85	63 (14%) 7 6	43, 77, 138, 211	0
All	All	3017/3024 (99%)	0.62	279 (9%) 16 14	42, 75, 124, 218	0

The worst 5 of 279 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	389	THR	6.3
1	B	126	ASP	6.2
1	F	141	ASP	6.1
1	A	134	TYR	6.0
1	G	326	VAL	5.9

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PCA	F	1	8/9	0.79	0.18	65,67,70,72	0
1	PCA	A	1	8/9	0.81	0.19	83,87,93,93	0
1	PCA	E	1	8/9	0.83	0.23	86,95,99,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PCA	C	1	8/9	0.90	0.21	76,88,94,96	0
1	PCA	G	1	8/9	0.90	0.18	74,76,80,81	0
1	PCA	B	1	8/9	0.91	0.17	68,77,80,82	0
1	PCA	D	1	8/9	0.92	0.15	76,82,87,88	0

6.3 Carbohydrates (i)

SUGAR-RSR INFOmissingINFO

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	F	511	1/1	0.85	0.12	127,127,127,127	0
3	CA	D	513	1/1	0.89	0.08	93,93,93,93	0
3	CA	F	513	1/1	0.91	0.06	93,93,93,93	0
3	CA	A	1013	1/1	0.91	0.11	96,96,96,96	0
3	CA	C	1013	1/1	0.92	0.09	94,94,94,94	0
3	CA	B	510	1/1	0.93	0.07	85,85,85,85	0
4	MG	G	512	1/1	0.93	0.07	108,108,108,108	0
3	CA	B	514	1/1	0.94	0.06	88,88,88,88	0
4	MG	A	1011	1/1	0.94	0.07	72,72,72,72	0
3	CA	E	514	1/1	0.94	0.06	88,88,88,88	0
3	CA	C	1008	1/1	0.95	0.09	69,69,69,69	0
3	CA	B	509	1/1	0.95	0.07	96,96,96,96	0
3	CA	E	510	1/1	0.95	0.06	95,95,95,95	0
3	CA	E	511	1/1	0.95	0.09	123,123,123,123	0
4	MG	E	513	1/1	0.95	0.06	109,109,109,109	0
3	CA	C	1007	1/1	0.96	0.06	64,64,64,64	0
3	CA	G	506	1/1	0.96	0.07	116,116,116,116	0
3	CA	G	508	1/1	0.96	0.07	84,84,84,84	0
4	MG	B	511	1/1	0.96	0.05	84,84,84,84	0
4	MG	F	510	1/1	0.96	0.06	68,68,68,68	0
3	CA	G	509	1/1	0.96	0.10	66,66,66,66	0
3	CA	G	513	1/1	0.97	0.06	87,87,87,87	0
3	CA	D	505	1/1	0.97	0.08	68,68,68,68	0
3	CA	D	508	1/1	0.97	0.06	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	D	509	1/1	0.97	0.06	97,97,97,97	0
3	CA	F	505	1/1	0.97	0.05	61,61,61,61	0
3	CA	F	506	1/1	0.97	0.08	92,92,92,92	0
4	MG	C	1011	1/1	0.97	0.04	86,86,86,86	0
3	CA	B	505	1/1	0.97	0.06	64,64,64,64	0
3	CA	B	506	1/1	0.97	0.06	75,75,75,75	0
3	CA	A	1007	1/1	0.97	0.06	67,67,67,67	0
3	CA	C	1010	1/1	0.97	0.05	91,91,91,91	0
4	MG	D	510	1/1	0.97	0.06	85,85,85,85	0
3	CA	D	503	1/1	0.98	0.04	73,73,73,73	0
3	CA	C	1014	1/1	0.98	0.07	60,60,60,60	0
3	CA	C	1006	1/1	0.98	0.08	65,65,65,65	0
3	CA	G	507	1/1	0.98	0.05	72,72,72,72	0
3	CA	A	1005	1/1	0.98	0.04	70,70,70,70	0
4	MG	A	1010	1/1	0.98	0.05	59,59,59,59	0
3	CA	A	1008	1/1	0.98	0.07	66,66,66,66	0
3	CA	G	510	1/1	0.98	0.05	83,83,83,83	0
4	MG	C	1012	1/1	0.98	0.04	67,67,67,67	0
3	CA	C	1009	1/1	0.98	0.04	75,75,75,75	0
3	CA	E	509	1/1	0.98	0.04	65,65,65,65	0
4	MG	B	512	1/1	0.98	0.04	70,70,70,70	0
4	MG	F	509	1/1	0.98	0.04	53,53,53,53	0
3	CA	A	1009	1/1	0.98	0.06	68,68,68,68	0
3	CA	A	1006	1/1	0.98	0.05	92,92,92,92	0
3	CA	B	508	1/1	0.98	0.08	79,79,79,79	0
4	MG	D	511	1/1	0.98	0.03	83,83,83,83	0
3	CA	E	515	1/1	0.99	0.08	37,37,37,37	1
3	CA	F	507	1/1	0.99	0.04	76,76,76,76	0
3	CA	D	504	1/1	0.99	0.04	84,84,84,84	0
3	CA	F	508	1/1	0.99	0.06	70,70,70,70	0
4	MG	E	512	1/1	0.99	0.03	54,54,54,54	0
3	CA	E	507	1/1	0.99	0.04	60,60,60,60	0
4	MG	G	511	1/1	0.99	0.05	74,74,74,74	0
3	CA	E	508	1/1	0.99	0.04	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.