wwPDB EM Validation Summary Report

Jun 28, 2026 – 01:09 AM JST

PDB ID	:	9UFE / pdb_00009ufe
EMDB ID	:	EMD-64106
Title	:	Cryo-EM structure of the tubular mastigoneme (the central tube) from golden algae 2.17 angstrom resolution
Authors	:	Huang, J.; Tao, H.; Chen, S.; Cui, Y.; Xu, Y.; Yan, C.; Yan, N.
Deposited on	:	2025-04-10
Resolution	:	2.17 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

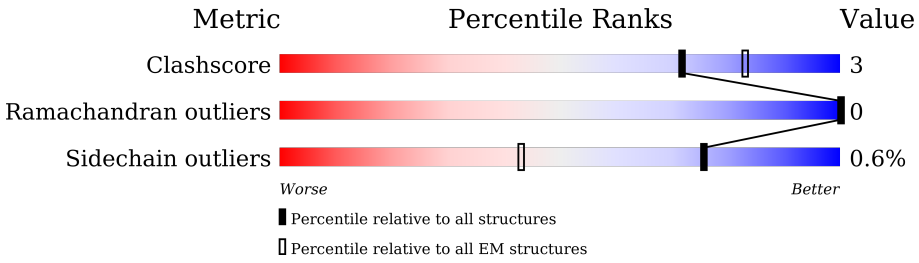
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	NOT EXECUTED
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.17 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	EA	368	87% 8% 5%
1	EB	368	88% 8% 5%
1	EC	368	89% 7% 5%
2	FA	723	89% 7% .
2	FB	723	88% 8% .
2	FC	723	89% 8% .
3	DA	209	82% 10% 8%
3	DB	209	86% 6% 8%
3	DC	209	84% 8% 8%

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Mol	Chain	Length	Quality of chain
4	CA	349	60% 5% 35%
4	CB	349	60% 5% 35%
4	CC	349	60% 5% 35%
5	AA	748	88% 9%
5	AB	748	90% 7%
5	AC	748	88% 9%
6	BA	366	88% 7% 5%
6	BB	366	88% 7% 5%
6	BC	366	87% 8% 5%
7	aA	14	29% 57% 14%
7	aF	14	7% 79% 14%
7	aK	14	21% 64% 14%
8	aB	16	38% 62%
8	aG	16	56% 44%
8	aL	16	50% 50%
9	aC	16	31% 69%
9	aH	16	38% 62%
9	aM	16	44% 56%
10	aD	9	22% 67% 11%
10	aI	9	33% 56% 11%
10	aN	9	33% 56% 11%
11	aE	15	47% 53%
11	aJ	15	53% 33% 13%
11	aO	15	53% 47%
12	bA	9	33% 67%

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Mol	Chain	Length	Quality of chain
12	bD	9	22% 67% 11%
12	bG	9	33% 67%
13	bB	5	40% 60%
13	bE	5	60% 40%
13	bH	5	20% 80%
14	bC	10	30% 70%
14	bF	10	30% 50% 20%
14	bI	10	20% 80%
15	cA	4	25% 75%
15	cB	4	25% 75%
15	cC	4	25% 75%
16	dA	7	14% 86%
16	dB	7	14% 86%
16	dC	7	14% 71% 14%
17	eA	11	18% 82%
17	eC	11	18% 73% 9%
17	eE	11	18% 82%
17	fC	11	27% 64% 9%
17	fD	11	27% 73%
17	fH	11	27% 73%
17	fI	11	27% 64% 9%
17	fM	11	18% 64% 18%
17	fN	11	9% 91%
18	eB	14	36% 64%
18	eD	14	50% 50%

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Mol	Chain	Length	Quality of chain
18	eF	14	57% 43%
19	fB	10	10% 90%
19	fE	10	30% 60% 10%
19	fG	10	20% 80%
19	fJ	10	20% 70% 10%
19	fL	10	20% 80%
19	fO	10	30% 60% 10%
20	fF	14	36% 64%
20	fK	14	36% 57% 7%
20	fP	14	43% 57%

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 71986 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 OCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	EA	351	Total	C	N	O	S	0	0
			2672	1651	460	532	29		
1	EB	351	Total	C	N	O	S	0	0
			2672	1651	460	532	29		
1	EC	351	Total	C	N	O	S	0	0
			2672	1651	460	532	29		

- Molecule 2 is a protein called OCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	FA	699	Total	C	N	O	S	0	0
			5350	3333	898	1078	41		
2	FB	699	Total	C	N	O	S	0	0
			5350	3333	898	1078	41		
2	FC	699	Total	C	N	O	S	0	0
			5350	3333	898	1078	41		

- Molecule 3 is a protein called Tubular mastigoneme protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	DA	192	Total	C	N	O	S	0	0
			1409	850	251	284	24		
3	DB	192	Total	C	N	O	S	0	0
			1409	850	251	284	24		
3	DC	192	Total	C	N	O	S	0	0
			1409	850	251	284	24		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	106	SER	PRO	conflict	UNP C4B7Q8
DB	106	SER	PRO	conflict	UNP C4B7Q8
DC	106	SER	PRO	conflict	UNP C4B7Q8

- Molecule 4 is a protein called OCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CA	227	Total	C	N	O	S	0	0
			1728	1047	313	343	25		
4	CB	227	Total	C	N	O	S	0	0
			1728	1047	313	343	25		
4	CC	227	Total	C	N	O	S	0	0
			1728	1047	313	343	25		

- Molecule 5 is a protein called Tubular mastigoneme protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AA	727	Total	C	N	O	S	0	0
			5689	3561	936	1150	42		
5	AB	727	Total	C	N	O	S	0	0
			5689	3561	936	1150	42		
5	AC	727	Total	C	N	O	S	0	0
			5689	3561	936	1150	42		

- Molecule 6 is a protein called Tubular mastigoneme protein.

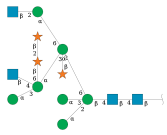
Mol	Chain	Residues	Atoms					AltConf	Trace
6	BA	348	Total	C	N	O	S	0	0
			2725	1678	462	558	27		
6	BB	348	Total	C	N	O	S	0	0
			2725	1678	462	558	27		
6	BC	348	Total	C	N	O	S	0	0
			2725	1678	462	558	27		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	72	GLY	VAL	conflict	UNP C4B7Q7
BA	112	ASP	ALA	conflict	UNP C4B7Q7
BB	72	GLY	VAL	conflict	UNP C4B7Q7
BB	112	ASP	ALA	conflict	UNP C4B7Q7
BC	72	GLY	VAL	conflict	UNP C4B7Q7
BC	112	ASP	ALA	conflict	UNP C4B7Q7

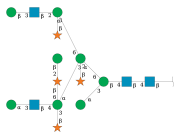
- Molecule 7 is an oligosaccharide called beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyra

nose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



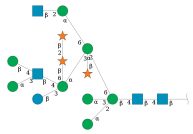
Mol	Chain	Residues	Atoms				AltConf	Trace
7	aA	14	Total	C	N	O	0	0
			160	89	4	67		
7	aF	14	Total	C	N	O	0	0
			160	89	4	67		
7	aK	14	Total	C	N	O	0	0
			160	89	4	67		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



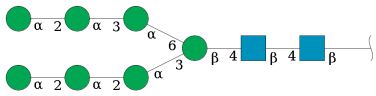
Mol	Chain	Residues	Atoms				AltConf	Trace
8	aB	16	Total	C	N	O	0	0
			180	100	4	76		
8	aG	16	Total	C	N	O	0	0
			180	100	4	76		
8	aL	16	Total	C	N	O	0	0
			180	100	4	76		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



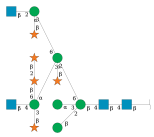
Mol	Chain	Residues	Atoms				AltConf	Trace
9	aC	16	Total 182	C 101	N 4	O 77	0	0
9	aH	16	Total 182	C 101	N 4	O 77	0	0
9	aM	16	Total 182	C 101	N 4	O 77	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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.



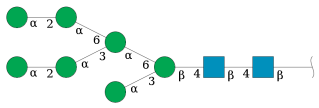
Mol	Chain	Residues	Atoms				AltConf	Trace
10	aD	9	Total 105	C 58	N 2	O 45	0	0
10	aI	9	Total 105	C 58	N 2	O 45	0	0
10	aN	9	Total 105	C 58	N 2	O 45	0	0

- Molecule 11 is an oligosaccharide called beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-xylopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



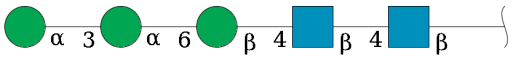
Mol	Chain	Residues	Atoms				AltConf	Trace
11	aE	15	Total	C	N	O	0	0
			167	93	4	70		
11	aJ	15	Total	C	N	O	0	0
			167	93	4	70		
11	aO	15	Total	C	N	O	0	0
			167	93	4	70		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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				AltConf	Trace
12	bA	9	Total	C	N	O	0	0
			105	58	2	45		
12	bD	9	Total	C	N	O	0	0
			105	58	2	45		
12	bG	9	Total	C	N	O	0	0
			105	58	2	45		

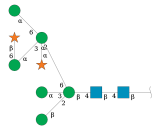
- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
13	bB	5	Total	C	N	O	0	0
			61	34	2	25		
13	bE	5	Total	C	N	O	0	0
			61	34	2	25		
13	bH	5	Total	C	N	O	0	0
			61	34	2	25		

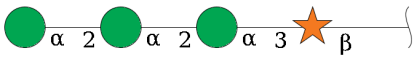
- Molecule 14 is an oligosaccharide called beta-D-xylopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-xylopyranose-(1-2)][alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(

1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



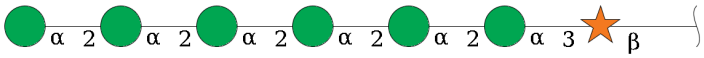
Mol	Chain	Residues	Atoms				AltConf	Trace
14	bC	10	Total	C	N	O	0	0
			112	62	2	48		
14	bF	10	Total	C	N	O	0	0
			112	62	2	48		
14	bI	10	Total	C	N	O	0	0
			112	62	2	48		

- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
15	cA	4	Total	C	O	0	0
			42	23	19		
15	cB	4	Total	C	O	0	0
			42	23	19		
15	cC	4	Total	C	O	0	0
			42	23	19		

- Molecule 16 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
16	dA	7	Total	C	O	0	0
			75	41	34		
16	dB	7	Total	C	O	0	0
			75	41	34		

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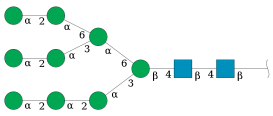
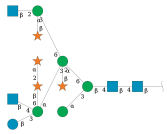
Mol	Chain	Residues	Atoms			AltConf	Trace
16	dC	7	Total 75	C 41	O 34	0	0

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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.



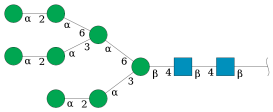
Mol	Chain	Residues	Atoms				AltConf	Trace
17	eA	11	Total 127	C 70	N 2	O 55	0	0
17	fC	11	Total 127	C 70	N 2	O 55	0	0
17	fD	11	Total 127	C 70	N 2	O 55	0	0
17	eC	11	Total 127	C 70	N 2	O 55	0	0
17	fH	11	Total 127	C 70	N 2	O 55	0	0
17	fI	11	Total 127	C 70	N 2	O 55	0	0
17	eE	11	Total 127	C 70	N 2	O 55	0	0
17	fM	11	Total 127	C 70	N 2	O 55	0	0
17	fN	11	Total 127	C 70	N 2	O 55	0	0

- Molecule 18 is an oligosaccharide called alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



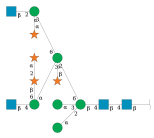
Mol	Chain	Residues	Atoms				AltConf	Trace
18	eB	14	Total	C	N	O	0	0
			158	88	4	66		
18	eD	14	Total	C	N	O	0	0
			158	88	4	66		
18	eF	14	Total	C	N	O	0	0
			158	88	4	66		

- Molecule 19 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]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				AltConf	Trace
19	fB	10	Total	C	N	O	0	0
			116	64	2	50		
19	fE	10	Total	C	N	O	0	0
			116	64	2	50		
19	fG	10	Total	C	N	O	0	0
			116	64	2	50		
19	fJ	10	Total	C	N	O	0	0
			116	64	2	50		
19	fL	10	Total	C	N	O	0	0
			116	64	2	50		
19	fO	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 20 is an oligosaccharide called alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]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	AltConf	Trace
20	fF	14	Total C N O 158 88 4 66	0	0
20	fK	14	Total C N O 158 88 4 66	0	0
20	fP	14	Total C N O 158 88 4 66	0	0

- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
21	EA	2	Total Ca 2 2	0
21	FA	6	Total Ca 6 6	0
21	CA	1	Total Ca 1 1	0
21	AA	7	Total Ca 7 7	0
21	BA	3	Total Ca 3 3	0
21	EB	1	Total Ca 1 1	0
21	FB	6	Total Ca 6 6	0
21	CB	1	Total Ca 1 1	0
21	AB	7	Total Ca 7 7	0
21	BB	3	Total Ca 3 3	0
21	EC	1	Total Ca 1 1	0
21	FC	6	Total Ca 6 6	0
21	CC	1	Total Ca 1 1	0
21	AC	7	Total Ca 7 7	0

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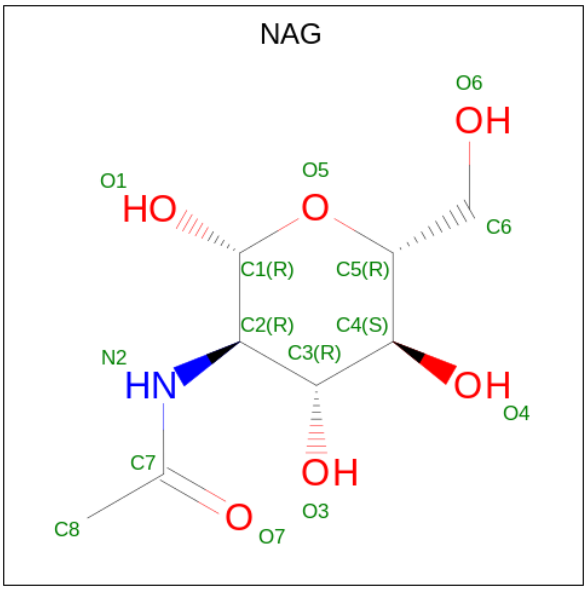
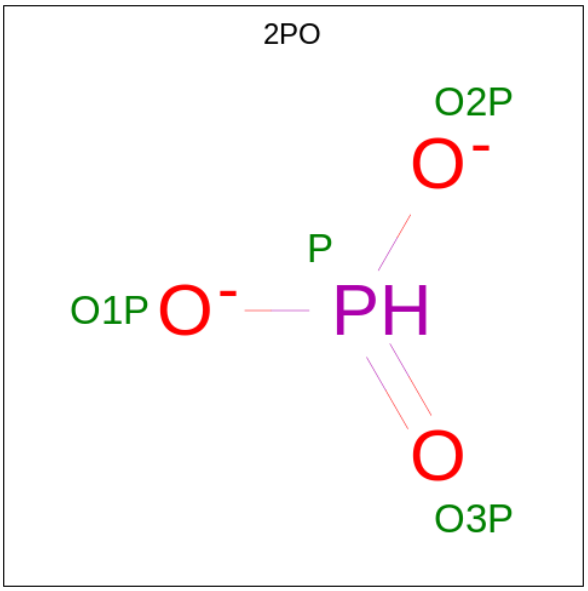
Mol	Chain	Residues	Atoms	AltConf
21	BC	3	Total Ca 3 3	0

- Molecule 22 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
22	EA	1	Total C N O 14 8 1 5	0
22	FA	1	Total C N O 14 8 1 5	0
22	EB	1	Total C N O 14 8 1 5	0
22	FB	1	Total C N O 14 8 1 5	0
22	EC	1	Total C N O 14 8 1 5	0
22	FC	1	Total C N O 14 8 1 5	0

- Molecule 23 is PHOSPHONATE (CCD ID: 2PO) (formula: HO_3P).



Mol	Chain	Residues	Atoms			AltConf
23	EA	1	Total	O	P	0
			4	3	1	
23	FA	1	Total	O	P	0
			4	3	1	
23	AA	1	Total	O	P	0
			4	3	1	
23	AA	1	Total	O	P	0
			4	3	1	
23	AA	1	Total	O	P	0
			4	3	1	
23	BA	1	Total	O	P	0
			4	3	1	
23	BA	1	Total	O	P	0
			4	3	1	
23	EB	1	Total	O	P	0
			4	3	1	
23	FB	1	Total	O	P	0
			4	3	1	
23	AB	1	Total	O	P	0
			4	3	1	
23	AB	1	Total	O	P	0
			4	3	1	
23	AB	1	Total	O	P	0
			4	3	1	
23	BB	1	Total	O	P	0
			4	3	1	
23	BB	1	Total	O	P	0
			4	3	1	

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Mol	Chain	Residues	Atoms	AltConf
23	EC	1	Total O P 4 3 1	0
23	FC	1	Total O P 4 3 1	0
23	AC	1	Total O P 4 3 1	0
23	AC	1	Total O P 4 3 1	0
23	AC	1	Total O P 4 3 1	0
23	BC	1	Total O P 4 3 1	0
23	BC	1	Total O P 4 3 1	0

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
24	DA	1	Total Cl 1 1	0
24	DB	1	Total Cl 1 1	0
24	DC	1	Total Cl 1 1	0

- Molecule 25 is water.

Mol	Chain	Residues	Atoms	AltConf
25	EA	293	Total O 293 293	0
25	FA	632	Total O 632 632	0
25	DA	167	Total O 167 167	0
25	CA	219	Total O 219 219	0
25	AA	610	Total O 610 610	0
25	BA	275	Total O 275 275	0
25	EB	294	Total O 294 294	0

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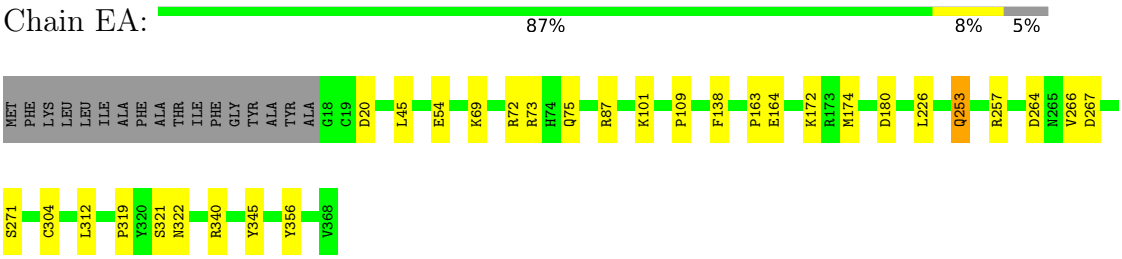
Mol	Chain	Residues	Atoms	AltConf
25	FB	635	Total O 635 635	0
25	DB	169	Total O 169 169	0
25	CB	217	Total O 217 217	0
25	AB	619	Total O 619 619	0
25	BB	300	Total O 300 300	0
25	EC	324	Total O 324 324	0
25	FC	636	Total O 636 636	0
25	DC	170	Total O 170 170	0
25	CC	209	Total O 209 209	0
25	AC	617	Total O 617 617	0
25	BC	301	Total O 301 301	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. 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. 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.

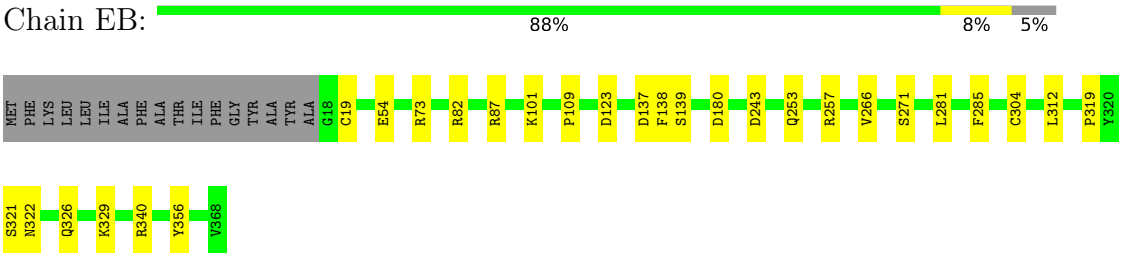
- Molecule 1: OCM5

Chain EA:



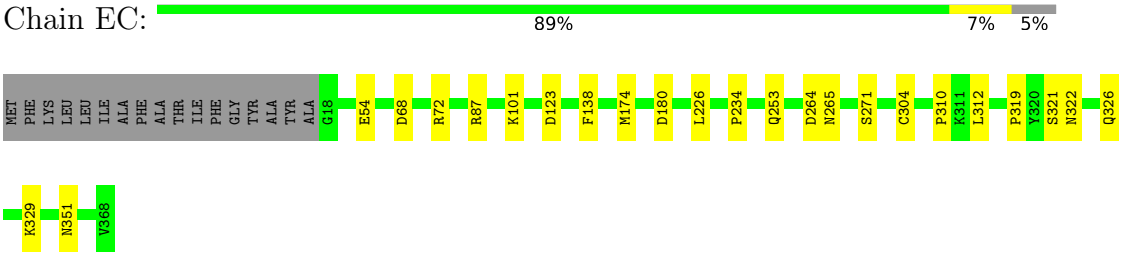
- Molecule 1: OCM5

Chain EB:



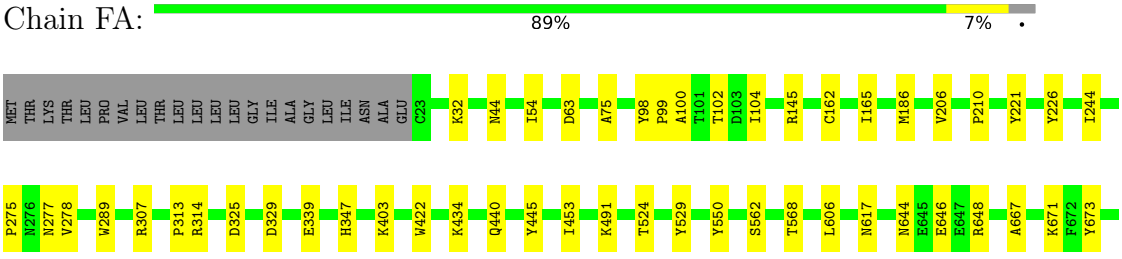
- Molecule 1: OCM5

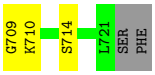
Chain EC:



- Molecule 2: OCM6

Chain FA:





• Molecule 2: OCM6

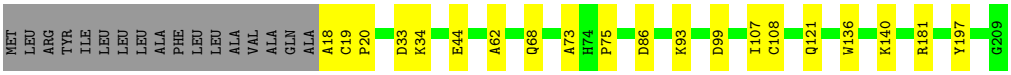
Chain FB:

• Molecule 2: OCM6

Chain FC:

• Molecule 3: Tubular mastigoneme protein

Chain DA:

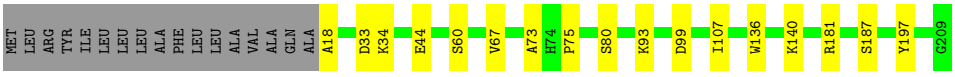


• Molecule 3: Tubular mastigoneme protein

Chain DB:

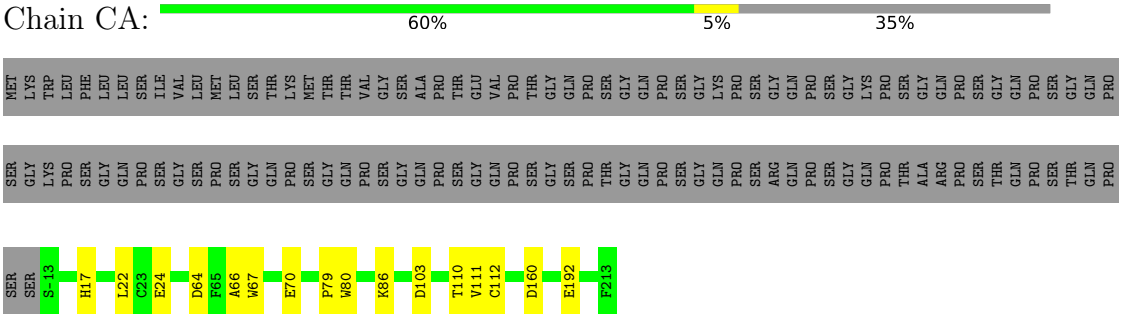
• Molecule 3: Tubular mastigoneme protein

Chain DC:



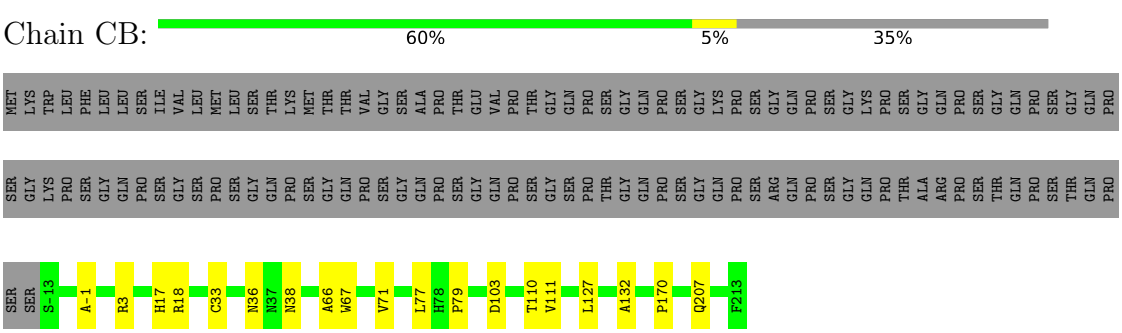
• Molecule 4: OCM3

Chain CA:



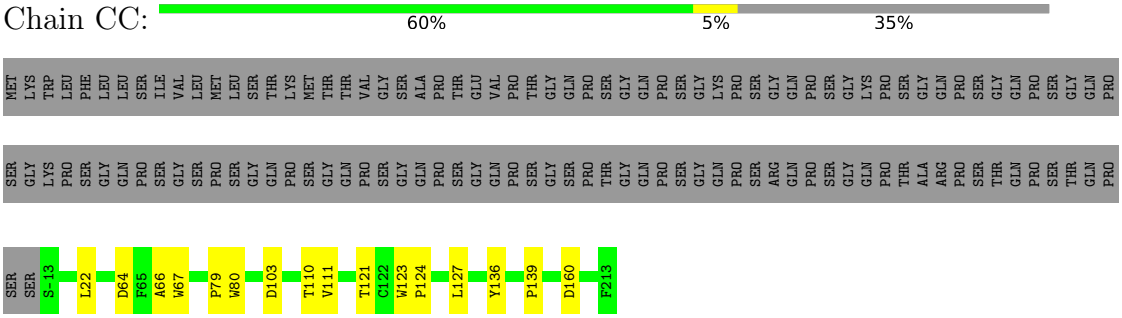
• Molecule 4: OCM3

Chain CB:



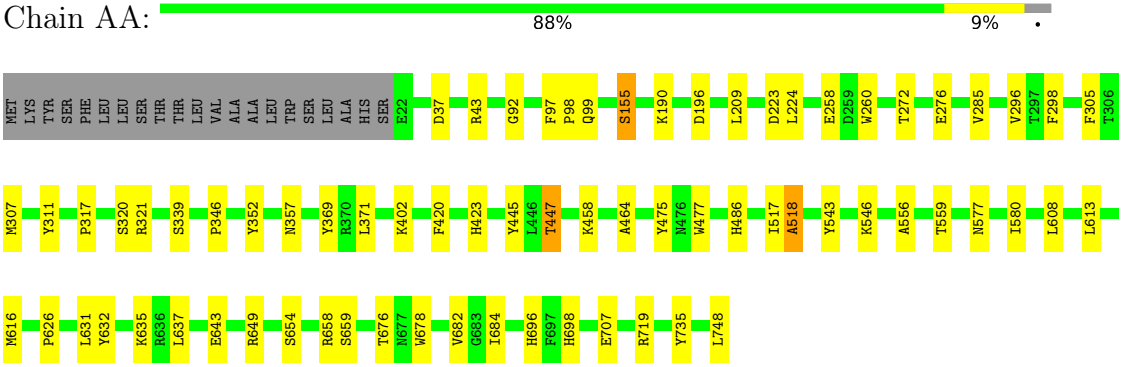
• Molecule 4: OCM3

Chain CC:



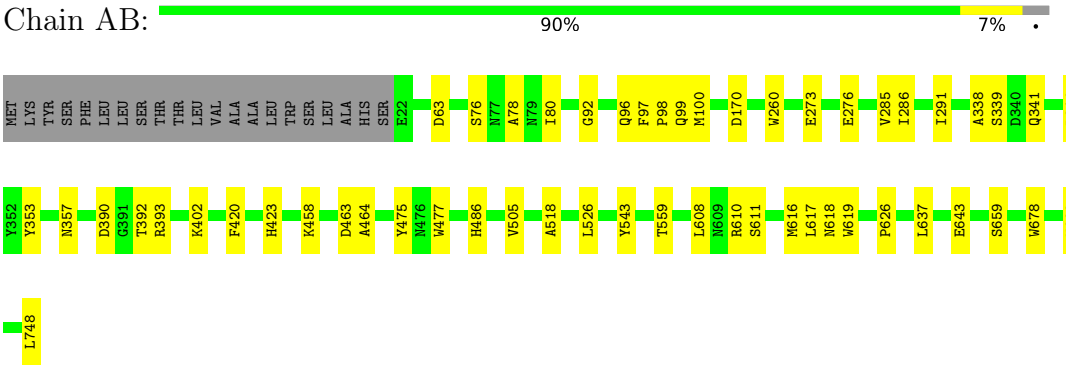
• Molecule 5: Tubular mastigoneme protein

Chain AA:



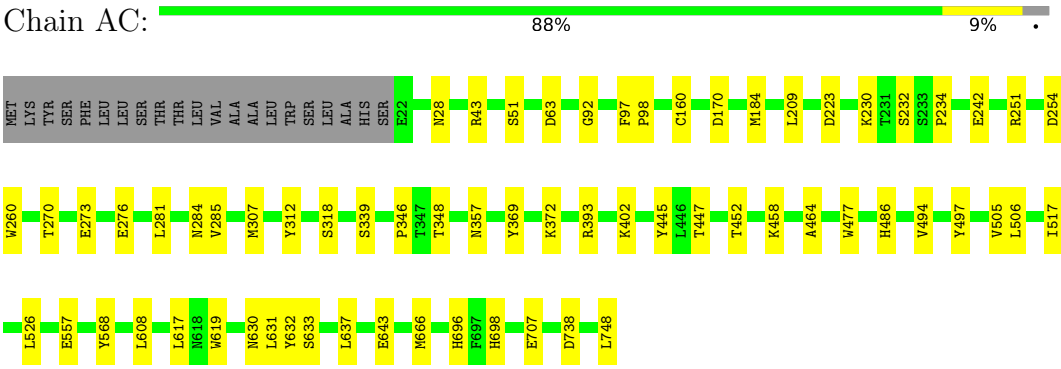
• Molecule 5: Tubular mastigoneme protein

Chain AB:



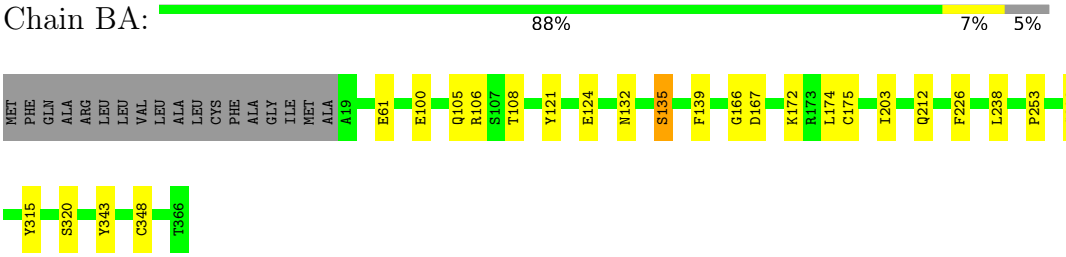
• Molecule 5: Tubular mastigoneme protein

Chain AC:



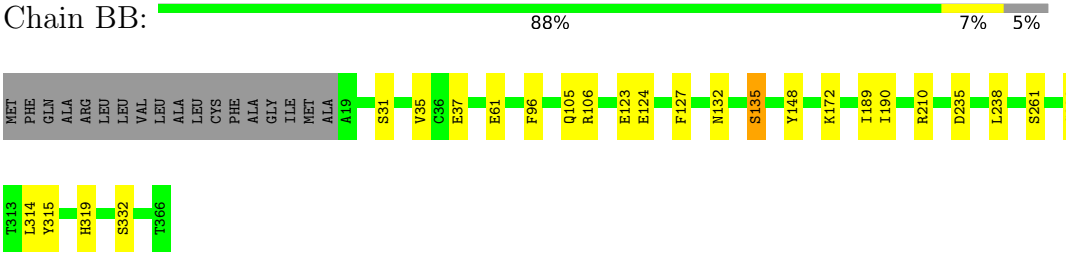
• Molecule 6: Tubular mastigoneme protein

Chain BA:



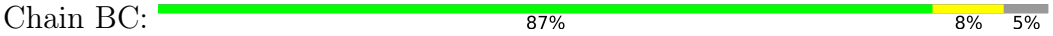
• Molecule 6: Tubular mastigoneme protein

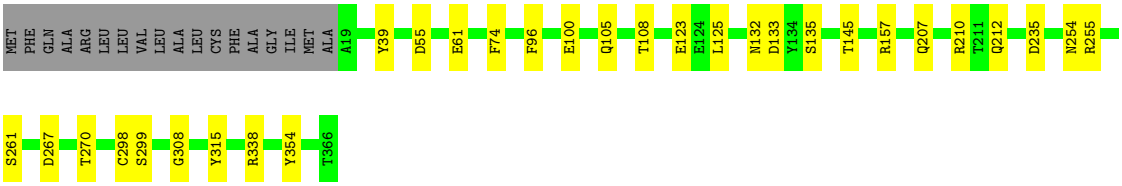
Chain BB:



• Molecule 6: Tubular mastigoneme protein

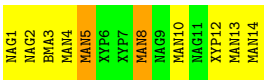
Chain BC:





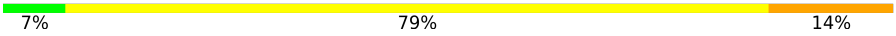
• Molecule 7: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

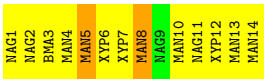
Chain aA:



• Molecule 7: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

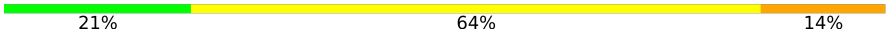
Chain aF:

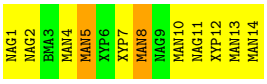




• Molecule 7: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

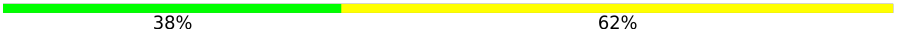
Chain aK:

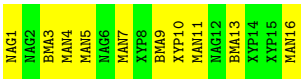




• Molecule 8: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

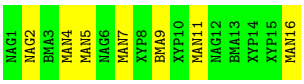
Chain aB:





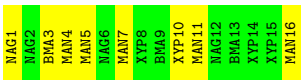
• Molecule 8: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain aG:



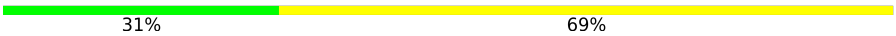
• Molecule 8: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

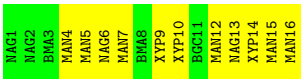
Chain aL:



• Molecule 9: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

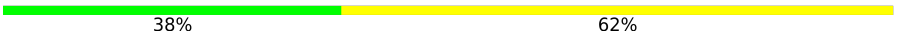
Chain aC:

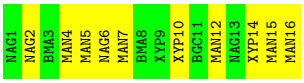




• Molecule 9: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

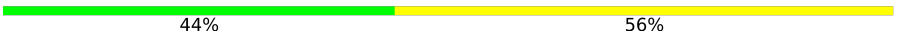
Chain aH:

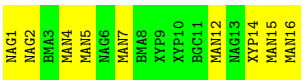




• Molecule 9: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

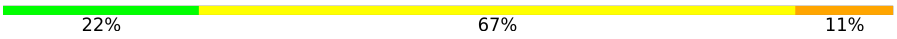
Chain aM:





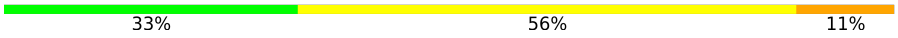
• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain aD:



• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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 aI:



• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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 aN:

• Molecule 11: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-xylopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-

D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][alpha-D-mann opyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain aE:

• Molecule 11: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-xylopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][alpha-D-mann opyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain aJ:

• Molecule 11: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-xylopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][alpha-D-mann opyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain aO:

• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain bA:

• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

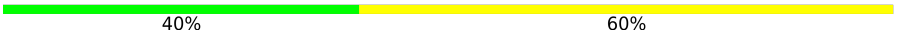
Chain bD:

• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain bG:

• Molecule 13: 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 bB:



• Molecule 13: 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

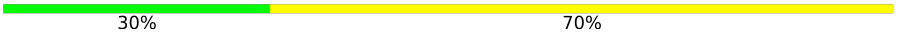
Chain bE:

• Molecule 13: 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 bH:

• Molecule 14: beta-D-xylopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-xylopyranose-(1-2)][alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

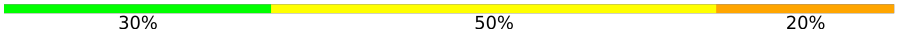
Chain bC:

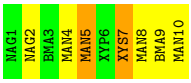


• Molecule 14: beta-D-xylopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-xylopyranose-(1-2)][alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][

alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

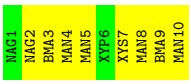
Chain bF:





• Molecule 14: beta-D-xylopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-xylopyranose-(1-2)][alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain bI:



• Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose

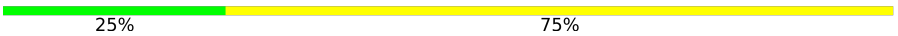
Chain cA:

• Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose

Chain cB:

• Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose

Chain cC:

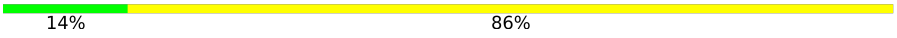


• Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose

Chain dA:

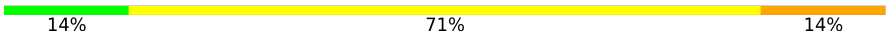
• Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose

Chain dB:



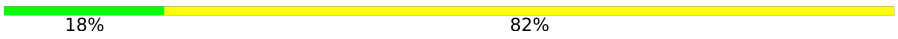
• Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose

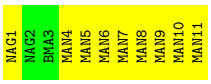
Chain dC:



• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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

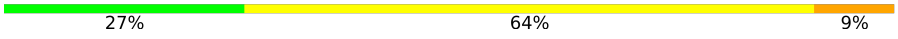
Chain eA:





• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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 fC:



• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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 fD:

• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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 eC:

• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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 fH:

• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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

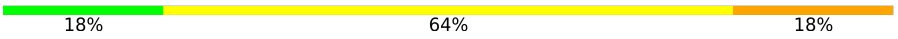
Chain fI:

• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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 eE:

• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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 fM:

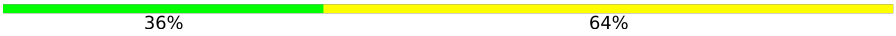


• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain fN:

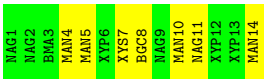
• Molecule 18: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain eB:



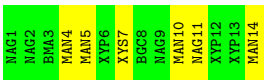
• Molecule 18: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain eD:



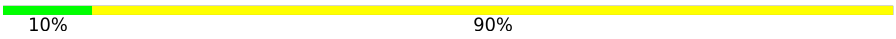
• Molecule 18: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain eF:



• Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain fB:

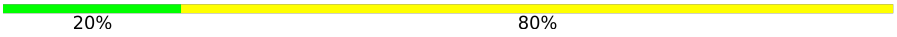


• Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain fE:

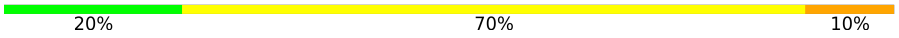
• Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

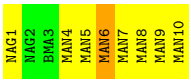
Chain fG:



• Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain fJ:



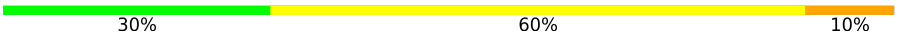


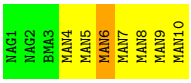
• Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain fL:

• Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

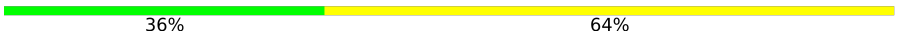
Chain fO:

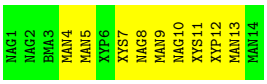




• Molecule 20: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

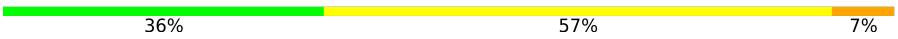
Chain fF:

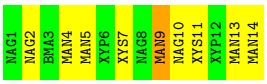




• Molecule 20: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

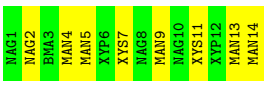
Chain fK:





• Molecule 20: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain fP:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104125	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYS, XYP, NAG, BGC, 2PO, BMA, CL, CA, MAN

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	EA	0.24	0/2733	0.41	0/3708
1	EB	0.24	0/2733	0.42	0/3708
1	EC	0.23	0/2733	0.43	0/3708
2	FA	0.22	0/5484	0.40	0/7488
2	FB	0.23	0/5484	0.42	0/7488
2	FC	0.24	0/5484	0.43	0/7488
3	DA	0.25	0/1439	0.45	0/1947
3	DB	0.27	0/1439	0.46	0/1947
3	DC	0.25	0/1439	0.47	0/1947
4	CA	0.24	0/1776	0.41	0/2413
4	CB	0.24	0/1776	0.45	0/2413
4	CC	0.26	0/1776	0.44	0/2413
5	AA	0.23	0/5841	0.40	0/7967
5	AB	0.24	0/5841	0.43	0/7967
5	AC	0.24	0/5841	0.43	2/7967 (0.0%)
6	BA	0.23	0/2782	0.42	0/3781
6	BB	0.25	0/2782	0.44	0/3781
6	BC	0.25	0/2782	0.44	0/3781
All	All	0.24	0/60165	0.42	2/81912 (0.0%)

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
5	AA	0	1
5	AB	0	1
5	AC	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AC	234	PRO	N-CD-CG	-8.23	93.92	103.80
5	AC	234	PRO	CA-N-CD	-5.62	103.62	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AA	518	ALA	Peptide
5	AB	518	ALA	Peptide
5	AC	518	ALA	Peptide

5.2 Too-close contacts (i)

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	EA	2672	0	2469	24	0
1	EB	2672	0	2470	20	0
1	EC	2672	0	2470	18	0
2	FA	5350	0	4914	35	0
2	FB	5350	0	4914	35	0
2	FC	5350	0	4913	41	0
3	DA	1409	0	1268	17	0
3	DB	1409	0	1268	11	0
3	DC	1409	0	1268	14	0
4	CA	1728	0	1530	12	0
4	CB	1728	0	1530	11	0
4	CC	1728	0	1530	9	0
5	AA	5689	0	5214	43	0
5	AB	5689	0	5214	36	0
5	AC	5689	0	5214	44	0
6	BA	2725	0	2484	16	0
6	BB	2725	0	2486	22	0
6	BC	2725	0	2485	22	0
7	aA	160	0	109	2	0
7	aF	160	0	109	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	aK	160	0	109	2	0
8	aB	180	0	117	0	0
8	aG	180	0	117	0	0
8	aL	180	0	117	1	0
9	aC	182	0	127	1	0
9	aH	182	0	127	0	0
9	aM	182	0	127	1	0
10	aD	105	0	88	1	0
10	aI	105	0	88	1	0
10	aN	105	0	88	1	0
11	aE	167	0	98	2	0
11	aJ	167	0	98	2	0
11	aO	167	0	98	1	0
12	bA	105	0	88	0	0
12	bD	105	0	88	1	0
12	bG	105	0	88	0	0
13	bB	61	0	52	0	0
13	bE	61	0	52	0	0
13	bH	61	0	52	0	0
14	bC	112	0	84	0	0
14	bF	112	0	84	1	0
14	bI	112	0	84	0	0
15	cA	42	0	28	0	0
15	cB	42	0	28	0	0
15	cC	42	0	28	0	0
16	dA	75	0	55	0	0
16	dB	75	0	55	0	0
16	dC	75	0	55	1	0
17	eA	127	0	106	0	0
17	eC	127	0	106	2	0
17	eE	127	0	106	0	0
17	fC	127	0	106	1	0
17	fD	127	0	106	0	0
17	fH	127	0	106	0	0
17	fI	127	0	106	1	0
17	fM	127	0	106	3	0
17	fN	127	0	106	1	0
18	eB	158	0	107	1	0
18	eD	158	0	107	0	0
18	eF	158	0	107	0	0
19	fB	116	0	97	0	0
19	fE	116	0	97	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	fG	116	0	97	0	0
19	fJ	116	0	97	1	0
19	fL	116	0	97	0	0
19	fO	116	0	97	1	0
20	fF	158	0	115	2	0
20	fK	158	0	115	1	0
20	fP	158	0	115	0	0
21	AA	7	0	0	0	0
21	AB	7	0	0	0	0
21	AC	7	0	0	0	0
21	BA	3	0	0	0	0
21	BB	3	0	0	1	0
21	BC	3	0	0	0	0
21	CA	1	0	0	0	0
21	CB	1	0	0	0	0
21	CC	1	0	0	0	0
21	EA	2	0	0	1	0
21	EB	1	0	0	0	0
21	EC	1	0	0	0	0
21	FA	6	0	0	0	0
21	FB	6	0	0	0	0
21	FC	6	0	0	0	0
22	EA	14	0	13	1	0
22	EB	14	0	13	1	0
22	EC	14	0	13	1	0
22	FA	14	0	13	0	0
22	FB	14	0	13	0	0
22	FC	14	0	13	0	0
23	AA	12	0	0	0	0
23	AB	12	0	0	0	0
23	AC	12	0	0	0	0
23	BA	8	0	0	0	0
23	BB	8	0	0	0	0
23	BC	8	0	0	0	0
23	EA	4	0	0	0	0
23	EB	4	0	0	0	0
23	EC	4	0	0	0	0
23	FA	4	0	0	0	0
23	FB	4	0	0	0	0
23	FC	4	0	0	0	0
24	DA	1	0	0	0	0
24	DB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	DC	1	0	0	0	0
25	AA	610	0	0	8	0
25	AB	619	0	0	8	0
25	AC	617	0	0	8	0
25	BA	275	0	0	1	0
25	BB	300	0	0	6	0
25	BC	301	0	0	9	0
25	CA	219	0	0	2	0
25	CB	217	0	0	2	0
25	CC	209	0	0	1	0
25	DA	167	0	0	5	0
25	DB	169	0	0	2	0
25	DC	170	0	0	3	0
25	EA	293	0	0	8	0
25	EB	294	0	0	7	0
25	EC	324	0	0	7	0
25	FA	632	0	0	4	0
25	FB	635	0	0	7	0
25	FC	636	0	0	14	0
All	All	71986	0	58459	415	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 3.

The worst 5 of 415 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)
2:FC:440:GLN:NE2	2:FC:491:LYS:O	2.05	0.89
2:FC:524:THR:HG1	17:fM:4:MAN:HO4	1.17	0.87
4:CB:17:HIS:ND1	25:AB:902:HOH:O	2.09	0.85
2:FB:440:GLN:NE2	2:FB:491:LYS:O	2.11	0.83
2:FA:524:THR:HG1	17:fC:4:MAN:HO4	1.25	0.80

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 PDB entries followed by that with respect to all EM entries.

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	EA	349/368 (95%)	345 (99%)	4 (1%)	0	100	100
1	EB	349/368 (95%)	343 (98%)	6 (2%)	0	100	100
1	EC	349/368 (95%)	343 (98%)	6 (2%)	0	100	100
2	FA	697/723 (96%)	677 (97%)	20 (3%)	0	100	100
2	FB	697/723 (96%)	674 (97%)	23 (3%)	0	100	100
2	FC	697/723 (96%)	681 (98%)	16 (2%)	0	100	100
3	DA	190/209 (91%)	181 (95%)	9 (5%)	0	100	100
3	DB	190/209 (91%)	184 (97%)	6 (3%)	0	100	100
3	DC	190/209 (91%)	184 (97%)	6 (3%)	0	100	100
4	CA	225/349 (64%)	218 (97%)	7 (3%)	0	100	100
4	CB	225/349 (64%)	220 (98%)	5 (2%)	0	100	100
4	CC	225/349 (64%)	219 (97%)	6 (3%)	0	100	100
5	AA	725/748 (97%)	705 (97%)	20 (3%)	0	100	100
5	AB	725/748 (97%)	700 (97%)	25 (3%)	0	100	100
5	AC	725/748 (97%)	708 (98%)	17 (2%)	0	100	100
6	BA	346/366 (94%)	332 (96%)	14 (4%)	0	100	100
6	BB	346/366 (94%)	334 (96%)	12 (4%)	0	100	100
6	BC	346/366 (94%)	336 (97%)	10 (3%)	0	100	100
All	All	7596/8289 (92%)	7384 (97%)	212 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	EA	294/306 (96%)	291 (99%)	3 (1%)	68	79
1	EB	294/306 (96%)	292 (99%)	2 (1%)	76	86
1	EC	294/306 (96%)	293 (100%)	1 (0%)	86	92
2	FA	582/602 (97%)	580 (100%)	2 (0%)	86	92
2	FB	582/602 (97%)	578 (99%)	4 (1%)	76	86
2	FC	582/602 (97%)	580 (100%)	2 (0%)	86	92
3	DA	152/165 (92%)	152 (100%)	0	100	100
3	DB	152/165 (92%)	152 (100%)	0	100	100
3	DC	152/165 (92%)	151 (99%)	1 (1%)	76	86
4	CA	187/287 (65%)	186 (100%)	1 (0%)	81	89
4	CB	187/287 (65%)	186 (100%)	1 (0%)	81	89
4	CC	187/287 (65%)	187 (100%)	0	100	100
5	AA	628/646 (97%)	623 (99%)	5 (1%)	73	83
5	AB	628/646 (97%)	625 (100%)	3 (0%)	81	89
5	AC	628/646 (97%)	623 (99%)	5 (1%)	73	83
6	BA	306/319 (96%)	305 (100%)	1 (0%)	86	92
6	BB	306/319 (96%)	303 (99%)	3 (1%)	68	79
6	BC	306/319 (96%)	303 (99%)	3 (1%)	68	79
All	All	6447/6975 (92%)	6410 (99%)	37 (1%)	76	87

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	DC	187	SER
6	BC	298	CYS
5	AC	357	ASN
5	AC	696	HIS
1	EB	243	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
5	AC	46	GLN

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Mol	Chain	Res	Type
5	AC	157	HIS
6	BC	153	ASN
2	FB	492	GLN
2	FB	315	ASN

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)

558 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	$\#\|Z\| > 2$
7	NAG	aA	1	7,5	14,14,15	0.34	0	17,19,21	0.81	0
7	MAN	aA	10	23,7	11,11,12	0.66	0	15,15,17	1.04	2 (13%)
7	NAG	aA	11	7	14,14,15	0.28	0	17,19,21	0.66	0
7	XYP	aA	12	7	9,9,10	1.89	3 (33%)	10,12,14	0.91	0
7	MAN	aA	13	7	11,11,12	0.67	1 (9%)	15,15,17	1.06	1 (6%)
7	MAN	aA	14	7	11,11,12	0.69	0	15,15,17	1.27	3 (20%)
7	NAG	aA	2	7	14,14,15	0.38	0	17,19,21	0.96	1 (5%)
7	BMA	aA	3	7	11,11,12	0.24	0	15,15,17	0.96	1 (6%)
7	MAN	aA	4	7	11,11,12	1.08	1 (9%)	15,15,17	1.29	3 (20%)
7	MAN	aA	5	7	11,11,12	0.64	0	15,15,17	1.33	3 (20%)
7	XYP	aA	6	7	9,9,10	0.19	0	10,12,14	0.90	0
7	XYP	aA	7	7	9,9,10	0.18	0	10,12,14	0.65	0
7	MAN	aA	8	7	11,11,12	0.79	1 (9%)	15,15,17	1.18	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	aA	9	7	14,14,15	0.27	0	17,19,21	0.65	0
8	NAG	aB	1	8,5	14,14,15	0.33	0	17,19,21	0.69	1 (5%)
8	XYP	aB	10	8	9,9,10	0.16	0	10,12,14	0.73	1 (10%)
8	MAN	aB	11	8	11,11,12	0.76	1 (9%)	15,15,17	1.04	1 (6%)
8	NAG	aB	12	8	14,14,15	0.35	0	17,19,21	0.81	0
8	BMA	aB	13	8	11,11,12	0.25	0	15,15,17	0.72	1 (6%)
8	XYP	aB	14	8	9,9,10	0.18	0	10,12,14	0.66	0
8	XYP	aB	15	8	9,9,10	0.17	0	10,12,14	0.61	0
8	MAN	aB	16	8	11,11,12	0.68	0	15,15,17	1.08	2 (13%)
8	NAG	aB	2	8	14,14,15	0.33	0	17,19,21	0.74	0
8	BMA	aB	3	8	11,11,12	0.22	0	15,15,17	0.93	1 (6%)
8	MAN	aB	4	8	11,11,12	0.87	1 (9%)	15,15,17	1.13	2 (13%)
8	MAN	aB	5	8	11,11,12	0.59	0	15,15,17	1.48	3 (20%)
8	NAG	aB	6	8	14,14,15	0.39	0	17,19,21	0.48	0
8	MAN	aB	7	8	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
8	XYP	aB	8	8	9,9,10	0.17	0	10,12,14	0.66	0
8	BMA	aB	9	8	11,11,12	0.28	0	15,15,17	1.35	2 (13%)
9	NAG	aC	1	5,9	14,14,15	0.29	0	17,19,21	0.78	0
9	XYP	aC	10	9	9,9,10	0.17	0	10,12,14	0.68	0
9	BGC	aC	11	9	11,11,12	0.22	0	15,15,17	0.59	0
9	MAN	aC	12	23,9	11,11,12	0.88	1 (9%)	15,15,17	1.28	2 (13%)
9	NAG	aC	13	9	14,14,15	0.30	0	17,19,21	0.89	1 (5%)
9	XYP	aC	14	9	9,9,10	1.78	3 (33%)	10,12,14	1.90	3 (30%)
9	MAN	aC	15	9	11,11,12	0.57	0	15,15,17	1.21	3 (20%)
9	MAN	aC	16	9	11,11,12	0.80	1 (9%)	15,15,17	1.11	2 (13%)
9	NAG	aC	2	9	14,14,15	0.28	0	17,19,21	0.78	0
9	BMA	aC	3	9	11,11,12	0.27	0	15,15,17	0.61	0
9	MAN	aC	4	9	11,11,12	0.94	1 (9%)	15,15,17	1.20	1 (6%)
9	MAN	aC	5	9	11,11,12	0.91	0	15,15,17	1.27	2 (13%)
9	NAG	aC	6	9	14,14,15	0.34	0	17,19,21	0.85	1 (5%)
9	MAN	aC	7	9	11,11,12	0.70	0	15,15,17	1.34	3 (20%)
9	BMA	aC	8	9	11,11,12	0.24	0	15,15,17	0.80	0
9	XYP	aC	9	9	9,9,10	0.15	0	10,12,14	0.59	0
10	NAG	aD	1	10,5	14,14,15	0.41	0	17,19,21	0.61	0
10	NAG	aD	2	10	14,14,15	0.40	0	17,19,21	0.78	0
10	BMA	aD	3	10	11,11,12	0.21	0	15,15,17	0.91	1 (6%)
10	MAN	aD	4	10	11,11,12	0.91	1 (9%)	15,15,17	1.16	1 (6%)
10	MAN	aD	5	10	11,11,12	0.85	1 (9%)	15,15,17	1.11	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	MAN	aD	6	10	11,11,12	0.83	0	15,15,17	1.13	2 (13%)
10	MAN	aD	7	10	11,11,12	0.73	0	15,15,17	1.29	3 (20%)
10	MAN	aD	8	10	11,11,12	0.91	1 (9%)	15,15,17	1.17	2 (13%)
10	MAN	aD	9	10	11,11,12	0.69	0	15,15,17	1.31	2 (13%)
11	NAG	aE	1	11,5	14,14,15	0.30	0	17,19,21	0.67	0
11	MAN	aE	10	23,11	11,11,12	0.93	1 (9%)	15,15,17	0.93	1 (6%)
11	NAG	aE	11	11	14,14,15	0.26	0	17,19,21	0.89	0
11	XYP	aE	12	11	9,9,10	0.19	0	10,12,14	0.67	0
11	XYP	aE	13	11	9,9,10	0.18	0	10,12,14	0.62	0
11	BMA	aE	14	11	11,11,12	0.88	1 (9%)	15,15,17	1.15	2 (13%)
11	MAN	aE	15	11	11,11,12	0.76	0	15,15,17	0.99	1 (6%)
11	NAG	aE	2	11	14,14,15	0.33	0	17,19,21	0.76	0
11	BMA	aE	3	11	11,11,12	0.36	0	15,15,17	0.95	0
11	MAN	aE	4	11	11,11,12	0.84	1 (9%)	15,15,17	1.03	1 (6%)
11	MAN	aE	5	11	11,11,12	0.60	0	15,15,17	1.56	3 (20%)
11	XYP	aE	6	11	9,9,10	0.20	0	10,12,14	0.70	0
11	XYP	aE	7	11	9,9,10	0.18	0	10,12,14	0.60	0
11	XYP	aE	8	11	9,9,10	0.20	0	10,12,14	0.64	0
11	NAG	aE	9	11	14,14,15	0.31	0	17,19,21	0.75	0
7	NAG	aF	1	7,5	14,14,15	0.35	0	17,19,21	0.89	1 (5%)
7	MAN	aF	10	23,7	11,11,12	0.71	0	15,15,17	1.01	1 (6%)
7	NAG	aF	11	7	14,14,15	0.26	0	17,19,21	0.83	1 (5%)
7	XYP	aF	12	7	9,9,10	1.86	3 (33%)	10,12,14	0.92	1 (10%)
7	MAN	aF	13	7	11,11,12	0.60	0	15,15,17	1.08	2 (13%)
7	MAN	aF	14	7	11,11,12	0.81	0	15,15,17	1.19	2 (13%)
7	NAG	aF	2	7	14,14,15	0.37	0	17,19,21	0.81	1 (5%)
7	BMA	aF	3	7	11,11,12	0.22	0	15,15,17	0.81	1 (6%)
7	MAN	aF	4	7	11,11,12	1.02	1 (9%)	15,15,17	1.15	1 (6%)
7	MAN	aF	5	7	11,11,12	0.56	0	15,15,17	1.44	3 (20%)
7	XYP	aF	6	7	9,9,10	0.19	0	10,12,14	1.00	1 (10%)
7	XYP	aF	7	7	9,9,10	0.17	0	10,12,14	0.72	1 (10%)
7	MAN	aF	8	7	11,11,12	0.81	1 (9%)	15,15,17	1.00	2 (13%)
7	NAG	aF	9	7	14,14,15	0.28	0	17,19,21	0.72	0
8	NAG	aG	1	8,5	14,14,15	0.36	0	17,19,21	0.79	0
8	XYP	aG	10	8	9,9,10	0.17	0	10,12,14	0.65	0
8	MAN	aG	11	8	11,11,12	0.72	0	15,15,17	1.25	1 (6%)
8	NAG	aG	12	8	14,14,15	0.33	0	17,19,21	0.75	0
8	BMA	aG	13	8	11,11,12	0.24	0	15,15,17	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	XYP	aG	14	8	9,9,10	0.19	0	10,12,14	0.68	0
8	XYP	aG	15	8	9,9,10	0.19	0	10,12,14	0.58	0
8	MAN	aG	16	8	11,11,12	0.86	1 (9%)	15,15,17	1.03	1 (6%)
8	NAG	aG	2	8	14,14,15	0.31	0	17,19,21	0.92	1 (5%)
8	BMA	aG	3	8	11,11,12	0.24	0	15,15,17	0.91	0
8	MAN	aG	4	8	11,11,12	0.63	0	15,15,17	1.22	2 (13%)
8	MAN	aG	5	8	11,11,12	0.64	0	15,15,17	1.53	3 (20%)
8	NAG	aG	6	8	14,14,15	0.35	0	17,19,21	0.49	0
8	MAN	aG	7	8	11,11,12	0.63	0	15,15,17	1.23	2 (13%)
8	XYP	aG	8	8	9,9,10	0.17	0	10,12,14	0.63	0
8	BMA	aG	9	8	11,11,12	0.27	0	15,15,17	1.30	3 (20%)
9	NAG	aH	1	5,9	14,14,15	0.35	0	17,19,21	0.79	0
9	XYP	aH	10	9	9,9,10	0.13	0	10,12,14	0.73	1 (10%)
9	BGC	aH	11	9	11,11,12	0.28	0	15,15,17	0.56	0
9	MAN	aH	12	9	11,11,12	1.07	1 (9%)	15,15,17	1.27	3 (20%)
9	NAG	aH	13	9	14,14,15	0.31	0	17,19,21	0.67	0
9	XYP	aH	14	9	9,9,10	1.94	4 (44%)	10,12,14	0.86	1 (10%)
9	MAN	aH	15	9	11,11,12	0.54	0	15,15,17	1.26	3 (20%)
9	MAN	aH	16	9	11,11,12	0.84	1 (9%)	15,15,17	0.89	1 (6%)
9	NAG	aH	2	9	14,14,15	0.34	0	17,19,21	1.04	1 (5%)
9	BMA	aH	3	9	11,11,12	0.26	0	15,15,17	0.66	0
9	MAN	aH	4	9	11,11,12	1.43	1 (9%)	15,15,17	1.32	3 (20%)
9	MAN	aH	5	9	11,11,12	1.02	1 (9%)	15,15,17	1.18	2 (13%)
9	NAG	aH	6	9	14,14,15	0.36	0	17,19,21	0.80	1 (5%)
9	MAN	aH	7	9	11,11,12	0.76	0	15,15,17	1.30	3 (20%)
9	BMA	aH	8	9	11,11,12	0.23	0	15,15,17	0.95	0
9	XYP	aH	9	9	9,9,10	0.17	0	10,12,14	0.67	0
10	NAG	aI	1	10,5	14,14,15	0.42	0	17,19,21	0.73	0
10	NAG	aI	2	10	14,14,15	0.40	0	17,19,21	0.75	0
10	BMA	aI	3	10	11,11,12	0.22	0	15,15,17	0.79	0
10	MAN	aI	4	10	11,11,12	0.83	1 (9%)	15,15,17	1.26	2 (13%)
10	MAN	aI	5	10	11,11,12	0.69	0	15,15,17	1.09	2 (13%)
10	MAN	aI	6	10	11,11,12	0.69	0	15,15,17	1.17	1 (6%)
10	MAN	aI	7	10	11,11,12	0.72	0	15,15,17	1.31	3 (20%)
10	MAN	aI	8	10	11,11,12	0.86	0	15,15,17	1.27	2 (13%)
10	MAN	aI	9	10	11,11,12	0.81	0	15,15,17	1.25	2 (13%)
11	NAG	aJ	1	11,5	14,14,15	0.38	0	17,19,21	0.75	0
11	MAN	aJ	10	11	11,11,12	0.85	1 (9%)	15,15,17	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	NAG	aJ	11	11	14,14,15	0.27	0	17,19,21	0.72	0
11	XYP	aJ	12	11	9,9,10	0.17	0	10,12,14	0.61	0
11	XYP	aJ	13	11	9,9,10	0.18	0	10,12,14	0.67	0
11	BMA	aJ	14	11	11,11,12	0.94	1 (9%)	15,15,17	0.99	2 (13%)
11	MAN	aJ	15	11	11,11,12	0.74	0	15,15,17	1.03	1 (6%)
11	NAG	aJ	2	11	14,14,15	0.32	0	17,19,21	0.62	0
11	BMA	aJ	3	11	11,11,12	0.33	0	15,15,17	0.92	1 (6%)
11	MAN	aJ	4	11	11,11,12	0.99	1 (9%)	15,15,17	1.08	2 (13%)
11	MAN	aJ	5	11	11,11,12	0.62	0	15,15,17	1.42	2 (13%)
11	XYP	aJ	6	11	9,9,10	0.18	0	10,12,14	0.62	0
11	XYP	aJ	7	11	9,9,10	0.20	0	10,12,14	0.58	0
11	XYP	aJ	8	11	9,9,10	0.21	0	10,12,14	0.62	0
11	NAG	aJ	9	11	14,14,15	0.34	0	17,19,21	0.75	0
7	NAG	aK	1	7,5	14,14,15	0.34	0	17,19,21	0.72	0
7	MAN	aK	10	23,7	11,11,12	0.60	0	15,15,17	1.28	2 (13%)
7	NAG	aK	11	7	14,14,15	0.28	0	17,19,21	0.84	1 (5%)
7	XYP	aK	12	7	9,9,10	1.93	3 (33%)	10,12,14	1.13	1 (10%)
7	MAN	aK	13	7	11,11,12	0.72	0	15,15,17	1.04	2 (13%)
7	MAN	aK	14	7	11,11,12	0.73	0	15,15,17	1.08	2 (13%)
7	NAG	aK	2	7	14,14,15	0.40	0	17,19,21	0.80	1 (5%)
7	BMA	aK	3	7	11,11,12	0.19	0	15,15,17	0.72	0
7	MAN	aK	4	7	11,11,12	0.99	1 (9%)	15,15,17	1.08	1 (6%)
7	MAN	aK	5	7	11,11,12	0.62	0	15,15,17	1.26	2 (13%)
7	XYP	aK	6	7	9,9,10	0.17	0	10,12,14	0.94	0
7	XYP	aK	7	7	9,9,10	0.17	0	10,12,14	0.79	1 (10%)
7	MAN	aK	8	7	11,11,12	0.67	0	15,15,17	1.17	3 (20%)
7	NAG	aK	9	7	14,14,15	0.35	0	17,19,21	0.72	0
8	NAG	aL	1	8,5	14,14,15	0.37	0	17,19,21	0.73	0
8	XYP	aL	10	8	9,9,10	0.18	0	10,12,14	0.73	1 (10%)
8	MAN	aL	11	23,8	11,11,12	0.70	0	15,15,17	1.21	2 (13%)
8	NAG	aL	12	8	14,14,15	0.35	0	17,19,21	0.84	0
8	BMA	aL	13	8	11,11,12	0.25	0	15,15,17	0.65	0
8	XYP	aL	14	8	9,9,10	0.17	0	10,12,14	0.68	0
8	XYP	aL	15	8	9,9,10	0.17	0	10,12,14	0.60	0
8	MAN	aL	16	8	11,11,12	0.73	1 (9%)	15,15,17	0.98	1 (6%)
8	NAG	aL	2	8	14,14,15	0.35	0	17,19,21	0.59	0
8	BMA	aL	3	8	11,11,12	0.22	0	15,15,17	0.97	1 (6%)
8	MAN	aL	4	8	11,11,12	0.77	0	15,15,17	1.31	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	MAN	aL	5	8	11,11,12	0.66	0	15,15,17	1.46	2 (13%)
8	NAG	aL	6	8	14,14,15	0.39	0	17,19,21	0.71	0
8	MAN	aL	7	8	11,11,12	0.63	0	15,15,17	1.36	3 (20%)
8	XYP	aL	8	8	9,9,10	0.17	0	10,12,14	0.61	0
8	BMA	aL	9	8	11,11,12	0.24	0	15,15,17	0.84	0
9	NAG	aM	1	5,9	14,14,15	0.38	0	17,19,21	0.68	0
9	XYP	aM	10	9	9,9,10	0.16	0	10,12,14	0.62	0
9	BGC	aM	11	9	11,11,12	0.28	0	15,15,17	0.56	0
9	MAN	aM	12	23,9	11,11,12	0.68	0	15,15,17	1.19	2 (13%)
9	NAG	aM	13	9	14,14,15	0.26	0	17,19,21	0.67	0
9	XYP	aM	14	9	9,9,10	1.85	3 (33%)	10,12,14	1.02	1 (10%)
9	MAN	aM	15	9	11,11,12	0.63	0	15,15,17	1.22	2 (13%)
9	MAN	aM	16	9	11,11,12	1.02	1 (9%)	15,15,17	0.83	0
9	NAG	aM	2	9	14,14,15	0.26	0	17,19,21	0.77	0
9	BMA	aM	3	9	11,11,12	0.25	0	15,15,17	0.62	0
9	MAN	aM	4	9	11,11,12	0.87	0	15,15,17	1.23	1 (6%)
9	MAN	aM	5	9	11,11,12	1.10	1 (9%)	15,15,17	1.25	3 (20%)
9	NAG	aM	6	9	14,14,15	0.37	0	17,19,21	0.52	0
9	MAN	aM	7	9	11,11,12	0.53	0	15,15,17	1.30	3 (20%)
9	BMA	aM	8	9	11,11,12	0.23	0	15,15,17	0.61	0
9	XYP	aM	9	9	9,9,10	0.17	0	10,12,14	0.51	0
10	NAG	aN	1	10,5	14,14,15	0.41	0	17,19,21	0.64	0
10	NAG	aN	2	10	14,14,15	0.38	0	17,19,21	0.91	0
10	BMA	aN	3	10	11,11,12	0.23	0	15,15,17	0.72	0
10	MAN	aN	4	10	11,11,12	0.88	0	15,15,17	1.06	2 (13%)
10	MAN	aN	5	10	11,11,12	0.89	1 (9%)	15,15,17	1.10	2 (13%)
10	MAN	aN	6	10	11,11,12	0.91	0	15,15,17	1.22	2 (13%)
10	MAN	aN	7	10	11,11,12	0.61	0	15,15,17	1.34	2 (13%)
10	MAN	aN	8	10	11,11,12	0.88	1 (9%)	15,15,17	1.11	2 (13%)
10	MAN	aN	9	10	11,11,12	0.82	0	15,15,17	1.21	2 (13%)
11	NAG	aO	1	11,5	14,14,15	0.33	0	17,19,21	0.80	0
11	MAN	aO	10	11	11,11,12	0.75	0	15,15,17	0.87	0
11	NAG	aO	11	11	14,14,15	0.31	0	17,19,21	1.07	1 (5%)
11	XYP	aO	12	11	9,9,10	0.20	0	10,12,14	0.62	0
11	XYP	aO	13	11	9,9,10	0.19	0	10,12,14	0.62	0
11	BMA	aO	14	11	11,11,12	0.74	0	15,15,17	1.05	1 (6%)
11	MAN	aO	15	11	11,11,12	0.90	1 (9%)	15,15,17	1.08	2 (13%)
11	NAG	aO	2	11	14,14,15	0.37	0	17,19,21	0.62	0
11	BMA	aO	3	11	11,11,12	0.29	0	15,15,17	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	MAN	aO	4	11	11,11,12	0.92	1 (9%)	15,15,17	1.05	1 (6%)
11	MAN	aO	5	11	11,11,12	0.57	0	15,15,17	1.37	2 (13%)
11	XYP	aO	6	11	9,9,10	0.18	0	10,12,14	0.63	0
11	XYP	aO	7	11	9,9,10	0.19	0	10,12,14	0.61	0
11	XYP	aO	8	11	9,9,10	0.19	0	10,12,14	0.67	0
11	NAG	aO	9	11	14,14,15	0.33	0	17,19,21	0.64	0
12	NAG	bA	1	12,6	14,14,15	0.44	0	17,19,21	0.73	0
12	NAG	bA	2	12	14,14,15	0.30	0	17,19,21	0.92	0
12	BMA	bA	3	12	11,11,12	0.25	0	15,15,17	0.79	1 (6%)
12	MAN	bA	4	12	11,11,12	0.89	1 (9%)	15,15,17	1.11	1 (6%)
12	MAN	bA	5	12	11,11,12	0.82	0	15,15,17	1.30	3 (20%)
12	MAN	bA	6	12	11,11,12	0.71	0	15,15,17	1.12	1 (6%)
12	MAN	bA	7	12	11,11,12	0.73	1 (9%)	15,15,17	1.11	2 (13%)
12	MAN	bA	8	12	11,11,12	0.70	0	15,15,17	1.14	2 (13%)
12	MAN	bA	9	12	11,11,12	0.73	0	15,15,17	0.98	0
13	NAG	bB	1	13,6	14,14,15	0.33	0	17,19,21	0.50	0
13	NAG	bB	2	13	14,14,15	0.28	0	17,19,21	0.89	1 (5%)
13	BMA	bB	3	13	11,11,12	0.18	0	15,15,17	0.57	0
13	MAN	bB	4	13	11,11,12	0.78	0	15,15,17	1.24	2 (13%)
13	MAN	bB	5	13	11,11,12	0.69	0	15,15,17	1.26	3 (20%)
14	NAG	bC	1	14,6	14,14,15	0.39	0	17,19,21	0.61	0
14	MAN	bC	10	14	11,11,12	0.79	1 (9%)	15,15,17	0.91	1 (6%)
14	NAG	bC	2	14	14,14,15	0.35	0	17,19,21	0.69	0
14	BMA	bC	3	14	11,11,12	0.23	0	15,15,17	1.13	2 (13%)
14	MAN	bC	4	14	11,11,12	0.92	1 (9%)	15,15,17	1.27	2 (13%)
14	MAN	bC	5	14	11,11,12	0.75	0	15,15,17	1.35	2 (13%)
14	XYP	bC	6	14	9,9,10	0.18	0	10,12,14	0.59	0
14	XYS	bC	7	14	9,9,10	1.93	3 (33%)	10,12,14	0.91	1 (10%)
14	MAN	bC	8	14,23	11,11,12	0.95	1 (9%)	15,15,17	0.92	1 (6%)
14	BMA	bC	9	14	11,11,12	0.84	1 (9%)	15,15,17	1.07	2 (13%)
12	NAG	bD	1	12,6	14,14,15	0.48	0	17,19,21	0.65	0
12	NAG	bD	2	12	14,14,15	0.35	0	17,19,21	0.84	0
12	BMA	bD	3	12	11,11,12	0.28	0	15,15,17	0.79	1 (6%)
12	MAN	bD	4	12	11,11,12	0.96	1 (9%)	15,15,17	1.17	1 (6%)
12	MAN	bD	5	12	11,11,12	1.03	1 (9%)	15,15,17	1.23	2 (13%)
12	MAN	bD	6	12	11,11,12	0.95	1 (9%)	15,15,17	1.19	2 (13%)
12	MAN	bD	7	12	11,11,12	0.79	1 (9%)	15,15,17	1.05	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	MAN	bD	8	12	11,11,12	0.74	0	15,15,17	1.14	2 (13%)
12	MAN	bD	9	12	11,11,12	0.75	0	15,15,17	1.12	1 (6%)
13	NAG	bE	1	13,6	14,14,15	0.32	0	17,19,21	0.54	0
13	NAG	bE	2	13	14,14,15	0.31	0	17,19,21	0.68	0
13	BMA	bE	3	13	11,11,12	0.20	0	15,15,17	0.61	0
13	MAN	bE	4	13	11,11,12	0.72	0	15,15,17	1.18	2 (13%)
13	MAN	bE	5	13	11,11,12	0.63	0	15,15,17	1.18	2 (13%)
14	NAG	bF	1	14,6	14,14,15	0.43	0	17,19,21	0.63	0
14	MAN	bF	10	14	11,11,12	0.90	1 (9%)	15,15,17	0.95	1 (6%)
14	NAG	bF	2	14	14,14,15	0.38	0	17,19,21	0.91	1 (5%)
14	BMA	bF	3	14	11,11,12	0.35	0	15,15,17	0.80	0
14	MAN	bF	4	14	11,11,12	0.83	1 (9%)	15,15,17	1.05	2 (13%)
14	MAN	bF	5	14	11,11,12	0.89	0	15,15,17	1.46	2 (13%)
14	XYP	bF	6	14	9,9,10	0.19	0	10,12,14	0.61	0
14	XYS	bF	7	14	9,9,10	1.93	3 (33%)	10,12,14	1.03	1 (10%)
14	MAN	bF	8	14,23	11,11,12	0.79	1 (9%)	15,15,17	1.04	2 (13%)
14	BMA	bF	9	14	11,11,12	1.09	1 (9%)	15,15,17	1.03	2 (13%)
12	NAG	bG	1	12,6	14,14,15	0.45	0	17,19,21	0.75	0
12	NAG	bG	2	12	14,14,15	0.35	0	17,19,21	0.81	0
12	BMA	bG	3	12	11,11,12	0.37	0	15,15,17	0.69	0
12	MAN	bG	4	12	11,11,12	0.81	0	15,15,17	1.30	2 (13%)
12	MAN	bG	5	12	11,11,12	0.87	0	15,15,17	1.27	2 (13%)
12	MAN	bG	6	12	11,11,12	0.79	0	15,15,17	1.14	2 (13%)
12	MAN	bG	7	12	11,11,12	0.82	1 (9%)	15,15,17	1.13	2 (13%)
12	MAN	bG	8	12	11,11,12	0.70	0	15,15,17	1.16	2 (13%)
12	MAN	bG	9	12	11,11,12	0.82	1 (9%)	15,15,17	0.93	1 (6%)
13	NAG	bH	1	13,6	14,14,15	0.35	0	17,19,21	0.60	1 (5%)
13	NAG	bH	2	13	14,14,15	0.29	0	17,19,21	0.79	1 (5%)
13	BMA	bH	3	13	11,11,12	0.28	0	15,15,17	0.49	0
13	MAN	bH	4	13	11,11,12	0.85	1 (9%)	15,15,17	1.11	2 (13%)
13	MAN	bH	5	13	11,11,12	0.62	0	15,15,17	1.48	3 (20%)
14	NAG	bI	1	14,6	14,14,15	0.42	0	17,19,21	0.67	0
14	MAN	bI	10	14	11,11,12	0.69	0	15,15,17	1.07	2 (13%)
14	NAG	bI	2	14	14,14,15	0.33	0	17,19,21	0.98	1 (5%)
14	BMA	bI	3	14	11,11,12	0.42	0	15,15,17	1.30	1 (6%)
14	MAN	bI	4	14	11,11,12	0.58	0	15,15,17	1.32	2 (13%)
14	MAN	bI	5	14	11,11,12	0.53	0	15,15,17	1.51	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	XYP	bI	6	14	9,9,10	0.18	0	10,12,14	0.58	0
14	XYS	bI	7	14	9,9,10	1.92	3 (33%)	10,12,14	1.37	1 (10%)
14	MAN	bI	8	14,23	11,11,12	0.82	1 (9%)	15,15,17	0.92	1 (6%)
14	BMA	bI	9	14	11,11,12	1.01	1 (9%)	15,15,17	0.99	1 (6%)
15	XYP	cA	1	15	9,9,10	0.16	0	10,12,14	0.63	0
15	MAN	cA	2	15	11,11,12	0.80	0	15,15,17	1.49	2 (13%)
15	MAN	cA	3	15	11,11,12	0.96	1 (9%)	15,15,17	1.09	2 (13%)
15	MAN	cA	4	15	11,11,12	0.64	0	15,15,17	1.39	3 (20%)
15	XYP	cB	1	15	9,9,10	0.21	0	10,12,14	0.71	0
15	MAN	cB	2	15	11,11,12	0.99	1 (9%)	15,15,17	1.09	1 (6%)
15	MAN	cB	3	15	11,11,12	0.95	1 (9%)	15,15,17	1.16	2 (13%)
15	MAN	cB	4	15	11,11,12	0.74	0	15,15,17	1.35	2 (13%)
15	XYP	cC	1	15	9,9,10	0.18	0	10,12,14	0.63	0
15	MAN	cC	2	15	11,11,12	0.78	0	15,15,17	1.43	2 (13%)
15	MAN	cC	3	15	11,11,12	0.85	0	15,15,17	1.24	2 (13%)
15	MAN	cC	4	15	11,11,12	0.78	0	15,15,17	1.44	3 (20%)
16	XYP	dA	1	16	9,9,10	0.16	0	10,12,14	0.74	0
16	MAN	dA	2	16	11,11,12	0.73	0	15,15,17	1.27	3 (20%)
16	MAN	dA	3	16	11,11,12	1.21	1 (9%)	15,15,17	1.25	2 (13%)
16	MAN	dA	4	16	11,11,12	1.08	1 (9%)	15,15,17	1.27	2 (13%)
16	MAN	dA	5	16	11,11,12	0.85	1 (9%)	15,15,17	1.22	2 (13%)
16	MAN	dA	6	16	11,11,12	0.94	1 (9%)	15,15,17	1.05	2 (13%)
16	MAN	dA	7	16	11,11,12	0.66	0	15,15,17	1.27	3 (20%)
16	XYP	dB	1	16	9,9,10	0.20	0	10,12,14	0.67	0
16	MAN	dB	2	16	11,11,12	0.96	1 (9%)	15,15,17	1.18	2 (13%)
16	MAN	dB	3	16	11,11,12	1.06	1 (9%)	15,15,17	1.31	2 (13%)
16	MAN	dB	4	16	11,11,12	0.87	1 (9%)	15,15,17	1.31	2 (13%)
16	MAN	dB	5	16	11,11,12	0.63	0	15,15,17	1.22	2 (13%)
16	MAN	dB	6	16	11,11,12	0.99	1 (9%)	15,15,17	1.01	1 (6%)
16	MAN	dB	7	16	11,11,12	0.72	0	15,15,17	1.23	2 (13%)
16	XYP	dC	1	16	9,9,10	0.15	0	10,12,14	0.65	0
16	MAN	dC	2	16	11,11,12	0.92	1 (9%)	15,15,17	1.11	2 (13%)
16	MAN	dC	3	16	11,11,12	1.02	1 (9%)	15,15,17	1.24	2 (13%)
16	MAN	dC	4	16	11,11,12	0.95	1 (9%)	15,15,17	1.35	3 (20%)
16	MAN	dC	5	16	11,11,12	0.75	0	15,15,17	1.30	2 (13%)
16	MAN	dC	6	16	11,11,12	0.93	1 (9%)	15,15,17	1.12	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	MAN	dC	7	16	11,11,12	0.86	1 (9%)	15,15,17	1.07	1 (6%)
17	NAG	eA	1	1,17	14,14,15	0.40	0	17,19,21	0.81	1 (5%)
17	MAN	eA	10	17	11,11,12	0.77	1 (9%)	15,15,17	1.13	2 (13%)
17	MAN	eA	11	17	11,11,12	0.77	0	15,15,17	1.20	2 (13%)
17	NAG	eA	2	17	14,14,15	0.38	0	17,19,21	0.72	0
17	BMA	eA	3	17	11,11,12	0.25	0	15,15,17	0.72	0
17	MAN	eA	4	17	11,11,12	0.57	0	15,15,17	1.23	2 (13%)
17	MAN	eA	5	17	11,11,12	0.82	1 (9%)	15,15,17	1.02	1 (6%)
17	MAN	eA	6	17	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
17	MAN	eA	7	17	11,11,12	0.76	0	15,15,17	1.30	3 (20%)
17	MAN	eA	8	17	11,11,12	1.00	1 (9%)	15,15,17	1.03	2 (13%)
17	MAN	eA	9	17	11,11,12	0.83	0	15,15,17	1.20	2 (13%)
18	NAG	eB	1	1,18	14,14,15	0.36	0	17,19,21	0.80	1 (5%)
18	MAN	eB	10	18	11,11,12	0.69	0	15,15,17	1.10	2 (13%)
18	NAG	eB	11	18	14,14,15	0.33	0	17,19,21	1.12	2 (11%)
18	XYP	eB	12	18	9,9,10	0.18	0	10,12,14	0.66	0
18	XYP	eB	13	18	9,9,10	0.16	0	10,12,14	0.63	0
18	MAN	eB	14	18	11,11,12	0.82	1 (9%)	15,15,17	1.14	2 (13%)
18	NAG	eB	2	18	14,14,15	0.31	0	17,19,21	0.76	0
18	BMA	eB	3	18	11,11,12	0.24	0	15,15,17	0.69	0
18	MAN	eB	4	18	11,11,12	0.98	0	15,15,17	1.25	1 (6%)
18	MAN	eB	5	18	11,11,12	1.00	1 (9%)	15,15,17	1.19	2 (13%)
18	XYP	eB	6	18	9,9,10	0.16	0	10,12,14	0.65	0
18	XYS	eB	7	18	9,9,10	1.85	3 (33%)	10,12,14	0.93	1 (10%)
18	BGC	eB	8	18	11,11,12	0.42	0	15,15,17	0.67	0
18	NAG	eB	9	18	14,14,15	0.32	0	17,19,21	0.61	0
17	NAG	eC	1	1,17	14,14,15	0.41	0	17,19,21	0.62	0
17	MAN	eC	10	17	11,11,12	0.70	0	15,15,17	1.19	3 (20%)
17	MAN	eC	11	17	11,11,12	0.69	0	15,15,17	1.08	1 (6%)
17	NAG	eC	2	17	14,14,15	0.38	0	17,19,21	0.71	0
17	BMA	eC	3	17	11,11,12	0.25	0	15,15,17	0.92	1 (6%)
17	MAN	eC	4	17	11,11,12	0.69	0	15,15,17	1.13	2 (13%)
17	MAN	eC	5	17	11,11,12	0.97	1 (9%)	15,15,17	1.02	2 (13%)
17	MAN	eC	6	17	11,11,12	0.63	0	15,15,17	1.37	3 (20%)
17	MAN	eC	7	17	11,11,12	0.69	0	15,15,17	1.33	3 (20%)
17	MAN	eC	8	17	11,11,12	1.02	1 (9%)	15,15,17	1.07	2 (13%)
17	MAN	eC	9	17	11,11,12	0.71	0	15,15,17	1.19	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	NAG	eD	1	1,18	14,14,15	0.37	0	17,19,21	0.59	0
18	MAN	eD	10	18,23	11,11,12	0.70	0	15,15,17	1.15	2 (13%)
18	NAG	eD	11	18	14,14,15	0.36	0	17,19,21	0.93	1 (5%)
18	XYP	eD	12	18	9,9,10	0.15	0	10,12,14	0.64	0
18	XYP	eD	13	18	9,9,10	0.17	0	10,12,14	0.61	0
18	MAN	eD	14	18	11,11,12	0.87	1 (9%)	15,15,17	1.08	2 (13%)
18	NAG	eD	2	18	14,14,15	0.39	0	17,19,21	0.68	0
18	BMA	eD	3	18	11,11,12	0.21	0	15,15,17	0.77	0
18	MAN	eD	4	18	11,11,12	0.89	0	15,15,17	1.52	3 (20%)
18	MAN	eD	5	18	11,11,12	0.99	1 (9%)	15,15,17	1.32	3 (20%)
18	XYP	eD	6	18	9,9,10	0.17	0	10,12,14	0.61	0
18	XYS	eD	7	18	9,9,10	1.84	3 (33%)	10,12,14	0.99	0
18	BGC	eD	8	18	11,11,12	0.23	0	15,15,17	0.73	1 (6%)
18	NAG	eD	9	18	14,14,15	0.33	0	17,19,21	0.56	0
17	NAG	eE	1	1,17	14,14,15	0.40	0	17,19,21	0.65	0
17	MAN	eE	10	17	11,11,12	0.80	0	15,15,17	1.05	1 (6%)
17	MAN	eE	11	17	11,11,12	0.80	1 (9%)	15,15,17	1.06	2 (13%)
17	NAG	eE	2	17	14,14,15	0.35	0	17,19,21	0.74	0
17	BMA	eE	3	17	11,11,12	0.29	0	15,15,17	0.89	1 (6%)
17	MAN	eE	4	17	11,11,12	0.68	0	15,15,17	1.14	2 (13%)
17	MAN	eE	5	17	11,11,12	0.95	1 (9%)	15,15,17	1.10	2 (13%)
17	MAN	eE	6	17	11,11,12	0.74	0	15,15,17	1.09	2 (13%)
17	MAN	eE	7	17	11,11,12	0.71	0	15,15,17	1.27	2 (13%)
17	MAN	eE	8	17	11,11,12	0.99	1 (9%)	15,15,17	0.99	1 (6%)
17	MAN	eE	9	17	11,11,12	0.73	0	15,15,17	1.15	2 (13%)
18	NAG	eF	1	1,18	14,14,15	0.38	0	17,19,21	0.62	0
18	MAN	eF	10	18	11,11,12	0.66	0	15,15,17	1.14	2 (13%)
18	NAG	eF	11	18	14,14,15	0.36	0	17,19,21	0.92	1 (5%)
18	XYP	eF	12	18	9,9,10	0.19	0	10,12,14	0.64	0
18	XYP	eF	13	18	9,9,10	0.16	0	10,12,14	0.63	0
18	MAN	eF	14	18	11,11,12	0.81	1 (9%)	15,15,17	1.03	2 (13%)
18	NAG	eF	2	18	14,14,15	0.31	0	17,19,21	0.56	0
18	BMA	eF	3	18	11,11,12	0.20	0	15,15,17	0.68	0
18	MAN	eF	4	18	11,11,12	0.91	0	15,15,17	1.54	3 (20%)
18	MAN	eF	5	18	11,11,12	1.02	1 (9%)	15,15,17	1.23	2 (13%)
18	XYP	eF	6	18	9,9,10	0.16	0	10,12,14	0.60	0
18	XYS	eF	7	18	9,9,10	1.93	3 (33%)	10,12,14	0.77	0
18	BGC	eF	8	18	11,11,12	0.29	0	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	NAG	eF	9	18	14,14,15	0.30	0	17,19,21	0.58	0
19	NAG	fB	1	19,2	14,14,15	0.40	0	17,19,21	0.75	1 (5%)
19	MAN	fB	10	19	11,11,12	0.76	1 (9%)	15,15,17	0.98	2 (13%)
19	NAG	fB	2	19	14,14,15	0.31	0	17,19,21	1.24	1 (5%)
19	BMA	fB	3	19	11,11,12	0.25	0	15,15,17	0.73	0
19	MAN	fB	4	19	11,11,12	0.97	1 (9%)	15,15,17	1.08	2 (13%)
19	MAN	fB	5	19	11,11,12	0.79	0	15,15,17	1.07	1 (6%)
19	MAN	fB	6	19	11,11,12	0.78	0	15,15,17	1.20	2 (13%)
19	MAN	fB	7	19	11,11,12	0.81	1 (9%)	15,15,17	1.33	2 (13%)
19	MAN	fB	8	19	11,11,12	0.83	1 (9%)	15,15,17	1.25	3 (20%)
19	MAN	fB	9	19	11,11,12	0.81	1 (9%)	15,15,17	1.07	2 (13%)
17	NAG	fC	1	17,2	14,14,15	0.41	0	17,19,21	0.75	0
17	MAN	fC	10	17	11,11,12	0.91	1 (9%)	15,15,17	1.07	2 (13%)
17	MAN	fC	11	17	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
17	NAG	fC	2	17	14,14,15	0.40	0	17,19,21	0.81	0
17	BMA	fC	3	17	11,11,12	0.26	0	15,15,17	0.96	0
17	MAN	fC	4	17	11,11,12	0.72	0	15,15,17	1.46	2 (13%)
17	MAN	fC	5	17	11,11,12	0.84	1 (9%)	15,15,17	1.10	1 (6%)
17	MAN	fC	6	17	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
17	MAN	fC	7	17	11,11,12	0.82	1 (9%)	15,15,17	1.08	1 (6%)
17	MAN	fC	8	17	11,11,12	0.79	1 (9%)	15,15,17	1.12	2 (13%)
17	MAN	fC	9	17	11,11,12	0.61	0	15,15,17	1.26	3 (20%)
17	NAG	fD	1	17,2	14,14,15	0.31	0	17,19,21	0.81	0
17	MAN	fD	10	17	11,11,12	0.73	0	15,15,17	1.21	2 (13%)
17	MAN	fD	11	17	11,11,12	0.96	1 (9%)	15,15,17	1.25	1 (6%)
17	NAG	fD	2	17	14,14,15	0.37	0	17,19,21	0.57	0
17	BMA	fD	3	17	11,11,12	0.27	0	15,15,17	0.75	0
17	MAN	fD	4	17	11,11,12	0.77	0	15,15,17	1.32	3 (20%)
17	MAN	fD	5	17	11,11,12	0.76	0	15,15,17	0.96	1 (6%)
17	MAN	fD	6	17	11,11,12	0.74	0	15,15,17	1.25	1 (6%)
17	MAN	fD	7	17	11,11,12	1.08	2 (18%)	15,15,17	1.11	1 (6%)
17	MAN	fD	8	17	11,11,12	0.76	0	15,15,17	1.20	2 (13%)
17	MAN	fD	9	17	11,11,12	0.73	0	15,15,17	1.16	3 (20%)
19	NAG	fE	1	19,2	14,14,15	0.36	0	17,19,21	0.57	0
19	MAN	fE	10	19	11,11,12	0.79	1 (9%)	15,15,17	0.97	1 (6%)
19	NAG	fE	2	19	14,14,15	0.32	0	17,19,21	0.58	0
19	BMA	fE	3	19	11,11,12	0.28	0	15,15,17	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	MAN	fE	4	19	11,11,12	0.86	0	15,15,17	1.31	3 (20%)
19	MAN	fE	5	19	11,11,12	0.89	1 (9%)	15,15,17	1.22	2 (13%)
19	MAN	fE	6	19	11,11,12	0.92	1 (9%)	15,15,17	1.02	2 (13%)
19	MAN	fE	7	19	11,11,12	0.77	0	15,15,17	1.25	2 (13%)
19	MAN	fE	8	19	11,11,12	0.81	1 (9%)	15,15,17	1.26	2 (13%)
19	MAN	fE	9	19	11,11,12	0.80	0	15,15,17	1.01	1 (6%)
20	NAG	fF	1	20,2	14,14,15	0.31	0	17,19,21	0.68	0
20	NAG	fF	10	20	14,14,15	0.32	0	17,19,21	0.75	0
20	XYS	fF	11	20	9,9,10	2.09	4 (44%)	10,12,14	1.04	1 (10%)
20	XYP	fF	12	20	9,9,10	0.17	0	10,12,14	0.65	0
20	MAN	fF	13	20	11,11,12	0.85	1 (9%)	15,15,17	1.03	2 (13%)
20	MAN	fF	14	20	11,11,12	0.73	0	15,15,17	0.92	0
20	NAG	fF	2	20	14,14,15	0.36	0	17,19,21	0.89	0
20	BMA	fF	3	20	11,11,12	0.16	0	15,15,17	0.88	0
20	MAN	fF	4	20	11,11,12	0.77	0	15,15,17	1.18	2 (13%)
20	MAN	fF	5	20	11,11,12	0.69	0	15,15,17	1.22	2 (13%)
20	XYP	fF	6	20	9,9,10	0.17	0	10,12,14	0.64	0
20	XYS	fF	7	20	9,9,10	1.89	3 (33%)	10,12,14	1.47	1 (10%)
20	NAG	fF	8	20	14,14,15	0.38	0	17,19,21	0.48	0
20	MAN	fF	9	20	11,11,12	0.80	1 (9%)	15,15,17	1.02	1 (6%)
19	NAG	fG	1	19,2	14,14,15	0.41	0	17,19,21	0.73	1 (5%)
19	MAN	fG	10	19	11,11,12	0.77	1 (9%)	15,15,17	1.04	1 (6%)
19	NAG	fG	2	19	14,14,15	0.33	0	17,19,21	0.93	0
19	BMA	fG	3	19	11,11,12	0.29	0	15,15,17	0.72	0
19	MAN	fG	4	19	11,11,12	0.91	1 (9%)	15,15,17	1.16	1 (6%)
19	MAN	fG	5	19	11,11,12	0.87	1 (9%)	15,15,17	1.29	1 (6%)
19	MAN	fG	6	19	11,11,12	0.82	0	15,15,17	1.23	2 (13%)
19	MAN	fG	7	19	11,11,12	0.89	1 (9%)	15,15,17	1.32	3 (20%)
19	MAN	fG	8	19	11,11,12	0.93	1 (9%)	15,15,17	1.14	2 (13%)
19	MAN	fG	9	19	11,11,12	0.82	1 (9%)	15,15,17	1.03	1 (6%)
17	NAG	fH	1	17,2	14,14,15	0.50	0	17,19,21	0.93	0
17	MAN	fH	10	17	11,11,12	0.90	1 (9%)	15,15,17	1.10	1 (6%)
17	MAN	fH	11	17	11,11,12	0.67	0	15,15,17	1.09	2 (13%)
17	NAG	fH	2	17	14,14,15	0.39	0	17,19,21	0.53	0
17	BMA	fH	3	17	11,11,12	0.28	0	15,15,17	0.75	0
17	MAN	fH	4	17	11,11,12	0.73	0	15,15,17	1.24	2 (13%)
17	MAN	fH	5	17	11,11,12	1.12	1 (9%)	15,15,17	1.01	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	MAN	fH	6	17	11,11,12	0.64	0	15,15,17	1.19	2 (13%)
17	MAN	fH	7	17	11,11,12	1.03	1 (9%)	15,15,17	1.11	1 (6%)
17	MAN	fH	8	17	11,11,12	0.74	0	15,15,17	1.10	2 (13%)
17	MAN	fH	9	17	11,11,12	0.56	0	15,15,17	1.21	2 (13%)
17	NAG	fI	1	17,2	14,14,15	0.35	0	17,19,21	0.79	0
17	MAN	fI	10	17	11,11,12	0.75	0	15,15,17	1.15	2 (13%)
17	MAN	fI	11	17	11,11,12	1.04	1 (9%)	15,15,17	1.04	2 (13%)
17	NAG	fI	2	17	14,14,15	0.40	0	17,19,21	0.48	0
17	BMA	fI	3	17	11,11,12	0.28	0	15,15,17	0.79	0
17	MAN	fI	4	17	11,11,12	0.72	0	15,15,17	1.24	3 (20%)
17	MAN	fI	5	17	11,11,12	0.95	1 (9%)	15,15,17	1.04	1 (6%)
17	MAN	fI	6	17	11,11,12	0.64	0	15,15,17	1.27	2 (13%)
17	MAN	fI	7	17	11,11,12	0.90	0	15,15,17	1.44	2 (13%)
17	MAN	fI	8	17	11,11,12	0.86	1 (9%)	15,15,17	1.11	2 (13%)
17	MAN	fI	9	17	11,11,12	0.84	1 (9%)	15,15,17	1.04	2 (13%)
19	NAG	fJ	1	19,2	14,14,15	0.36	0	17,19,21	0.67	1 (5%)
19	MAN	fJ	10	19	11,11,12	0.92	1 (9%)	15,15,17	0.99	1 (6%)
19	NAG	fJ	2	19	14,14,15	0.34	0	17,19,21	0.51	0
19	BMA	fJ	3	19	11,11,12	0.24	0	15,15,17	0.80	0
19	MAN	fJ	4	19	11,11,12	0.85	0	15,15,17	1.31	2 (13%)
19	MAN	fJ	5	19	11,11,12	0.93	1 (9%)	15,15,17	1.12	2 (13%)
19	MAN	fJ	6	19	11,11,12	0.85	1 (9%)	15,15,17	1.14	2 (13%)
19	MAN	fJ	7	19	11,11,12	0.95	1 (9%)	15,15,17	1.28	1 (6%)
19	MAN	fJ	8	19	11,11,12	0.90	1 (9%)	15,15,17	1.12	1 (6%)
19	MAN	fJ	9	19	11,11,12	0.87	1 (9%)	15,15,17	1.09	1 (6%)
20	NAG	fK	1	20,2	14,14,15	0.34	0	17,19,21	0.78	0
20	NAG	fK	10	20	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
20	XYS	fK	11	20	9,9,10	1.99	4 (44%)	10,12,14	1.59	1 (10%)
20	XYP	fK	12	20	9,9,10	0.17	0	10,12,14	0.66	0
20	MAN	fK	13	20	11,11,12	0.58	0	15,15,17	1.15	2 (13%)
20	MAN	fK	14	20	11,11,12	0.66	0	15,15,17	0.98	2 (13%)
20	NAG	fK	2	20	14,14,15	0.36	0	17,19,21	0.97	1 (5%)
20	BMA	fK	3	20	11,11,12	0.22	0	15,15,17	0.75	0
20	MAN	fK	4	20	11,11,12	0.89	1 (9%)	15,15,17	1.12	2 (13%)
20	MAN	fK	5	20	11,11,12	0.55	0	15,15,17	1.16	1 (6%)
20	XYP	fK	6	20	9,9,10	0.17	0	10,12,14	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	XYS	fK	7	20	9,9,10	1.94	3 (33%)	10,12,14	1.20	1 (10%)
20	NAG	fK	8	20	14,14,15	0.41	0	17,19,21	0.59	0
20	MAN	fK	9	23,20	11,11,12	0.70	0	15,15,17	1.11	1 (6%)
19	NAG	fL	1	19,2	14,14,15	0.41	0	17,19,21	0.57	0
19	MAN	fL	10	19	11,11,12	0.75	0	15,15,17	1.00	2 (13%)
19	NAG	fL	2	19	14,14,15	0.34	0	17,19,21	1.16	1 (5%)
19	BMA	fL	3	19	11,11,12	0.21	0	15,15,17	0.62	0
19	MAN	fL	4	19	11,11,12	0.85	1 (9%)	15,15,17	1.33	2 (13%)
19	MAN	fL	5	19	11,11,12	0.94	1 (9%)	15,15,17	1.19	1 (6%)
19	MAN	fL	6	19	11,11,12	0.80	0	15,15,17	1.34	2 (13%)
19	MAN	fL	7	19	11,11,12	0.95	1 (9%)	15,15,17	1.44	3 (20%)
19	MAN	fL	8	19	11,11,12	1.14	1 (9%)	15,15,17	1.19	2 (13%)
19	MAN	fL	9	19	11,11,12	0.83	1 (9%)	15,15,17	1.03	1 (6%)
17	NAG	fM	1	17,2	14,14,15	0.55	0	17,19,21	0.83	0
17	MAN	fM	10	17	11,11,12	0.68	0	15,15,17	1.45	3 (20%)
17	MAN	fM	11	17	11,11,12	0.73	0	15,15,17	1.17	2 (13%)
17	NAG	fM	2	17	14,14,15	0.37	0	17,19,21	1.03	1 (5%)
17	BMA	fM	3	17	11,11,12	0.29	0	15,15,17	0.85	0
17	MAN	fM	4	17	11,11,12	0.73	0	15,15,17	1.48	3 (20%)
17	MAN	fM	5	17	11,11,12	0.85	1 (9%)	15,15,17	1.16	1 (6%)
17	MAN	fM	6	17	11,11,12	0.58	0	15,15,17	1.26	2 (13%)
17	MAN	fM	7	17	11,11,12	1.00	1 (9%)	15,15,17	1.11	2 (13%)
17	MAN	fM	8	17	11,11,12	0.86	1 (9%)	15,15,17	1.13	1 (6%)
17	MAN	fM	9	17	11,11,12	0.73	0	15,15,17	1.12	2 (13%)
17	NAG	fN	1	17,2	14,14,15	0.31	0	17,19,21	0.86	0
17	MAN	fN	10	17	11,11,12	0.76	0	15,15,17	1.20	2 (13%)
17	MAN	fN	11	17	11,11,12	0.95	1 (9%)	15,15,17	1.23	2 (13%)
17	NAG	fN	2	17	14,14,15	0.36	0	17,19,21	0.67	0
17	BMA	fN	3	17	11,11,12	0.27	0	15,15,17	0.85	1 (6%)
17	MAN	fN	4	17	11,11,12	0.84	1 (9%)	15,15,17	1.21	2 (13%)
17	MAN	fN	5	17	11,11,12	0.78	0	15,15,17	1.05	2 (13%)
17	MAN	fN	6	17	11,11,12	0.68	0	15,15,17	1.19	1 (6%)
17	MAN	fN	7	17	11,11,12	0.86	0	15,15,17	1.30	2 (13%)
17	MAN	fN	8	17	11,11,12	0.85	0	15,15,17	1.27	2 (13%)
17	MAN	fN	9	17	11,11,12	0.75	1 (9%)	15,15,17	1.08	2 (13%)
19	NAG	fO	1	19,2	14,14,15	0.44	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	MAN	fO	10	19	11,11,12	0.83	1 (9%)	15,15,17	1.04	2 (13%)
19	NAG	fO	2	19	14,14,15	0.34	0	17,19,21	0.65	0
19	BMA	fO	3	19	11,11,12	0.32	0	15,15,17	0.73	0
19	MAN	fO	4	19	11,11,12	0.90	0	15,15,17	1.29	3 (20%)
19	MAN	fO	5	19	11,11,12	1.05	1 (9%)	15,15,17	1.11	2 (13%)
19	MAN	fO	6	19	11,11,12	0.91	1 (9%)	15,15,17	1.15	2 (13%)
19	MAN	fO	7	19	11,11,12	0.82	1 (9%)	15,15,17	1.27	2 (13%)
19	MAN	fO	8	19	11,11,12	0.67	0	15,15,17	1.18	2 (13%)
19	MAN	fO	9	19	11,11,12	0.84	1 (9%)	15,15,17	1.02	1 (6%)
20	NAG	fP	1	20,2	14,14,15	0.38	0	17,19,21	0.67	0
20	NAG	fP	10	20	14,14,15	0.36	0	17,19,21	0.80	0
20	XYS	fP	11	20	9,9,10	1.99	3 (33%)	10,12,14	1.27	2 (20%)
20	XYP	fP	12	20	9,9,10	0.20	0	10,12,14	0.66	0
20	MAN	fP	13	20	11,11,12	0.77	1 (9%)	15,15,17	1.07	1 (6%)
20	MAN	fP	14	20	11,11,12	0.71	1 (9%)	15,15,17	0.99	1 (6%)
20	NAG	fP	2	20	14,14,15	0.36	0	17,19,21	0.79	1 (5%)
20	BMA	fP	3	20	11,11,12	0.22	0	15,15,17	0.87	0
20	MAN	fP	4	20	11,11,12	0.74	0	15,15,17	1.17	3 (20%)
20	MAN	fP	5	20	11,11,12	0.63	0	15,15,17	1.33	3 (20%)
20	XYP	fP	6	20	9,9,10	0.17	0	10,12,14	0.62	0
20	XYS	fP	7	20	9,9,10	1.90	3 (33%)	10,12,14	1.12	1 (10%)
20	NAG	fP	8	20	14,14,15	0.34	0	17,19,21	0.70	0
20	MAN	fP	9	23,20	11,11,12	0.67	0	15,15,17	1.09	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	aA	1	7,5	-	0/6/23/26	0/1/1/1
7	MAN	aA	10	23,7	-	0/2/19/22	0/1/1/1
7	NAG	aA	11	7	-	0/6/23/26	0/1/1/1
7	XYP	aA	12	7	-	-	0/1/1/1
7	MAN	aA	13	7	-	0/2/19/22	0/1/1/1
7	MAN	aA	14	7	-	2/2/19/22	0/1/1/1
7	NAG	aA	2	7	-	0/6/23/26	0/1/1/1
7	BMA	aA	3	7	-	0/2/19/22	0/1/1/1
7	MAN	aA	4	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	aA	5	7	-	0/2/19/22	0/1/1/1
7	XYP	aA	6	7	-	-	0/1/1/1
7	XYP	aA	7	7	-	-	0/1/1/1
7	MAN	aA	8	7	-	0/2/19/22	0/1/1/1
7	NAG	aA	9	7	-	0/6/23/26	0/1/1/1
8	NAG	aB	1	8,5	-	0/6/23/26	0/1/1/1
8	XYP	aB	10	8	-	-	0/1/1/1
8	MAN	aB	11	8	-	0/2/19/22	0/1/1/1
8	NAG	aB	12	8	-	2/6/23/26	0/1/1/1
8	BMA	aB	13	8	-	0/2/19/22	0/1/1/1
8	XYP	aB	14	8	-	-	0/1/1/1
8	XYP	aB	15	8	-	-	0/1/1/1
8	MAN	aB	16	8	-	0/2/19/22	0/1/1/1
8	NAG	aB	2	8	-	2/6/23/26	0/1/1/1
8	BMA	aB	3	8	-	0/2/19/22	0/1/1/1
8	MAN	aB	4	8	-	0/2/19/22	0/1/1/1
8	MAN	aB	5	8	-	0/2/19/22	0/1/1/1
8	NAG	aB	6	8	-	0/6/23/26	0/1/1/1
8	MAN	aB	7	8	-	2/2/19/22	0/1/1/1
8	XYP	aB	8	8	-	-	0/1/1/1
8	BMA	aB	9	8	-	0/2/19/22	0/1/1/1
9	NAG	aC	1	5,9	-	0/6/23/26	0/1/1/1
9	XYP	aC	10	9	-	-	0/1/1/1
9	BGC	aC	11	9	-	1/2/19/22	0/1/1/1
9	MAN	aC	12	23,9	-	0/2/19/22	0/1/1/1
9	NAG	aC	13	9	-	0/6/23/26	0/1/1/1
9	XYP	aC	14	9	-	-	0/1/1/1
9	MAN	aC	15	9	-	0/2/19/22	0/1/1/1
9	MAN	aC	16	9	-	0/2/19/22	0/1/1/1
9	NAG	aC	2	9	-	0/6/23/26	0/1/1/1
9	BMA	aC	3	9	-	0/2/19/22	0/1/1/1
9	MAN	aC	4	9	-	0/2/19/22	0/1/1/1
9	MAN	aC	5	9	-	0/2/19/22	0/1/1/1
9	NAG	aC	6	9	-	2/6/23/26	0/1/1/1
9	MAN	aC	7	9	-	0/2/19/22	0/1/1/1
9	BMA	aC	8	9	-	0/2/19/22	0/1/1/1
9	XYP	aC	9	9	-	-	0/1/1/1
10	NAG	aD	1	10,5	-	0/6/23/26	0/1/1/1
10	NAG	aD	2	10	-	0/6/23/26	0/1/1/1
10	BMA	aD	3	10	-	0/2/19/22	0/1/1/1
10	MAN	aD	4	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	aD	5	10	-	1/2/19/22	0/1/1/1
10	MAN	aD	6	10	-	0/2/19/22	0/1/1/1
10	MAN	aD	7	10	-	2/2/19/22	0/1/1/1
10	MAN	aD	8	10	-	2/2/19/22	0/1/1/1
10	MAN	aD	9	10	-	0/2/19/22	0/1/1/1
11	NAG	aE	1	11,5	-	0/6/23/26	0/1/1/1
11	MAN	aE	10	23,11	-	0/2/19/22	0/1/1/1
11	NAG	aE	11	11	-	3/6/23/26	0/1/1/1
11	XYP	aE	12	11	-	-	0/1/1/1
11	XYP	aE	13	11	-	-	0/1/1/1
11	BMA	aE	14	11	-	0/2/19/22	0/1/1/1
11	MAN	aE	15	11	-	2/2/19/22	0/1/1/1
11	NAG	aE	2	11	-	0/6/23/26	0/1/1/1
11	BMA	aE	3	11	-	0/2/19/22	0/1/1/1
11	MAN	aE	4	11	-	2/2/19/22	0/1/1/1
11	MAN	aE	5	11	-	2/2/19/22	0/1/1/1
11	XYP	aE	6	11	-	-	0/1/1/1
11	XYP	aE	7	11	-	-	0/1/1/1
11	XYP	aE	8	11	-	-	0/1/1/1
11	NAG	aE	9	11	-	2/6/23/26	0/1/1/1
7	NAG	aF	1	7,5	-	0/6/23/26	0/1/1/1
7	MAN	aF	10	23,7	-	1/2/19/22	0/1/1/1
7	NAG	aF	11	7	-	0/6/23/26	0/1/1/1
7	XYP	aF	12	7	-	-	0/1/1/1
7	MAN	aF	13	7	-	0/2/19/22	0/1/1/1
7	MAN	aF	14	7	-	2/2/19/22	0/1/1/1
7	NAG	aF	2	7	-	0/6/23/26	0/1/1/1
7	BMA	aF	3	7	-	0/2/19/22	0/1/1/1
7	MAN	aF	4	7	-	1/2/19/22	0/1/1/1
7	MAN	aF	5	7	-	0/2/19/22	0/1/1/1
7	XYP	aF	6	7	-	-	0/1/1/1
7	XYP	aF	7	7	-	-	0/1/1/1
7	MAN	aF	8	7	-	0/2/19/22	0/1/1/1
7	NAG	aF	9	7	-	0/6/23/26	0/1/1/1
8	NAG	aG	1	8,5	-	0/6/23/26	0/1/1/1
8	XYP	aG	10	8	-	-	0/1/1/1
8	MAN	aG	11	8	-	0/2/19/22	0/1/1/1
8	NAG	aG	12	8	-	0/6/23/26	0/1/1/1
8	BMA	aG	13	8	-	0/2/19/22	0/1/1/1
8	XYP	aG	14	8	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	XYP	aG	15	8	-	-	0/1/1/1
8	MAN	aG	16	8	-	0/2/19/22	0/1/1/1
8	NAG	aG	2	8	-	0/6/23/26	0/1/1/1
8	BMA	aG	3	8	-	0/2/19/22	0/1/1/1
8	MAN	aG	4	8	-	0/2/19/22	0/1/1/1
8	MAN	aG	5	8	-	0/2/19/22	0/1/1/1
8	NAG	aG	6	8	-	0/6/23/26	0/1/1/1
8	MAN	aG	7	8	-	0/2/19/22	0/1/1/1
8	XYP	aG	8	8	-	-	0/1/1/1
8	BMA	aG	9	8	-	0/2/19/22	0/1/1/1
9	NAG	aH	1	5,9	-	0/6/23/26	0/1/1/1
9	XYP	aH	10	9	-	-	0/1/1/1
9	BGC	aH	11	9	-	2/2/19/22	0/1/1/1
9	MAN	aH	12	9	-	2/2/19/22	0/1/1/1
9	NAG	aH	13	9	-	0/6/23/26	0/1/1/1
9	XYP	aH	14	9	-	-	0/1/1/1
9	MAN	aH	15	9	-	1/2/19/22	0/1/1/1
9	MAN	aH	16	9	-	0/2/19/22	0/1/1/1
9	NAG	aH	2	9	-	0/6/23/26	0/1/1/1
9	BMA	aH	3	9	-	1/2/19/22	0/1/1/1
9	MAN	aH	4	9	-	2/2/19/22	0/1/1/1
9	MAN	aH	5	9	-	1/2/19/22	0/1/1/1
9	NAG	aH	6	9	-	2/6/23/26	0/1/1/1
9	MAN	aH	7	9	-	0/2/19/22	0/1/1/1
9	BMA	aH	8	9	-	0/2/19/22	0/1/1/1
9	XYP	aH	9	9	-	-	0/1/1/1
10	NAG	aI	1	10,5	-	2/6/23/26	0/1/1/1
10	NAG	aI	2	10	-	0/6/23/26	0/1/1/1
10	BMA	aI	3	10	-	0/2/19/22	0/1/1/1
10	MAN	aI	4	10	-	0/2/19/22	0/1/1/1
10	MAN	aI	5	10	-	1/2/19/22	0/1/1/1
10	MAN	aI	6	10	-	2/2/19/22	0/1/1/1
10	MAN	aI	7	10	-	0/2/19/22	0/1/1/1
10	MAN	aI	8	10	-	0/2/19/22	0/1/1/1
10	MAN	aI	9	10	-	0/2/19/22	0/1/1/1
11	NAG	aJ	1	11,5	-	0/6/23/26	0/1/1/1
11	MAN	aJ	10	11	-	0/2/19/22	0/1/1/1
11	NAG	aJ	11	11	-	3/6/23/26	0/1/1/1
11	XYP	aJ	12	11	-	-	0/1/1/1
11	XYP	aJ	13	11	-	-	0/1/1/1
11	BMA	aJ	14	11	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	aJ	15	11	-	1/2/19/22	0/1/1/1
11	NAG	aJ	2	11	-	0/6/23/26	0/1/1/1
11	BMA	aJ	3	11	-	0/2/19/22	0/1/1/1
11	MAN	aJ	4	11	-	1/2/19/22	0/1/1/1
11	MAN	aJ	5	11	-	0/2/19/22	0/1/1/1
11	XYP	aJ	6	11	-	-	0/1/1/1
11	XYP	aJ	7	11	-	-	0/1/1/1
11	XYP	aJ	8	11	-	-	0/1/1/1
11	NAG	aJ	9	11	-	2/6/23/26	0/1/1/1
7	NAG	aK	1	7,5	-	0/6/23/26	0/1/1/1
7	MAN	aK	10	23,7	-	0/2/19/22	0/1/1/1
7	NAG	aK	11	7	-	0/6/23/26	0/1/1/1
7	XYP	aK	12	7	-	-	0/1/1/1
7	MAN	aK	13	7	-	0/2/19/22	0/1/1/1
7	MAN	aK	14	7	-	0/2/19/22	0/1/1/1
7	NAG	aK	2	7	-	0/6/23/26	0/1/1/1
7	BMA	aK	3	7	-	0/2/19/22	0/1/1/1
7	MAN	aK	4	7	-	0/2/19/22	0/1/1/1
7	MAN	aK	5	7	-	2/2/19/22	0/1/1/1
7	XYP	aK	6	7	-	-	0/1/1/1
7	XYP	aK	7	7	-	-	0/1/1/1
7	MAN	aK	8	7	-	0/2/19/22	0/1/1/1
7	NAG	aK	9	7	-	0/6/23/26	0/1/1/1
8	NAG	aL	1	8,5	-	0/6/23/26	0/1/1/1
8	XYP	aL	10	8	-	-	0/1/1/1
8	MAN	aL	11	23,8	-	0/2/19/22	0/1/1/1
8	NAG	aL	12	8	-	0/6/23/26	0/1/1/1
8	BMA	aL	13	8	-	0/2/19/22	0/1/1/1
8	XYP	aL	14	8	-	-	0/1/1/1
8	XYP	aL	15	8	-	-	0/1/1/1
8	MAN	aL	16	8	-	0/2/19/22	0/1/1/1
8	NAG	aL	2	8	-	2/6/23/26	0/1/1/1
8	BMA	aL	3	8	-	0/2/19/22	0/1/1/1
8	MAN	aL	4	8	-	0/2/19/22	0/1/1/1
8	MAN	aL	5	8	-	0/2/19/22	0/1/1/1
8	NAG	aL	6	8	-	0/6/23/26	0/1/1/1
8	MAN	aL	7	8	-	0/2/19/22	0/1/1/1
8	XYP	aL	8	8	-	-	0/1/1/1
8	BMA	aL	9	8	-	0/2/19/22	0/1/1/1
9	NAG	aM	1	5,9	-	0/6/23/26	0/1/1/1
9	XYP	aM	10	9	-	-	0/1/1/1
9	BGC	aM	11	9	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	aM	12	23,9	-	0/2/19/22	0/1/1/1
9	NAG	aM	13	9	-	2/6/23/26	0/1/1/1
9	XYP	aM	14	9	-	-	0/1/1/1
9	MAN	aM	15	9	-	0/2/19/22	0/1/1/1
9	MAN	aM	16	9	-	1/2/19/22	0/1/1/1
9	NAG	aM	2	9	-	0/6/23/26	0/1/1/1
9	BMA	aM	3	9	-	0/2/19/22	0/1/1/1
9	MAN	aM	4	9	-	0/2/19/22	0/1/1/1
9	MAN	aM	5	9	-	2/2/19/22	0/1/1/1
9	NAG	aM	6	9	-	0/6/23/26	0/1/1/1
9	MAN	aM	7	9	-	0/2/19/22	0/1/1/1
9	BMA	aM	8	9	-	0/2/19/22	0/1/1/1
9	XYP	aM	9	9	-	-	0/1/1/1
10	NAG	aN	1	10,5	-	0/6/23/26	0/1/1/1
10	NAG	aN	2	10	-	0/6/23/26	0/1/1/1
10	BMA	aN	3	10	-	0/2/19/22	0/1/1/1
10	MAN	aN	4	10	-	0/2/19/22	0/1/1/1
10	MAN	aN	5	10	-	1/2/19/22	0/1/1/1
10	MAN	aN	6	10	-	0/2/19/22	0/1/1/1
10	MAN	aN	7	10	-	2/2/19/22	0/1/1/1
10	MAN	aN	8	10	-	2/2/19/22	0/1/1/1
10	MAN	aN	9	10	-	0/2/19/22	0/1/1/1
11	NAG	aO	1	11,5	-	0/6/23/26	0/1/1/1
11	MAN	aO	10	11	-	0/2/19/22	0/1/1/1
11	NAG	aO	11	11	-	3/6/23/26	0/1/1/1
11	XYP	aO	12	11	-	-	0/1/1/1
11	XYP	aO	13	11	-	-	0/1/1/1
11	BMA	aO	14	11	-	0/2/19/22	0/1/1/1
11	MAN	aO	15	11	-	0/2/19/22	0/1/1/1
11	NAG	aO	2	11	-	0/6/23/26	0/1/1/1
11	BMA	aO	3	11	-	0/2/19/22	0/1/1/1
11	MAN	aO	4	11	-	2/2/19/22	0/1/1/1
11	MAN	aO	5	11	-	2/2/19/22	0/1/1/1
11	XYP	aO	6	11	-	-	0/1/1/1
11	XYP	aO	7	11	-	-	0/1/1/1
11	XYP	aO	8	11	-	-	0/1/1/1
11	NAG	aO	9	11	-	0/6/23/26	0/1/1/1
12	NAG	bA	1	12,6	-	0/6/23/26	0/1/1/1
12	NAG	bA	2	12	-	0/6/23/26	0/1/1/1
12	BMA	bA	3	12	-	0/2/19/22	0/1/1/1
12	MAN	bA	4	12	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	bA	5	12	-	0/2/19/22	0/1/1/1
12	MAN	bA	6	12	-	2/2/19/22	0/1/1/1
12	MAN	bA	7	12	-	2/2/19/22	0/1/1/1
12	MAN	bA	8	12	-	2/2/19/22	0/1/1/1
12	MAN	bA	9	12	-	2/2/19/22	0/1/1/1
13	NAG	bB	1	13,6	-	0/6/23/26	0/1/1/1
13	NAG	bB	2	13	-	0/6/23/26	0/1/1/1
13	BMA	bB	3	13	-	1/2/19/22	0/1/1/1
13	MAN	bB	4	13	-	1/2/19/22	0/1/1/1
13	MAN	bB	5	13	-	0/2/19/22	0/1/1/1
14	NAG	bC	1	14,6	-	0/6/23/26	0/1/1/1
14	MAN	bC	10	14	-	2/2/19/22	0/1/1/1
14	NAG	bC	2	14	-	0/6/23/26	0/1/1/1
14	BMA	bC	3	14	-	0/2/19/22	0/1/1/1
14	MAN	bC	4	14	-	2/2/19/22	0/1/1/1
14	MAN	bC	5	14	-	0/2/19/22	0/1/1/1
14	XYP	bC	6	14	-	-	0/1/1/1
14	XYS	bC	7	14	-	-	0/1/1/1
14	MAN	bC	8	14,23	-	0/2/19/22	0/1/1/1
14	BMA	bC	9	14	-	0/2/19/22	0/1/1/1
12	NAG	bD	1	12,6	-	0/6/23/26	0/1/1/1
12	NAG	bD	2	12	-	0/6/23/26	0/1/1/1
12	BMA	bD	3	12	-	0/2/19/22	0/1/1/1
12	MAN	bD	4	12	-	0/2/19/22	0/1/1/1
12	MAN	bD	5	12	-	0/2/19/22	0/1/1/1
12	MAN	bD	6	12	-	2/2/19/22	0/1/1/1
12	MAN	bD	7	12	-	0/2/19/22	0/1/1/1
12	MAN	bD	8	12	-	0/2/19/22	0/1/1/1
12	MAN	bD	9	12	-	2/2/19/22	0/1/1/1
13	NAG	bE	1	13,6	-	0/6/23/26	0/1/1/1
13	NAG	bE	2	13	-	0/6/23/26	0/1/1/1
13	BMA	bE	3	13	-	1/2/19/22	0/1/1/1
13	MAN	bE	4	13	-	2/2/19/22	0/1/1/1
13	MAN	bE	5	13	-	0/2/19/22	0/1/1/1
14	NAG	bF	1	14,6	-	0/6/23/26	0/1/1/1
14	MAN	bF	10	14	-	1/2/19/22	0/1/1/1
14	NAG	bF	2	14	-	0/6/23/26	0/1/1/1
14	BMA	bF	3	14	-	0/2/19/22	0/1/1/1
14	MAN	bF	4	14	-	2/2/19/22	0/1/1/1
14	MAN	bF	5	14	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	XYP	bF	6	14	-	-	0/1/1/1
14	XYS	bF	7	14	-	-	0/1/1/1
14	MAN	bF	8	14,23	-	0/2/19/22	0/1/1/1
14	BMA	bF	9	14	-	0/2/19/22	0/1/1/1
12	NAG	bG	1	12,6	-	0/6/23/26	0/1/1/1
12	NAG	bG	2	12	-	0/6/23/26	0/1/1/1
12	BMA	bG	3	12	-	0/2/19/22	0/1/1/1
12	MAN	bG	4	12	-	0/2/19/22	0/1/1/1
12	MAN	bG	5	12	-	0/2/19/22	0/1/1/1
12	MAN	bG	6	12	-	0/2/19/22	0/1/1/1
12	MAN	bG	7	12	-	0/2/19/22	0/1/1/1
12	MAN	bG	8	12	-	0/2/19/22	0/1/1/1
12	MAN	bG	9	12	-	0/2/19/22	0/1/1/1
13	NAG	bH	1	13,6	-	0/6/23/26	0/1/1/1
13	NAG	bH	2	13	-	0/6/23/26	0/1/1/1
13	BMA	bH	3	13	-	2/2/19/22	0/1/1/1
13	MAN	bH	4	13	-	1/2/19/22	0/1/1/1
13	MAN	bH	5	13	-	2/2/19/22	0/1/1/1
14	NAG	bI	1	14,6	-	0/6/23/26	0/1/1/1
14	MAN	bI	10	14	-	2/2/19/22	0/1/1/1
14	NAG	bI	2	14	-	1/6/23/26	0/1/1/1
14	BMA	bI	3	14	-	0/2/19/22	0/1/1/1
14	MAN	bI	4	14	-	2/2/19/22	0/1/1/1
14	MAN	bI	5	14	-	0/2/19/22	0/1/1/1
14	XYP	bI	6	14	-	-	0/1/1/1
14	XYS	bI	7	14	-	-	0/1/1/1
14	MAN	bI	8	14,23	-	0/2/19/22	0/1/1/1
14	BMA	bI	9	14	-	0/2/19/22	0/1/1/1
15	XYP	cA	1	15	-	-	0/1/1/1
15	MAN	cA	2	15	-	0/2/19/22	0/1/1/1
15	MAN	cA	3	15	-	0/2/19/22	0/1/1/1
15	MAN	cA	4	15	-	2/2/19/22	0/1/1/1
15	XYP	cB	1	15	-	-	0/1/1/1
15	MAN	cB	2	15	-	0/2/19/22	0/1/1/1
15	MAN	cB	3	15	-	1/2/19/22	0/1/1/1
15	MAN	cB	4	15	-	0/2/19/22	0/1/1/1
15	XYP	cC	1	15	-	-	0/1/1/1
15	MAN	cC	2	15	-	0/2/19/22	0/1/1/1
15	MAN	cC	3	15	-	0/2/19/22	0/1/1/1
15	MAN	cC	4	15	-	0/2/19/22	0/1/1/1
16	XYP	dA	1	16	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	MAN	dA	2	16	-	0/2/19/22	0/1/1/1
16	MAN	dA	3	16	-	1/2/19/22	0/1/1/1
16	MAN	dA	4	16	-	1/2/19/22	0/1/1/1
16	MAN	dA	5	16	-	0/2/19/22	0/1/1/1
16	MAN	dA	6	16	-	2/2/19/22	0/1/1/1
16	MAN	dA	7	16	-	1/2/19/22	0/1/1/1
16	XYP	dB	1	16	-	-	0/1/1/1
16	MAN	dB	2	16	-	0/2/19/22	0/1/1/1
16	MAN	dB	3	16	-	2/2/19/22	0/1/1/1
16	MAN	dB	4	16	-	0/2/19/22	0/1/1/1
16	MAN	dB	5	16	-	0/2/19/22	0/1/1/1
16	MAN	dB	6	16	-	2/2/19/22	0/1/1/1
16	MAN	dB	7	16	-	0/2/19/22	0/1/1/1
16	XYP	dC	1	16	-	-	0/1/1/1
16	MAN	dC	2	16	-	2/2/19/22	0/1/1/1
16	MAN	dC	3	16	-	2/2/19/22	0/1/1/1
16	MAN	dC	4	16	-	0/2/19/22	0/1/1/1
16	MAN	dC	5	16	-	0/2/19/22	0/1/1/1
16	MAN	dC	6	16	-	2/2/19/22	0/1/1/1
16	MAN	dC	7	16	-	1/2/19/22	0/1/1/1
17	NAG	eA	1	1,17	-	0/6/23/26	0/1/1/1
17	MAN	eA	10	17	-	0/2/19/22	0/1/1/1
17	MAN	eA	11	17	-	0/2/19/22	0/1/1/1
17	NAG	eA	2	17	-	0/6/23/26	0/1/1/1
17	BMA	eA	3	17	-	0/2/19/22	0/1/1/1
17	MAN	eA	4	17	-	0/2/19/22	0/1/1/1
17	MAN	eA	5	17	-	1/2/19/22	0/1/1/1
17	MAN	eA	6	17	-	0/2/19/22	0/1/1/1
17	MAN	eA	7	17	-	2/2/19/22	0/1/1/1
17	MAN	eA	8	17	-	1/2/19/22	0/1/1/1
17	MAN	eA	9	17	-	0/2/19/22	0/1/1/1
18	NAG	eB	1	1,18	-	0/6/23/26	0/1/1/1
18	MAN	eB	10	18	-	0/2/19/22	0/1/1/1
18	NAG	eB	11	18	-	3/6/23/26	0/1/1/1
18	XYP	eB	12	18	-	-	0/1/1/1
18	XYP	eB	13	18	-	-	0/1/1/1
18	MAN	eB	14	18	-	2/2/19/22	0/1/1/1
18	NAG	eB	2	18	-	0/6/23/26	0/1/1/1
18	BMA	eB	3	18	-	0/2/19/22	0/1/1/1
18	MAN	eB	4	18	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MAN	eB	5	18	-	0/2/19/22	0/1/1/1
18	XYP	eB	6	18	-	-	0/1/1/1
18	XYS	eB	7	18	-	-	0/1/1/1
18	BGC	eB	8	18	-	2/2/19/22	0/1/1/1
18	NAG	eB	9	18	-	0/6/23/26	0/1/1/1
17	NAG	eC	1	1,17	-	0/6/23/26	0/1/1/1
17	MAN	eC	10	17	-	0/2/19/22	0/1/1/1
17	MAN	eC	11	17	-	0/2/19/22	0/1/1/1
17	NAG	eC	2	17	-	2/6/23/26	0/1/1/1
17	BMA	eC	3	17	-	0/2/19/22	0/1/1/1
17	MAN	eC	4	17	-	0/2/19/22	0/1/1/1
17	MAN	eC	5	17	-	1/2/19/22	0/1/1/1
17	MAN	eC	6	17	-	0/2/19/22	0/1/1/1
17	MAN	eC	7	17	-	0/2/19/22	0/1/1/1
17	MAN	eC	8	17	-	0/2/19/22	0/1/1/1
17	MAN	eC	9	17	-	2/2/19/22	0/1/1/1
18	NAG	eD	1	1,18	-	0/6/23/26	0/1/1/1
18	MAN	eD	10	18,23	-	0/2/19/22	0/1/1/1
18	NAG	eD	11	18	-	0/6/23/26	0/1/1/1
18	XYP	eD	12	18	-	-	0/1/1/1
18	XYP	eD	13	18	-	-	0/1/1/1
18	MAN	eD	14	18	-	2/2/19/22	0/1/1/1
18	NAG	eD	2	18	-	0/6/23/26	0/1/1/1
18	BMA	eD	3	18	-	0/2/19/22	0/1/1/1
18	MAN	eD	4	18	-	0/2/19/22	0/1/1/1
18	MAN	eD	5	18	-	0/2/19/22	0/1/1/1
18	XYP	eD	6	18	-	-	0/1/1/1
18	XYS	eD	7	18	-	-	0/1/1/1
18	BGC	eD	8	18	-	2/2/19/22	0/1/1/1
18	NAG	eD	9	18	-	0/6/23/26	0/1/1/1
17	NAG	eE	1	1,17	-	0/6/23/26	0/1/1/1
17	MAN	eE	10	17	-	0/2/19/22	0/1/1/1
17	MAN	eE	11	17	-	0/2/19/22	0/1/1/1
17	NAG	eE	2	17	-	1/6/23/26	0/1/1/1
17	BMA	eE	3	17	-	0/2/19/22	0/1/1/1
17	MAN	eE	4	17	-	0/2/19/22	0/1/1/1
17	MAN	eE	5	17	-	2/2/19/22	0/1/1/1
17	MAN	eE	6	17	-	0/2/19/22	0/1/1/1
17	MAN	eE	7	17	-	0/2/19/22	0/1/1/1
17	MAN	eE	8	17	-	1/2/19/22	0/1/1/1
17	MAN	eE	9	17	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	NAG	eF	1	1,18	-	0/6/23/26	0/1/1/1
18	MAN	eF	10	18	-	0/2/19/22	0/1/1/1
18	NAG	eF	11	18	-	0/6/23/26	0/1/1/1
18	XYP	eF	12	18	-	-	0/1/1/1
18	XYP	eF	13	18	-	-	0/1/1/1
18	MAN	eF	14	18	-	2/2/19/22	0/1/1/1
18	NAG	eF	2	18	-	0/6/23/26	0/1/1/1
18	BMA	eF	3	18	-	0/2/19/22	0/1/1/1
18	MAN	eF	4	18	-	0/2/19/22	0/1/1/1
18	MAN	eF	5	18	-	0/2/19/22	0/1/1/1
18	XYP	eF	6	18	-	-	0/1/1/1
18	XYS	eF	7	18	-	-	0/1/1/1
18	BGC	eF	8	18	-	0/2/19/22	0/1/1/1
18	NAG	eF	9	18	-	0/6/23/26	0/1/1/1
19	NAG	fB	1	19,2	-	0/6/23/26	0/1/1/1
19	MAN	fB	10	19	-	2/2/19/22	0/1/1/1
19	NAG	fB	2	19	-	1/6/23/26	0/1/1/1
19	BMA	fB	3	19	-	0/2/19/22	0/1/1/1
19	MAN	fB	4	19	-	0/2/19/22	0/1/1/1
19	MAN	fB	5	19	-	2/2/19/22	0/1/1/1
19	MAN	fB	6	19	-	0/2/19/22	0/1/1/1
19	MAN	fB	7	19	-	2/2/19/22	0/1/1/1
19	MAN	fB	8	19	-	0/2/19/22	0/1/1/1
19	MAN	fB	9	19	-	1/2/19/22	0/1/1/1
17	NAG	fC	1	17,2	-	1/6/23/26	0/1/1/1
17	MAN	fC	10	17	-	0/2/19/22	0/1/1/1
17	MAN	fC	11	17	-	2/2/19/22	0/1/1/1
17	NAG	fC	2	17	-	0/6/23/26	0/1/1/1
17	BMA	fC	3	17	-	0/2/19/22	0/1/1/1
17	MAN	fC	4	17	-	0/2/19/22	0/1/1/1
17	MAN	fC	5	17	-	0/2/19/22	0/1/1/1
17	MAN	fC	6	17	-	0/2/19/22	0/1/1/1
17	MAN	fC	7	17	-	2/2/19/22	0/1/1/1
17	MAN	fC	8	17	-	0/2/19/22	0/1/1/1
17	MAN	fC	9	17	-	1/2/19/22	0/1/1/1
17	NAG	fD	1	17,2	-	2/6/23/26	0/1/1/1
17	MAN	fD	10	17	-	0/2/19/22	0/1/1/1
17	MAN	fD	11	17	-	0/2/19/22	0/1/1/1
17	NAG	fD	2	17	-	0/6/23/26	0/1/1/1
17	BMA	fD	3	17	-	0/2/19/22	0/1/1/1
17	MAN	fD	4	17	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MAN	fD	5	17	-	0/2/19/22	0/1/1/1
17	MAN	fD	6	17	-	0/2/19/22	0/1/1/1
17	MAN	fD	7	17	-	0/2/19/22	0/1/1/1
17	MAN	fD	8	17	-	2/2/19/22	0/1/1/1
17	MAN	fD	9	17	-	2/2/19/22	0/1/1/1
19	NAG	fE	1	19,2	-	2/6/23/26	0/1/1/1
19	MAN	fE	10	19	-	2/2/19/22	0/1/1/1
19	NAG	fE	2	19	-	0/6/23/26	0/1/1/1
19	BMA	fE	3	19	-	0/2/19/22	0/1/1/1
19	MAN	fE	4	19	-	0/2/19/22	0/1/1/1
19	MAN	fE	5	19	-	0/2/19/22	0/1/1/1
19	MAN	fE	6	19	-	0/2/19/22	0/1/1/1
19	MAN	fE	7	19	-	0/2/19/22	0/1/1/1
19	MAN	fE	8	19	-	2/2/19/22	0/1/1/1
19	MAN	fE	9	19	-	0/2/19/22	0/1/1/1
20	NAG	fF	1	20,2	-	0/6/23/26	0/1/1/1
20	NAG	fF	10	20	-	0/6/23/26	0/1/1/1
20	XYS	fF	11	20	-	-	0/1/1/1
20	XYP	fF	12	20	-	-	0/1/1/1
20	MAN	fF	13	20	-	0/2/19/22	0/1/1/1
20	MAN	fF	14	20	-	0/2/19/22	0/1/1/1
20	NAG	fF	2	20	-	0/6/23/26	0/1/1/1
20	BMA	fF	3	20	-	0/2/19/22	0/1/1/1
20	MAN	fF	4	20	-	0/2/19/22	0/1/1/1
20	MAN	fF	5	20	-	0/2/19/22	0/1/1/1
20	XYP	fF	6	20	-	-	0/1/1/1
20	XYS	fF	7	20	-	-	0/1/1/1
20	NAG	fF	8	20	-	0/6/23/26	0/1/1/1
20	MAN	fF	9	20	-	0/2/19/22	0/1/1/1
19	NAG	fG	1	19,2	-	0/6/23/26	0/1/1/1
19	MAN	fG	10	19	-	2/2/19/22	0/1/1/1
19	NAG	fG	2	19	-	3/6/23/26	0/1/1/1
19	BMA	fG	3	19	-	0/2/19/22	0/1/1/1
19	MAN	fG	4	19	-	0/2/19/22	0/1/1/1
19	MAN	fG	5	19	-	2/2/19/22	0/1/1/1
19	MAN	fG	6	19	-	0/2/19/22	0/1/1/1
19	MAN	fG	7	19	-	2/2/19/22	0/1/1/1
19	MAN	fG	8	19	-	1/2/19/22	0/1/1/1
19	MAN	fG	9	19	-	1/2/19/22	0/1/1/1
17	NAG	fH	1	17,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MAN	fH	10	17	-	0/2/19/22	0/1/1/1
17	MAN	fH	11	17	-	0/2/19/22	0/1/1/1
17	NAG	fH	2	17	-	0/6/23/26	0/1/1/1
17	BMA	fH	3	17	-	0/2/19/22	0/1/1/1
17	MAN	fH	4	17	-	2/2/19/22	0/1/1/1
17	MAN	fH	5	17	-	0/2/19/22	0/1/1/1
17	MAN	fH	6	17	-	0/2/19/22	0/1/1/1
17	MAN	fH	7	17	-	2/2/19/22	0/1/1/1
17	MAN	fH	8	17	-	2/2/19/22	0/1/1/1
17	MAN	fH	9	17	-	2/2/19/22	0/1/1/1
17	NAG	fI	1	17,2	-	1/6/23/26	0/1/1/1
17	MAN	fI	10	17	-	0/2/19/22	0/1/1/1
17	MAN	fI	11	17	-	0/2/19/22	0/1/1/1
17	NAG	fI	2	17	-	0/6/23/26	0/1/1/1
17	BMA	fI	3	17	-	0/2/19/22	0/1/1/1
17	MAN	fI	4	17	-	2/2/19/22	0/1/1/1
17	MAN	fI	5	17	-	0/2/19/22	0/1/1/1
17	MAN	fI	6	17	-	0/2/19/22	0/1/1/1
17	MAN	fI	7	17	-	0/2/19/22	0/1/1/1
17	MAN	fI	8	17	-	0/2/19/22	0/1/1/1
17	MAN	fI	9	17	-	2/2/19/22	0/1/1/1
19	NAG	fJ	1	19,2	-	2/6/23/26	0/1/1/1
19	MAN	fJ	10	19	-	0/2/19/22	0/1/1/1
19	NAG	fJ	2	19	-	0/6/23/26	0/1/1/1
19	BMA	fJ	3	19	-	0/2/19/22	0/1/1/1
19	MAN	fJ	4	19	-	0/2/19/22	0/1/1/1
19	MAN	fJ	5	19	-	0/2/19/22	0/1/1/1
19	MAN	fJ	6	19	-	0/2/19/22	0/1/1/1
19	MAN	fJ	7	19	-	2/2/19/22	0/1/1/1
19	MAN	fJ	8	19	-	0/2/19/22	0/1/1/1
19	MAN	fJ	9	19	-	2/2/19/22	0/1/1/1
20	NAG	fK	1	20,2	-	0/6/23/26	0/1/1/1
20	NAG	fK	10	20	-	0/6/23/26	0/1/1/1
20	XYS	fK	11	20	-	-	0/1/1/1
20	XYP	fK	12	20	-	-	0/1/1/1
20	MAN	fK	13	20	-	0/2/19/22	0/1/1/1
20	MAN	fK	14	20	-	1/2/19/22	0/1/1/1
20	NAG	fK	2	20	-	0/6/23/26	0/1/1/1
20	BMA	fK	3	20	-	0/2/19/22	0/1/1/1
20	MAN	fK	4	20	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	MAN	fK	5	20	-	0/2/19/22	0/1/1/1
20	XYP	fK	6	20	-	-	0/1/1/1
20	XYS	fK	7	20	-	-	0/1/1/1
20	NAG	fK	8	20	-	2/6/23/26	0/1/1/1
20	MAN	fK	9	23,20	-	0/2/19/22	0/1/1/1
19	NAG	fL	1	19,2	-	0/6/23/26	0/1/1/1
19	MAN	fL	10	19	-	0/2/19/22	0/1/1/1
19	NAG	fL	2	19	-	1/6/23/26	0/1/1/1
19	BMA	fL	3	19	-	0/2/19/22	0/1/1/1
19	MAN	fL	4	19	-	0/2/19/22	0/1/1/1
19	MAN	fL	5	19	-	0/2/19/22	0/1/1/1
19	MAN	fL	6	19	-	0/2/19/22	0/1/1/1
19	MAN	fL	7	19	-	2/2/19/22	0/1/1/1
19	MAN	fL	8	19	-	2/2/19/22	0/1/1/1
19	MAN	fL	9	19	-	2/2/19/22	0/1/1/1
17	NAG	fM	1	17,2	-	0/6/23/26	0/1/1/1
17	MAN	fM	10	17	-	1/2/19/22	0/1/1/1
17	MAN	fM	11	17	-	0/2/19/22	0/1/1/1
17	NAG	fM	2	17	-	0/6/23/26	0/1/1/1
17	BMA	fM	3	17	-	0/2/19/22	0/1/1/1
17	MAN	fM	4	17	-	1/2/19/22	0/1/1/1
17	MAN	fM	5	17	-	0/2/19/22	0/1/1/1
17	MAN	fM	6	17	-	2/2/19/22	0/1/1/1
17	MAN	fM	7	17	-	0/2/19/22	0/1/1/1
17	MAN	fM	8	17	-	2/2/19/22	0/1/1/1
17	MAN	fM	9	17	-	0/2/19/22	0/1/1/1
17	NAG	fN	1	17,2	-	2/6/23/26	0/1/1/1
17	MAN	fN	10	17	-	0/2/19/22	0/1/1/1
17	MAN	fN	11	17	-	0/2/19/22	0/1/1/1
17	NAG	fN	2	17	-	0/6/23/26	0/1/1/1
17	BMA	fN	3	17	-	0/2/19/22	0/1/1/1
17	MAN	fN	4	17	-	0/2/19/22	0/1/1/1
17	MAN	fN	5	17	-	2/2/19/22	0/1/1/1
17	MAN	fN	6	17	-	0/2/19/22	0/1/1/1
17	MAN	fN	7	17	-	0/2/19/22	0/1/1/1
17	MAN	fN	8	17	-	0/2/19/22	0/1/1/1
17	MAN	fN	9	17	-	2/2/19/22	0/1/1/1
19	NAG	fO	1	19,2	-	2/6/23/26	0/1/1/1
19	MAN	fO	10	19	-	0/2/19/22	0/1/1/1
19	NAG	fO	2	19	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BMA	fO	3	19	-	0/2/19/22	0/1/1/1
19	MAN	fO	4	19	-	0/2/19/22	0/1/1/1
19	MAN	fO	5	19	-	0/2/19/22	0/1/1/1
19	MAN	fO	6	19	-	0/2/19/22	0/1/1/1
19	MAN	fO	7	19	-	1/2/19/22	0/1/1/1
19	MAN	fO	8	19	-	2/2/19/22	0/1/1/1
19	MAN	fO	9	19	-	0/2/19/22	0/1/1/1
20	NAG	fP	1	20,2	-	0/6/23/26	0/1/1/1
20	NAG	fP	10	20	-	0/6/23/26	0/1/1/1
20	XYS	fP	11	20	-	-	0/1/1/1
20	XYP	fP	12	20	-	-	0/1/1/1
20	MAN	fP	13	20	-	0/2/19/22	0/1/1/1
20	MAN	fP	14	20	-	0/2/19/22	0/1/1/1
20	NAG	fP	2	20	-	0/6/23/26	0/1/1/1
20	BMA	fP	3	20	-	0/2/19/22	0/1/1/1
20	MAN	fP	4	20	-	0/2/19/22	0/1/1/1
20	MAN	fP	5	20	-	0/2/19/22	0/1/1/1
20	XYP	fP	6	20	-	-	0/1/1/1
20	XYS	fP	7	20	-	-	0/1/1/1
20	NAG	fP	8	20	-	0/6/23/26	0/1/1/1
20	MAN	fP	9	23,20	-	0/2/19/22	0/1/1/1

The worst 5 of 195 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	fP	11	XYS	O5-C1	4.13	1.50	1.42
20	fF	11	XYS	O5-C1	4.13	1.50	1.42
9	aH	4	MAN	O5-C1	-4.07	1.37	1.43
20	fK	11	XYS	O5-C1	4.03	1.50	1.42
14	bF	7	XYS	O5-C1	3.99	1.50	1.42

The worst 5 of 629 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	2	MAN	C1-O5-C5	4.65	118.49	112.19
17	fC	4	MAN	C1-O5-C5	4.45	118.22	112.19
8	aG	5	MAN	C1-O5-C5	4.32	118.04	112.19
8	aB	5	MAN	C1-O5-C5	4.25	117.95	112.19
17	fM	10	MAN	C1-O5-C5	4.08	117.72	112.19

There are no chirality outliers.

5 of 241 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	aE	11	NAG	C8-C7-N2-C2
11	aE	11	NAG	O7-C7-N2-C2
11	aJ	11	NAG	C3-C2-N2-C7
11	aJ	11	NAG	C8-C7-N2-C2
11	aJ	11	NAG	O7-C7-N2-C2

There are no ring outliers.

43 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	fC	4	MAN	1	0
11	aE	1	NAG	1	0
11	aJ	4	MAN	1	0
11	aO	6	XYP	1	0
14	bF	7	XYS	1	0
12	bD	5	MAN	1	0
7	aK	1	NAG	1	0
9	aC	10	XYP	1	0
20	fF	8	NAG	1	0
7	aA	1	NAG	1	0
7	aA	5	MAN	1	0
19	fJ	6	MAN	1	0
20	fK	9	MAN	1	0
11	aJ	1	NAG	1	0
17	eC	11	MAN	2	0
18	eB	9	NAG	1	0
9	aM	1	NAG	1	0
7	aK	5	MAN	1	0
20	fF	10	NAG	1	0
10	aN	8	MAN	1	0
8	aL	1	NAG	1	0
9	aC	9	XYP	1	0
17	fM	2	NAG	1	0
16	dC	2	MAN	1	0
11	aO	7	XYP	1	0
11	aJ	10	MAN	1	0
10	aD	8	MAN	1	0
17	fM	4	MAN	2	0
7	aF	5	MAN	1	0
9	aM	2	NAG	1	0
7	aK	8	MAN	1	0
14	bF	5	MAN	1	0
19	fO	6	MAN	1	0

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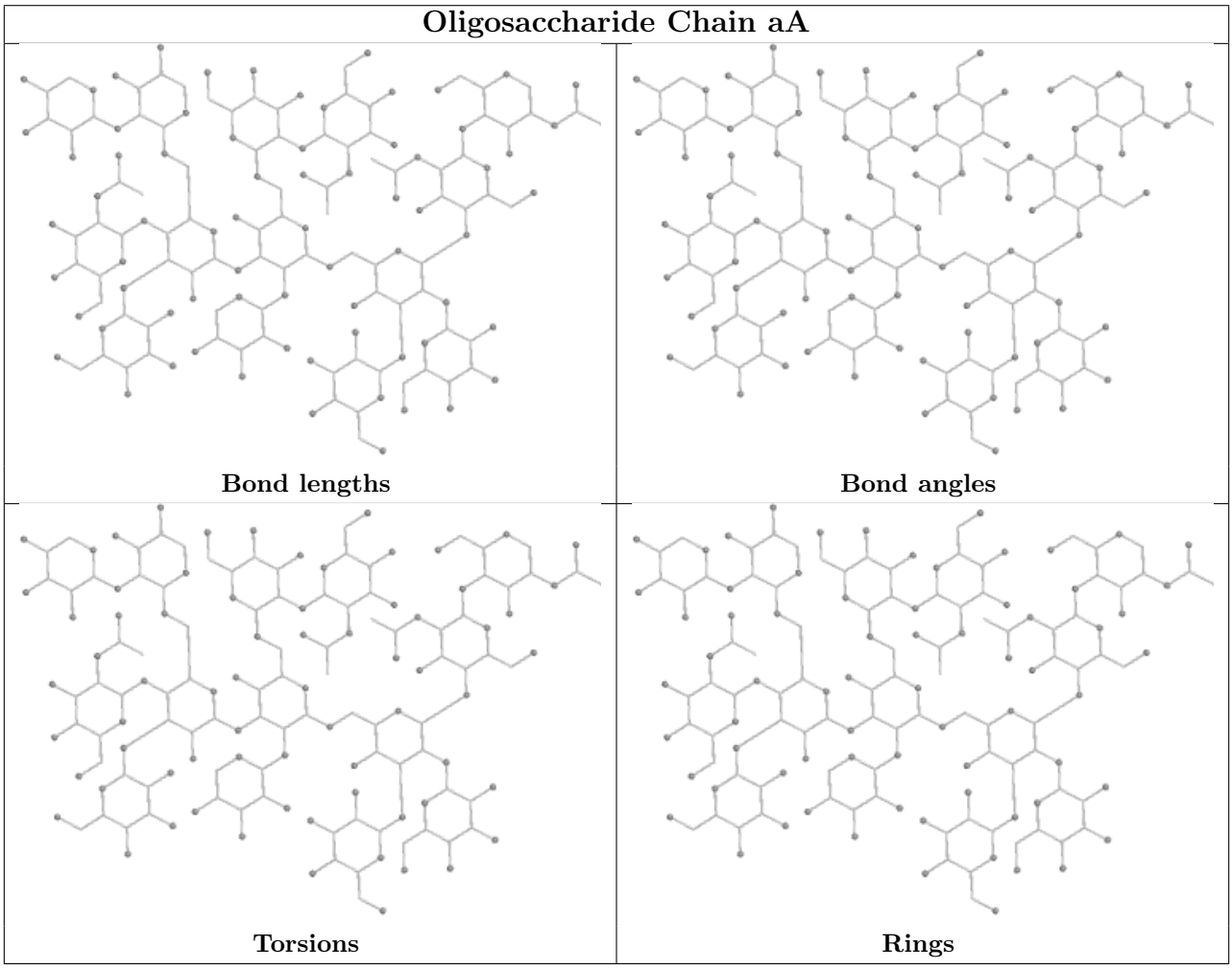
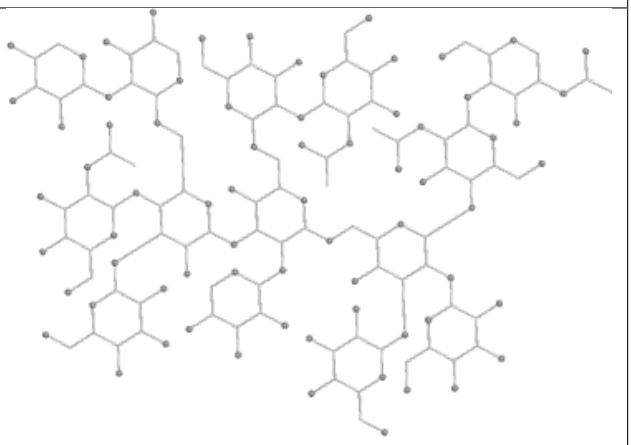
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	aF	8	MAN	1	0
17	fI	10	MAN	1	0
20	fF	12	XYP	1	0
18	eB	8	BGC	1	0
11	aE	6	XYP	1	0
10	aI	8	MAN	1	0
17	fN	2	NAG	1	0
11	aE	7	XYP	1	0
19	fE	6	MAN	1	0
7	aA	8	MAN	1	0

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

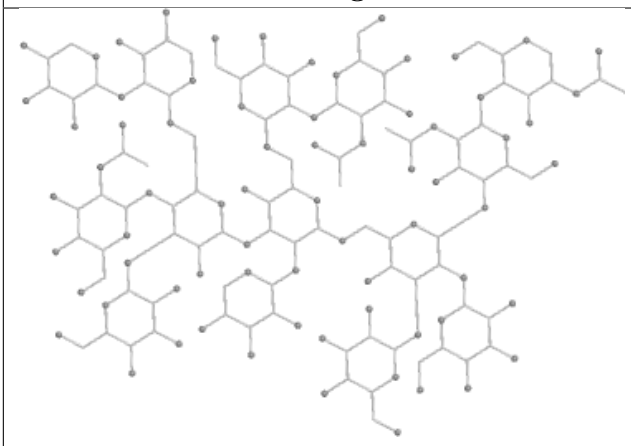


Oligosaccharide Chain aF

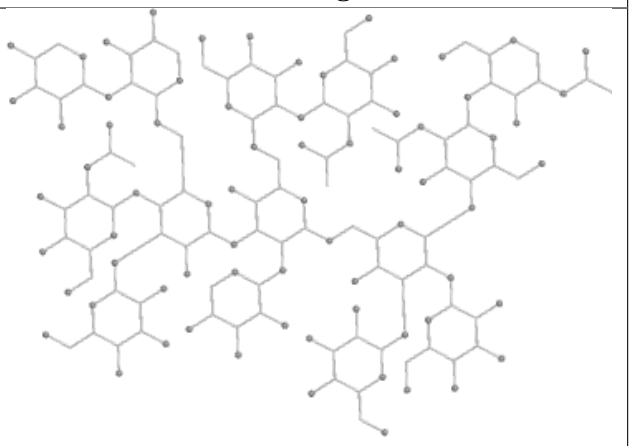
Bond lengths



Bond angles



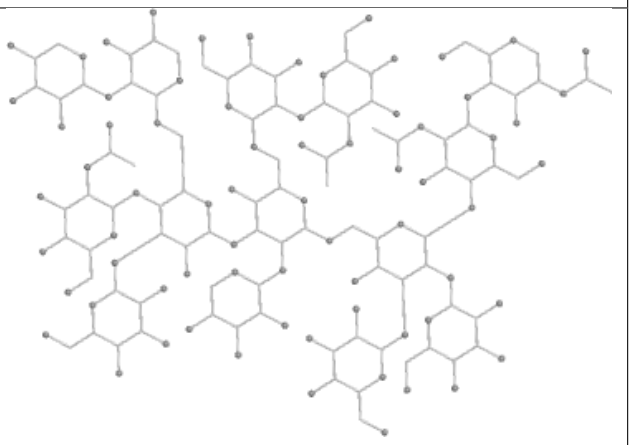
Torsions



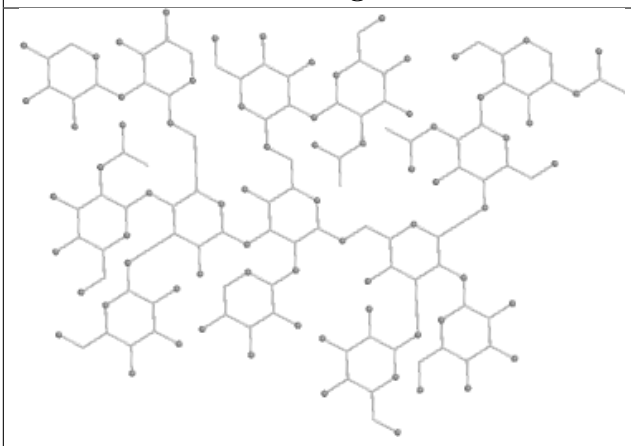
Rings

Oligosaccharide Chain aK

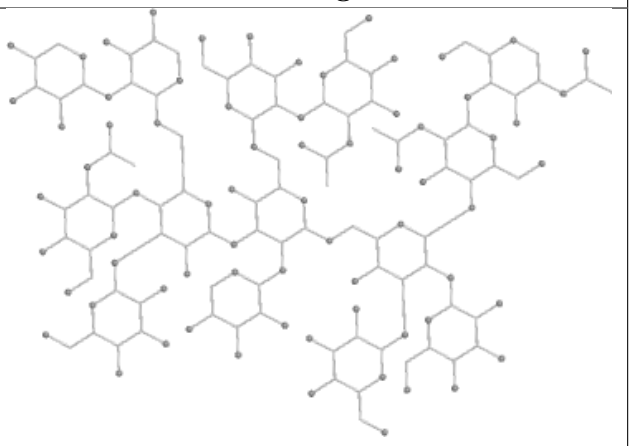
Bond lengths



Bond angles

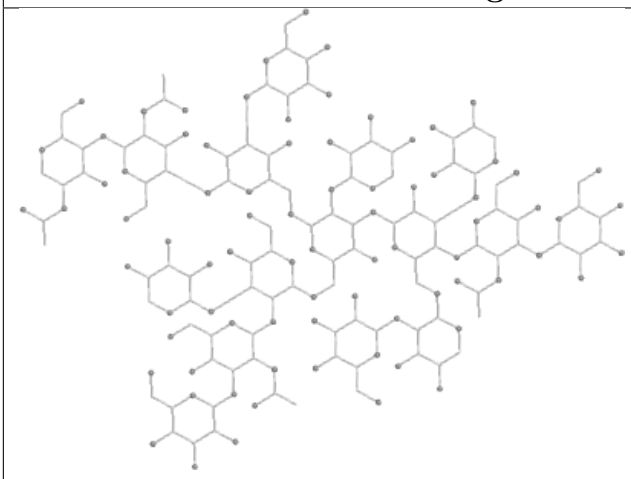


Torsions

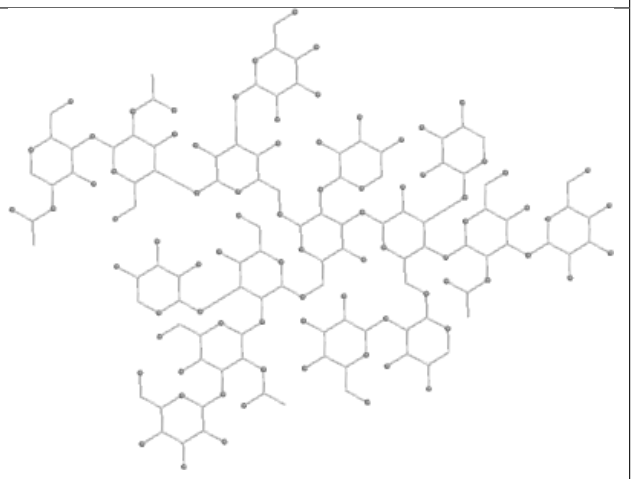


Rings

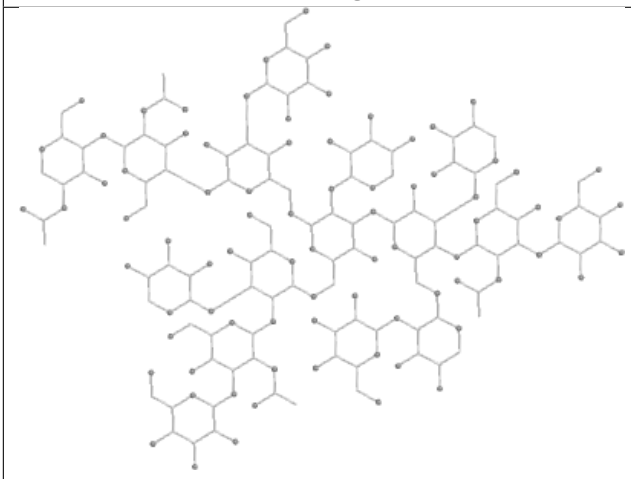
Oligosaccharide Chain aB



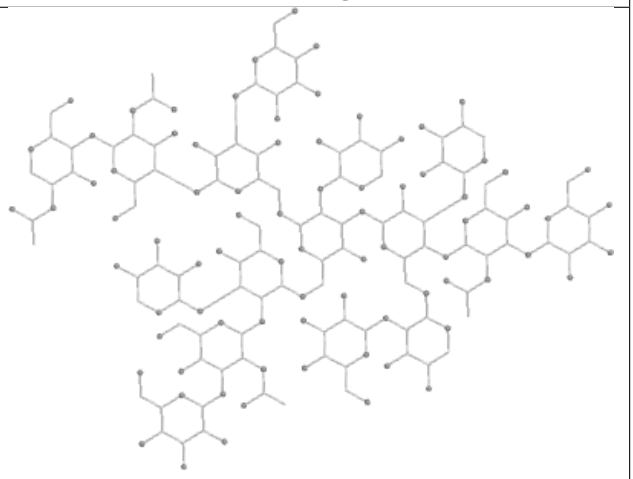
Bond lengths



Bond angles

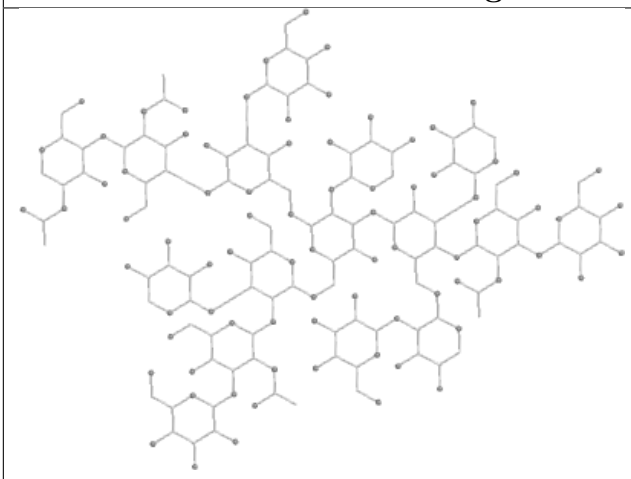


Torsions

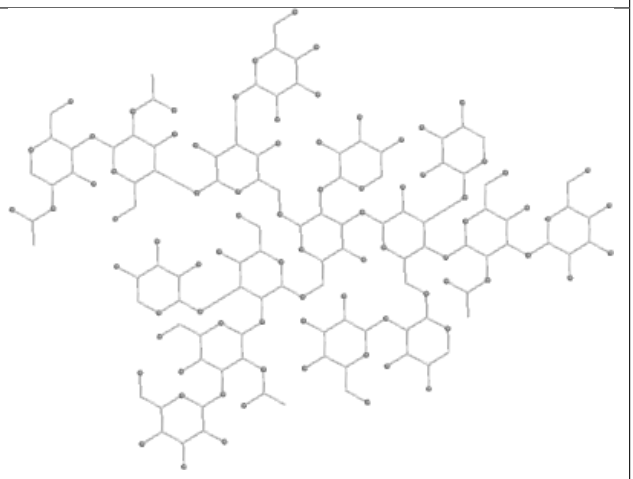


Rings

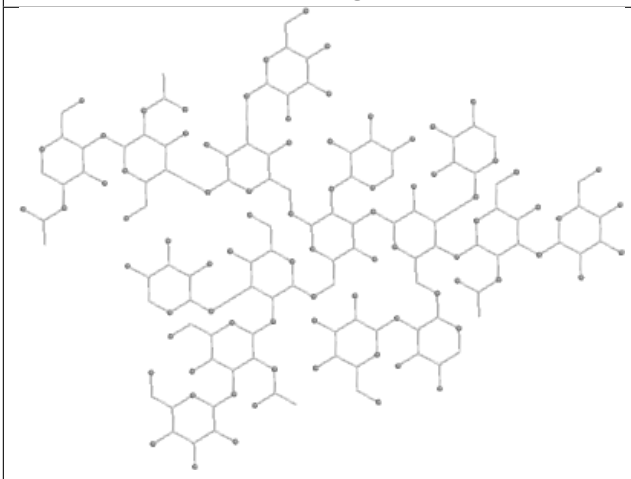
Oligosaccharide Chain aG



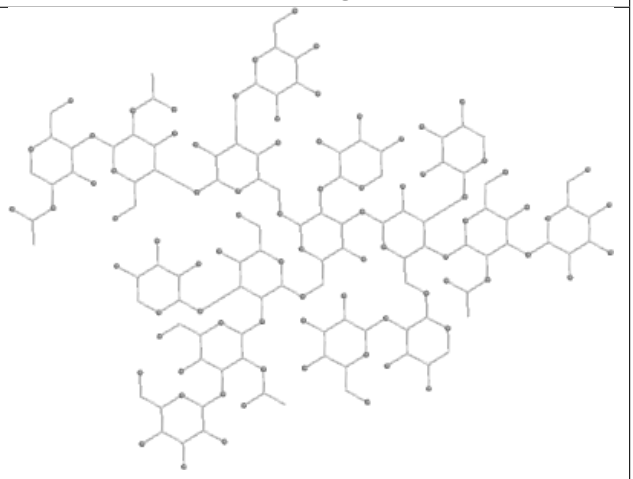
Bond lengths



Bond angles

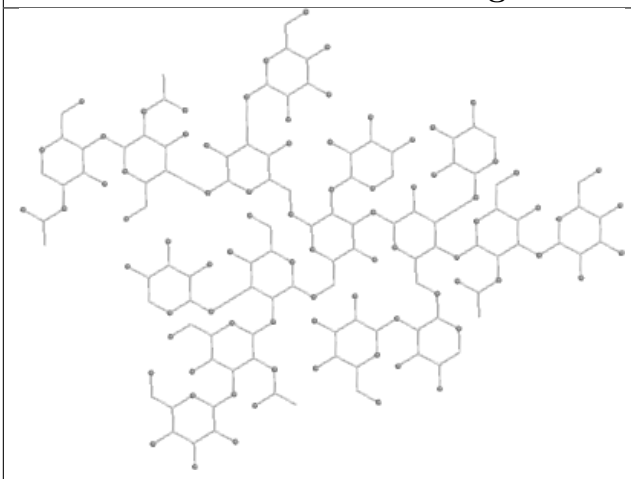


Torsions

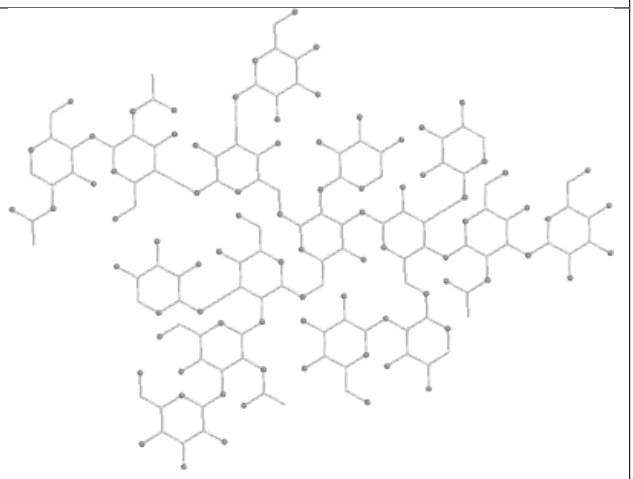


Rings

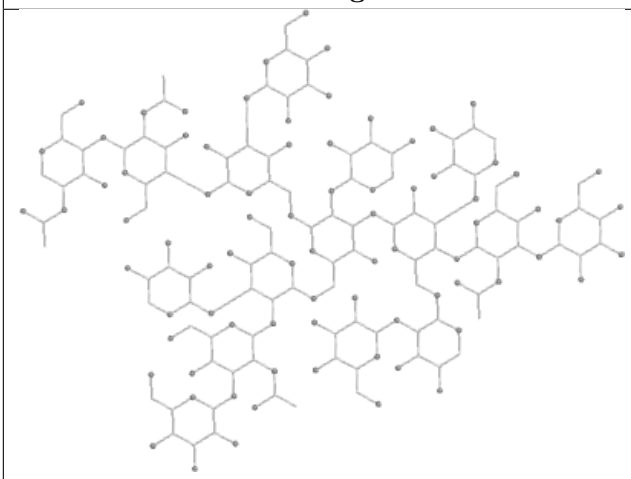
Oligosaccharide Chain aL



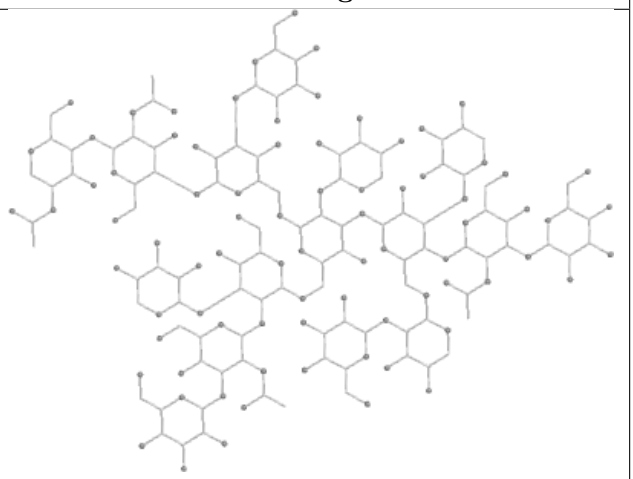
Bond lengths



Bond angles

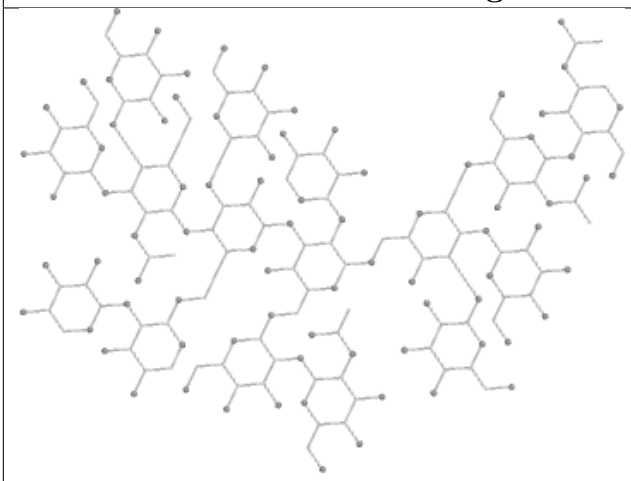


Torsions

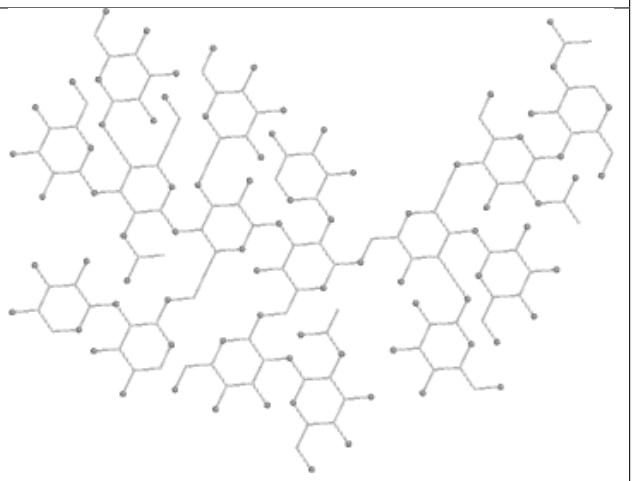


Rings

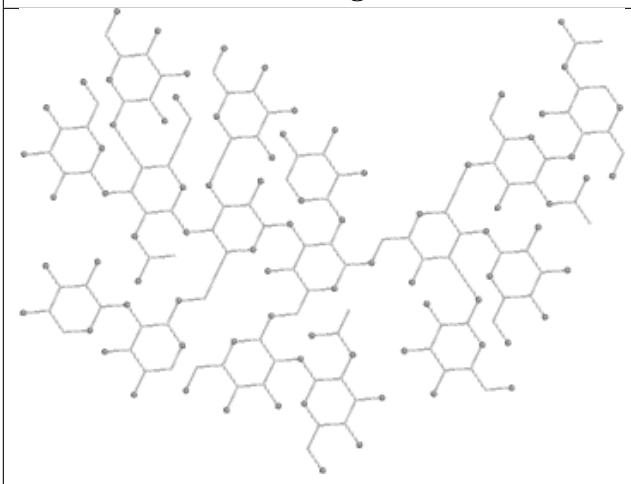
Oligosaccharide Chain aC



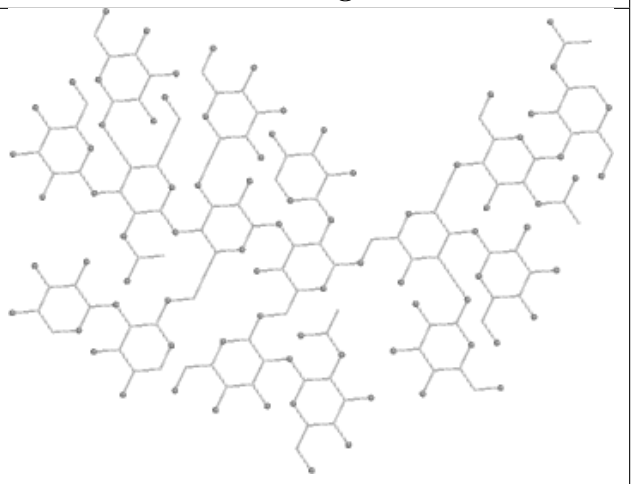
Bond lengths



Bond angles

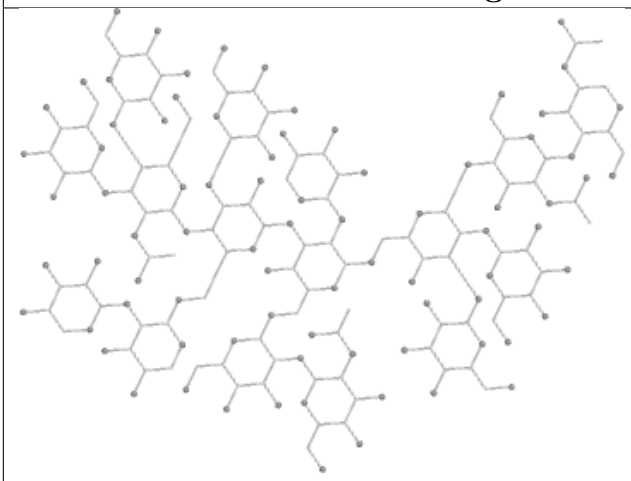


Torsions

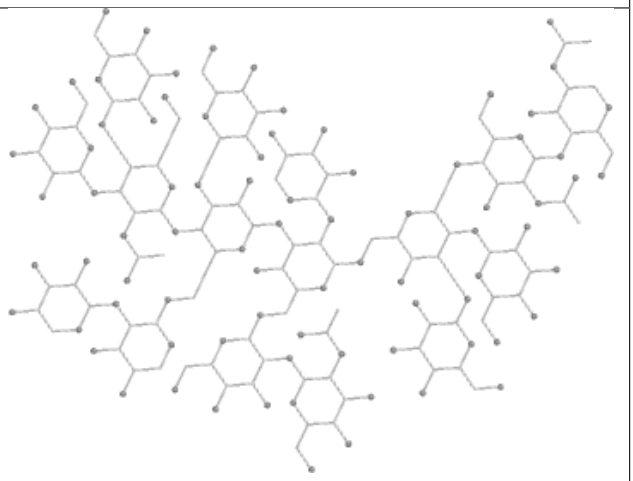


Rings

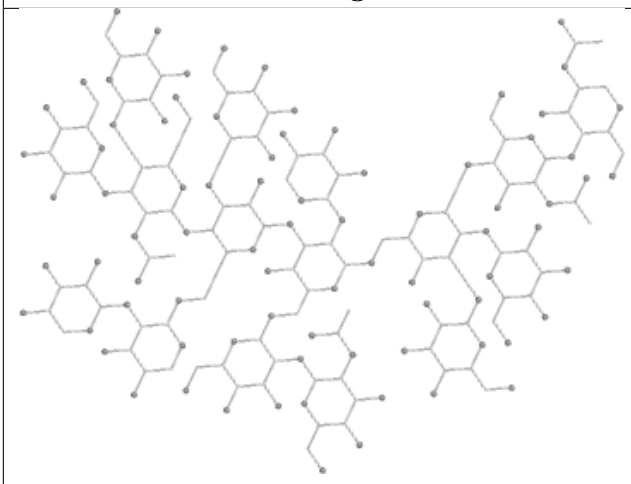
Oligosaccharide Chain aH



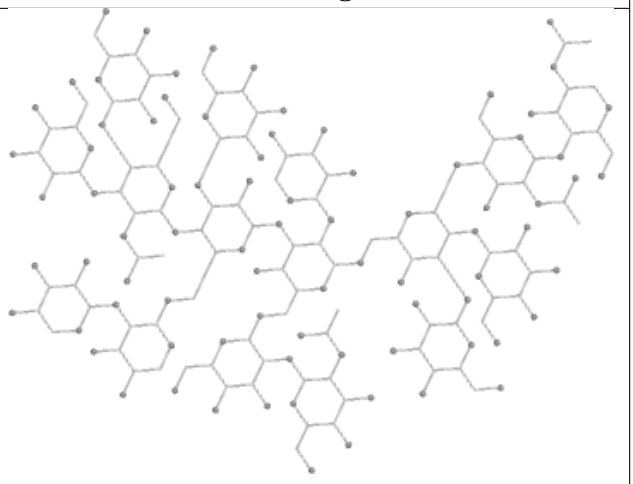
Bond lengths



Bond angles

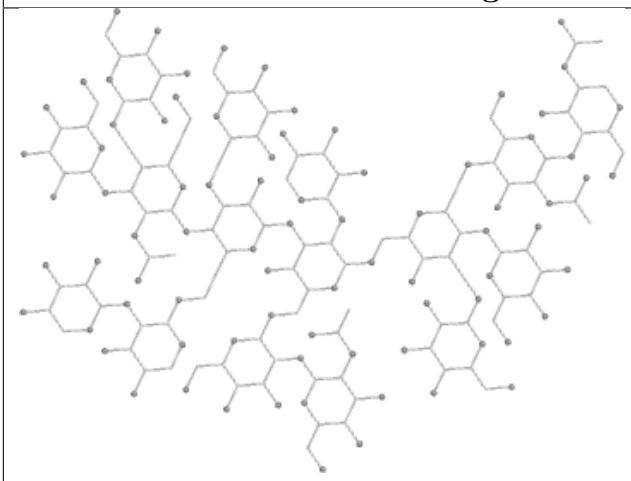


Torsions

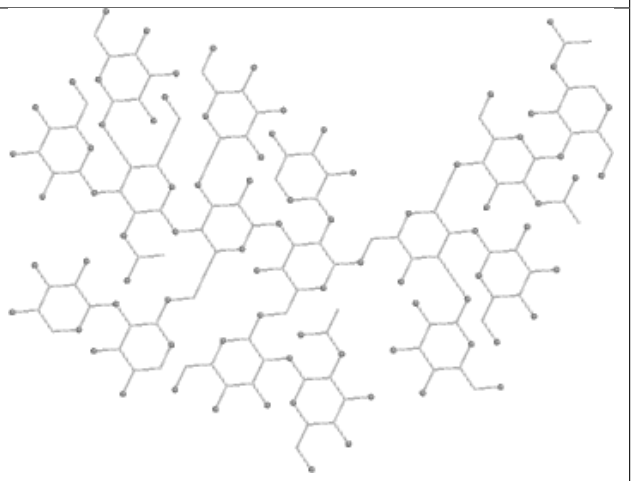


Rings

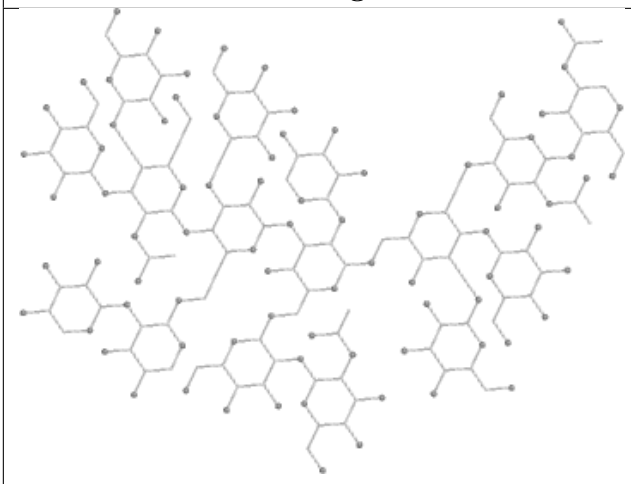
Oligosaccharide Chain aM



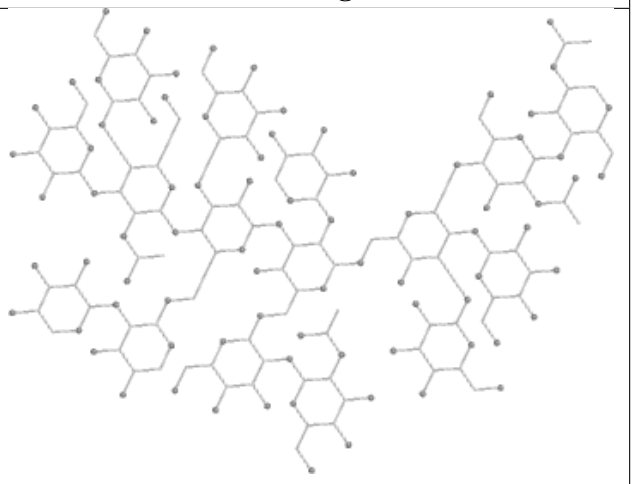
Bond lengths



Bond angles

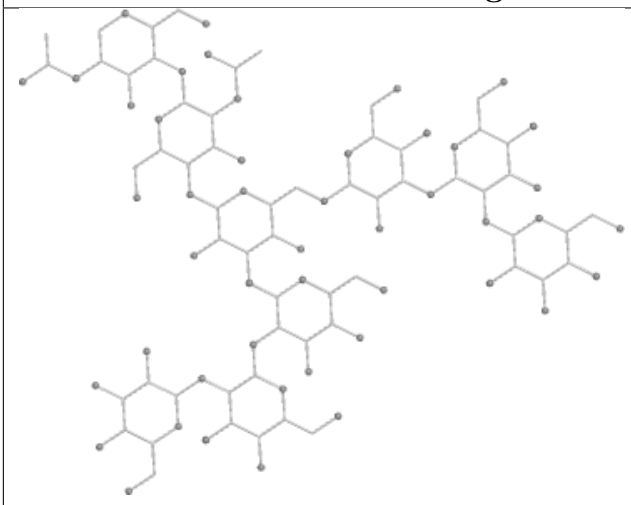


Torsions

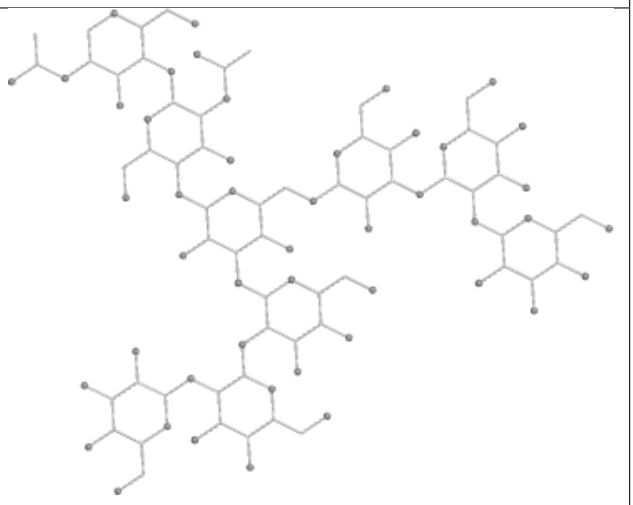


Rings

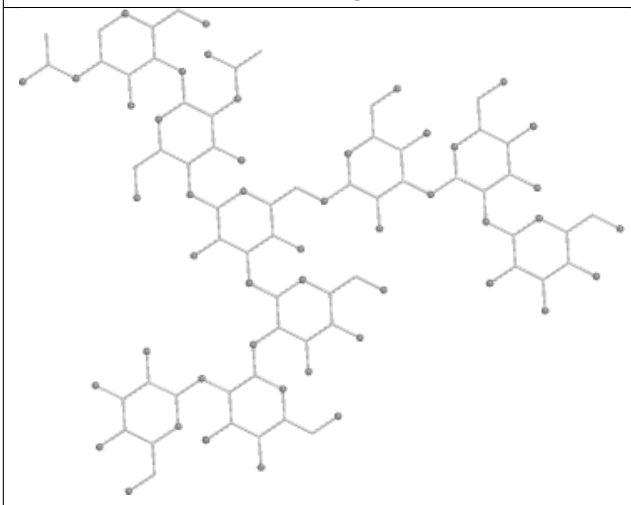
Oligosaccharide Chain aD



Bond lengths



Bond angles



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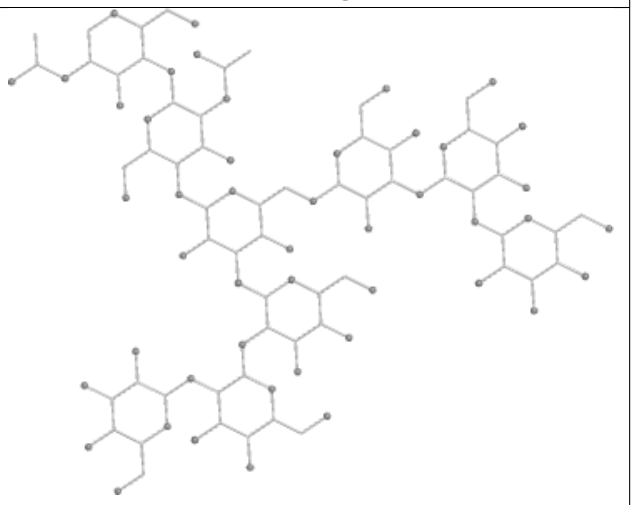
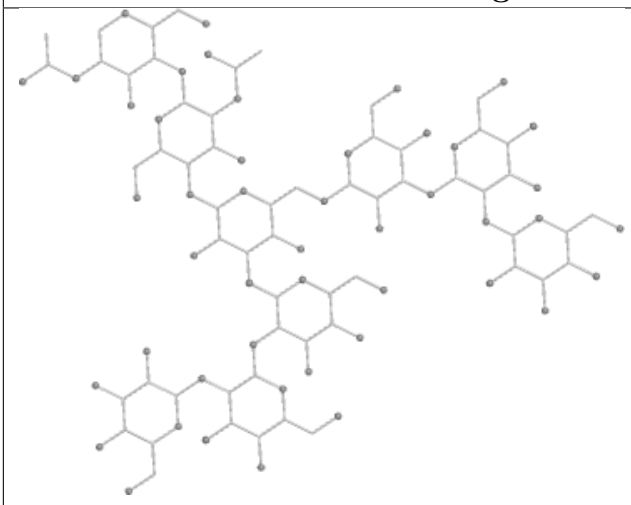
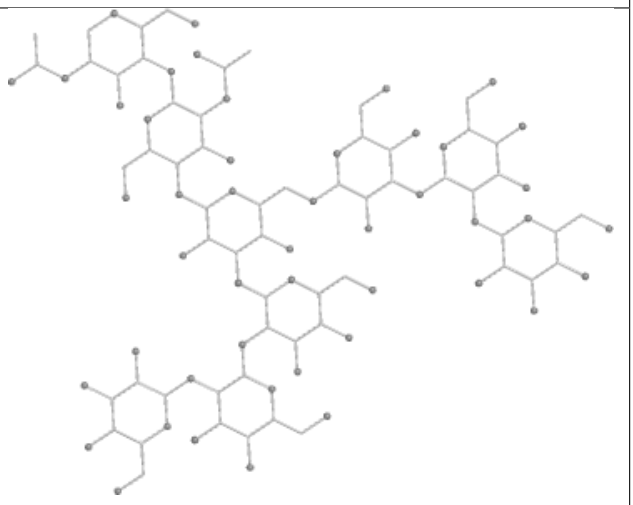
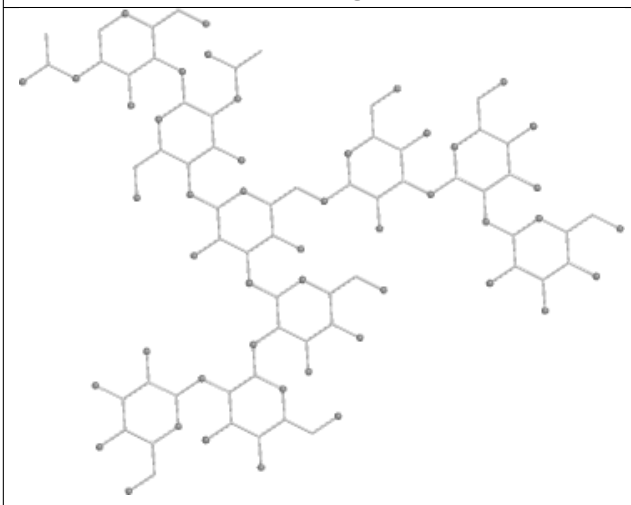
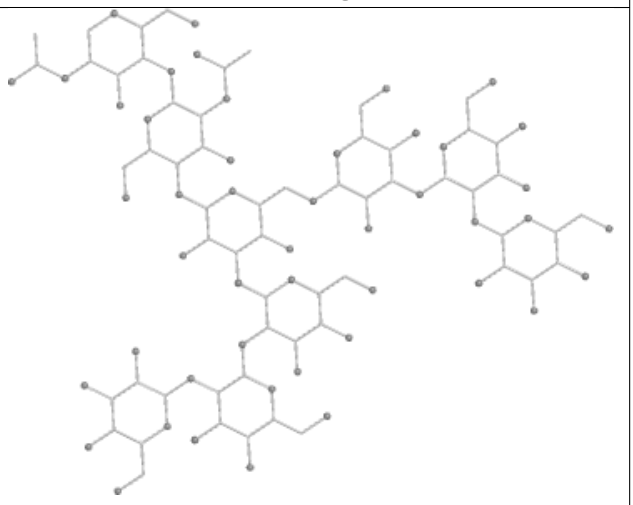
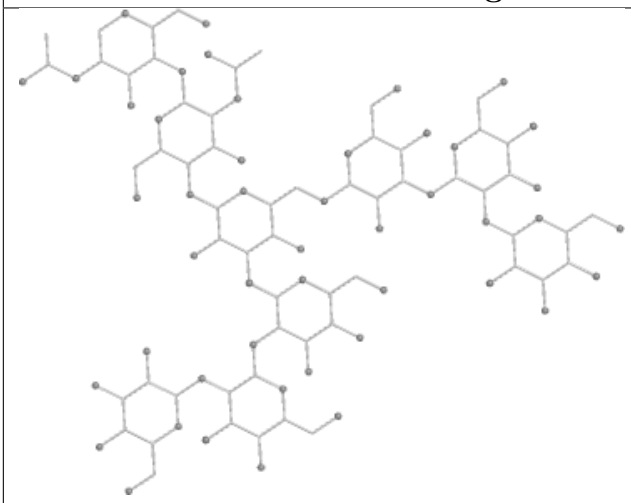


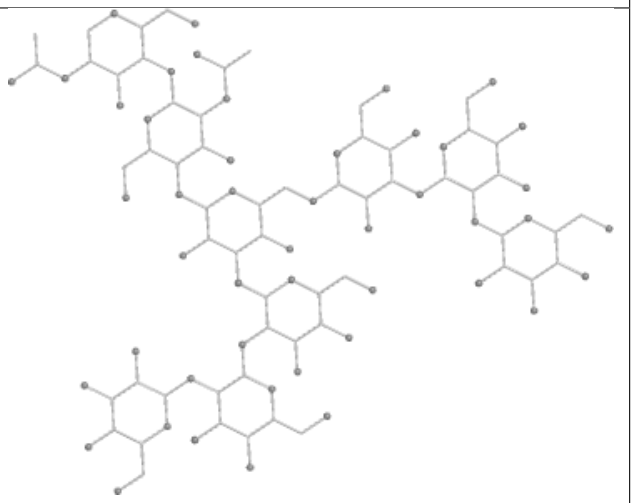
Rings

Oligosaccharide Chain aI	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

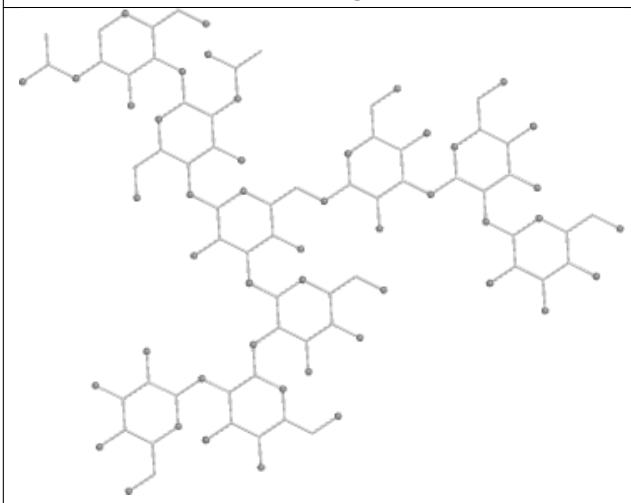
Oligosaccharide Chain aN



Bond lengths



Bond angles



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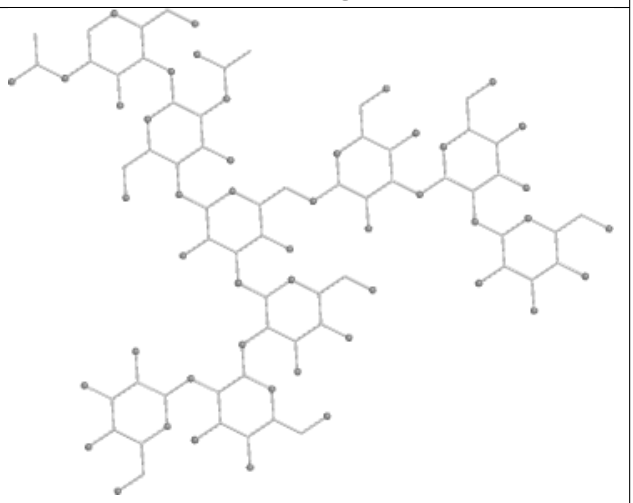
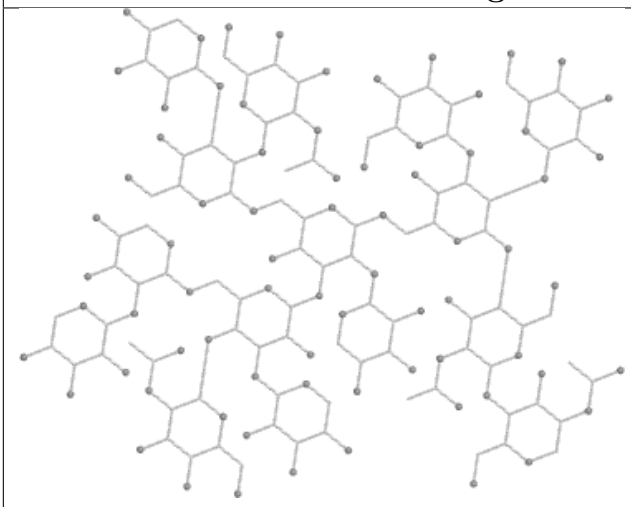
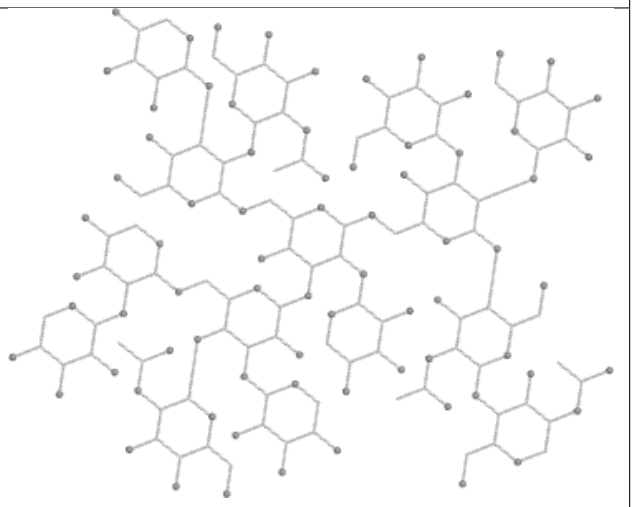


Rings

Oligosaccharide Chain aE



Bond lengths



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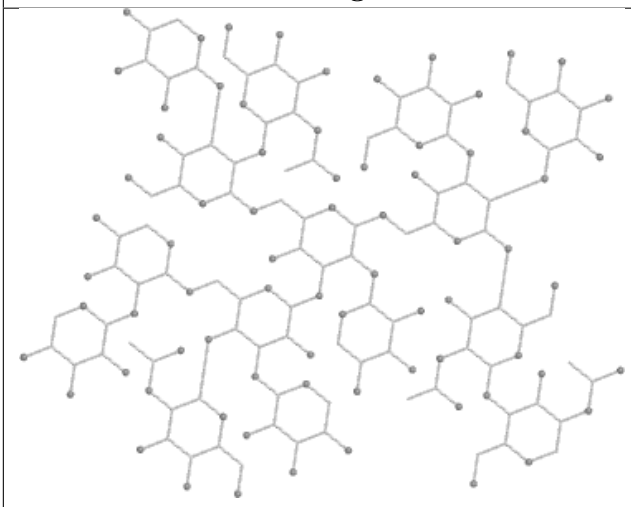

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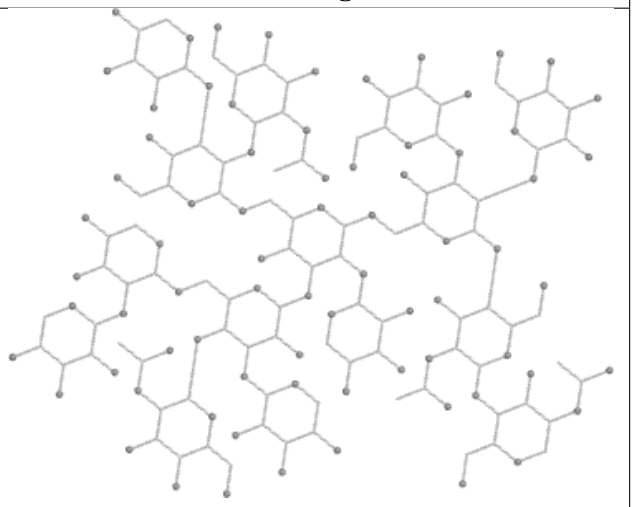
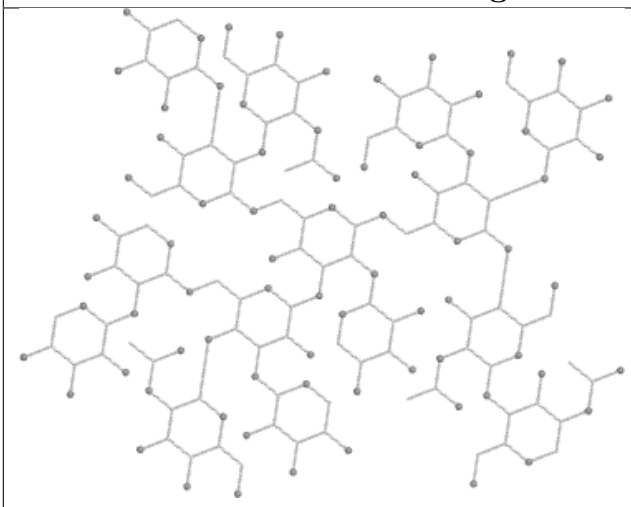


Rings

Oligosaccharide Chain aJ



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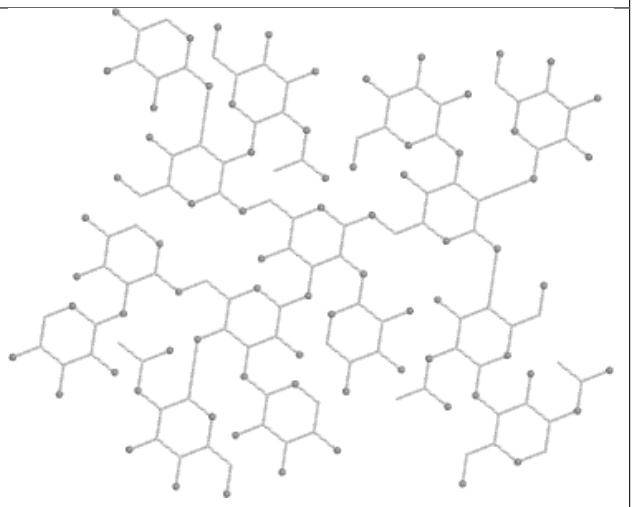
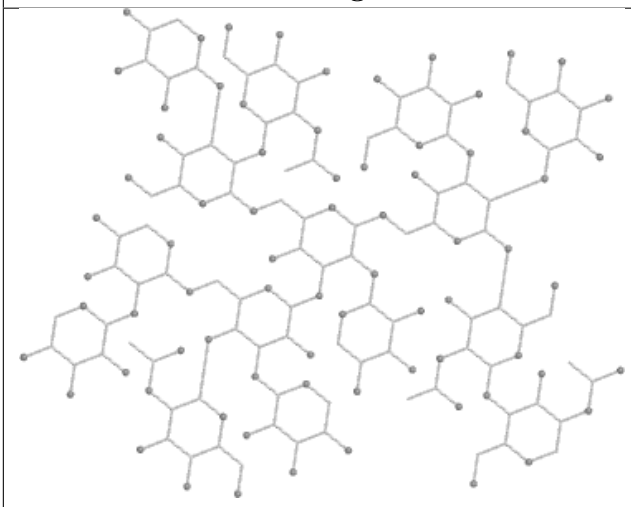


Bond angles



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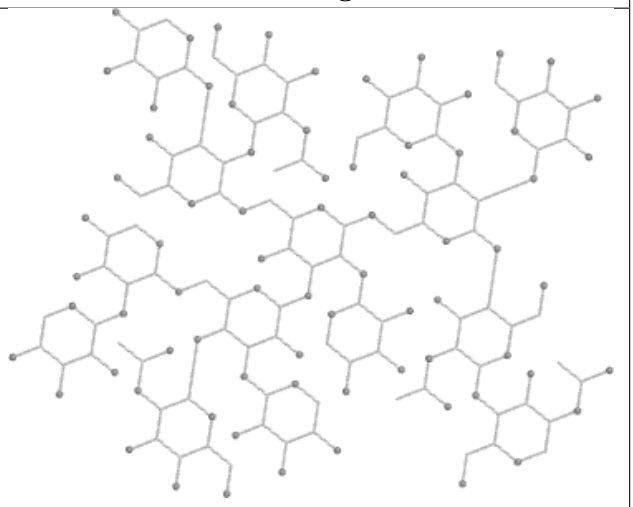
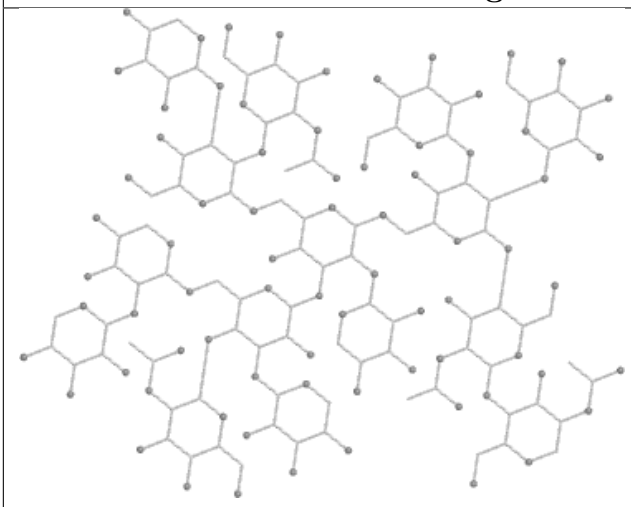
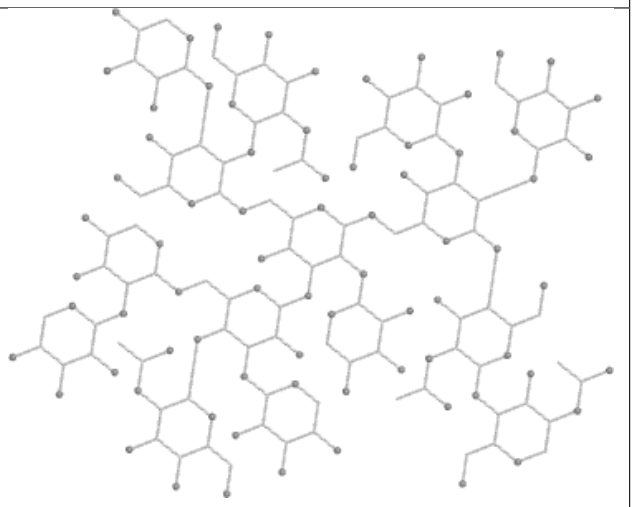


Rings

Oligosaccharide Chain aO



Bond lengths



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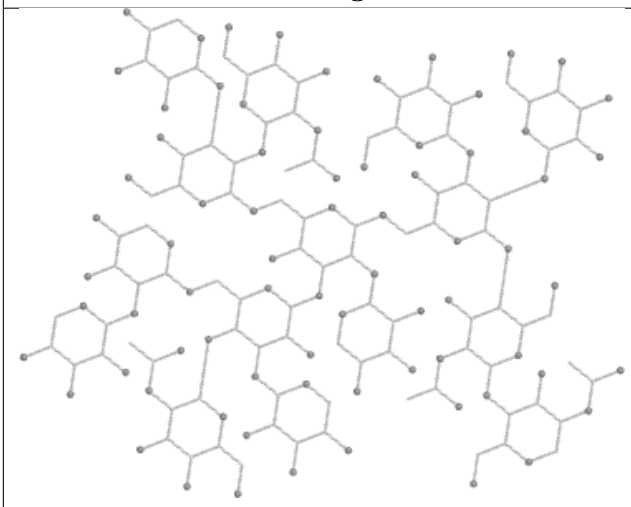

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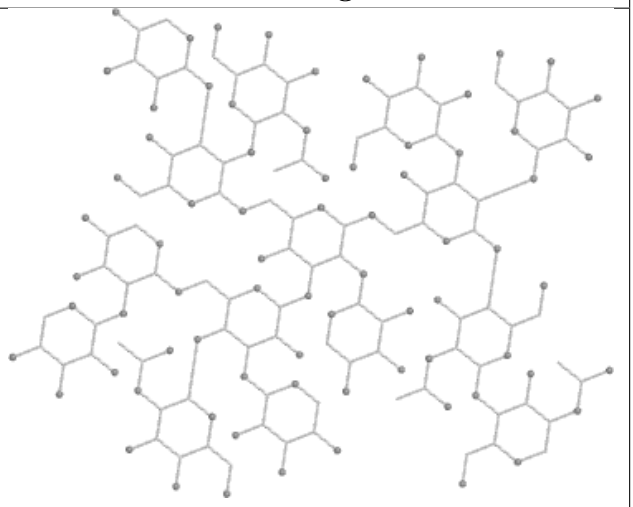
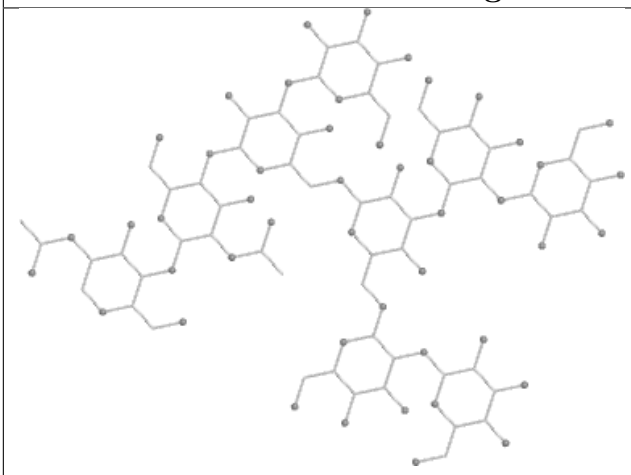


Rings

Oligosaccharide Chain bA



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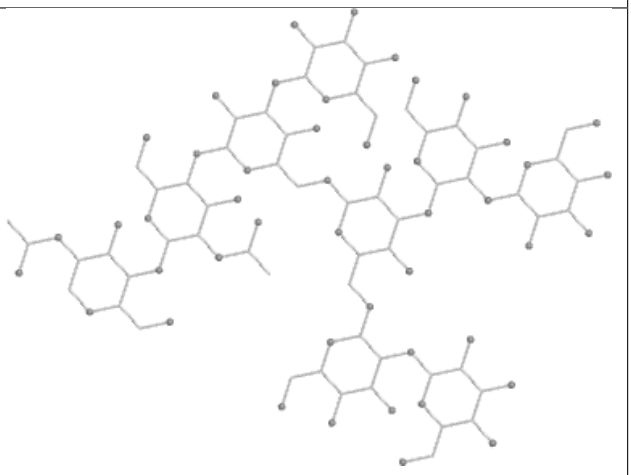

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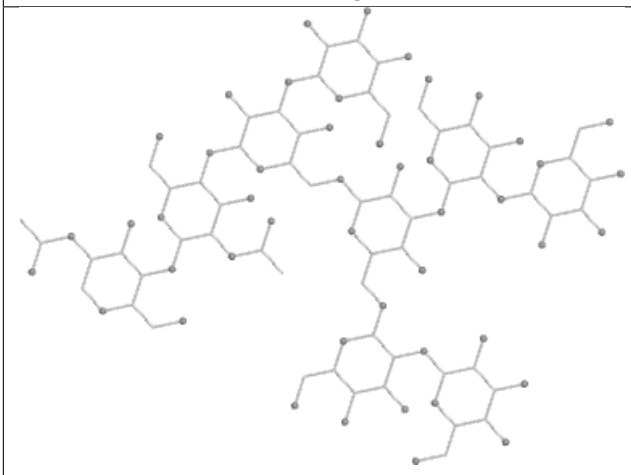

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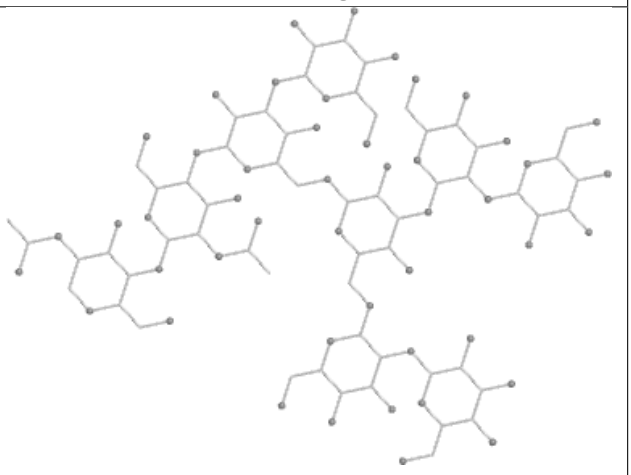
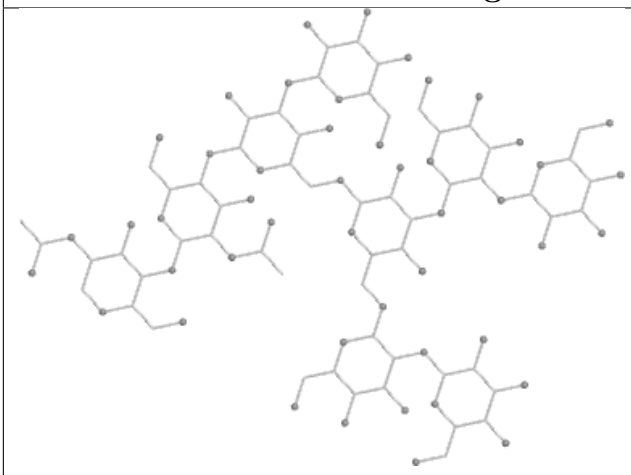


Rings

Oligosaccharide Chain bD



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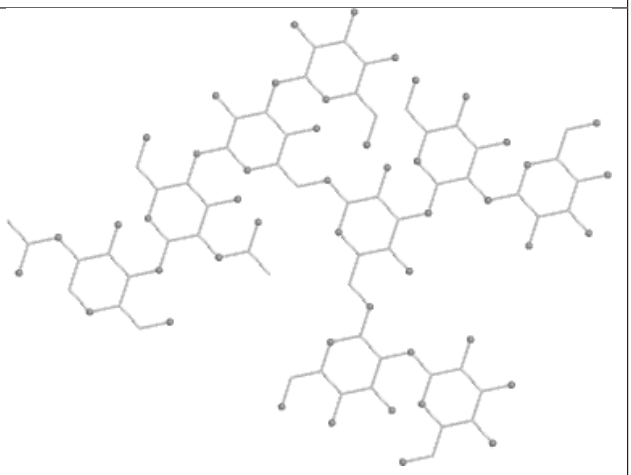
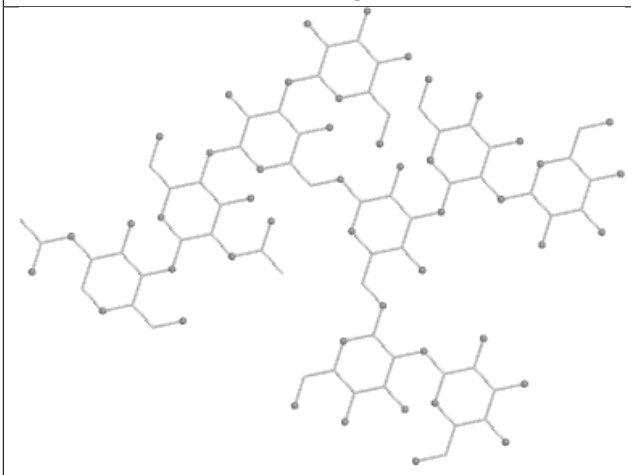


Bond angles



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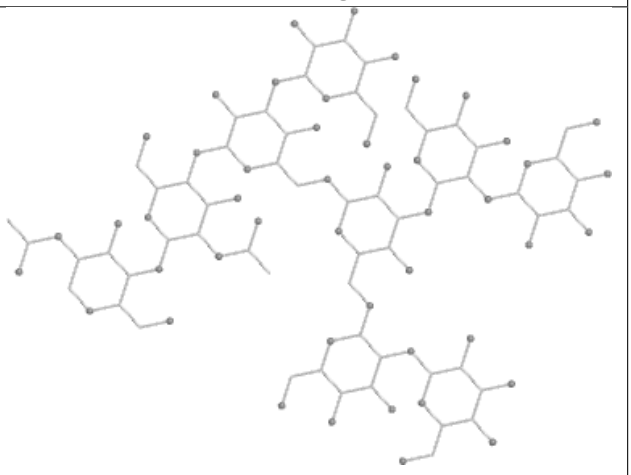
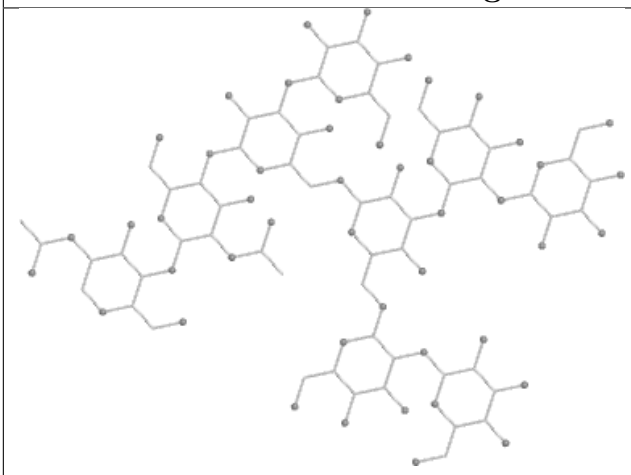
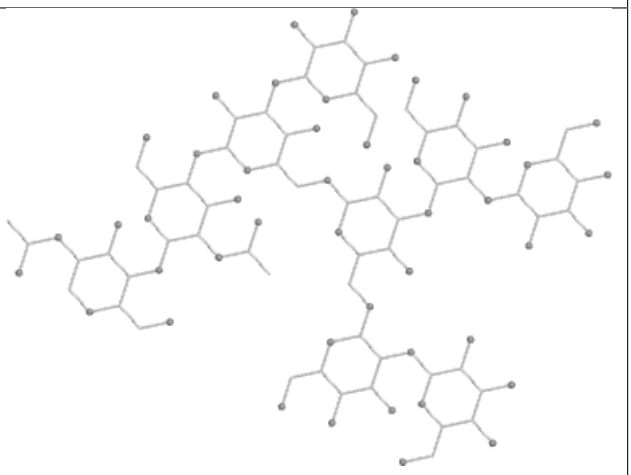


Rings

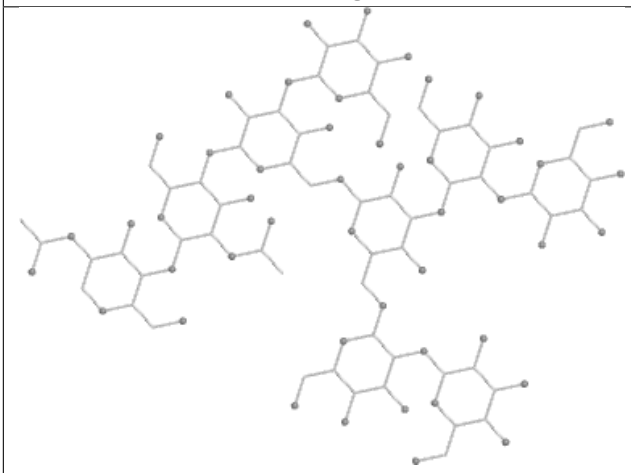
Oligosaccharide Chain bG



Bond lengths



Bond angles



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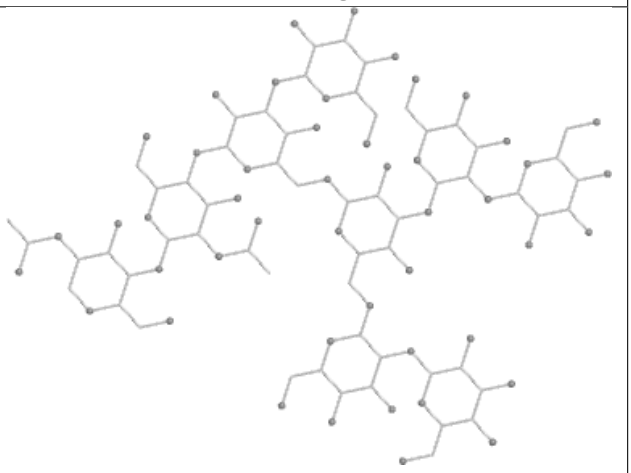
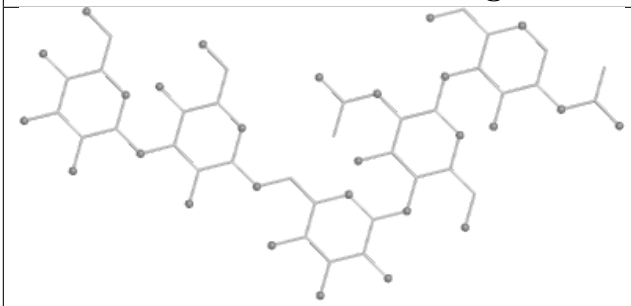
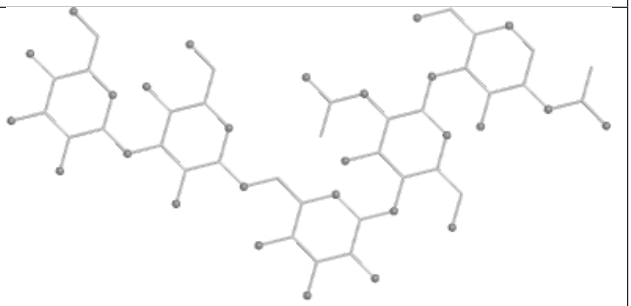


Rings

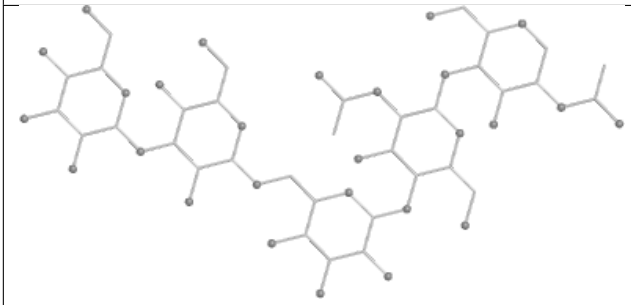
Oligosaccharide Chain bB



Bond lengths



Bond angles



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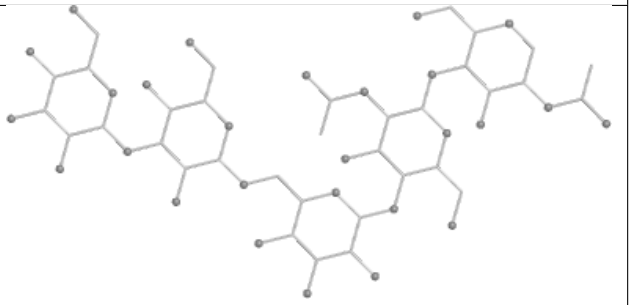
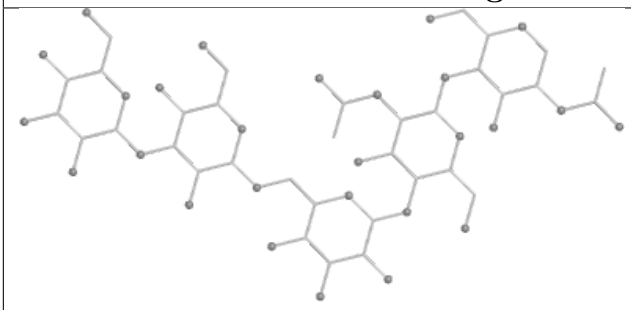
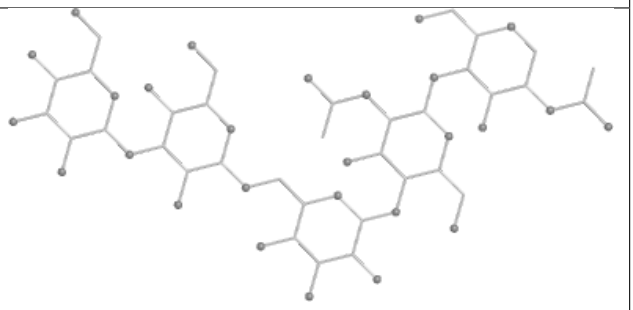
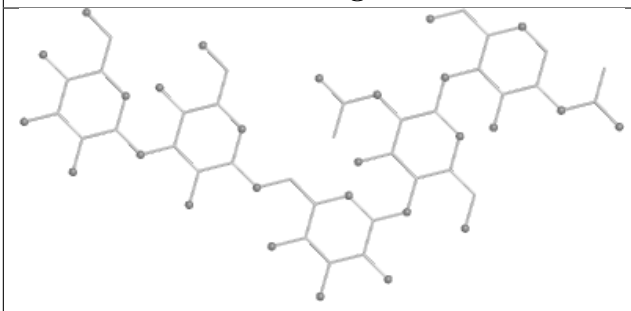
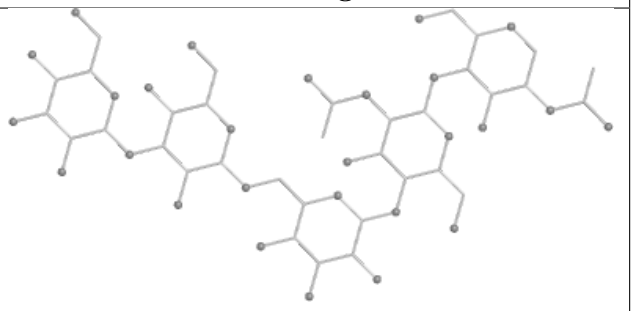
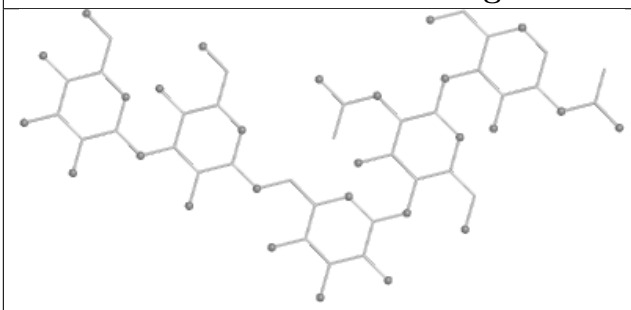
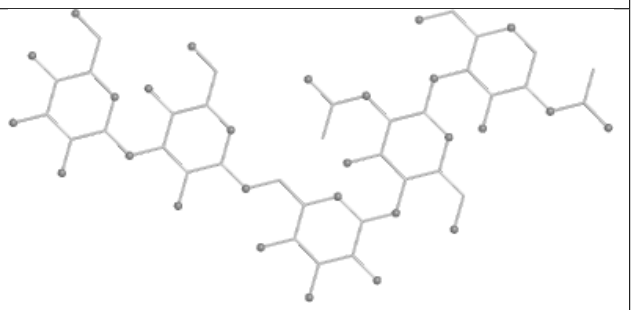
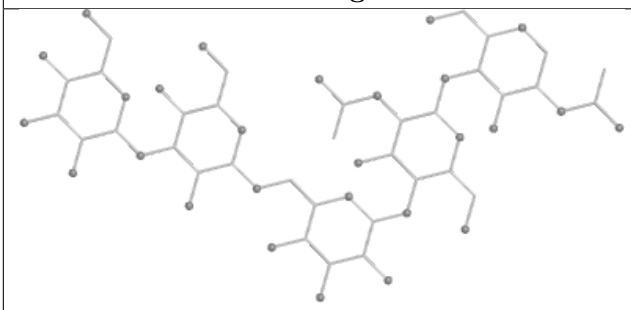
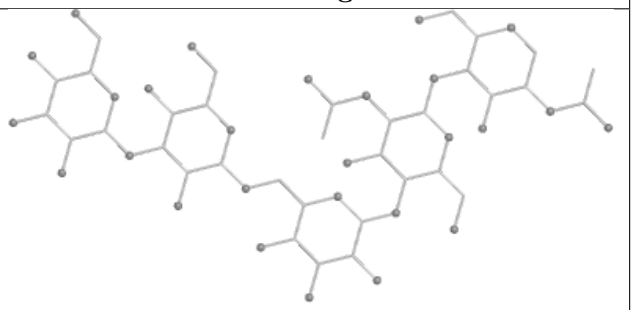
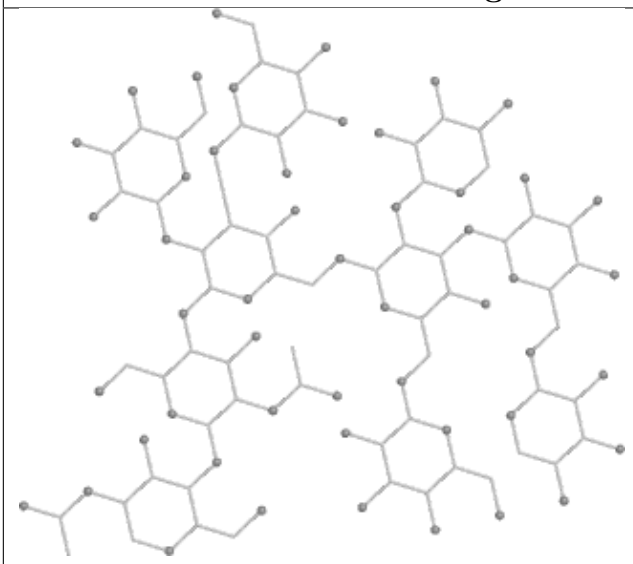


Rings

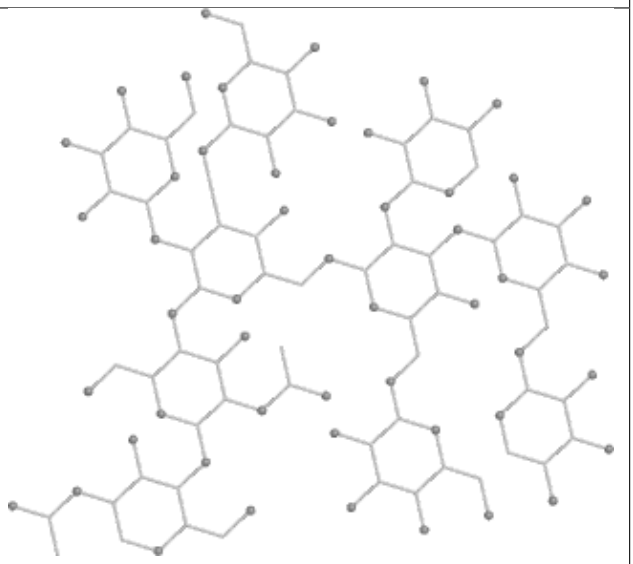
Oligosaccharide Chain bE	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain bH	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

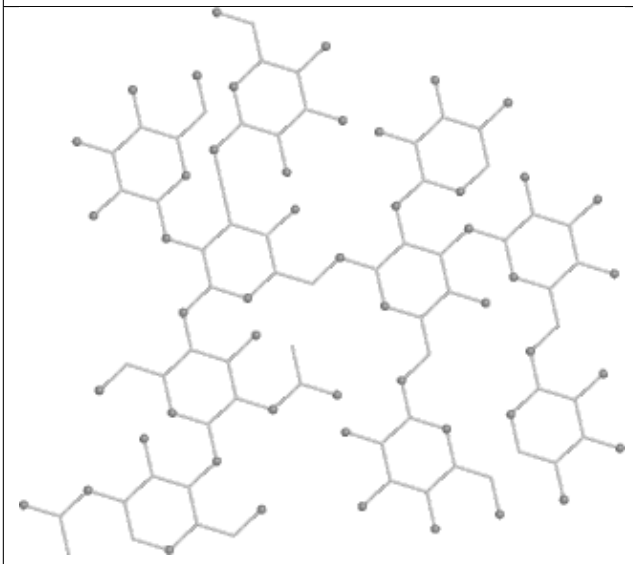
Oligosaccharide Chain bC



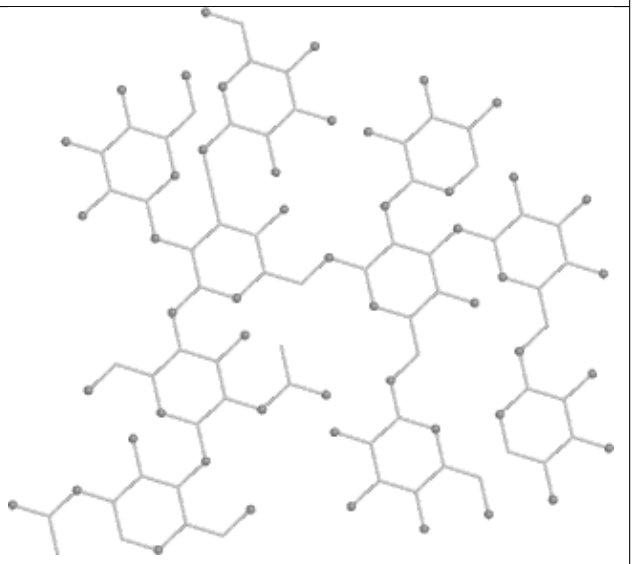
Bond lengths



Bond angles

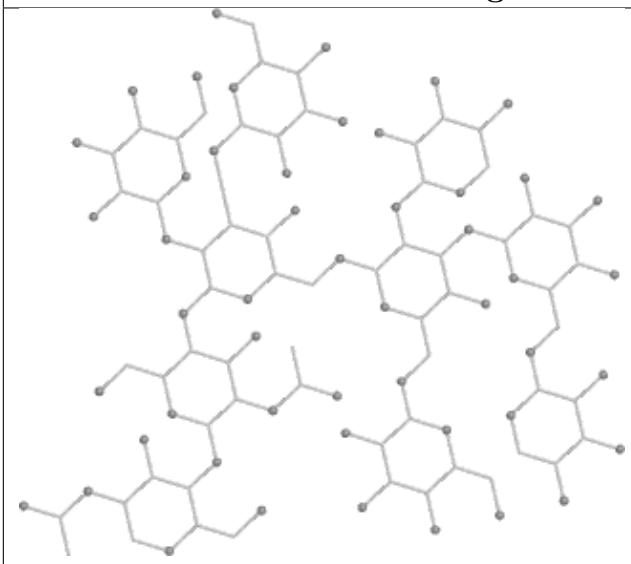


Torsions

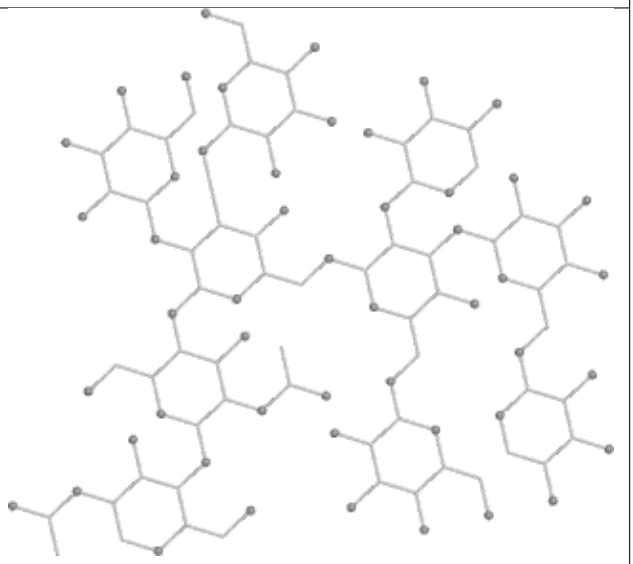


Rings

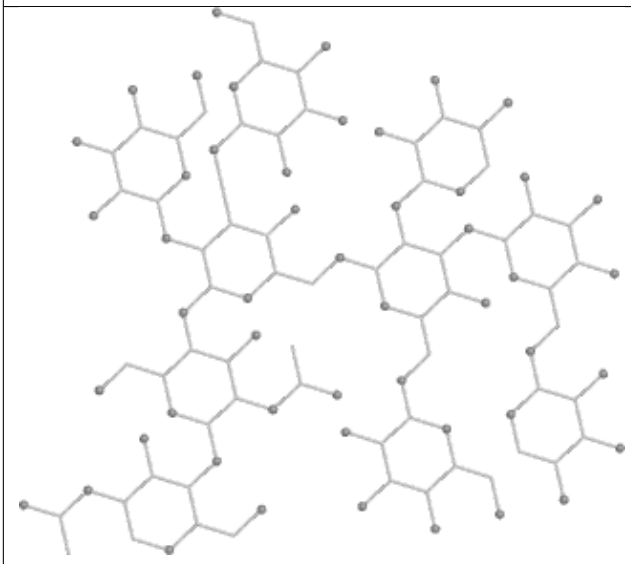
Oligosaccharide Chain bF



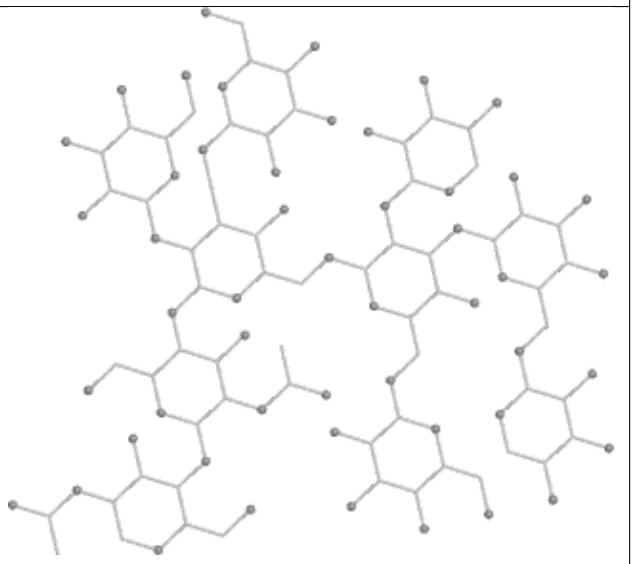
Bond lengths



Bond angles

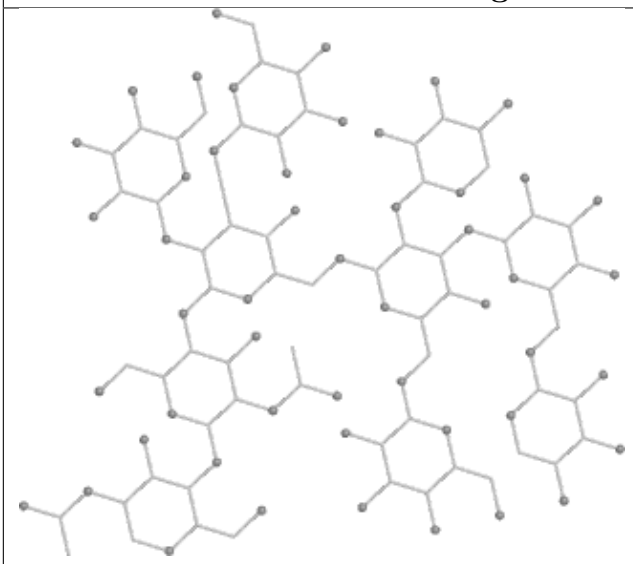


Torsions

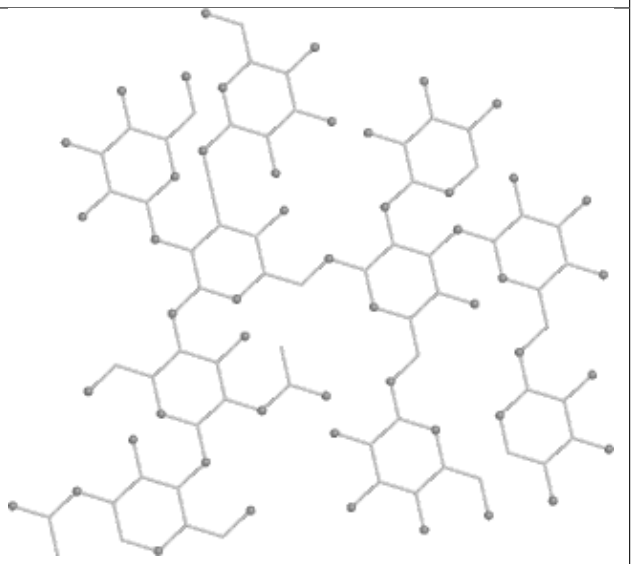


Rings

Oligosaccharide Chain bI



Bond lengths



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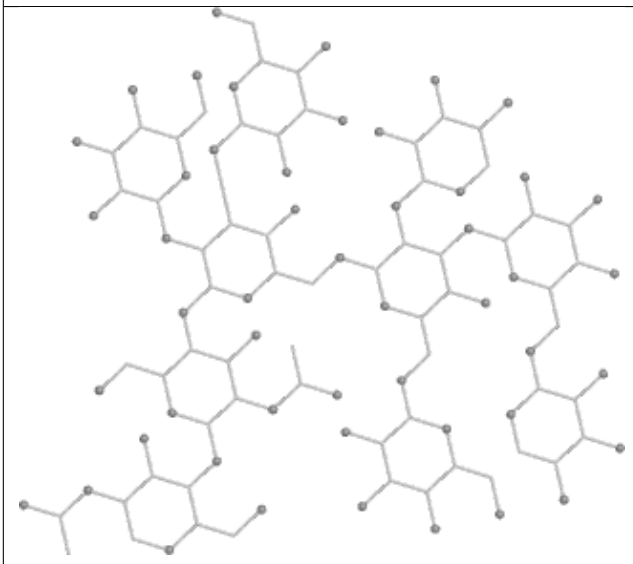

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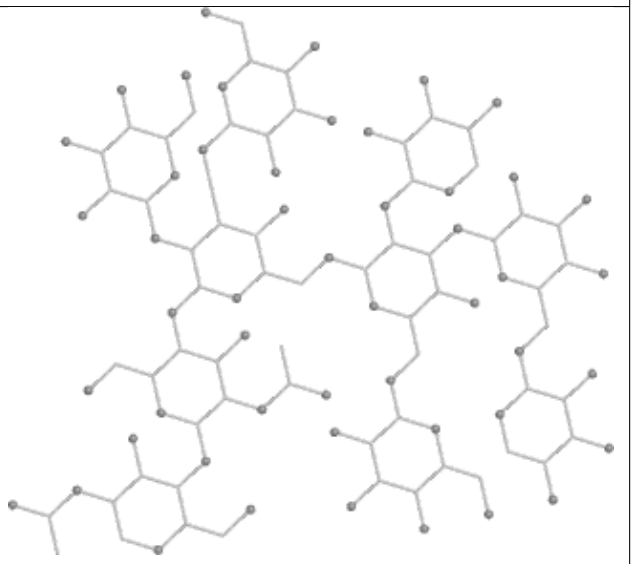
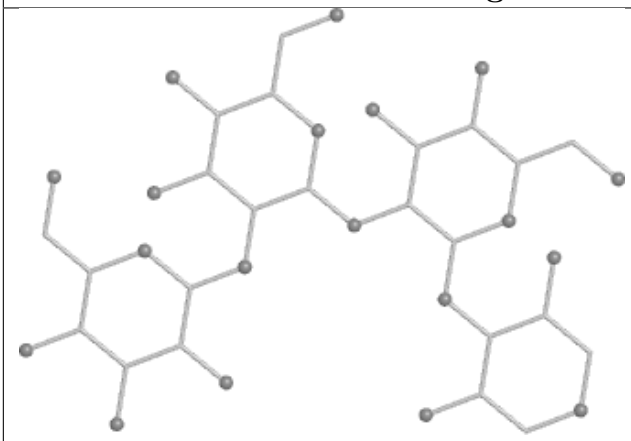


Rings

Oligosaccharide Chain cA



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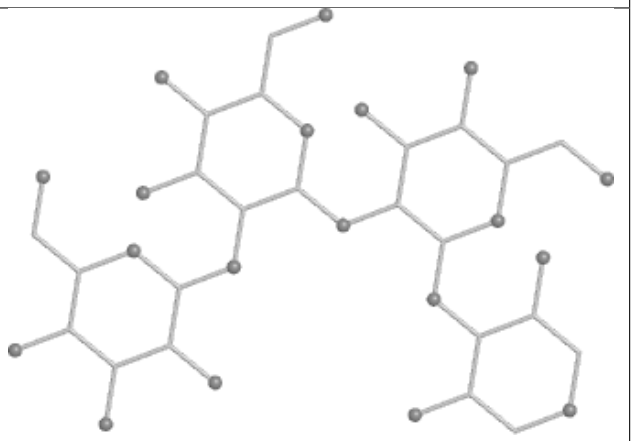

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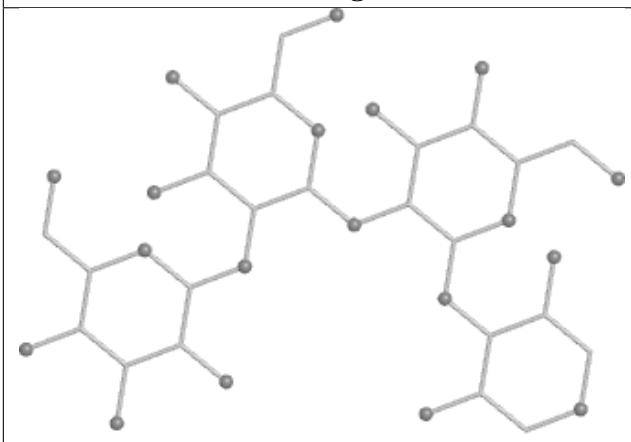

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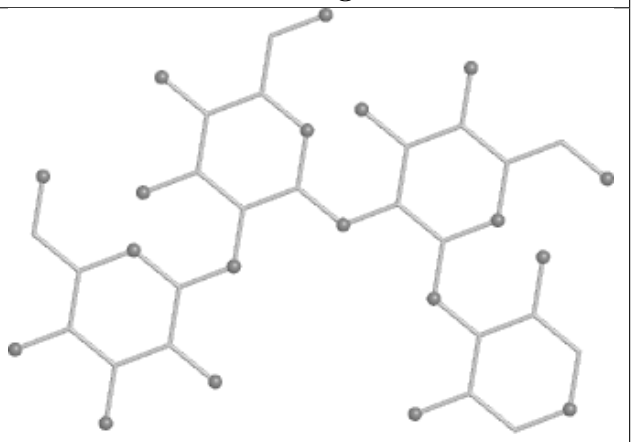
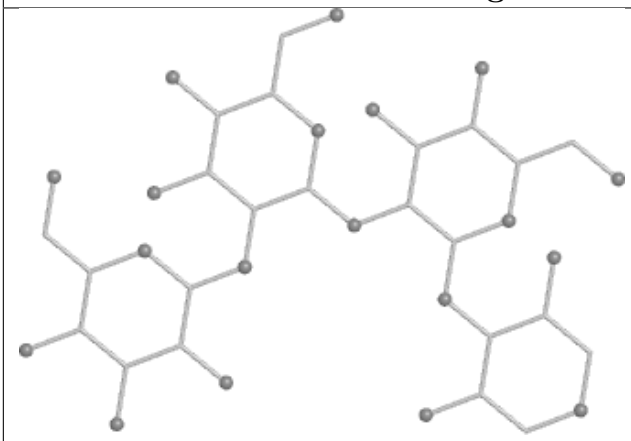


Rings

Oligosaccharide Chain cB



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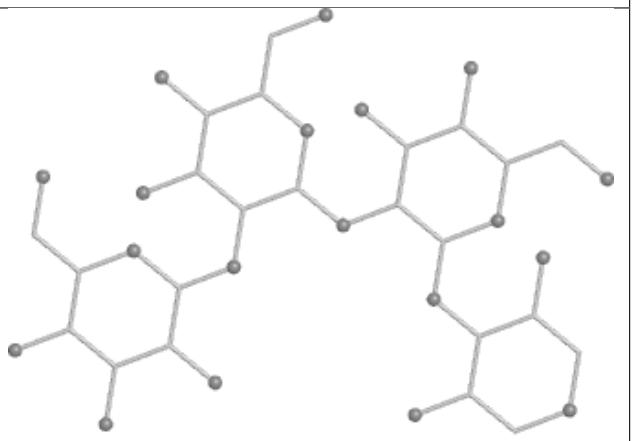

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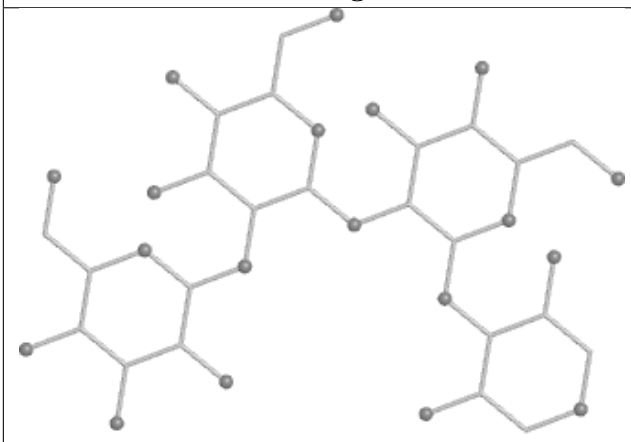

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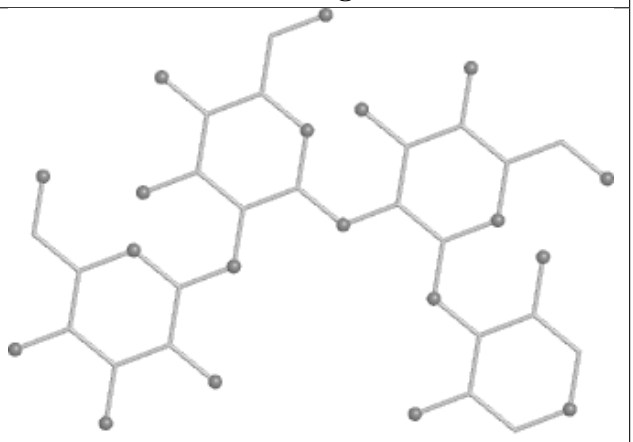
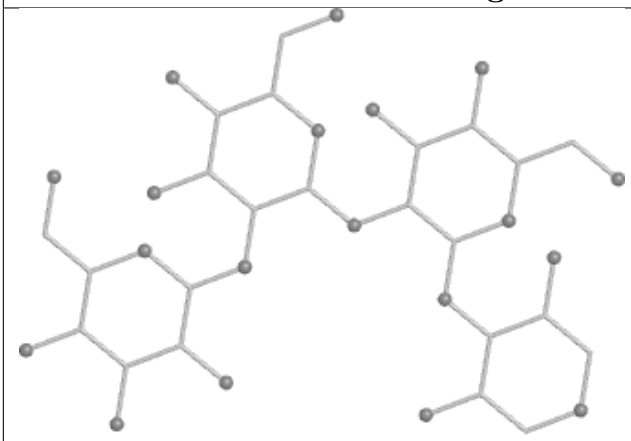


Rings

Oligosaccharide Chain cC



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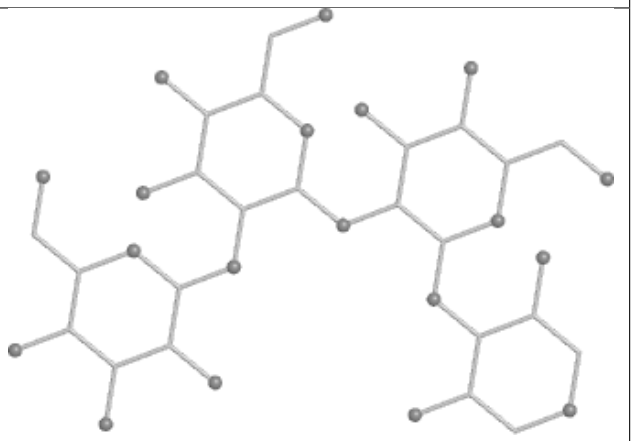

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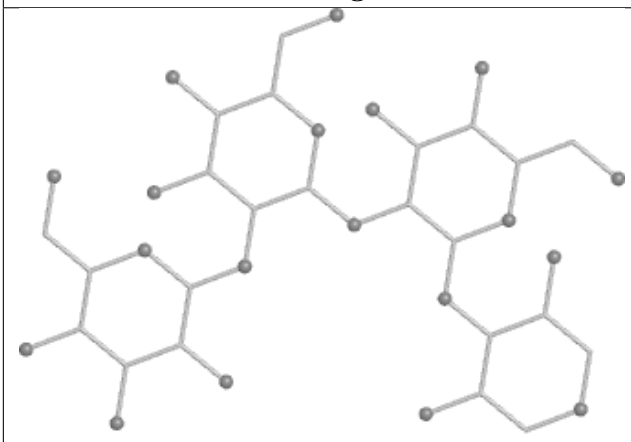

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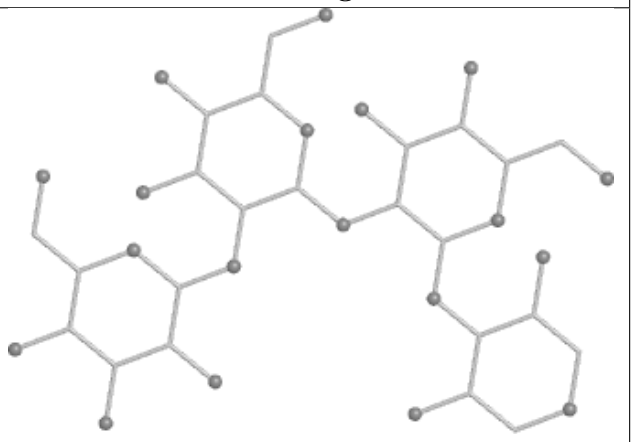
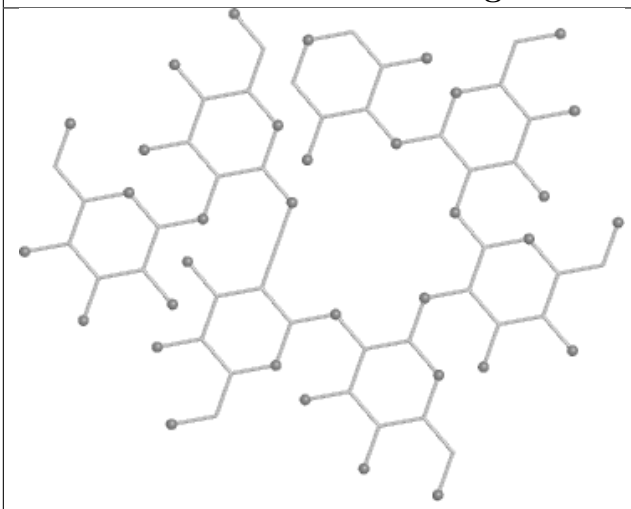


Rings

Oligosaccharide Chain dA



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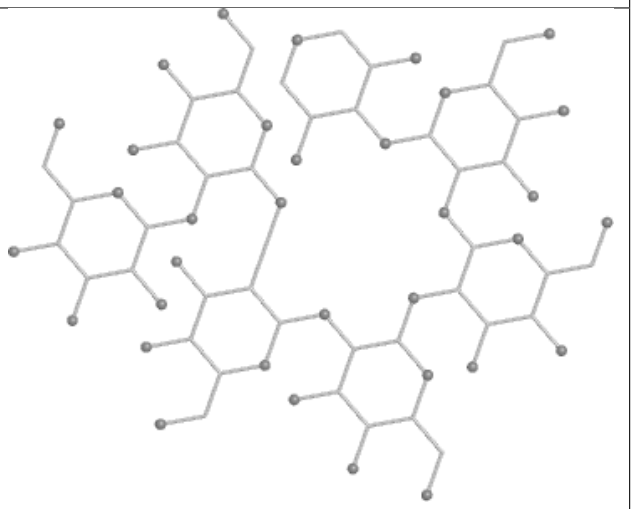

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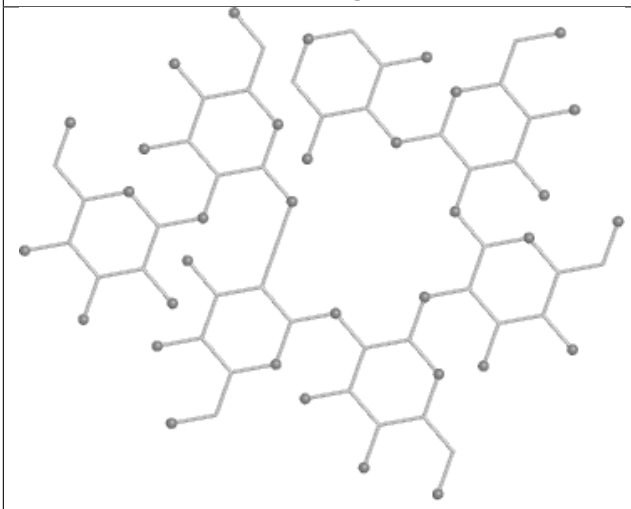

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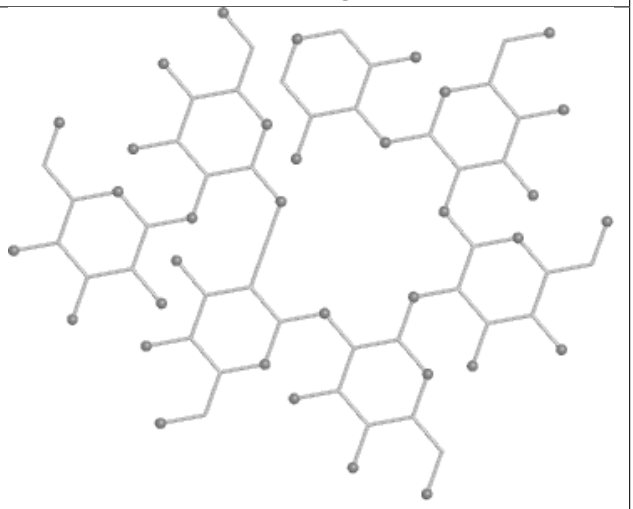
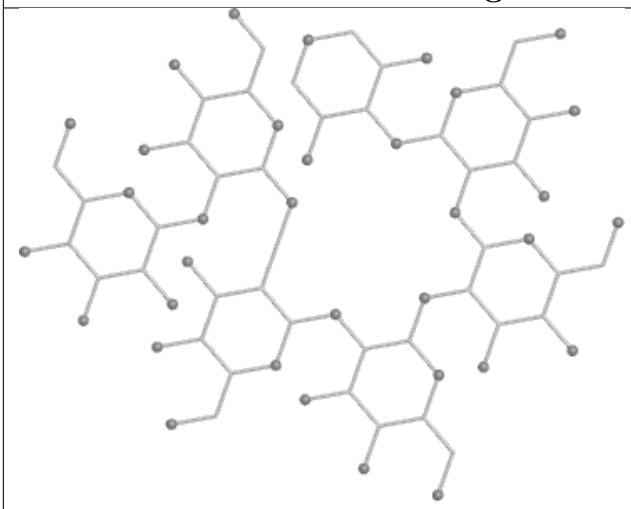


Rings

Oligosaccharide Chain dB



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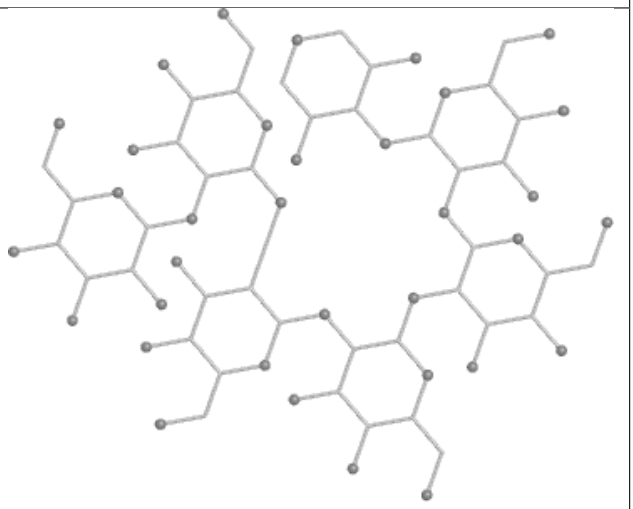

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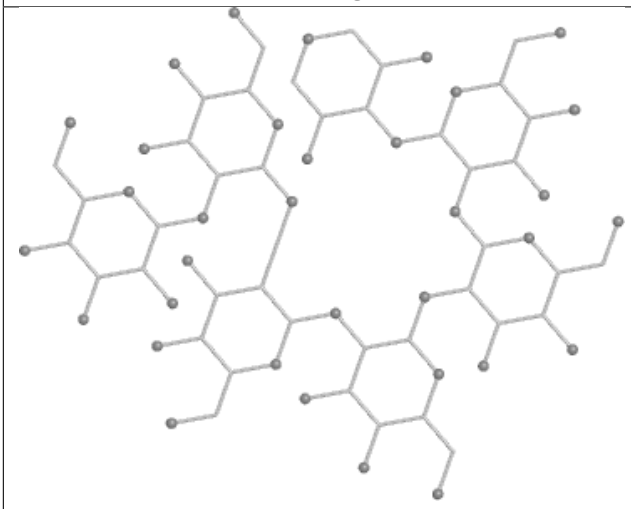

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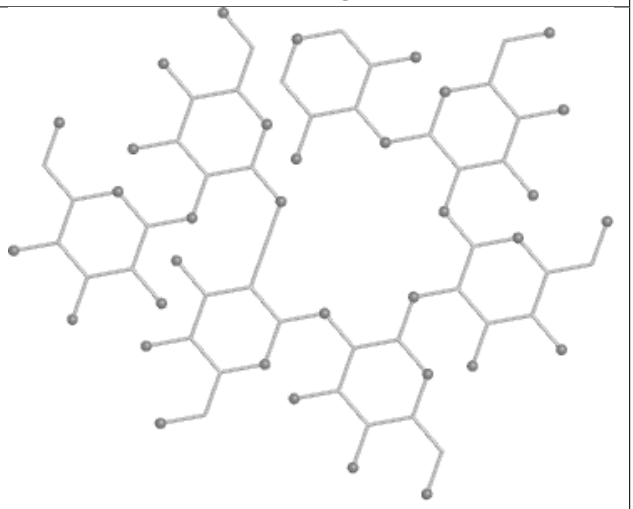
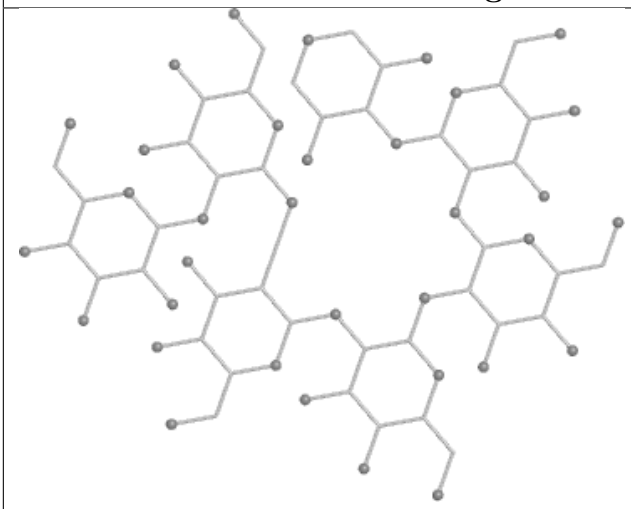


Rings

Oligosaccharide Chain dC



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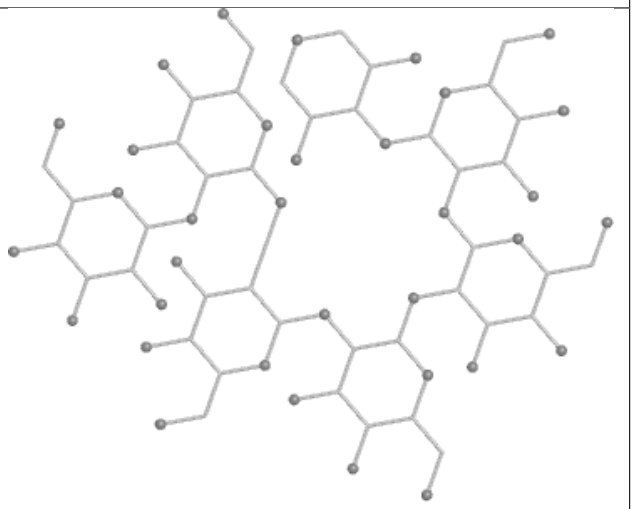

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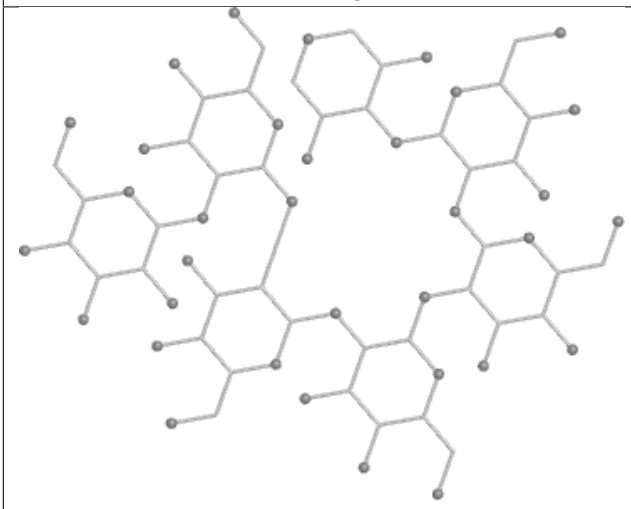

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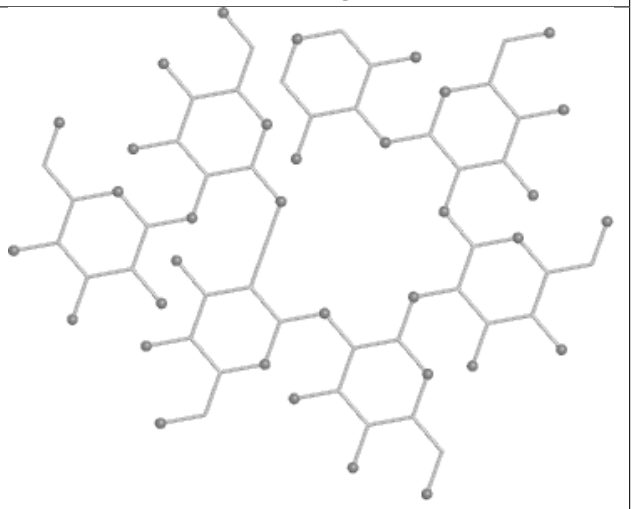
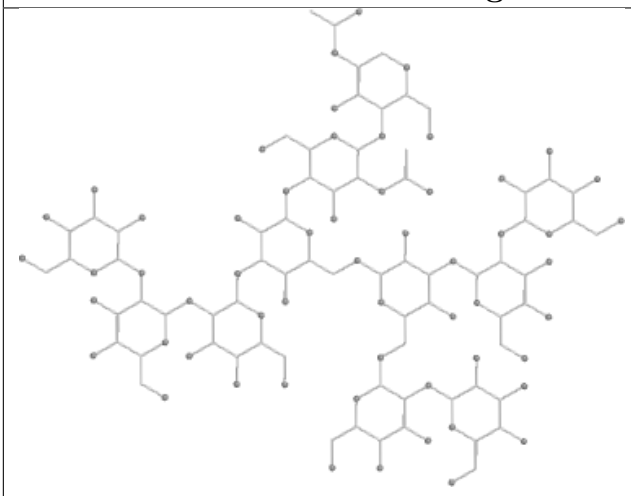


Rings

Oligosaccharide Chain eA



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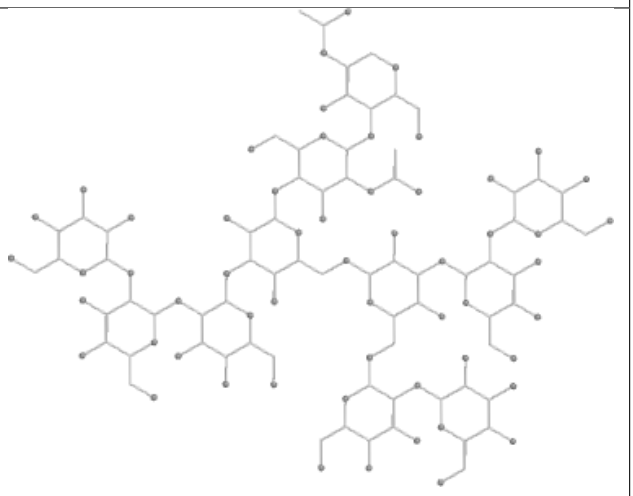
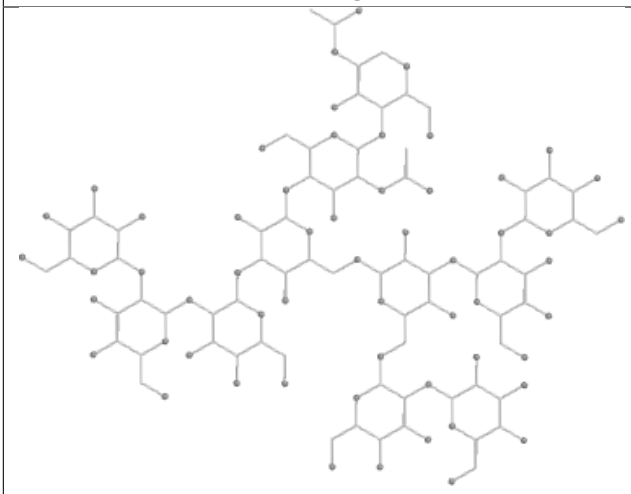


Bond angles



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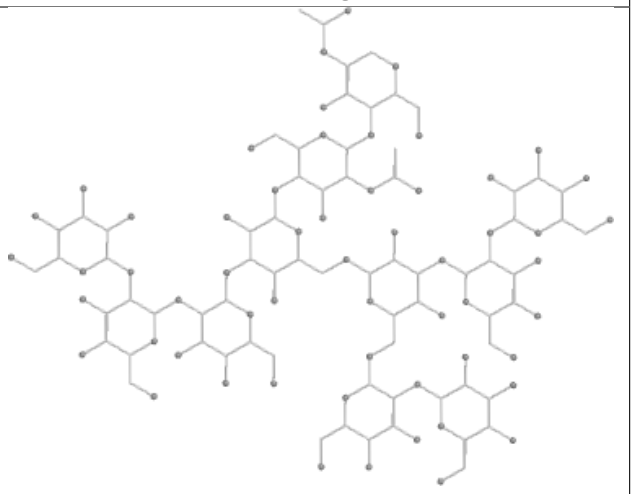
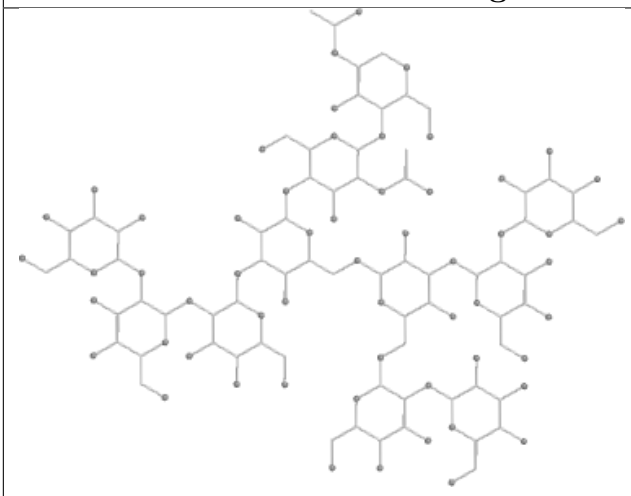


Rings

Oligosaccharide Chain fC



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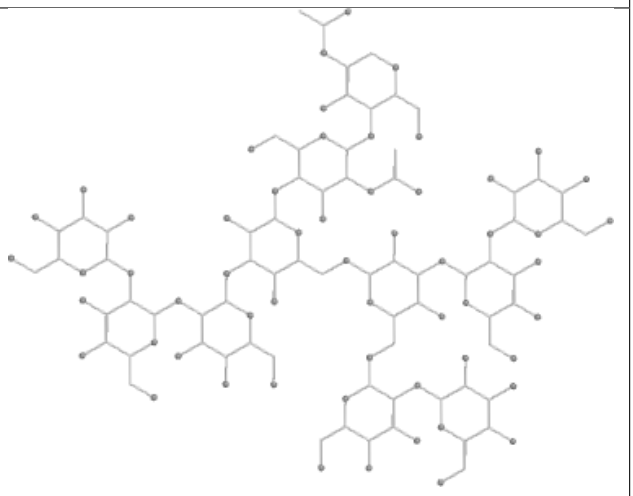

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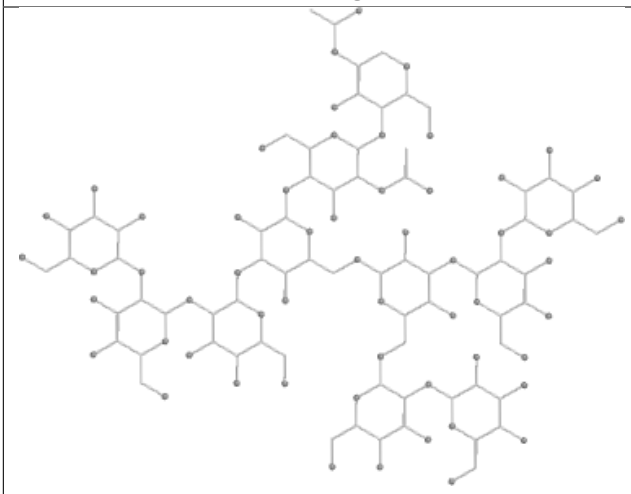

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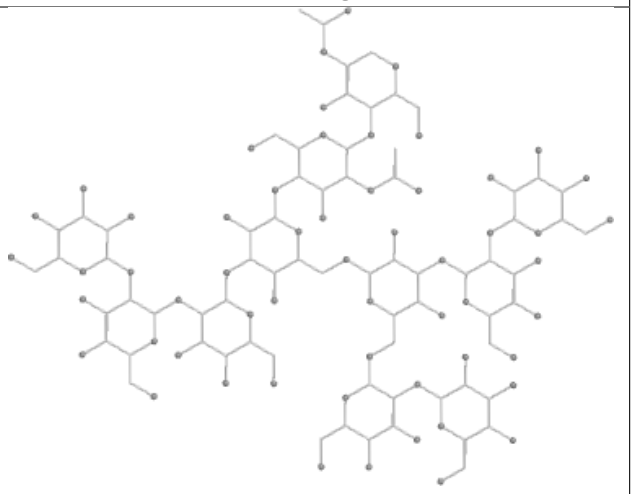
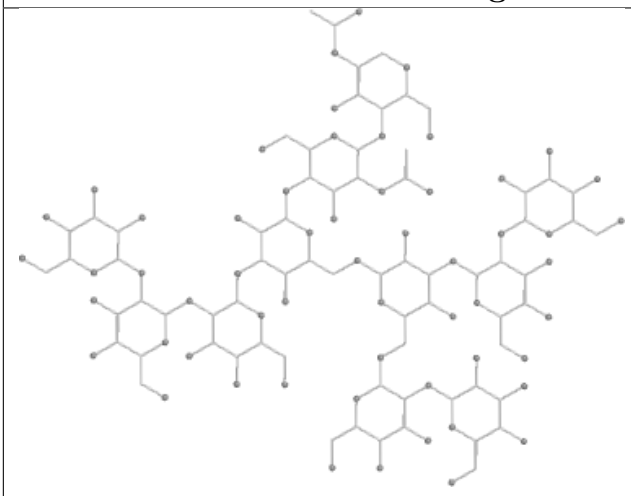


Rings

Oligosaccharide Chain fD



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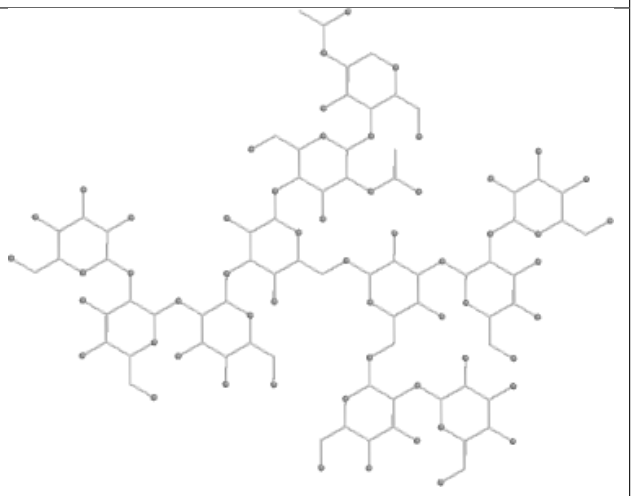
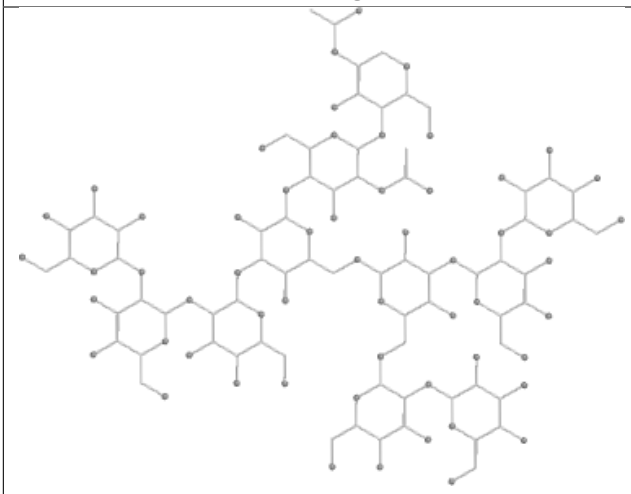


Bond angles



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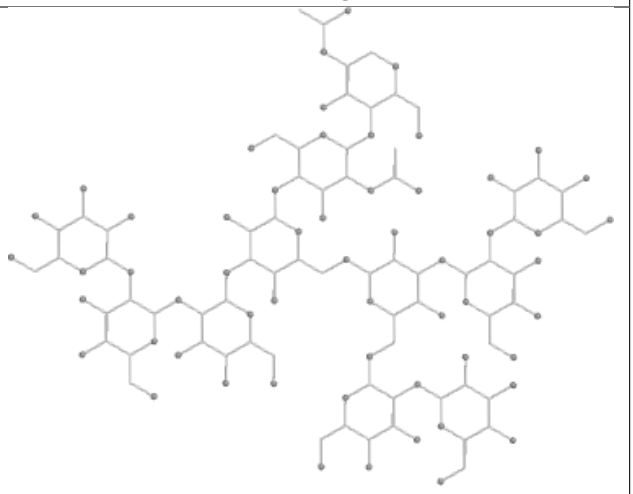
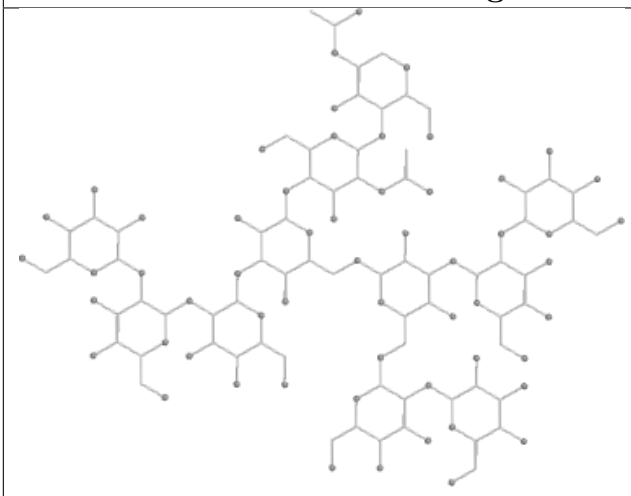


Rings

Oligosaccharide Chain eC



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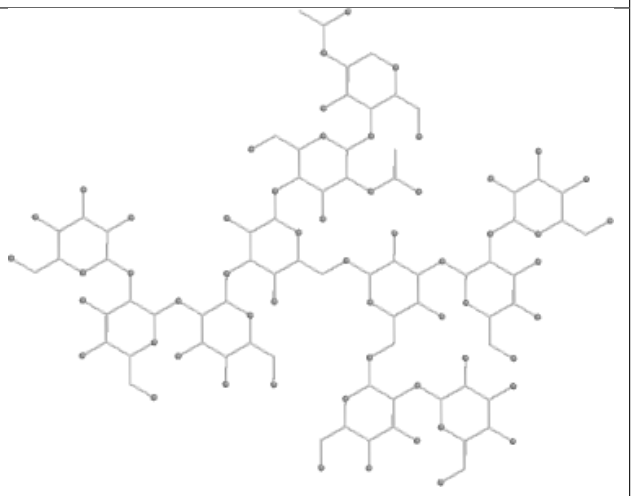
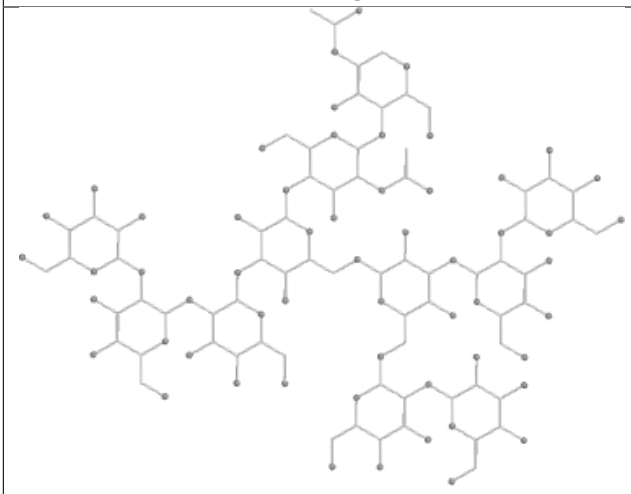


Bond angles



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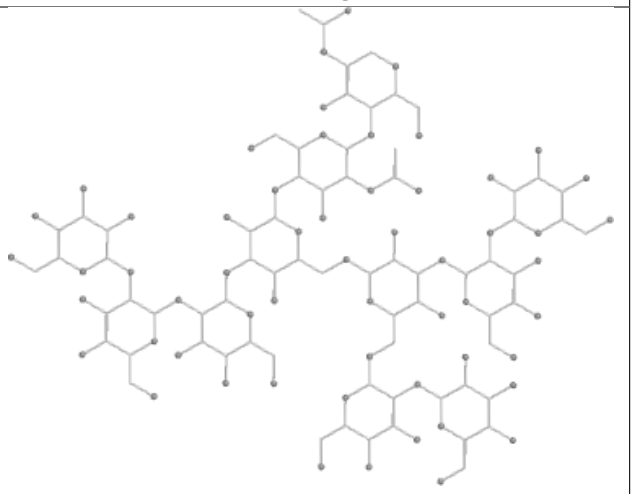
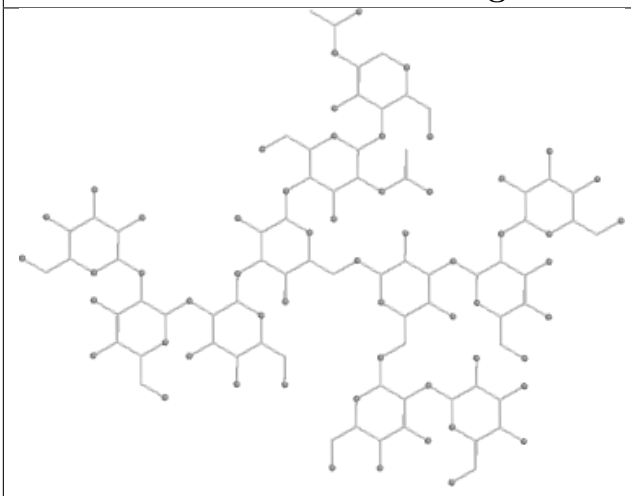
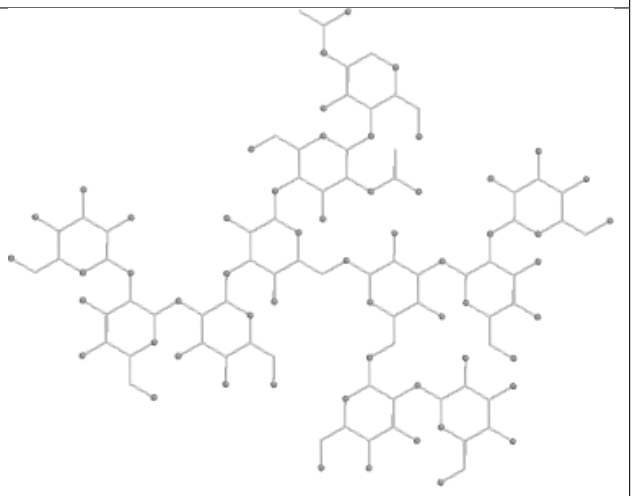


Rings

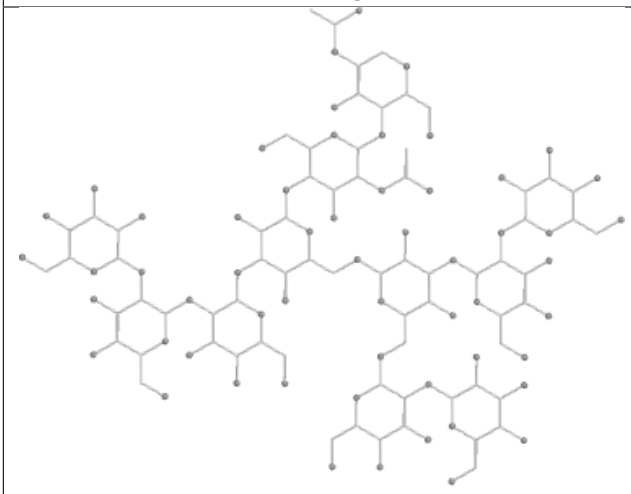
Oligosaccharide Chain fH



Bond lengths



Bond angles



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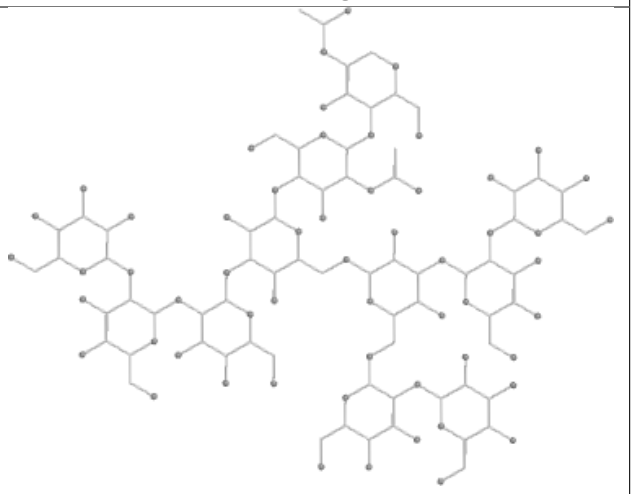
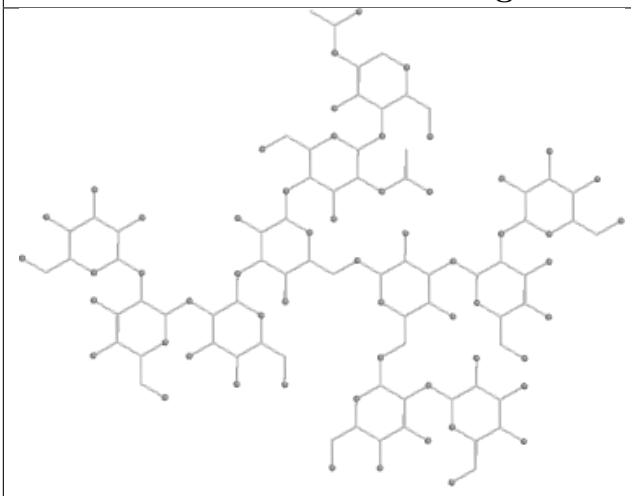
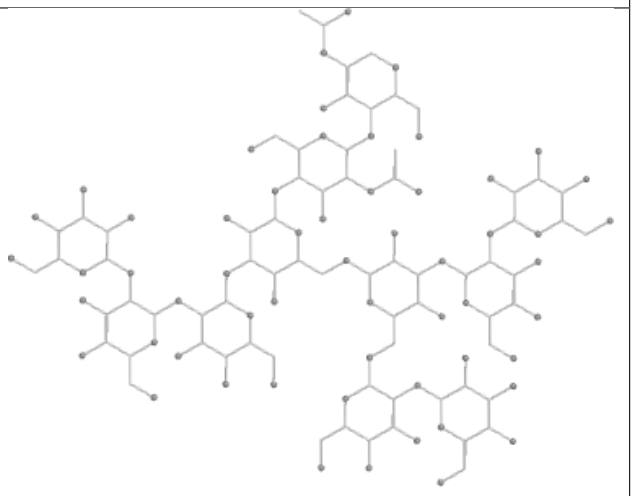


Rings

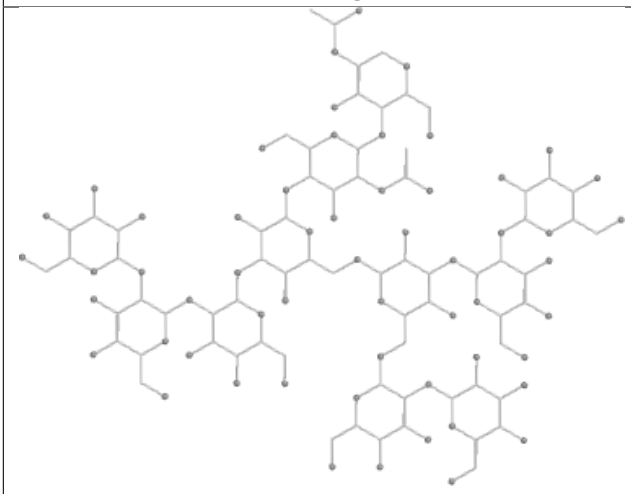
Oligosaccharide Chain fI



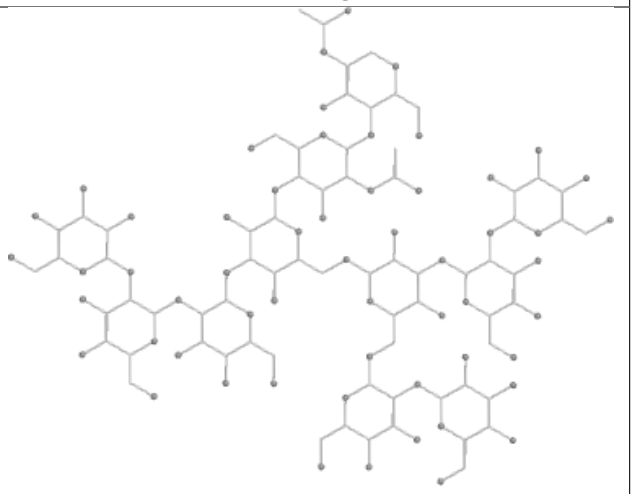
Bond lengths



Bond angles

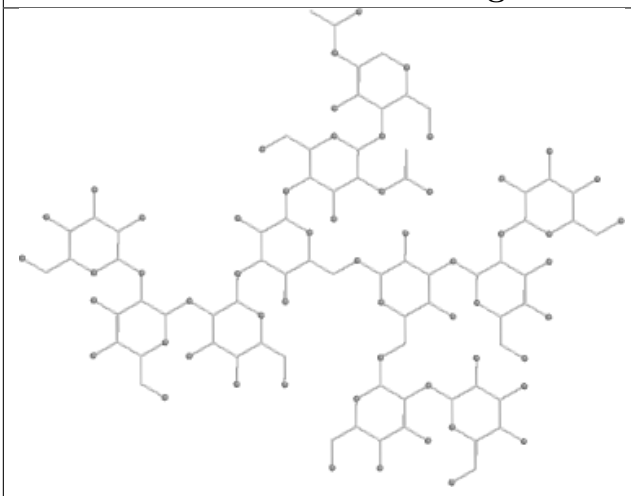


Torsions

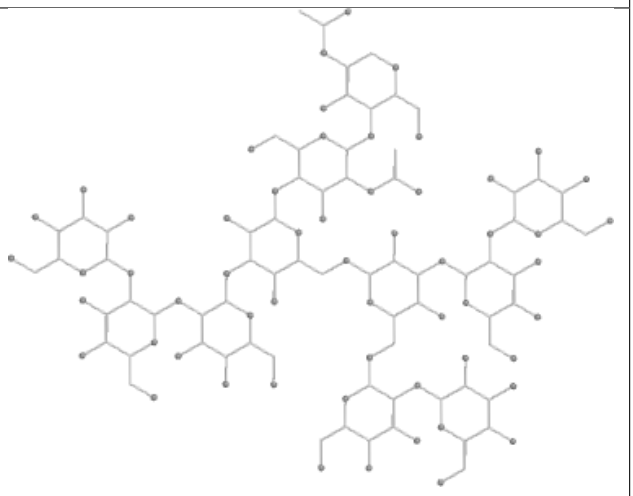


Rings

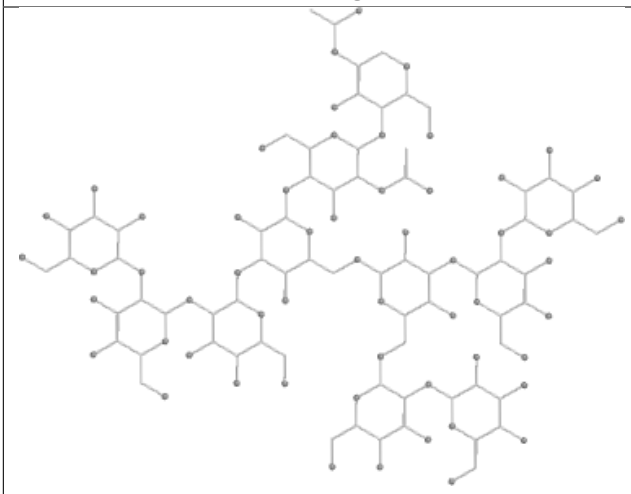
Oligosaccharide Chain eE



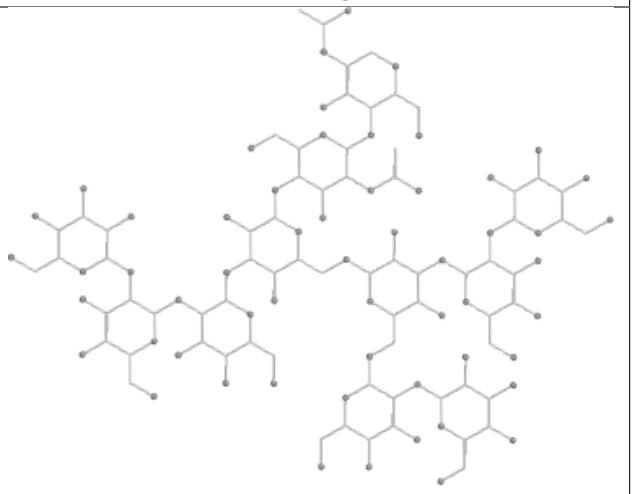
Bond lengths



Bond angles

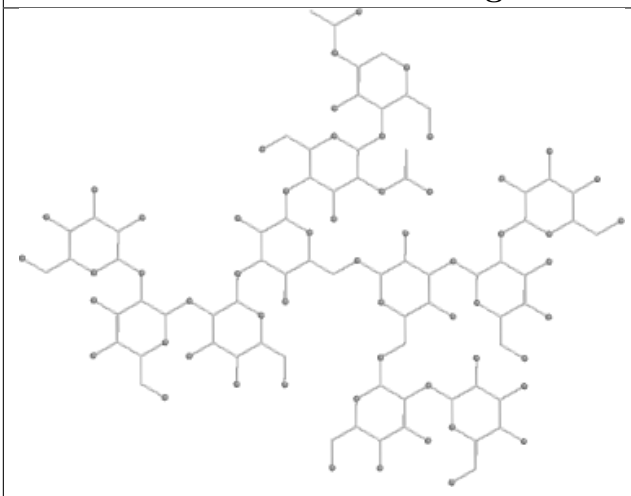


Torsions



Rings

Oligosaccharide Chain fM



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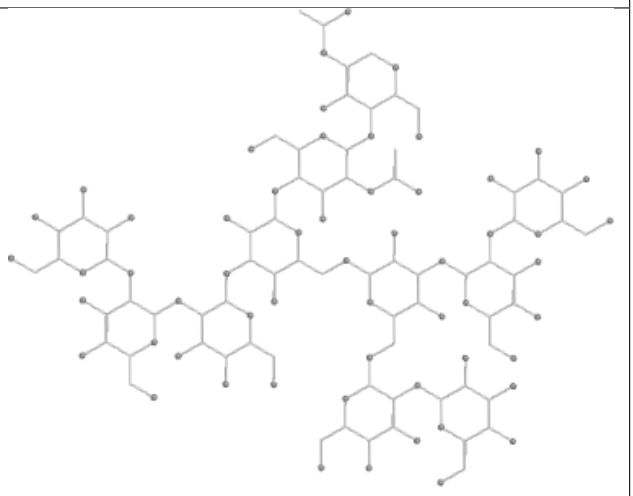
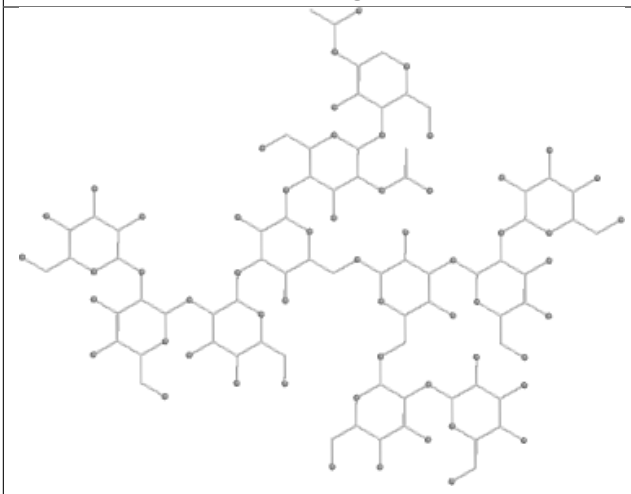


Bond angles



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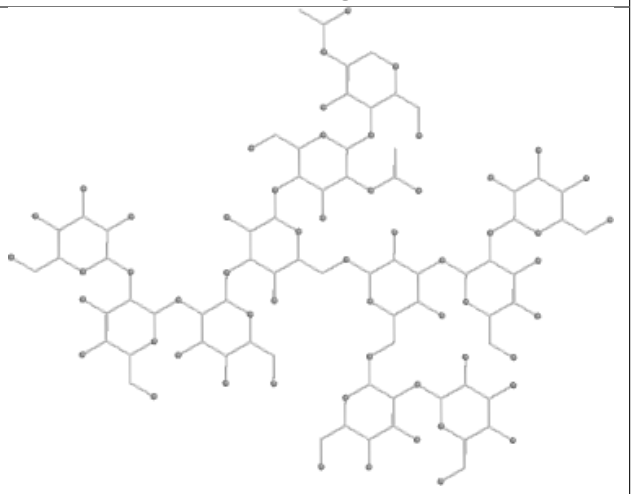
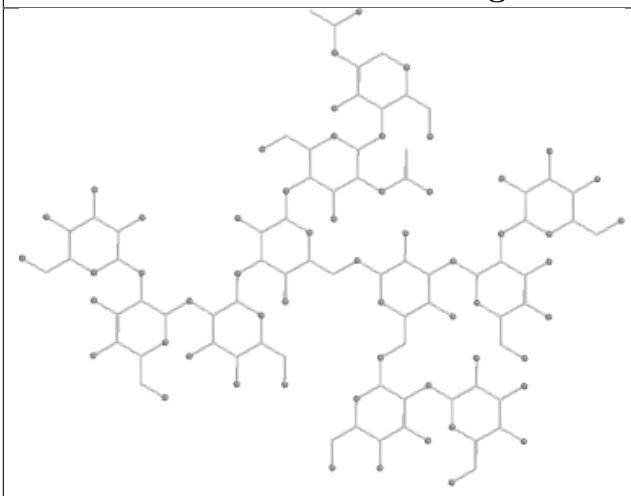


Rings

Oligosaccharide Chain fN



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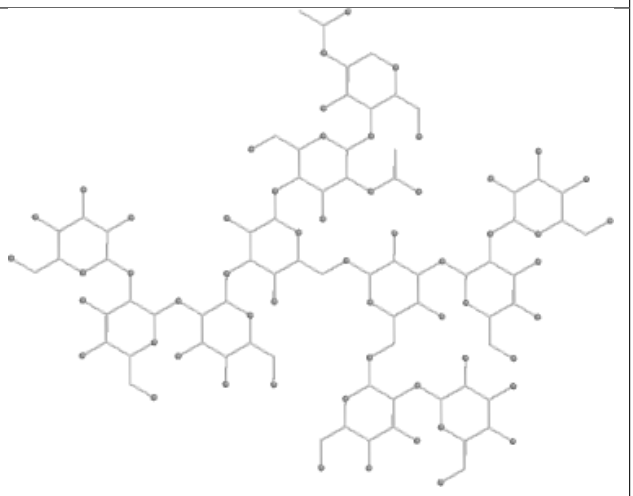
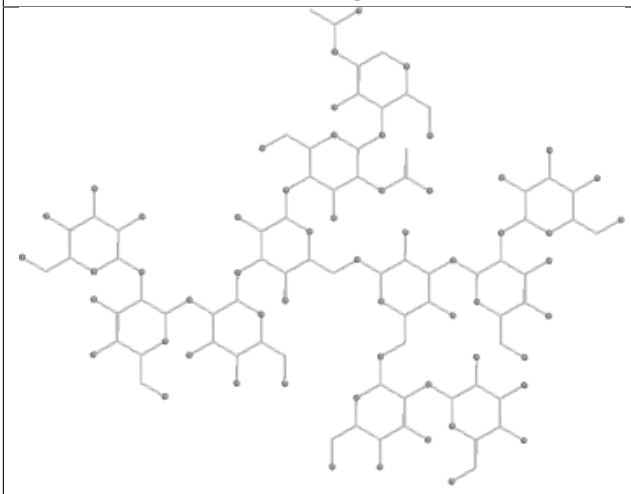


Bond angles



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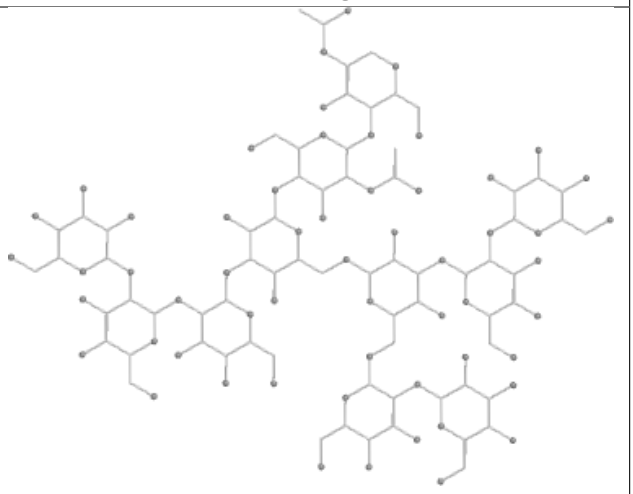
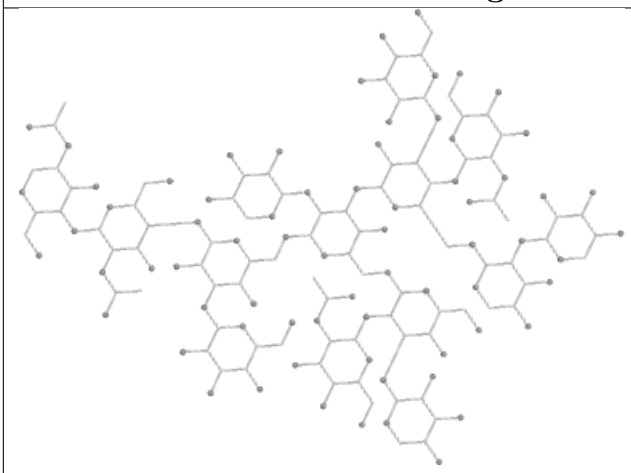


Rings

Oligosaccharide Chain eB



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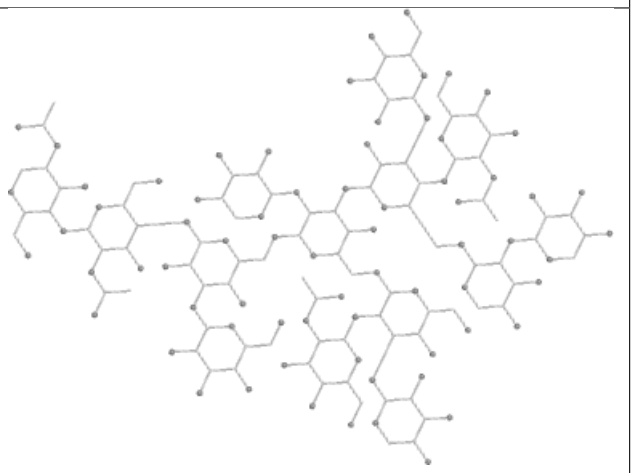
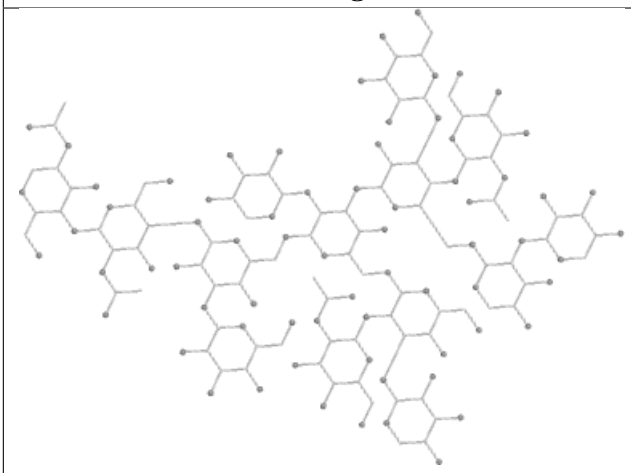


Bond angles



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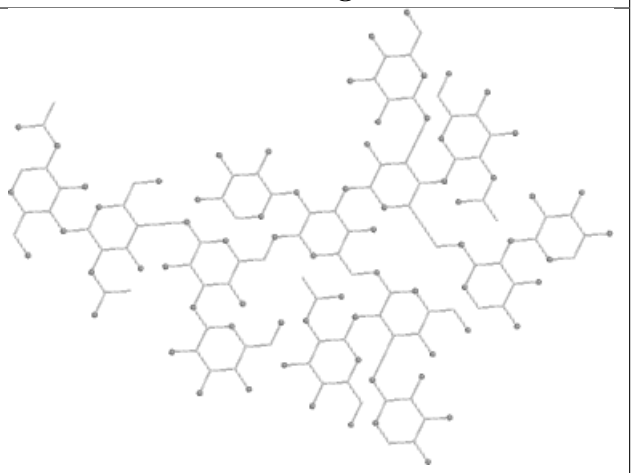
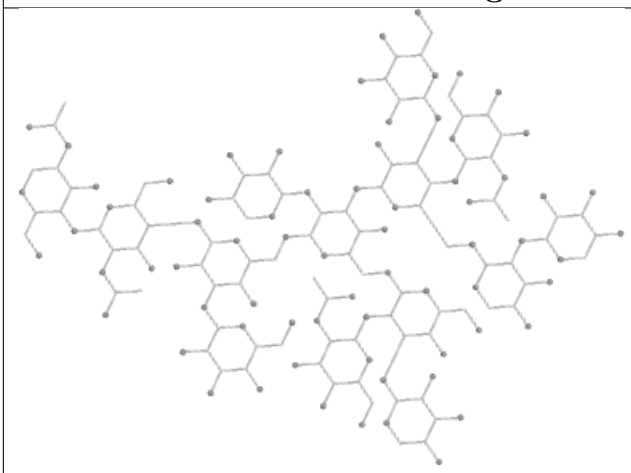


Rings

Oligosaccharide Chain eD



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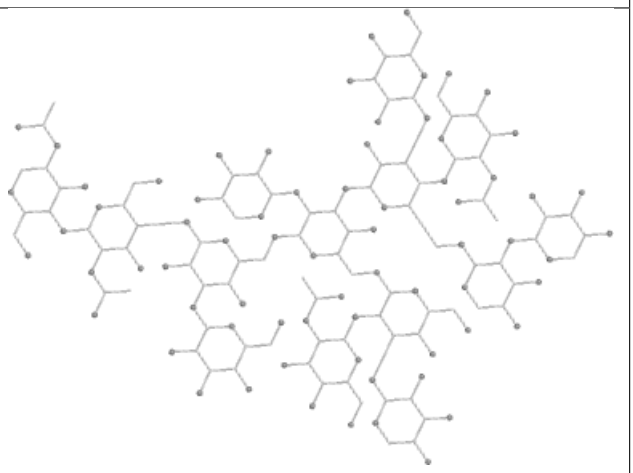
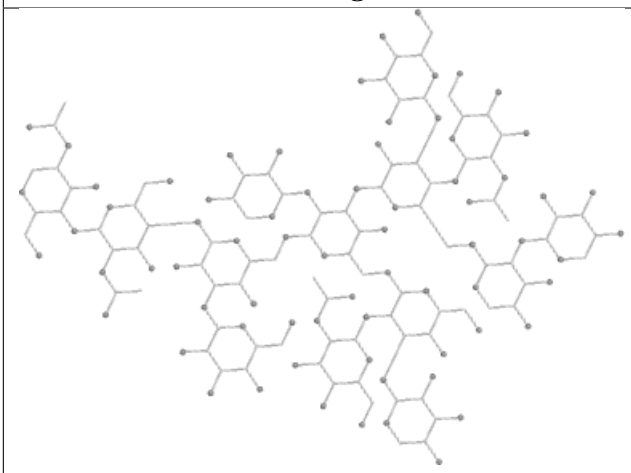


Bond angles



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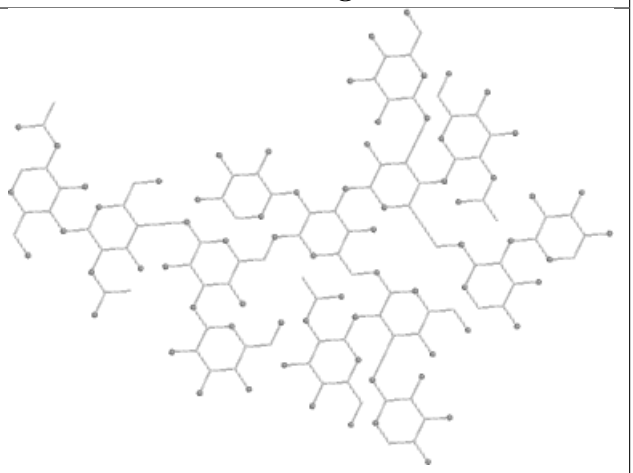
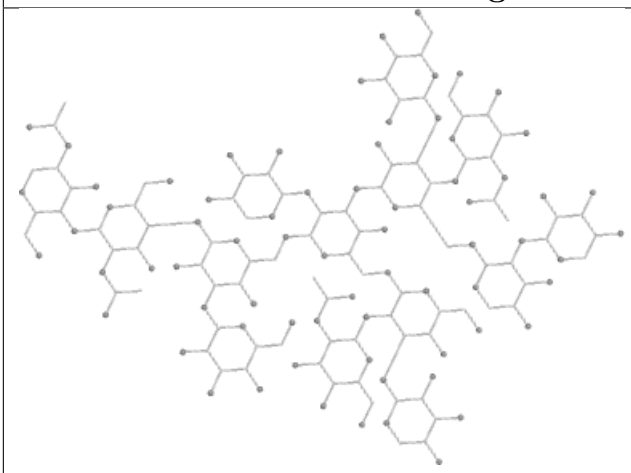


Rings

Oligosaccharide Chain eF



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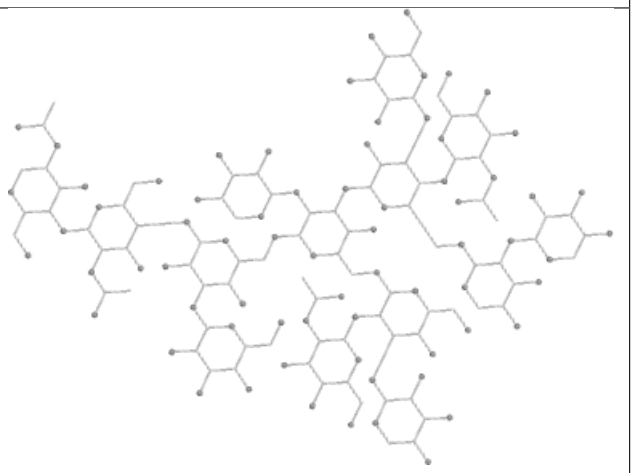
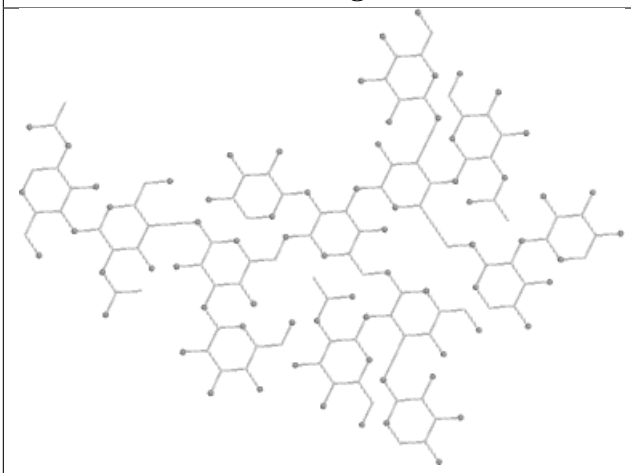


Bond angles



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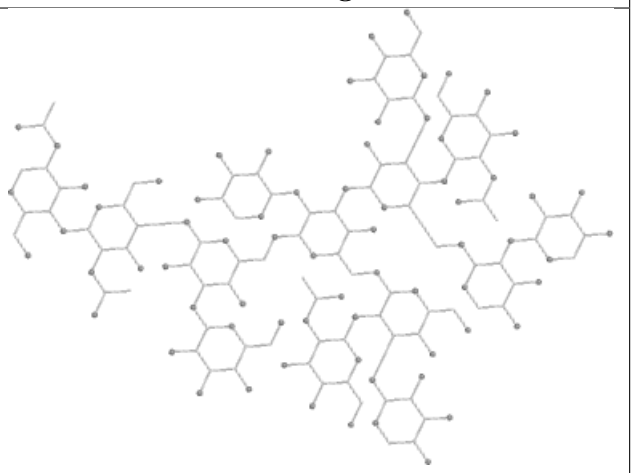
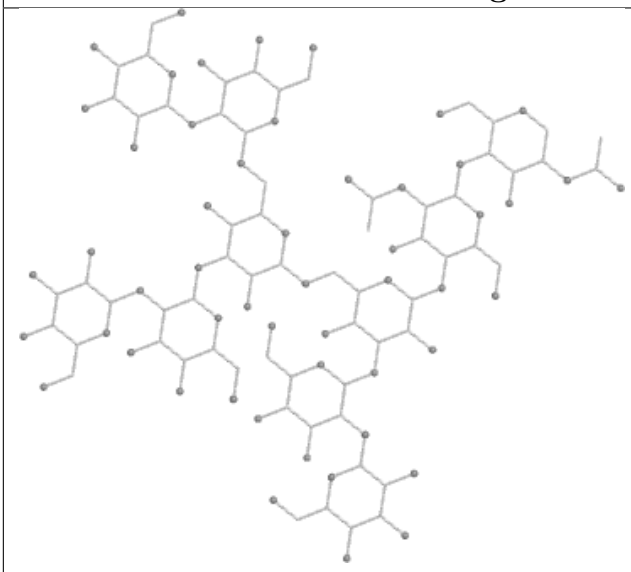


Rings

Oligosaccharide Chain fB



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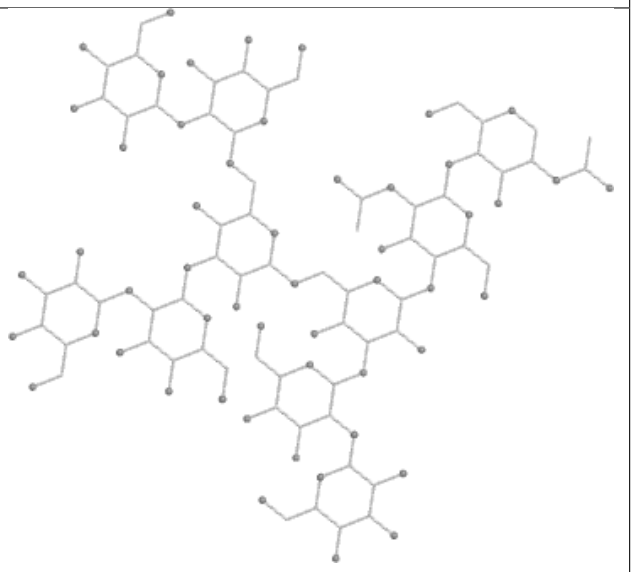

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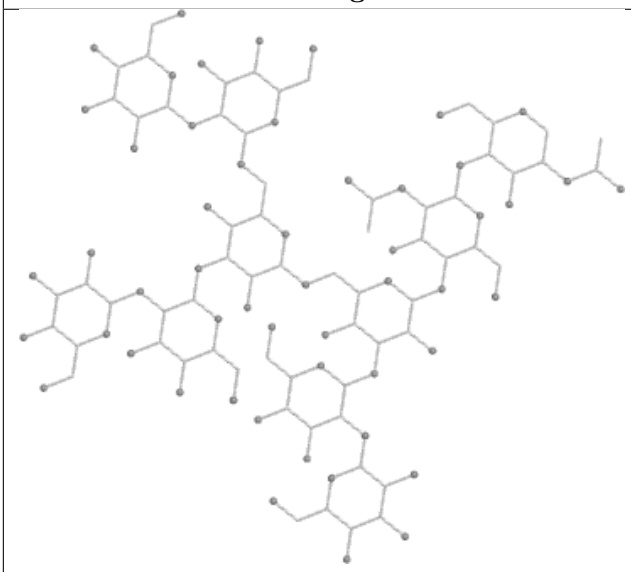

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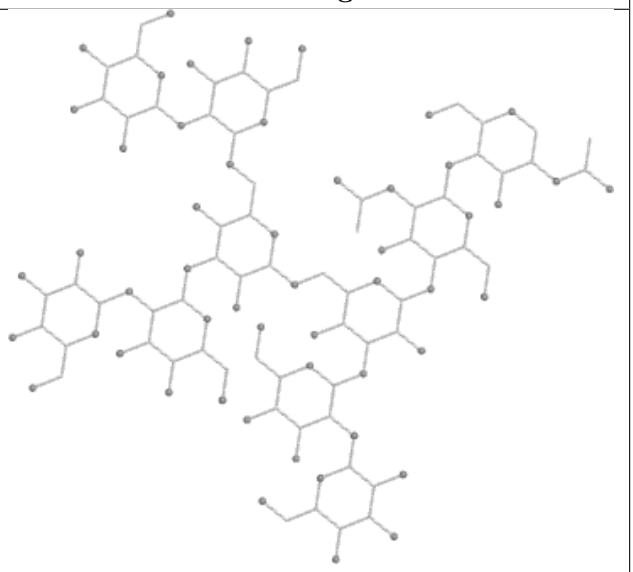
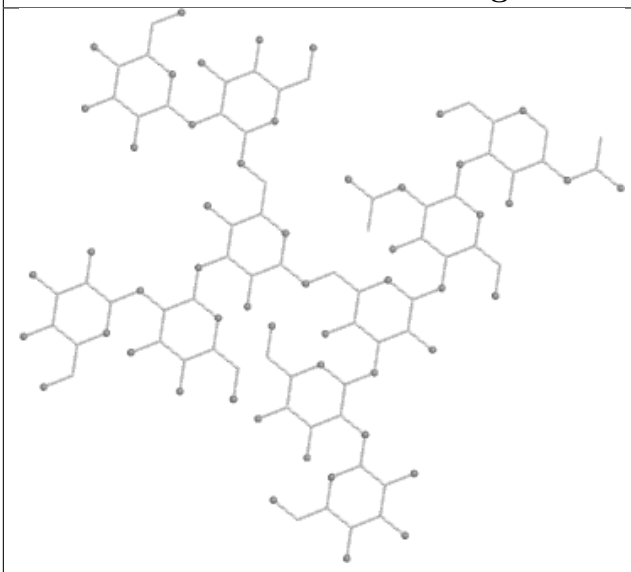


Rings

Oligosaccharide Chain fE



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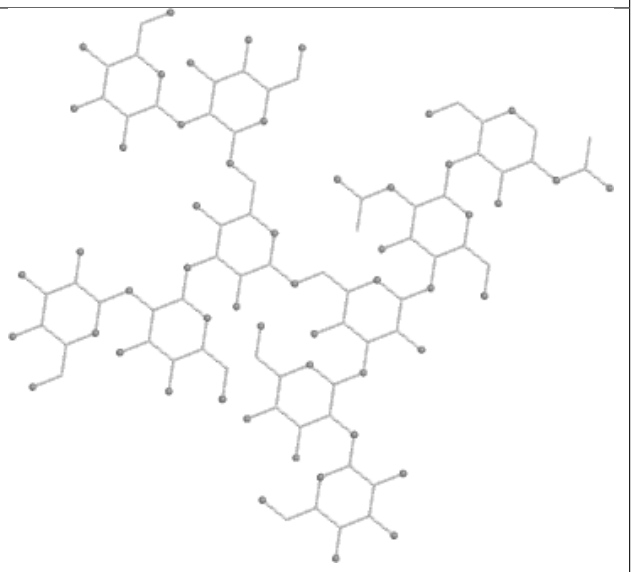
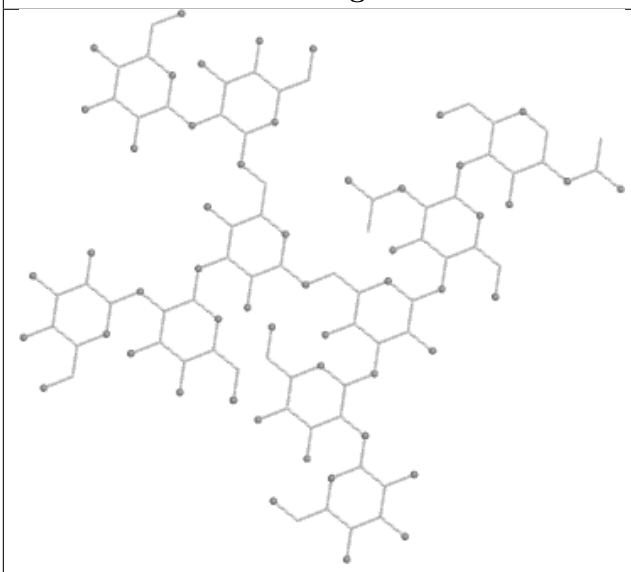


Bond angles



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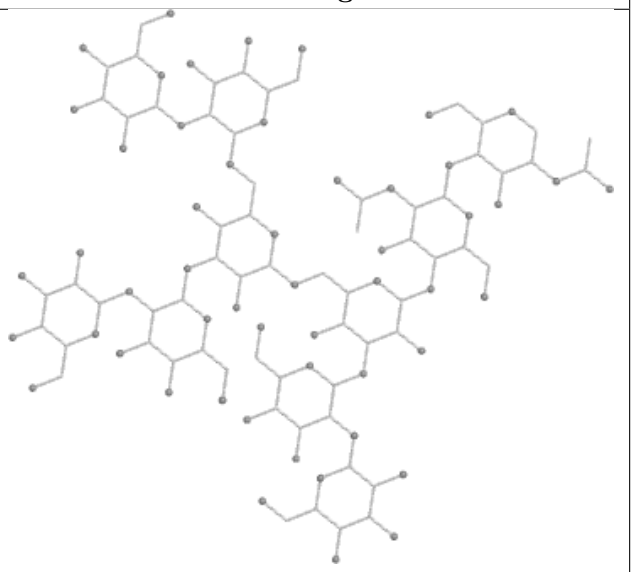
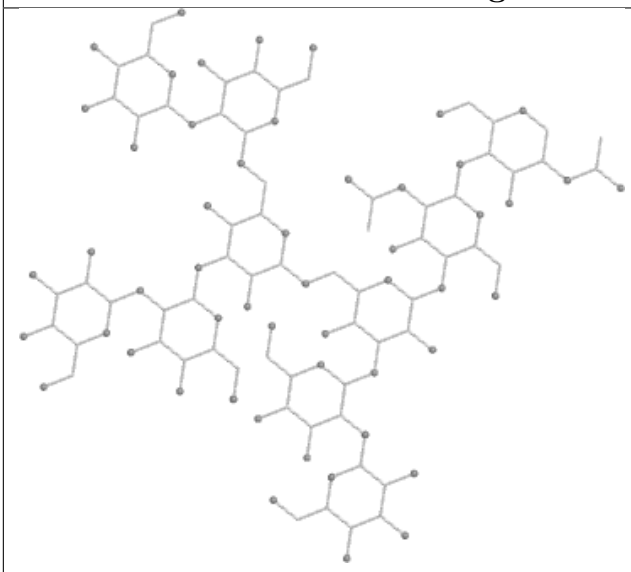


Rings

Oligosaccharide Chain fG



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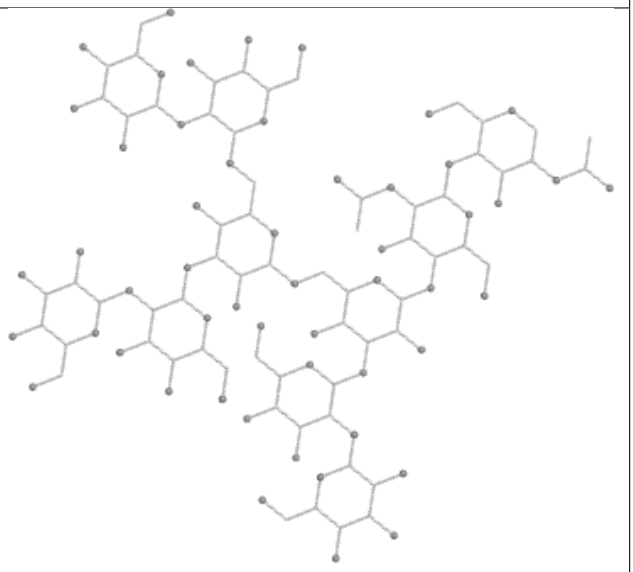
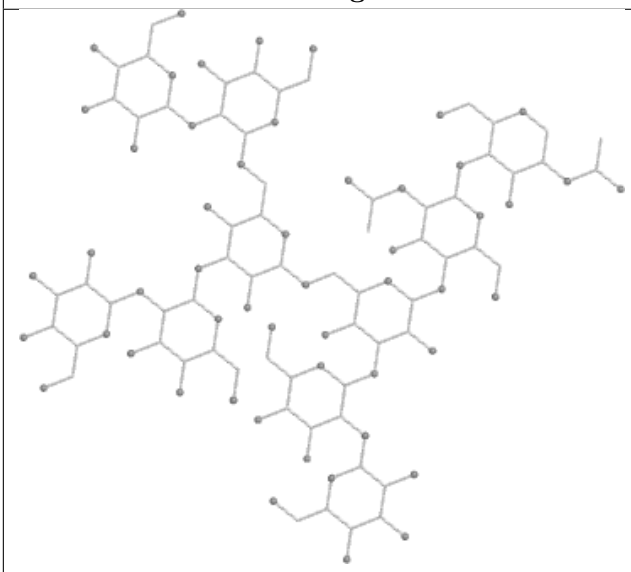


Bond angles



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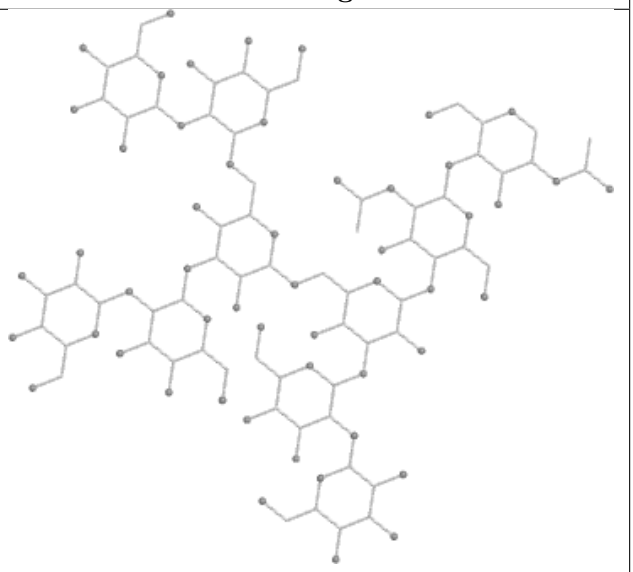
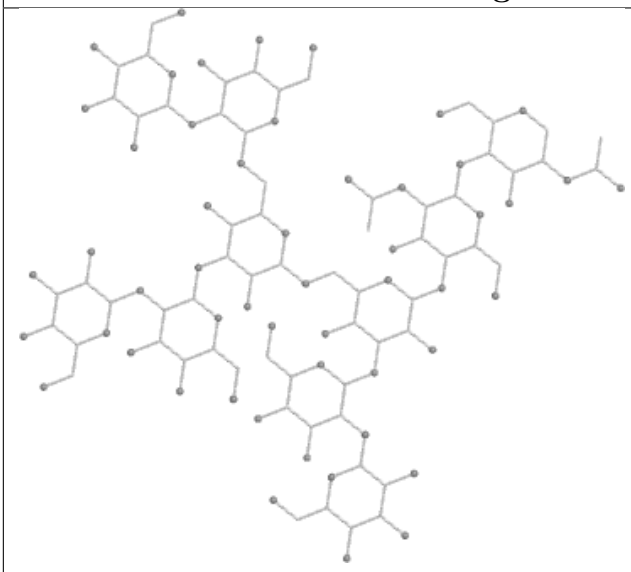


Rings

Oligosaccharide Chain fJ



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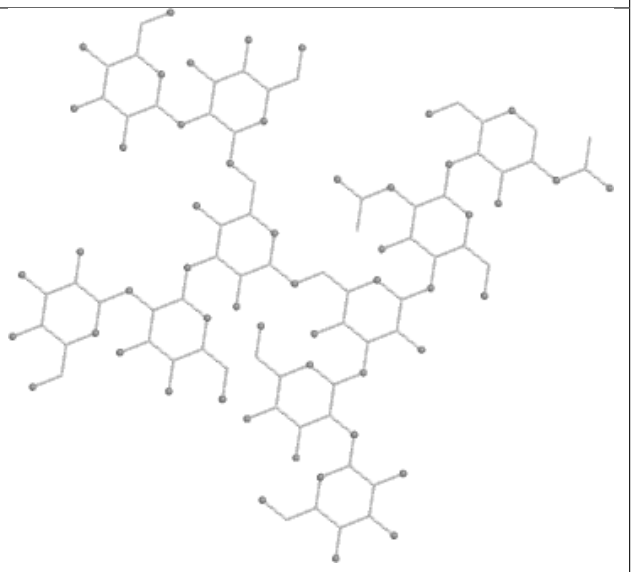
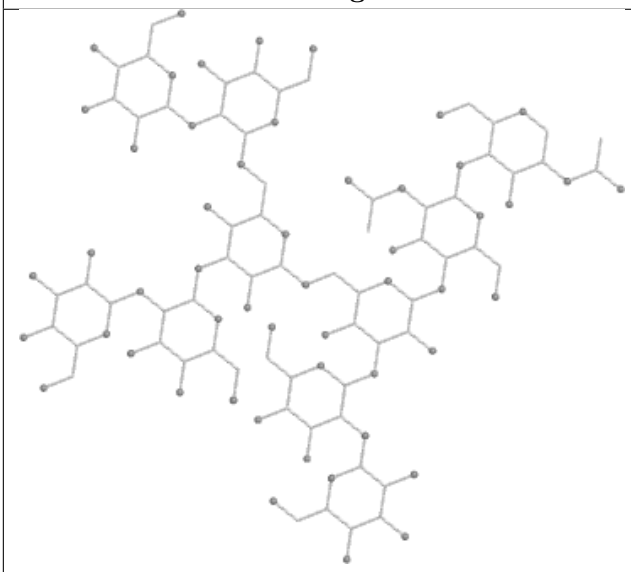


Bond angles



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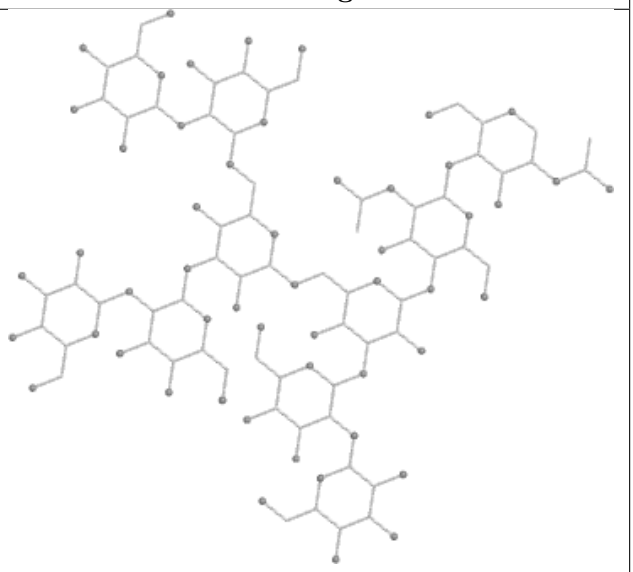
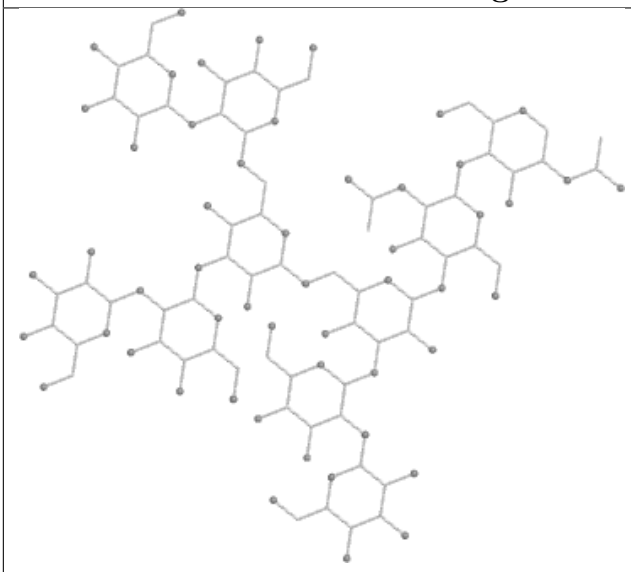


Rings

Oligosaccharide Chain fL



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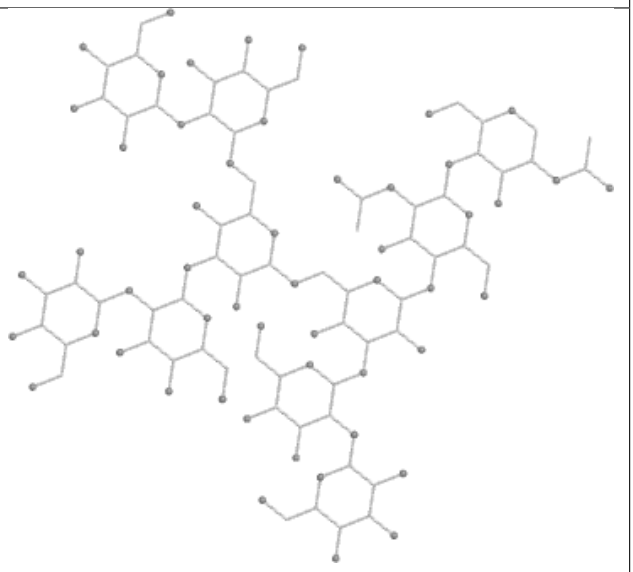
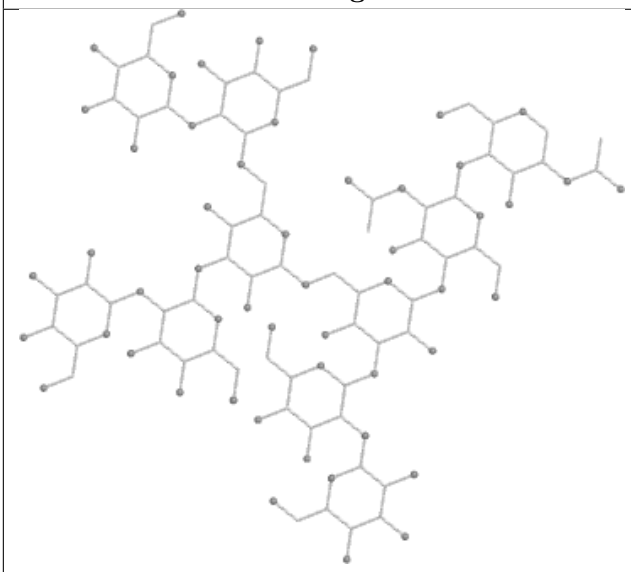


Bond angles



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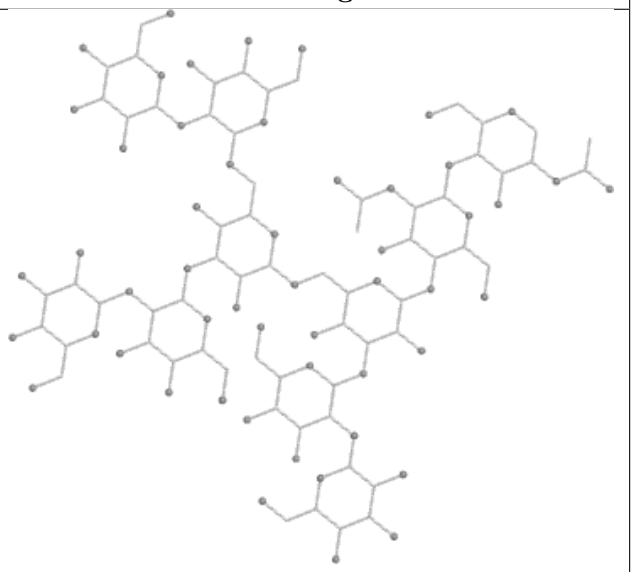
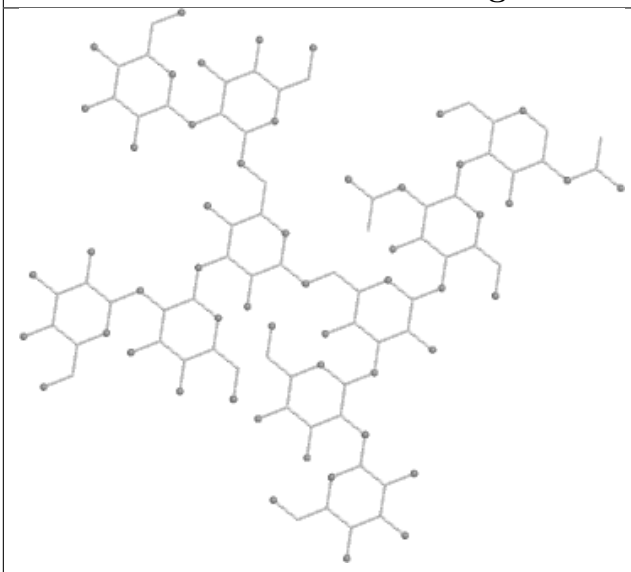
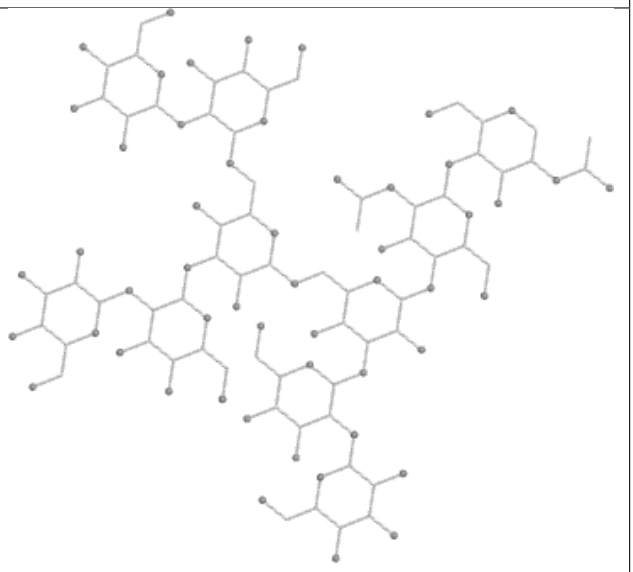


Rings

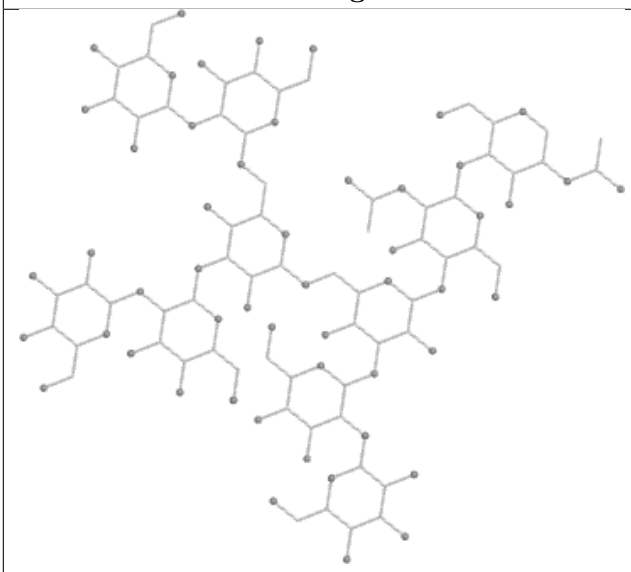
Oligosaccharide Chain fO



Bond lengths



Bond angles



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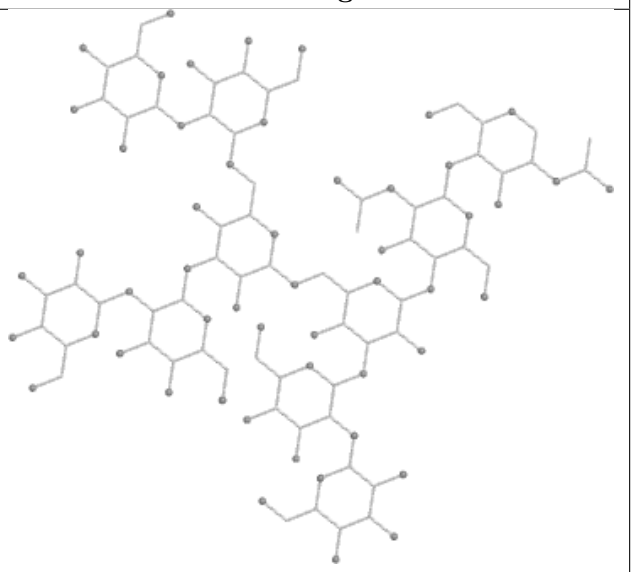
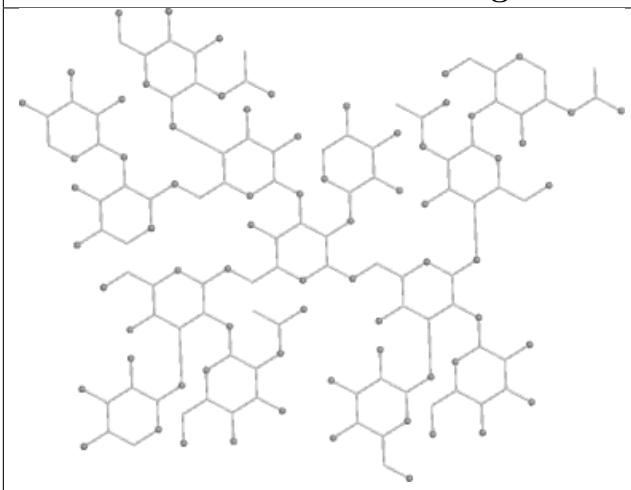


Rings

Oligosaccharide Chain fF



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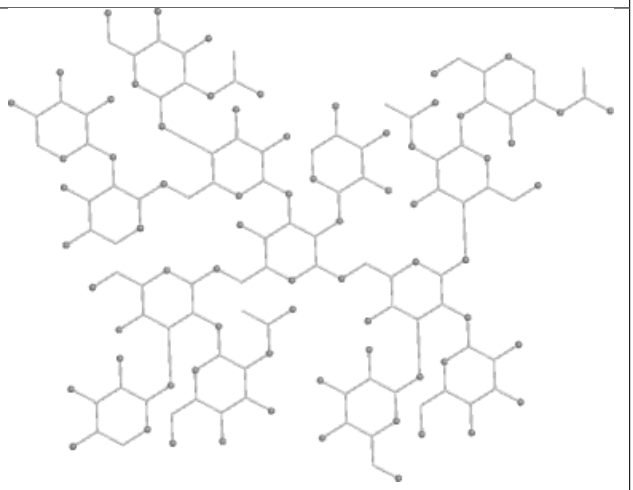
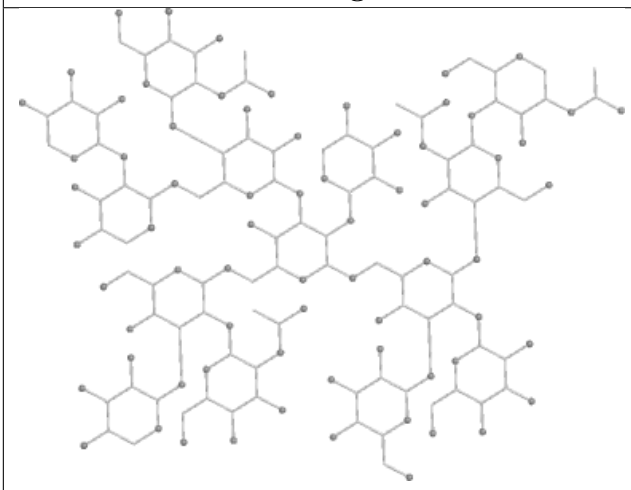


Bond angles



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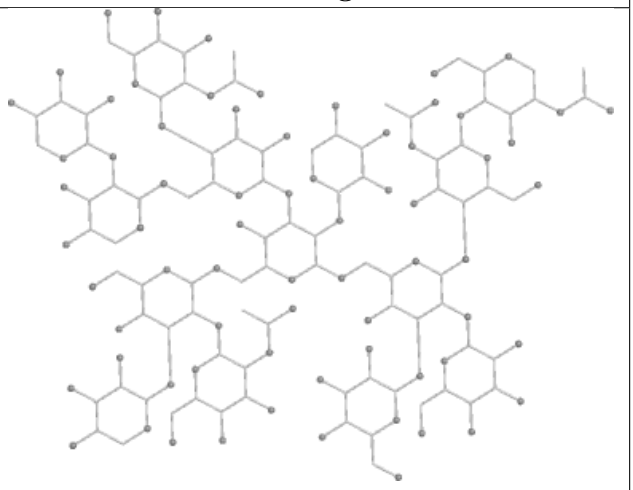
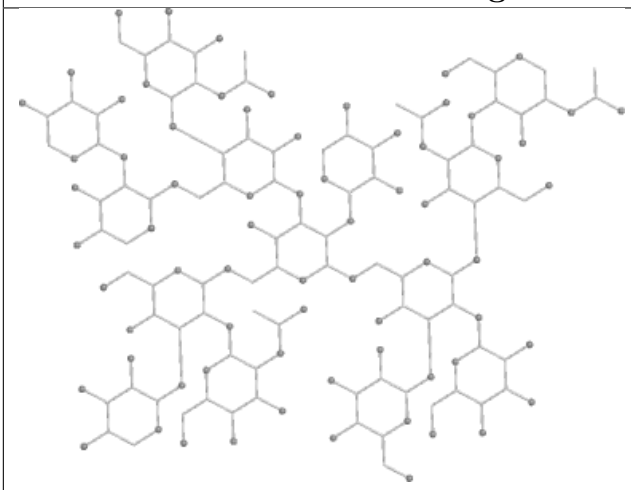
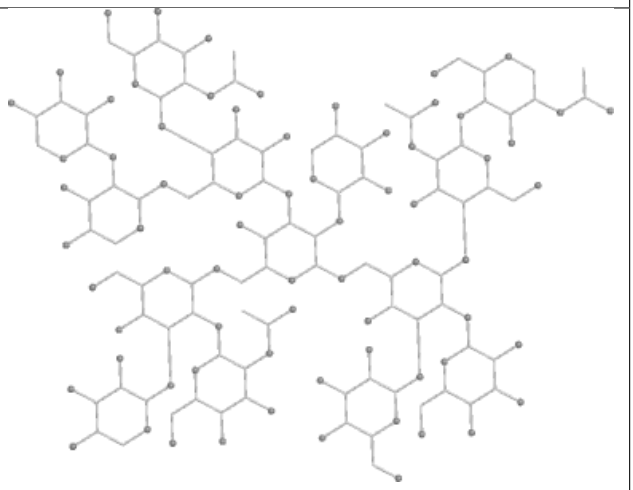


Rings

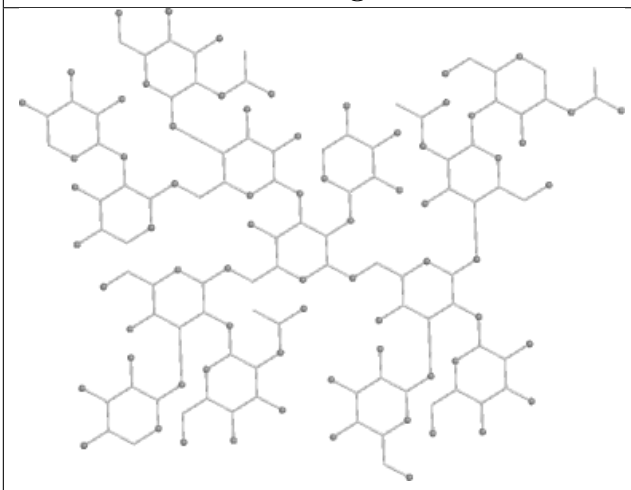
Oligosaccharide Chain fK



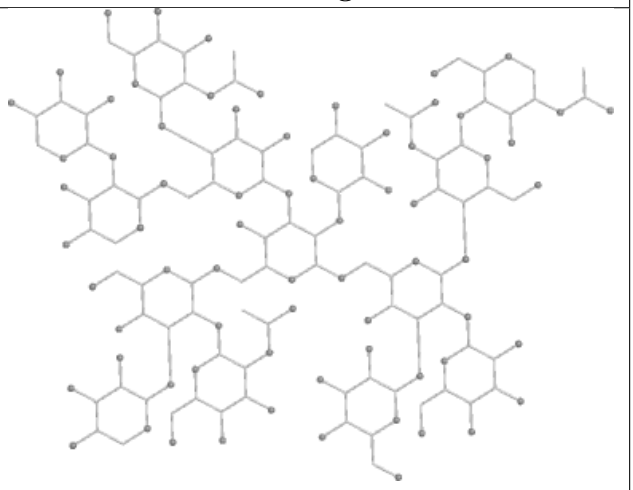
Bond lengths



Bond angles

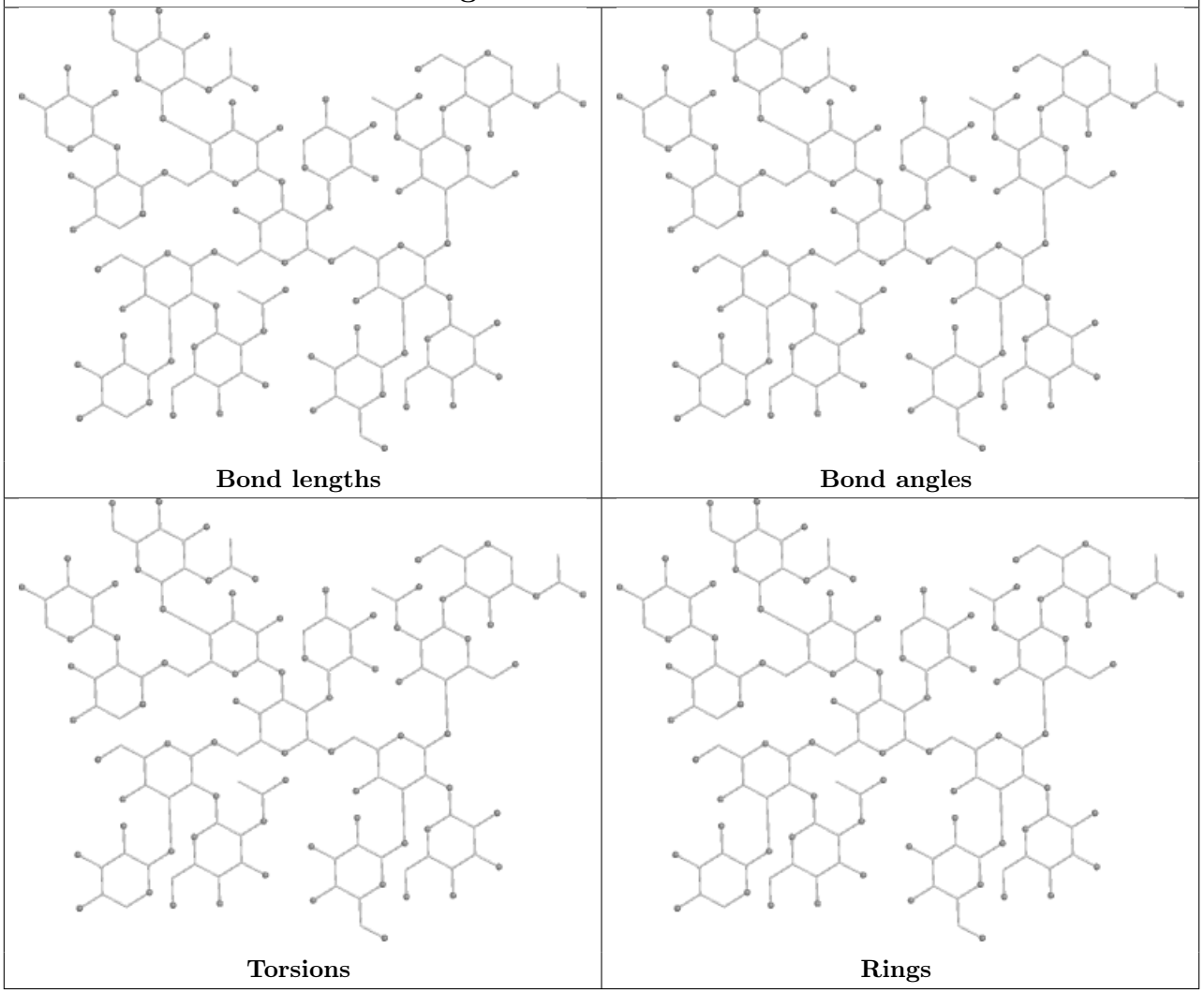


Torsions



Rings

Oligosaccharide Chain fP



5.6 Ligand geometry (i)

Of 85 ligands modelled in this entry, 58 are monoatomic - leaving 27 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	2PO	EC	402	-	0,3,3	-	-	0,3,3	-	-
23	2PO	AA	801	7	0,3,3	-	-	0,3,3	-	-
23	2PO	BA	401	21,11	0,3,3	-	-	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	2PO	BB	401	21	0,3,3	-	-	0,3,3	-	-
23	2PO	AB	801	7	0,3,3	-	-	0,3,3	-	-
23	2PO	AC	803	9	0,3,3	-	-	0,3,3	-	-
23	2PO	AA	803	9	0,3,3	-	-	0,3,3	-	-
22	NAG	FA	801	2	14,14,15	0.37	0	17,19,21	0.63	0
23	2PO	EB	402	18	0,3,3	-	-	0,3,3	-	-
23	2PO	AA	802	-	0,3,3	-	-	0,3,3	-	-
23	2PO	EA	403	-	0,3,3	-	-	0,3,3	-	-
23	2PO	BA	402	14	0,3,3	-	-	0,3,3	-	-
22	NAG	EA	402	1	14,14,15	0.39	0	17,19,21	1.04	1 (5%)
23	2PO	BB	402	14	0,3,3	-	-	0,3,3	-	-
23	2PO	BC	402	14	0,3,3	-	-	0,3,3	-	-
23	2PO	FA	802	-	0,3,3	-	-	0,3,3	-	-
22	NAG	EC	401	1	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
23	2PO	AC	801	7	0,3,3	-	-	0,3,3	-	-
23	2PO	AB	802	-	0,3,3	-	-	0,3,3	-	-
23	2PO	AC	802	8	0,3,3	-	-	0,3,3	-	-
22	NAG	FC	801	2	14,14,15	0.35	0	17,19,21	0.64	0
23	2PO	FC	802	20	0,3,3	-	-	0,3,3	-	-
22	NAG	FB	801	2	14,14,15	0.34	0	17,19,21	0.81	0
23	2PO	BC	401	21	0,3,3	-	-	0,3,3	-	-
23	2PO	FB	802	20	0,3,3	-	-	0,3,3	-	-
23	2PO	AB	803	-	0,3,3	-	-	0,3,3	-	-
22	NAG	EB	401	1	14,14,15	0.34	0	17,19,21	1.03	1 (5%)

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
22	NAG	FB	801	2	-	0/6/23/26	0/1/1/1
22	NAG	FA	801	2	-	0/6/23/26	0/1/1/1
22	NAG	EC	401	1	-	0/6/23/26	0/1/1/1
22	NAG	EB	401	1	-	0/6/23/26	0/1/1/1
22	NAG	FC	801	2	-	0/6/23/26	0/1/1/1
22	NAG	EA	402	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	EA	402	NAG	C1-O5-C5	3.44	116.85	112.19
22	EB	401	NAG	C1-O5-C5	2.96	116.20	112.19
22	EC	401	NAG	C1-O5-C5	2.72	115.88	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	EA	402	NAG	C4-C5-C6-O6

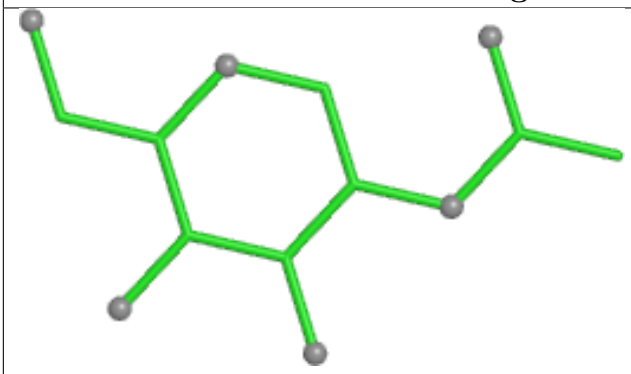
There are no ring outliers.

3 monomers are involved in 3 short contacts:

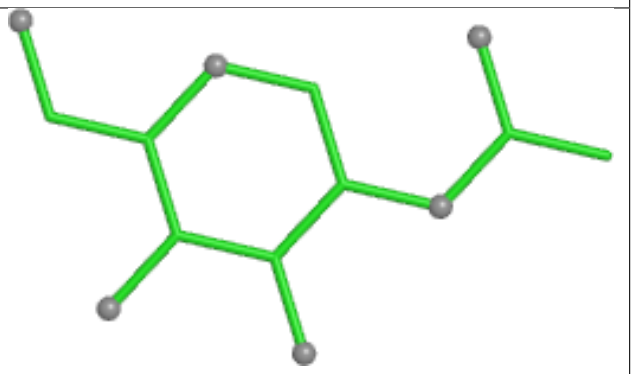
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	EA	402	NAG	1	0
22	EC	401	NAG	1	0
22	EB	401	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

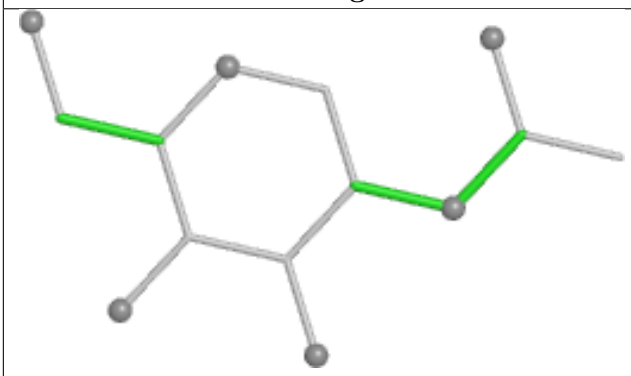
Ligand NAG FA 801



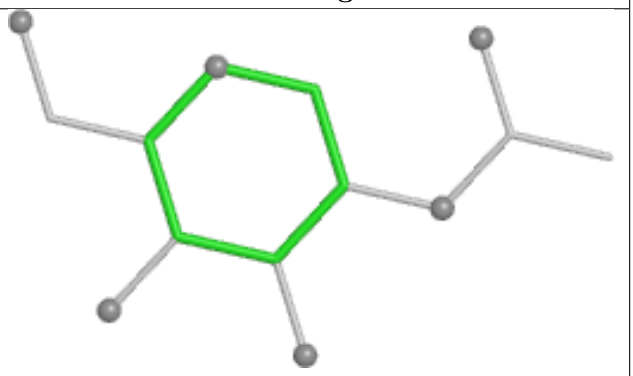
Bond lengths



Bond angles

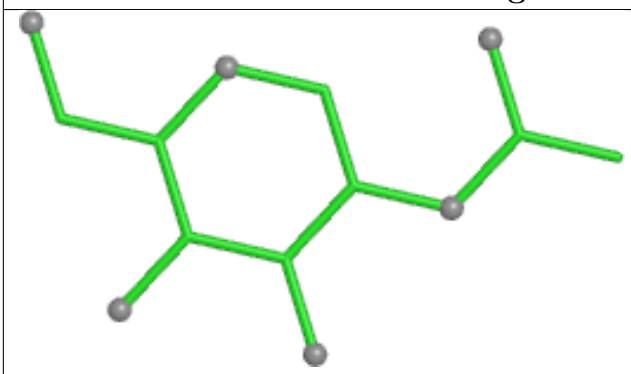


Torsions

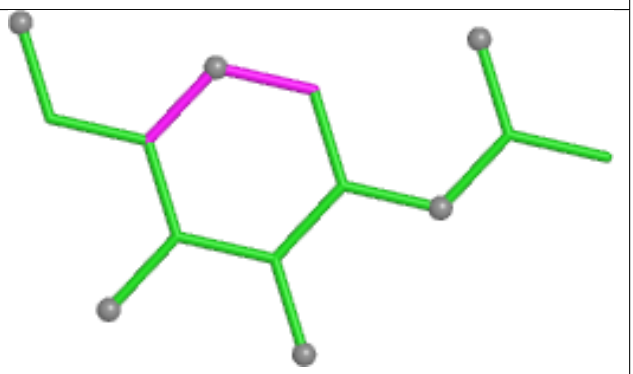


Rings

Ligand NAG EA 402



Bond lengths



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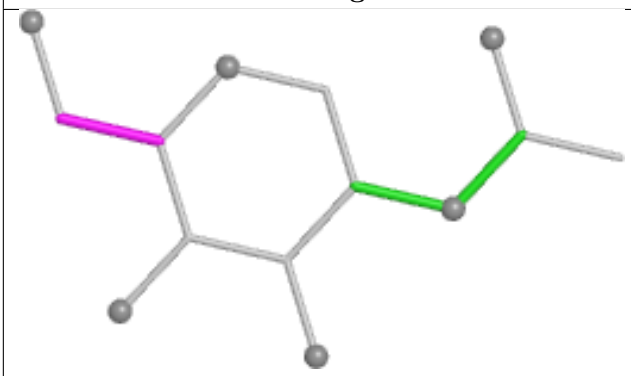
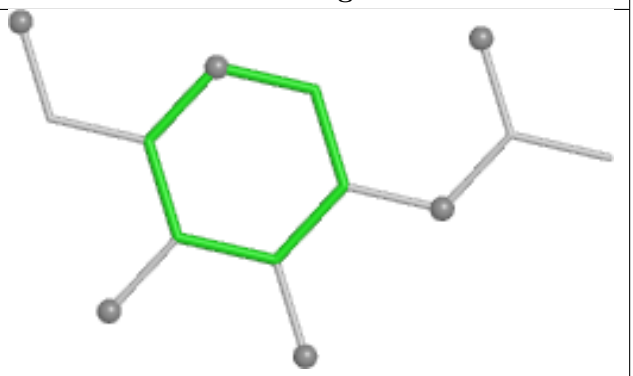


Torsions



Rings

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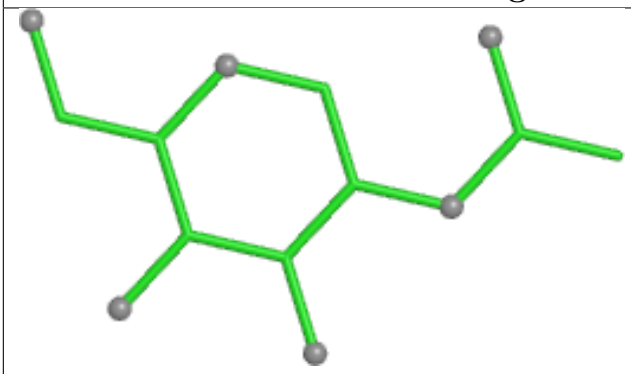

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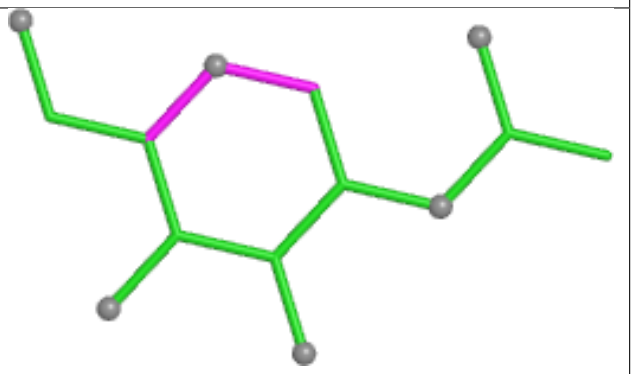

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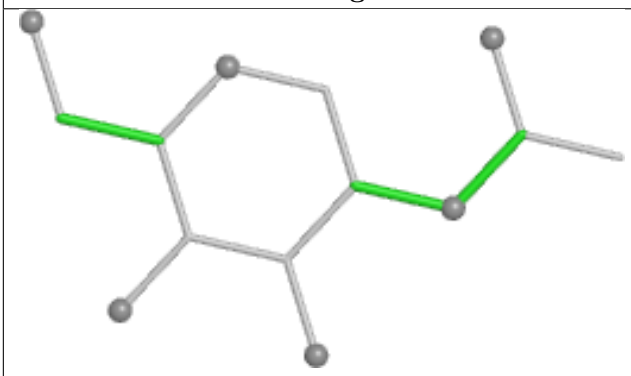

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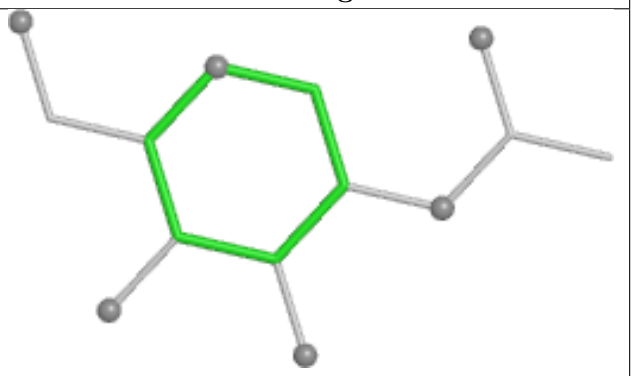
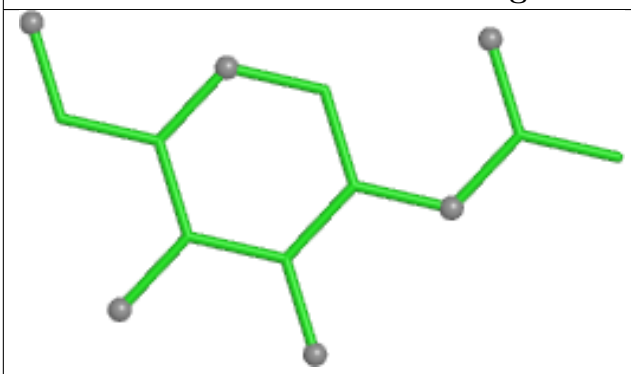


Rings

Ligand NAG FC 801



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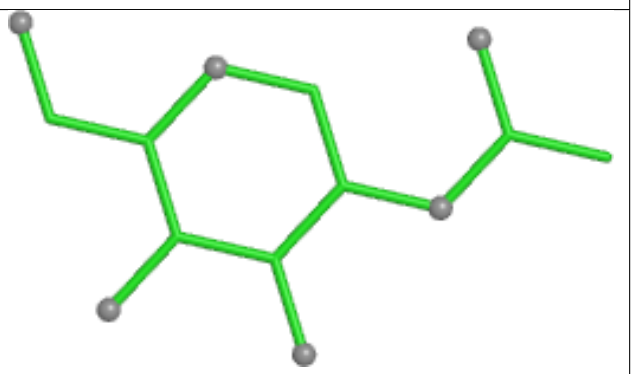

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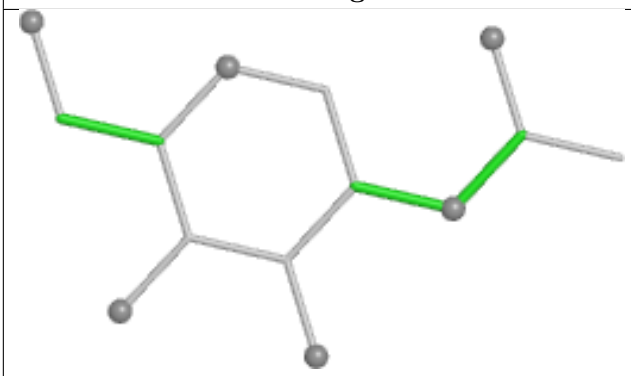

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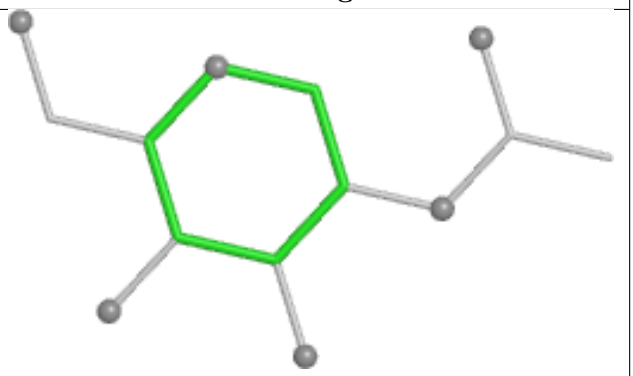
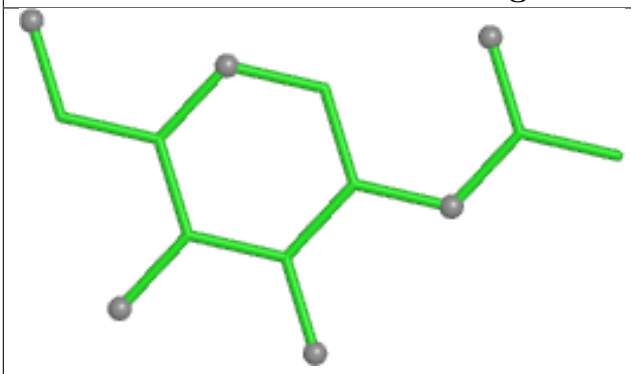
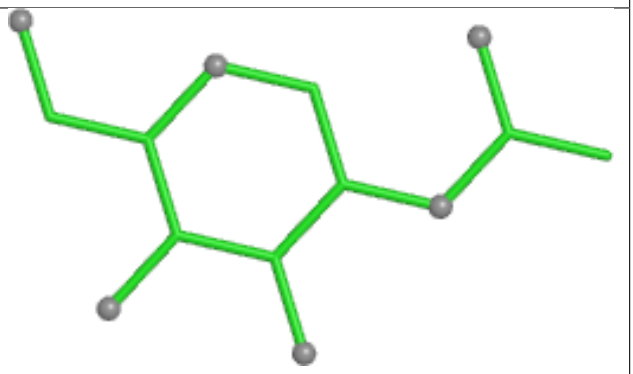


Rings

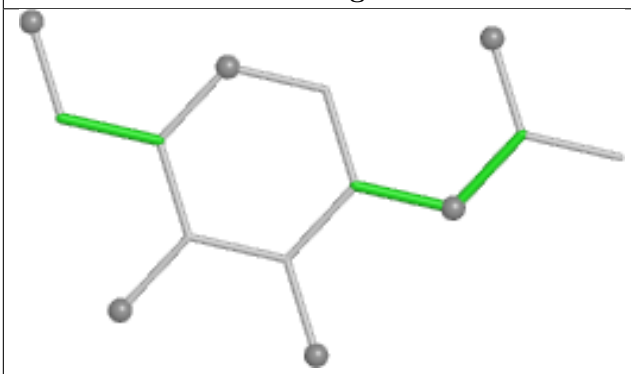
Ligand NAG FB 801



Bond lengths



Bond angles



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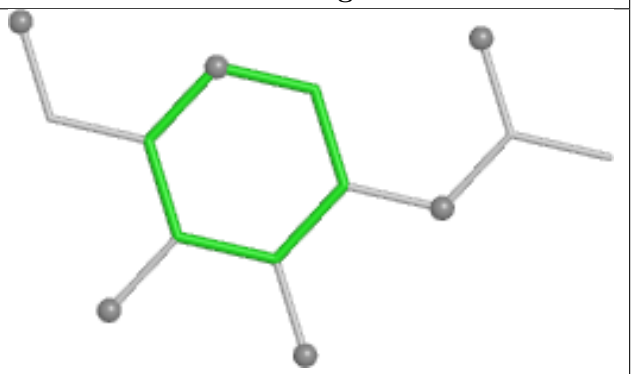
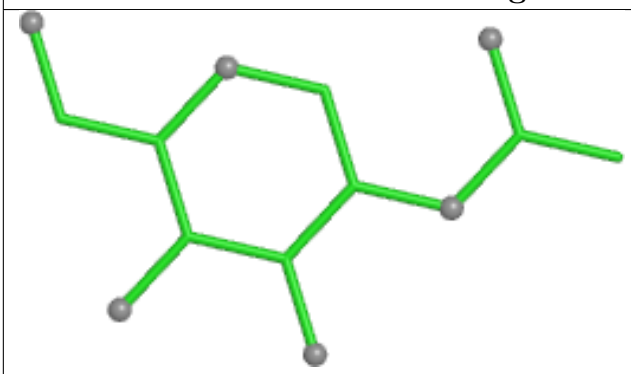
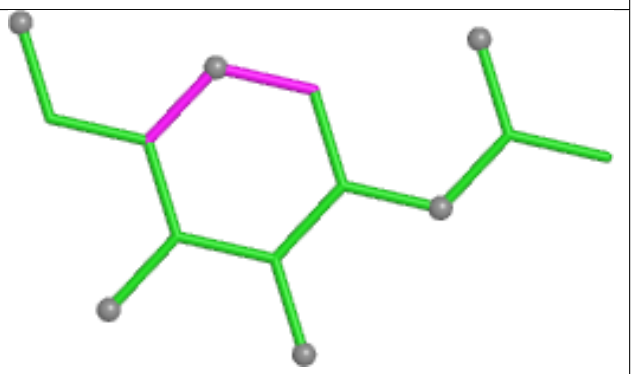


Rings

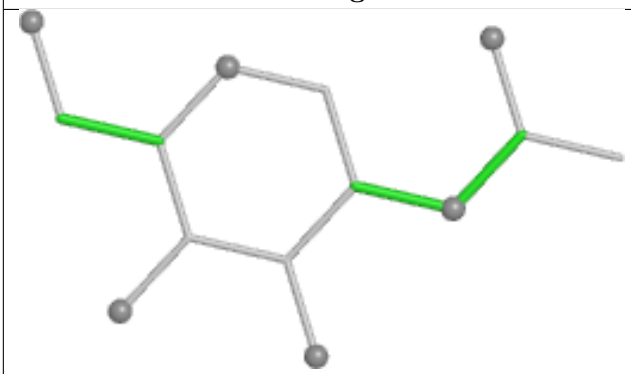
Ligand NAG EB 401



Bond lengths



Bond angles



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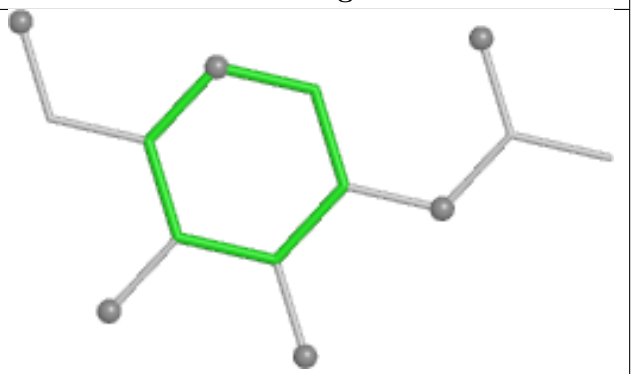

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.