wwPDB X-ray Structure Validation Summary Report (i)

Oct 28, 2024 – 02:50 am GMT

PDB ID	:	6FB3
Title	:	Teneurin 2 Partial Extracellular Domain
Authors	:	Jackson, V.A.; Carrasquero, M.; Lowe, E.D.; Seiradake, E.
Deposited on	:	2017-12-18
Resolution	:	2.38 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 (1)) were used in the production of this report:

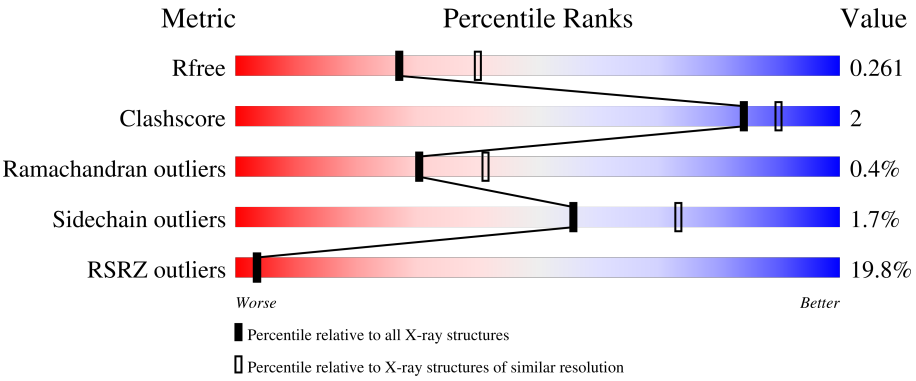
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.38 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	6699 (2.40-2.36)
Clashscore	180529	7414 (2.40-2.36)
Ramachandran outliers	177936	7337 (2.40-2.36)
Sidechain outliers	177891	7338 (2.40-2.36)
RSRZ outliers	164620	6699 (2.40-2.36)

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	1859	24% 91% 7%
1	B	1859	21% 91% 8%
1	C	1859	13% 91% 7%
1	D	1859	21% 91% 7%
2	E	8	25% 75%

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Mol	Chain	Length	Quality of chain
2	K	8	25% 75%
2	Q	8	12% 88%
2	W	8	25% 75%
3	F	2	100%
3	G	2	100%
3	H	2	50% 50%
3	I	2	100%
3	J	2	50% 50%
3	L	2	100%
3	M	2	100%
3	N	2	50% 50%
3	O	2	100%
3	P	2	100%
3	R	2	50% 50%
3	S	2	100%
3	T	2	50% 50%
3	U	2	50% 50%
3	V	2	50% 50%
3	X	2	100%
3	Y	2	100%
3	Z	2	50% 50%
3	a	2	100%
3	b	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 59451 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 Teneurin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1836	Total	C	N	O	S	0	1	0
			14513	9168	2508	2774	63			
1	B	1836	Total	C	N	O	S	0	1	0
			14513	9168	2508	2774	63			
1	C	1836	Total	C	N	O	S	0	1	0
			14513	9168	2508	2774	63			
1	D	1836	Total	C	N	O	S	0	1	0
			14513	9168	2508	2774	63			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	953	THR	-	expression tag	UNP Q9DER5
A	954	GLY	-	expression tag	UNP Q9DER5
A	2803	GLY	-	expression tag	UNP Q9DER5
A	2804	THR	-	expression tag	UNP Q9DER5
A	2805	LYS	-	expression tag	UNP Q9DER5
A	2806	HIS	-	expression tag	UNP Q9DER5
A	2807	HIS	-	expression tag	UNP Q9DER5
A	2808	HIS	-	expression tag	UNP Q9DER5
A	2809	HIS	-	expression tag	UNP Q9DER5
A	2810	HIS	-	expression tag	UNP Q9DER5
A	2811	HIS	-	expression tag	UNP Q9DER5
B	953	THR	-	expression tag	UNP Q9DER5
B	954	GLY	-	expression tag	UNP Q9DER5
B	2803	GLY	-	expression tag	UNP Q9DER5
B	2804	THR	-	expression tag	UNP Q9DER5
B	2805	LYS	-	expression tag	UNP Q9DER5
B	2806	HIS	-	expression tag	UNP Q9DER5
B	2807	HIS	-	expression tag	UNP Q9DER5
B	2808	HIS	-	expression tag	UNP Q9DER5
B	2809	HIS	-	expression tag	UNP Q9DER5
B	2810	HIS	-	expression tag	UNP Q9DER5

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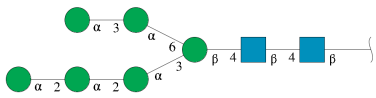
Chain	Residue	Modelled	Actual	Comment	Reference
B	2811	HIS	-	expression tag	UNP Q9DER5
C	953	THR	-	expression tag	UNP Q9DER5
C	954	GLY	-	expression tag	UNP Q9DER5
C	2803	GLY	-	expression tag	UNP Q9DER5
C	2804	THR	-	expression tag	UNP Q9DER5
C	2805	LYS	-	expression tag	UNP Q9DER5
C	2806	HIS	-	expression tag	UNP Q9DER5
C	2807	HIS	-	expression tag	UNP Q9DER5
C	2808	HIS	-	expression tag	UNP Q9DER5
C	2809	HIS	-	expression tag	UNP Q9DER5
C	2810	HIS	-	expression tag	UNP Q9DER5
C	2811	HIS	-	expression tag	UNP Q9DER5
D	953	THR	-	expression tag	UNP Q9DER5
D	954	GLY	-	expression tag	UNP Q9DER5
D	2803	GLY	-	expression tag	UNP Q9DER5
D	2804	THR	-	expression tag	UNP Q9DER5
D	2805	LYS	-	expression tag	UNP Q9DER5
D	2806	HIS	-	expression tag	UNP Q9DER5
D	2807	HIS	-	expression tag	UNP Q9DER5
D	2808	HIS	-	expression tag	UNP Q9DER5
D	2809	HIS	-	expression tag	UNP Q9DER5
D	2810	HIS	-	expression tag	UNP Q9DER5
D	2811	HIS	-	expression tag	UNP Q9DER5

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	0	0	0
			94	52	2	40			
2	K	8	Total	C	N	O	0	0	0
			94	52	2	40			
2	Q	8	Total	C	N	O	0	0	0
			94	52	2	40			
2	W	8	Total	C	N	O	0	0	0
			94	52	2	40			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			

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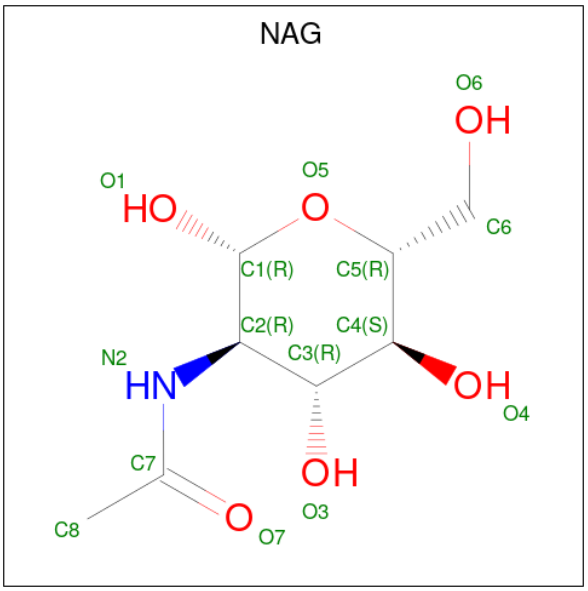
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	a	2	Total C N O 28 16 2 10	0	0	0
3	b	2	Total C N O 28 16 2 10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 5 is water.

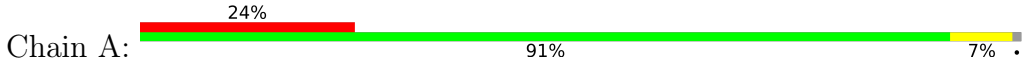
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	17	Total O 17 17	0	0
5	B	29	Total O 29 29	0	0
5	C	105	Total O 105 105	0	0
5	D	32	Total O 32 32	0	0

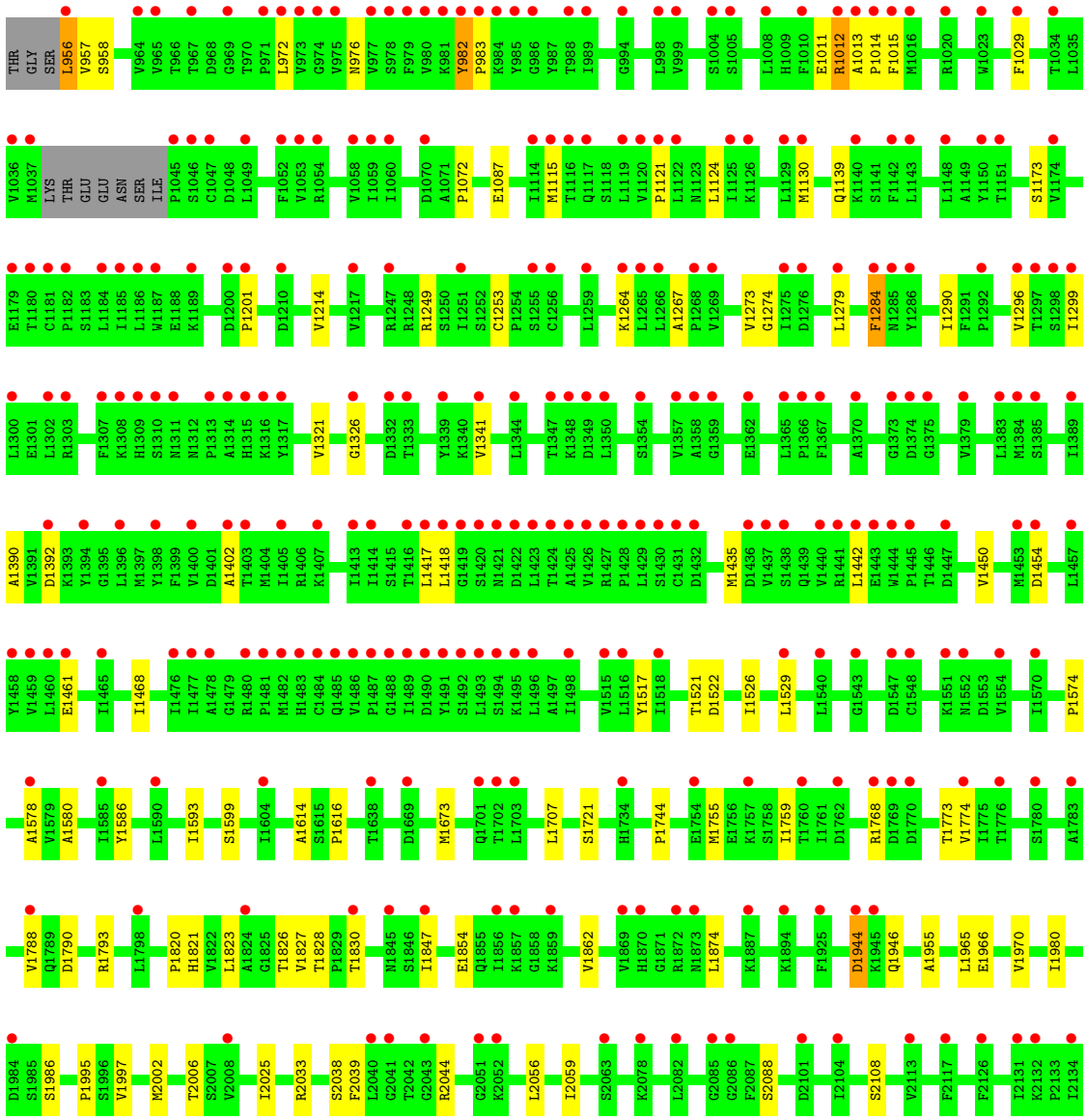
3 Residue-property plots (i)

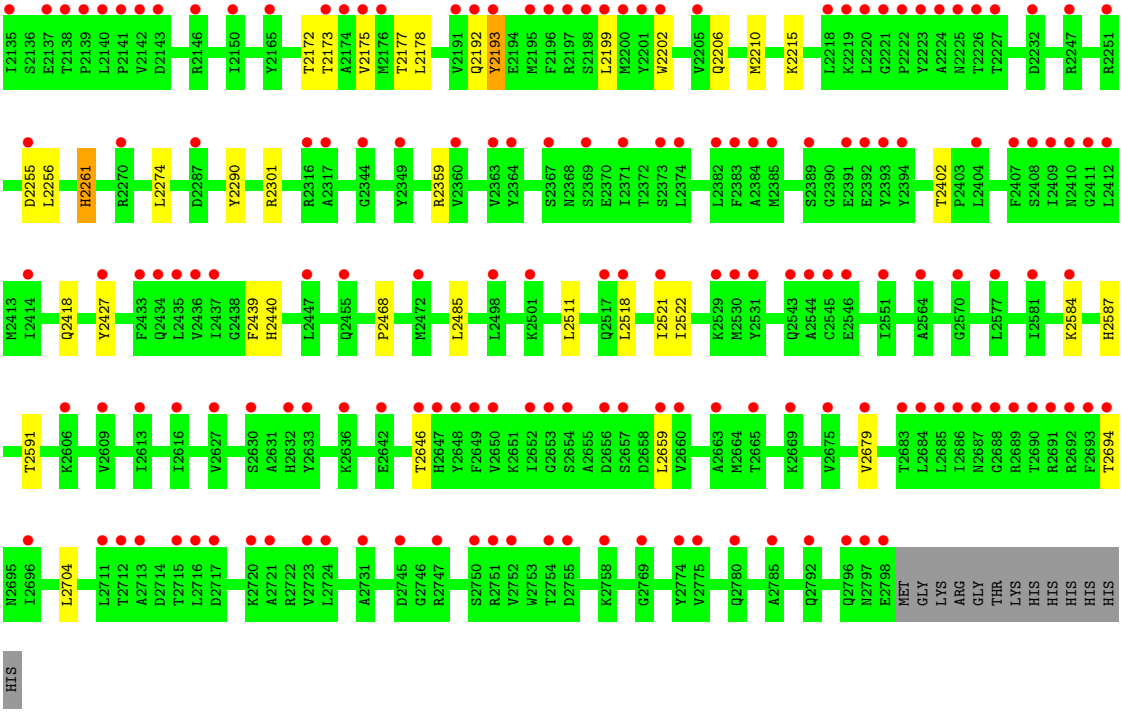
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Teneurin-2

Chain A:

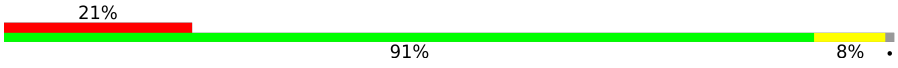


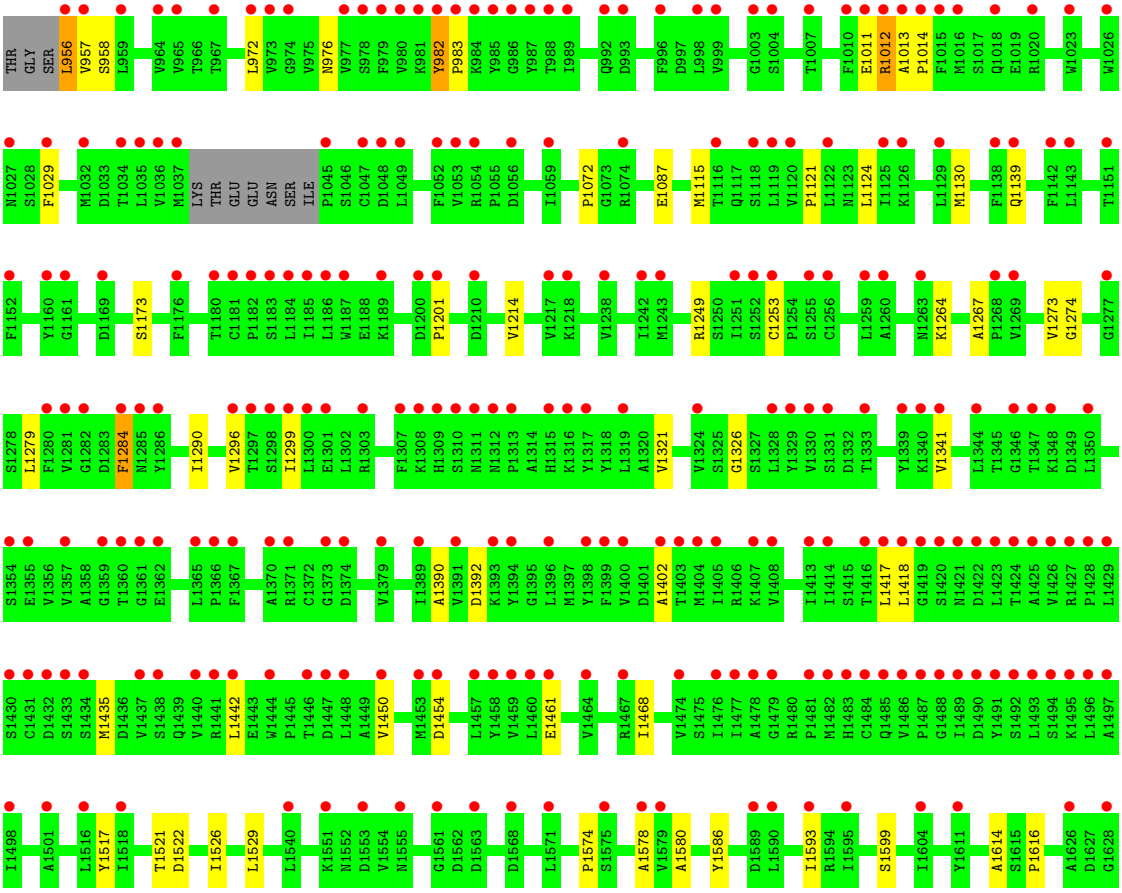


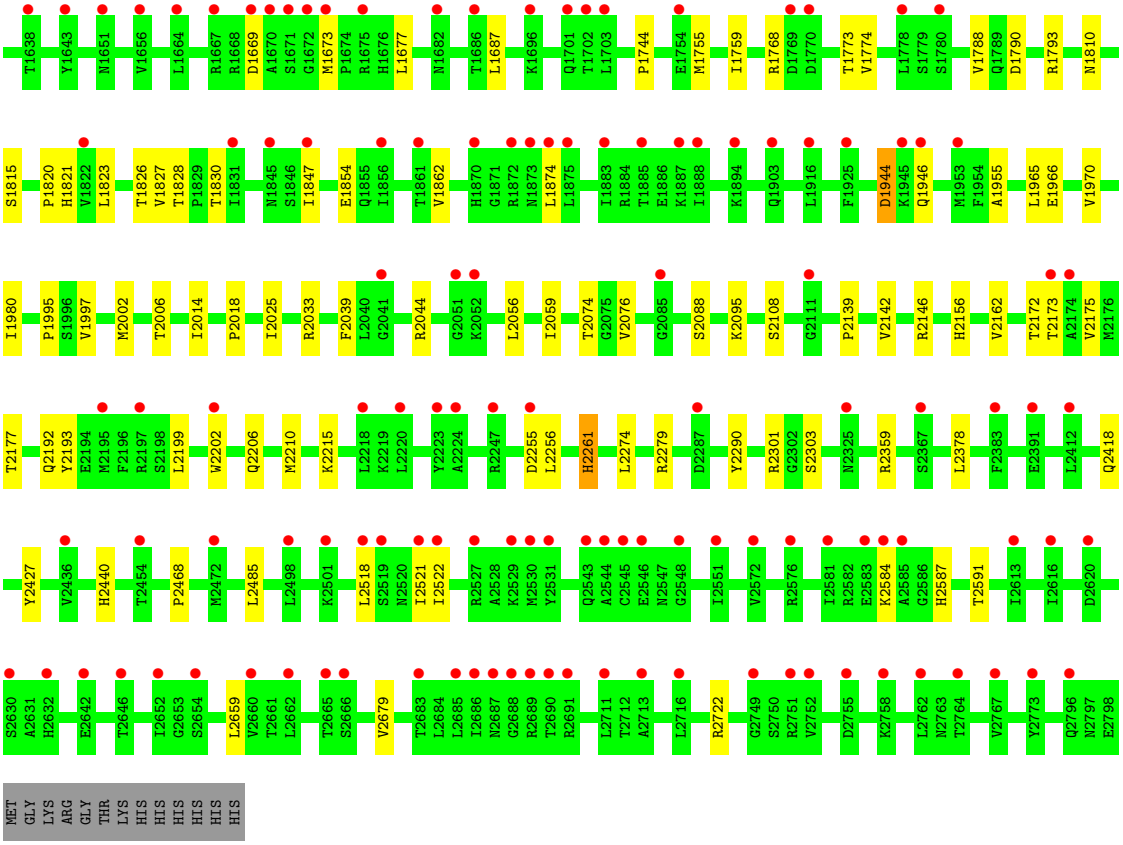


- Molecule 1: Teneurin-2

Chain B:

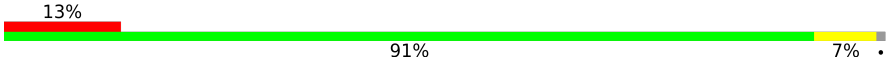


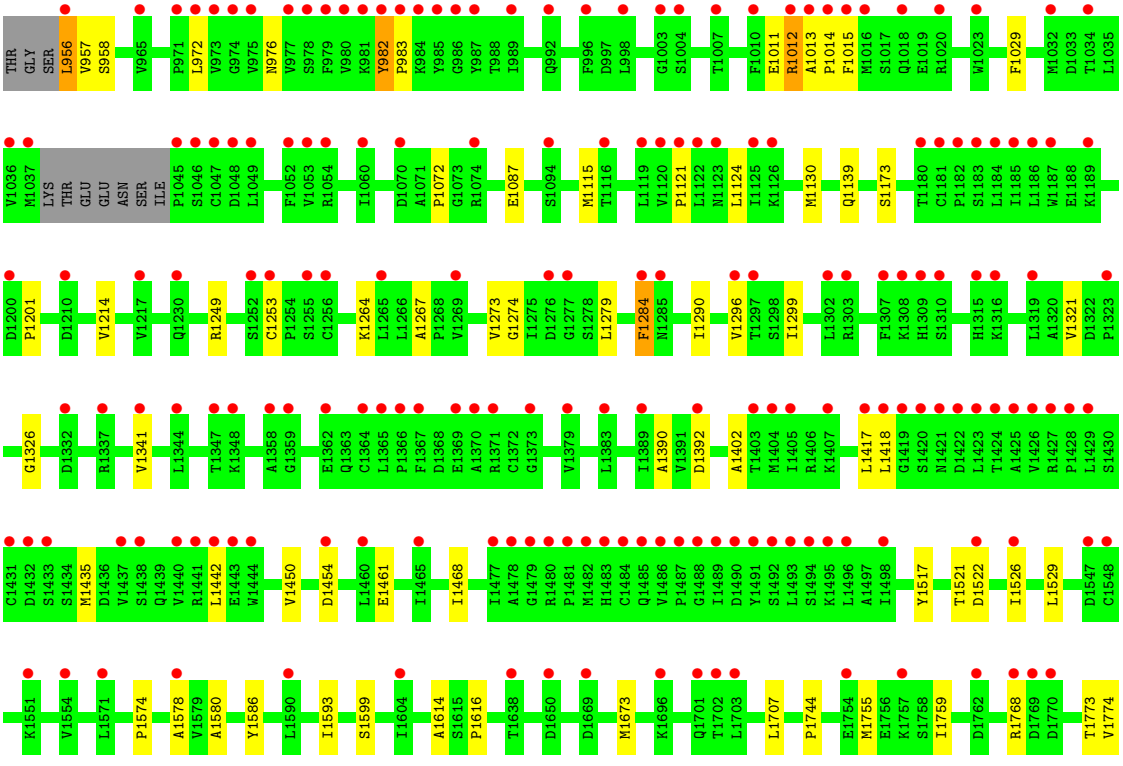


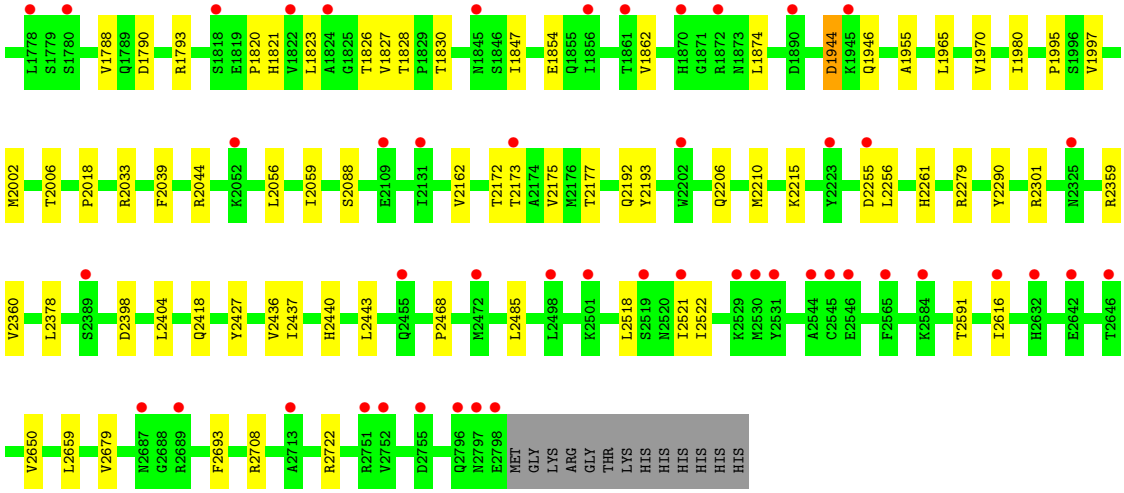


• Molecule 1: Teneurin-2

Chain C:

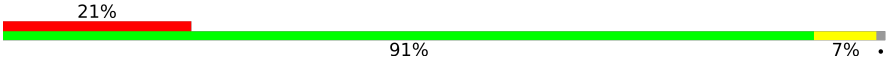


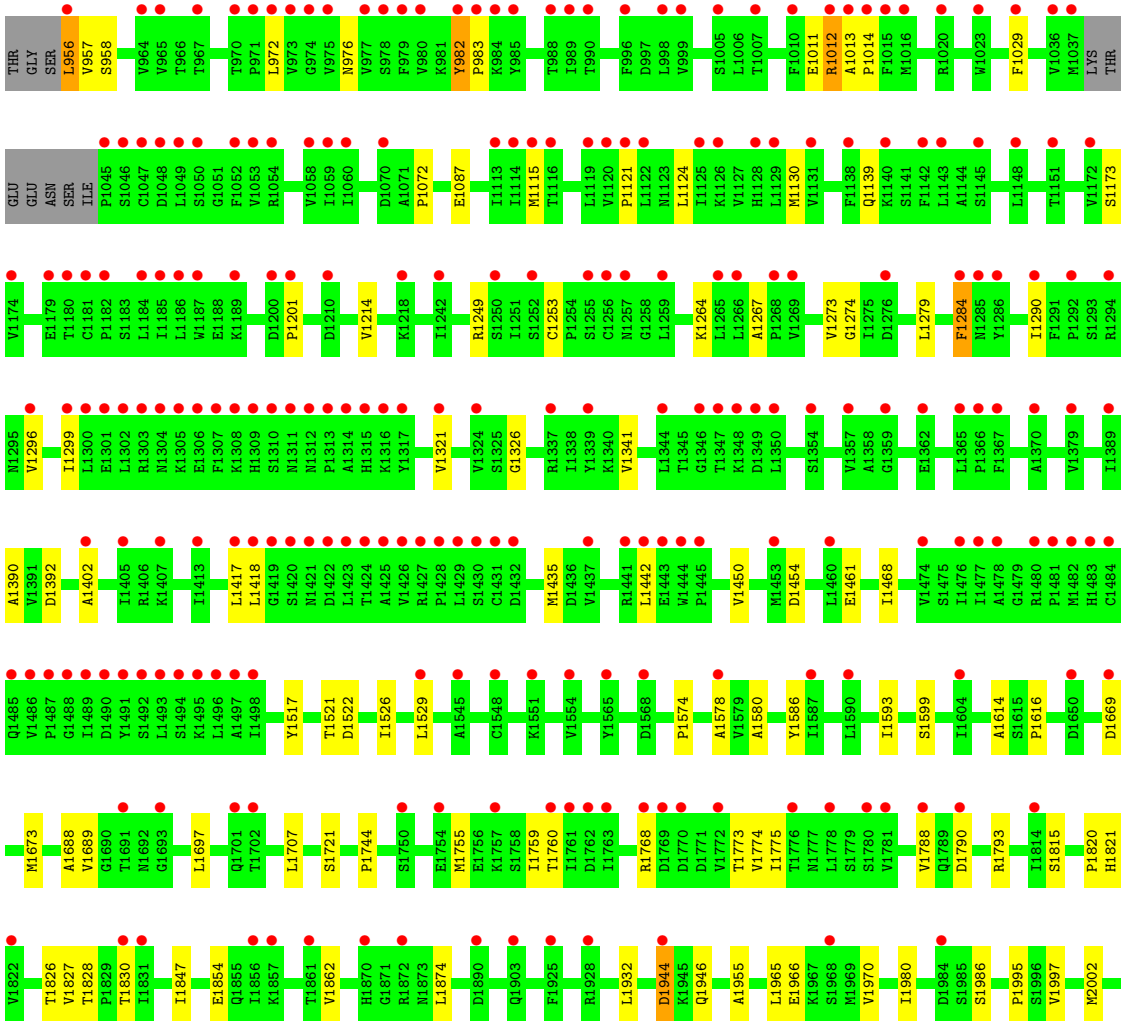


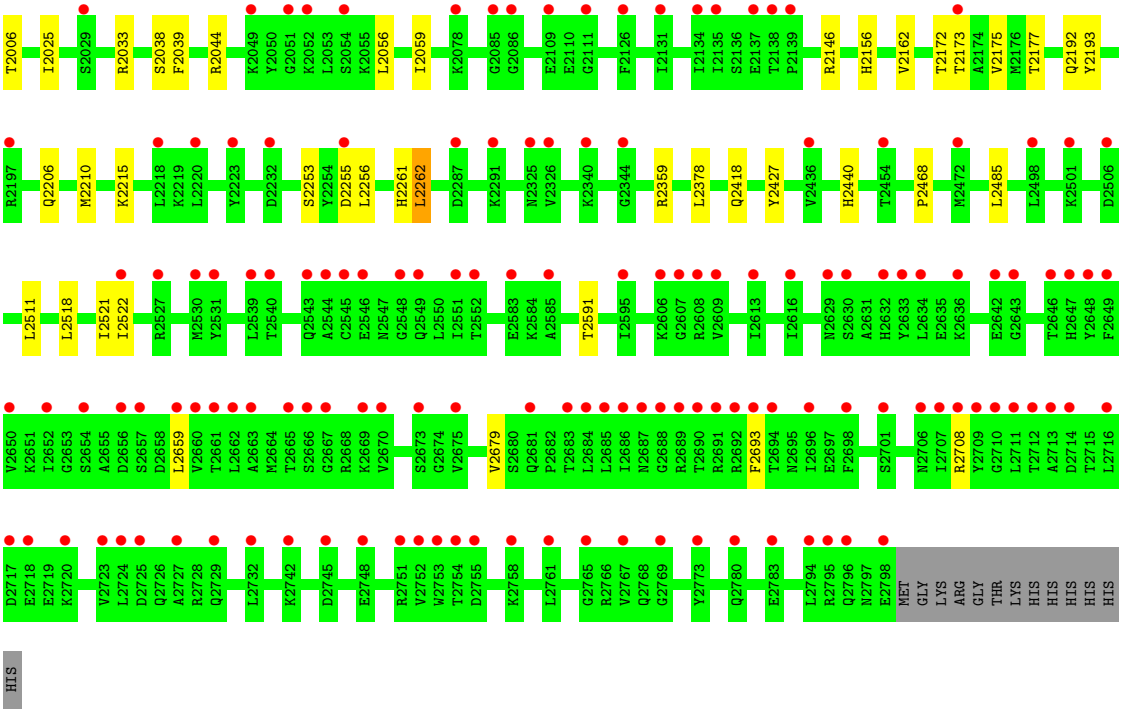


• Molecule 1: Teneurin-2

Chain D:

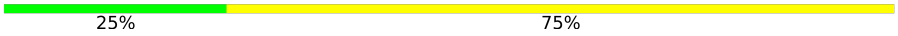






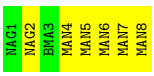
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



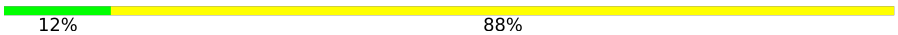
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



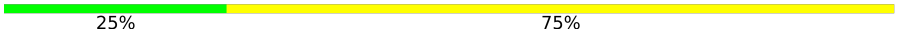
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



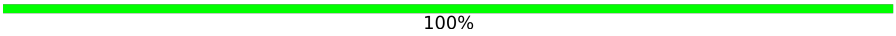
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



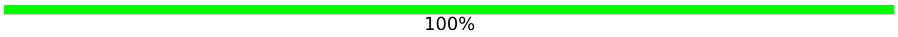
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

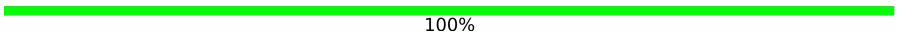


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

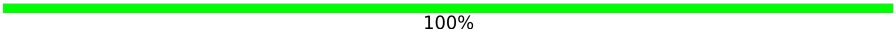
Chain J:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

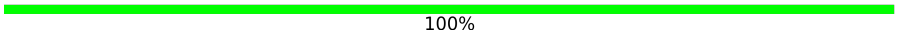


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

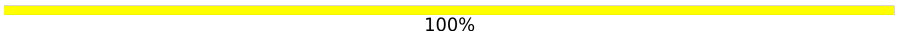
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

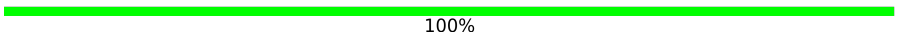


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 

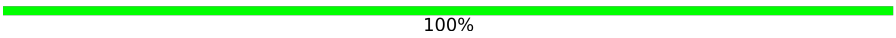
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 

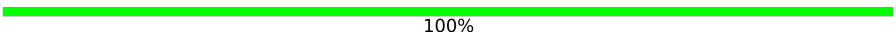
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 

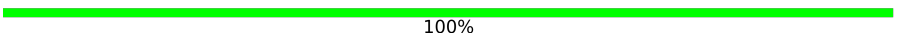
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

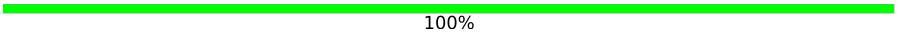
Chain Z: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.56Å 452.56Å 146.36Å 90.00° 95.12° 90.00°	Depositor
Resolution (Å)	89.38 – 2.38 89.38 – 2.38	Depositor EDS
% Data completeness (in resolution range)	94.3 (89.38-2.38) 94.3 (89.38-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.37Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.225 , 0.242 0.242 , 0.261	Depositor DCC
R_{free} test set	21455 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	59451	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2374e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MAN, BMA, NAG

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	0.37	0/14827	0.62	0/20108
1	B	0.37	0/14827	0.62	0/20108
1	C	0.37	0/14827	0.62	0/20108
1	D	0.37	0/14827	0.62	0/20108
All	All	0.37	0/59308	0.62	0/80432

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14513	0	14253	66	0
1	B	14513	0	14253	69	0
1	C	14513	0	14253	63	0
1	D	14513	0	14253	64	0
2	E	94	0	79	0	0
2	K	94	0	79	0	0
2	Q	94	0	79	0	0
2	W	94	0	79	0	0
3	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
4	A	70	0	65	0	0
4	B	70	0	65	0	0
4	C	70	0	65	0	0
4	D	70	0	65	0	0
5	A	17	0	0	0	0
5	B	29	0	0	0	0
5	C	105	0	0	0	0
5	D	32	0	0	0	0
All	All	59451	0	58088	260	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 260 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1821:HIS:HD2	1:C:1830:THR:HG21	1.41	0.85
1:A:1821:HIS:HD2	1:A:1830:THR:HG21	1.41	0.85
1:B:1821:HIS:HD2	1:B:1830:THR:HG21	1.41	0.83
1:D:1821:HIS:HD2	1:D:1830:THR:HG21	1.42	0.82
1:D:982:TYR:HB3	1:D:983:PRO:HD3	1.65	0.79

There are no symmetry-related clashes.

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	1833/1859 (99%)	1769 (96%)	57 (3%)	7 (0%)	30	41
1	B	1833/1859 (99%)	1763 (96%)	63 (3%)	7 (0%)	30	41
1	C	1833/1859 (99%)	1768 (96%)	59 (3%)	6 (0%)	37	49
1	D	1833/1859 (99%)	1765 (96%)	61 (3%)	7 (0%)	30	41
All	All	7332/7436 (99%)	7065 (96%)	240 (3%)	27 (0%)	30	41

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	982	TYR
1	B	982	TYR
1	C	982	TYR
1	D	982	TYR
1	A	1997	VAL

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	1601/1620 (99%)	1574 (98%)	27 (2%)	56	73
1	B	1601/1620 (99%)	1573 (98%)	28 (2%)	56	73
1	C	1601/1620 (99%)	1574 (98%)	27 (2%)	56	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	1601/1620 (99%)	1572 (98%)	29 (2%)	54 72
All	All	6404/6480 (99%)	6293 (98%)	111 (2%)	56 73

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1012	ARG
1	D	2591	THR
1	C	1965	LEU
1	D	2440	HIS
1	D	1944	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2185	HIS
1	D	2587	HIS
1	D	2362	HIS
1	C	1311	ASN
1	D	1892	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

72 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	E	1	2,1	14,14,15	0.42	0	17,19,21	0.69	1 (5%)
2	NAG	E	2	2	14,14,15	0.42	0	17,19,21	0.86	0
2	BMA	E	3	2	11,11,12	0.50	0	15,15,17	0.72	0
2	MAN	E	4	2	11,11,12	0.59	0	15,15,17	0.93	1 (6%)
2	MAN	E	5	2	11,11,12	0.65	0	15,15,17	0.76	1 (6%)
2	MAN	E	6	2	11,11,12	0.61	0	15,15,17	0.91	1 (6%)
2	MAN	E	7	2	11,11,12	0.67	0	15,15,17	1.06	1 (6%)
2	MAN	E	8	2	11,11,12	0.48	0	15,15,17	1.07	2 (13%)
3	NAG	F	1	3,1	14,14,15	0.41	0	17,19,21	0.69	0
3	NAG	F	2	3	14,14,15	0.43	0	17,19,21	0.61	0
3	NAG	G	1	3,1	14,14,15	0.43	0	17,19,21	0.59	0
3	NAG	G	2	3	14,14,15	0.44	0	17,19,21	0.68	0
3	NAG	H	1	3,1	14,14,15	0.43	0	17,19,21	0.91	2 (11%)
3	NAG	H	2	3	14,14,15	0.43	0	17,19,21	0.62	0
3	NAG	I	1	3,1	14,14,15	0.43	0	17,19,21	0.78	0
3	NAG	I	2	3	14,14,15	0.42	0	17,19,21	0.56	0
3	NAG	J	1	3,1	14,14,15	0.42	0	17,19,21	0.78	0
3	NAG	J	2	3	14,14,15	0.44	0	17,19,21	0.72	1 (5%)
2	NAG	K	1	2,1	14,14,15	0.42	0	17,19,21	0.69	0
2	NAG	K	2	2	14,14,15	0.41	0	17,19,21	0.87	1 (5%)
2	BMA	K	3	2	11,11,12	0.50	0	15,15,17	0.71	0
2	MAN	K	4	2	11,11,12	0.58	0	15,15,17	0.92	1 (6%)
2	MAN	K	5	2	11,11,12	0.63	0	15,15,17	0.76	1 (6%)
2	MAN	K	6	2	11,11,12	0.62	0	15,15,17	0.90	1 (6%)
2	MAN	K	7	2	11,11,12	0.67	0	15,15,17	1.05	1 (6%)
2	MAN	K	8	2	11,11,12	0.55	0	15,15,17	1.02	2 (13%)
3	NAG	L	1	3,1	14,14,15	0.41	0	17,19,21	0.71	0
3	NAG	L	2	3	14,14,15	0.42	0	17,19,21	0.71	0
3	NAG	M	1	3,1	14,14,15	0.43	0	17,19,21	0.58	0
3	NAG	M	2	3	14,14,15	0.42	0	17,19,21	0.65	0
3	NAG	N	1	3,1	14,14,15	0.41	0	17,19,21	0.88	2 (11%)
3	NAG	N	2	3	14,14,15	0.43	0	17,19,21	0.60	0
3	NAG	O	1	3,1	14,14,15	0.43	0	17,19,21	0.81	0
3	NAG	O	2	3	14,14,15	0.43	0	17,19,21	0.56	0
3	NAG	P	1	3,1	14,14,15	0.42	0	17,19,21	0.79	1 (5%)
3	NAG	P	2	3	14,14,15	0.45	0	17,19,21	0.69	1 (5%)
2	NAG	Q	1	2,1	14,14,15	0.42	0	17,19,21	0.72	1 (5%)
2	NAG	Q	2	2	14,14,15	0.42	0	17,19,21	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMA	Q	3	2	11,11,12	0.48	0	15,15,17	0.71	0
2	MAN	Q	4	2	11,11,12	0.62	0	15,15,17	0.89	1 (6%)
2	MAN	Q	5	2	11,11,12	0.68	0	15,15,17	0.77	1 (6%)
2	MAN	Q	6	2	11,11,12	0.66	0	15,15,17	0.90	1 (6%)
2	MAN	Q	7	2	11,11,12	0.67	0	15,15,17	1.06	1 (6%)
2	MAN	Q	8	2	11,11,12	0.56	0	15,15,17	1.03	2 (13%)
3	NAG	R	1	3,1	14,14,15	0.43	0	17,19,21	0.75	1 (5%)
3	NAG	R	2	3	14,14,15	0.42	0	17,19,21	0.58	0
3	NAG	S	1	3,1	14,14,15	0.41	0	17,19,21	0.58	0
3	NAG	S	2	3	14,14,15	0.42	0	17,19,21	0.64	0
3	NAG	T	1	3,1	14,14,15	0.45	0	17,19,21	0.86	2 (11%)
3	NAG	T	2	3	14,14,15	0.42	0	17,19,21	0.61	0
3	NAG	U	1	3,1	14,14,15	0.44	0	17,19,21	0.83	1 (5%)
3	NAG	U	2	3	14,14,15	0.43	0	17,19,21	0.58	0
3	NAG	V	1	3,1	14,14,15	0.43	0	17,19,21	0.80	1 (5%)
3	NAG	V	2	3	14,14,15	0.44	0	17,19,21	0.76	0
2	NAG	W	1	2,1	14,14,15	0.41	0	17,19,21	0.71	1 (5%)
2	NAG	W	2	2	14,14,15	0.40	0	17,19,21	0.83	0
2	BMA	W	3	2	11,11,12	0.54	0	15,15,17	0.68	0
2	MAN	W	4	2	11,11,12	0.58	0	15,15,17	0.91	1 (6%)
2	MAN	W	5	2	11,11,12	0.68	0	15,15,17	0.76	1 (6%)
2	MAN	W	6	2	11,11,12	0.62	0	15,15,17	0.86	1 (6%)
2	MAN	W	7	2	11,11,12	0.65	0	15,15,17	1.03	1 (6%)
2	MAN	W	8	2	11,11,12	0.61	0	15,15,17	1.05	2 (13%)
3	NAG	X	1	3,1	14,14,15	0.43	0	17,19,21	0.71	0
3	NAG	X	2	3	14,14,15	0.44	0	17,19,21	0.62	0
3	NAG	Y	1	3,1	14,14,15	0.43	0	17,19,21	0.60	0
3	NAG	Y	2	3	14,14,15	0.43	0	17,19,21	0.64	0
3	NAG	Z	1	3,1	14,14,15	0.45	0	17,19,21	0.86	2 (11%)
3	NAG	Z	2	3	14,14,15	0.42	0	17,19,21	0.58	0
3	NAG	a	1	3,1	14,14,15	0.43	0	17,19,21	0.79	0
3	NAG	a	2	3	14,14,15	0.42	0	17,19,21	0.56	0
3	NAG	b	1	3,1	14,14,15	0.42	0	17,19,21	0.77	0
3	NAG	b	2	3	14,14,15	0.44	0	17,19,21	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	0/2/19/22	0/1/1/1
2	MAN	E	7	2	-	2/2/19/22	0/1/1/1
2	MAN	E	8	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	BMA	K	3	2	-	2/2/19/22	0/1/1/1
2	MAN	K	4	2	-	0/2/19/22	0/1/1/1
2	MAN	K	5	2	-	0/2/19/22	0/1/1/1
2	MAN	K	6	2	-	0/2/19/22	0/1/1/1
2	MAN	K	7	2	-	2/2/19/22	0/1/1/1
2	MAN	K	8	2	-	2/2/19/22	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	4/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	Q	3	2	-	2/2/19/22	0/1/1/1
2	MAN	Q	4	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	5	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	6	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	7	2	-	2/2/19/22	0/1/1/1
2	MAN	Q	8	2	-	2/2/19/22	0/1/1/1
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	U	2	3	-	4/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
2	NAG	W	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	BMA	W	3	2	-	2/2/19/22	0/1/1/1
2	MAN	W	4	2	-	0/2/19/22	0/1/1/1
2	MAN	W	5	2	-	0/2/19/22	0/1/1/1
2	MAN	W	6	2	-	0/2/19/22	0/1/1/1
2	MAN	W	7	2	-	2/2/19/22	0/1/1/1
2	MAN	W	8	2	-	2/2/19/22	0/1/1/1
3	NAG	X	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Y	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Z	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
3	NAG	a	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	3/6/23/26	0/1/1/1
3	NAG	b	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	7	MAN	C1-O5-C5	3.32	116.69	112.19
2	K	7	MAN	C1-O5-C5	3.29	116.65	112.19
2	Q	7	MAN	C1-O5-C5	3.24	116.58	112.19
2	W	7	MAN	C1-O5-C5	3.20	116.53	112.19
2	K	4	MAN	C1-O5-C5	2.90	116.12	112.19

There are no chirality outliers.

5 of 95 torsion outliers are listed below:

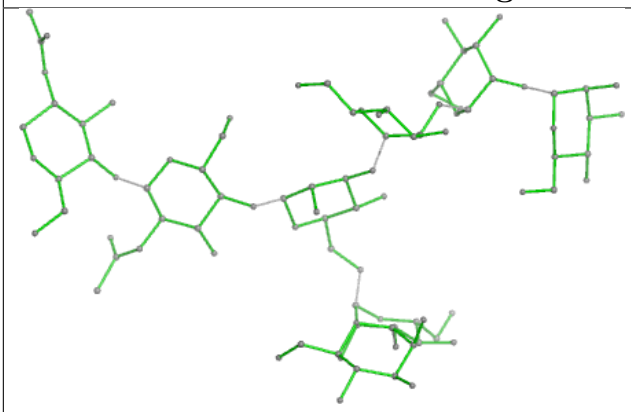
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2

There are no ring outliers.

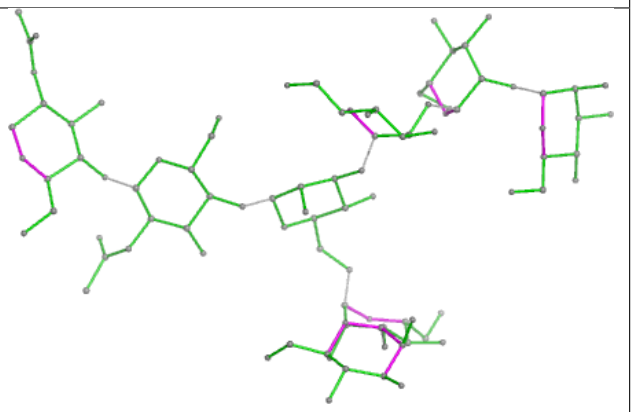
No monomer is involved in short contacts.

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

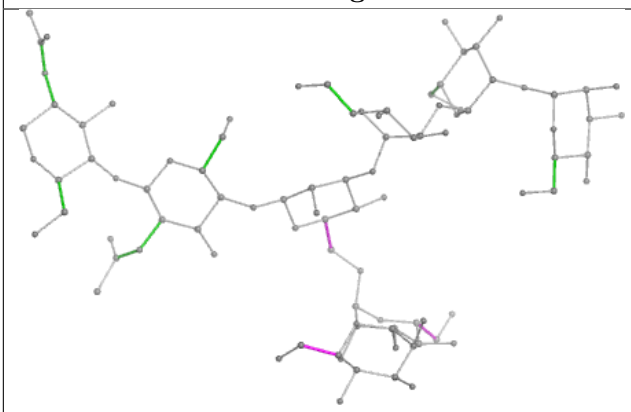
Oligosaccharide Chain E



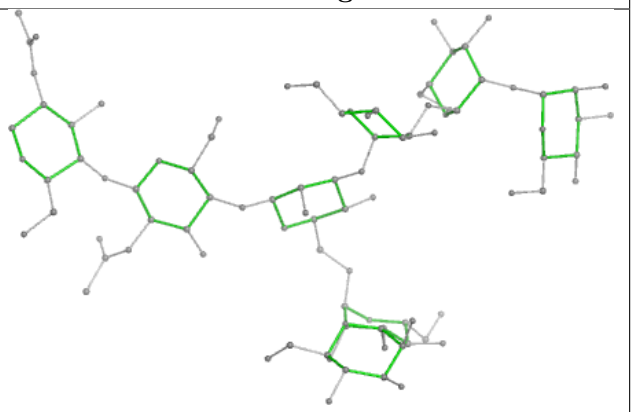
Bond lengths



Bond angles

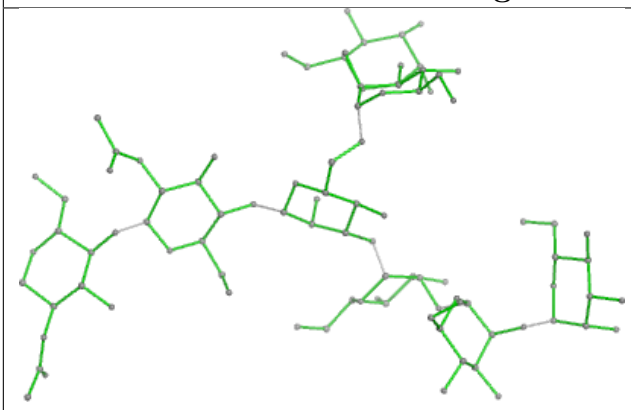


Torsions

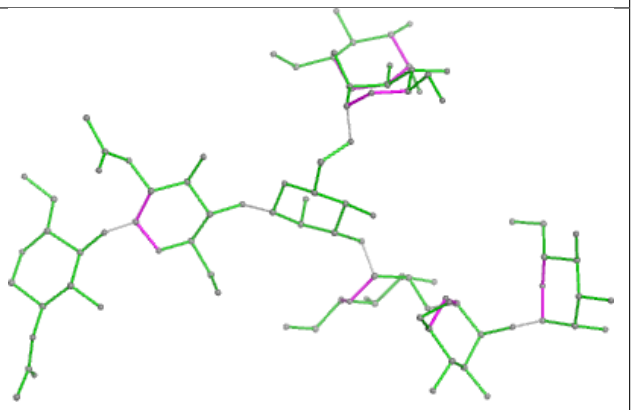


Rings

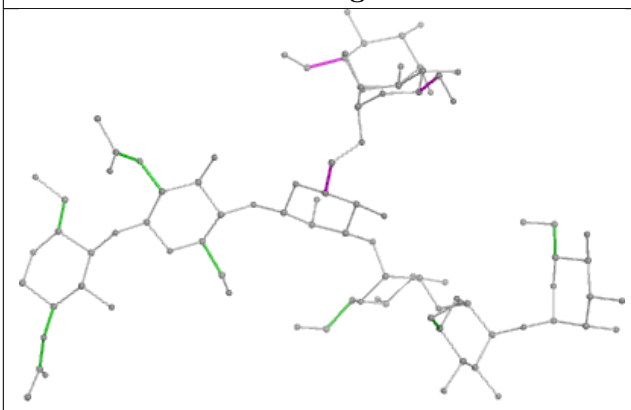
Oligosaccharide Chain K



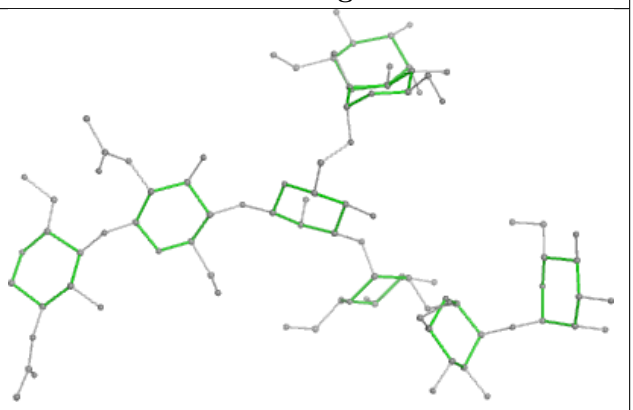
Bond lengths



Bond angles

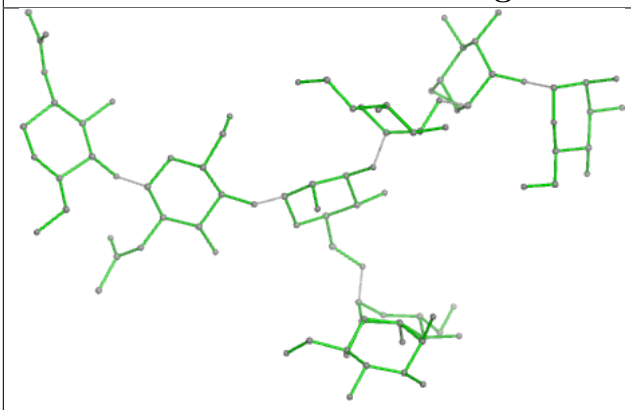


Torsions

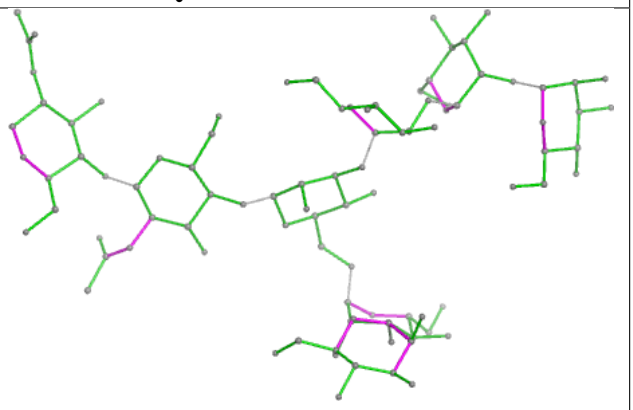


Rings

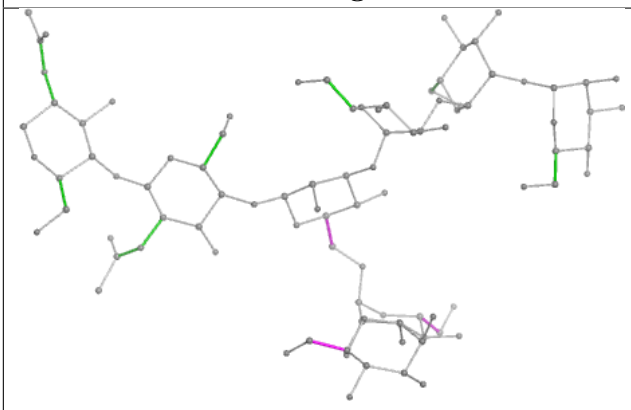
Oligosaccharide Chain Q



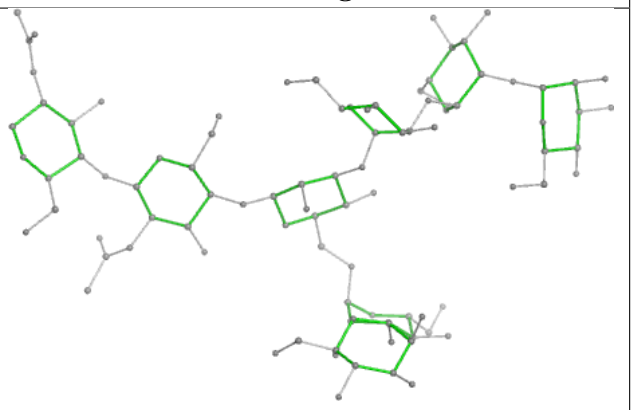
Bond lengths



Bond angles

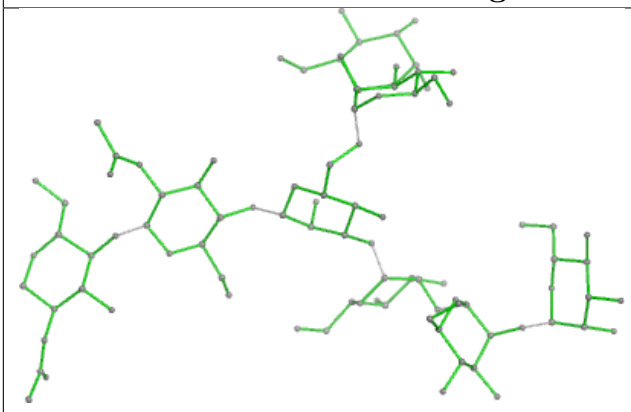


Torsions

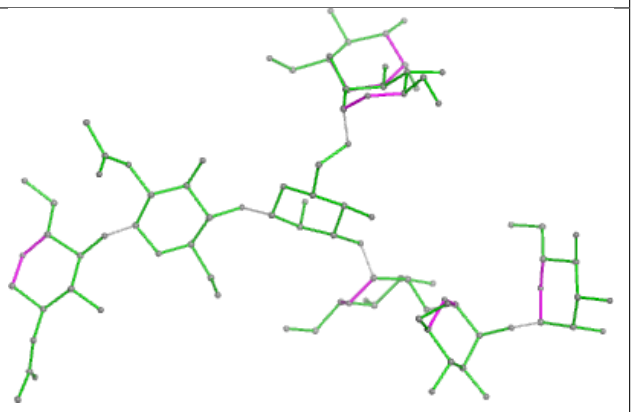


Rings

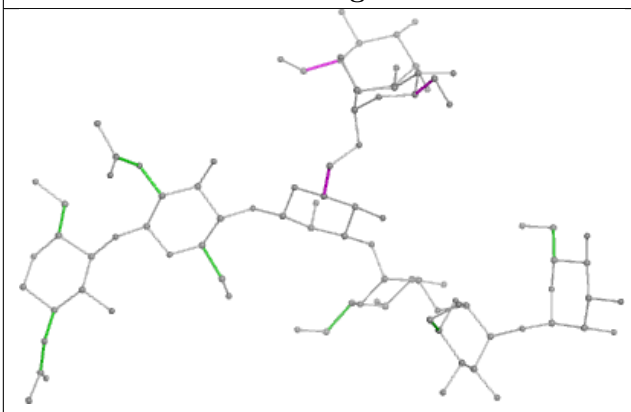
Oligosaccharide Chain W



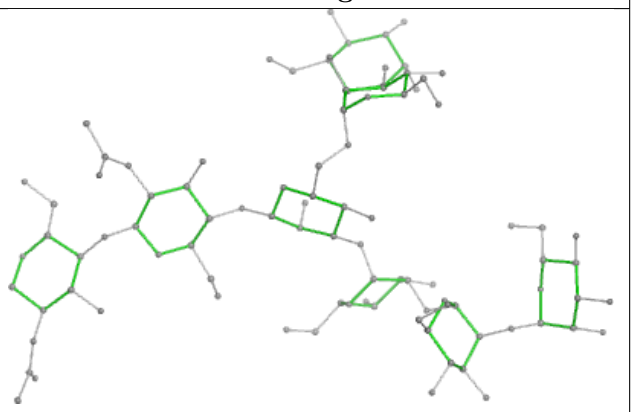
Bond lengths



Bond angles

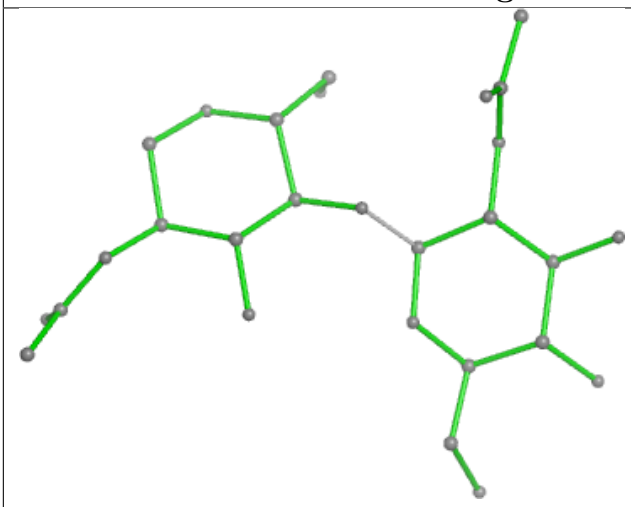


Torsions

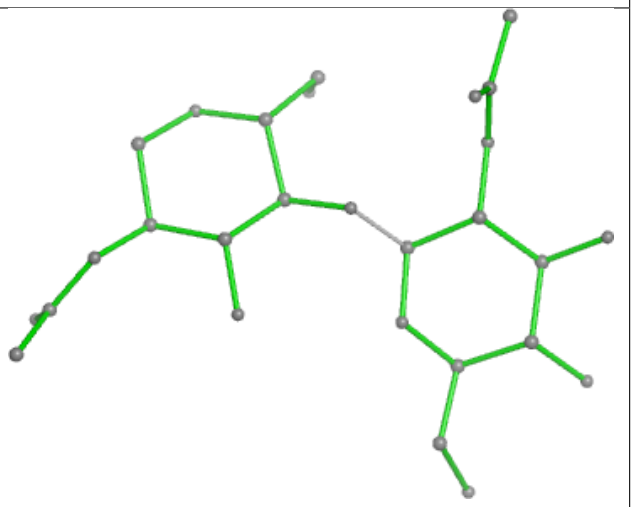


Rings

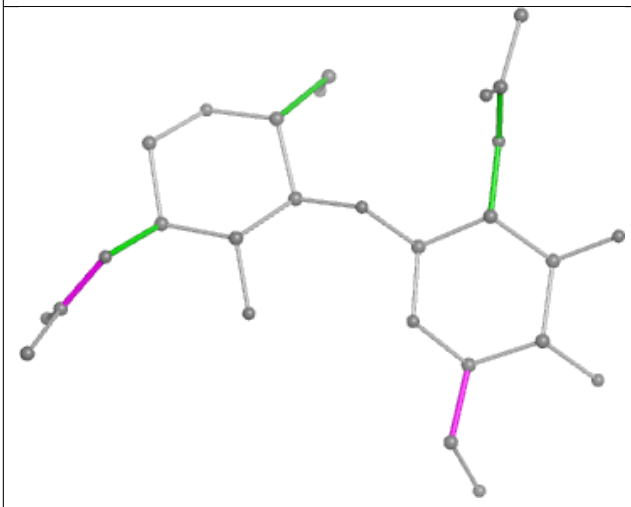
Oligosaccharide Chain F



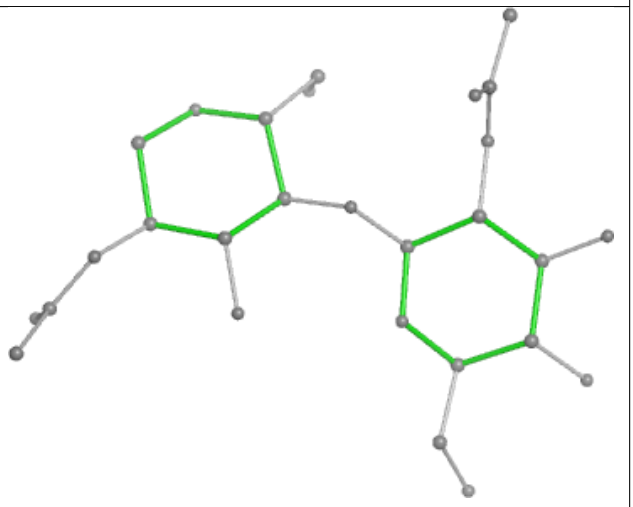
Bond lengths



Bond angles

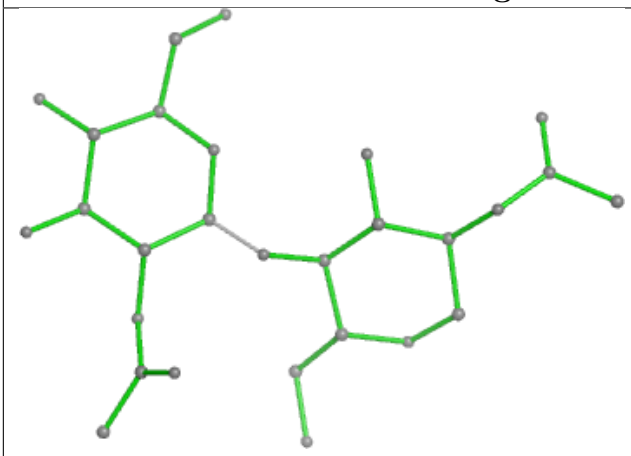


Torsions

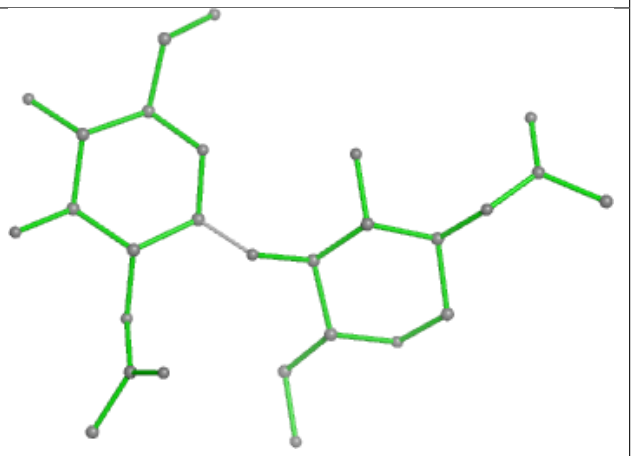


Rings

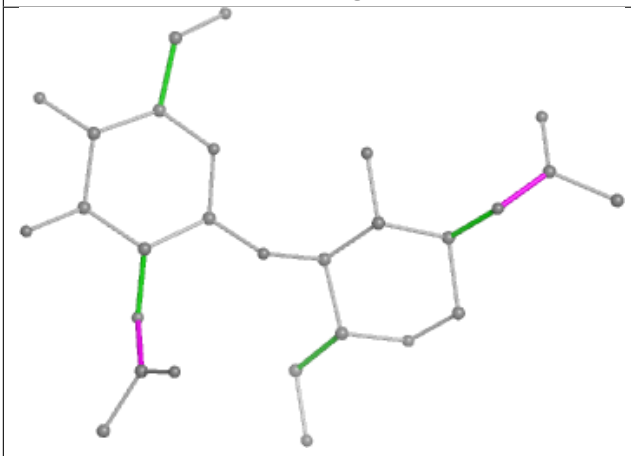
Oligosaccharide Chain G



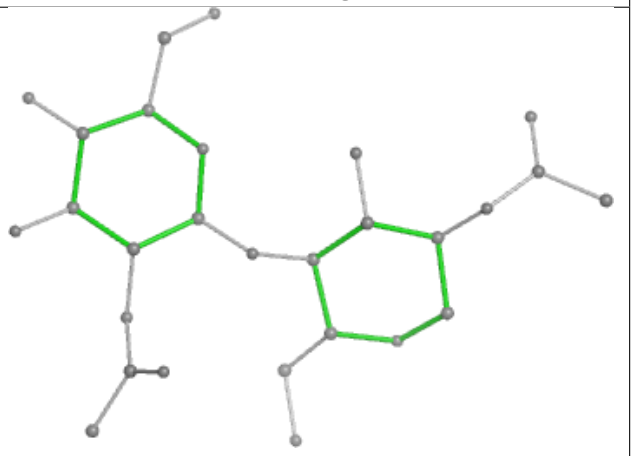
Bond lengths



Bond angles

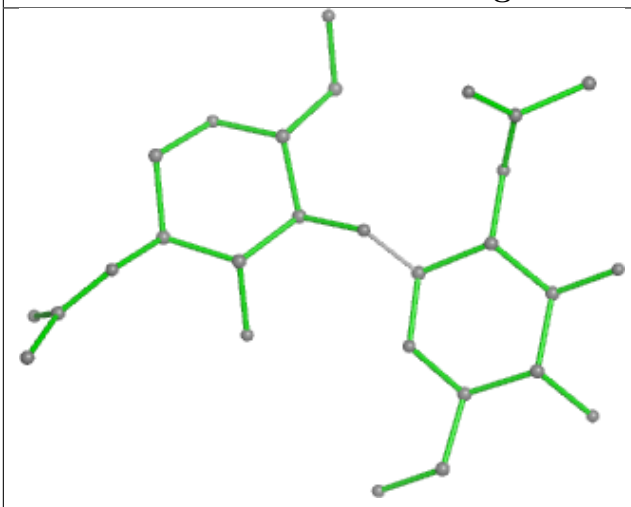


Torsions

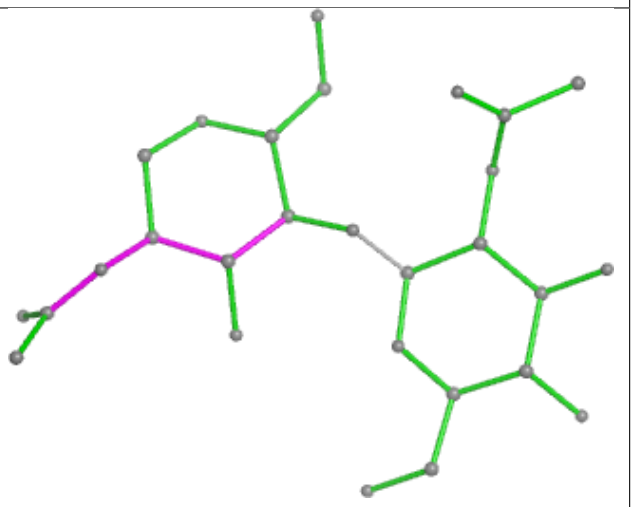


Rings

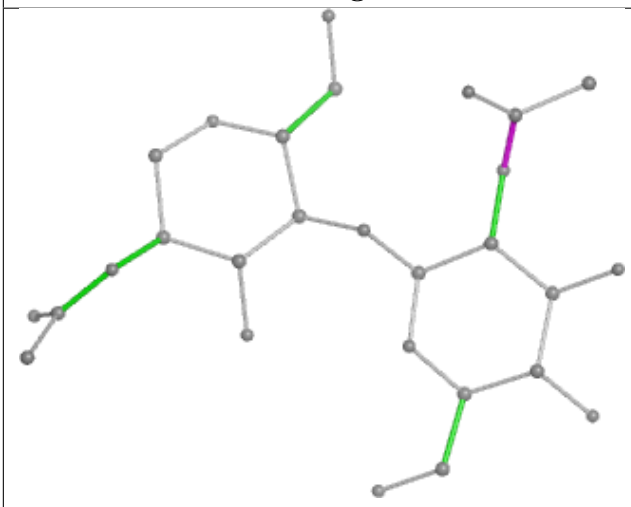
Oligosaccharide Chain H



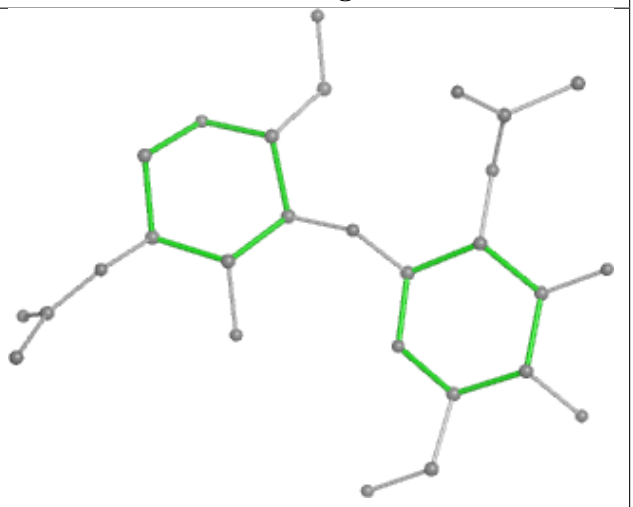
Bond lengths



Bond angles

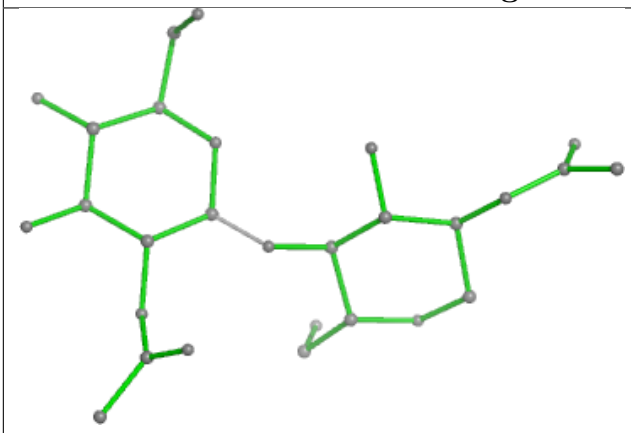


Torsions

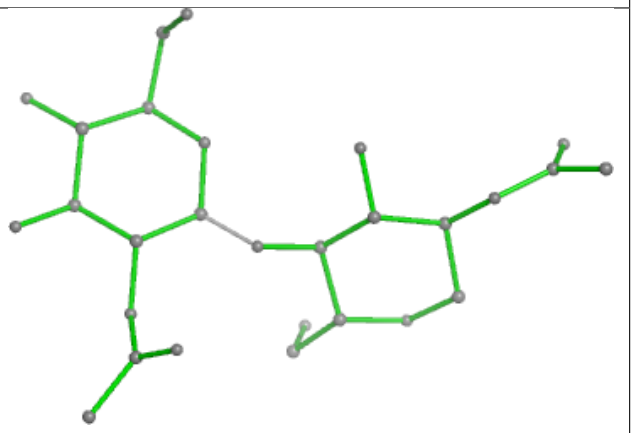


Rings

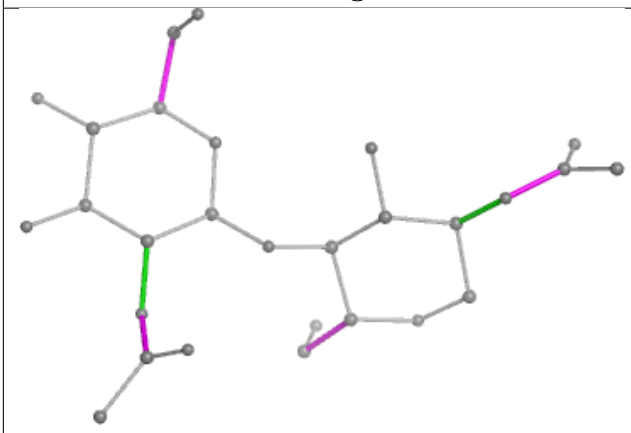
Oligosaccharide Chain I



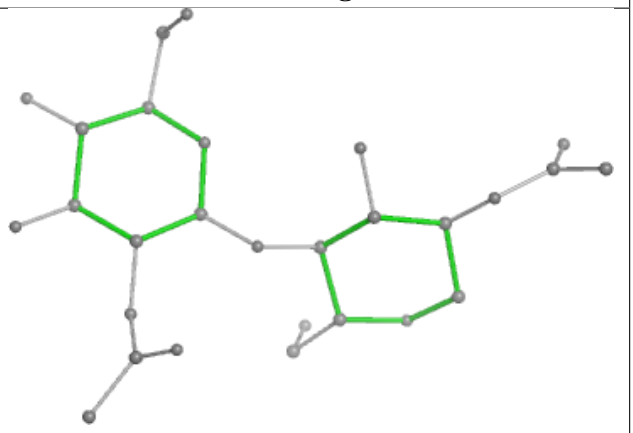
Bond lengths



Bond angles

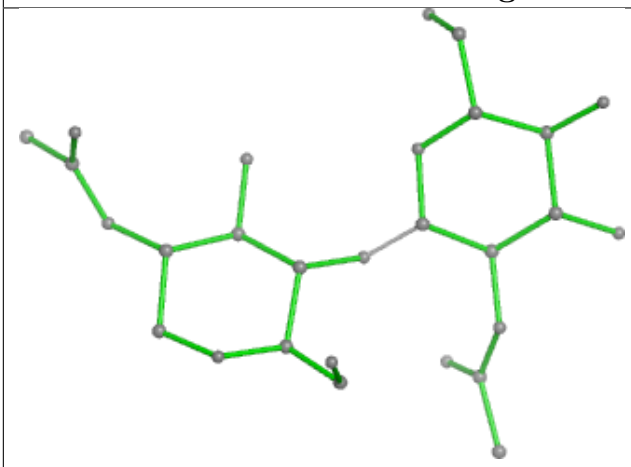


Torsions

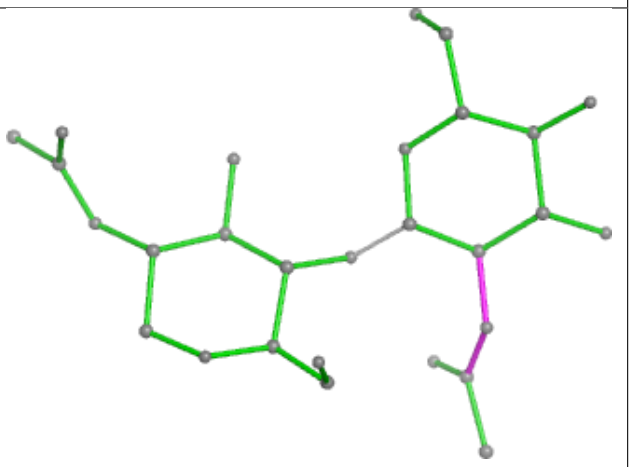


Rings

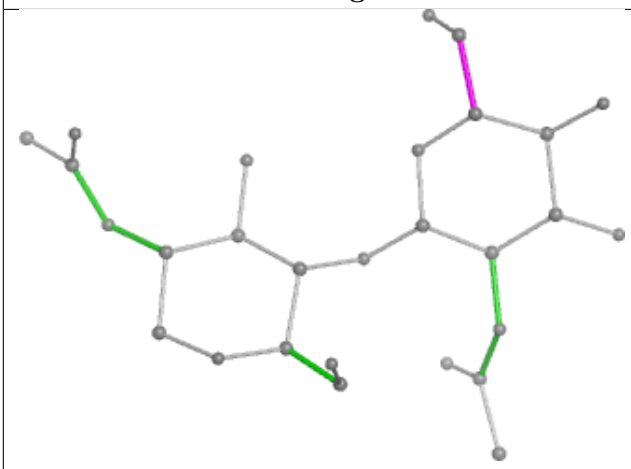
Oligosaccharide Chain J



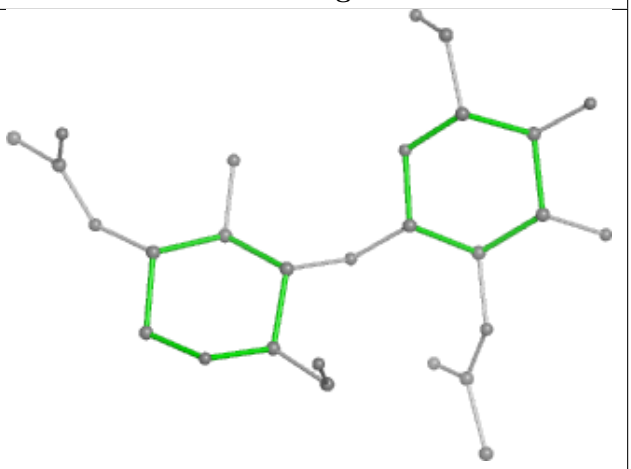
Bond lengths



Bond angles

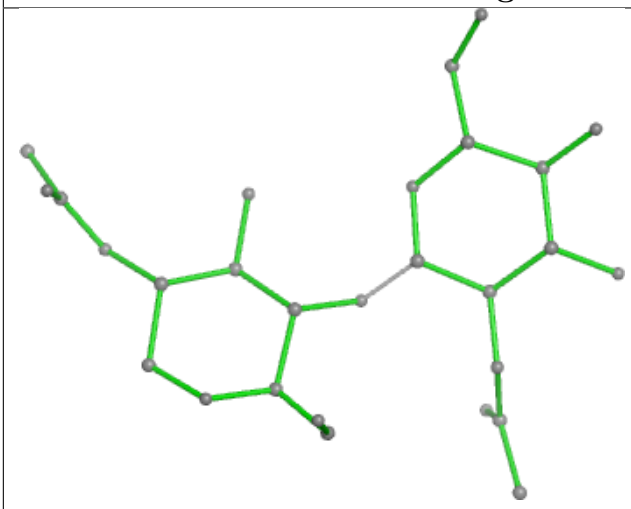


Torsions

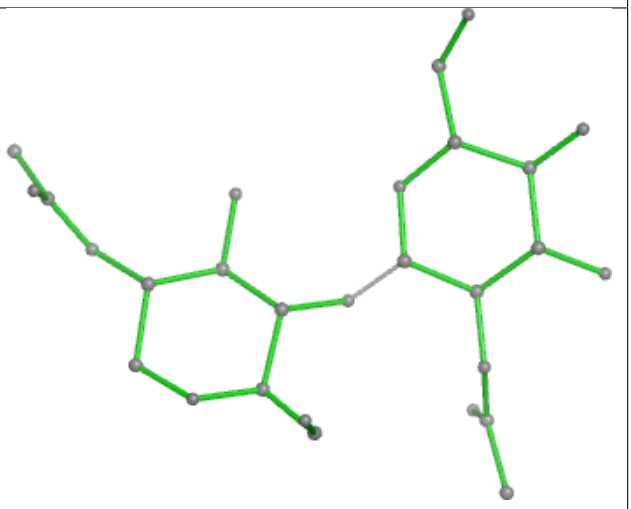


Rings

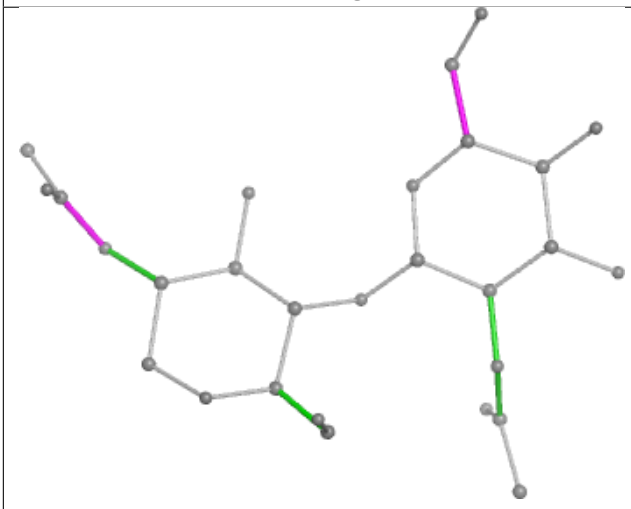
Oligosaccharide Chain L



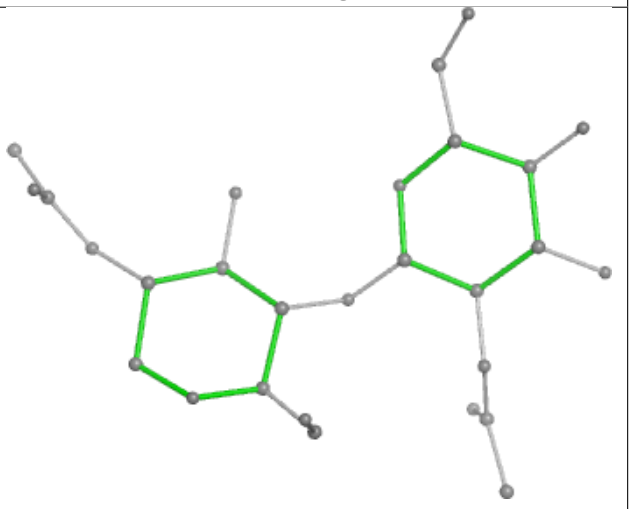
Bond lengths



Bond angles

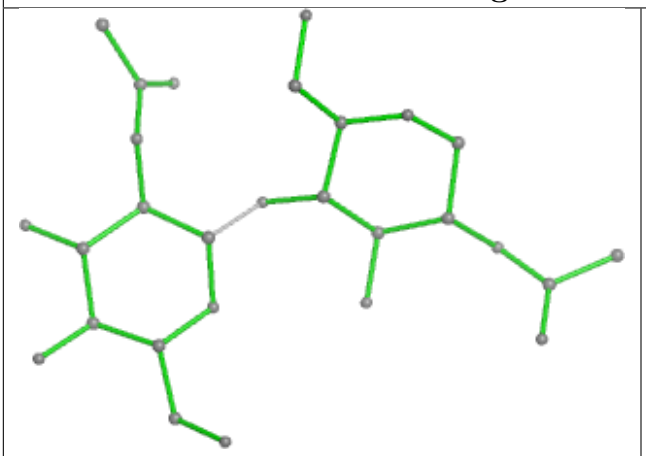


Torsions

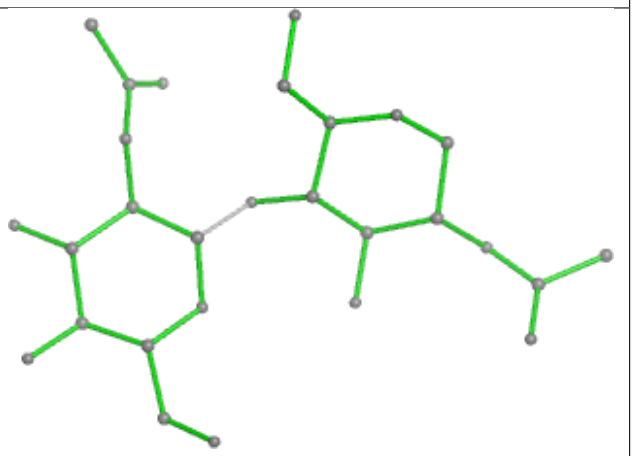


Rings

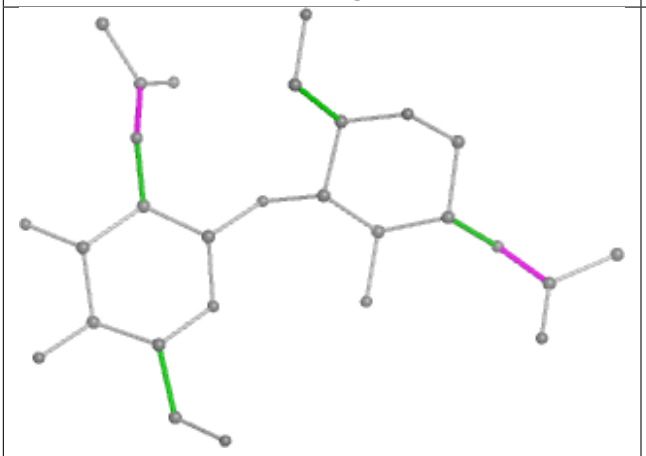
Oligosaccharide Chain M



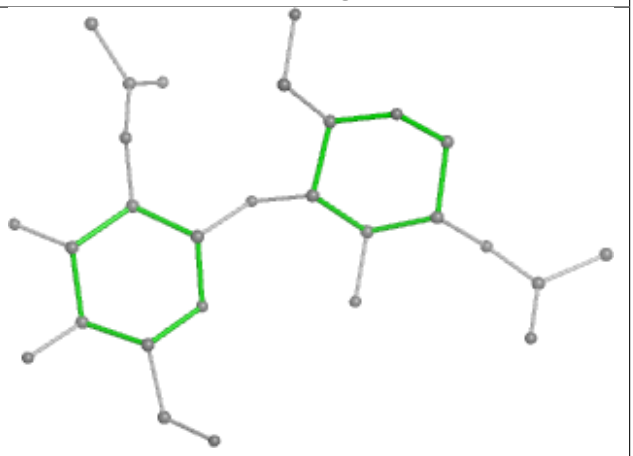
Bond lengths



Bond angles

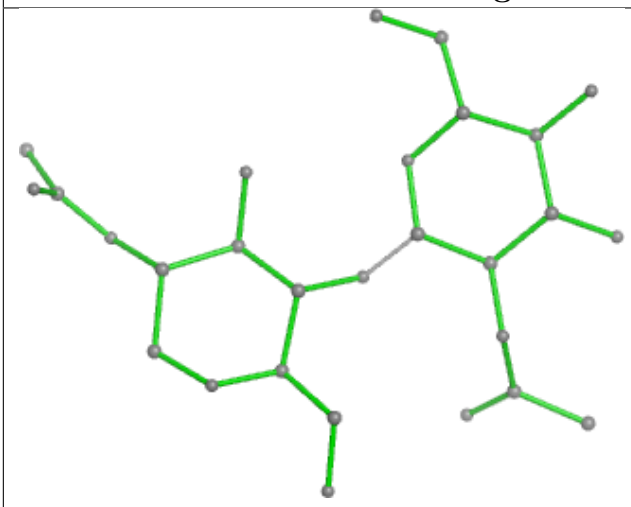


Torsions

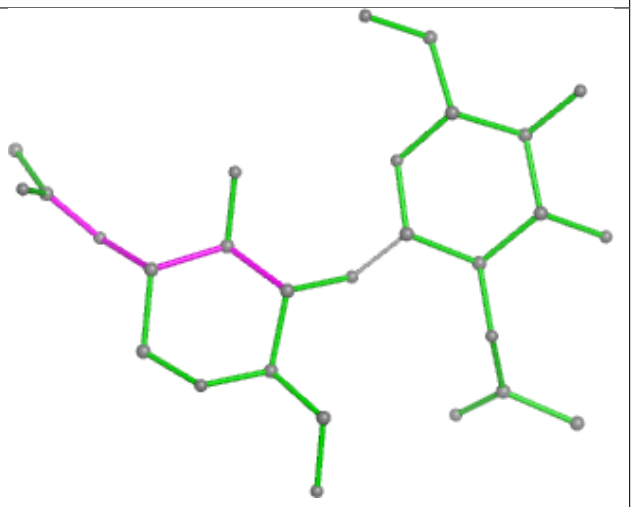


Rings

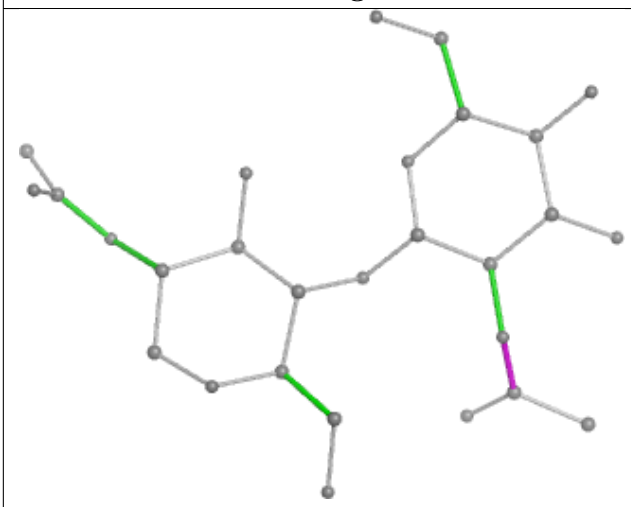
Oligosaccharide Chain N



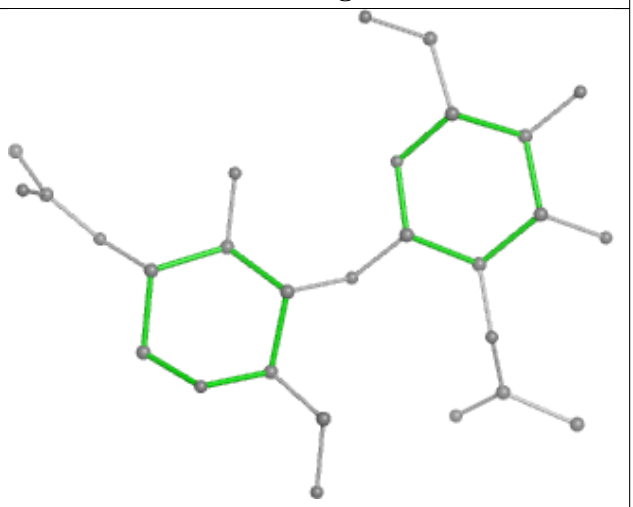
Bond lengths



Bond angles

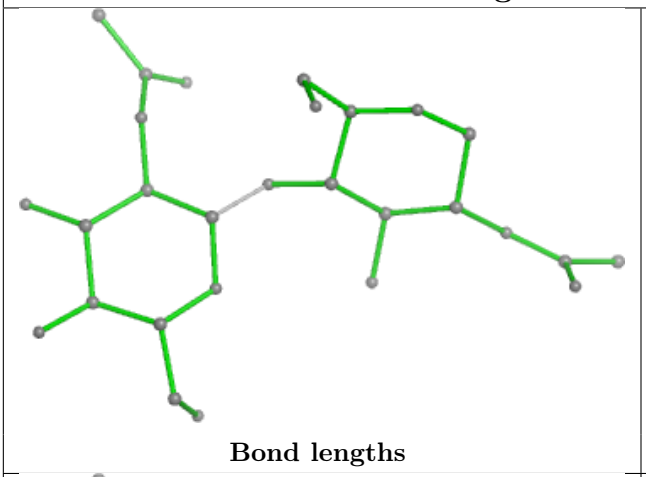


Torsions

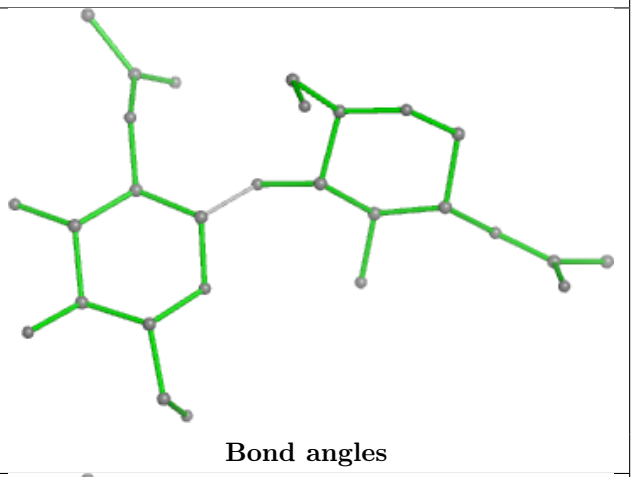


Rings

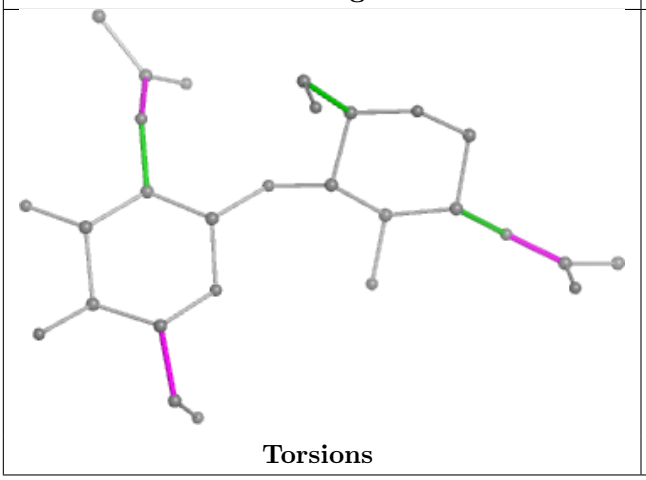
Oligosaccharide Chain O



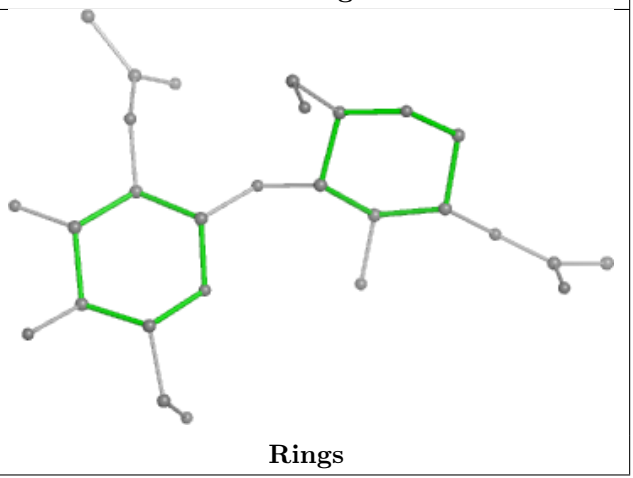
Bond lengths



Bond angles

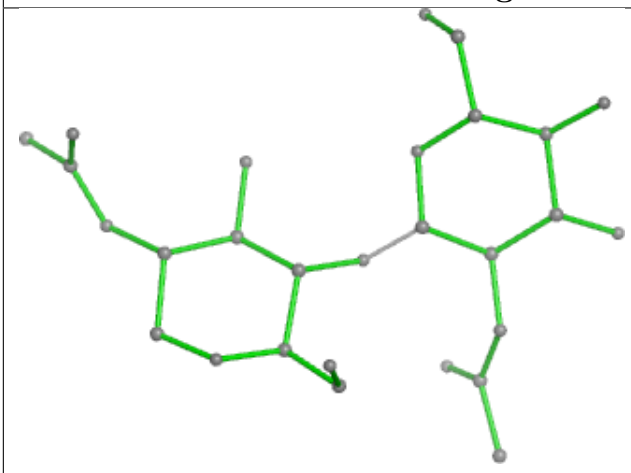


Torsions

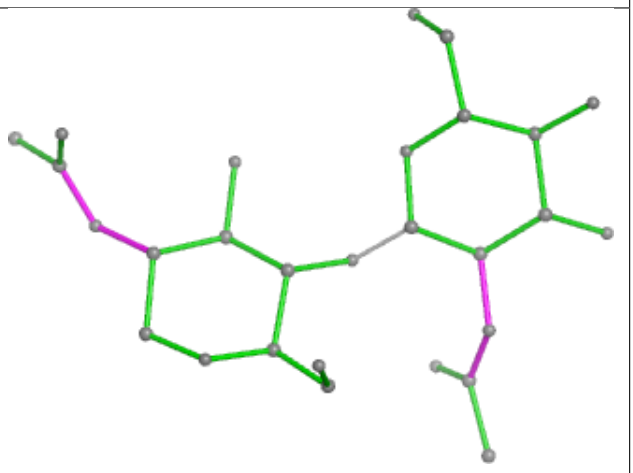


Rings

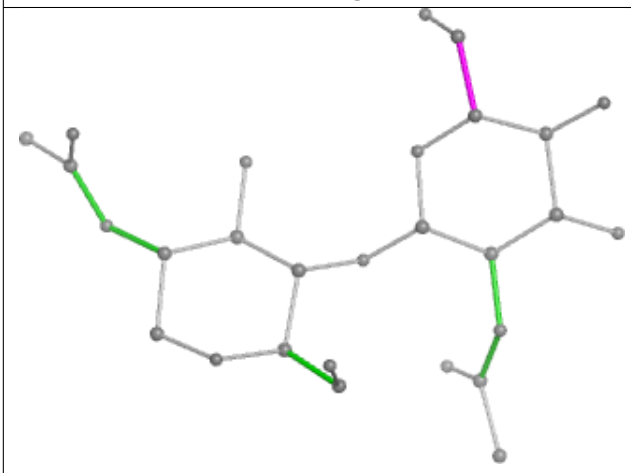
Oligosaccharide Chain P



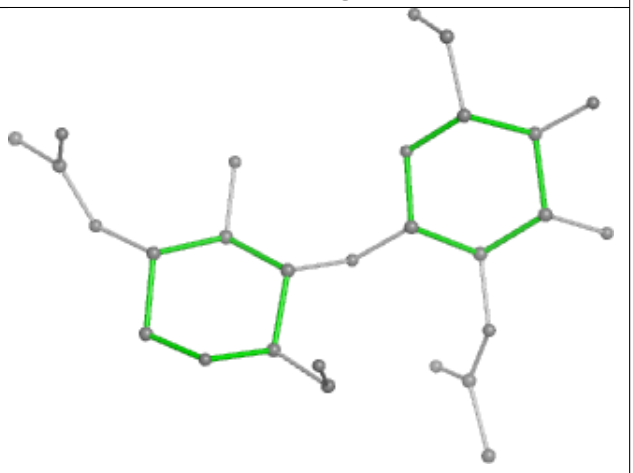
Bond lengths



Bond angles

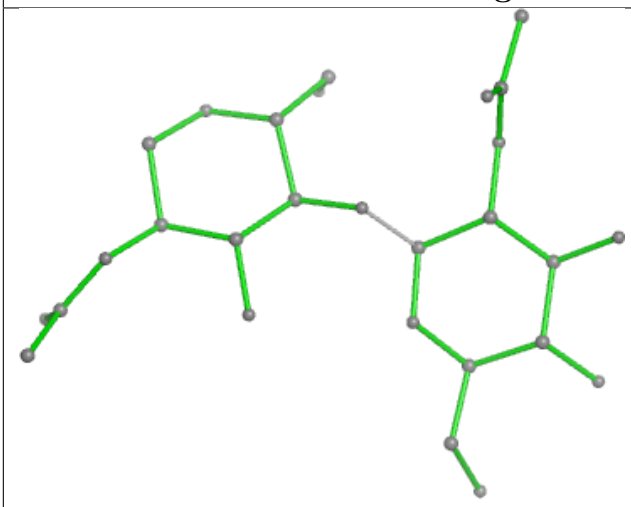


Torsions

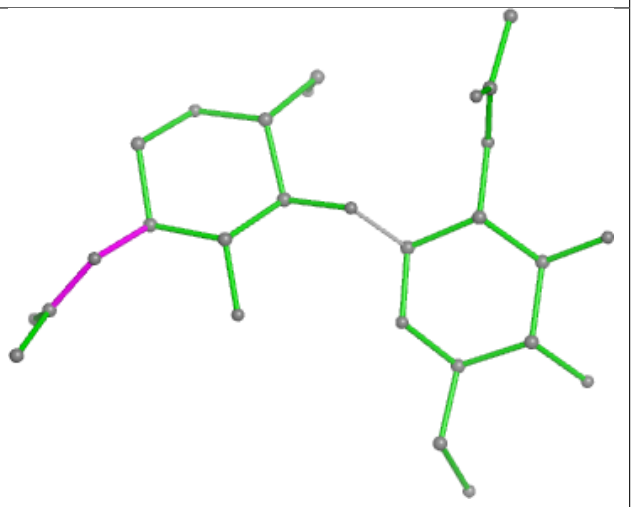


Rings

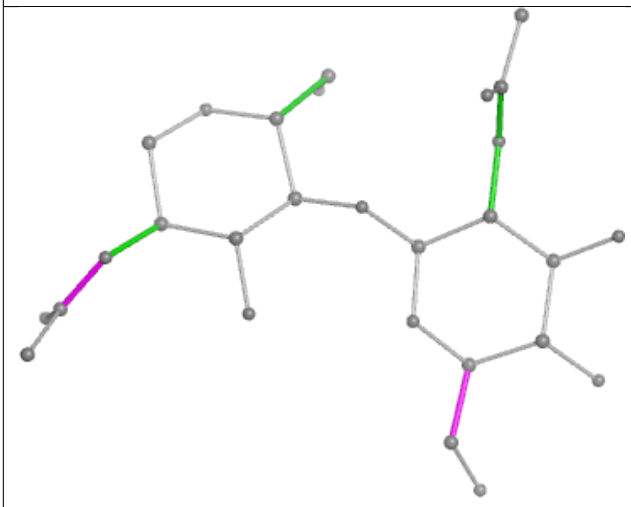
Oligosaccharide Chain R



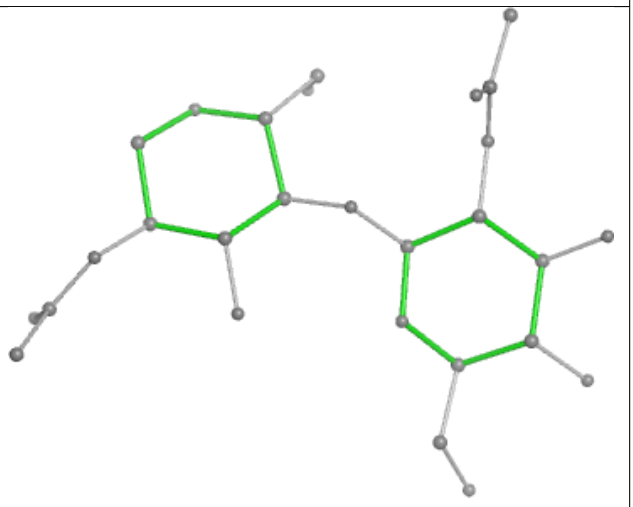
Bond lengths



Bond angles

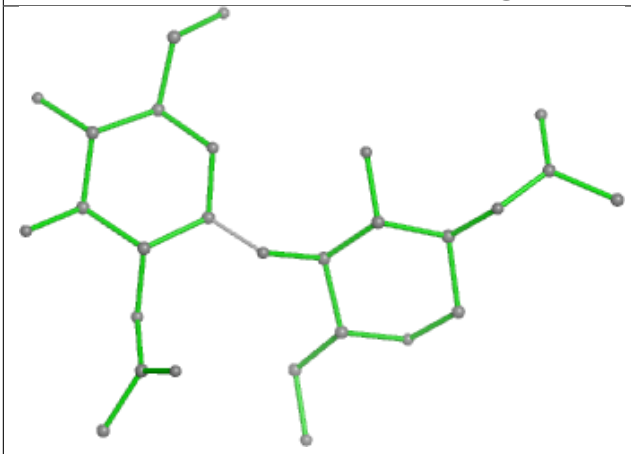


Torsions

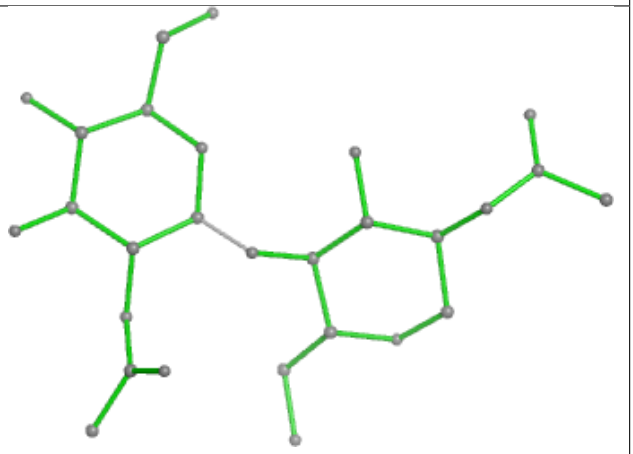


Rings

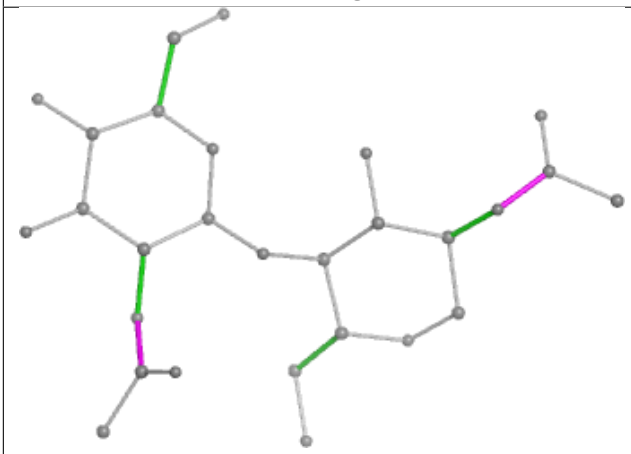
Oligosaccharide Chain S



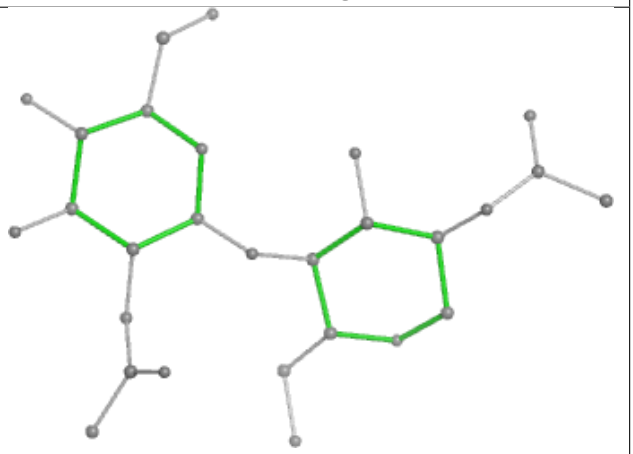
Bond lengths



Bond angles

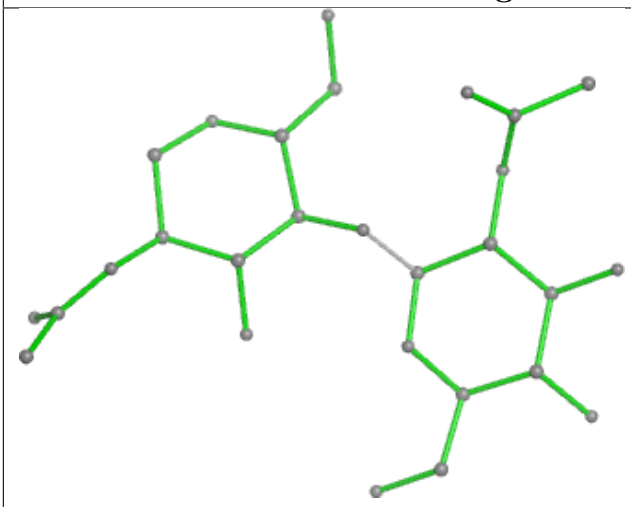


Torsions

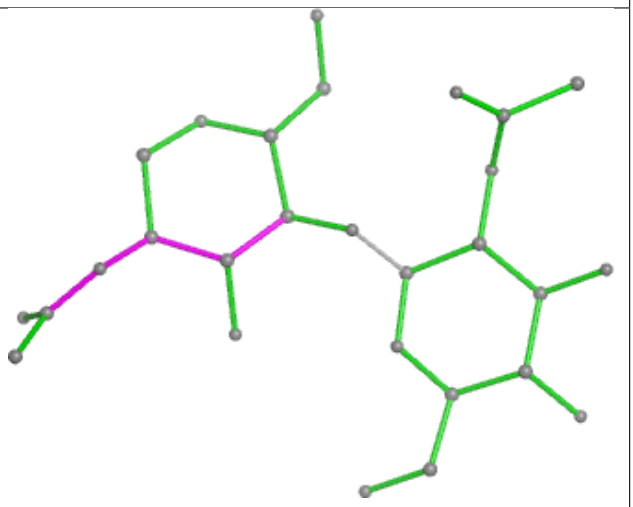


Rings

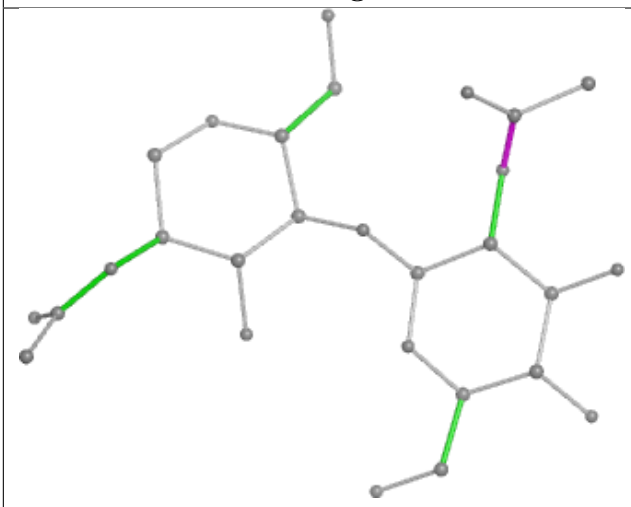
Oligosaccharide Chain T



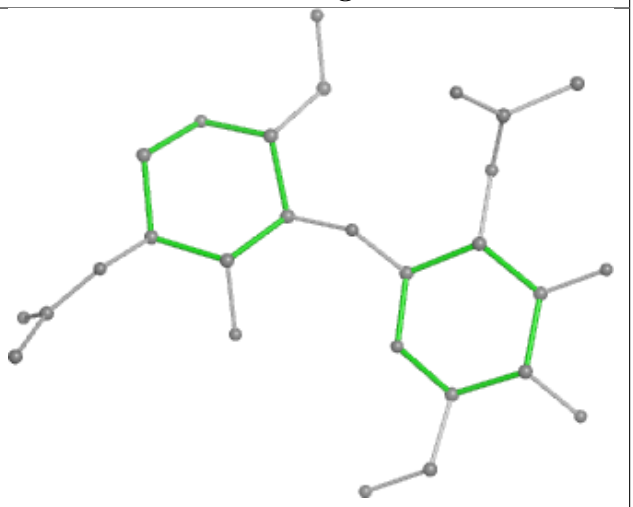
Bond lengths



Bond angles

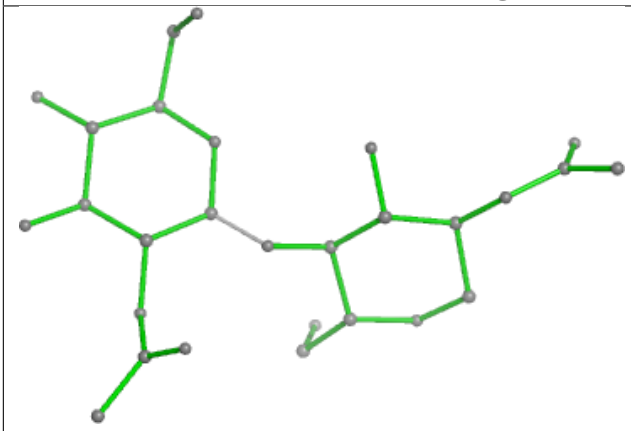


Torsions

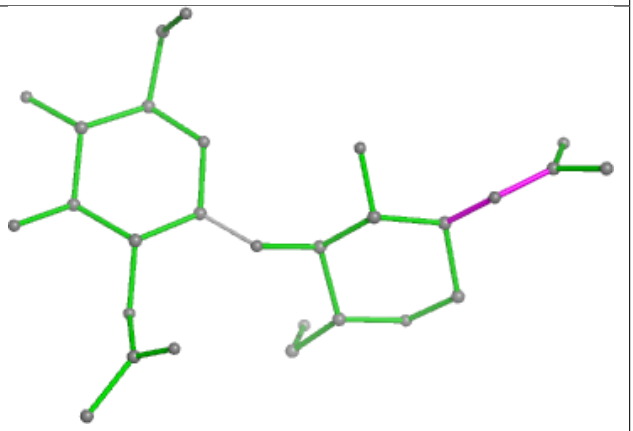


Rings

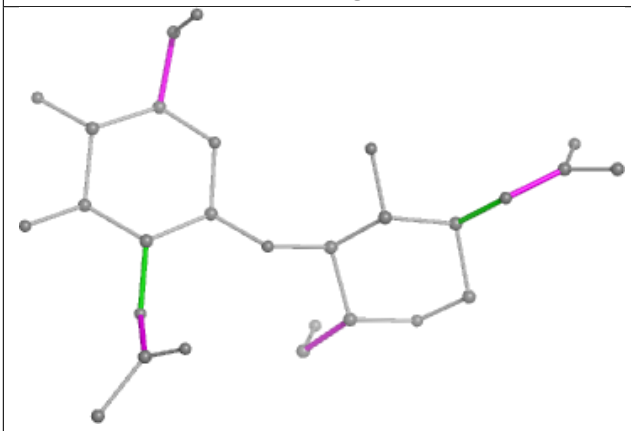
Oligosaccharide Chain U



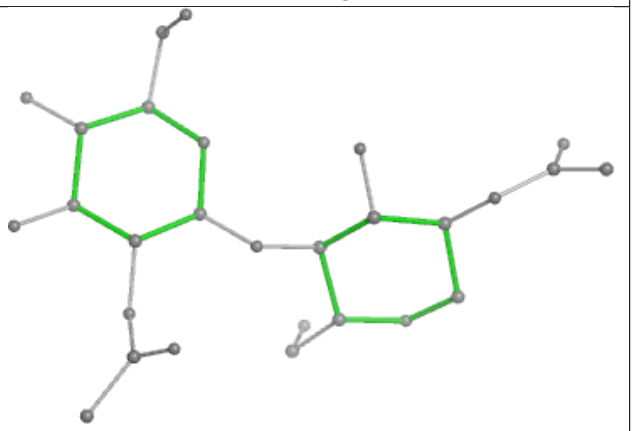
Bond lengths



Bond angles

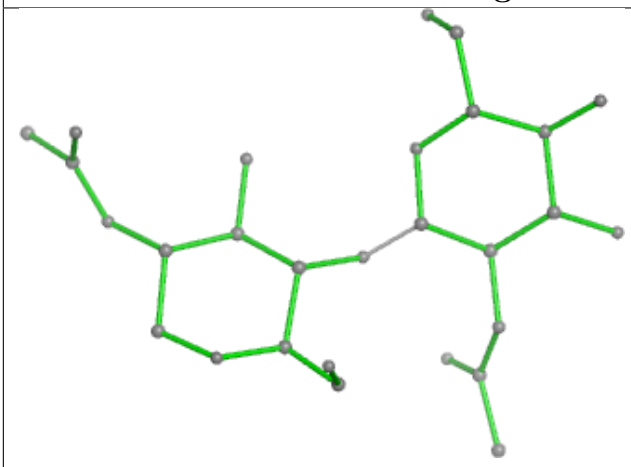


Torsions

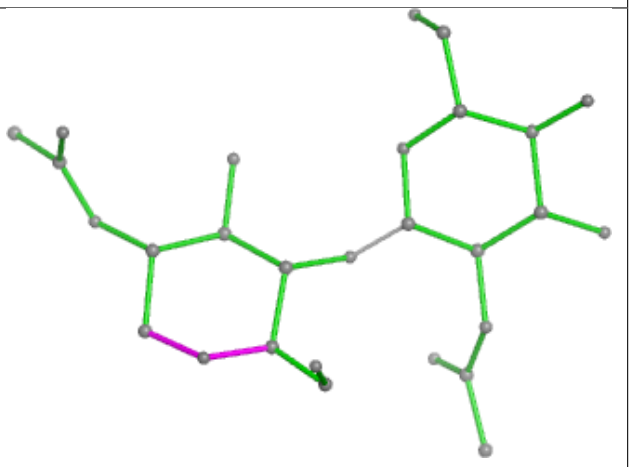


Rings

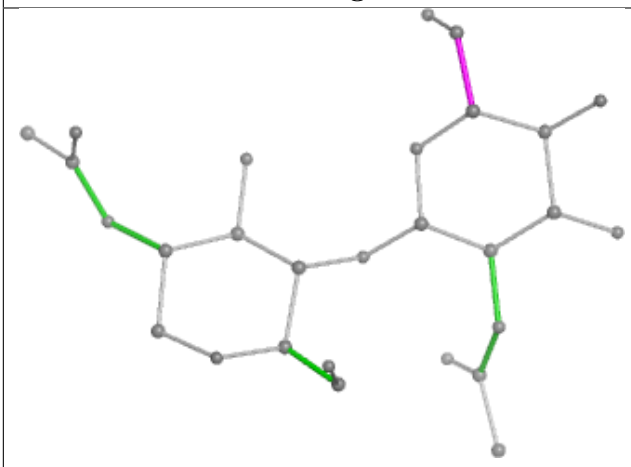
Oligosaccharide Chain V



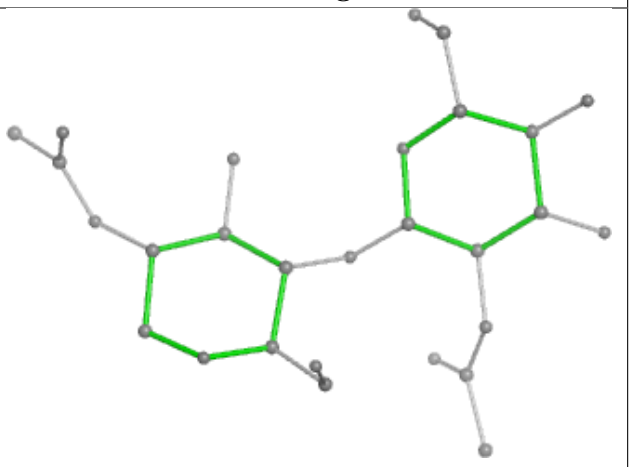
Bond lengths



Bond angles

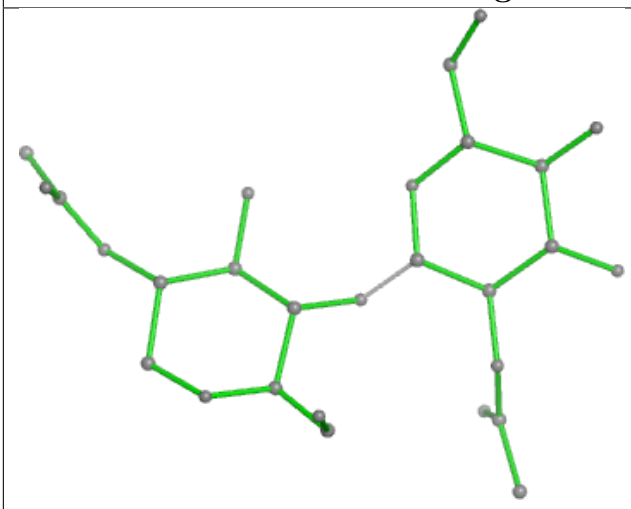


Torsions

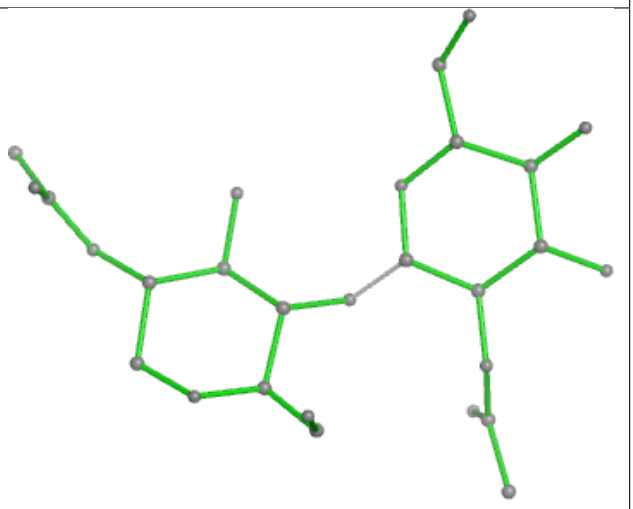


Rings

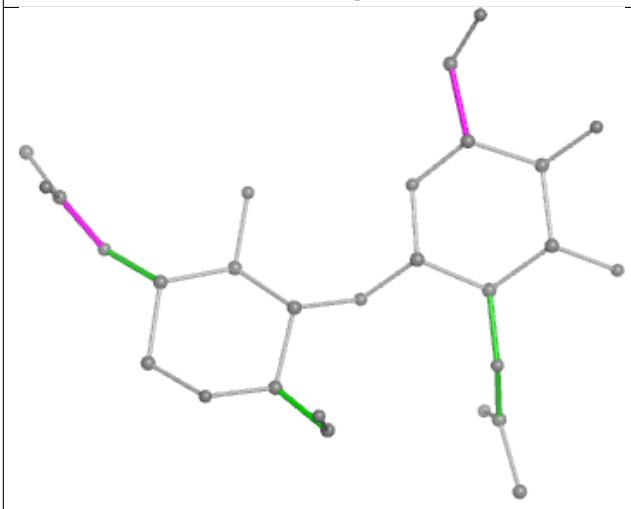
Oligosaccharide Chain X



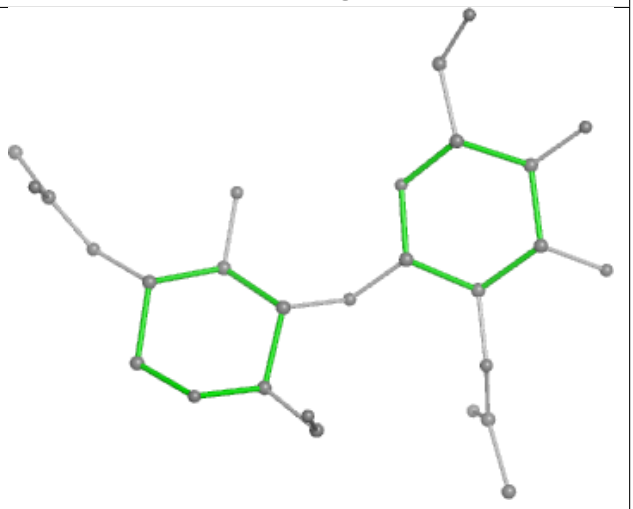
Bond lengths



Bond angles

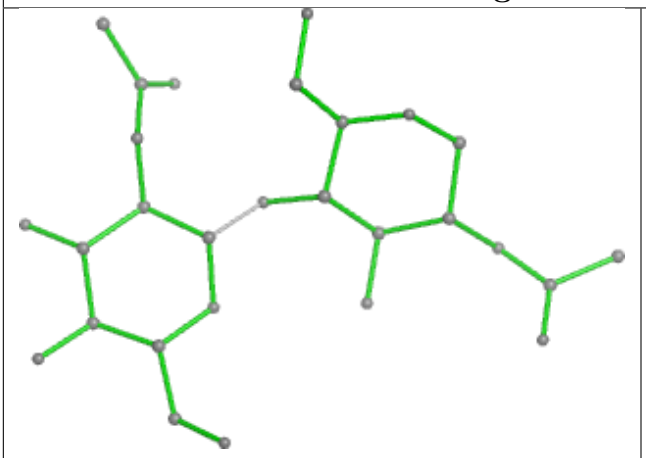


Torsions

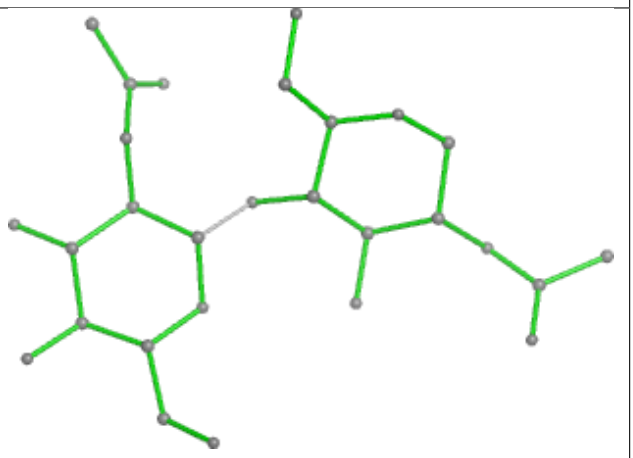


Rings

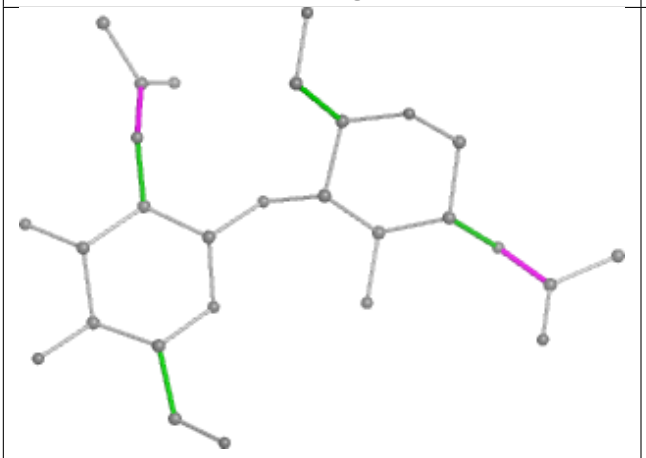
Oligosaccharide Chain Y



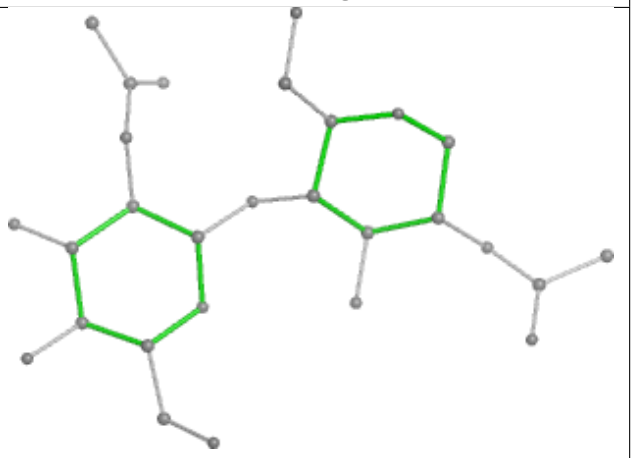
Bond lengths



Bond angles

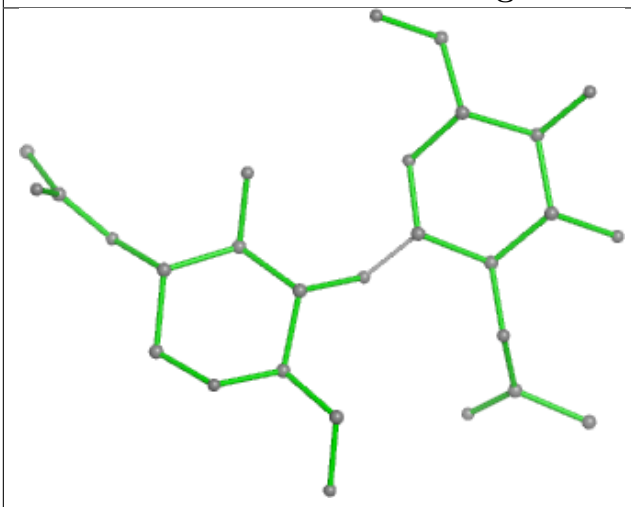


Torsions

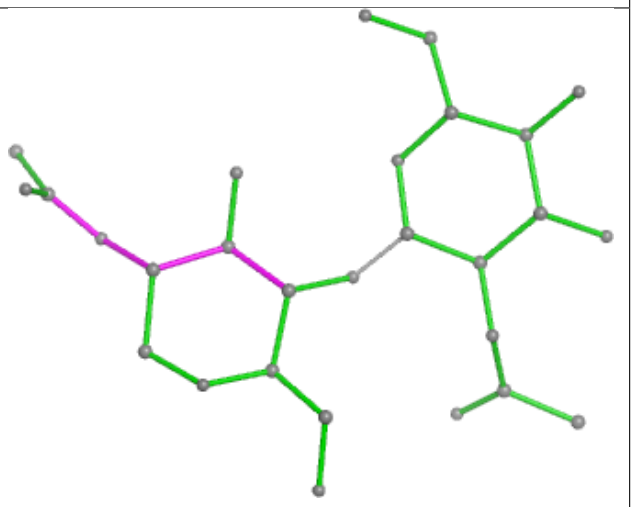


Rings

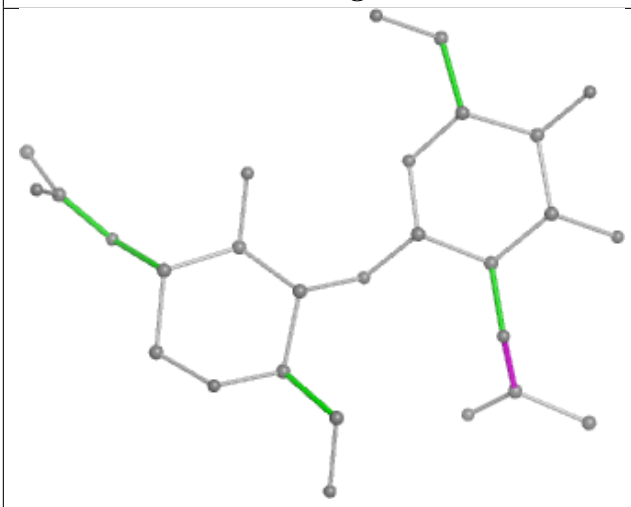
Oligosaccharide Chain Z



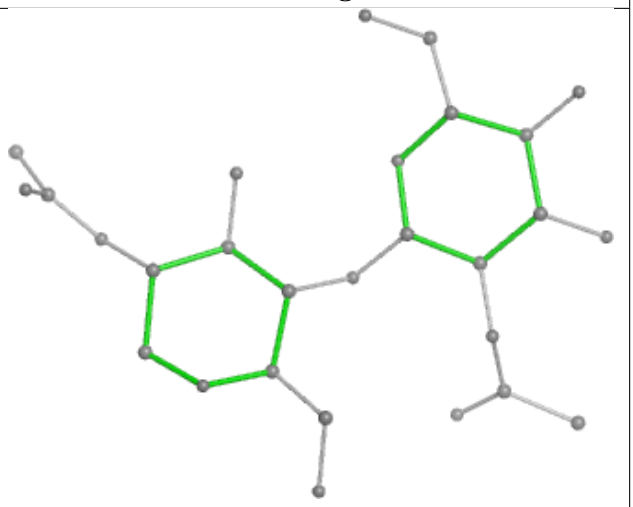
Bond lengths



Bond angles

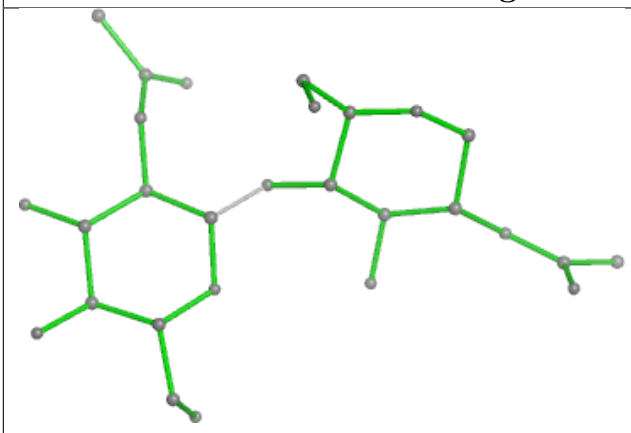


Torsions

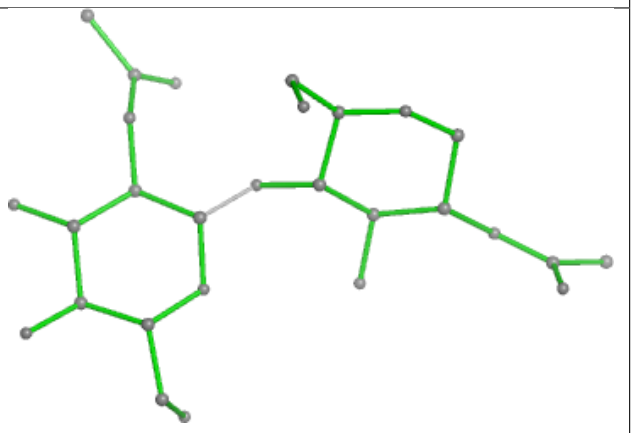


Rings

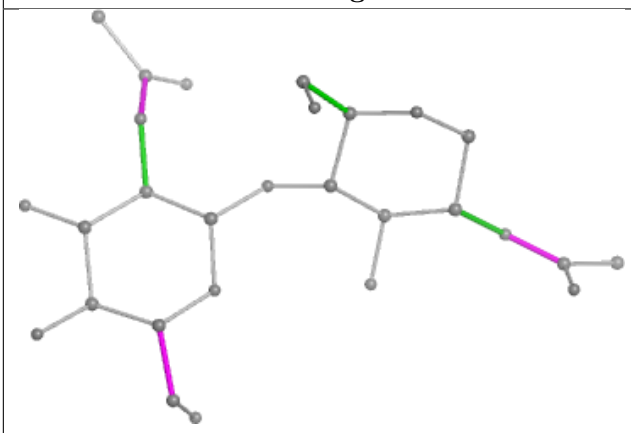
Oligosaccharide Chain a



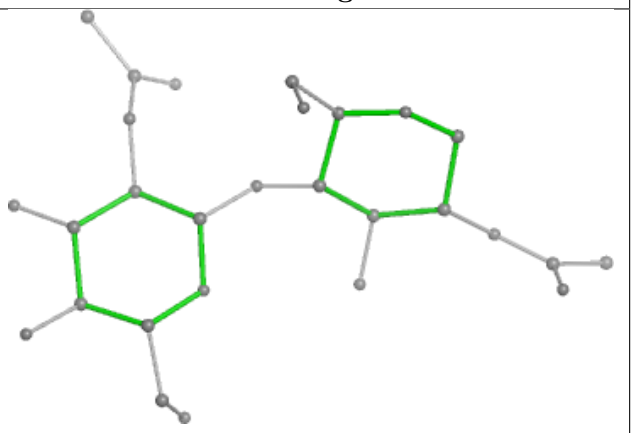
Bond lengths



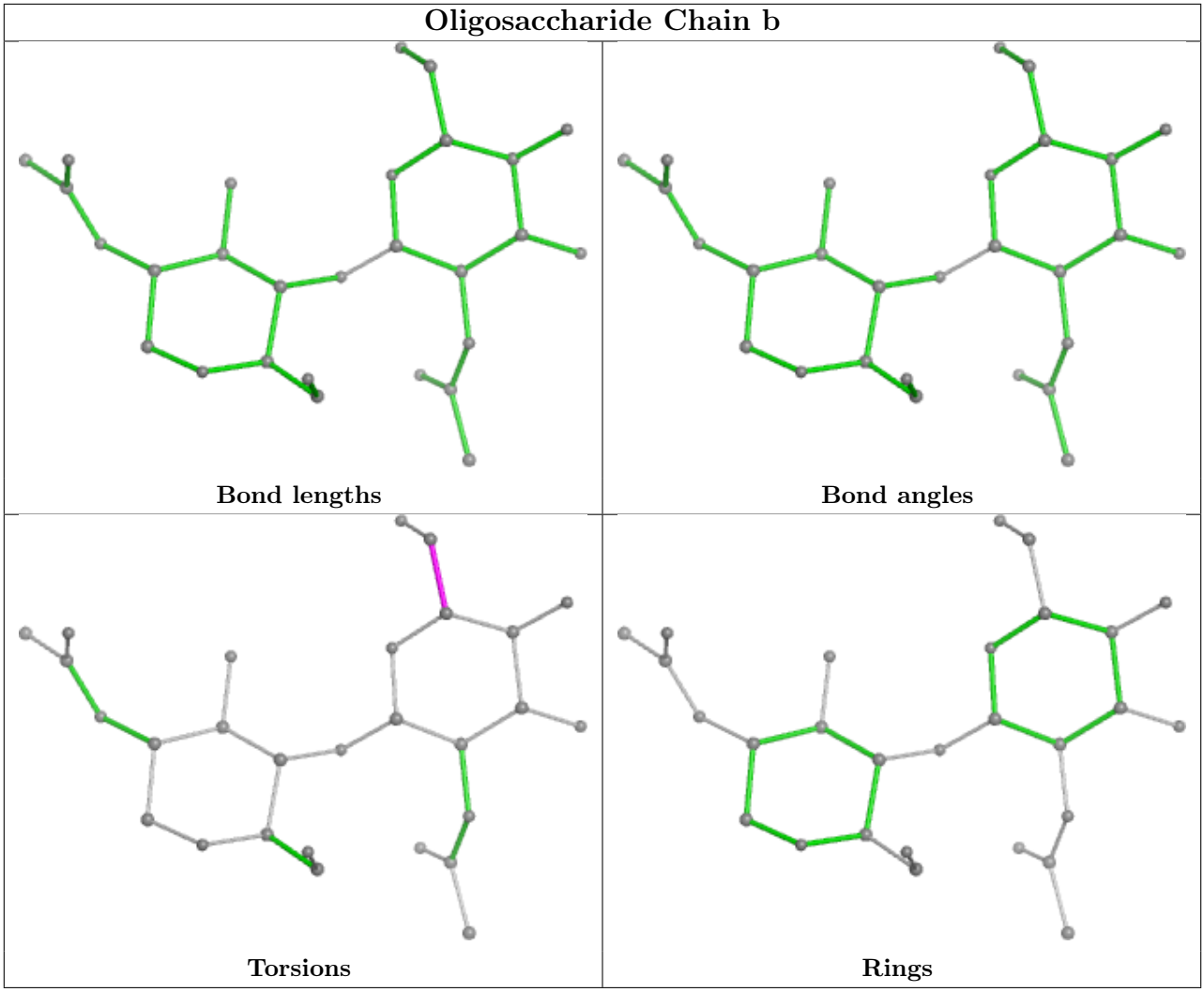
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

20 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	$\#\|Z\| > 2$
4	NAG	A	3019	1	14,14,15	0.44	0	17,19,21	0.68	0
4	NAG	B	3000	1	14,14,15	0.41	0	17,19,21	1.35	2 (11%)
4	NAG	A	3011	1	14,14,15	0.42	0	17,19,21	0.71	0
4	NAG	B	3014	1	14,14,15	0.44	0	17,19,21	1.47	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	3000	1	14,14,15	0.41	0	17,19,21	1.35	2 (11%)
4	NAG	A	3022	1	14,14,15	0.43	0	17,19,21	0.67	0
4	NAG	B	3019	1	14,14,15	0.44	0	17,19,21	0.70	0
4	NAG	A	3014	1	14,14,15	0.45	0	17,19,21	1.46	3 (17%)
4	NAG	D	3011	1	14,14,15	0.42	0	17,19,21	0.72	0
4	NAG	C	3011	1	14,14,15	0.42	0	17,19,21	0.72	0
4	NAG	D	3000	1	14,14,15	0.41	0	17,19,21	1.34	2 (11%)
4	NAG	D	3022	1	14,14,15	0.42	0	17,19,21	0.67	0
4	NAG	D	3014	1	14,14,15	0.45	0	17,19,21	1.45	3 (17%)
4	NAG	C	3000	1	14,14,15	0.42	0	17,19,21	1.35	2 (11%)
4	NAG	C	3014	1	14,14,15	0.45	0	17,19,21	1.43	3 (17%)
4	NAG	C	3022	1	14,14,15	0.42	0	17,19,21	0.70	0
4	NAG	B	3022	1	14,14,15	0.42	0	17,19,21	0.70	0
4	NAG	D	3019	1	14,14,15	0.44	0	17,19,21	0.69	0
4	NAG	C	3019	1	14,14,15	0.42	0	17,19,21	0.68	0
4	NAG	B	3011	1	14,14,15	0.43	0	17,19,21	0.69	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
4	NAG	A	3019	1	-	2/6/23/26	0/1/1/1
4	NAG	B	3000	1	-	3/6/23/26	0/1/1/1
4	NAG	A	3011	1	-	4/6/23/26	0/1/1/1
4	NAG	B	3014	1	-	5/6/23/26	0/1/1/1
4	NAG	A	3000	1	-	3/6/23/26	0/1/1/1
4	NAG	A	3022	1	-	2/6/23/26	0/1/1/1
4	NAG	B	3019	1	-	3/6/23/26	0/1/1/1
4	NAG	A	3014	1	-	5/6/23/26	0/1/1/1
4	NAG	D	3011	1	-	4/6/23/26	0/1/1/1
4	NAG	C	3011	1	-	4/6/23/26	0/1/1/1
4	NAG	D	3000	1	-	3/6/23/26	0/1/1/1
4	NAG	D	3022	1	-	2/6/23/26	0/1/1/1
4	NAG	D	3014	1	-	5/6/23/26	0/1/1/1
4	NAG	C	3000	1	-	3/6/23/26	0/1/1/1
4	NAG	C	3014	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	3022	1	-	2/6/23/26	0/1/1/1
4	NAG	B	3022	1	-	2/6/23/26	0/1/1/1
4	NAG	D	3019	1	-	3/6/23/26	0/1/1/1
4	NAG	C	3019	1	-	2/6/23/26	0/1/1/1
4	NAG	B	3011	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3014	NAG	C2-N2-C7	4.17	128.84	122.90
4	B	3014	NAG	C2-N2-C7	4.07	128.70	122.90
4	D	3014	NAG	C2-N2-C7	4.07	128.70	122.90
4	A	3000	NAG	C1-C2-N2	4.02	117.36	110.49
4	B	3000	NAG	C1-C2-N2	4.02	117.35	110.49

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3000	NAG	C8-C7-N2-C2
4	A	3000	NAG	O7-C7-N2-C2
4	A	3019	NAG	C8-C7-N2-C2
4	A	3019	NAG	O7-C7-N2-C2
4	A	3022	NAG	O7-C7-N2-C2

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

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	1836/1859 (98%)	1.37	449 (24%)	2	2	22, 80, 142, 183	1 (0%)
1	B	1836/1859 (98%)	1.25	382 (20%)	3	3	28, 74, 129, 163	1 (0%)
1	C	1836/1859 (98%)	0.87	236 (12%)	9	9	21, 57, 103, 143	1 (0%)
1	D	1836/1859 (98%)	1.23	387 (21%)	3	3	28, 72, 136, 176	1 (0%)
All	All	7344/7436 (98%)	1.18	1454 (19%)	3	3	21, 71, 130, 183	4 (0%)

The worst 5 of 1454 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2202	TRP	8.2
1	B	1493	LEU	7.6
1	A	2220	LEU	7.1
1	A	1493	LEU	7.0
1	C	1486	VAL	6.9

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

SUGAR-RSR INFOmissingINFO

6.4 Ligands

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
4	NAG	A	3019	14/15	0.42	0.19	183,185,186,186	0
4	NAG	B	3019	14/15	0.49	0.17	128,131,135,135	0
4	NAG	D	3019	14/15	0.50	0.19	123,126,128,130	0
4	NAG	C	3019	14/15	0.53	0.18	116,118,120,121	0
4	NAG	A	3014	14/15	0.64	0.21	110,113,116,116	0
4	NAG	B	3022	14/15	0.64	0.16	145,148,152,152	0
4	NAG	B	3011	14/15	0.65	0.22	106,109,111,112	0
4	NAG	B	3014	14/15	0.66	0.19	91,95,100,102	0
4	NAG	C	3014	14/15	0.67	0.20	92,96,96,96	0
4	NAG	C	3011	14/15	0.68	0.20	87,92,93,95	0
4	NAG	A	3000	14/15	0.69	0.19	184,187,188,188	0
4	NAG	A	3022	14/15	0.69	0.16	134,137,139,139	0
4	NAG	B	3000	14/15	0.70	0.19	166,170,173,174	0
4	NAG	C	3000	14/15	0.70	0.18	121,122,124,124	0
4	NAG	D	3000	14/15	0.70	0.18	150,156,159,160	0
4	NAG	D	3014	14/15	0.70	0.18	96,100,101,102	0
4	NAG	A	3011	14/15	0.70	0.18	98,103,107,108	0
4	NAG	D	3022	14/15	0.75	0.14	124,127,128,128	0
4	NAG	D	3011	14/15	0.77	0.17	117,120,124,125	0
4	NAG	C	3022	14/15	0.78	0.13	111,113,114,115	0

6.5 Other polymers (i)

There are no such residues in this entry.