Full wwPDB EM Validation Report ⓘ

Nov 1, 2022 – 11:42 PM EDT

PDB ID	:	5SZS
EMDB ID	:	EMD-8331
Title	:	Glycan shield and epitope masking of a coronavirus spike protein observed by cryo-electron microscopy
Authors	:	Walls, A.C.; Tortorici, M.A.; Frenz, B.; Snijder, J.; Li, W.; Rey, F.A.; DiMaio, F.; Bosch, B.J.; Veesler, D.
Deposited on	:	2016-08-15
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

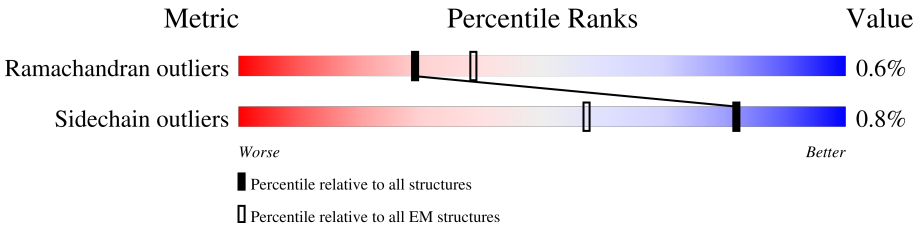
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.40 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1325	5% 86% · 11%
1	B	1325	5% 86% · 11%
1	C	1325	5% 86% · 11%
2	D	6	17% 100%
2	Y	6	17% 100%
2	t	6	17% 100%
3	2	2	50% 100%
3	5	2	100% 100%
3	6	2	50% 100%

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Mol	Chain	Length	Quality of chain
3	7	2	50% 100%
3	8	2	50% 100%
3	9	2	100% 100%
3	CA	2	100%
3	E	2	50% 100%
3	G	2	50% 100%
3	I	2	100% 100%
3	J	2	50% 100%
3	M	2	100% 100%
3	P	2	100% 100%
3	Q	2	50% 100%
3	R	2	50% 100%
3	S	2	50% 100%
3	T	2	100% 100%
3	W	2	100%
3	Z	2	100%
3	b	2	50% 100%
3	d	2	100% 100%
3	e	2	50% 100%
3	h	2	50% 100%
3	k	2	100% 100%
3	l	2	50% 100%
3	m	2	50% 100%
3	n	2	50% 100%
3	o	2	100% 100%

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Mol	Chain	Length	Quality of chain
3	r	2	100%
3	u	2	50% 100%
3	w	2	50% 100%
3	y	2	100% 100%
3	z	2	50% 100%
4	AA	4	75% 100%
4	F	4	50% 100%
4	U	4	75% 100%
4	a	4	50% 100%
4	p	4	75% 100%
4	v	4	50% 100%
5	H	4	50% 100%
5	c	4	50% 100%
5	x	4	50% 100%
6	0	8	38% 100%
6	K	8	38% 100%
6	f	8	38% 100%
7	1	3	67% 100%
7	4	3	67% 100%
7	DA	3	67% 100%
7	L	3	67% 100%
7	O	3	67% 100%
7	X	3	67% 100%
7	g	3	67% 100%
7	j	3	67% 100%

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Mol	Chain	Length	Quality of chain
7	s	3	67% 100%
8	3	5	80% 100%
8	BA	5	80% 100%
8	N	5	80% 100%
8	V	5	80% 100%
8	i	5	80% 100%
8	q	5	80% 100%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 30306 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1177	Total	C	N	O	S	0	0
			9141	5821	1532	1745	43		
1	B	1177	Total	C	N	O	S	0	0
			9141	5821	1532	1745	43		
1	C	1177	Total	C	N	O	S	0	0
			9141	5821	1532	1745	43		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1292	LEU	-	expression tag	UNP Q6Q1S2
A	1293	ILE	-	expression tag	UNP Q6Q1S2
A	1294	LYS	-	expression tag	UNP Q6Q1S2
A	1295	ARG	-	expression tag	UNP Q6Q1S2
A	1296	MET	-	expression tag	UNP Q6Q1S2
A	1297	LYS	-	expression tag	UNP Q6Q1S2
A	1298	GLN	-	expression tag	UNP Q6Q1S2
A	1299	ILE	-	expression tag	UNP Q6Q1S2
A	1300	GLU	-	expression tag	UNP Q6Q1S2
A	1301	ASP	-	expression tag	UNP Q6Q1S2
A	1302	LYS	-	expression tag	UNP Q6Q1S2
A	1303	ILE	-	expression tag	UNP Q6Q1S2
A	1304	GLU	-	expression tag	UNP Q6Q1S2
A	1305	GLU	-	expression tag	UNP Q6Q1S2
A	1306	ILE	-	expression tag	UNP Q6Q1S2
A	1307	GLU	-	expression tag	UNP Q6Q1S2
A	1308	SER	-	expression tag	UNP Q6Q1S2
A	1309	LYS	-	expression tag	UNP Q6Q1S2
A	1310	GLN	-	expression tag	UNP Q6Q1S2
A	1311	LYS	-	expression tag	UNP Q6Q1S2
A	1312	LYS	-	expression tag	UNP Q6Q1S2
A	1313	ILE	-	expression tag	UNP Q6Q1S2
A	1314	GLU	-	expression tag	UNP Q6Q1S2
A	1315	ASN	-	expression tag	UNP Q6Q1S2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1316	GLU	-	expression tag	UNP Q6Q1S2
A	1317	ILE	-	expression tag	UNP Q6Q1S2
A	1318	ALA	-	expression tag	UNP Q6Q1S2
A	1319	ARG	-	expression tag	UNP Q6Q1S2
A	1320	ILE	-	expression tag	UNP Q6Q1S2
A	1321	LYS	-	expression tag	UNP Q6Q1S2
A	1322	LYS	-	expression tag	UNP Q6Q1S2
A	1323	ILE	-	expression tag	UNP Q6Q1S2
A	1324	LYS	-	expression tag	UNP Q6Q1S2
A	1325	LEU	-	expression tag	UNP Q6Q1S2
A	1326	VAL	-	expression tag	UNP Q6Q1S2
A	1327	PRO	-	expression tag	UNP Q6Q1S2
A	1328	ARG	-	expression tag	UNP Q6Q1S2
A	1329	GLY	-	expression tag	UNP Q6Q1S2
A	1330	SER	-	expression tag	UNP Q6Q1S2
A	1331	LEU	-	expression tag	UNP Q6Q1S2
A	1332	GLU	-	expression tag	UNP Q6Q1S2
A	1333	TRP	-	expression tag	UNP Q6Q1S2
A	1334	SER	-	expression tag	UNP Q6Q1S2
A	1335	HIS	-	expression tag	UNP Q6Q1S2
A	1336	PRO	-	expression tag	UNP Q6Q1S2
A	1337	GLN	-	expression tag	UNP Q6Q1S2
A	1338	PHE	-	expression tag	UNP Q6Q1S2
A	1339	GLU	-	expression tag	UNP Q6Q1S2
A	1340	LYS	-	expression tag	UNP Q6Q1S2
B	1292	LEU	-	expression tag	UNP Q6Q1S2
B	1293	ILE	-	expression tag	UNP Q6Q1S2
B	1294	LYS	-	expression tag	UNP Q6Q1S2
B	1295	ARG	-	expression tag	UNP Q6Q1S2
B	1296	MET	-	expression tag	UNP Q6Q1S2
B	1297	LYS	-	expression tag	UNP Q6Q1S2
B	1298	GLN	-	expression tag	UNP Q6Q1S2
B	1299	ILE	-	expression tag	UNP Q6Q1S2
B	1300	GLU	-	expression tag	UNP Q6Q1S2
B	1301	ASP	-	expression tag	UNP Q6Q1S2
B	1302	LYS	-	expression tag	UNP Q6Q1S2
B	1303	ILE	-	expression tag	UNP Q6Q1S2
B	1304	GLU	-	expression tag	UNP Q6Q1S2
B	1305	GLU	-	expression tag	UNP Q6Q1S2
B	1306	ILE	-	expression tag	UNP Q6Q1S2
B	1307	GLU	-	expression tag	UNP Q6Q1S2
B	1308	SER	-	expression tag	UNP Q6Q1S2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1309	LYS	-	expression tag	UNP Q6Q1S2
B	1310	GLN	-	expression tag	UNP Q6Q1S2
B	1311	LYS	-	expression tag	UNP Q6Q1S2
B	1312	LYS	-	expression tag	UNP Q6Q1S2
B	1313	ILE	-	expression tag	UNP Q6Q1S2
B	1314	GLU	-	expression tag	UNP Q6Q1S2
B	1315	ASN	-	expression tag	UNP Q6Q1S2
B	1316	GLU	-	expression tag	UNP Q6Q1S2
B	1317	ILE	-	expression tag	UNP Q6Q1S2
B	1318	ALA	-	expression tag	UNP Q6Q1S2
B	1319	ARG	-	expression tag	UNP Q6Q1S2
B	1320	ILE	-	expression tag	UNP Q6Q1S2
B	1321	LYS	-	expression tag	UNP Q6Q1S2
B	1322	LYS	-	expression tag	UNP Q6Q1S2
B	1323	ILE	-	expression tag	UNP Q6Q1S2
B	1324	LYS	-	expression tag	UNP Q6Q1S2
B	1325	LEU	-	expression tag	UNP Q6Q1S2
B	1326	VAL	-	expression tag	UNP Q6Q1S2
B	1327	PRO	-	expression tag	UNP Q6Q1S2
B	1328	ARG	-	expression tag	UNP Q6Q1S2
B	1329	GLY	-	expression tag	UNP Q6Q1S2
B	1330	SER	-	expression tag	UNP Q6Q1S2
B	1331	LEU	-	expression tag	UNP Q6Q1S2
B	1332	GLU	-	expression tag	UNP Q6Q1S2
B	1333	TRP	-	expression tag	UNP Q6Q1S2
B	1334	SER	-	expression tag	UNP Q6Q1S2
B	1335	HIS	-	expression tag	UNP Q6Q1S2
B	1336	PRO	-	expression tag	UNP Q6Q1S2
B	1337	GLN	-	expression tag	UNP Q6Q1S2
B	1338	PHE	-	expression tag	UNP Q6Q1S2
B	1339	GLU	-	expression tag	UNP Q6Q1S2
B	1340	LYS	-	expression tag	UNP Q6Q1S2
C	1292	LEU	-	expression tag	UNP Q6Q1S2
C	1293	ILE	-	expression tag	UNP Q6Q1S2
C	1294	LYS	-	expression tag	UNP Q6Q1S2
C	1295	ARG	-	expression tag	UNP Q6Q1S2
C	1296	MET	-	expression tag	UNP Q6Q1S2
C	1297	LYS	-	expression tag	UNP Q6Q1S2
C	1298	GLN	-	expression tag	UNP Q6Q1S2
C	1299	ILE	-	expression tag	UNP Q6Q1S2
C	1300	GLU	-	expression tag	UNP Q6Q1S2
C	1301	ASP	-	expression tag	UNP Q6Q1S2

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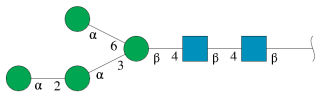
Chain	Residue	Modelled	Actual	Comment	Reference
C	1302	LYS	-	expression tag	UNP Q6Q1S2
C	1303	ILE	-	expression tag	UNP Q6Q1S2
C	1304	GLU	-	expression tag	UNP Q6Q1S2
C	1305	GLU	-	expression tag	UNP Q6Q1S2
C	1306	ILE	-	expression tag	UNP Q6Q1S2
C	1307	GLU	-	expression tag	UNP Q6Q1S2
C	1308	SER	-	expression tag	UNP Q6Q1S2
C	1309	LYS	-	expression tag	UNP Q6Q1S2
C	1310	GLN	-	expression tag	UNP Q6Q1S2
C	1311	LYS	-	expression tag	UNP Q6Q1S2
C	1312	LYS	-	expression tag	UNP Q6Q1S2
C	1313	ILE	-	expression tag	UNP Q6Q1S2
C	1314	GLU	-	expression tag	UNP Q6Q1S2
C	1315	ASN	-	expression tag	UNP Q6Q1S2
C	1316	GLU	-	expression tag	UNP Q6Q1S2
C	1317	ILE	-	expression tag	UNP Q6Q1S2
C	1318	ALA	-	expression tag	UNP Q6Q1S2
C	1319	ARG	-	expression tag	UNP Q6Q1S2
C	1320	ILE	-	expression tag	UNP Q6Q1S2
C	1321	LYS	-	expression tag	UNP Q6Q1S2
C	1322	LYS	-	expression tag	UNP Q6Q1S2
C	1323	ILE	-	expression tag	UNP Q6Q1S2
C	1324	LYS	-	expression tag	UNP Q6Q1S2
C	1325	LEU	-	expression tag	UNP Q6Q1S2
C	1326	VAL	-	expression tag	UNP Q6Q1S2
C	1327	PRO	-	expression tag	UNP Q6Q1S2
C	1328	ARG	-	expression tag	UNP Q6Q1S2
C	1329	GLY	-	expression tag	UNP Q6Q1S2
C	1330	SER	-	expression tag	UNP Q6Q1S2
C	1331	LEU	-	expression tag	UNP Q6Q1S2
C	1332	GLU	-	expression tag	UNP Q6Q1S2
C	1333	TRP	-	expression tag	UNP Q6Q1S2
C	1334	SER	-	expression tag	UNP Q6Q1S2
C	1335	HIS	-	expression tag	UNP Q6Q1S2
C	1336	PRO	-	expression tag	UNP Q6Q1S2
C	1337	GLN	-	expression tag	UNP Q6Q1S2
C	1338	PHE	-	expression tag	UNP Q6Q1S2
C	1339	GLU	-	expression tag	UNP Q6Q1S2
C	1340	LYS	-	expression tag	UNP Q6Q1S2

- Molecule 2 is an oligosaccharide called 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
2	D	6	Total	C	N	O	0	0
			72	40	2	30		
2	Y	6	Total	C	N	O	0	0
			72	40	2	30		
2	t	6	Total	C	N	O	0	0
			72	40	2	30		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	b	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	2	Total	C	N	O	0	0
			28	16	2	10		
3	e	2	Total	C	N	O	0	0
			28	16	2	10		
3	h	2	Total	C	N	O	0	0
			28	16	2	10		
3	k	2	Total	C	N	O	0	0
			28	16	2	10		
3	l	2	Total	C	N	O	0	0
			28	16	2	10		
3	m	2	Total	C	N	O	0	0
			28	16	2	10		
3	n	2	Total	C	N	O	0	0
			28	16	2	10		
3	o	2	Total	C	N	O	0	0
			28	16	2	10		
3	r	2	Total	C	N	O	0	0
			28	16	2	10		
3	u	2	Total	C	N	O	0	0
			28	16	2	10		
3	w	2	Total	C	N	O	0	0
			28	16	2	10		
3	y	2	Total	C	N	O	0	0
			28	16	2	10		
3	z	2	Total	C	N	O	0	0
			28	16	2	10		
3	2	2	Total	C	N	O	0	0
			28	16	2	10		
3	5	2	Total	C	N	O	0	0
			28	16	2	10		
3	6	2	Total	C	N	O	0	0
			28	16	2	10		
3	7	2	Total	C	N	O	0	0
			28	16	2	10		
3	8	2	Total	C	N	O	0	0
			28	16	2	10		
3	9	2	Total	C	N	O	0	0
			28	16	2	10		
3	CA	2	Total	C	N	O	0	0
			28	16	2	10		

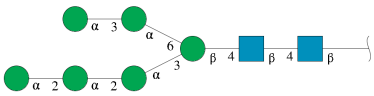
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	4	Total	C	N	O	0	0
			50	28	2	20		
4	U	4	Total	C	N	O	0	0
			50	28	2	20		
4	a	4	Total	C	N	O	0	0
			50	28	2	20		
4	p	4	Total	C	N	O	0	0
			50	28	2	20		
4	v	4	Total	C	N	O	0	0
			50	28	2	20		
4	AA	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is an oligosaccharide called 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.

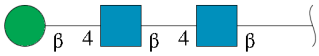
Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	4	Total	C	N	O	0	0
			50	28	2	20		
5	c	4	Total	C	N	O	0	0
			50	28	2	20		
5	x	4	Total	C	N	O	0	0
			50	28	2	20		

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



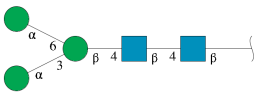
Mol	Chain	Residues	Atoms	AltConf	Trace
6	K	8	Total C N O 94 52 2 40	0	0
6	f	8	Total C N O 94 52 2 40	0	0
6	0	8	Total C N O 94 52 2 40	0	0

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



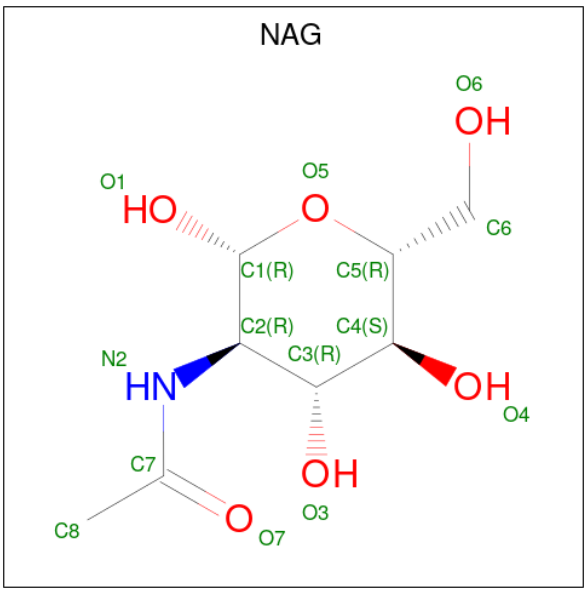
Mol	Chain	Residues	Atoms	AltConf	Trace
7	L	3	Total C N O 39 22 2 15	0	0
7	O	3	Total C N O 39 22 2 15	0	0
7	X	3	Total C N O 39 22 2 15	0	0
7	g	3	Total C N O 39 22 2 15	0	0
7	j	3	Total C N O 39 22 2 15	0	0
7	s	3	Total C N O 39 22 2 15	0	0
7	1	3	Total C N O 39 22 2 15	0	0
7	4	3	Total C N O 39 22 2 15	0	0
7	DA	3	Total C N O 39 22 2 15	0	0

- Molecule 8 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
8	N	5	Total C N O 61 34 2 25	0	0
8	V	5	Total C N O 61 34 2 25	0	0
8	i	5	Total C N O 61 34 2 25	0	0
8	q	5	Total C N O 61 34 2 25	0	0
8	3	5	Total C N O 61 34 2 25	0	0
8	BA	5	Total C N O 61 34 2 25	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C N O 98 56 7 35	0
9	A	1	Total C N O 98 56 7 35	0
9	A	1	Total C N O 98 56 7 35	0

Continued on next page...

Continued from previous page...

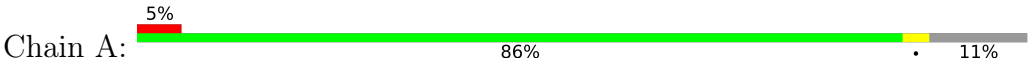
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			98	56	7	35	
9	A	1	Total	C	N	O	0
			98	56	7	35	
9	A	1	Total	C	N	O	0
			98	56	7	35	
9	A	1	Total	C	N	O	0
			98	56	7	35	
9	B	1	Total	C	N	O	0
			98	56	7	35	
9	B	1	Total	C	N	O	0
			98	56	7	35	
9	B	1	Total	C	N	O	0
			98	56	7	35	
9	B	1	Total	C	N	O	0
			98	56	7	35	
9	B	1	Total	C	N	O	0
			98	56	7	35	
9	B	1	Total	C	N	O	0
			98	56	7	35	
9	B	1	Total	C	N	O	0
			98	56	7	35	
9	C	1	Total	C	N	O	0
			98	56	7	35	
9	C	1	Total	C	N	O	0
			98	56	7	35	
9	C	1	Total	C	N	O	0
			98	56	7	35	
9	C	1	Total	C	N	O	0
			98	56	7	35	
9	C	1	Total	C	N	O	0
			98	56	7	35	
9	C	1	Total	C	N	O	0
			98	56	7	35	
9	C	1	Total	C	N	O	0
			98	56	7	35	

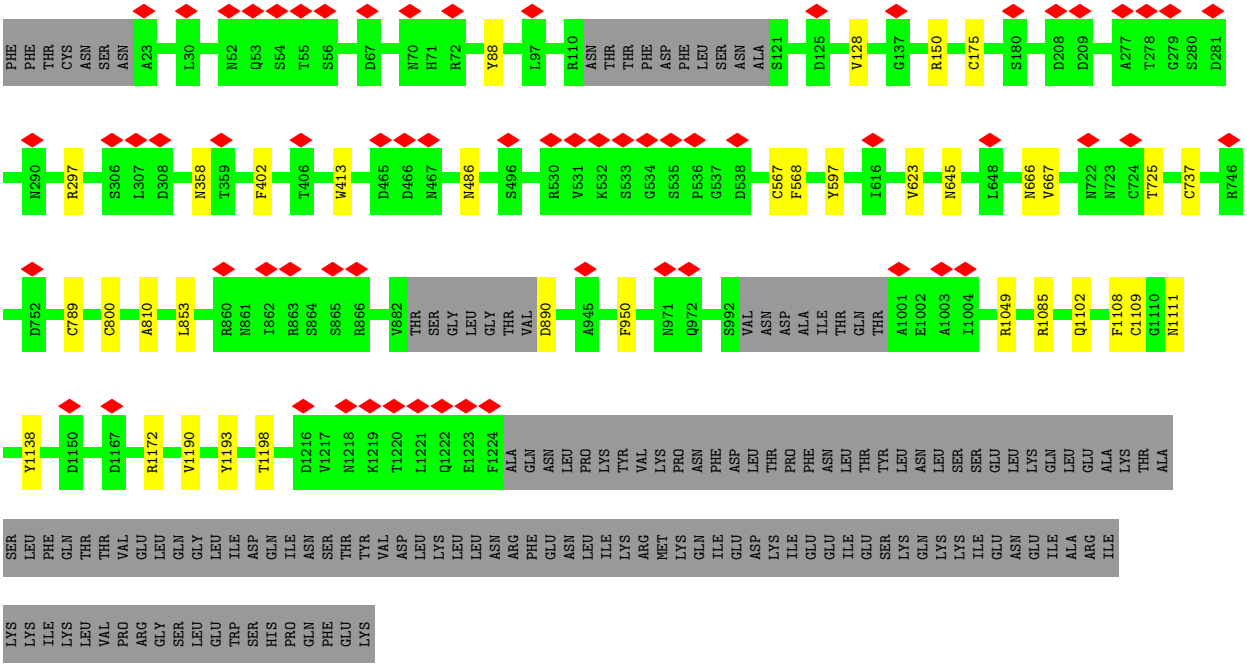
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Spike glycoprotein

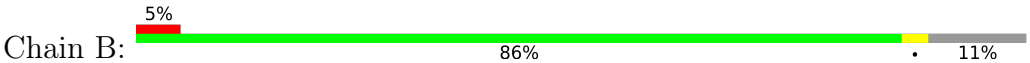
Chain A:

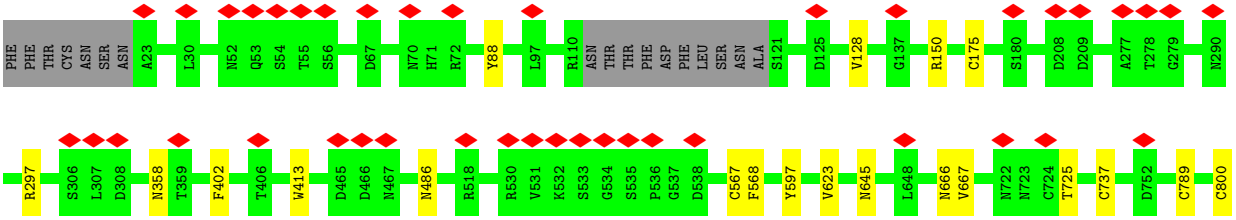


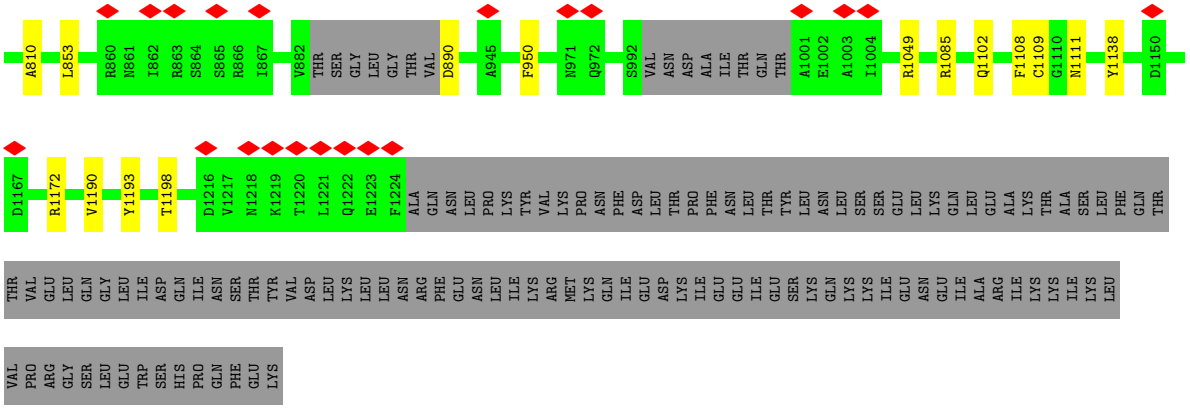


• Molecule 1: Spike glycoprotein

Chain B:

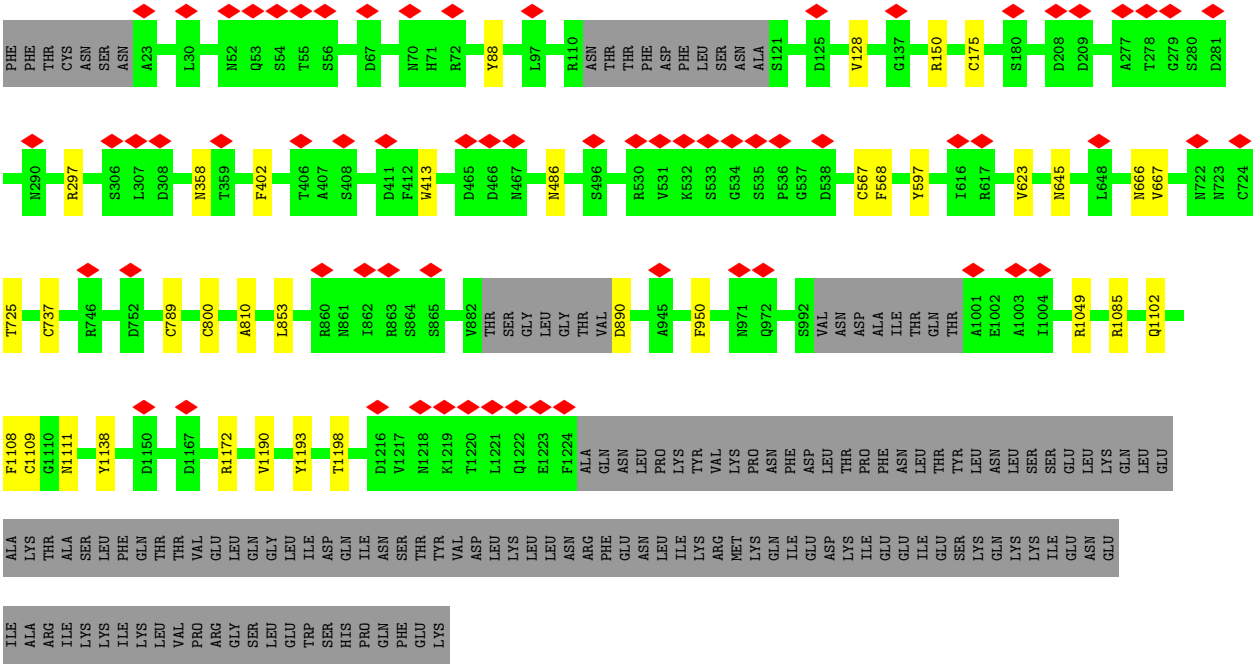






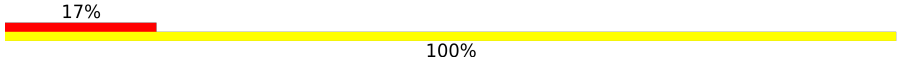
• Molecule 1: Spike glycoprotein

Chain C:



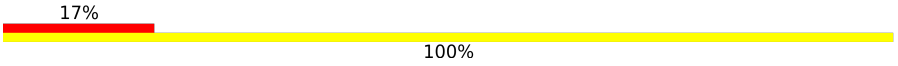
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



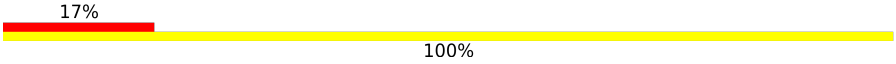
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



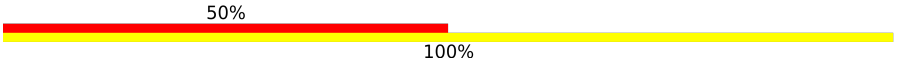
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:



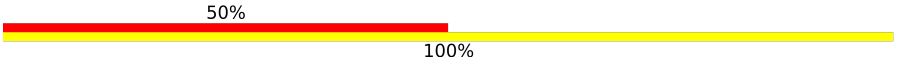
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



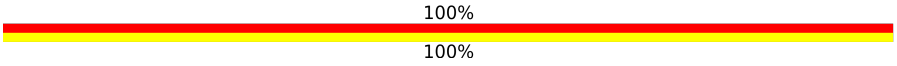
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



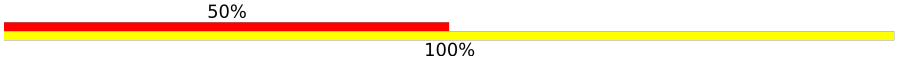
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



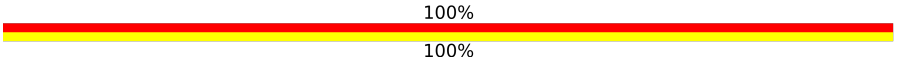
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



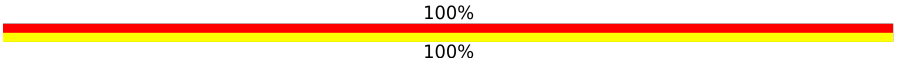
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



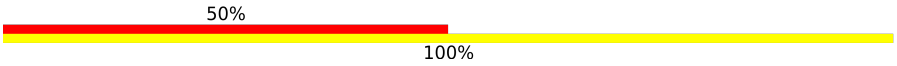
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



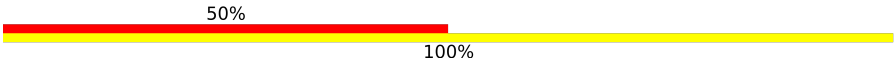
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



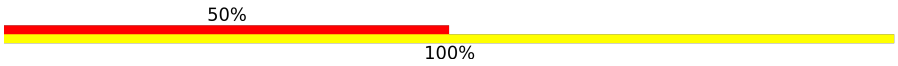
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



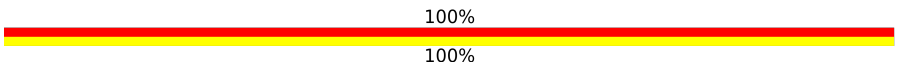
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



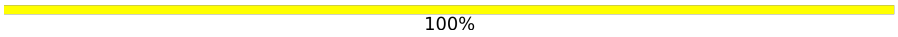
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



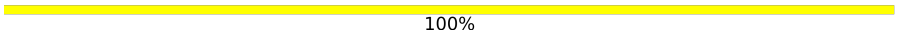
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



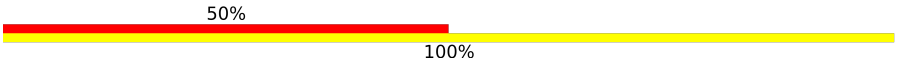
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



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

Chain b:

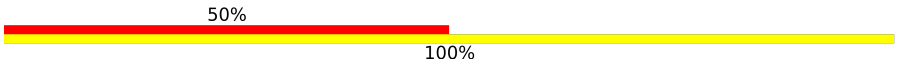


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

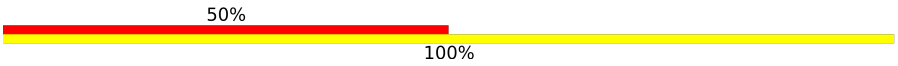
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



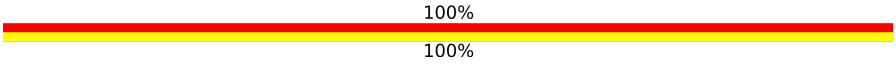
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



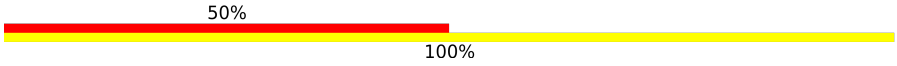
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



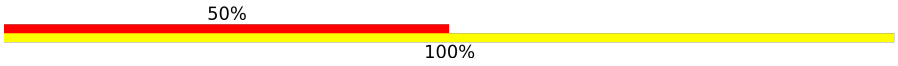
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



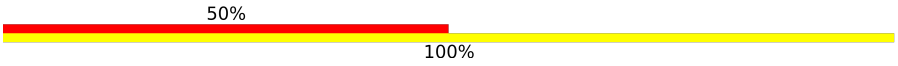
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



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

Chain n:

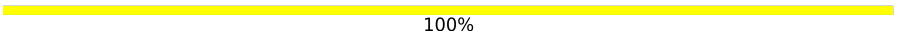


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:

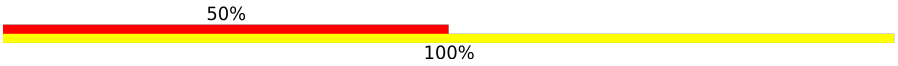
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



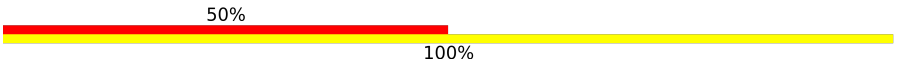
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



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

Chain w:



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

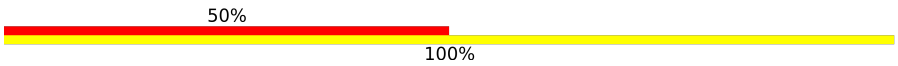
Chain y:

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

Chain z:

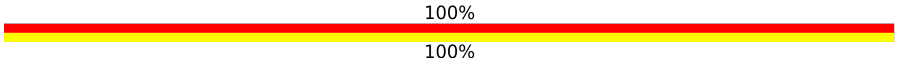
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:



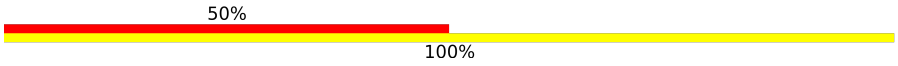
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5:



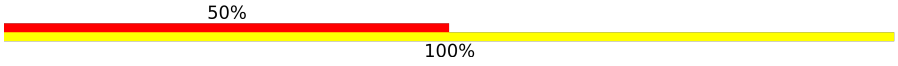
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6:



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

Chain 7:

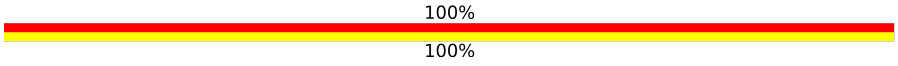


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8:

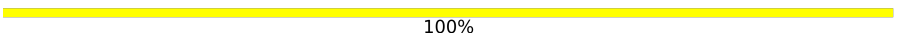
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9:



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

Chain CA:

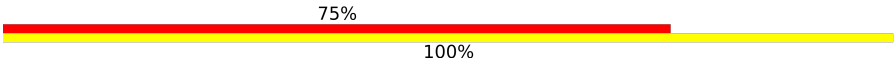


• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

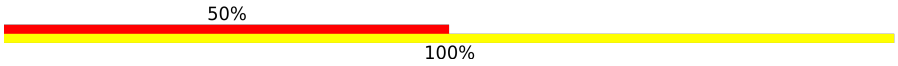
• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



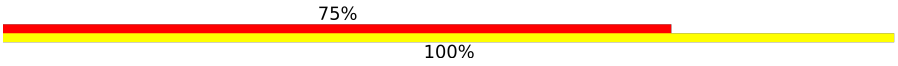
• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 4: 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 p:

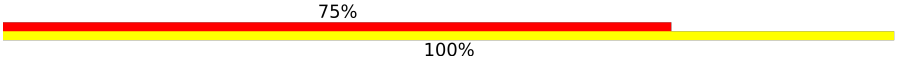


• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:

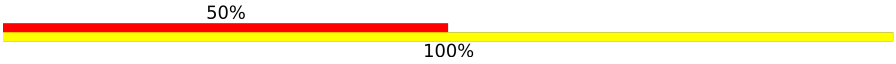
• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:



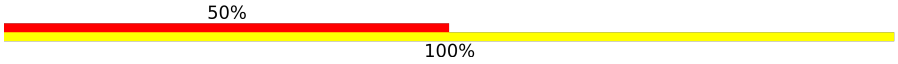
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



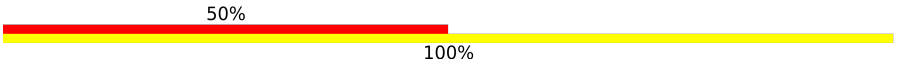
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



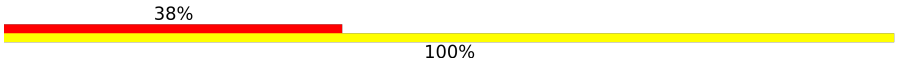
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:



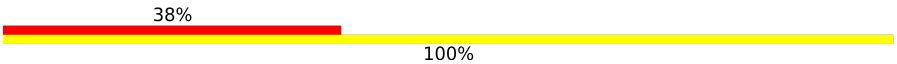
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

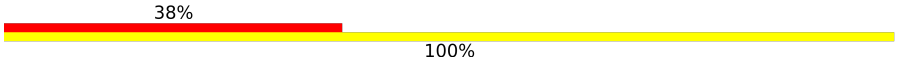
Chain f:



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

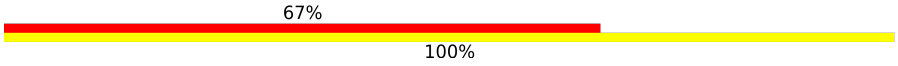
-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos
e

Chain 0:



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain L:

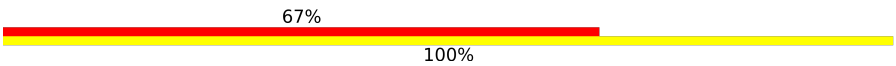


• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain O:

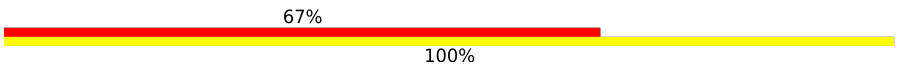
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain X:



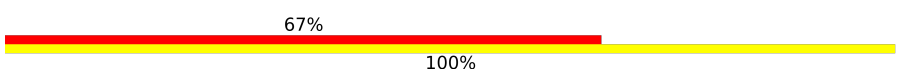
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain g:



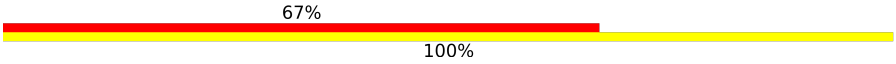
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac
etamido-2-deoxy-beta-D-glucopyranose

Chain j:



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:

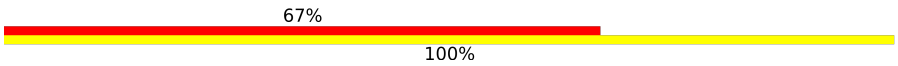


• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:

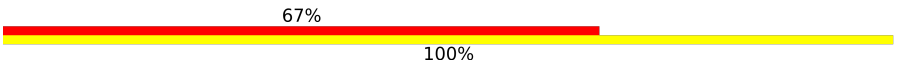
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:



• Molecule 8: 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 N:

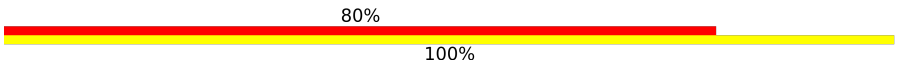
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra

nose

Chain V:

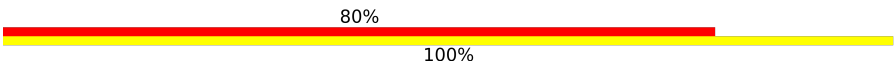
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain i:



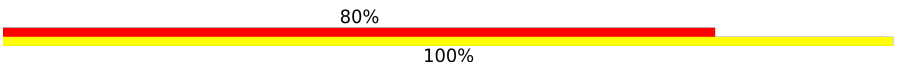
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain q:



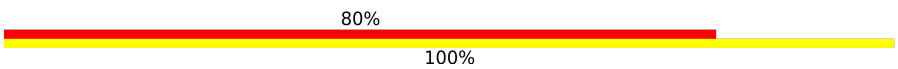
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain 3:



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

Chain BA:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	79667	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.299	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.95	10/9345 (0.1%)	0.82	12/12747 (0.1%)
1	B	0.95	10/9345 (0.1%)	0.82	12/12747 (0.1%)
1	C	0.95	10/9345 (0.1%)	0.82	12/12747 (0.1%)
All	All	0.95	30/28035 (0.1%)	0.82	36/38241 (0.1%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	737	CYS	CB-SG	-8.38	1.68	1.82
1	C	737	CYS	CB-SG	-8.37	1.68	1.82
1	B	737	CYS	CB-SG	-8.34	1.68	1.82
1	C	800	CYS	CB-SG	-7.71	1.69	1.82
1	A	800	CYS	CB-SG	-7.70	1.69	1.82
1	B	800	CYS	CB-SG	-7.69	1.69	1.82
1	C	1193	TYR	CB-CG	-6.75	1.41	1.51
1	A	1193	TYR	CB-CG	-6.69	1.41	1.51
1	B	1193	TYR	CB-CG	-6.65	1.41	1.51
1	B	1190	VAL	C-N	5.62	1.47	1.34
1	B	666	ASN	CB-CG	5.61	1.64	1.51
1	C	666	ASN	CB-CG	5.61	1.64	1.51
1	A	666	ASN	CB-CG	5.61	1.64	1.51
1	A	1190	VAL	C-N	5.61	1.47	1.34
1	C	1190	VAL	C-N	5.61	1.47	1.34
1	C	128	VAL	CB-CG2	-5.58	1.41	1.52
1	A	128	VAL	CB-CG2	-5.58	1.41	1.52
1	B	128	VAL	CB-CG2	-5.56	1.41	1.52
1	A	950	PHE	CB-CG	-5.39	1.42	1.51
1	C	950	PHE	CB-CG	-5.38	1.42	1.51
1	B	950	PHE	CB-CG	-5.37	1.42	1.51
1	B	568	PHE	CB-CG	-5.33	1.42	1.51
1	C	568	PHE	CB-CG	-5.31	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	568	PHE	CB-CG	-5.31	1.42	1.51
1	C	413	TRP	CB-CG	-5.22	1.40	1.50
1	A	413	TRP	CB-CG	-5.21	1.40	1.50
1	C	597	TYR	CB-CG	-5.19	1.43	1.51
1	B	413	TRP	CB-CG	-5.18	1.41	1.50
1	B	597	TYR	CB-CG	-5.17	1.43	1.51
1	A	597	TYR	CB-CG	-5.16	1.44	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	297	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	C	297	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	B	297	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	C	1172	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	B	1172	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	B	810	ALA	CB-CA-C	8.49	122.84	110.10
1	A	1172	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	C	810	ALA	CB-CA-C	8.48	122.83	110.10
1	A	810	ALA	CB-CA-C	8.46	122.79	110.10
1	A	1193	TYR	CB-CG-CD2	-8.06	116.16	121.00
1	B	1193	TYR	CB-CG-CD2	-8.06	116.17	121.00
1	C	1193	TYR	CB-CG-CD2	-8.01	116.20	121.00
1	B	1085	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	C	1085	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	A	1085	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	C	1198	THR	C-N-CA	7.10	139.45	121.70
1	A	1198	THR	C-N-CA	7.09	139.42	121.70
1	B	1198	THR	C-N-CA	7.08	139.40	121.70
1	B	297	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	297	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	297	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	1049	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	1049	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	1049	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	88	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	B	88	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	A	88	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	623	VAL	O-C-N	5.50	131.50	122.70
1	C	623	VAL	O-C-N	5.50	131.51	122.70
1	B	623	VAL	O-C-N	5.50	131.50	122.70
1	B	150	ARG	NE-CZ-NH2	-5.38	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	150	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	C	150	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	890	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	890	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	890	ASP	CB-CG-OD2	5.22	123.00	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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	A	1169/1325 (88%)	1095 (94%)	67 (6%)	7 (1%)	25	57
1	B	1169/1325 (88%)	1096 (94%)	66 (6%)	7 (1%)	25	57
1	C	1169/1325 (88%)	1095 (94%)	67 (6%)	7 (1%)	25	57
All	All	3507/3975 (88%)	3286 (94%)	200 (6%)	21 (1%)	29	57

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	667	VAL
1	A	853	LEU
1	B	667	VAL
1	B	853	LEU
1	C	667	VAL
1	C	853	LEU

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Mol	Chain	Res	Type
1	A	567	CYS
1	A	725	THR
1	A	1102	GLN
1	B	567	CYS
1	B	725	THR
1	B	1102	GLN
1	C	567	CYS
1	C	725	THR
1	C	1102	GLN
1	A	1109	CYS
1	B	1109	CYS
1	C	1109	CYS
1	A	1108	PHE
1	B	1108	PHE
1	C	1108	PHE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	1031/1169 (88%)	1023 (99%)	8 (1%)	81	91
1	B	1031/1169 (88%)	1023 (99%)	8 (1%)	81	91
1	C	1031/1169 (88%)	1023 (99%)	8 (1%)	81	91
All	All	3093/3507 (88%)	3069 (99%)	24 (1%)	82	91

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	CYS
1	A	358	ASN
1	A	402	PHE
1	A	486	ASN
1	A	645	ASN
1	A	789	CYS
1	A	1111	ASN

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Mol	Chain	Res	Type
1	A	1138	TYR
1	B	175	CYS
1	B	358	ASN
1	B	402	PHE
1	B	486	ASN
1	B	645	ASN
1	B	789	CYS
1	B	1111	ASN
1	B	1138	TYR
1	C	175	CYS
1	C	358	ASN
1	C	402	PHE
1	C	486	ASN
1	C	645	ASN
1	C	789	CYS
1	C	1111	ASN
1	C	1138	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	660	ASN
1	B	660	ASN
1	C	660	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)

201 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	$\#\|Z\| > 2$
6	NAG	0	1	1,6	14,14,15	2.73	3 (21%)	17,19,21	4.08	6 (35%)
6	NAG	0	2	6	14,14,15	2.85	4 (28%)	17,19,21	3.64	4 (23%)
6	BMA	0	3	6	11,11,12	1.86	2 (18%)	15,15,17	6.02	6 (40%)
6	MAN	0	4	6	11,11,12	1.71	2 (18%)	15,15,17	8.79	6 (40%)
6	MAN	0	5	6	11,11,12	1.72	3 (27%)	15,15,17	4.79	5 (33%)
6	MAN	0	6	6	11,11,12	1.99	3 (27%)	15,15,17	2.94	1 (6%)
6	MAN	0	7	6	11,11,12	1.95	4 (36%)	15,15,17	5.68	7 (46%)
6	MAN	0	8	6	11,11,12	2.60	6 (54%)	15,15,17	4.21	7 (46%)
7	NAG	1	1	1,7	14,14,15	3.30	4 (28%)	17,19,21	5.85	6 (35%)
7	NAG	1	2	7	14,14,15	3.04	4 (28%)	17,19,21	2.85	7 (41%)
7	BMA	1	3	7	11,11,12	2.08	4 (36%)	15,15,17	3.81	5 (33%)
3	NAG	2	1	1,3	14,14,15	2.84	3 (21%)	17,19,21	4.71	6 (35%)
3	NAG	2	2	3	14,14,15	2.87	3 (21%)	17,19,21	2.36	3 (17%)
8	NAG	3	1	1,8	14,14,15	2.66	3 (21%)	17,19,21	3.55	6 (35%)
8	NAG	3	2	8	14,14,15	2.83	3 (21%)	17,19,21	6.75	7 (41%)
8	BMA	3	3	8	11,11,12	1.88	2 (18%)	15,15,17	3.38	5 (33%)
8	MAN	3	4	8	11,11,12	2.10	4 (36%)	15,15,17	3.02	6 (40%)
8	MAN	3	5	8	11,11,12	1.97	3 (27%)	15,15,17	3.37	5 (33%)
7	NAG	4	1	1,7	14,14,15	2.88	3 (21%)	17,19,21	3.36	4 (23%)
7	NAG	4	2	7	14,14,15	2.95	4 (28%)	17,19,21	4.17	8 (47%)
7	BMA	4	3	7	11,11,12	1.97	3 (27%)	15,15,17	4.25	5 (33%)
3	NAG	5	1	1,3	14,14,15	2.81	3 (21%)	17,19,21	3.75	5 (29%)
3	NAG	5	2	3	14,14,15	2.83	4 (28%)	17,19,21	2.86	5 (29%)
3	NAG	6	1	1,3	14,14,15	2.81	4 (28%)	17,19,21	4.78	7 (41%)
3	NAG	6	2	3	14,14,15	2.86	3 (21%)	17,19,21	2.93	3 (17%)
3	NAG	7	1	1,3	14,14,15	2.72	3 (21%)	17,19,21	4.12	6 (35%)
3	NAG	7	2	3	14,14,15	2.98	3 (21%)	17,19,21	3.92	4 (23%)
3	NAG	8	1	1,3	14,14,15	2.81	3 (21%)	17,19,21	4.04	4 (23%)
3	NAG	8	2	3	14,14,15	2.72	4 (28%)	17,19,21	2.52	2 (11%)
3	NAG	9	1	1,3	14,14,15	2.77	3 (21%)	17,19,21	4.62	3 (17%)
3	NAG	9	2	3	14,14,15	2.95	4 (28%)	17,19,21	3.43	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	AA	1	1,4	14,14,15	2.67	3 (21%)	17,19,21	5.91	5 (29%)
4	NAG	AA	2	4	14,14,15	2.90	3 (21%)	17,19,21	3.77	6 (35%)
4	BMA	AA	3	4	11,11,12	1.84	2 (18%)	15,15,17	4.68	4 (26%)
4	MAN	AA	4	4	11,11,12	2.02	3 (27%)	15,15,17	3.78	6 (40%)
8	NAG	BA	1	1,8	14,14,15	2.73	3 (21%)	17,19,21	4.43	7 (41%)
8	NAG	BA	2	8	14,14,15	2.79	4 (28%)	17,19,21	5.64	8 (47%)
8	BMA	BA	3	8	11,11,12	1.87	3 (27%)	15,15,17	4.71	6 (40%)
8	MAN	BA	4	8	11,11,12	2.08	4 (36%)	15,15,17	3.17	5 (33%)
8	MAN	BA	5	8	11,11,12	2.04	3 (27%)	15,15,17	4.27	4 (26%)
3	NAG	CA	1	1,3	14,14,15	2.86	4 (28%)	17,19,21	6.18	6 (35%)
3	NAG	CA	2	3	14,14,15	2.92	2 (14%)	17,19,21	1.65	3 (17%)
2	NAG	D	1	1,2	14,14,15	2.70	3 (21%)	17,19,21	3.64	5 (29%)
2	NAG	D	2	2	14,14,15	2.86	4 (28%)	17,19,21	5.73	7 (41%)
2	BMA	D	3	2	11,11,12	2.00	4 (36%)	15,15,17	3.47	5 (33%)
2	MAN	D	4	2	11,11,12	1.96	4 (36%)	15,15,17	4.66	5 (33%)
2	MAN	D	5	2	11,11,12	2.69	7 (63%)	15,15,17	2.68	7 (46%)
2	MAN	D	6	2	11,11,12	2.61	6 (54%)	15,15,17	3.71	5 (33%)
7	NAG	DA	1	1,7	14,14,15	2.77	3 (21%)	17,19,21	4.55	6 (35%)
7	NAG	DA	2	7	14,14,15	2.85	3 (21%)	17,19,21	6.35	9 (52%)
7	BMA	DA	3	7	11,11,12	2.06	3 (27%)	15,15,17	3.43	5 (33%)
3	NAG	E	1	1,3	14,14,15	2.91	3 (21%)	17,19,21	4.19	6 (35%)
3	NAG	E	2	3	14,14,15	3.27	5 (35%)	17,19,21	4.05	6 (35%)
4	NAG	F	1	1,4	14,14,15	2.77	3 (21%)	17,19,21	5.52	6 (35%)
4	NAG	F	2	4	14,14,15	2.77	3 (21%)	17,19,21	7.75	6 (35%)
4	BMA	F	3	4	11,11,12	1.86	3 (27%)	15,15,17	3.12	4 (26%)
4	MAN	F	4	4	11,11,12	2.03	3 (27%)	15,15,17	3.82	5 (33%)
3	NAG	G	1	1,3	14,14,15	2.80	3 (21%)	17,19,21	2.52	4 (23%)
3	NAG	G	2	3	14,14,15	2.86	4 (28%)	17,19,21	5.01	4 (23%)
5	NAG	H	1	1,5	14,14,15	2.73	3 (21%)	17,19,21	2.96	5 (29%)
5	NAG	H	2	5	14,14,15	2.99	3 (21%)	17,19,21	5.22	8 (47%)
5	BMA	H	3	5	11,11,12	1.89	3 (27%)	15,15,17	3.57	4 (26%)
5	MAN	H	4	5	11,11,12	1.93	3 (27%)	15,15,17	3.97	5 (33%)
3	NAG	I	1	1,3	14,14,15	2.77	3 (21%)	17,19,21	5.11	6 (35%)
3	NAG	I	2	3	14,14,15	2.97	4 (28%)	17,19,21	2.14	3 (17%)
3	NAG	J	1	1,3	14,14,15	2.62	3 (21%)	17,19,21	5.95	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	J	2	3	14,14,15	2.74	3 (21%)	17,19,21	2.21	4 (23%)
6	NAG	K	1	1,6	14,14,15	2.74	3 (21%)	17,19,21	4.09	6 (35%)
6	NAG	K	2	6	14,14,15	2.86	4 (28%)	17,19,21	3.64	4 (23%)
6	BMA	K	3	6	11,11,12	1.86	2 (18%)	15,15,17	6.02	6 (40%)
6	MAN	K	4	6	11,11,12	1.72	2 (18%)	15,15,17	8.78	6 (40%)
6	MAN	K	5	6	11,11,12	1.72	3 (27%)	15,15,17	4.79	5 (33%)
6	MAN	K	6	6	11,11,12	1.98	3 (27%)	15,15,17	2.94	1 (6%)
6	MAN	K	7	6	11,11,12	1.95	4 (36%)	15,15,17	5.68	7 (46%)
6	MAN	K	8	6	11,11,12	2.60	7 (63%)	15,15,17	4.21	7 (46%)
7	NAG	L	1	1,7	14,14,15	3.30	4 (28%)	17,19,21	5.85	6 (35%)
7	NAG	L	2	7	14,14,15	3.05	4 (28%)	17,19,21	2.85	7 (41%)
7	BMA	L	3	7	11,11,12	2.09	4 (36%)	15,15,17	3.80	5 (33%)
3	NAG	M	1	1,3	14,14,15	2.83	3 (21%)	17,19,21	4.71	6 (35%)
3	NAG	M	2	3	14,14,15	2.88	3 (21%)	17,19,21	2.35	3 (17%)
8	NAG	N	1	1,8	14,14,15	2.66	3 (21%)	17,19,21	3.55	6 (35%)
8	NAG	N	2	8	14,14,15	2.83	3 (21%)	17,19,21	6.75	7 (41%)
8	BMA	N	3	8	11,11,12	1.89	3 (27%)	15,15,17	3.38	5 (33%)
8	MAN	N	4	8	11,11,12	2.10	4 (36%)	15,15,17	3.01	6 (40%)
8	MAN	N	5	8	11,11,12	1.98	4 (36%)	15,15,17	3.37	5 (33%)
7	NAG	O	1	1,7	14,14,15	2.89	3 (21%)	17,19,21	3.36	4 (23%)
7	NAG	O	2	7	14,14,15	2.96	4 (28%)	17,19,21	4.17	8 (47%)
7	BMA	O	3	7	11,11,12	1.97	3 (27%)	15,15,17	4.25	5 (33%)
3	NAG	P	1	1,3	14,14,15	2.82	3 (21%)	17,19,21	3.75	5 (29%)
3	NAG	P	2	3	14,14,15	2.84	4 (28%)	17,19,21	2.87	5 (29%)
3	NAG	Q	1	1,3	14,14,15	2.81	4 (28%)	17,19,21	4.78	7 (41%)
3	NAG	Q	2	3	14,14,15	2.86	2 (14%)	17,19,21	2.93	3 (17%)
3	NAG	R	1	1,3	14,14,15	2.72	3 (21%)	17,19,21	4.13	6 (35%)
3	NAG	R	2	3	14,14,15	2.98	3 (21%)	17,19,21	3.92	4 (23%)
3	NAG	S	1	1,3	14,14,15	2.80	3 (21%)	17,19,21	4.04	4 (23%)
3	NAG	S	2	3	14,14,15	2.73	4 (28%)	17,19,21	2.53	2 (11%)
3	NAG	T	1	1,3	14,14,15	2.76	3 (21%)	17,19,21	4.62	3 (17%)
3	NAG	T	2	3	14,14,15	2.95	4 (28%)	17,19,21	3.43	4 (23%)
4	NAG	U	1	1,4	14,14,15	2.68	3 (21%)	17,19,21	5.91	5 (29%)
4	NAG	U	2	4	14,14,15	2.90	3 (21%)	17,19,21	3.77	6 (35%)
4	BMA	U	3	4	11,11,12	1.84	2 (18%)	15,15,17	4.68	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MAN	U	4	4	11,11,12	2.03	3 (27%)	15,15,17	3.78	6 (40%)
8	NAG	V	1	1,8	14,14,15	2.73	3 (21%)	17,19,21	4.43	7 (41%)
8	NAG	V	2	8	14,14,15	2.79	4 (28%)	17,19,21	5.64	8 (47%)
8	BMA	V	3	8	11,11,12	1.87	3 (27%)	15,15,17	4.71	6 (40%)
8	MAN	V	4	8	11,11,12	2.08	4 (36%)	15,15,17	3.17	5 (33%)
8	MAN	V	5	8	11,11,12	2.04	3 (27%)	15,15,17	4.25	4 (26%)
3	NAG	W	1	1,3	14,14,15	2.87	4 (28%)	17,19,21	6.18	6 (35%)
3	NAG	W	2	3	14,14,15	2.92	2 (14%)	17,19,21	1.65	3 (17%)
7	NAG	X	1	1,7	14,14,15	2.78	3 (21%)	17,19,21	4.55	6 (35%)
7	NAG	X	2	7	14,14,15	2.85	3 (21%)	17,19,21	6.35	9 (52%)
7	BMA	X	3	7	11,11,12	2.06	3 (27%)	15,15,17	3.43	5 (33%)
2	NAG	Y	1	1,2	14,14,15	2.71	3 (21%)	17,19,21	3.64	5 (29%)
2	NAG	Y	2	2	14,14,15	2.87	4 (28%)	17,19,21	5.73	7 (41%)
2	BMA	Y	3	2	11,11,12	2.01	3 (27%)	15,15,17	3.47	5 (33%)
2	MAN	Y	4	2	11,11,12	1.96	4 (36%)	15,15,17	4.66	5 (33%)
2	MAN	Y	5	2	11,11,12	2.68	6 (54%)	15,15,17	2.68	7 (46%)
2	MAN	Y	6	2	11,11,12	2.61	6 (54%)	15,15,17	3.71	5 (33%)
3	NAG	Z	1	1,3	14,14,15	2.91	3 (21%)	17,19,21	4.20	6 (35%)
3	NAG	Z	2	3	14,14,15	3.27	5 (35%)	17,19,21	4.06	6 (35%)
4	NAG	a	1	1,4	14,14,15	2.76	3 (21%)	17,19,21	5.52	6 (35%)
4	NAG	a	2	4	14,14,15	2.77	3 (21%)	17,19,21	7.75	6 (35%)
4	BMA	a	3	4	11,11,12	1.86	3 (27%)	15,15,17	3.12	4 (26%)
4	MAN	a	4	4	11,11,12	2.03	3 (27%)	15,15,17	3.82	5 (33%)
3	NAG	b	1	1,3	14,14,15	2.80	3 (21%)	17,19,21	2.52	4 (23%)
3	NAG	b	2	3	14,14,15	2.86	4 (28%)	17,19,21	5.01	4 (23%)
5	NAG	c	1	1,5	14,14,15	2.74	3 (21%)	17,19,21	2.96	5 (29%)
5	NAG	c	2	5	14,14,15	2.98	3 (21%)	17,19,21	5.22	8 (47%)
5	BMA	c	3	5	11,11,12	1.89	3 (27%)	15,15,17	3.57	4 (26%)
5	MAN	c	4	5	11,11,12	1.94	3 (27%)	15,15,17	3.98	5 (33%)
3	NAG	d	1	1,3	14,14,15	2.76	3 (21%)	17,19,21	5.11	6 (35%)
3	NAG	d	2	3	14,14,15	2.96	4 (28%)	17,19,21	2.14	3 (17%)
3	NAG	e	1	1,3	14,14,15	2.62	3 (21%)	17,19,21	5.95	6 (35%)
3	NAG	e	2	3	14,14,15	2.74	3 (21%)	17,19,21	2.21	4 (23%)
6	NAG	f	1	1,6	14,14,15	2.73	3 (21%)	17,19,21	4.09	6 (35%)
6	NAG	f	2	6	14,14,15	2.86	4 (28%)	17,19,21	3.64	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BMA	f	3	6	11,11,12	1.85	2 (18%)	15,15,17	6.02	6 (40%)
6	MAN	f	4	6	11,11,12	1.72	2 (18%)	15,15,17	8.79	6 (40%)
6	MAN	f	5	6	11,11,12	1.73	3 (27%)	15,15,17	4.79	5 (33%)
6	MAN	f	6	6	11,11,12	1.98	3 (27%)	15,15,17	2.95	1 (6%)
6	MAN	f	7	6	11,11,12	1.94	4 (36%)	15,15,17	5.68	7 (46%)
6	MAN	f	8	6	11,11,12	2.60	6 (54%)	15,15,17	4.21	7 (46%)
7	NAG	g	1	1,7	14,14,15	3.29	4 (28%)	17,19,21	5.85	6 (35%)
7	NAG	g	2	7	14,14,15	3.05	4 (28%)	17,19,21	2.85	7 (41%)
7	BMA	g	3	7	11,11,12	2.09	4 (36%)	15,15,17	3.80	5 (33%)
3	NAG	h	1	1,3	14,14,15	2.83	3 (21%)	17,19,21	4.71	6 (35%)
3	NAG	h	2	3	14,14,15	2.87	3 (21%)	17,19,21	2.35	3 (17%)
8	NAG	i	1	1,8	14,14,15	2.65	3 (21%)	17,19,21	3.54	6 (35%)
8	NAG	i	2	8	14,14,15	2.83	3 (21%)	17,19,21	6.75	7 (41%)
8	BMA	i	3	8	11,11,12	1.88	2 (18%)	15,15,17	3.38	5 (33%)
8	MAN	i	4	8	11,11,12	2.10	4 (36%)	15,15,17	3.02	6 (40%)
8	MAN	i	5	8	11,11,12	1.98	4 (36%)	15,15,17	3.37	5 (33%)
7	NAG	j	1	1,7	14,14,15	2.88	3 (21%)	17,19,21	3.36	4 (23%)
7	NAG	j	2	7	14,14,15	2.95	4 (28%)	17,19,21	4.16	8 (47%)
7	BMA	j	3	7	11,11,12	1.98	3 (27%)	15,15,17	4.25	5 (33%)
3	NAG	k	1	1,3	14,14,15	2.81	3 (21%)	17,19,21	3.75	5 (29%)
3	NAG	k	2	3	14,14,15	2.83	4 (28%)	17,19,21	2.86	5 (29%)
3	NAG	l	1	1,3	14,14,15	2.81	4 (28%)	17,19,21	4.78	7 (41%)
3	NAG	l	2	3	14,14,15	2.85	3 (21%)	17,19,21	2.93	3 (17%)
3	NAG	m	1	1,3	14,14,15	2.72	3 (21%)	17,19,21	4.12	6 (35%)
3	NAG	m	2	3	14,14,15	2.99	3 (21%)	17,19,21	3.92	4 (23%)
3	NAG	n	1	1,3	14,14,15	2.80	3 (21%)	17,19,21	4.04	4 (23%)
3	NAG	n	2	3	14,14,15	2.73	4 (28%)	17,19,21	2.54	2 (11%)
3	NAG	o	1	1,3	14,14,15	2.77	3 (21%)	17,19,21	4.62	3 (17%)
3	NAG	o	2	3	14,14,15	2.95	4 (28%)	17,19,21	3.43	4 (23%)
4	NAG	p	1	1,4	14,14,15	2.68	3 (21%)	17,19,21	5.91	5 (29%)
4	NAG	p	2	4	14,14,15	2.91	3 (21%)	17,19,21	3.77	6 (35%)
4	BMA	p	3	4	11,11,12	1.84	2 (18%)	15,15,17	4.68	4 (26%)
4	MAN	p	4	4	11,11,12	2.02	3 (27%)	15,15,17	3.78	6 (40%)
8	NAG	q	1	1,8	14,14,15	2.73	3 (21%)	17,19,21	4.43	7 (41%)
8	NAG	q	2	8	14,14,15	2.78	4 (28%)	17,19,21	5.64	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BMA	q	3	8	11,11,12	1.87	3 (27%)	15,15,17	4.71	6 (40%)
8	MAN	q	4	8	11,11,12	2.07	4 (36%)	15,15,17	3.17	5 (33%)
8	MAN	q	5	8	11,11,12	2.04	4 (36%)	15,15,17	4.26	4 (26%)
3	NAG	r	1	1,3	14,14,15	2.88	4 (28%)	17,19,21	6.18	6 (35%)
3	NAG	r	2	3	14,14,15	2.91	2 (14%)	17,19,21	1.65	3 (17%)
7	NAG	s	1	1,7	14,14,15	2.76	3 (21%)	17,19,21	4.55	6 (35%)
7	NAG	s	2	7	14,14,15	2.86	3 (21%)	17,19,21	6.35	9 (52%)
7	BMA	s	3	7	11,11,12	2.07	3 (27%)	15,15,17	3.43	5 (33%)
2	NAG	t	1	1,2	14,14,15	2.70	3 (21%)	17,19,21	3.64	5 (29%)
2	NAG	t	2	2	14,14,15	2.86	4 (28%)	17,19,21	5.73	7 (41%)
2	BMA	t	3	2	11,11,12	2.01	4 (36%)	15,15,17	3.47	5 (33%)
2	MAN	t	4	2	11,11,12	1.96	4 (36%)	15,15,17	4.67	5 (33%)
2	MAN	t	5	2	11,11,12	2.70	7 (63%)	15,15,17	2.67	7 (46%)
2	MAN	t	6	2	11,11,12	2.60	6 (54%)	15,15,17	3.71	5 (33%)
3	NAG	u	1	1,3	14,14,15	2.91	3 (21%)	17,19,21	4.20	6 (35%)
3	NAG	u	2	3	14,14,15	3.27	5 (35%)	17,19,21	4.05	6 (35%)
4	NAG	v	1	1,4	14,14,15	2.76	3 (21%)	17,19,21	5.52	6 (35%)
4	NAG	v	2	4	14,14,15	2.78	3 (21%)	17,19,21	7.75	6 (35%)
4	BMA	v	3	4	11,11,12	1.86	3 (27%)	15,15,17	3.11	4 (26%)
4	MAN	v	4	4	11,11,12	2.03	3 (27%)	15,15,17	3.82	5 (33%)
3	NAG	w	1	1,3	14,14,15	2.80	3 (21%)	17,19,21	2.52	4 (23%)
3	NAG	w	2	3	14,14,15	2.87	4 (28%)	17,19,21	5.01	4 (23%)
5	NAG	x	1	1,5	14,14,15	2.74	3 (21%)	17,19,21	2.96	4 (23%)
5	NAG	x	2	5	14,14,15	2.98	3 (21%)	17,19,21	5.22	8 (47%)
5	BMA	x	3	5	11,11,12	1.89	3 (27%)	15,15,17	3.57	4 (26%)
5	MAN	x	4	5	11,11,12	1.93	3 (27%)	15,15,17	3.97	5 (33%)
3	NAG	y	1	1,3	14,14,15	2.76	3 (21%)	17,19,21	5.11	6 (35%)
3	NAG	y	2	3	14,14,15	2.96	4 (28%)	17,19,21	2.14	3 (17%)
3	NAG	z	1	1,3	14,14,15	2.63	3 (21%)	17,19,21	5.95	6 (35%)
3	NAG	z	2	3	14,14,15	2.74	3 (21%)	17,19,21	2.21	4 (23%)

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
6	NAG	0	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	0	2	6	-	2/6/23/26	0/1/1/1
6	BMA	0	3	6	-	2/2/19/22	0/1/1/1
6	MAN	0	4	6	-	0/2/19/22	0/1/1/1
6	MAN	0	5	6	-	0/2/19/22	0/1/1/1
6	MAN	0	6	6	-	0/2/19/22	0/1/1/1
6	MAN	0	7	6	-	1/2/19/22	0/1/1/1
6	MAN	0	8	6	-	1/2/19/22	0/1/1/1
7	NAG	1	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	1	2	7	-	0/6/23/26	0/1/1/1
7	BMA	1	3	7	-	0/2/19/22	0/1/1/1
3	NAG	2	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	2	2	3	-	0/6/23/26	0/1/1/1
8	NAG	3	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	3	2	8	-	1/6/23/26	0/1/1/1
8	BMA	3	3	8	-	2/2/19/22	0/1/1/1
8	MAN	3	4	8	-	0/2/19/22	0/1/1/1
8	MAN	3	5	8	-	1/2/19/22	0/1/1/1
7	NAG	4	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	4	2	7	-	0/6/23/26	0/1/1/1
7	BMA	4	3	7	-	0/2/19/22	0/1/1/1
3	NAG	5	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	5	2	3	-	0/6/23/26	0/1/1/1
3	NAG	6	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	6	2	3	-	2/6/23/26	0/1/1/1
3	NAG	7	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	7	2	3	-	1/6/23/26	0/1/1/1
3	NAG	8	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	8	2	3	-	1/6/23/26	0/1/1/1
3	NAG	9	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	9	2	3	-	1/6/23/26	0/1/1/1
4	NAG	AA	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	AA	2	4	-	0/6/23/26	0/1/1/1
4	BMA	AA	3	4	-	1/2/19/22	0/1/1/1
4	MAN	AA	4	4	-	0/2/19/22	0/1/1/1
8	NAG	BA	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	BA	2	8	-	2/6/23/26	0/1/1/1
8	BMA	BA	3	8	-	2/2/19/22	0/1/1/1
8	MAN	BA	4	8	-	0/2/19/22	0/1/1/1
8	MAN	BA	5	8	-	1/2/19/22	0/1/1/1
3	NAG	CA	1	1,3	-	1/6/23/26	0/1/1/1

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	a	3	4	-	1/2/19/22	0/1/1/1
4	MAN	a	4	4	-	0/2/19/22	0/1/1/1
3	NAG	b	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	1/6/23/26	0/1/1/1
5	NAG	c	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	BMA	c	3	5	-	2/2/19/22	0/1/1/1
5	MAN	c	4	5	-	0/2/19/22	0/1/1/1
3	NAG	d	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
3	NAG	e	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	e	2	3	-	1/6/23/26	0/1/1/1
6	NAG	f	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	BMA	f	3	6	-	2/2/19/22	0/1/1/1
6	MAN	f	4	6	-	0/2/19/22	0/1/1/1
6	MAN	f	5	6	-	0/2/19/22	0/1/1/1
6	MAN	f	6	6	-	0/2/19/22	0/1/1/1
6	MAN	f	7	6	-	1/2/19/22	0/1/1/1
6	MAN	f	8	6	-	1/2/19/22	0/1/1/1
7	NAG	g	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	g	2	7	-	0/6/23/26	0/1/1/1
7	BMA	g	3	7	-	0/2/19/22	0/1/1/1
3	NAG	h	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	h	2	3	-	0/6/23/26	0/1/1/1
8	NAG	i	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	i	2	8	-	1/6/23/26	0/1/1/1
8	BMA	i	3	8	-	2/2/19/22	0/1/1/1
8	MAN	i	4	8	-	0/2/19/22	0/1/1/1
8	MAN	i	5	8	-	1/2/19/22	0/1/1/1
7	NAG	j	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	j	2	7	-	0/6/23/26	0/1/1/1
7	BMA	j	3	7	-	0/2/19/22	0/1/1/1
3	NAG	k	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	k	2	3	-	0/6/23/26	0/1/1/1
3	NAG	l	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	l	2	3	-	2/6/23/26	0/1/1/1
3	NAG	m	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	m	2	3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	n	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	n	2	3	-	1/6/23/26	0/1/1/1
3	NAG	o	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	o	2	3	-	1/6/23/26	0/1/1/1
4	NAG	p	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	p	2	4	-	0/6/23/26	0/1/1/1
4	BMA	p	3	4	-	1/2/19/22	0/1/1/1
4	MAN	p	4	4	-	0/2/19/22	0/1/1/1
8	NAG	q	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	q	2	8	-	2/6/23/26	0/1/1/1
8	BMA	q	3	8	-	2/2/19/22	0/1/1/1
8	MAN	q	4	8	-	0/2/19/22	0/1/1/1
8	MAN	q	5	8	-	1/2/19/22	0/1/1/1
3	NAG	r	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	r	2	3	-	1/6/23/26	0/1/1/1
7	NAG	s	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	s	2	7	-	1/6/23/26	0/1/1/1
7	BMA	s	3	7	-	0/2/19/22	0/1/1/1
2	NAG	t	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	t	2	2	-	1/6/23/26	0/1/1/1
2	BMA	t	3	2	-	1/2/19/22	0/1/1/1
2	MAN	t	4	2	-	1/2/19/22	0/1/1/1
2	MAN	t	5	2	-	1/2/19/22	0/1/1/1
2	MAN	t	6	2	-	1/2/19/22	0/1/1/1
3	NAG	u	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	u	2	3	-	0/6/23/26	0/1/1/1
4	NAG	v	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	v	2	4	-	1/6/23/26	0/1/1/1
4	BMA	v	3	4	-	1/2/19/22	0/1/1/1
4	MAN	v	4	4	-	0/2/19/22	0/1/1/1
3	NAG	w	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	w	2	3	-	1/6/23/26	0/1/1/1
5	NAG	x	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	x	2	5	-	2/6/23/26	0/1/1/1
5	BMA	x	3	5	-	2/2/19/22	0/1/1/1
5	MAN	x	4	5	-	0/2/19/22	0/1/1/1
3	NAG	y	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	y	2	3	-	2/6/23/26	0/1/1/1
3	NAG	z	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	z	2	3	-	1/6/23/26	0/1/1/1

All (683) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	O5-C1	9.24	1.58	1.43
3	u	2	NAG	O5-C1	9.24	1.58	1.43
3	Z	2	NAG	O5-C1	9.23	1.58	1.43
7	1	1	NAG	O5-C1	8.96	1.58	1.43
7	L	1	NAG	O5-C1	8.94	1.58	1.43
7	g	1	NAG	O5-C1	8.92	1.58	1.43
7	g	2	NAG	O5-C1	8.77	1.57	1.43
7	L	2	NAG	O5-C1	8.76	1.57	1.43
7	1	2	NAG	O5-C1	8.72	1.57	1.43
3	I	2	NAG	O5-C1	8.47	1.57	1.43
3	y	2	NAG	O5-C1	8.45	1.57	1.43
3	d	2	NAG	O5-C1	8.44	1.57	1.43
3	m	2	NAG	O5-C1	8.22	1.56	1.43
3	7	2	NAG	O5-C1	8.19	1.56	1.43
3	R	2	NAG	O5-C1	8.18	1.56	1.43
3	6	2	NAG	O5-C1	8.16	1.56	1.43
3	2	2	NAG	O5-C1	8.15	1.56	1.43
3	Q	2	NAG	O5-C1	8.14	1.56	1.43
3	l	2	NAG	O5-C1	8.14	1.56	1.43
3	M	2	NAG	O5-C1	8.12	1.56	1.43
3	h	2	NAG	O5-C1	8.10	1.56	1.43
3	o	2	NAG	O5-C1	7.95	1.56	1.43
3	9	2	NAG	O5-C1	7.95	1.56	1.43
3	T	2	NAG	O5-C1	7.95	1.56	1.43
3	w	2	NAG	O5-C1	7.89	1.56	1.43
3	G	2	NAG	O5-C1	7.84	1.56	1.43
3	P	2	NAG	O5-C1	7.83	1.56	1.43
3	b	2	NAG	O5-C1	7.83	1.56	1.43
3	k	2	NAG	O5-C1	7.80	1.56	1.43
3	z	2	NAG	O5-C1	7.80	1.56	1.43
3	J	2	NAG	O5-C1	7.79	1.56	1.43
3	5	2	NAG	O5-C1	7.78	1.56	1.43
3	e	2	NAG	O5-C1	7.78	1.56	1.43
7	O	2	NAG	O5-C1	7.77	1.56	1.43
7	j	2	NAG	O5-C1	7.76	1.56	1.43
7	4	2	NAG	O5-C1	7.75	1.56	1.43
2	Y	2	NAG	O5-C1	7.66	1.55	1.43
2	t	2	NAG	O5-C1	7.65	1.55	1.43
2	D	2	NAG	O5-C1	7.64	1.55	1.43
4	p	2	NAG	O5-C1	7.53	1.55	1.43
4	U	2	NAG	O5-C1	7.52	1.55	1.43
6	K	2	NAG	O5-C1	7.49	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	2	NAG	O5-C1	7.49	1.55	1.43
4	AA	2	NAG	O5-C1	7.49	1.55	1.43
5	x	2	NAG	O5-C1	7.48	1.55	1.43
5	c	2	NAG	O5-C1	7.48	1.55	1.43
6	f	2	NAG	O5-C1	7.47	1.55	1.43
6	0	2	NAG	O5-C1	7.47	1.55	1.43
3	CA	2	NAG	C2-N2	-7.46	1.33	1.46
3	W	2	NAG	C2-N2	-7.44	1.33	1.46
3	r	2	NAG	C2-N2	-7.41	1.33	1.46
3	r	1	NAG	C2-N2	-7.40	1.33	1.46
3	W	1	NAG	C2-N2	-7.38	1.33	1.46
3	CA	1	NAG	C2-N2	-7.35	1.33	1.46
3	l	1	NAG	O5-C1	7.32	1.55	1.43
3	Q	1	NAG	O5-C1	7.32	1.55	1.43
3	6	1	NAG	O5-C1	7.32	1.55	1.43
3	b	1	NAG	O5-C1	7.31	1.55	1.43
3	w	1	NAG	O5-C1	7.30	1.55	1.43
3	G	1	NAG	O5-C1	7.30	1.55	1.43
3	k	1	NAG	O5-C1	7.29	1.55	1.43
3	u	1	NAG	O5-C1	7.28	1.55	1.43
3	P	1	NAG	O5-C1	7.28	1.55	1.43
3	E	1	NAG	O5-C1	7.28	1.55	1.43
3	Z	1	NAG	O5-C1	7.28	1.55	1.43
3	5	1	NAG	O5-C1	7.27	1.55	1.43
7	s	2	NAG	O5-C1	7.26	1.55	1.43
3	2	1	NAG	O5-C1	7.26	1.55	1.43
7	X	1	NAG	O5-C1	7.25	1.55	1.43
3	9	1	NAG	O5-C1	7.25	1.55	1.43
3	M	1	NAG	O5-C1	7.24	1.55	1.43
7	DA	2	NAG	O5-C1	7.23	1.55	1.43
3	h	1	NAG	O5-C1	7.23	1.55	1.43
7	X	2	NAG	O5-C1	7.23	1.55	1.43
7	DA	1	NAG	O5-C1	7.23	1.55	1.43
7	s	1	NAG	O5-C1	7.22	1.55	1.43
3	T	1	NAG	O5-C1	7.21	1.55	1.43
8	BA	2	NAG	O5-C1	7.20	1.55	1.43
3	o	1	NAG	O5-C1	7.19	1.55	1.43
8	V	2	NAG	O5-C1	7.19	1.55	1.43
3	m	1	NAG	O5-C1	7.17	1.55	1.43
8	q	2	NAG	O5-C1	7.17	1.55	1.43
6	0	1	NAG	O5-C1	7.15	1.55	1.43
3	7	1	NAG	O5-C1	7.15	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	1	NAG	O5-C1	7.14	1.55	1.43
3	R	1	NAG	O5-C1	7.14	1.55	1.43
6	K	1	NAG	O5-C1	7.14	1.55	1.43
8	N	2	NAG	O5-C1	7.14	1.55	1.43
7	4	1	NAG	O5-C1	7.14	1.55	1.43
8	3	2	NAG	O5-C1	7.13	1.55	1.43
7	j	1	NAG	O5-C1	7.13	1.55	1.43
6	f	1	NAG	O5-C1	7.11	1.55	1.43
8	i	2	NAG	O5-C1	7.11	1.55	1.43
3	n	2	NAG	O5-C1	7.08	1.55	1.43
3	S	2	NAG	O5-C1	7.07	1.55	1.43
3	I	1	NAG	O5-C1	7.07	1.55	1.43
3	y	1	NAG	O5-C1	7.06	1.55	1.43
3	d	1	NAG	O5-C1	7.06	1.55	1.43
8	V	1	NAG	O5-C1	7.05	1.55	1.43
5	H	2	NAG	C2-N2	-7.05	1.34	1.46
5	c	2	NAG	C2-N2	-7.04	1.34	1.46
3	8	2	NAG	O5-C1	7.04	1.55	1.43
3	Z	1	NAG	C2-N2	-7.04	1.34	1.46
8	q	1	NAG	O5-C1	7.03	1.54	1.43
3	E	1	NAG	C2-N2	-7.03	1.34	1.46
5	x	2	NAG	C2-N2	-7.03	1.34	1.46
8	BA	1	NAG	O5-C1	7.02	1.54	1.43
3	u	1	NAG	C2-N2	-7.02	1.34	1.46
5	c	1	NAG	O5-C1	7.00	1.54	1.43
7	O	1	NAG	C2-N2	-7.00	1.34	1.46
5	x	1	NAG	O5-C1	7.00	1.54	1.43
2	Y	1	NAG	O5-C1	6.99	1.54	1.43
3	8	1	NAG	O5-C1	6.99	1.54	1.43
7	4	1	NAG	C2-N2	-6.98	1.34	1.46
3	CA	2	NAG	O5-C1	6.98	1.54	1.43
4	v	2	NAG	O5-C1	6.98	1.54	1.43
5	H	1	NAG	O5-C1	6.98	1.54	1.43
7	j	1	NAG	C2-N2	-6.98	1.34	1.46
4	F	1	NAG	O5-C1	6.97	1.54	1.43
4	a	1	NAG	O5-C1	6.97	1.54	1.43
4	v	1	NAG	O5-C1	6.97	1.54	1.43
3	W	2	NAG	O5-C1	6.95	1.54	1.43
4	F	2	NAG	O5-C1	6.95	1.54	1.43
2	D	1	NAG	O5-C1	6.95	1.54	1.43
3	S	1	NAG	O5-C1	6.95	1.54	1.43
3	r	2	NAG	O5-C1	6.95	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	2	NAG	O5-C1	6.95	1.54	1.43
3	n	1	NAG	O5-C1	6.93	1.54	1.43
2	t	1	NAG	O5-C1	6.92	1.54	1.43
8	N	1	NAG	O5-C1	6.86	1.54	1.43
8	3	1	NAG	O5-C1	6.86	1.54	1.43
8	i	1	NAG	O5-C1	6.82	1.54	1.43
4	p	1	NAG	O5-C1	6.74	1.54	1.43
4	p	2	NAG	C2-N2	-6.74	1.34	1.46
4	U	1	NAG	O5-C1	6.73	1.54	1.43
4	AA	2	NAG	C2-N2	-6.71	1.34	1.46
4	U	2	NAG	C2-N2	-6.71	1.34	1.46
4	AA	1	NAG	O5-C1	6.70	1.54	1.43
7	O	2	NAG	C2-N2	-6.65	1.35	1.46
3	8	1	NAG	C2-N2	-6.65	1.35	1.46
7	j	2	NAG	C2-N2	-6.65	1.35	1.46
7	4	2	NAG	C2-N2	-6.65	1.35	1.46
3	z	1	NAG	O5-C1	6.64	1.54	1.43
3	S	1	NAG	C2-N2	-6.64	1.35	1.46
3	n	1	NAG	C2-N2	-6.64	1.35	1.46
3	J	1	NAG	O5-C1	6.62	1.54	1.43
3	2	1	NAG	C2-N2	-6.61	1.35	1.46
3	M	1	NAG	C2-N2	-6.61	1.35	1.46
3	h	1	NAG	C2-N2	-6.60	1.35	1.46
3	e	1	NAG	O5-C1	6.59	1.54	1.43
7	s	2	NAG	C2-N2	-6.58	1.35	1.46
8	3	2	NAG	C2-N2	-6.57	1.35	1.46
8	i	2	NAG	C2-N2	-6.57	1.35	1.46
7	X	2	NAG	C2-N2	-6.55	1.35	1.46
4	F	1	NAG	C2-N2	-6.55	1.35	1.46
8	N	2	NAG	C2-N2	-6.54	1.35	1.46
4	a	1	NAG	C2-N2	-6.54	1.35	1.46
7	DA	2	NAG	C2-N2	-6.54	1.35	1.46
4	v	1	NAG	C2-N2	-6.54	1.35	1.46
3	r	1	NAG	O5-C1	6.53	1.54	1.43
3	W	1	NAG	O5-C1	6.51	1.54	1.43
4	a	2	NAG	C2-N2	-6.49	1.35	1.46
4	F	2	NAG	C2-N2	-6.48	1.35	1.46
4	v	2	NAG	C2-N2	-6.47	1.35	1.46
3	CA	1	NAG	O5-C1	6.47	1.54	1.43
3	R	2	NAG	C2-N2	-6.45	1.35	1.46
3	9	2	NAG	C2-N2	-6.43	1.35	1.46
3	m	2	NAG	C2-N2	-6.43	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	d	1	NAG	C2-N2	-6.43	1.35	1.46
3	P	1	NAG	C2-N2	-6.43	1.35	1.46
3	T	2	NAG	C2-N2	-6.42	1.35	1.46
3	o	2	NAG	C2-N2	-6.41	1.35	1.46
3	I	1	NAG	C2-N2	-6.41	1.35	1.46
3	7	2	NAG	C2-N2	-6.41	1.35	1.46
3	y	1	NAG	C2-N2	-6.40	1.35	1.46
3	5	1	NAG	C2-N2	-6.40	1.35	1.46
3	w	1	NAG	C2-N2	-6.40	1.35	1.46
7	L	1	NAG	C2-N2	-6.39	1.35	1.46
3	k	1	NAG	C2-N2	-6.38	1.35	1.46
7	1	1	NAG	C2-N2	-6.38	1.35	1.46
3	G	1	NAG	C2-N2	-6.38	1.35	1.46
3	6	1	NAG	C2-N2	-6.38	1.35	1.46
7	DA	1	NAG	C2-N2	-6.37	1.35	1.46
7	X	1	NAG	C2-N2	-6.36	1.35	1.46
7	g	1	NAG	C2-N2	-6.36	1.35	1.46
3	l	1	NAG	C2-N2	-6.36	1.35	1.46
3	Q	1	NAG	C2-N2	-6.36	1.35	1.46
3	b	1	NAG	C2-N2	-6.35	1.35	1.46
6	f	2	NAG	C2-N2	-6.34	1.35	1.46
7	s	1	NAG	C2-N2	-6.34	1.35	1.46
6	K	2	NAG	C2-N2	-6.33	1.35	1.46
5	x	1	NAG	C2-N2	-6.32	1.35	1.46
5	H	1	NAG	C2-N2	-6.31	1.35	1.46
6	0	2	NAG	C2-N2	-6.31	1.35	1.46
2	t	1	NAG	C2-N2	-6.30	1.35	1.46
5	c	1	NAG	C2-N2	-6.29	1.35	1.46
2	D	1	NAG	C2-N2	-6.28	1.35	1.46
8	BA	1	NAG	C2-N2	-6.25	1.35	1.46
2	Y	1	NAG	C2-N2	-6.25	1.35	1.46
8	V	1	NAG	C2-N2	-6.23	1.35	1.46
8	q	1	NAG	C2-N2	-6.23	1.35	1.46
3	o	1	NAG	C2-N2	-6.22	1.35	1.46
4	U	1	NAG	C2-N2	-6.20	1.35	1.46
4	AA	1	NAG	C2-N2	-6.20	1.35	1.46
8	V	2	NAG	C2-N2	-6.19	1.35	1.46
4	p	1	NAG	C2-N2	-6.18	1.35	1.46
8	3	1	NAG	C2-N2	-6.17	1.35	1.46
8	N	1	NAG	C2-N2	-6.17	1.35	1.46
8	BA	2	NAG	C2-N2	-6.17	1.35	1.46
8	i	1	NAG	C2-N2	-6.17	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9	1	NAG	C2-N2	-6.17	1.35	1.46
3	T	1	NAG	C2-N2	-6.16	1.35	1.46
8	q	2	NAG	C2-N2	-6.16	1.35	1.46
6	f	1	NAG	C2-N2	-6.15	1.35	1.46
6	K	1	NAG	C2-N2	-6.14	1.35	1.46
3	z	1	NAG	C2-N2	-6.13	1.35	1.46
6	0	1	NAG	C2-N2	-6.13	1.35	1.46
3	e	1	NAG	C2-N2	-6.11	1.35	1.46
3	J	1	NAG	C2-N2	-6.09	1.35	1.46
3	S	2	NAG	C2-N2	-6.07	1.36	1.46
3	8	2	NAG	C2-N2	-6.07	1.36	1.46
3	n	2	NAG	C2-N2	-6.07	1.36	1.46
3	7	1	NAG	C2-N2	-6.06	1.36	1.46
3	R	1	NAG	C2-N2	-6.06	1.36	1.46
3	m	1	NAG	C2-N2	-6.04	1.36	1.46
3	G	2	NAG	C2-N2	-5.99	1.36	1.46
3	b	2	NAG	C2-N2	-5.98	1.36	1.46
3	w	2	NAG	C2-N2	-5.96	1.36	1.46
3	5	2	NAG	C2-N2	-5.96	1.36	1.46
3	k	2	NAG	C2-N2	-5.95	1.36	1.46
3	P	2	NAG	C2-N2	-5.94	1.36	1.46
3	h	2	NAG	C2-N2	-5.91	1.36	1.46
3	M	2	NAG	C2-N2	-5.89	1.36	1.46
3	2	2	NAG	C2-N2	-5.84	1.36	1.46
3	d	2	NAG	C2-N2	-5.81	1.36	1.46
3	I	2	NAG	C2-N2	-5.81	1.36	1.46
3	y	2	NAG	C2-N2	-5.80	1.36	1.46
3	6	2	NAG	C2-N2	-5.64	1.36	1.46
3	Q	2	NAG	C2-N2	-5.64	1.36	1.46
3	l	2	NAG	C2-N2	-5.63	1.36	1.46
2	Y	2	NAG	C2-N2	-5.62	1.36	1.46
2	D	2	NAG	C2-N2	-5.60	1.36	1.46
2	t	2	NAG	C2-N2	-5.60	1.36	1.46
3	z	2	NAG	C2-N2	-5.49	1.37	1.46
3	J	2	NAG	C2-N2	-5.48	1.37	1.46
3	e	2	NAG	C2-N2	-5.47	1.37	1.46
7	g	2	NAG	C2-N2	-5.46	1.37	1.46
7	L	2	NAG	C2-N2	-5.43	1.37	1.46
7	1	2	NAG	C2-N2	-5.43	1.37	1.46
3	Z	2	NAG	C2-N2	-4.88	1.38	1.46
3	E	2	NAG	C2-N2	-4.88	1.38	1.46
3	u	2	NAG	C2-N2	-4.86	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	0	3	BMA	O2-C2	-4.26	1.34	1.43
6	K	3	BMA	O2-C2	-4.25	1.34	1.43
6	0	8	MAN	O5-C1	4.23	1.50	1.43
6	K	8	MAN	O5-C1	4.23	1.50	1.43
6	f	8	MAN	O5-C1	4.22	1.50	1.43
6	f	3	BMA	O2-C2	-4.20	1.34	1.43
8	q	5	MAN	O2-C2	-4.19	1.34	1.43
2	t	5	MAN	O5-C1	4.19	1.50	1.43
8	V	5	MAN	O2-C2	-4.19	1.34	1.43
2	D	5	MAN	O5-C1	4.18	1.50	1.43
7	s	3	BMA	O2-C2	-4.18	1.34	1.43
7	X	3	BMA	O2-C2	-4.17	1.34	1.43
8	BA	5	MAN	O2-C2	-4.17	1.34	1.43
7	DA	3	BMA	O2-C2	-4.14	1.34	1.43
4	v	4	MAN	O2-C2	-4.14	1.34	1.43
4	F	4	MAN	O2-C2	-4.14	1.34	1.43
2	Y	5	MAN	O5-C1	4.12	1.50	1.43
4	a	4	MAN	O2-C2	-4.12	1.34	1.43
2	t	6	MAN	C4-C5	4.09	1.61	1.53
6	0	6	MAN	O2-C2	-4.09	1.34	1.43
2	Y	5	MAN	C4-C5	4.09	1.61	1.53
2	t	5	MAN	C4-C5	4.08	1.61	1.53
6	f	6	MAN	O2-C2	-4.08	1.34	1.43
6	K	6	MAN	O2-C2	-4.08	1.34	1.43
7	4	3	BMA	O2-C2	-4.08	1.34	1.43
2	Y	6	MAN	C4-C5	4.07	1.61	1.53
2	D	6	MAN	C4-C5	4.07	1.61	1.53
8	V	3	BMA	O2-C2	-4.06	1.34	1.43
8	q	3	BMA	O2-C2	-4.06	1.34	1.43
2	D	5	MAN	C4-C5	4.06	1.61	1.53
7	O	3	BMA	O2-C2	-4.05	1.34	1.43
8	BA	3	BMA	O2-C2	-4.05	1.34	1.43
7	j	3	BMA	O2-C2	-4.04	1.34	1.43
4	p	4	MAN	O2-C2	-4.04	1.34	1.43
4	U	4	MAN	O2-C2	-4.04	1.34	1.43
2	Y	3	BMA	O2-C2	-4.02	1.34	1.43
4	AA	4	MAN	O2-C2	-4.02	1.34	1.43
8	3	3	BMA	O2-C2	-4.01	1.34	1.43
8	N	3	BMA	O2-C2	-3.99	1.34	1.43
8	i	3	BMA	O2-C2	-3.99	1.34	1.43
2	t	3	BMA	O2-C2	-3.99	1.34	1.43
2	D	3	BMA	O2-C2	-3.98	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1	3	BMA	O2-C2	-3.97	1.35	1.43
7	L	3	BMA	O2-C2	-3.96	1.35	1.43
5	H	4	MAN	O2-C2	-3.96	1.35	1.43
5	c	4	MAN	O2-C2	-3.96	1.35	1.43
7	g	3	BMA	O2-C2	-3.96	1.35	1.43
5	H	3	BMA	O2-C2	-3.95	1.35	1.43
5	c	3	BMA	O2-C2	-3.95	1.35	1.43
5	x	4	MAN	O2-C2	-3.95	1.35	1.43
5	x	3	BMA	O2-C2	-3.94	1.35	1.43
8	3	4	MAN	O2-C2	-3.94	1.35	1.43
8	N	4	MAN	O2-C2	-3.93	1.35	1.43
8	i	4	MAN	O2-C2	-3.92	1.35	1.43
8	BA	4	MAN	O2-C2	-3.92	1.35	1.43
4	a	3	BMA	O2-C2	-3.92	1.35	1.43
8	i	5	MAN	O2-C2	-3.91	1.35	1.43
4	p	3	BMA	O2-C2	-3.91	1.35	1.43
8	N	5	MAN	O2-C2	-3.90	1.35	1.43
4	F	3	BMA	O2-C2	-3.90	1.35	1.43
8	V	4	MAN	O2-C2	-3.90	1.35	1.43
4	v	3	BMA	O2-C2	-3.90	1.35	1.43
6	f	8	MAN	O2-C2	-3.89	1.35	1.43
8	3	5	MAN	O2-C2	-3.89	1.35	1.43
8	q	4	MAN	O2-C2	-3.89	1.35	1.43
4	U	3	BMA	O2-C2	-3.88	1.35	1.43
4	AA	3	BMA	O2-C2	-3.88	1.35	1.43
6	0	8	MAN	O2-C2	-3.88	1.35	1.43
6	K	8	MAN	O2-C2	-3.87	1.35	1.43
7	1	1	NAG	C4-C3	3.84	1.62	1.52
7	L	1	NAG	C4-C3	3.82	1.62	1.52
7	g	1	NAG	C4-C3	3.80	1.62	1.52
2	D	6	MAN	O2-C2	-3.80	1.35	1.43
2	Y	6	MAN	O2-C2	-3.79	1.35	1.43
2	Y	5	MAN	O2-C2	-3.79	1.35	1.43
2	D	5	MAN	O2-C2	-3.79	1.35	1.43
2	t	5	MAN	O2-C2	-3.78	1.35	1.43
2	t	6	MAN	O2-C2	-3.75	1.35	1.43
6	0	8	MAN	C4-C5	3.74	1.60	1.53
6	f	8	MAN	C4-C5	3.74	1.60	1.53
6	K	8	MAN	C4-C5	3.73	1.60	1.53
6	0	7	MAN	O2-C2	-3.68	1.35	1.43
6	K	7	MAN	O2-C2	-3.67	1.35	1.43
6	f	7	MAN	O2-C2	-3.67	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	MAN	O5-C1	3.56	1.49	1.43
2	t	6	MAN	O5-C1	3.52	1.49	1.43
2	Y	6	MAN	O5-C1	3.52	1.49	1.43
7	g	3	BMA	O5-C1	3.51	1.49	1.43
7	L	3	BMA	O5-C1	3.50	1.49	1.43
7	1	3	BMA	O5-C1	3.47	1.49	1.43
3	E	2	NAG	C4-C5	3.44	1.60	1.53
3	u	2	NAG	C4-C5	3.44	1.60	1.53
3	Z	2	NAG	C4-C5	3.44	1.60	1.53
8	3	4	MAN	O5-C1	3.36	1.49	1.43
8	N	4	MAN	O5-C1	3.35	1.49	1.43
8	i	4	MAN	O5-C1	3.35	1.49	1.43
8	BA	4	MAN	O5-C1	3.32	1.49	1.43
8	V	4	MAN	O5-C1	3.31	1.49	1.43
8	q	4	MAN	O5-C1	3.30	1.49	1.43
3	u	2	NAG	C4-C3	3.29	1.60	1.52
3	Z	2	NAG	C4-C3	3.28	1.60	1.52
2	D	2	NAG	C4-C3	3.27	1.60	1.52
3	E	2	NAG	C4-C3	3.27	1.60	1.52
2	Y	2	NAG	C4-C3	3.26	1.60	1.52
2	t	2	NAG	C4-C3	3.25	1.60	1.52
2	t	4	MAN	O5-C1	3.24	1.48	1.43
2	D	4	MAN	O5-C1	3.23	1.48	1.43
4	F	4	MAN	O5-C1	3.19	1.48	1.43
4	v	4	MAN	O5-C1	3.18	1.48	1.43
4	a	4	MAN	O5-C1	3.18	1.48	1.43
2	Y	4	MAN	O5-C1	3.18	1.48	1.43
6	K	4	MAN	O2-C2	-3.17	1.36	1.43
6	f	4	MAN	O2-C2	-3.17	1.36	1.43
6	0	4	MAN	O2-C2	-3.15	1.36	1.43
6	0	6	MAN	O5-C1	3.15	1.48	1.43
6	K	6	MAN	O5-C1	3.12	1.48	1.43
6	f	6	MAN	O5-C1	3.11	1.48	1.43
7	DA	2	NAG	C4-C3	3.07	1.60	1.52
7	s	2	NAG	C4-C3	3.06	1.60	1.52
7	X	2	NAG	C4-C3	3.05	1.60	1.52
2	t	4	MAN	O2-C2	-3.04	1.36	1.43
2	t	5	MAN	O5-C5	3.04	1.49	1.43
7	j	3	BMA	O5-C1	3.04	1.48	1.43
2	Y	4	MAN	O2-C2	-3.03	1.36	1.43
7	O	3	BMA	O5-C1	3.02	1.48	1.43
2	D	5	MAN	O5-C5	3.00	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	MAN	O2-C2	-3.00	1.37	1.43
2	Y	5	MAN	O5-C5	2.99	1.49	1.43
7	4	3	BMA	O5-C1	2.98	1.48	1.43
6	f	5	MAN	O2-C2	-2.98	1.37	1.43
6	K	5	MAN	O2-C2	-2.97	1.37	1.43
7	s	3	BMA	O5-C1	2.96	1.48	1.43
7	DA	3	BMA	O5-C1	2.96	1.48	1.43
6	0	5	MAN	O2-C2	-2.96	1.37	1.43
2	Y	6	MAN	O5-C5	2.95	1.49	1.43
2	D	6	MAN	O5-C5	2.94	1.49	1.43
4	p	4	MAN	O5-C1	2.94	1.48	1.43
7	X	3	BMA	O5-C1	2.94	1.48	1.43
4	U	4	MAN	O5-C1	2.93	1.48	1.43
4	AA	4	MAN	O5-C1	2.93	1.48	1.43
6	f	8	MAN	O5-C5	2.93	1.49	1.43
2	t	6	MAN	O5-C5	2.92	1.49	1.43
6	K	8	MAN	O5-C5	2.91	1.49	1.43
6	0	8	MAN	O5-C5	2.91	1.49	1.43
2	t	6	MAN	C1-C2	2.90	1.58	1.52
7	1	2	NAG	C4-C5	2.89	1.59	1.53
7	L	2	NAG	C4-C5	2.89	1.59	1.53
7	g	2	NAG	C4-C5	2.88	1.59	1.53
2	Y	6	MAN	C1-C2	2.88	1.58	1.52
2	D	6	MAN	C1-C2	2.87	1.58	1.52
8	q	2	NAG	C4-C3	2.86	1.59	1.52
8	V	2	NAG	C4-C3	2.84	1.59	1.52
8	BA	2	NAG	C4-C3	2.81	1.59	1.52
5	H	2	NAG	C4-C3	2.80	1.59	1.52
5	c	2	NAG	C4-C3	2.80	1.59	1.52
2	D	2	NAG	C4-C5	2.80	1.58	1.53
2	Y	4	MAN	C4-C5	2.80	1.58	1.53
5	x	2	NAG	C4-C3	2.80	1.59	1.52
2	t	2	NAG	C4-C5	2.78	1.58	1.53
2	Y	2	NAG	C4-C5	2.78	1.58	1.53
2	D	4	MAN	C4-C5	2.77	1.58	1.53
2	t	4	MAN	C4-C5	2.75	1.58	1.53
2	t	5	MAN	C1-C2	2.73	1.58	1.52
2	D	5	MAN	C1-C2	2.72	1.58	1.52
2	Y	5	MAN	C1-C2	2.72	1.58	1.52
6	f	7	MAN	O5-C1	2.69	1.48	1.43
3	Q	1	NAG	C4-C3	2.69	1.59	1.52
7	1	2	NAG	C4-C3	2.69	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	2	NAG	C4-C3	2.69	1.59	1.52
8	BA	5	MAN	O5-C1	2.69	1.48	1.43
7	g	2	NAG	C4-C3	2.69	1.59	1.52
3	6	1	NAG	C4-C3	2.68	1.59	1.52
3	l	1	NAG	C4-C3	2.68	1.59	1.52
6	0	7	MAN	O5-C1	2.67	1.48	1.43
6	K	7	MAN	O5-C1	2.67	1.48	1.43
5	c	4	MAN	O5-C1	2.64	1.47	1.43
8	q	5	MAN	O5-C1	2.64	1.47	1.43
8	V	5	MAN	O5-C1	2.63	1.47	1.43
3	8	2	NAG	C4-C3	2.63	1.59	1.52
2	D	3	BMA	O5-C1	2.63	1.47	1.43
2	t	3	BMA	O5-C1	2.63	1.47	1.43
5	H	4	MAN	O5-C1	2.63	1.47	1.43
3	S	2	NAG	C4-C3	2.62	1.59	1.52
5	x	4	MAN	O5-C1	2.61	1.47	1.43
3	b	2	NAG	C4-C3	2.61	1.59	1.52
3	G	2	NAG	C4-C3	2.60	1.59	1.52
3	w	2	NAG	C4-C3	2.60	1.58	1.52
3	n	2	NAG	C4-C3	2.59	1.58	1.52
2	Y	3	BMA	O5-C1	2.58	1.47	1.43
8	3	5	MAN	O5-C1	2.58	1.47	1.43
8	i	5	MAN	O5-C1	2.58	1.47	1.43
4	F	2	NAG	C4-C3	2.55	1.58	1.52
8	N	5	MAN	O5-C1	2.54	1.47	1.43
4	v	2	NAG	C4-C3	2.54	1.58	1.52
4	a	2	NAG	C4-C3	2.53	1.58	1.52
8	V	5	MAN	C4-C5	2.52	1.58	1.53
7	L	1	NAG	C4-C5	2.52	1.58	1.53
3	m	2	NAG	C4-C3	2.52	1.58	1.52
7	1	1	NAG	C4-C5	2.52	1.58	1.53
8	3	5	MAN	C4-C5	2.52	1.58	1.53
3	7	2	NAG	C4-C3	2.51	1.58	1.52
3	R	2	NAG	C4-C3	2.50	1.58	1.52
7	g	1	NAG	C4-C5	2.50	1.58	1.53
7	O	2	NAG	C4-C3	2.50	1.58	1.52
3	e	1	NAG	C4-C3	2.49	1.58	1.52
3	z	1	NAG	C4-C3	2.49	1.58	1.52
8	BA	5	MAN	C4-C5	2.49	1.58	1.53
7	4	2	NAG	C4-C3	2.49	1.58	1.52
8	N	5	MAN	C4-C5	2.49	1.58	1.53
8	q	5	MAN	C4-C5	2.48	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1	NAG	C4-C3	2.48	1.58	1.52
8	i	5	MAN	C4-C5	2.47	1.58	1.53
8	i	2	NAG	C4-C3	2.47	1.58	1.52
7	j	2	NAG	C4-C3	2.47	1.58	1.52
6	K	1	NAG	C4-C3	2.46	1.58	1.52
6	f	1	NAG	C4-C3	2.46	1.58	1.52
6	0	1	NAG	C4-C3	2.45	1.58	1.52
3	T	2	NAG	C4-C3	2.45	1.58	1.52
3	9	2	NAG	C4-C3	2.45	1.58	1.52
3	o	2	NAG	C4-C3	2.45	1.58	1.52
4	AA	4	MAN	C4-C5	2.45	1.58	1.53
4	U	4	MAN	C4-C5	2.44	1.58	1.53
8	N	2	NAG	C4-C3	2.43	1.58	1.52
8	i	4	MAN	C4-C5	2.43	1.58	1.53
3	I	2	NAG	C4-C3	2.43	1.58	1.52
3	y	2	NAG	C4-C3	2.43	1.58	1.52
3	d	2	NAG	C4-C3	2.43	1.58	1.52
8	3	4	MAN	C4-C5	2.42	1.58	1.53
4	p	4	MAN	C4-C5	2.42	1.58	1.53
8	N	4	MAN	C4-C5	2.42	1.58	1.53
3	W	1	NAG	C1-C2	-2.42	1.48	1.52
6	K	7	MAN	C4-C5	2.41	1.58	1.53
3	CA	1	NAG	C1-C2	-2.41	1.48	1.52
8	BA	1	NAG	C4-C3	2.41	1.58	1.52
6	0	7	MAN	C4-C5	2.41	1.58	1.53
8	3	2	NAG	C4-C3	2.41	1.58	1.52
3	r	1	NAG	C1-C2	-2.40	1.48	1.52
6	K	2	NAG	C4-C3	2.40	1.58	1.52
8	V	1	NAG	C4-C3	2.39	1.58	1.52
6	f	2	NAG	C4-C3	2.39	1.58	1.52
6	f	7	MAN	C4-C5	2.39	1.58	1.53
3	E	2	NAG	C1-C2	2.39	1.55	1.52
6	0	2	NAG	C4-C3	2.39	1.58	1.52
3	u	2	NAG	C1-C2	2.39	1.55	1.52
8	q	1	NAG	C4-C3	2.38	1.58	1.52
3	8	1	NAG	C4-C3	2.38	1.58	1.52
3	k	1	NAG	C4-C3	2.38	1.58	1.52
2	t	3	BMA	C4-C5	2.38	1.58	1.53
3	Z	2	NAG	C1-C2	2.38	1.55	1.52
3	5	1	NAG	C4-C3	2.38	1.58	1.52
3	P	1	NAG	C4-C3	2.37	1.58	1.52
8	V	4	MAN	C4-C5	2.37	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	BMA	C4-C5	2.37	1.58	1.53
8	q	4	MAN	C4-C5	2.37	1.58	1.53
3	E	1	NAG	C4-C3	2.36	1.58	1.52
3	S	1	NAG	C4-C3	2.36	1.58	1.52
3	n	1	NAG	C4-C3	2.36	1.58	1.52
3	Z	1	NAG	C4-C3	2.36	1.58	1.52
3	5	2	NAG	C4-C3	2.36	1.58	1.52
2	Y	3	BMA	C4-C5	2.36	1.58	1.53
3	u	1	NAG	C4-C3	2.35	1.58	1.52
4	U	1	NAG	C4-C3	2.35	1.58	1.52
3	k	2	NAG	C4-C3	2.34	1.58	1.52
7	X	1	NAG	C4-C3	2.34	1.58	1.52
3	P	2	NAG	C4-C3	2.34	1.58	1.52
4	AA	1	NAG	C4-C3	2.34	1.58	1.52
3	M	1	NAG	C4-C3	2.34	1.58	1.52
3	2	1	NAG	C4-C3	2.34	1.58	1.52
4	p	1	NAG	C4-C3	2.34	1.58	1.52
3	9	1	NAG	C4-C3	2.33	1.58	1.52
8	BA	4	MAN	C4-C5	2.33	1.57	1.53
3	h	1	NAG	C4-C3	2.33	1.58	1.52
3	o	1	NAG	C4-C3	2.33	1.58	1.52
3	I	1	NAG	C4-C3	2.33	1.58	1.52
3	z	2	NAG	C4-C3	2.33	1.58	1.52
3	J	2	NAG	C4-C3	2.33	1.58	1.52
7	s	1	NAG	C4-C3	2.33	1.58	1.52
3	T	1	NAG	C4-C3	2.33	1.58	1.52
3	e	2	NAG	C4-C3	2.32	1.58	1.52
3	d	1	NAG	C4-C3	2.32	1.58	1.52
7	DA	1	NAG	C4-C3	2.32	1.58	1.52
4	a	3	BMA	O5-C1	2.32	1.47	1.43
4	F	3	BMA	O5-C1	2.32	1.47	1.43
3	y	1	NAG	C4-C3	2.31	1.58	1.52
3	m	1	NAG	C4-C3	2.31	1.58	1.52
2	Y	5	MAN	C6-C5	2.31	1.59	1.51
2	D	5	MAN	C6-C5	2.30	1.59	1.51
2	t	5	MAN	C6-C5	2.30	1.59	1.51
4	v	3	BMA	O5-C1	2.30	1.47	1.43
6	0	4	MAN	O5-C1	2.30	1.47	1.43
3	M	2	NAG	C4-C3	2.30	1.58	1.52
3	R	1	NAG	C4-C3	2.29	1.58	1.52
3	7	1	NAG	C4-C3	2.28	1.58	1.52
6	K	4	MAN	O5-C1	2.28	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	4	MAN	O5-C1	2.28	1.47	1.43
5	x	4	MAN	C4-C5	2.28	1.57	1.53
3	2	2	NAG	C4-C3	2.27	1.58	1.52
5	c	4	MAN	C4-C5	2.27	1.57	1.53
3	h	2	NAG	C4-C3	2.27	1.58	1.52
5	H	4	MAN	C4-C5	2.27	1.57	1.53
6	0	8	MAN	C6-C5	2.25	1.59	1.51
4	a	4	MAN	C4-C5	2.25	1.57	1.53
4	AA	2	NAG	C4-C3	2.25	1.58	1.52
2	Y	6	MAN	C6-C5	2.25	1.59	1.51
6	K	8	MAN	C6-C5	2.25	1.59	1.51
4	F	4	MAN	C4-C5	2.25	1.57	1.53
6	f	8	MAN	C6-C5	2.25	1.59	1.51
8	BA	4	MAN	C6-C5	2.25	1.59	1.51
4	p	2	NAG	C4-C3	2.25	1.58	1.52
4	v	4	MAN	C4-C5	2.25	1.57	1.53
8	q	4	MAN	C6-C5	2.24	1.59	1.51
4	U	2	NAG	C4-C3	2.24	1.58	1.52
2	D	6	MAN	C6-C5	2.24	1.59	1.51
8	V	4	MAN	C6-C5	2.24	1.59	1.51
4	F	1	NAG	C4-C3	2.22	1.58	1.52
3	n	2	NAG	C4-C5	2.22	1.57	1.53
2	t	6	MAN	C6-C5	2.22	1.59	1.51
7	DA	3	BMA	C4-C5	2.22	1.57	1.53
7	s	3	BMA	C4-C5	2.21	1.57	1.53
3	S	2	NAG	C4-C5	2.21	1.57	1.53
4	v	1	NAG	C4-C3	2.21	1.58	1.52
7	X	3	BMA	C4-C5	2.21	1.57	1.53
4	a	1	NAG	C4-C3	2.21	1.58	1.52
7	g	3	BMA	C4-C5	2.21	1.57	1.53
3	8	2	NAG	C4-C5	2.20	1.57	1.53
7	L	3	BMA	C4-C5	2.19	1.57	1.53
6	0	6	MAN	C4-C5	2.19	1.57	1.53
6	K	6	MAN	C4-C5	2.19	1.57	1.53
5	c	3	BMA	O5-C1	2.19	1.47	1.43
5	H	3	BMA	O5-C1	2.19	1.47	1.43
6	K	8	MAN	C1-C2	2.18	1.57	1.52
7	1	3	BMA	C4-C5	2.18	1.57	1.53
2	Y	1	NAG	C4-C3	2.18	1.57	1.52
8	i	3	BMA	C2-C3	-2.18	1.49	1.52
5	x	1	NAG	C4-C3	2.18	1.57	1.52
5	x	3	BMA	O5-C1	2.18	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	8	MAN	C1-C2	2.17	1.57	1.52
2	t	1	NAG	C4-C3	2.17	1.57	1.52
5	H	1	NAG	C4-C3	2.17	1.57	1.52
8	N	3	BMA	C2-C3	-2.17	1.49	1.52
6	0	8	MAN	C1-C2	2.17	1.57	1.52
5	c	1	NAG	C4-C3	2.17	1.57	1.52
8	3	3	BMA	C2-C3	-2.17	1.49	1.52
6	f	6	MAN	C4-C5	2.16	1.57	1.53
2	D	1	NAG	C4-C3	2.16	1.57	1.52
6	f	2	NAG	C4-C5	2.15	1.57	1.53
3	G	1	NAG	C4-C3	2.15	1.57	1.52
7	4	1	NAG	C4-C3	2.15	1.57	1.52
7	O	1	NAG	C4-C3	2.15	1.57	1.52
3	w	1	NAG	C4-C3	2.15	1.57	1.52
7	j	1	NAG	C4-C3	2.14	1.57	1.52
7	1	3	BMA	C6-C5	2.14	1.59	1.51
6	K	2	NAG	C4-C5	2.14	1.57	1.53
7	L	3	BMA	C6-C5	2.14	1.59	1.51
3	b	1	NAG	C4-C3	2.14	1.57	1.52
7	g	3	BMA	C6-C5	2.14	1.59	1.51
6	f	5	MAN	O5-C1	2.14	1.47	1.43
6	K	5	MAN	O5-C1	2.14	1.47	1.43
6	0	2	NAG	C4-C5	2.12	1.57	1.53
8	3	1	NAG	C4-C3	2.12	1.57	1.52
6	K	7	MAN	C6-C5	2.12	1.59	1.51
6	0	7	MAN	C6-C5	2.11	1.58	1.51
8	BA	2	NAG	C4-C5	2.11	1.57	1.53
5	H	3	BMA	C6-C5	2.11	1.58	1.51
3	6	1	NAG	C4-C5	2.11	1.57	1.53
6	0	5	MAN	O5-C1	2.11	1.47	1.43
6	f	5	MAN	C6-C5	2.10	1.58	1.51
8	N	1	NAG	C4-C3	2.10	1.57	1.52
8	BA	3	BMA	C2-C3	-2.10	1.49	1.52
8	q	3	BMA	C2-C3	-2.10	1.49	1.52
4	U	3	BMA	O5-C1	2.10	1.47	1.43
3	Q	1	NAG	C4-C5	2.10	1.57	1.53
8	i	1	NAG	C4-C3	2.10	1.57	1.52
8	V	3	BMA	C2-C3	-2.10	1.49	1.52
2	t	4	MAN	C6-C5	2.09	1.58	1.51
2	Y	4	MAN	C6-C5	2.09	1.58	1.51
5	c	3	BMA	C6-C5	2.09	1.58	1.51
8	V	2	NAG	C4-C5	2.09	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	5	MAN	C6-C5	2.09	1.58	1.51
6	f	7	MAN	C6-C5	2.09	1.58	1.51
4	p	3	BMA	O5-C1	2.09	1.47	1.43
6	0	5	MAN	C6-C5	2.09	1.58	1.51
3	I	2	NAG	C4-C5	2.09	1.57	1.53
3	l	1	NAG	C4-C5	2.09	1.57	1.53
5	x	3	BMA	C6-C5	2.08	1.58	1.51
2	D	4	MAN	C6-C5	2.08	1.58	1.51
4	AA	3	BMA	O5-C1	2.08	1.47	1.43
3	d	2	NAG	C4-C5	2.08	1.57	1.53
3	y	2	NAG	C4-C5	2.08	1.57	1.53
3	CA	1	NAG	C3-C2	-2.08	1.48	1.52
8	q	2	NAG	C4-C5	2.08	1.57	1.53
7	j	2	NAG	C4-C5	2.07	1.57	1.53
3	W	1	NAG	C3-C2	-2.07	1.48	1.52
3	r	1	NAG	C3-C2	-2.06	1.48	1.52
7	O	2	NAG	C4-C5	2.06	1.57	1.53
7	4	2	NAG	C4-C5	2.06	1.57	1.53
8	N	4	MAN	C6-C5	2.06	1.58	1.51
3	k	2	NAG	C4-C5	2.05	1.57	1.53
7	O	3	BMA	C4-C5	2.05	1.57	1.53
8	i	4	MAN	C6-C5	2.05	1.58	1.51
3	5	2	NAG	C4-C5	2.05	1.57	1.53
7	j	3	BMA	C4-C5	2.05	1.57	1.53
8	3	4	MAN	C6-C5	2.05	1.58	1.51
3	P	2	NAG	C4-C5	2.05	1.57	1.53
7	4	3	BMA	C4-C5	2.04	1.57	1.53
4	a	3	BMA	C6-C5	2.04	1.58	1.51
2	t	5	MAN	C4-C3	2.04	1.57	1.52
8	BA	3	BMA	C6-C5	2.04	1.58	1.51
8	q	3	BMA	C6-C5	2.04	1.58	1.51
8	V	3	BMA	C6-C5	2.03	1.58	1.51
4	F	3	BMA	C6-C5	2.03	1.58	1.51
6	K	3	BMA	C4-C5	2.03	1.57	1.53
6	f	3	BMA	C4-C5	2.03	1.57	1.53
2	t	3	BMA	C6-C5	2.03	1.58	1.51
8	i	5	MAN	C6-C5	2.03	1.58	1.51
2	D	5	MAN	C4-C3	2.02	1.57	1.52
6	0	3	BMA	C4-C5	2.02	1.57	1.53
8	q	5	MAN	C6-C5	2.02	1.58	1.51
3	o	2	NAG	C4-C5	2.02	1.57	1.53
4	v	3	BMA	C6-C5	2.02	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	5	MAN	C6-C5	2.02	1.58	1.51
2	D	3	BMA	C6-C5	2.02	1.58	1.51
3	b	2	NAG	C4-C5	2.01	1.57	1.53
3	G	2	NAG	C4-C5	2.01	1.57	1.53
3	T	2	NAG	C4-C5	2.01	1.57	1.53
3	9	2	NAG	C4-C5	2.01	1.57	1.53
3	l	2	NAG	C4-C3	2.01	1.57	1.52
3	6	2	NAG	C4-C3	2.01	1.57	1.52
8	N	3	BMA	C6-C5	2.01	1.58	1.51
3	w	2	NAG	C4-C5	2.01	1.57	1.53
6	K	8	MAN	C4-C3	2.00	1.57	1.52

All (1061) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	e	1	NAG	O5-C5-C6	-22.93	71.26	107.20
3	z	1	NAG	O5-C5-C6	-22.92	71.27	107.20
3	J	1	NAG	O5-C5-C6	-22.92	71.27	107.20
6	0	4	MAN	O3-C3-C2	21.80	151.74	109.99
6	f	4	MAN	O3-C3-C2	21.80	151.73	109.99
6	K	4	MAN	O3-C3-C2	21.78	151.70	109.99
4	F	2	NAG	O5-C5-C6	-20.58	74.93	107.20
4	a	2	NAG	O5-C5-C6	-20.58	74.94	107.20
4	v	2	NAG	O5-C5-C6	-20.56	74.97	107.20
8	i	2	NAG	O5-C5-C6	-20.46	75.13	107.20
8	N	2	NAG	O5-C5-C6	-20.45	75.14	107.20
8	3	2	NAG	O5-C5-C6	-20.45	75.15	107.20
3	W	1	NAG	O5-C5-C6	-19.84	76.11	107.20
3	r	1	NAG	O5-C5-C6	-19.83	76.12	107.20
3	CA	1	NAG	O5-C5-C6	-19.83	76.12	107.20
7	s	2	NAG	O5-C5-C6	-19.77	76.21	107.20
7	DA	2	NAG	O5-C5-C6	-19.77	76.21	107.20
7	X	2	NAG	O5-C5-C6	-19.76	76.23	107.20
4	p	1	NAG	O5-C5-C6	-19.38	76.82	107.20
4	U	1	NAG	O5-C5-C6	-19.38	76.83	107.20
4	AA	1	NAG	O5-C5-C6	-19.35	76.86	107.20
4	v	1	NAG	C1-C2-N2	18.74	142.51	110.49
4	F	1	NAG	C1-C2-N2	18.74	142.50	110.49
4	a	1	NAG	C1-C2-N2	18.73	142.49	110.49
3	I	1	NAG	O5-C5-C6	-18.32	78.48	107.20
3	d	1	NAG	O5-C5-C6	-18.32	78.49	107.20
3	y	1	NAG	O5-C5-C6	-18.30	78.52	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	2	NAG	O5-C5-C6	-18.14	78.77	107.20
2	D	2	NAG	O5-C5-C6	-18.13	78.78	107.20
2	t	2	NAG	O5-C5-C6	-18.13	78.79	107.20
7	L	1	NAG	O4-C4-C3	-17.73	69.36	110.35
7	g	1	NAG	O4-C4-C3	-17.73	69.37	110.35
7	1	1	NAG	O4-C4-C3	-17.72	69.37	110.35
6	f	4	MAN	O3-C3-C4	-17.23	70.52	110.35
6	0	4	MAN	O3-C3-C4	-17.23	70.53	110.35
6	K	4	MAN	O3-C3-C4	-17.22	70.54	110.35
3	w	2	NAG	O5-C5-C6	-16.16	81.87	107.20
3	G	2	NAG	O5-C5-C6	-16.14	81.90	107.20
3	b	2	NAG	O5-C5-C6	-16.14	81.91	107.20
3	M	1	NAG	O5-C5-C6	-15.66	82.66	107.20
3	2	1	NAG	O5-C5-C6	-15.65	82.66	107.20
3	h	1	NAG	O5-C5-C6	-15.65	82.67	107.20
4	v	2	NAG	C6-C5-C4	15.44	149.18	113.00
4	F	2	NAG	C6-C5-C4	15.44	149.17	113.00
4	a	2	NAG	C6-C5-C4	15.44	149.16	113.00
6	K	4	MAN	O5-C5-C6	-15.16	83.44	107.20
6	f	4	MAN	O5-C5-C6	-15.16	83.44	107.20
6	0	4	MAN	O5-C5-C6	-15.14	83.46	107.20
6	f	7	MAN	O5-C5-C6	-14.74	84.10	107.20
6	0	7	MAN	O5-C5-C6	-14.73	84.12	107.20
6	K	7	MAN	O5-C5-C6	-14.72	84.12	107.20
3	T	1	NAG	O5-C5-C6	-14.50	84.47	107.20
3	9	1	NAG	O5-C5-C6	-14.50	84.47	107.20
3	o	1	NAG	O5-C5-C6	-14.49	84.50	107.20
6	f	5	MAN	O5-C5-C6	-14.48	84.51	107.20
6	K	5	MAN	O5-C5-C6	-14.47	84.52	107.20
6	0	5	MAN	O5-C5-C6	-14.47	84.53	107.20
5	c	2	NAG	O5-C5-C6	-14.12	85.07	107.20
5	H	2	NAG	O5-C5-C6	-14.11	85.08	107.20
5	x	2	NAG	O5-C5-C6	-14.11	85.09	107.20
6	0	3	BMA	O3-C3-C2	14.06	136.92	109.99
6	K	3	BMA	O3-C3-C2	14.03	136.87	109.99
6	f	3	BMA	O3-C3-C2	14.03	136.85	109.99
3	W	1	NAG	C1-C2-N2	13.69	133.87	110.49
3	r	1	NAG	C1-C2-N2	13.68	133.86	110.49
3	CA	1	NAG	C1-C2-N2	13.68	133.85	110.49
6	f	7	MAN	O3-C3-C2	-13.39	84.36	109.99
6	K	7	MAN	O3-C3-C2	-13.38	84.37	109.99
6	0	7	MAN	O3-C3-C2	-13.37	84.38	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	AA	3	BMA	O3-C3-C2	-13.37	84.39	109.99
4	U	3	BMA	O3-C3-C2	-13.36	84.40	109.99
4	p	3	BMA	O3-C3-C2	-13.36	84.40	109.99
3	8	1	NAG	O4-C4-C3	-13.03	80.22	110.35
3	n	1	NAG	O4-C4-C3	-13.03	80.22	110.35
3	S	1	NAG	O4-C4-C3	-13.03	80.23	110.35
2	t	4	MAN	O5-C5-C6	-12.76	87.20	107.20
3	Z	2	NAG	O5-C5-C6	-12.76	87.21	107.20
3	E	2	NAG	O5-C5-C6	-12.74	87.23	107.20
8	BA	5	MAN	O5-C5-C6	-12.74	87.23	107.20
2	D	4	MAN	O5-C5-C6	-12.73	87.25	107.20
2	Y	4	MAN	O5-C5-C6	-12.72	87.26	107.20
8	q	5	MAN	O5-C5-C6	-12.72	87.26	107.20
3	u	2	NAG	O5-C5-C6	-12.71	87.27	107.20
8	V	5	MAN	O5-C5-C6	-12.71	87.28	107.20
5	c	4	MAN	O5-C5-C6	-12.62	87.43	107.20
5	H	4	MAN	O5-C5-C6	-12.61	87.43	107.20
5	x	4	MAN	O5-C5-C6	-12.59	87.47	107.20
4	U	2	NAG	O5-C5-C6	-12.40	87.76	107.20
4	AA	2	NAG	O5-C5-C6	-12.40	87.77	107.20
4	p	2	NAG	O5-C5-C6	-12.39	87.77	107.20
8	N	2	NAG	C6-C5-C4	12.36	141.94	113.00
8	3	2	NAG	C6-C5-C4	12.36	141.94	113.00
8	i	2	NAG	C6-C5-C4	12.35	141.94	113.00
3	R	2	NAG	O5-C5-C6	-12.09	88.25	107.20
3	7	2	NAG	O5-C5-C6	-12.09	88.26	107.20
6	K	3	BMA	C6-C5-C4	12.08	141.30	113.00
3	m	2	NAG	O5-C5-C6	-12.08	88.27	107.20
6	0	3	BMA	C6-C5-C4	12.08	141.29	113.00
6	f	3	BMA	C6-C5-C4	12.07	141.28	113.00
6	f	3	BMA	O5-C5-C6	-11.99	88.40	107.20
6	K	3	BMA	O5-C5-C6	-11.98	88.42	107.20
6	0	3	BMA	O5-C5-C6	-11.97	88.43	107.20
2	Y	1	NAG	O5-C5-C6	-11.94	88.49	107.20
2	D	1	NAG	O5-C5-C6	-11.94	88.49	107.20
2	t	1	NAG	O5-C5-C6	-11.93	88.50	107.20
6	f	1	NAG	C6-C5-C4	11.71	140.42	113.00
6	K	1	NAG	C6-C5-C4	11.70	140.40	113.00
6	0	1	NAG	C6-C5-C4	11.69	140.38	113.00
3	u	1	NAG	O5-C5-C6	-11.64	88.95	107.20
3	Z	1	NAG	O5-C5-C6	-11.64	88.96	107.20
3	E	1	NAG	O5-C5-C6	-11.63	88.97	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	1	NAG	O4-C4-C3	11.56	137.08	110.35
3	l	1	NAG	O4-C4-C3	11.56	137.07	110.35
3	6	1	NAG	O4-C4-C3	11.56	137.06	110.35
7	DA	2	NAG	O4-C4-C3	11.55	137.06	110.35
7	X	2	NAG	O4-C4-C3	11.54	137.03	110.35
7	s	2	NAG	O4-C4-C3	11.53	137.01	110.35
6	K	8	MAN	O5-C5-C6	-11.42	89.30	107.20
6	f	8	MAN	O5-C5-C6	-11.42	89.30	107.20
6	0	8	MAN	O5-C5-C6	-11.41	89.31	107.20
8	q	2	NAG	O5-C5-C6	-11.38	89.36	107.20
8	V	2	NAG	O5-C5-C6	-11.37	89.39	107.20
8	BA	2	NAG	O5-C5-C6	-11.36	89.39	107.20
7	1	1	NAG	O5-C5-C6	-11.36	89.40	107.20
7	L	1	NAG	O5-C5-C6	-11.35	89.41	107.20
7	g	1	NAG	O5-C5-C6	-11.35	89.42	107.20
4	a	2	NAG	O3-C3-C2	-11.33	86.02	109.47
4	F	2	NAG	O3-C3-C2	-11.32	86.04	109.47
4	v	2	NAG	O3-C3-C2	-11.32	86.05	109.47
3	9	1	NAG	C6-C5-C4	11.30	139.46	113.00
3	T	1	NAG	C6-C5-C4	11.29	139.45	113.00
3	o	1	NAG	C6-C5-C4	11.27	139.40	113.00
7	s	1	NAG	O4-C4-C3	-11.27	84.30	110.35
7	X	1	NAG	O4-C4-C3	-11.26	84.31	110.35
7	DA	1	NAG	O4-C4-C3	-11.26	84.33	110.35
3	l	1	NAG	O3-C3-C2	-11.16	86.37	109.47
3	6	1	NAG	O3-C3-C2	-11.15	86.39	109.47
8	BA	2	NAG	O4-C4-C3	11.15	136.13	110.35
3	Q	1	NAG	O3-C3-C2	-11.14	86.41	109.47
8	V	2	NAG	O4-C4-C3	11.13	136.09	110.35
8	q	2	NAG	O4-C4-C3	11.12	136.07	110.35
3	m	1	NAG	O5-C5-C6	-11.03	89.92	107.20
3	R	1	NAG	O5-C5-C6	-11.02	89.93	107.20
3	7	1	NAG	O5-C5-C6	-11.01	89.94	107.20
3	G	2	NAG	C6-C5-C4	10.89	138.51	113.00
3	w	2	NAG	C6-C5-C4	10.89	138.50	113.00
3	b	2	NAG	C6-C5-C4	10.88	138.49	113.00
6	f	2	NAG	O4-C4-C3	10.77	135.25	110.35
6	K	2	NAG	O4-C4-C3	10.76	135.23	110.35
6	0	2	NAG	O4-C4-C3	10.74	135.18	110.35
6	f	6	MAN	O5-C5-C6	-10.72	90.40	107.20
6	0	6	MAN	O5-C5-C6	-10.71	90.42	107.20
6	K	6	MAN	O5-C5-C6	-10.70	90.43	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	2	NAG	O3-C3-C2	-10.66	87.40	109.47
8	BA	2	NAG	O3-C3-C2	-10.66	87.41	109.47
8	V	2	NAG	O3-C3-C2	-10.65	87.42	109.47
8	3	1	NAG	O5-C5-C6	-10.59	90.60	107.20
8	N	1	NAG	O5-C5-C6	-10.58	90.62	107.20
8	i	1	NAG	O5-C5-C6	-10.57	90.64	107.20
3	R	1	NAG	C6-C5-C4	10.50	137.60	113.00
3	m	1	NAG	C6-C5-C4	10.49	137.57	113.00
8	q	3	BMA	O2-C2-C3	10.48	131.14	110.14
3	7	1	NAG	C6-C5-C4	10.48	137.55	113.00
8	BA	3	BMA	O2-C2-C3	10.48	131.12	110.14
8	V	3	BMA	O2-C2-C3	10.47	131.12	110.14
7	O	3	BMA	O5-C5-C6	-10.43	90.86	107.20
7	j	3	BMA	O5-C5-C6	-10.42	90.86	107.20
7	4	3	BMA	O5-C5-C6	-10.41	90.88	107.20
4	v	2	NAG	C1-C2-N2	-10.41	92.71	110.49
8	BA	2	NAG	C1-C2-N2	-10.40	92.72	110.49
8	V	2	NAG	C1-C2-N2	-10.40	92.72	110.49
4	F	2	NAG	C1-C2-N2	-10.39	92.73	110.49
8	q	2	NAG	C1-C2-N2	-10.39	92.74	110.49
4	a	2	NAG	C1-C2-N2	-10.39	92.74	110.49
8	q	1	NAG	O4-C4-C3	-10.38	86.35	110.35
8	V	1	NAG	O4-C4-C3	-10.38	86.36	110.35
8	BA	1	NAG	O4-C4-C3	-10.37	86.38	110.35
4	a	2	NAG	O4-C4-C3	10.35	134.28	110.35
4	v	2	NAG	O4-C4-C3	10.34	134.26	110.35
2	Y	6	MAN	O5-C5-C6	-10.34	90.99	107.20
4	F	2	NAG	O4-C4-C3	10.34	134.25	110.35
2	D	6	MAN	O5-C5-C6	-10.34	91.00	107.20
7	s	2	NAG	C1-C2-N2	-10.32	92.86	110.49
7	X	2	NAG	C1-C2-N2	-10.32	92.86	110.49
2	t	6	MAN	O5-C5-C6	-10.31	91.04	107.20
7	DA	2	NAG	C1-C2-N2	-10.31	92.88	110.49
4	AA	3	BMA	O5-C5-C6	-10.30	91.05	107.20
4	p	3	BMA	O5-C5-C6	-10.30	91.06	107.20
4	U	3	BMA	O5-C5-C6	-10.30	91.06	107.20
7	4	2	NAG	O4-C4-C3	10.18	133.88	110.35
2	Y	2	NAG	O4-C4-C3	-10.17	86.84	110.35
7	O	2	NAG	O4-C4-C3	10.17	133.85	110.35
4	U	1	NAG	O4-C4-C3	-10.16	86.85	110.35
2	D	2	NAG	O4-C4-C3	-10.16	86.86	110.35
4	p	1	NAG	O4-C4-C3	-10.16	86.86	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	AA	1	NAG	O4-C4-C3	-10.16	86.86	110.35
7	j	2	NAG	O4-C4-C3	10.16	133.83	110.35
2	t	2	NAG	O4-C4-C3	-10.15	86.88	110.35
8	i	3	BMA	O5-C5-C6	-10.10	91.37	107.20
4	F	1	NAG	O5-C5-C6	-10.10	91.37	107.20
4	a	1	NAG	O5-C5-C6	-10.10	91.37	107.20
8	N	3	BMA	O5-C5-C6	-10.10	91.37	107.20
8	3	3	BMA	O5-C5-C6	-10.10	91.37	107.20
4	v	1	NAG	O5-C5-C6	-10.09	91.39	107.20
7	DA	1	NAG	O3-C3-C2	-10.04	88.70	109.47
7	s	1	NAG	O3-C3-C2	-10.03	88.70	109.47
7	X	1	NAG	O3-C3-C2	-10.03	88.71	109.47
7	O	1	NAG	O5-C5-C6	-9.98	91.56	107.20
5	c	3	BMA	O3-C3-C4	-9.97	87.29	110.35
7	4	1	NAG	O5-C5-C6	-9.97	91.57	107.20
7	j	1	NAG	O5-C5-C6	-9.97	91.57	107.20
5	x	3	BMA	O3-C3-C4	-9.96	87.31	110.35
5	H	3	BMA	O3-C3-C4	-9.96	87.31	110.35
3	k	1	NAG	O5-C5-C6	-9.84	91.77	107.20
3	P	1	NAG	O5-C5-C6	-9.84	91.77	107.20
3	5	1	NAG	O5-C5-C6	-9.83	91.79	107.20
3	Z	1	NAG	O4-C4-C3	9.74	132.88	110.35
3	u	1	NAG	O4-C4-C3	9.74	132.86	110.35
3	E	1	NAG	O4-C4-C3	9.72	132.83	110.35
8	N	2	NAG	O4-C4-C3	-9.68	87.97	110.35
8	i	2	NAG	O4-C4-C3	-9.68	87.97	110.35
8	3	2	NAG	O4-C4-C3	-9.67	87.98	110.35
3	5	1	NAG	O4-C4-C3	-9.67	88.00	110.35
3	k	1	NAG	O4-C4-C3	-9.67	88.00	110.35
3	P	1	NAG	O4-C4-C3	-9.67	88.00	110.35
8	q	1	NAG	C6-C5-C4	9.55	135.36	113.00
8	V	1	NAG	C6-C5-C4	9.54	135.36	113.00
8	BA	1	NAG	C6-C5-C4	9.54	135.36	113.00
3	o	2	NAG	O5-C5-C6	-9.48	92.35	107.20
3	9	2	NAG	O5-C5-C6	-9.47	92.35	107.20
3	T	2	NAG	O5-C5-C6	-9.47	92.36	107.20
5	H	2	NAG	O3-C3-C4	9.46	132.22	110.35
5	x	2	NAG	O3-C3-C4	9.46	132.21	110.35
5	c	2	NAG	O3-C3-C4	9.45	132.19	110.35
8	BA	3	BMA	O2-C2-C1	-9.45	89.82	109.15
8	q	3	BMA	O2-C2-C1	-9.44	89.83	109.15
8	V	3	BMA	O2-C2-C1	-9.43	89.86	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	2	NAG	O5-C5-C6	-9.41	92.46	107.20
3	k	2	NAG	O5-C5-C6	-9.39	92.48	107.20
3	5	2	NAG	O5-C5-C6	-9.36	92.53	107.20
7	s	3	BMA	O2-C2-C3	9.36	128.89	110.14
7	X	3	BMA	O2-C2-C3	9.34	128.86	110.14
7	DA	3	BMA	O2-C2-C3	9.34	128.84	110.14
8	i	2	NAG	C1-C2-N2	-9.26	94.67	110.49
8	N	2	NAG	C1-C2-N2	-9.26	94.68	110.49
8	3	2	NAG	C1-C2-N2	-9.25	94.68	110.49
5	c	1	NAG	O3-C3-C2	-9.20	90.42	109.47
5	H	1	NAG	O3-C3-C2	-9.20	90.42	109.47
5	x	1	NAG	O3-C3-C2	-9.20	90.43	109.47
4	F	4	MAN	O5-C5-C6	-9.09	92.95	107.20
4	a	4	MAN	O5-C5-C6	-9.09	92.96	107.20
4	v	4	MAN	O5-C5-C6	-9.08	92.97	107.20
8	BA	1	NAG	O5-C5-C6	-8.99	93.11	107.20
8	V	1	NAG	O5-C5-C6	-8.98	93.12	107.20
8	q	1	NAG	O5-C5-C6	-8.98	93.13	107.20
3	M	1	NAG	C6-C5-C4	8.89	133.81	113.00
3	h	1	NAG	C6-C5-C4	8.88	133.81	113.00
3	2	1	NAG	C6-C5-C4	8.87	133.79	113.00
4	a	3	BMA	O5-C5-C6	-8.86	93.31	107.20
4	F	3	BMA	O5-C5-C6	-8.85	93.33	107.20
4	U	1	NAG	C6-C5-C4	8.85	133.73	113.00
4	AA	1	NAG	C6-C5-C4	8.85	133.73	113.00
4	p	1	NAG	C6-C5-C4	8.85	133.73	113.00
4	v	3	BMA	O5-C5-C6	-8.84	93.34	107.20
8	3	5	MAN	O5-C5-C6	-8.80	93.42	107.20
8	N	5	MAN	O5-C5-C6	-8.79	93.42	107.20
8	i	5	MAN	O5-C5-C6	-8.79	93.43	107.20
4	p	4	MAN	O5-C5-C6	-8.67	93.61	107.20
7	1	1	NAG	O3-C3-C4	-8.67	90.31	110.35
4	AA	4	MAN	O5-C5-C6	-8.66	93.63	107.20
4	U	4	MAN	O5-C5-C6	-8.66	93.63	107.20
7	g	1	NAG	O3-C3-C4	-8.65	90.35	110.35
7	L	1	NAG	O3-C3-C4	-8.65	90.36	110.35
3	n	2	NAG	O5-C5-C6	-8.62	93.69	107.20
4	v	4	MAN	O3-C3-C2	-8.62	93.49	109.99
4	a	4	MAN	O3-C3-C2	-8.61	93.51	109.99
7	O	2	NAG	O5-C5-C6	-8.61	93.71	107.20
4	F	4	MAN	O3-C3-C2	-8.60	93.52	109.99
3	S	2	NAG	O5-C5-C6	-8.59	93.73	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	j	2	NAG	O5-C5-C6	-8.59	93.74	107.20
7	4	2	NAG	O5-C5-C6	-8.59	93.74	107.20
3	8	2	NAG	O5-C5-C6	-8.56	93.78	107.20
6	K	4	MAN	O4-C4-C5	-8.34	88.58	109.30
6	f	4	MAN	O4-C4-C5	-8.34	88.59	109.30
6	0	4	MAN	O4-C4-C5	-8.33	88.61	109.30
5	c	2	NAG	O4-C4-C3	8.25	129.43	110.35
5	x	2	NAG	O4-C4-C3	8.25	129.43	110.35
5	H	2	NAG	O4-C4-C3	8.25	129.42	110.35
3	8	1	NAG	O5-C5-C6	-8.24	94.28	107.20
3	S	1	NAG	O5-C5-C6	-8.24	94.29	107.20
3	n	1	NAG	O5-C5-C6	-8.23	94.30	107.20
2	t	4	MAN	O2-C2-C1	8.13	125.80	109.15
3	6	1	NAG	O5-C5-C6	-8.10	94.50	107.20
3	Q	1	NAG	O5-C5-C6	-8.10	94.51	107.20
3	l	1	NAG	O5-C5-C6	-8.09	94.52	107.20
2	D	4	MAN	O2-C2-C1	8.09	125.70	109.15
2	Y	4	MAN	O2-C2-C1	8.09	125.70	109.15
6	K	5	MAN	O3-C3-C4	-8.09	91.65	110.35
6	0	5	MAN	O3-C3-C4	-8.08	91.66	110.35
6	f	5	MAN	O3-C3-C4	-8.07	91.69	110.35
3	w	1	NAG	O3-C3-C2	-7.90	93.11	109.47
3	G	1	NAG	O3-C3-C2	-7.89	93.14	109.47
3	b	1	NAG	O3-C3-C2	-7.88	93.15	109.47
3	2	2	NAG	O5-C5-C6	-7.87	94.87	107.20
3	M	2	NAG	O5-C5-C6	-7.86	94.89	107.20
3	h	2	NAG	O5-C5-C6	-7.84	94.91	107.20
7	4	3	BMA	O2-C2-C3	7.83	125.82	110.14
8	BA	5	MAN	C6-C5-C4	7.82	131.33	113.00
8	V	5	MAN	C6-C5-C4	7.80	131.28	113.00
7	O	3	BMA	O2-C2-C3	7.80	125.76	110.14
8	q	5	MAN	C6-C5-C4	7.79	131.25	113.00
7	j	3	BMA	O2-C2-C3	7.79	125.74	110.14
2	t	3	BMA	O2-C2-C1	7.58	124.66	109.15
8	V	4	MAN	O3-C3-C2	-7.58	95.48	109.99
8	q	4	MAN	O3-C3-C2	-7.58	95.49	109.99
2	Y	3	BMA	O2-C2-C1	7.57	124.65	109.15
2	D	3	BMA	O2-C2-C1	7.57	124.64	109.15
8	BA	4	MAN	O3-C3-C2	-7.56	95.52	109.99
6	0	8	MAN	O3-C3-C2	-7.52	95.59	109.99
6	K	8	MAN	O3-C3-C2	-7.51	95.61	109.99
6	f	8	MAN	O3-C3-C2	-7.49	95.65	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	1	NAG	O3-C3-C4	-7.49	93.04	110.35
7	DA	1	NAG	O3-C3-C4	-7.48	93.06	110.35
3	l	2	NAG	C1-C2-N2	-7.48	97.71	110.49
7	s	1	NAG	O3-C3-C4	-7.48	93.06	110.35
2	t	3	BMA	O5-C5-C6	-7.47	95.49	107.20
2	D	3	BMA	O5-C5-C6	-7.47	95.49	107.20
2	Y	3	BMA	O5-C5-C6	-7.47	95.49	107.20
3	Q	2	NAG	C1-C2-N2	-7.46	97.74	110.49
3	6	2	NAG	C1-C2-N2	-7.46	97.75	110.49
2	t	4	MAN	O3-C3-C4	-7.45	93.12	110.35
2	Y	4	MAN	O3-C3-C4	-7.45	93.13	110.35
7	j	1	NAG	O4-C4-C3	-7.44	93.14	110.35
2	D	4	MAN	O3-C3-C4	-7.44	93.15	110.35
7	4	1	NAG	O4-C4-C3	-7.44	93.15	110.35
7	O	1	NAG	O4-C4-C3	-7.44	93.15	110.35
7	1	3	BMA	O3-C3-C2	-7.42	95.78	109.99
7	g	3	BMA	O3-C3-C2	-7.42	95.79	109.99
7	L	3	BMA	O3-C3-C2	-7.42	95.79	109.99
6	K	1	NAG	O3-C3-C2	-7.40	94.16	109.47
6	f	1	NAG	O3-C3-C2	-7.38	94.19	109.47
6	0	1	NAG	O3-C3-C2	-7.38	94.19	109.47
3	9	2	NAG	C1-C2-N2	-7.25	98.11	110.49
7	1	3	BMA	O2-C2-C1	-7.24	94.34	109.15
3	T	2	NAG	C1-C2-N2	-7.23	98.13	110.49
3	o	2	NAG	C1-C2-N2	-7.23	98.14	110.49
7	L	3	BMA	O2-C2-C1	-7.23	94.37	109.15
7	g	3	BMA	O2-C2-C1	-7.21	94.40	109.15
8	i	4	MAN	O3-C3-C2	-7.16	96.29	109.99
8	3	4	MAN	O3-C3-C2	-7.15	96.30	109.99
8	N	4	MAN	O3-C3-C2	-7.15	96.31	109.99
3	R	2	NAG	C1-C2-N2	7.13	122.66	110.49
3	7	2	NAG	C1-C2-N2	7.12	122.65	110.49
3	u	2	NAG	C1-C2-N2	-7.12	98.33	110.49
3	m	2	NAG	C1-C2-N2	7.12	122.64	110.49
3	Z	2	NAG	C1-C2-N2	-7.10	98.35	110.49
6	0	2	NAG	O3-C3-C4	7.10	126.77	110.35
3	E	2	NAG	C1-C2-N2	-7.10	98.36	110.49
6	K	2	NAG	O3-C3-C4	7.09	126.75	110.35
6	f	2	NAG	O3-C3-C4	7.08	126.73	110.35
7	1	3	BMA	O4-C4-C3	-6.98	94.22	110.35
7	L	3	BMA	O4-C4-C3	-6.97	94.24	110.35
7	g	3	BMA	O4-C4-C3	-6.96	94.26	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	p	2	NAG	C6-C5-C4	6.96	129.30	113.00
4	AA	2	NAG	C6-C5-C4	6.95	129.29	113.00
8	i	4	MAN	O5-C5-C6	-6.95	96.31	107.20
4	U	2	NAG	C6-C5-C4	6.95	129.27	113.00
8	3	4	MAN	O5-C5-C6	-6.94	96.32	107.20
7	O	3	BMA	O2-C2-C1	-6.94	94.95	109.15
7	4	3	BMA	O2-C2-C1	-6.94	94.96	109.15
8	N	4	MAN	O5-C5-C6	-6.94	96.33	107.20
7	j	3	BMA	O2-C2-C1	-6.93	94.97	109.15
8	q	3	BMA	O5-C5-C6	-6.93	96.34	107.20
8	V	3	BMA	O5-C5-C6	-6.93	96.35	107.20
8	BA	3	BMA	O5-C5-C6	-6.92	96.36	107.20
4	a	3	BMA	O2-C2-C3	6.88	123.92	110.14
4	F	3	BMA	O2-C2-C3	6.86	123.89	110.14
4	v	3	BMA	O2-C2-C3	6.86	123.88	110.14
2	t	2	NAG	C1-C2-N2	-6.75	98.95	110.49
2	D	2	NAG	C1-C2-N2	-6.75	98.95	110.49
6	f	4	MAN	O4-C4-C3	6.75	125.95	110.35
2	Y	2	NAG	C1-C2-N2	-6.75	98.97	110.49
6	0	4	MAN	O4-C4-C3	6.74	125.94	110.35
6	K	4	MAN	O4-C4-C3	6.74	125.93	110.35
5	x	2	NAG	C1-C2-N2	-6.72	99.01	110.49
7	O	2	NAG	C1-C2-N2	-6.71	99.02	110.49
7	4	2	NAG	C1-C2-N2	-6.71	99.03	110.49
5	H	2	NAG	C1-C2-N2	-6.71	99.03	110.49
5	c	2	NAG	C1-C2-N2	-6.71	99.03	110.49
7	j	2	NAG	C1-C2-N2	-6.69	99.06	110.49
7	s	1	NAG	C1-C2-N2	-6.63	99.15	110.49
7	X	1	NAG	C1-C2-N2	-6.63	99.16	110.49
7	DA	1	NAG	C1-C2-N2	-6.61	99.19	110.49
8	BA	4	MAN	O5-C5-C6	-6.58	96.90	107.20
8	q	4	MAN	O5-C5-C6	-6.56	96.92	107.20
8	V	4	MAN	O5-C5-C6	-6.56	96.93	107.20
5	H	3	BMA	O3-C3-C2	6.47	122.38	109.99
5	c	3	BMA	O3-C3-C2	6.46	122.36	109.99
5	x	3	BMA	O3-C3-C2	6.46	122.36	109.99
3	J	2	NAG	O5-C5-C6	-6.35	97.24	107.20
3	e	2	NAG	O5-C5-C6	-6.35	97.25	107.20
3	z	2	NAG	O5-C5-C6	-6.34	97.26	107.20
8	q	3	BMA	O4-C4-C5	-6.30	93.65	109.30
8	V	3	BMA	O4-C4-C5	-6.30	93.66	109.30
8	BA	3	BMA	O4-C4-C5	-6.29	93.67	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	1	NAG	O4-C4-C3	-6.27	95.86	110.35
8	i	1	NAG	O4-C4-C3	-6.26	95.87	110.35
8	3	1	NAG	O4-C4-C3	-6.26	95.88	110.35
7	1	1	NAG	C1-C2-N2	6.25	121.17	110.49
7	g	1	NAG	C1-C2-N2	6.25	121.17	110.49
7	L	1	NAG	C1-C2-N2	6.25	121.16	110.49
3	Q	2	NAG	O5-C5-C6	-6.18	97.52	107.20
3	6	2	NAG	O5-C5-C6	-6.18	97.52	107.20
3	R	2	NAG	O4-C4-C5	-6.18	93.96	109.30
3	m	2	NAG	O4-C4-C5	-6.18	93.96	109.30
3	7	2	NAG	O4-C4-C5	-6.17	93.97	109.30
3	l	2	NAG	O5-C5-C6	-6.17	97.53	107.20
7	g	2	NAG	O5-C5-C6	-6.14	97.59	107.20
7	1	2	NAG	O5-C5-C6	-6.13	97.59	107.20
4	U	4	MAN	O3-C3-C2	-6.13	98.26	109.99
7	L	2	NAG	O5-C5-C6	-6.13	97.60	107.20
4	AA	4	MAN	O3-C3-C2	-6.13	98.26	109.99
4	p	4	MAN	O3-C3-C2	-6.12	98.28	109.99
3	Q	1	NAG	C6-C5-C4	6.11	127.31	113.00
3	6	1	NAG	C6-C5-C4	6.10	127.30	113.00
3	l	1	NAG	C6-C5-C4	6.10	127.30	113.00
3	I	2	NAG	O4-C4-C3	-6.08	96.29	110.35
3	d	2	NAG	O4-C4-C3	-6.08	96.29	110.35
3	y	2	NAG	O4-C4-C3	-6.08	96.29	110.35
2	D	6	MAN	O2-C2-C1	6.05	121.53	109.15
3	y	1	NAG	C8-C7-N2	6.04	126.33	116.10
3	I	1	NAG	C8-C7-N2	6.04	126.33	116.10
2	Y	6	MAN	O2-C2-C1	6.04	121.50	109.15
2	t	6	MAN	O2-C2-C1	6.03	121.50	109.15
3	d	1	NAG	C8-C7-N2	6.03	126.31	116.10
7	s	3	BMA	O5-C5-C6	-6.03	97.75	107.20
8	N	5	MAN	O3-C3-C2	-6.03	98.46	109.99
8	i	5	MAN	O3-C3-C2	-6.02	98.46	109.99
7	DA	3	BMA	O5-C5-C6	-6.02	97.77	107.20
7	X	3	BMA	O5-C5-C6	-6.01	97.77	107.20
8	3	5	MAN	O3-C3-C2	-6.01	98.48	109.99
5	x	2	NAG	O3-C3-C2	-5.98	97.10	109.47
7	O	3	BMA	O3-C3-C2	-5.98	98.55	109.99
7	j	3	BMA	O3-C3-C2	-5.98	98.55	109.99
5	H	2	NAG	O3-C3-C2	-5.97	97.10	109.47
7	1	3	BMA	O2-C2-C3	5.96	122.09	110.14
5	c	2	NAG	O3-C3-C2	-5.96	97.13	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	4	3	BMA	O3-C3-C2	-5.96	98.58	109.99
7	L	3	BMA	O2-C2-C3	5.95	122.06	110.14
7	g	3	BMA	O2-C2-C3	5.94	122.04	110.14
8	q	2	NAG	C6-C5-C4	5.92	126.87	113.00
8	V	2	NAG	C6-C5-C4	5.92	126.86	113.00
3	d	1	NAG	C6-C5-C4	5.91	126.85	113.00
8	BA	2	NAG	C6-C5-C4	5.91	126.85	113.00
3	I	1	NAG	C6-C5-C4	5.90	126.81	113.00
3	y	1	NAG	C6-C5-C4	5.90	126.81	113.00
5	H	4	MAN	O2-C2-C1	5.86	121.15	109.15
5	x	4	MAN	O2-C2-C1	5.86	121.15	109.15
5	c	4	MAN	O2-C2-C1	5.86	121.15	109.15
4	p	4	MAN	O2-C2-C1	5.85	121.12	109.15
4	AA	4	MAN	O2-C2-C1	5.85	121.12	109.15
4	U	4	MAN	O2-C2-C1	5.84	121.10	109.15
6	0	1	NAG	C1-C2-N2	-5.84	100.52	110.49
2	Y	5	MAN	O3-C3-C2	-5.84	98.82	109.99
3	6	2	NAG	C6-C5-C4	5.83	126.66	113.00
6	f	1	NAG	C1-C2-N2	-5.83	100.53	110.49
6	K	1	NAG	C1-C2-N2	-5.83	100.53	110.49
2	D	5	MAN	O3-C3-C2	-5.83	98.83	109.99
2	t	5	MAN	O3-C3-C2	-5.83	98.84	109.99
3	Q	2	NAG	C6-C5-C4	5.82	126.64	113.00
3	l	2	NAG	C6-C5-C4	5.82	126.64	113.00
6	K	5	MAN	C6-C5-C4	5.78	126.55	113.00
6	K	4	MAN	O2-C2-C1	5.78	120.98	109.15
6	0	5	MAN	C6-C5-C4	5.78	126.54	113.00
6	f	4	MAN	O2-C2-C1	5.78	120.98	109.15
6	0	4	MAN	O2-C2-C1	5.78	120.97	109.15
6	f	5	MAN	C6-C5-C4	5.77	126.51	113.00
6	f	1	NAG	O5-C5-C6	-5.71	98.25	107.20
6	K	1	NAG	O5-C5-C6	-5.70	98.27	107.20
6	0	1	NAG	O5-C5-C6	-5.69	98.29	107.20
2	D	3	BMA	C6-C5-C4	5.61	126.15	113.00
2	Y	3	BMA	C6-C5-C4	5.61	126.13	113.00
7	L	2	NAG	O3-C3-C4	-5.60	97.40	110.35
7	g	2	NAG	O3-C3-C4	-5.59	97.42	110.35
2	t	3	BMA	C6-C5-C4	5.59	126.11	113.00
7	1	2	NAG	O3-C3-C4	-5.59	97.42	110.35
6	f	8	MAN	C6-C5-C4	5.55	126.01	113.00
6	0	8	MAN	C6-C5-C4	5.55	126.00	113.00
6	K	8	MAN	C6-C5-C4	5.55	126.00	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	1	NAG	O3-C3-C2	-5.52	98.05	109.47
8	BA	1	NAG	O3-C3-C2	-5.51	98.07	109.47
8	V	1	NAG	O3-C3-C2	-5.50	98.08	109.47
3	CA	1	NAG	O4-C4-C3	-5.49	97.65	110.35
3	W	1	NAG	O4-C4-C3	-5.48	97.67	110.35
3	r	1	NAG	O4-C4-C3	-5.48	97.68	110.35
6	f	7	MAN	O2-C2-C3	5.47	121.09	110.14
6	0	7	MAN	O2-C2-C3	5.45	121.06	110.14
6	K	7	MAN	O2-C2-C3	5.45	121.06	110.14
8	i	5	MAN	C6-C5-C4	5.42	125.71	113.00
8	N	5	MAN	C6-C5-C4	5.42	125.71	113.00
8	3	5	MAN	C6-C5-C4	5.42	125.70	113.00
2	t	2	NAG	C6-C5-C4	5.40	125.66	113.00
2	Y	2	NAG	C6-C5-C4	5.40	125.64	113.00
2	D	2	NAG	C6-C5-C4	5.39	125.63	113.00
2	Y	4	MAN	C6-C5-C4	5.36	125.57	113.00
2	t	4	MAN	C6-C5-C4	5.35	125.55	113.00
2	D	4	MAN	C6-C5-C4	5.34	125.51	113.00
8	BA	3	BMA	O4-C4-C3	5.34	122.69	110.35
8	V	3	BMA	O4-C4-C3	5.33	122.68	110.35
7	j	2	NAG	C6-C5-C4	5.32	125.47	113.00
7	4	2	NAG	C6-C5-C4	5.32	125.47	113.00
8	q	3	BMA	O4-C4-C3	5.32	122.64	110.35
7	O	2	NAG	C6-C5-C4	5.31	125.45	113.00
8	3	1	NAG	C6-C5-C4	5.30	125.43	113.00
8	N	1	NAG	C6-C5-C4	5.30	125.42	113.00
8	i	1	NAG	C6-C5-C4	5.30	125.42	113.00
2	Y	5	MAN	C1-O5-C5	5.26	119.32	112.19
4	F	4	MAN	C6-C5-C4	5.26	125.32	113.00
4	a	4	MAN	C6-C5-C4	5.25	125.31	113.00
4	a	1	NAG	O4-C4-C3	-5.25	98.21	110.35
4	v	4	MAN	C6-C5-C4	5.25	125.29	113.00
4	F	1	NAG	O4-C4-C3	-5.24	98.22	110.35
4	v	1	NAG	O4-C4-C3	-5.24	98.24	110.35
2	D	5	MAN	C1-O5-C5	5.23	119.28	112.19
2	t	5	MAN	C1-O5-C5	5.23	119.28	112.19
6	f	3	BMA	O2-C2-C1	-5.18	98.56	109.15
6	K	3	BMA	O2-C2-C1	-5.17	98.57	109.15
6	0	3	BMA	O2-C2-C1	-5.16	98.60	109.15
8	i	3	BMA	C6-C5-C4	5.14	125.04	113.00
8	3	3	BMA	C6-C5-C4	5.13	125.01	113.00
8	N	3	BMA	C6-C5-C4	5.12	125.00	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	x	1	NAG	C6-C5-C4	5.10	124.96	113.00
5	H	1	NAG	C6-C5-C4	5.10	124.95	113.00
5	c	1	NAG	C6-C5-C4	5.10	124.95	113.00
3	u	2	NAG	O4-C4-C5	-5.09	96.65	109.30
3	E	2	NAG	O4-C4-C5	-5.09	96.65	109.30
3	Z	2	NAG	O4-C4-C5	-5.08	96.67	109.30
4	p	4	MAN	C6-C5-C4	5.04	124.81	113.00
6	0	2	NAG	C6-C5-C4	5.04	124.81	113.00
3	E	1	NAG	C1-C2-N2	5.04	119.09	110.49
3	u	1	NAG	C1-C2-N2	5.03	119.09	110.49
6	K	2	NAG	C6-C5-C4	5.03	124.79	113.00
4	U	4	MAN	C6-C5-C4	5.03	124.79	113.00
6	f	2	NAG	C6-C5-C4	5.03	124.78	113.00
4	AA	4	MAN	C6-C5-C4	5.03	124.78	113.00
3	Z	1	NAG	C1-C2-N2	5.02	119.07	110.49
3	w	2	NAG	C1-C2-N2	-5.00	101.95	110.49
3	G	2	NAG	C1-C2-N2	-4.98	101.98	110.49
3	b	2	NAG	C1-C2-N2	-4.98	101.98	110.49
3	9	2	NAG	C6-C5-C4	4.98	124.66	113.00
3	e	1	NAG	O3-C3-C4	4.97	121.84	110.35
3	z	1	NAG	O3-C3-C4	4.97	121.84	110.35
3	o	2	NAG	C6-C5-C4	4.97	124.64	113.00
3	J	1	NAG	O3-C3-C4	4.97	121.83	110.35
3	T	2	NAG	C6-C5-C4	4.97	124.64	113.00
2	D	1	NAG	O3-C3-C2	-4.84	99.45	109.47
2	t	1	NAG	O3-C3-C2	-4.84	99.45	109.47
2	Y	1	NAG	O3-C3-C2	-4.83	99.47	109.47
6	0	7	MAN	C6-C5-C4	4.74	124.10	113.00
6	f	7	MAN	C6-C5-C4	4.74	124.09	113.00
3	P	1	NAG	C6-C5-C4	4.73	124.07	113.00
3	5	1	NAG	C6-C5-C4	4.72	124.06	113.00
6	K	7	MAN	C6-C5-C4	4.72	124.06	113.00
3	k	1	NAG	C6-C5-C4	4.71	124.04	113.00
3	9	2	NAG	O4-C4-C3	-4.67	99.56	110.35
3	T	2	NAG	O4-C4-C3	-4.66	99.57	110.35
3	o	2	NAG	O4-C4-C3	-4.66	99.58	110.35
5	x	3	BMA	O2-C2-C3	4.61	119.36	110.14
5	H	3	BMA	O2-C2-C3	4.60	119.36	110.14
5	c	3	BMA	O2-C2-C3	4.60	119.36	110.14
4	U	4	MAN	O4-C4-C3	-4.55	99.84	110.35
4	AA	4	MAN	O4-C4-C3	-4.55	99.84	110.35
2	Y	6	MAN	C6-C5-C4	4.54	123.64	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	t	6	MAN	C6-C5-C4	4.54	123.64	113.00
4	p	4	MAN	O4-C4-C3	-4.53	99.88	110.35
2	D	6	MAN	C6-C5-C4	4.53	123.61	113.00
3	n	2	NAG	O4-C4-C5	-4.50	98.11	109.30
4	AA	3	BMA	O2-C2-C3	4.49	119.13	110.14
4	p	3	BMA	O2-C2-C3	4.49	119.12	110.14
4	U	3	BMA	O2-C2-C3	4.48	119.12	110.14
2	Y	1	NAG	C6-C5-C4	4.48	123.50	113.00
3	S	2	NAG	O4-C4-C5	-4.48	98.17	109.30
2	t	1	NAG	C6-C5-C4	4.48	123.50	113.00
2	D	1	NAG	C6-C5-C4	4.48	123.50	113.00
3	8	2	NAG	O4-C4-C5	-4.47	98.20	109.30
4	F	4	MAN	O2-C2-C3	4.46	119.08	110.14
4	a	4	MAN	O2-C2-C3	4.46	119.07	110.14
4	v	4	MAN	O2-C2-C3	4.46	119.07	110.14
8	BA	5	MAN	O2-C2-C3	4.38	118.92	110.14
8	q	5	MAN	O2-C2-C3	4.38	118.90	110.14
8	V	5	MAN	O2-C2-C3	4.37	118.89	110.14
7	s	3	BMA	O3-C3-C2	-4.37	101.63	109.99
7	DA	3	BMA	O3-C3-C2	-4.36	101.64	109.99
7	X	3	BMA	O3-C3-C2	-4.36	101.64	109.99
6	0	2	NAG	O5-C5-C6	-4.34	100.39	107.20
8	i	3	BMA	O2-C2-C3	4.34	118.83	110.14
8	3	3	BMA	O2-C2-C3	4.34	118.83	110.14
8	N	3	BMA	O2-C2-C3	4.34	118.83	110.14
6	K	2	NAG	O5-C5-C6	-4.32	100.42	107.20
6	f	2	NAG	O5-C5-C6	-4.32	100.43	107.20
3	R	1	NAG	C1-C2-N2	4.32	117.86	110.49
3	m	1	NAG	C1-C2-N2	4.31	117.86	110.49
4	p	1	NAG	C1-C2-N2	-4.30	103.14	110.49
8	q	5	MAN	O3-C3-C2	-4.29	101.77	109.99
3	7	1	NAG	C1-C2-N2	4.29	117.82	110.49
4	U	1	NAG	C1-C2-N2	-4.28	103.18	110.49
4	AA	1	NAG	C1-C2-N2	-4.28	103.18	110.49
8	V	5	MAN	O3-C3-C2	-4.26	101.83	109.99
8	BA	5	MAN	O3-C3-C2	-4.25	101.85	109.99
7	1	2	NAG	O4-C4-C3	4.22	120.11	110.35
7	L	2	NAG	O4-C4-C3	4.22	120.11	110.35
3	J	2	NAG	C1-C2-N2	4.22	117.70	110.49
3	e	2	NAG	C1-C2-N2	4.22	117.69	110.49
3	z	2	NAG	C1-C2-N2	4.22	117.69	110.49
7	g	2	NAG	O4-C4-C3	4.21	120.08	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	y	2	NAG	O3-C3-C2	4.21	118.17	109.47
3	I	2	NAG	O3-C3-C2	4.20	118.16	109.47
3	d	2	NAG	O3-C3-C2	4.20	118.16	109.47
2	t	1	NAG	O4-C4-C3	-4.18	100.68	110.35
2	D	1	NAG	O4-C4-C3	-4.18	100.68	110.35
6	K	7	MAN	O4-C4-C5	-4.18	98.91	109.30
6	0	7	MAN	O4-C4-C5	-4.18	98.91	109.30
2	Y	1	NAG	O4-C4-C3	-4.18	100.68	110.35
6	f	7	MAN	O4-C4-C5	-4.18	98.92	109.30
8	BA	4	MAN	O4-C4-C3	-4.14	100.78	110.35
8	q	4	MAN	O4-C4-C3	-4.13	100.79	110.35
8	V	4	MAN	O4-C4-C3	-4.13	100.79	110.35
2	t	6	MAN	C1-O5-C5	4.12	117.78	112.19
5	H	3	BMA	O4-C4-C3	4.11	119.84	110.35
5	x	3	BMA	O4-C4-C3	4.10	119.83	110.35
5	c	3	BMA	O4-C4-C3	4.10	119.83	110.35
5	c	4	MAN	O3-C3-C2	-4.10	102.14	109.99
5	H	4	MAN	O3-C3-C2	-4.10	102.15	109.99
7	L	2	NAG	C6-C5-C4	4.10	122.60	113.00
5	x	4	MAN	O3-C3-C2	-4.10	102.15	109.99
2	Y	6	MAN	C1-O5-C5	4.08	117.72	112.19
2	D	6	MAN	C1-O5-C5	4.07	117.71	112.19
7	g	2	NAG	C6-C5-C4	4.07	122.54	113.00
7	1	2	NAG	C6-C5-C4	4.07	122.54	113.00
3	u	2	NAG	C1-O5-C5	4.07	117.70	112.19
3	b	1	NAG	O5-C5-C6	4.06	113.56	107.20
3	E	2	NAG	C1-O5-C5	4.05	117.68	112.19
6	0	8	MAN	C1-O5-C5	4.05	117.68	112.19
3	w	1	NAG	O5-C5-C6	4.05	113.55	107.20
6	f	8	MAN	C1-O5-C5	4.05	117.67	112.19
3	G	1	NAG	O5-C5-C6	4.04	113.55	107.20
3	Z	2	NAG	C1-O5-C5	4.04	117.67	112.19
6	K	8	MAN	C1-O5-C5	4.04	117.67	112.19
3	Z	1	NAG	O3-C3-C4	-4.02	101.05	110.35
3	u	1	NAG	O3-C3-C4	-4.01	101.08	110.35
3	E	1	NAG	O3-C3-C4	-4.01	101.08	110.35
4	U	4	MAN	O4-C4-C5	3.98	119.19	109.30
4	AA	4	MAN	O4-C4-C5	3.97	119.16	109.30
7	4	2	NAG	O3-C3-C2	-3.96	101.26	109.47
4	p	4	MAN	O4-C4-C5	3.96	119.13	109.30
7	O	2	NAG	O3-C3-C2	-3.96	101.27	109.47
7	j	2	NAG	O3-C3-C2	-3.96	101.28	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	3	BMA	O4-C4-C5	3.91	119.00	109.30
7	L	3	BMA	O4-C4-C5	3.90	118.98	109.30
7	1	3	BMA	O4-C4-C5	3.89	118.97	109.30
2	Y	3	BMA	O3-C3-C2	-3.89	102.54	109.99
2	D	3	BMA	O3-C3-C2	-3.89	102.55	109.99
3	5	2	NAG	C1-C2-N2	3.89	117.13	110.49
2	t	3	BMA	O3-C3-C2	-3.89	102.55	109.99
3	P	2	NAG	C1-C2-N2	3.87	117.10	110.49
3	k	2	NAG	C1-C2-N2	3.87	117.10	110.49
3	M	1	NAG	O3-C3-C2	3.83	117.39	109.47
6	0	5	MAN	O4-C4-C3	-3.83	101.50	110.35
6	K	5	MAN	O4-C4-C3	-3.82	101.51	110.35
3	2	1	NAG	O3-C3-C2	3.82	117.37	109.47
3	h	1	NAG	O3-C3-C2	3.82	117.36	109.47
6	f	5	MAN	O4-C4-C3	-3.81	101.55	110.35
5	c	1	NAG	O5-C5-C6	-3.74	101.34	107.20
5	H	4	MAN	C6-C5-C4	3.74	121.76	113.00
5	c	4	MAN	C6-C5-C4	3.73	121.75	113.00
3	y	1	NAG	C1-C2-N2	3.73	116.87	110.49
3	8	1	NAG	C6-C5-C4	3.73	121.75	113.00
5	x	4	MAN	C6-C5-C4	3.73	121.74	113.00
5	H	1	NAG	O5-C5-C6	-3.73	101.36	107.20
3	I	1	NAG	C1-C2-N2	3.72	116.85	110.49
5	x	1	NAG	O5-C5-C6	-3.72	101.37	107.20
3	d	1	NAG	C1-C2-N2	3.72	116.85	110.49
3	S	1	NAG	C6-C5-C4	3.72	121.72	113.00
3	n	1	NAG	C6-C5-C4	3.71	121.70	113.00
2	D	5	MAN	C6-C5-C4	3.71	121.69	113.00
3	h	1	NAG	O3-C3-C4	-3.70	101.80	110.35
2	Y	5	MAN	C6-C5-C4	3.69	121.66	113.00
3	M	1	NAG	O3-C3-C4	-3.69	101.81	110.35
3	2	1	NAG	O3-C3-C4	-3.69	101.82	110.35
2	t	5	MAN	C6-C5-C4	3.68	121.63	113.00
3	CA	2	NAG	O4-C4-C3	-3.68	101.85	110.35
3	W	2	NAG	O4-C4-C3	-3.67	101.86	110.35
3	r	2	NAG	O4-C4-C3	-3.67	101.87	110.35
4	U	2	NAG	O3-C3-C4	3.64	118.76	110.35
3	z	1	NAG	O4-C4-C3	-3.64	101.94	110.35
4	p	2	NAG	O3-C3-C4	3.63	118.75	110.35
3	e	1	NAG	O4-C4-C3	-3.63	101.95	110.35
7	X	3	BMA	O4-C4-C5	3.63	118.31	109.30
7	DA	3	BMA	O4-C4-C5	3.63	118.31	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	s	3	BMA	O4-C4-C5	3.62	118.30	109.30
3	J	1	NAG	O4-C4-C3	-3.62	101.97	110.35
4	AA	2	NAG	O3-C3-C4	3.62	118.73	110.35
3	h	2	NAG	C6-C5-C4	3.60	121.44	113.00
3	2	2	NAG	C6-C5-C4	3.60	121.43	113.00
3	M	2	NAG	C6-C5-C4	3.59	121.42	113.00
8	V	4	MAN	C6-C5-C4	3.59	121.41	113.00
8	q	4	MAN	C6-C5-C4	3.59	121.40	113.00
2	t	2	NAG	O3-C3-C2	-3.58	102.06	109.47
8	BA	4	MAN	C6-C5-C4	3.58	121.39	113.00
2	D	2	NAG	O3-C3-C2	-3.58	102.06	109.47
2	Y	2	NAG	O3-C3-C2	-3.57	102.09	109.47
7	X	2	NAG	C6-C5-C4	3.54	121.30	113.00
7	DA	2	NAG	C6-C5-C4	3.54	121.30	113.00
7	s	2	NAG	C6-C5-C4	3.54	121.29	113.00
2	Y	6	MAN	O3-C3-C2	-3.52	103.25	109.99
7	4	1	NAG	O3-C3-C4	3.52	118.49	110.35
7	O	1	NAG	O3-C3-C4	3.51	118.47	110.35
7	j	1	NAG	O3-C3-C4	3.51	118.47	110.35
6	f	5	MAN	O3-C3-C2	3.51	116.71	109.99
2	t	6	MAN	O3-C3-C2	-3.49	103.31	109.99
8	i	3	BMA	O2-C2-C1	3.49	116.29	109.15
8	N	3	BMA	O2-C2-C1	3.49	116.29	109.15
6	K	5	MAN	O3-C3-C2	3.49	116.67	109.99
8	3	3	BMA	O2-C2-C1	3.49	116.28	109.15
6	0	5	MAN	O3-C3-C2	3.49	116.67	109.99
2	D	6	MAN	O3-C3-C2	-3.47	103.34	109.99
8	N	1	NAG	O3-C3-C4	-3.47	102.34	110.35
8	3	1	NAG	O3-C3-C4	-3.46	102.34	110.35
8	i	1	NAG	O3-C3-C4	-3.46	102.34	110.35
3	d	1	NAG	O7-C7-N2	-3.45	115.60	121.95
3	y	1	NAG	O7-C7-N2	-3.45	115.60	121.95
3	I	1	NAG	O7-C7-N2	-3.45	115.61	121.95
3	R	1	NAG	O4-C4-C3	-3.43	102.42	110.35
3	7	1	NAG	O4-C4-C3	-3.43	102.42	110.35
3	m	1	NAG	O4-C4-C3	-3.43	102.42	110.35
7	4	2	NAG	O3-C3-C4	-3.43	102.43	110.35
7	j	2	NAG	O3-C3-C4	-3.42	102.44	110.35
7	O	2	NAG	O3-C3-C4	-3.42	102.44	110.35
3	e	1	NAG	O3-C3-C2	-3.42	102.39	109.47
3	z	1	NAG	O3-C3-C2	-3.42	102.40	109.47
3	J	1	NAG	O3-C3-C2	-3.41	102.40	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	3	5	MAN	O2-C2-C1	3.41	116.13	109.15
8	N	5	MAN	O2-C2-C1	3.41	116.13	109.15
8	i	5	MAN	O2-C2-C1	3.40	116.12	109.15
7	X	3	BMA	O4-C4-C3	-3.35	102.60	110.35
7	DA	3	BMA	O4-C4-C3	-3.35	102.61	110.35
7	s	3	BMA	O4-C4-C3	-3.34	102.62	110.35
6	K	1	NAG	O3-C3-C4	-3.25	102.83	110.35
6	0	1	NAG	O3-C3-C4	-3.24	102.85	110.35
6	f	1	NAG	O3-C3-C4	-3.23	102.87	110.35
3	w	1	NAG	C6-C5-C4	3.23	120.57	113.00
4	F	1	NAG	C8-C7-N2	3.23	121.56	116.10
4	v	1	NAG	C8-C7-N2	3.22	121.56	116.10
4	a	1	NAG	C8-C7-N2	3.22	121.55	116.10
3	b	1	NAG	C6-C5-C4	3.22	120.54	113.00
3	G	1	NAG	C6-C5-C4	3.21	120.51	113.00
3	k	2	NAG	O4-C4-C5	-3.18	101.41	109.30
3	u	2	NAG	O5-C1-C2	-3.18	106.27	111.29
3	P	2	NAG	O4-C4-C5	-3.17	101.42	109.30
3	5	2	NAG	O4-C4-C5	-3.17	101.43	109.30
3	Z	2	NAG	O5-C1-C2	-3.16	106.29	111.29
3	E	2	NAG	O5-C1-C2	-3.16	106.29	111.29
2	D	5	MAN	O5-C5-C6	-3.13	102.30	107.20
8	q	2	NAG	O3-C3-C4	3.12	117.57	110.35
3	R	2	NAG	O3-C3-C2	3.12	115.92	109.47
3	7	2	NAG	O3-C3-C2	3.12	115.92	109.47
3	m	2	NAG	O3-C3-C2	3.12	115.92	109.47
8	V	2	NAG	O3-C3-C4	3.12	117.56	110.35
2	Y	2	NAG	C1-O5-C5	3.12	116.42	112.19
8	BA	2	NAG	O3-C3-C4	3.11	117.55	110.35
2	t	5	MAN	O5-C5-C6	-3.11	102.33	107.20
2	D	2	NAG	C1-O5-C5	3.11	116.41	112.19
2	t	2	NAG	C1-O5-C5	3.11	116.40	112.19
8	BA	3	BMA	O3-C3-C2	-3.10	104.06	109.99
3	P	2	NAG	C6-C5-C4	3.10	120.26	113.00
8	V	3	BMA	O3-C3-C2	-3.10	104.06	109.99
8	q	3	BMA	O3-C3-C2	-3.10	104.06	109.99
3	k	2	NAG	C6-C5-C4	3.10	120.25	113.00
3	5	2	NAG	C6-C5-C4	3.09	120.25	113.00
6	0	3	BMA	O2-C2-C3	3.09	116.34	110.14
2	Y	5	MAN	O5-C5-C6	-3.08	102.38	107.20
6	K	3	BMA	O2-C2-C3	3.08	116.30	110.14
3	r	1	NAG	C6-C5-C4	-3.07	105.81	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CA	1	NAG	C6-C5-C4	-3.07	105.82	113.00
2	D	2	NAG	O3-C3-C4	-3.06	103.27	110.35
3	W	1	NAG	C6-C5-C4	-3.06	105.84	113.00
4	p	3	BMA	O4-C4-C3	-3.06	103.28	110.35
6	f	3	BMA	O2-C2-C3	3.06	116.26	110.14
8	N	4	MAN	C6-C5-C4	3.06	120.17	113.00
7	DA	2	NAG	C2-N2-C7	-3.06	118.55	122.90
8	3	4	MAN	C6-C5-C4	3.05	120.16	113.00
3	8	1	NAG	O3-C3-C4	-3.05	103.29	110.35
4	U	3	BMA	O4-C4-C3	-3.05	103.29	110.35
4	AA	3	BMA	O4-C4-C3	-3.05	103.29	110.35
7	X	2	NAG	C2-N2-C7	-3.05	118.56	122.90
7	s	2	NAG	C2-N2-C7	-3.05	118.56	122.90
2	t	2	NAG	O3-C3-C4	-3.05	103.30	110.35
8	i	4	MAN	C6-C5-C4	3.05	120.15	113.00
2	Y	2	NAG	O3-C3-C4	-3.05	103.30	110.35
3	S	1	NAG	O3-C3-C4	-3.05	103.31	110.35
3	7	1	NAG	O3-C3-C2	-3.04	103.17	109.47
3	n	1	NAG	O3-C3-C4	-3.04	103.33	110.35
3	R	1	NAG	O3-C3-C2	-3.02	103.22	109.47
3	m	1	NAG	O3-C3-C2	-3.02	103.22	109.47
3	CA	1	NAG	O3-C3-C4	-3.00	103.40	110.35
3	r	1	NAG	O3-C3-C4	-3.00	103.41	110.35
6	0	8	MAN	O2-C2-C3	3.00	116.14	110.14
3	W	1	NAG	O3-C3-C4	-2.99	103.44	110.35
6	K	8	MAN	O2-C2-C3	2.99	116.13	110.14
6	f	8	MAN	O2-C2-C3	2.98	116.10	110.14
3	r	2	NAG	O5-C1-C2	-2.98	106.59	111.29
3	W	2	NAG	O5-C1-C2	-2.97	106.60	111.29
3	CA	2	NAG	O5-C1-C2	-2.97	106.60	111.29
7	s	2	NAG	O3-C3-C2	-2.95	103.36	109.47
7	X	2	NAG	O3-C3-C2	-2.95	103.36	109.47
7	DA	2	NAG	O3-C3-C2	-2.94	103.38	109.47
2	Y	3	BMA	O2-C2-C3	2.92	116.00	110.14
2	D	3	BMA	O2-C2-C3	2.91	115.97	110.14
6	0	3	BMA	C2-C3-C4	-2.91	105.86	110.89
2	t	3	BMA	O2-C2-C3	2.91	115.96	110.14
7	g	2	NAG	C1-C2-N2	2.90	115.44	110.49
7	L	2	NAG	C1-C2-N2	2.89	115.43	110.49
8	BA	4	MAN	O2-C2-C1	2.89	115.07	109.15
7	1	2	NAG	C1-C2-N2	2.89	115.42	110.49
6	K	3	BMA	C2-C3-C4	-2.88	105.91	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	4	MAN	O2-C2-C1	2.88	115.04	109.15
6	f	3	BMA	C2-C3-C4	-2.87	105.94	110.89
2	Y	5	MAN	O2-C2-C3	2.86	115.87	110.14
2	D	5	MAN	O2-C2-C3	2.86	115.86	110.14
8	q	4	MAN	O2-C2-C1	2.85	114.99	109.15
2	t	5	MAN	O2-C2-C3	2.85	115.85	110.14
8	i	4	MAN	O2-C2-C1	2.84	114.96	109.15
7	X	1	NAG	C6-C5-C4	2.83	119.64	113.00
8	N	4	MAN	O2-C2-C1	2.83	114.94	109.15
8	3	4	MAN	O2-C2-C1	2.83	114.94	109.15
7	s	1	NAG	C6-C5-C4	2.83	119.62	113.00
7	DA	1	NAG	C6-C5-C4	2.82	119.62	113.00
5	x	2	NAG	C2-N2-C7	-2.79	118.93	122.90
7	X	2	NAG	C8-C7-N2	2.78	120.81	116.10
7	s	2	NAG	C8-C7-N2	2.78	120.81	116.10
5	H	2	NAG	C2-N2-C7	-2.78	118.95	122.90
8	i	4	MAN	O4-C4-C3	-2.77	103.94	110.35
3	5	1	NAG	O3-C3-C4	2.77	116.76	110.35
8	3	4	MAN	O4-C4-C3	-2.77	103.94	110.35
5	c	2	NAG	C2-N2-C7	-2.77	118.96	122.90
7	DA	2	NAG	C8-C7-N2	2.77	120.78	116.10
8	N	4	MAN	O4-C4-C3	-2.76	103.96	110.35
3	k	1	NAG	O3-C3-C4	2.76	116.73	110.35
3	J	1	NAG	C6-C5-C4	2.76	119.47	113.00
3	e	1	NAG	C6-C5-C4	2.76	119.46	113.00
3	P	1	NAG	O3-C3-C4	2.76	116.72	110.35
8	BA	2	NAG	C8-C7-N2	2.75	120.76	116.10
3	z	1	NAG	C6-C5-C4	2.75	119.45	113.00
8	q	2	NAG	C8-C7-N2	2.75	120.76	116.10
8	V	2	NAG	C8-C7-N2	2.75	120.75	116.10
7	j	3	BMA	C6-C5-C4	2.73	119.41	113.00
7	O	3	BMA	C6-C5-C4	2.73	119.40	113.00
7	1	1	NAG	C1-O5-C5	2.73	115.89	112.19
7	4	3	BMA	C6-C5-C4	2.73	119.39	113.00
7	L	1	NAG	C1-O5-C5	2.73	115.89	112.19
3	E	1	NAG	C8-C7-N2	2.71	120.69	116.10
3	J	1	NAG	C8-C7-N2	2.71	120.69	116.10
3	z	1	NAG	C8-C7-N2	2.71	120.69	116.10
3	e	1	NAG	C8-C7-N2	2.71	120.68	116.10
3	u	1	NAG	C8-C7-N2	2.71	120.68	116.10
7	g	1	NAG	C1-O5-C5	2.70	115.86	112.19
4	v	1	NAG	C6-C5-C4	2.70	119.33	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	1	NAG	C8-C7-N2	2.70	120.67	116.10
3	CA	2	NAG	O5-C5-C6	-2.70	102.98	107.20
3	Z	1	NAG	C8-C7-N2	2.69	120.65	116.10
3	h	1	NAG	C8-C7-N2	2.68	120.64	116.10
3	T	1	NAG	C8-C7-N2	2.68	120.64	116.10
3	2	1	NAG	C8-C7-N2	2.68	120.64	116.10
3	o	1	NAG	C8-C7-N2	2.68	120.64	116.10
4	a	1	NAG	C6-C5-C4	2.68	119.29	113.00
4	F	1	NAG	C6-C5-C4	2.68	119.29	113.00
3	W	2	NAG	O5-C5-C6	-2.68	103.00	107.20
5	c	1	NAG	C8-C7-N2	2.68	120.63	116.10
5	H	1	NAG	C8-C7-N2	2.67	120.62	116.10
4	a	1	NAG	C2-N2-C7	-2.67	119.10	122.90
6	0	8	MAN	O2-C2-C1	2.67	114.61	109.15
4	F	1	NAG	C2-N2-C7	-2.67	119.10	122.90
3	9	1	NAG	C8-C7-N2	2.67	120.61	116.10
4	v	1	NAG	C2-N2-C7	-2.66	119.11	122.90
3	r	2	NAG	O5-C5-C6	-2.65	103.04	107.20
6	f	8	MAN	O2-C2-C1	2.65	114.58	109.15
5	x	1	NAG	C8-C7-N2	2.65	120.59	116.10
6	K	8	MAN	O2-C2-C1	2.65	114.57	109.15
8	3	1	NAG	C8-C7-N2	2.65	120.58	116.10
7	O	1	NAG	C6-C5-C4	2.64	119.18	113.00
7	j	1	NAG	C6-C5-C4	2.64	119.18	113.00
3	2	2	NAG	O3-C3-C2	-2.64	104.01	109.47
3	I	2	NAG	O4-C4-C5	2.63	115.83	109.30
8	N	1	NAG	C8-C7-N2	2.63	120.55	116.10
3	d	2	NAG	O4-C4-C5	2.63	115.83	109.30
3	y	2	NAG	O4-C4-C5	2.63	115.83	109.30
6	f	7	MAN	C1-O5-C5	2.63	115.75	112.19
7	4	1	NAG	C6-C5-C4	2.63	119.16	113.00
3	h	2	NAG	O3-C3-C2	-2.62	104.04	109.47
8	i	1	NAG	C8-C7-N2	2.62	120.54	116.10
6	K	7	MAN	C1-O5-C5	2.62	115.75	112.19
3	M	2	NAG	O3-C3-C2	-2.62	104.05	109.47
7	DA	1	NAG	C8-C7-N2	2.62	120.53	116.10
3	CA	1	NAG	C3-C4-C5	-2.61	105.59	110.24
6	0	7	MAN	C1-O5-C5	2.61	115.72	112.19
3	m	1	NAG	C8-C7-N2	2.60	120.50	116.10
3	R	1	NAG	C8-C7-N2	2.60	120.49	116.10
3	7	1	NAG	C8-C7-N2	2.60	120.49	116.10
3	r	1	NAG	C3-C4-C5	-2.59	105.61	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	1	NAG	C8-C7-N2	2.59	120.48	116.10
3	W	1	NAG	C3-C4-C5	-2.58	105.64	110.24
7	s	1	NAG	C8-C7-N2	2.58	120.46	116.10
4	a	3	BMA	O3-C3-C2	2.57	114.92	109.99
4	F	3	BMA	O3-C3-C2	2.57	114.91	109.99
4	v	3	BMA	O3-C3-C2	2.56	114.90	109.99
4	a	4	MAN	O4-C4-C5	-2.54	102.98	109.30
4	v	4	MAN	O4-C4-C5	-2.54	102.99	109.30
4	F	4	MAN	O4-C4-C5	-2.54	102.99	109.30
2	Y	5	MAN	O5-C1-C2	-2.51	106.90	110.77
2	t	5	MAN	O5-C1-C2	-2.51	106.90	110.77
2	D	5	MAN	O5-C1-C2	-2.50	106.91	110.77
7	s	2	NAG	O3-C3-C4	2.50	116.13	110.35
7	X	2	NAG	O3-C3-C4	2.50	116.12	110.35
3	6	1	NAG	C3-C4-C5	-2.50	105.79	110.24
7	DA	2	NAG	O3-C3-C4	2.49	116.11	110.35
3	Q	1	NAG	C3-C4-C5	-2.49	105.80	110.24
3	l	1	NAG	C3-C4-C5	-2.49	105.81	110.24
3	w	2	NAG	O4-C4-C5	-2.46	103.19	109.30
3	G	2	NAG	O4-C4-C5	-2.45	103.20	109.30
3	b	2	NAG	O4-C4-C5	-2.45	103.21	109.30
3	z	2	NAG	O4-C4-C5	-2.45	103.22	109.30
3	e	2	NAG	O4-C4-C5	-2.44	103.23	109.30
3	J	2	NAG	O4-C4-C5	-2.44	103.25	109.30
3	Z	1	NAG	C2-N2-C7	-2.42	119.45	122.90
7	g	2	NAG	C1-O5-C5	2.42	115.47	112.19
7	L	2	NAG	C1-O5-C5	2.42	115.47	112.19
3	u	1	NAG	C2-N2-C7	-2.42	119.46	122.90
7	1	2	NAG	C1-O5-C5	2.40	115.45	112.19
3	E	1	NAG	C2-N2-C7	-2.40	119.48	122.90
3	6	1	NAG	C8-C7-N2	2.39	120.15	116.10
6	0	1	NAG	C8-C7-N2	2.39	120.14	116.10
6	K	1	NAG	C8-C7-N2	2.39	120.14	116.10
4	AA	1	NAG	C8-C7-N2	2.38	120.14	116.10
3	l	1	NAG	C8-C7-N2	2.38	120.13	116.10
6	f	1	NAG	C8-C7-N2	2.38	120.13	116.10
3	Q	1	NAG	C8-C7-N2	2.38	120.13	116.10
4	U	1	NAG	C8-C7-N2	2.38	120.13	116.10
4	p	1	NAG	C8-C7-N2	2.37	120.12	116.10
8	3	3	BMA	O4-C4-C5	2.37	115.18	109.30
8	N	3	BMA	O4-C4-C5	2.36	115.15	109.30
5	x	4	MAN	O4-C4-C3	-2.35	104.91	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	4	MAN	O4-C4-C3	-2.35	104.91	110.35
5	H	4	MAN	O4-C4-C3	-2.35	104.92	110.35
8	i	3	BMA	O4-C4-C5	2.34	115.10	109.30
5	x	2	NAG	C8-C7-N2	2.31	120.01	116.10
5	c	2	NAG	C8-C7-N2	2.31	120.01	116.10
7	DA	2	NAG	C3-C4-C5	-2.31	106.12	110.24
7	1	2	NAG	O5-C1-C2	-2.31	107.65	111.29
5	H	2	NAG	C8-C7-N2	2.31	120.00	116.10
4	v	3	BMA	O2-C2-C1	-2.30	104.44	109.15
3	w	1	NAG	C8-C7-N2	2.30	120.00	116.10
4	F	3	BMA	O2-C2-C1	-2.30	104.44	109.15
3	b	1	NAG	C8-C7-N2	2.30	119.99	116.10
7	s	2	NAG	C3-C4-C5	-2.30	106.14	110.24
3	G	1	NAG	C8-C7-N2	2.29	119.98	116.10
7	X	2	NAG	C3-C4-C5	-2.29	106.15	110.24
7	g	2	NAG	O5-C1-C2	-2.29	107.67	111.29
7	L	2	NAG	O5-C1-C2	-2.29	107.67	111.29
7	4	2	NAG	C2-N2-C7	-2.29	119.65	122.90
4	a	3	BMA	O2-C2-C1	-2.28	104.48	109.15
8	N	2	NAG	C2-N2-C7	-2.28	119.66	122.90
8	i	2	NAG	C2-N2-C7	-2.28	119.66	122.90
8	3	2	NAG	C2-N2-C7	-2.27	119.67	122.90
2	Y	4	MAN	C1-O5-C5	2.27	115.27	112.19
7	O	2	NAG	C2-N2-C7	-2.26	119.68	122.90
2	t	5	MAN	O5-C5-C4	-2.26	105.33	110.83
2	Y	5	MAN	O5-C5-C4	-2.25	105.35	110.83
7	j	2	NAG	C2-N2-C7	-2.25	119.70	122.90
2	t	4	MAN	C1-O5-C5	2.24	115.23	112.19
2	D	5	MAN	O5-C5-C4	-2.24	105.38	110.83
8	3	2	NAG	C8-C7-N2	2.23	119.88	116.10
6	0	8	MAN	O5-C1-C2	-2.23	107.33	110.77
8	i	2	NAG	C8-C7-N2	2.22	119.87	116.10
6	f	8	MAN	O5-C1-C2	-2.22	107.34	110.77
2	D	4	MAN	C1-O5-C5	2.22	115.20	112.19
8	N	2	NAG	C8-C7-N2	2.22	119.86	116.10
6	K	8	MAN	O5-C1-C2	-2.22	107.35	110.77
3	P	1	NAG	C8-C7-N2	2.22	119.85	116.10
3	5	1	NAG	C8-C7-N2	2.21	119.85	116.10
2	t	1	NAG	C1-C2-N2	2.21	114.27	110.49
8	q	1	NAG	O3-C3-C4	2.21	115.45	110.35
8	BA	1	NAG	O3-C3-C4	2.20	115.44	110.35
8	V	1	NAG	O3-C3-C4	2.20	115.44	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	h	1	NAG	C2-N2-C7	-2.19	119.78	122.90
2	D	1	NAG	C1-C2-N2	2.19	114.23	110.49
3	k	1	NAG	C8-C7-N2	2.19	119.80	116.10
8	N	1	NAG	C1-C2-N2	-2.19	106.75	110.49
4	U	2	NAG	C8-C7-N2	2.19	119.80	116.10
4	p	2	NAG	C8-C7-N2	2.19	119.80	116.10
8	3	1	NAG	C1-C2-N2	-2.18	106.76	110.49
4	AA	2	NAG	C8-C7-N2	2.18	119.79	116.10
3	6	1	NAG	C1-C2-N2	2.18	114.21	110.49
8	q	1	NAG	C1-C2-N2	-2.18	106.77	110.49
3	Q	1	NAG	C1-C2-N2	2.18	114.20	110.49
8	i	1	NAG	C1-C2-N2	-2.17	106.77	110.49
2	Y	1	NAG	C1-C2-N2	2.17	114.19	110.49
3	l	1	NAG	C1-C2-N2	2.17	114.19	110.49
4	AA	2	NAG	O3-C3-C2	-2.17	104.98	109.47
8	BA	1	NAG	C1-C2-N2	-2.16	106.79	110.49
3	2	1	NAG	C2-N2-C7	-2.16	119.82	122.90
8	V	1	NAG	C1-C2-N2	-2.16	106.80	110.49
3	M	1	NAG	C2-N2-C7	-2.16	119.83	122.90
8	i	2	NAG	O3-C3-C4	-2.15	105.37	110.35
3	I	1	NAG	O7-C7-C8	-2.15	118.06	122.06
4	U	2	NAG	O3-C3-C2	-2.15	105.02	109.47
3	y	1	NAG	O7-C7-C8	-2.15	118.07	122.06
8	N	2	NAG	O3-C3-C4	-2.15	105.39	110.35
8	3	2	NAG	O3-C3-C4	-2.14	105.40	110.35
7	1	1	NAG	O7-C7-C8	-2.14	118.08	122.06
4	p	2	NAG	O3-C3-C2	-2.14	105.03	109.47
3	d	1	NAG	O7-C7-C8	-2.14	118.09	122.06
7	L	1	NAG	O7-C7-C8	-2.14	118.09	122.06
8	BA	2	NAG	C3-C4-C5	-2.12	106.45	110.24
7	g	1	NAG	O7-C7-C8	-2.12	118.11	122.06
7	j	2	NAG	C8-C7-N2	2.11	119.68	116.10
8	V	2	NAG	C3-C4-C5	-2.11	106.47	110.24
7	O	2	NAG	C8-C7-N2	2.11	119.67	116.10
5	H	2	NAG	C3-C4-C5	-2.11	106.48	110.24
8	i	4	MAN	O2-C2-C3	2.10	114.35	110.14
8	N	4	MAN	O2-C2-C3	2.10	114.35	110.14
8	3	4	MAN	O2-C2-C3	2.10	114.35	110.14
5	x	2	NAG	C3-C4-C5	-2.10	106.49	110.24
3	J	2	NAG	C8-C7-N2	2.10	119.66	116.10
8	i	5	MAN	O4-C4-C5	2.10	114.51	109.30
7	4	2	NAG	C8-C7-N2	2.10	119.65	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	2	NAG	C3-C4-C5	-2.10	106.50	110.24
3	Z	2	NAG	C2-N2-C7	2.09	125.88	122.90
5	c	2	NAG	C3-C4-C5	-2.09	106.51	110.24
3	e	2	NAG	C8-C7-N2	2.09	119.63	116.10
8	N	5	MAN	O4-C4-C5	2.08	114.47	109.30
3	z	2	NAG	C8-C7-N2	2.08	119.62	116.10
3	u	2	NAG	C2-N2-C7	2.08	125.86	122.90
3	E	2	NAG	C2-N2-C7	2.07	125.85	122.90
6	f	7	MAN	O5-C1-C2	-2.07	107.58	110.77
8	3	5	MAN	O4-C4-C5	2.07	114.43	109.30
4	v	2	NAG	C8-C7-N2	2.06	119.59	116.10
4	F	2	NAG	C8-C7-N2	2.06	119.58	116.10
4	a	2	NAG	C8-C7-N2	2.06	119.58	116.10
6	K	7	MAN	O5-C1-C2	-2.05	107.61	110.77
3	P	2	NAG	O5-C1-C2	-2.04	108.07	111.29
6	0	7	MAN	O5-C1-C2	-2.03	107.63	110.77
3	k	2	NAG	O5-C1-C2	-2.03	108.09	111.29
8	BA	1	NAG	C8-C7-N2	2.03	119.53	116.10
5	c	1	NAG	O7-C7-C8	-2.02	118.31	122.06
8	V	1	NAG	C8-C7-N2	2.02	119.52	116.10
4	p	2	NAG	O4-C4-C3	2.01	115.00	110.35
4	U	2	NAG	O4-C4-C3	2.01	115.00	110.35
4	AA	2	NAG	O4-C4-C3	2.01	115.00	110.35
3	5	2	NAG	O5-C1-C2	-2.01	108.11	111.29
5	H	1	NAG	O7-C7-C8	-2.01	118.33	122.06
8	q	1	NAG	C8-C7-N2	2.01	119.50	116.10

There are no chirality outliers.

All (186) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	1	NAG	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
5	x	1	NAG	C4-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	x	2	NAG	O5-C5-C6-O6
8	V	3	BMA	C4-C5-C6-O6
8	q	3	BMA	C4-C5-C6-O6
8	BA	3	BMA	C4-C5-C6-O6
6	K	3	BMA	C4-C5-C6-O6
6	f	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	0	3	BMA	C4-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	f	2	NAG	O5-C5-C6-O6
6	0	2	NAG	O5-C5-C6-O6
8	V	3	BMA	O5-C5-C6-O6
8	q	3	BMA	O5-C5-C6-O6
8	BA	3	BMA	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
3	y	2	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	f	2	NAG	C4-C5-C6-O6
6	0	2	NAG	C4-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	x	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	l	1	NAG	C4-C5-C6-O6
3	6	1	NAG	C4-C5-C6-O6
8	V	2	NAG	O5-C5-C6-O6
8	q	2	NAG	O5-C5-C6-O6
8	BA	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	d	2	NAG	C4-C5-C6-O6
3	y	2	NAG	C4-C5-C6-O6
8	V	2	NAG	C4-C5-C6-O6
8	q	2	NAG	C4-C5-C6-O6
8	BA	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	d	1	NAG	C8-C7-N2-C2
3	d	1	NAG	O7-C7-N2-C2
3	y	1	NAG	C8-C7-N2-C2
3	y	1	NAG	O7-C7-N2-C2
5	H	3	BMA	C4-C5-C6-O6
5	c	3	BMA	C4-C5-C6-O6
5	x	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	l	2	NAG	O5-C5-C6-O6
3	6	2	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	x	3	BMA	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	w	1	NAG	O5-C5-C6-O6
6	K	3	BMA	O5-C5-C6-O6
6	f	3	BMA	O5-C5-C6-O6
6	0	3	BMA	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	m	1	NAG	O5-C5-C6-O6
3	7	1	NAG	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	l	2	NAG	C4-C5-C6-O6
3	6	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6
2	t	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	l	1	NAG	O5-C5-C6-O6
3	6	1	NAG	O5-C5-C6-O6
8	N	3	BMA	O5-C5-C6-O6
8	i	3	BMA	O5-C5-C6-O6
8	3	3	BMA	O5-C5-C6-O6
6	K	7	MAN	O5-C5-C6-O6
6	f	7	MAN	O5-C5-C6-O6
6	0	7	MAN	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	d	1	NAG	C4-C5-C6-O6
3	y	1	NAG	C4-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
7	j	1	NAG	O5-C5-C6-O6
7	4	1	NAG	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	f	1	NAG	O5-C5-C6-O6
6	0	1	NAG	O5-C5-C6-O6
8	i	2	NAG	C4-C5-C6-O6
8	N	2	NAG	C4-C5-C6-O6
8	3	2	NAG	C4-C5-C6-O6
8	N	1	NAG	O5-C5-C6-O6
8	i	1	NAG	O5-C5-C6-O6
8	3	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	e	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	z	2	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	n	2	NAG	O5-C5-C6-O6
3	o	2	NAG	O5-C5-C6-O6
3	8	2	NAG	O5-C5-C6-O6
3	9	2	NAG	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	a	3	BMA	O5-C5-C6-O6
4	v	3	BMA	O5-C5-C6-O6
2	D	5	MAN	O5-C5-C6-O6
2	Y	5	MAN	O5-C5-C6-O6
2	t	5	MAN	O5-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
5	x	3	BMA	O5-C5-C6-O6
4	U	3	BMA	O5-C5-C6-O6
4	p	3	BMA	O5-C5-C6-O6
4	AA	3	BMA	O5-C5-C6-O6
8	N	3	BMA	C4-C5-C6-O6
8	i	3	BMA	C4-C5-C6-O6
8	3	3	BMA	C4-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	o	1	NAG	O5-C5-C6-O6
3	9	1	NAG	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	Y	3	BMA	O5-C5-C6-O6
2	t	3	BMA	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
3	m	2	NAG	O5-C5-C6-O6
3	r	2	NAG	O5-C5-C6-O6
3	7	2	NAG	O5-C5-C6-O6
3	CA	2	NAG	O5-C5-C6-O6
8	N	5	MAN	O5-C5-C6-O6
8	i	5	MAN	O5-C5-C6-O6
8	3	5	MAN	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6
2	t	1	NAG	O5-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
8	V	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
8	q	1	NAG	C3-C2-N2-C7
8	BA	1	NAG	C3-C2-N2-C7
2	Y	4	MAN	O5-C5-C6-O6
2	t	4	MAN	O5-C5-C6-O6
3	m	1	NAG	C4-C5-C6-O6
3	7	1	NAG	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	k	1	NAG	C4-C5-C6-O6
3	5	1	NAG	C4-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6
7	j	1	NAG	C4-C5-C6-O6
7	4	1	NAG	C4-C5-C6-O6
3	W	1	NAG	C1-C2-N2-C7
3	r	1	NAG	C1-C2-N2-C7
3	CA	1	NAG	C1-C2-N2-C7
3	G	2	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
3	w	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C3-C2-N2-C7
3	Q	1	NAG	C3-C2-N2-C7
3	b	1	NAG	C3-C2-N2-C7
3	l	1	NAG	C3-C2-N2-C7
3	w	1	NAG	C3-C2-N2-C7
3	6	1	NAG	C3-C2-N2-C7
7	L	1	NAG	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
7	1	1	NAG	O5-C5-C6-O6
8	q	5	MAN	O5-C5-C6-O6
8	V	5	MAN	O5-C5-C6-O6
8	BA	5	MAN	O5-C5-C6-O6
3	d	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	y	1	NAG	O5-C5-C6-O6
6	f	8	MAN	O5-C5-C6-O6
6	K	8	MAN	O5-C5-C6-O6
6	0	8	MAN	O5-C5-C6-O6
7	X	2	NAG	O5-C5-C6-O6
7	s	2	NAG	O5-C5-C6-O6
7	DA	2	NAG	O5-C5-C6-O6
2	D	6	MAN	O5-C5-C6-O6
2	t	6	MAN	O5-C5-C6-O6

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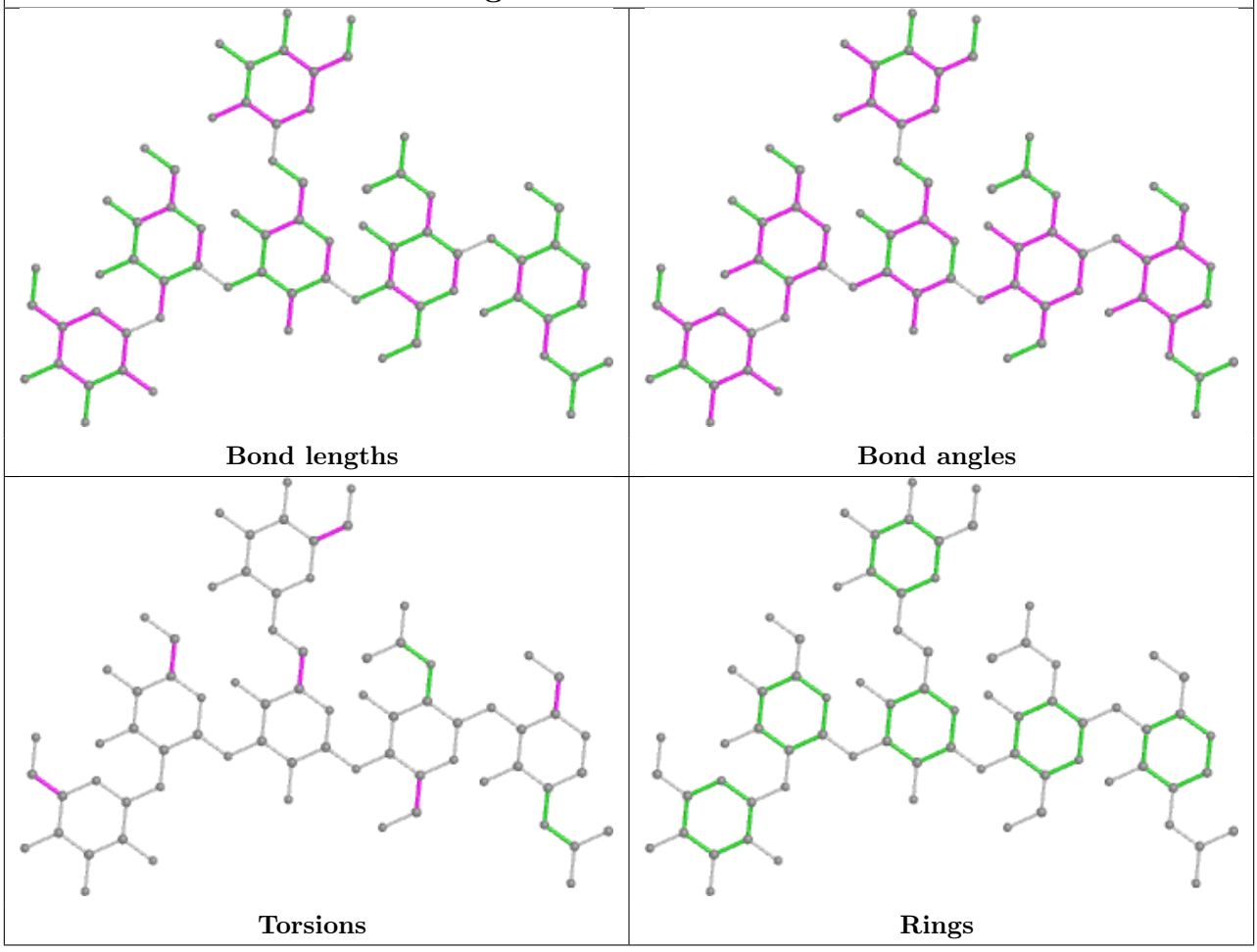
Mol	Chain	Res	Type	Atoms
2	Y	6	MAN	O5-C5-C6-O6
4	v	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	R	1	NAG	C3-C2-N2-C7
3	m	1	NAG	C3-C2-N2-C7
3	7	1	NAG	C3-C2-N2-C7
4	a	2	NAG	O5-C5-C6-O6

There are no ring outliers.

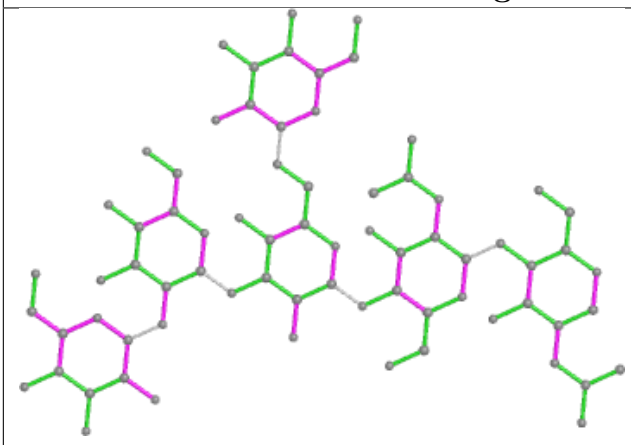
No monomer is involved in short contacts.

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

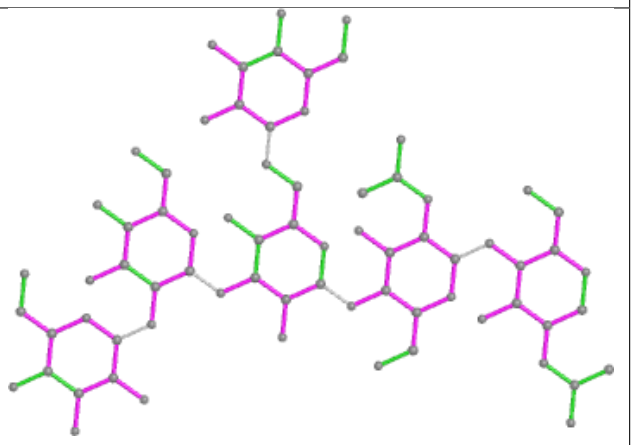
Oligosaccharide Chain D



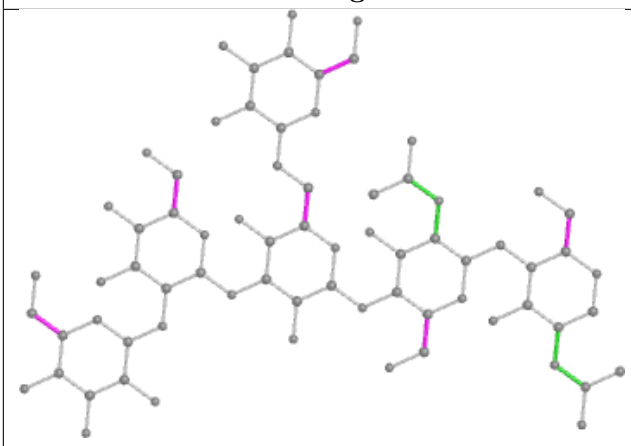
Oligosaccharide Chain Y



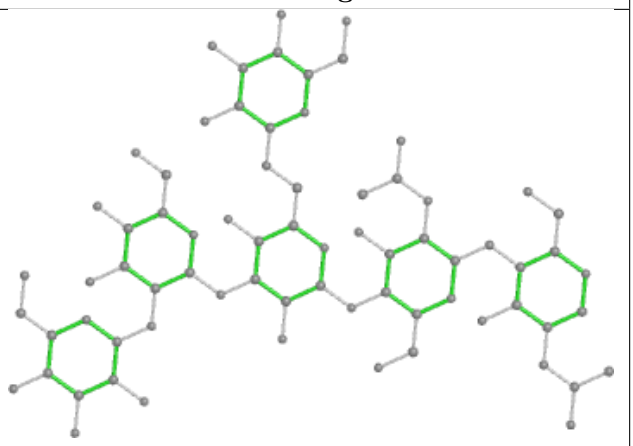
Bond lengths



Bond angles

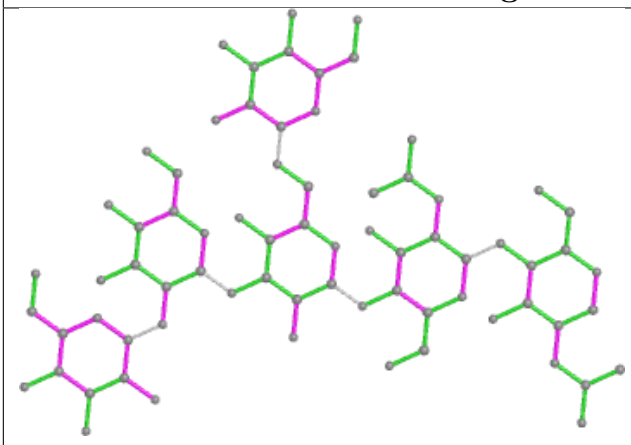


Torsions

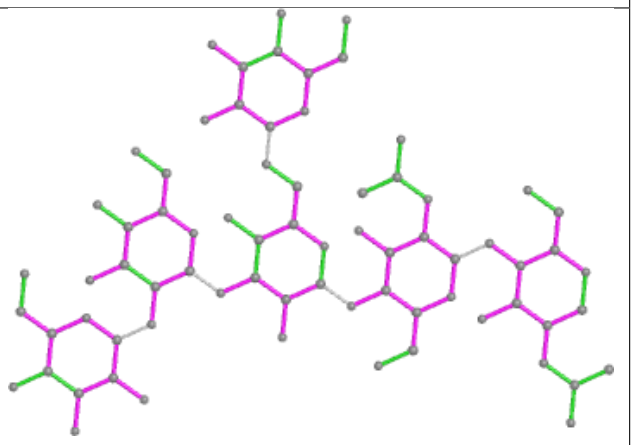


Rings

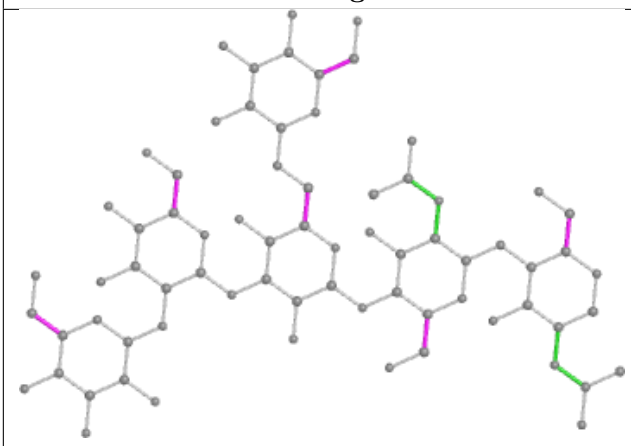
Oligosaccharide Chain t



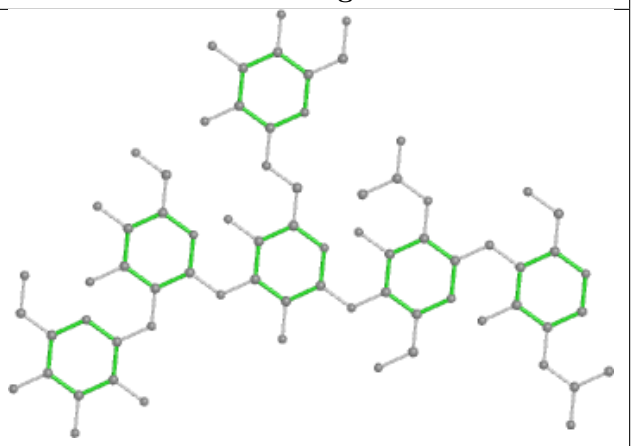
Bond lengths



Bond angles

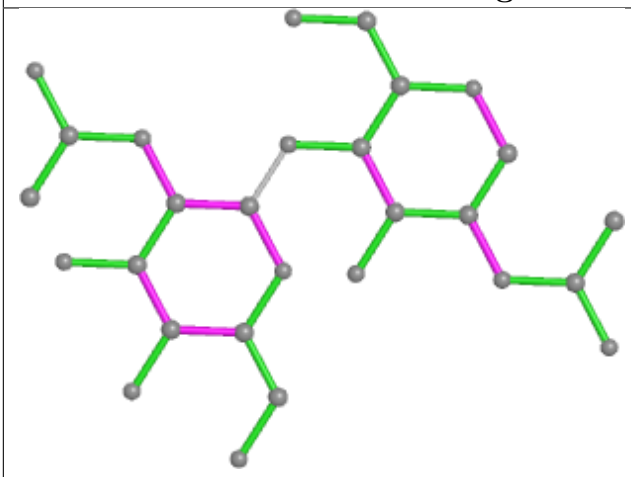


Torsions

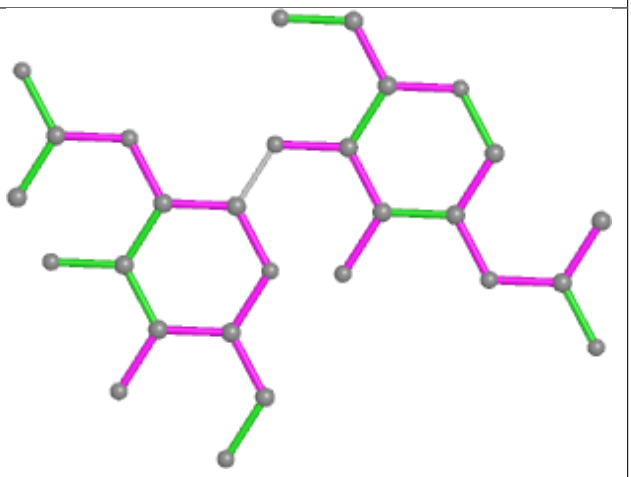


Rings

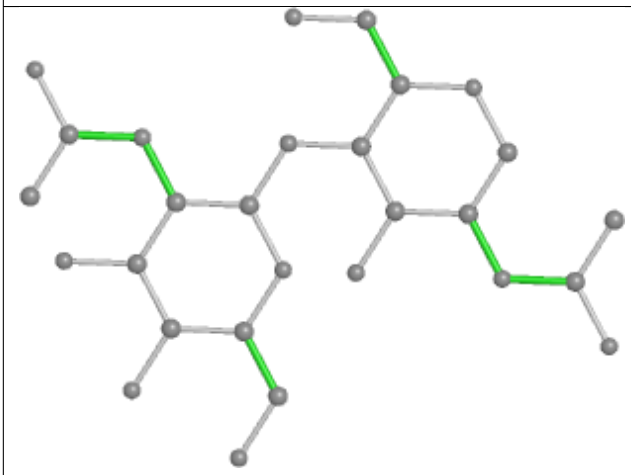
Oligosaccharide Chain E



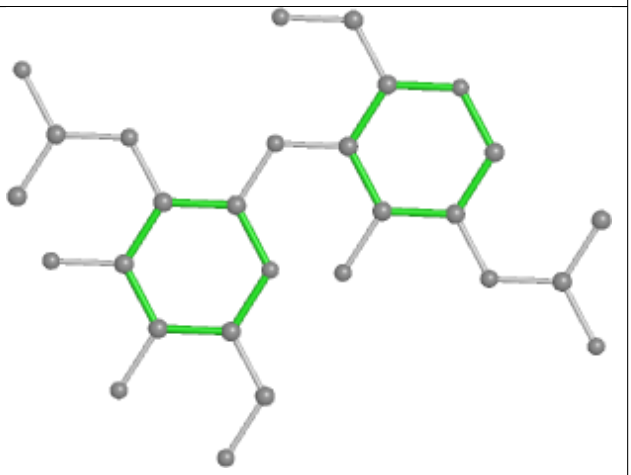
Bond lengths



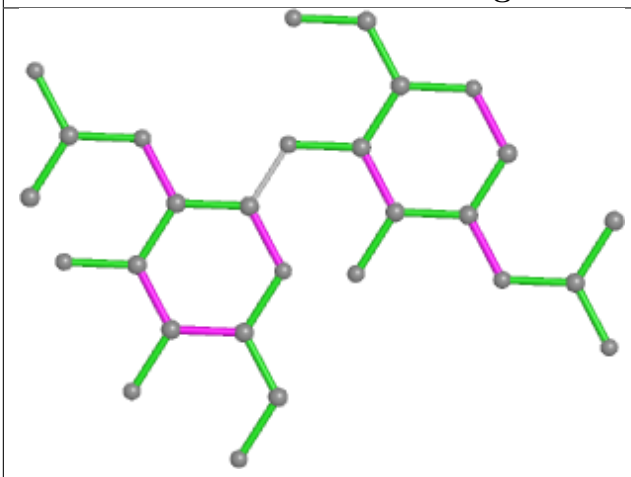
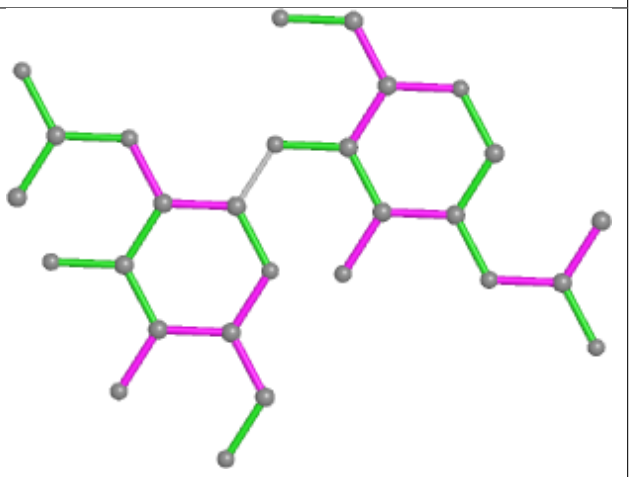
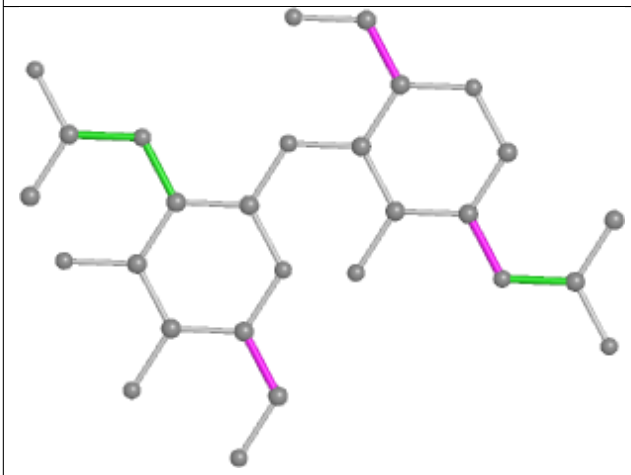
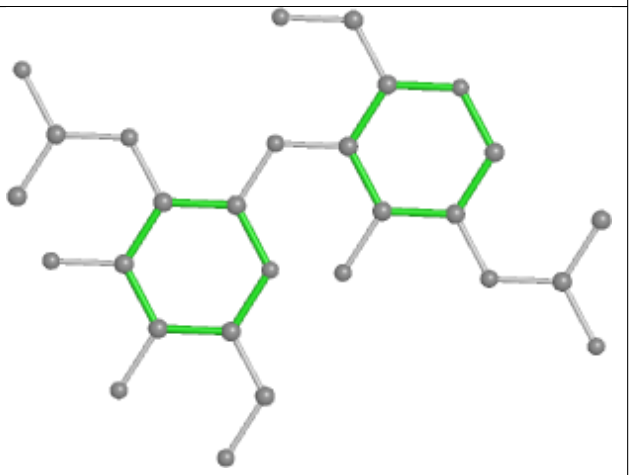
Bond angles



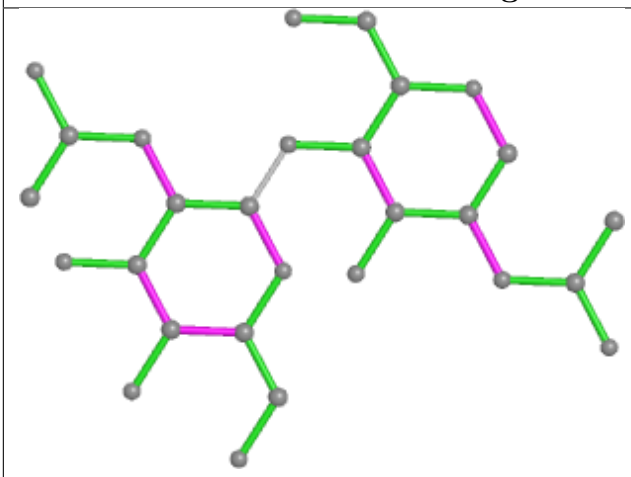
Torsions



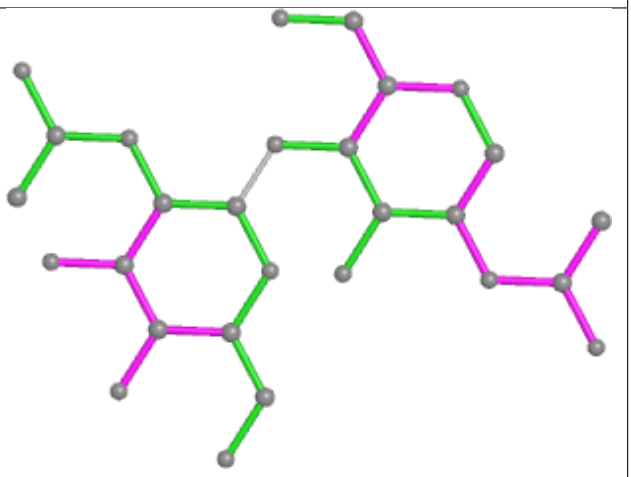
Rings

Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

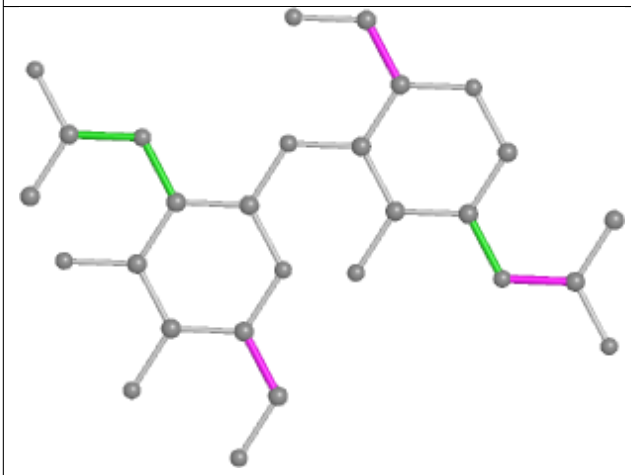
Oligosaccharide Chain I



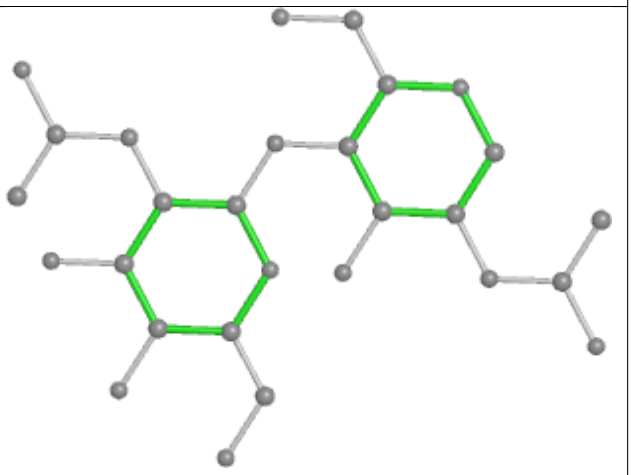
Bond lengths



Bond angles

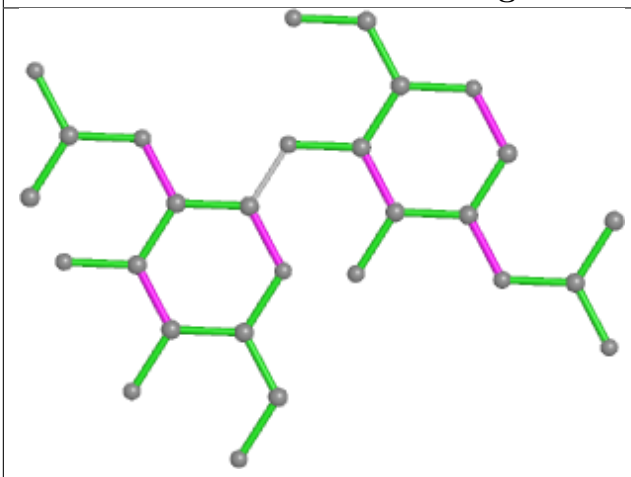


Torsions

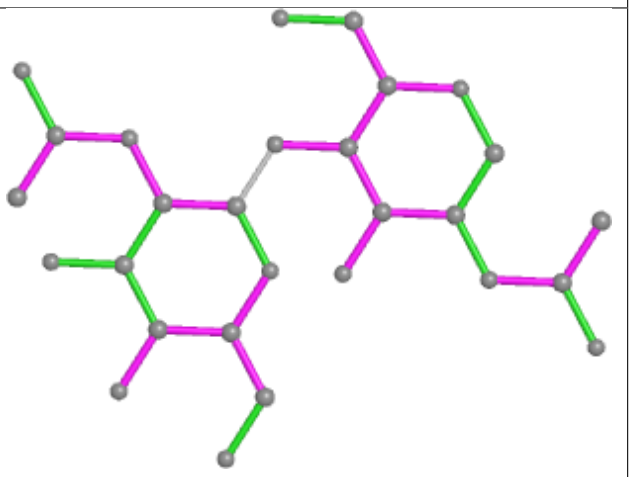


Rings

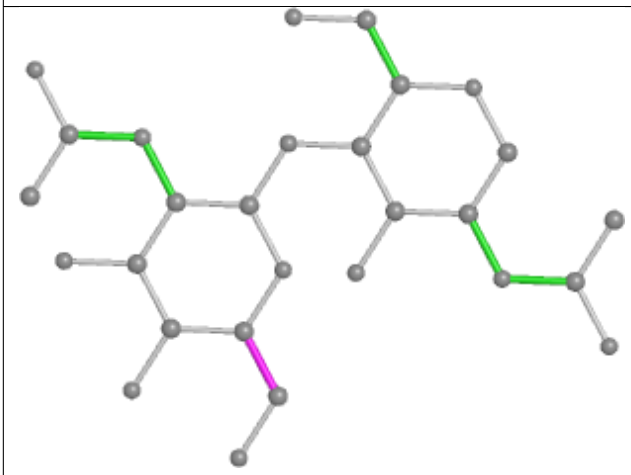
Oligosaccharide Chain J



Bond lengths



Bond angles



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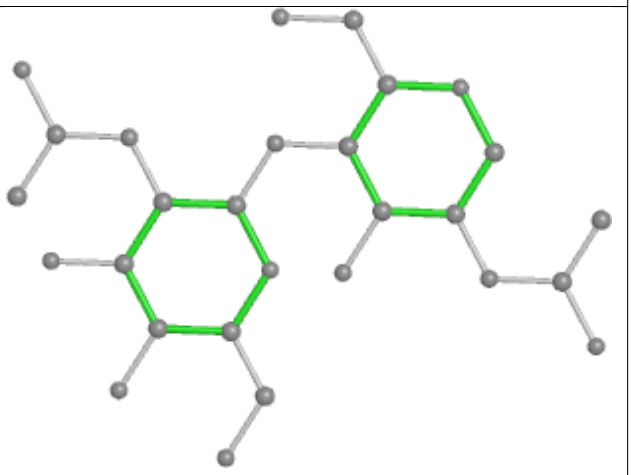
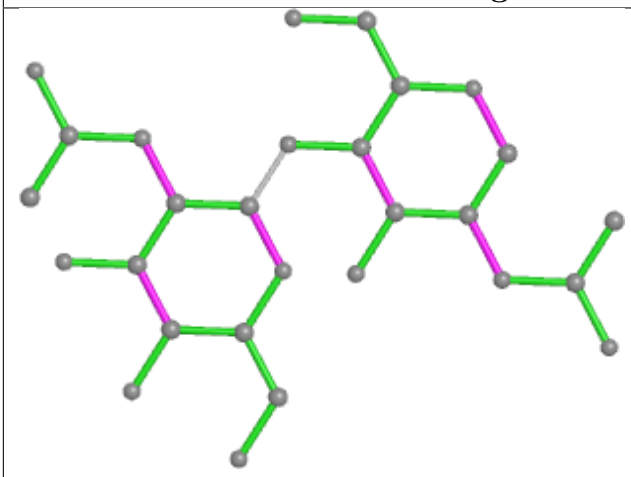
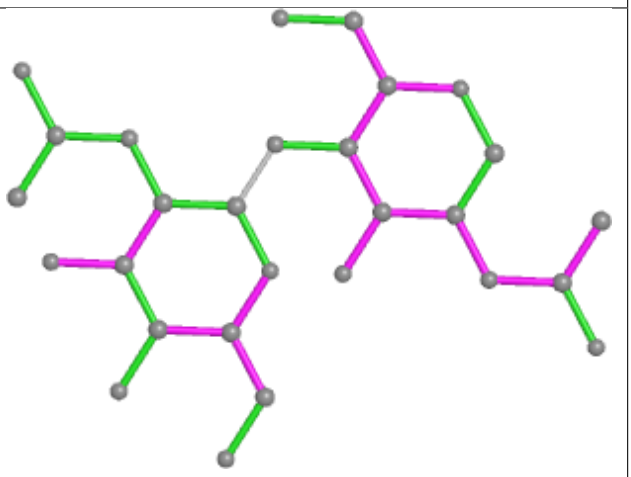


Rings

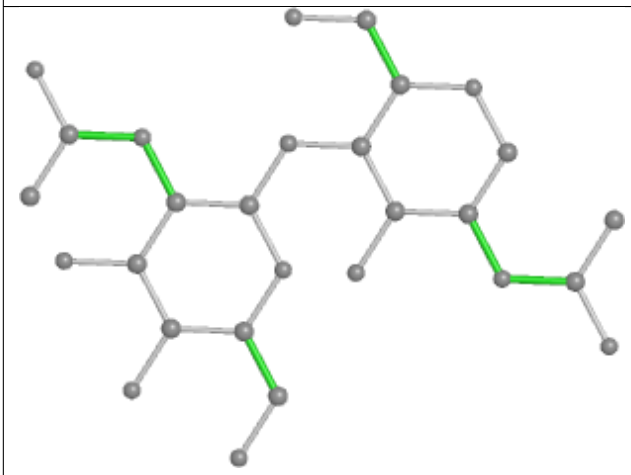
Oligosaccharide Chain M



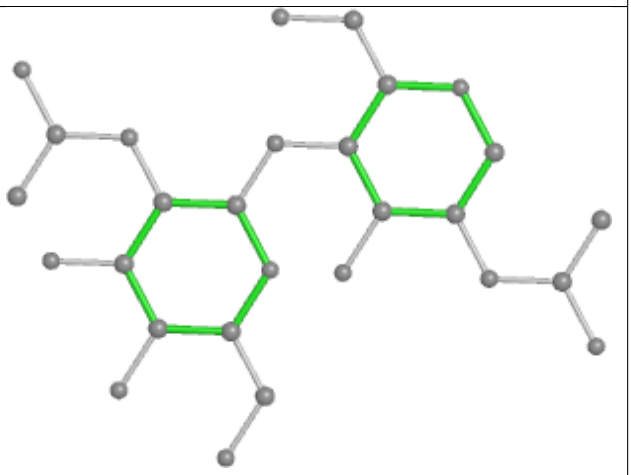
Bond lengths



Bond angles

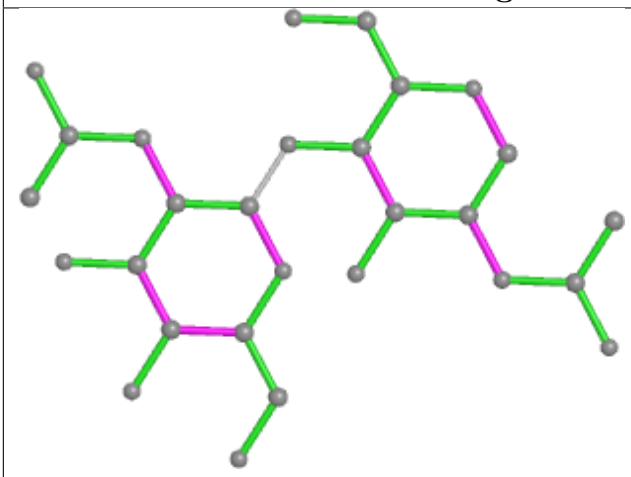


Torsions

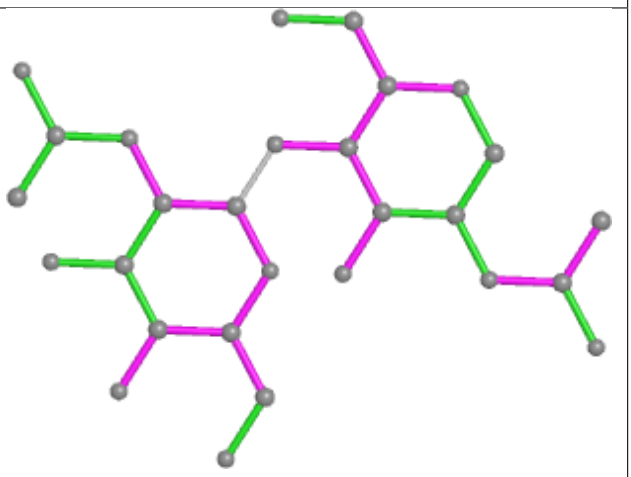


Rings

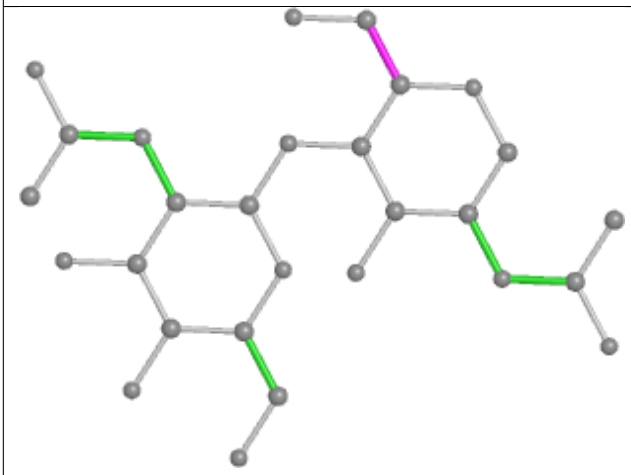
Oligosaccharide Chain P



Bond lengths



Bond angles



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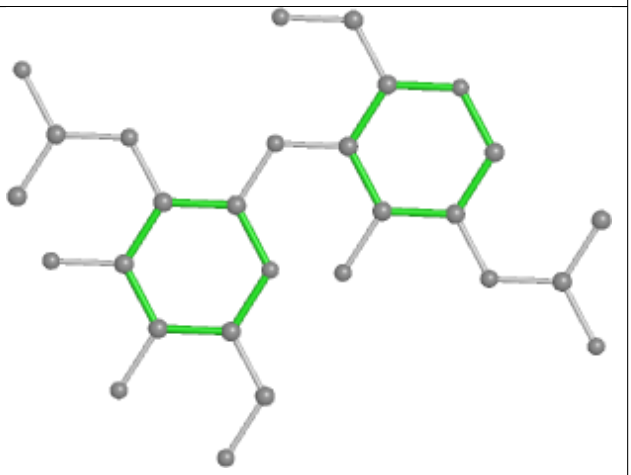
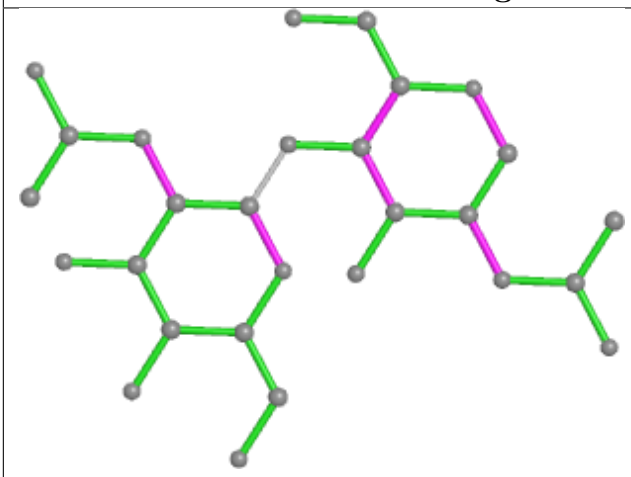
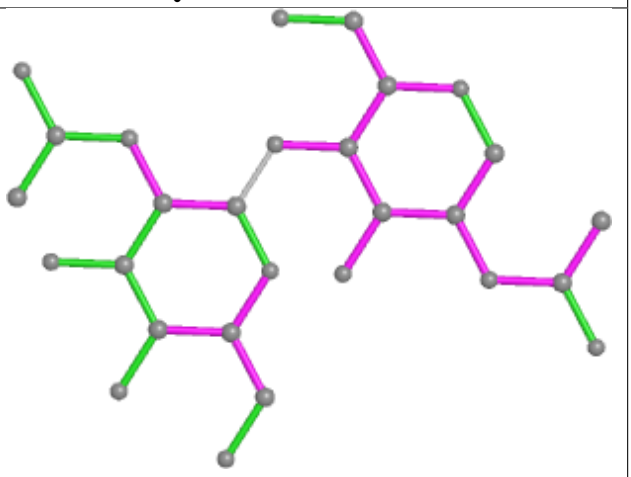


Rings

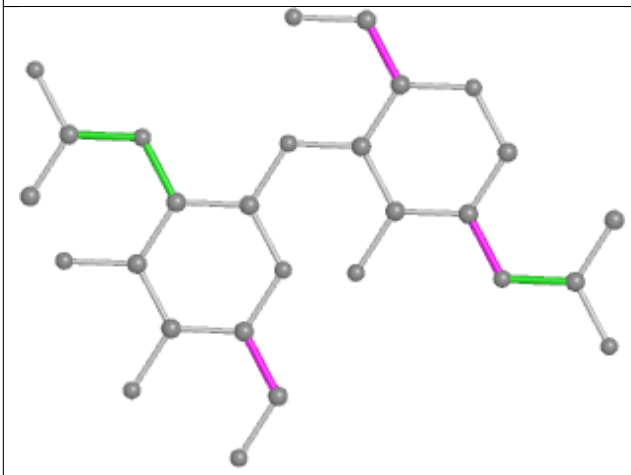
Oligosaccharide Chain Q



Bond lengths



Bond angles



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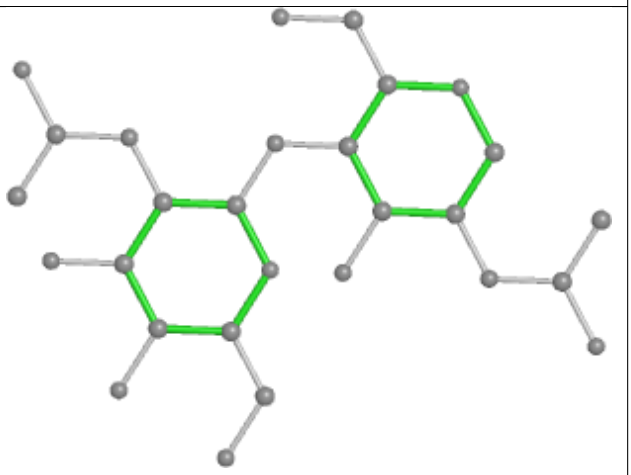
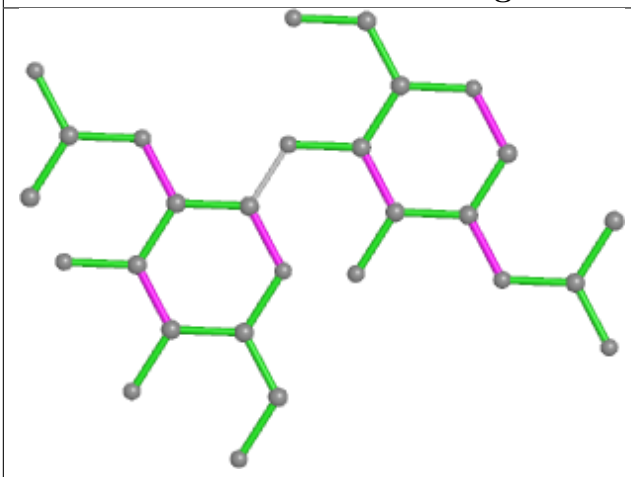
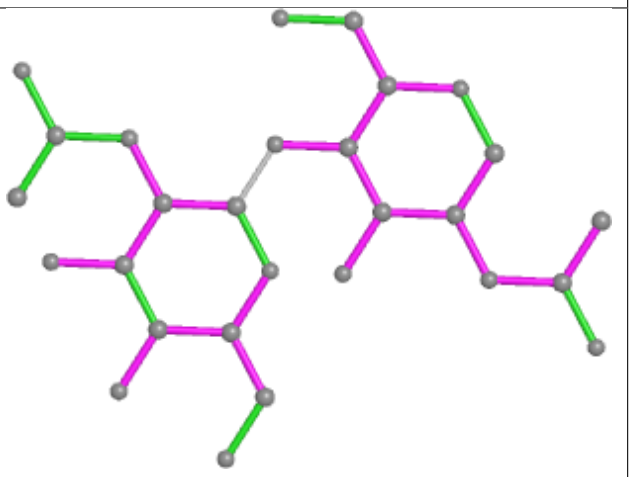


Rings

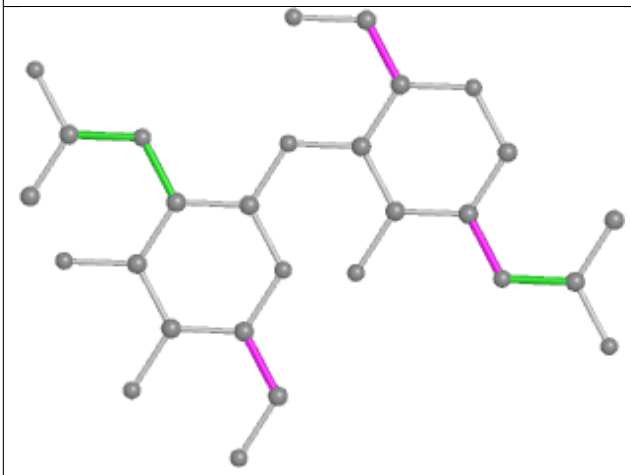
Oligosaccharide Chain R



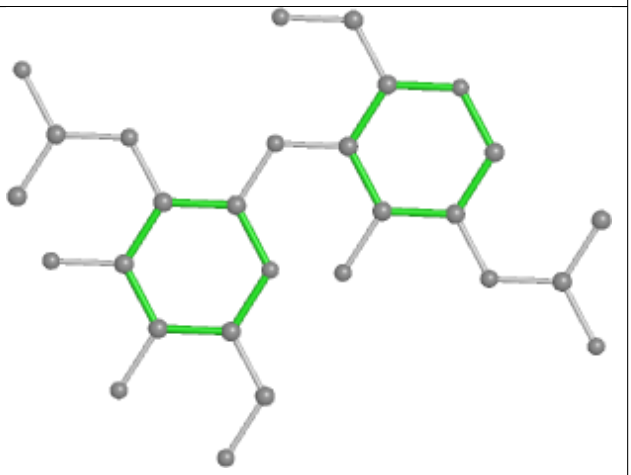
Bond lengths



Bond angles

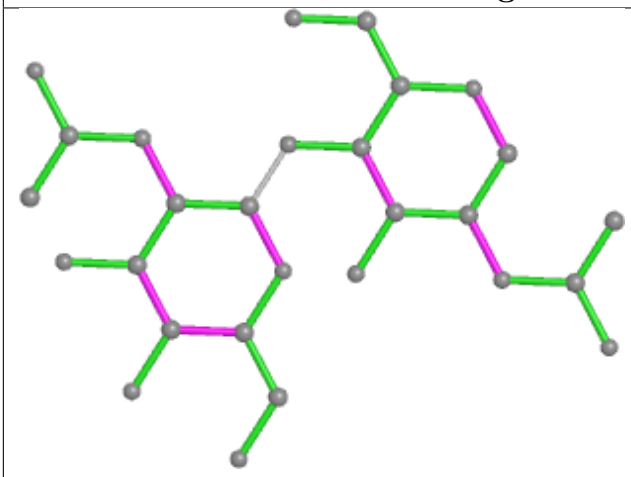


Torsions

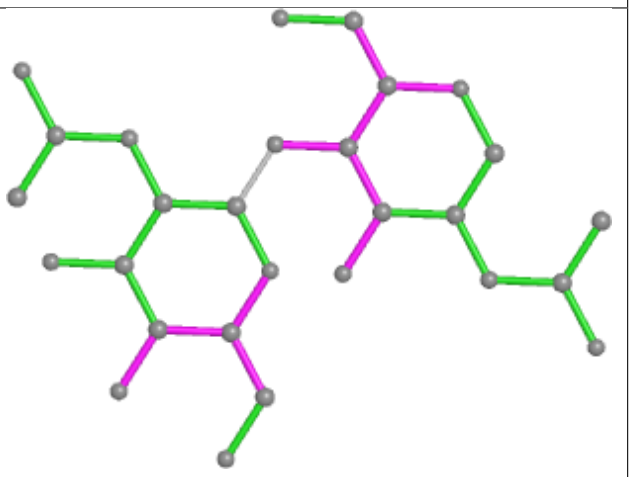


Rings

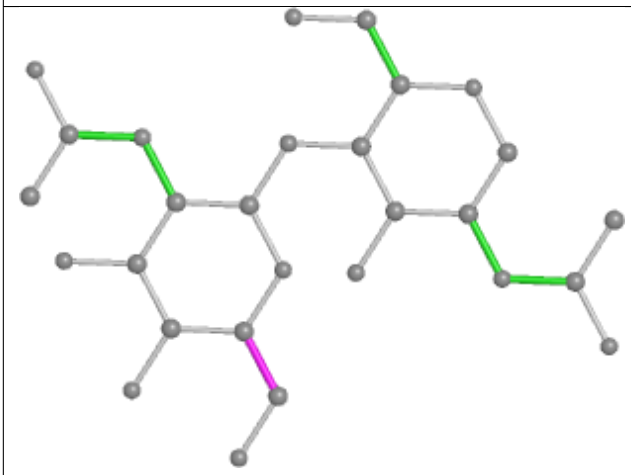
Oligosaccharide Chain S



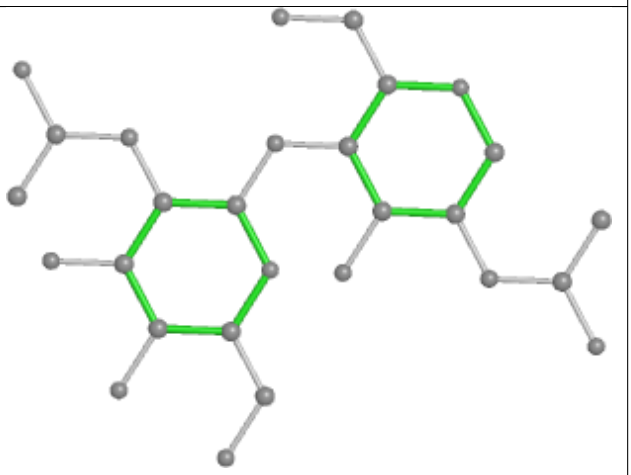
Bond lengths



Bond angles

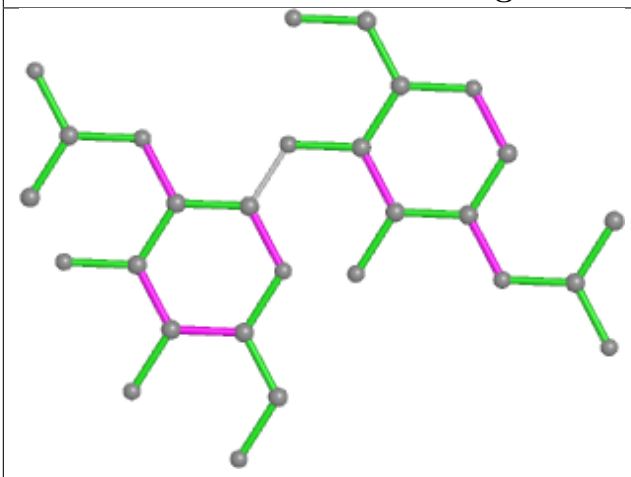


Torsions



Rings

Oligosaccharide Chain T



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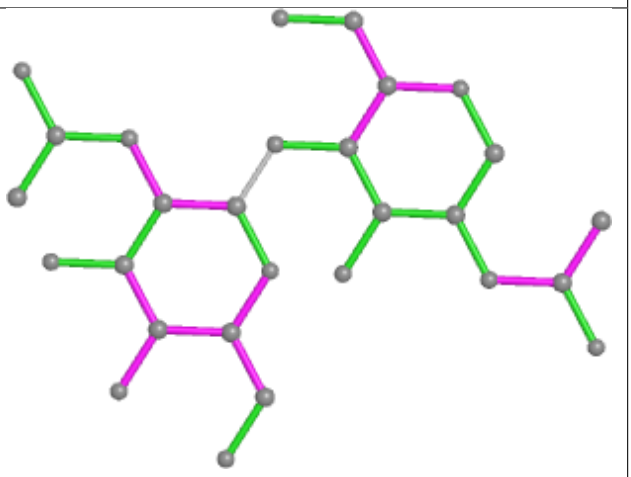

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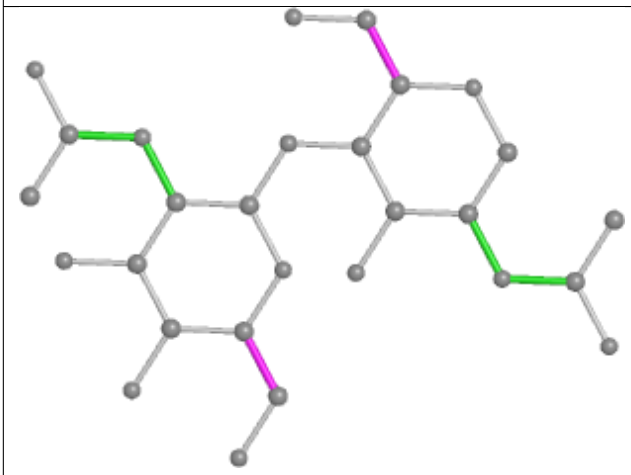

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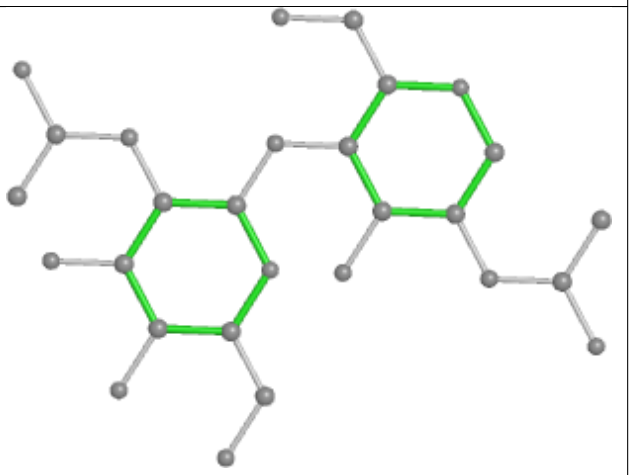
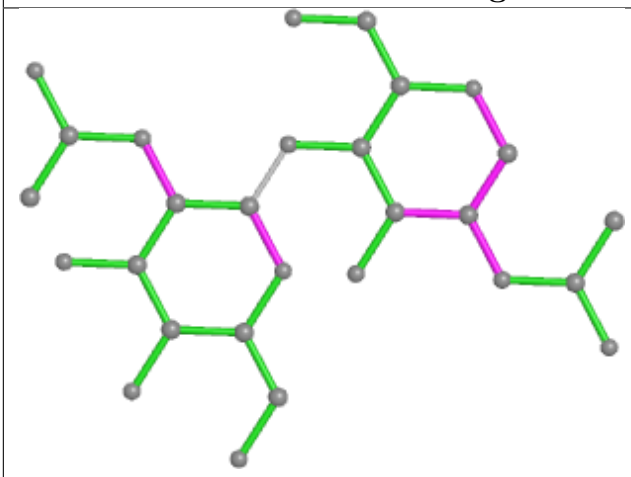


Rings

Oligosaccharide Chain W



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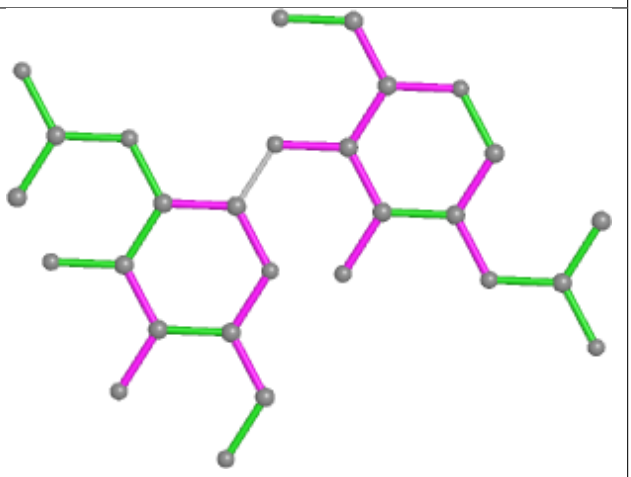

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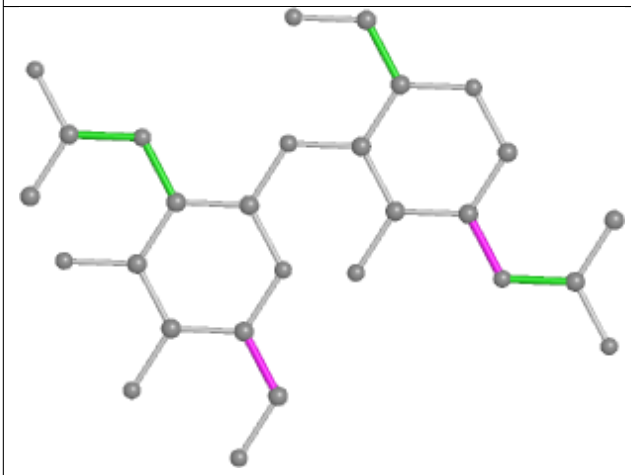

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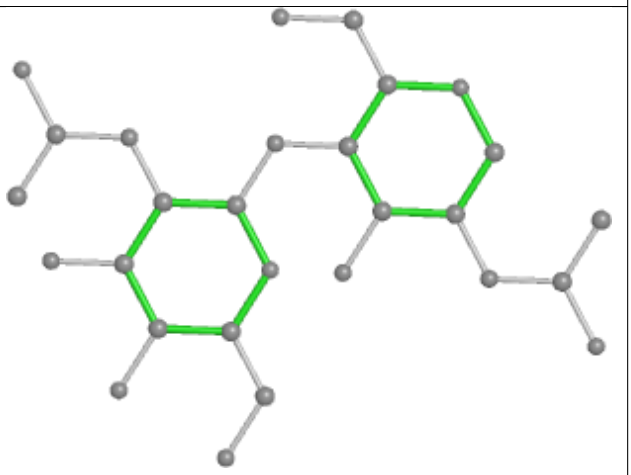
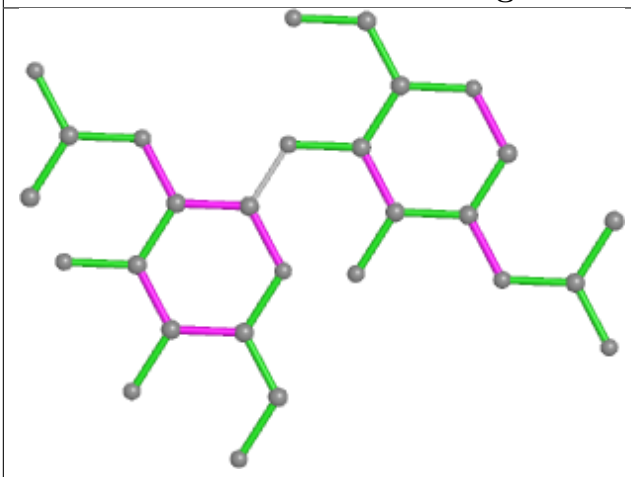


Rings

Oligosaccharide Chain Z



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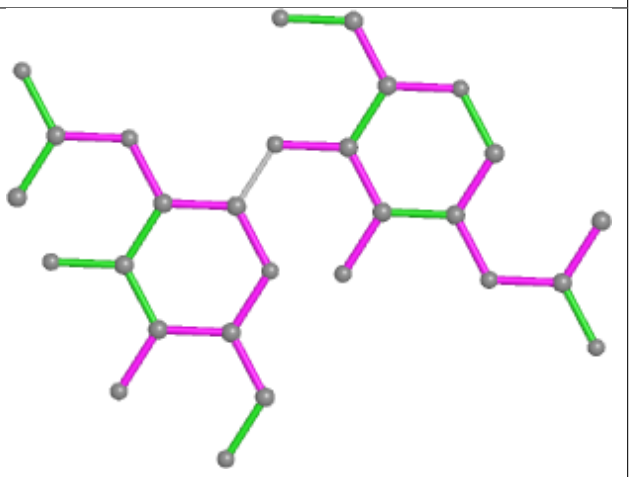

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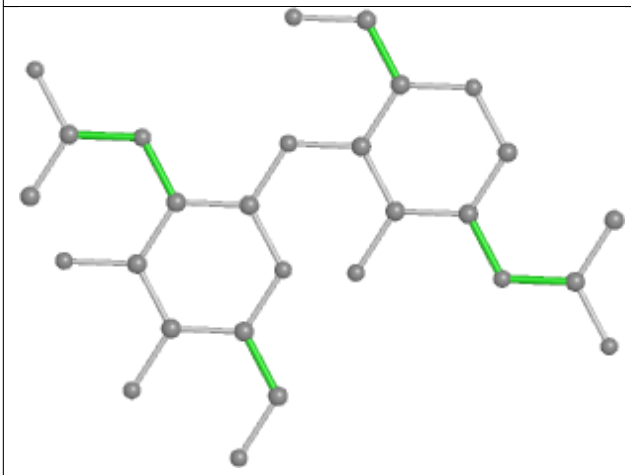

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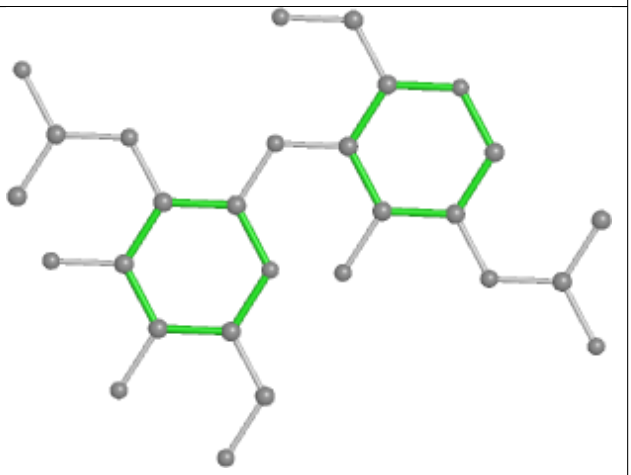
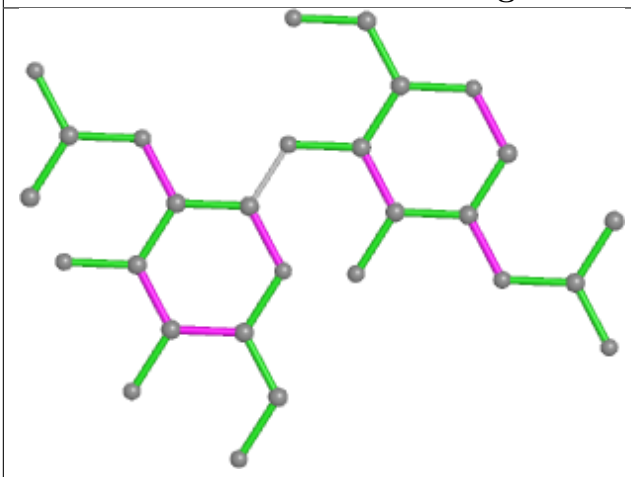
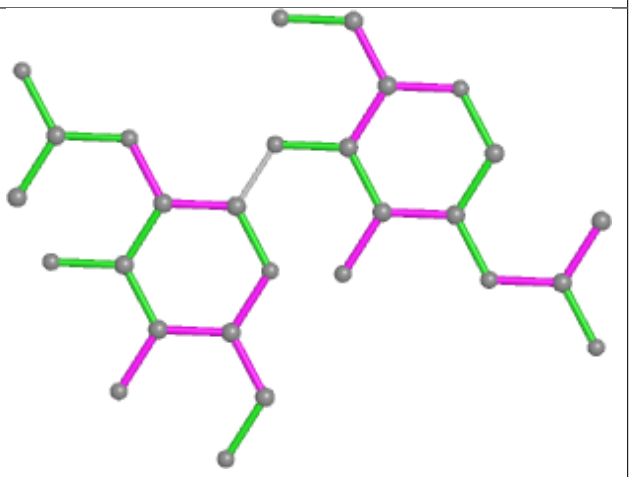


Rings

Oligosaccharide Chain b	
	
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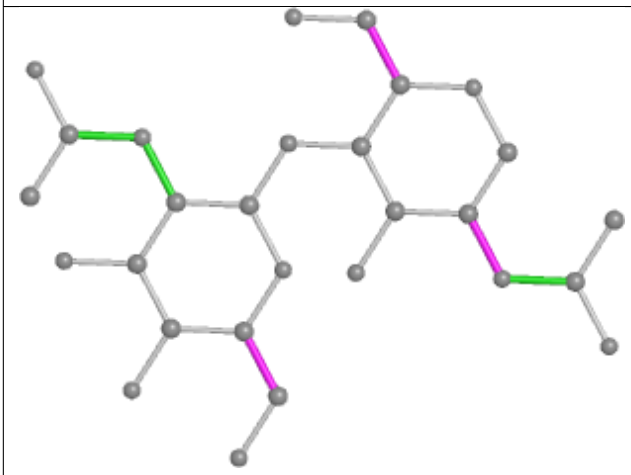
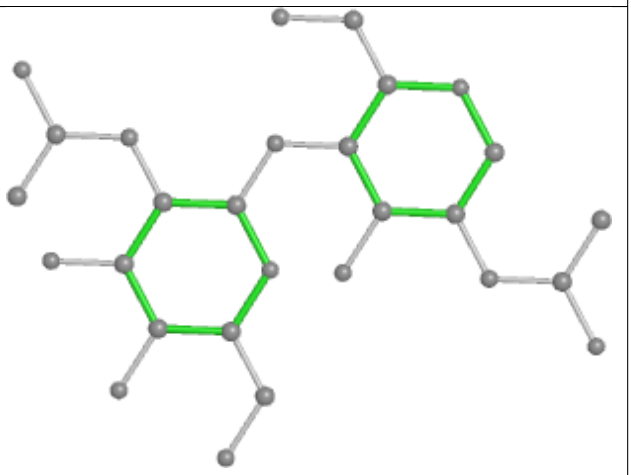
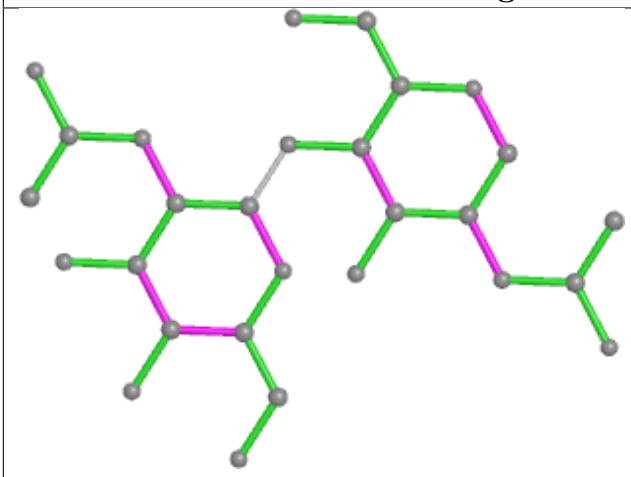
	
Torsions	**Rings**

Oligosaccharide Chain d



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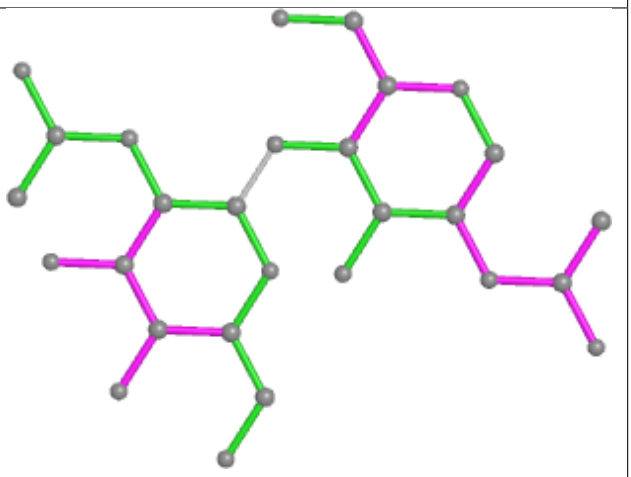
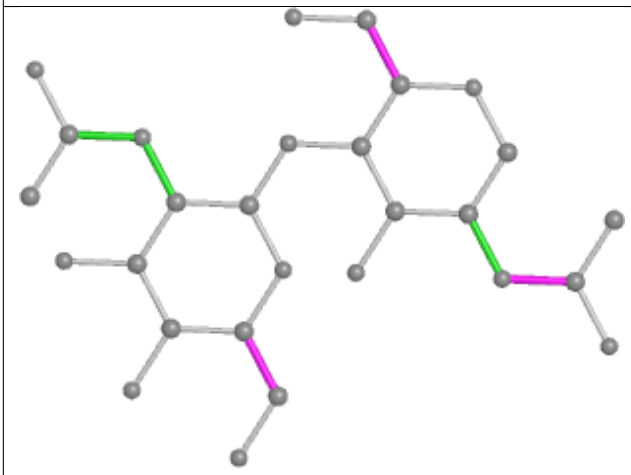


Bond angles



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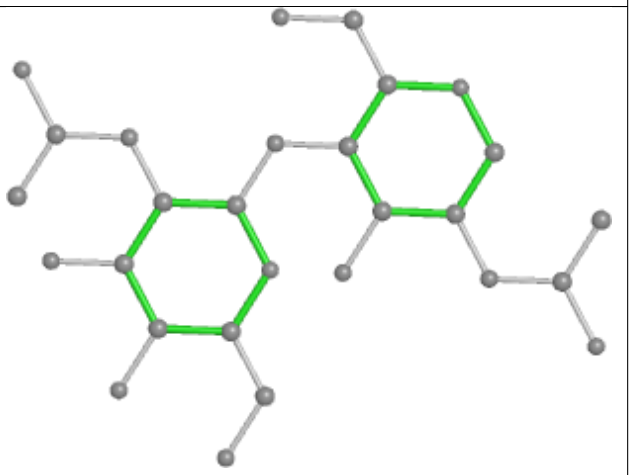
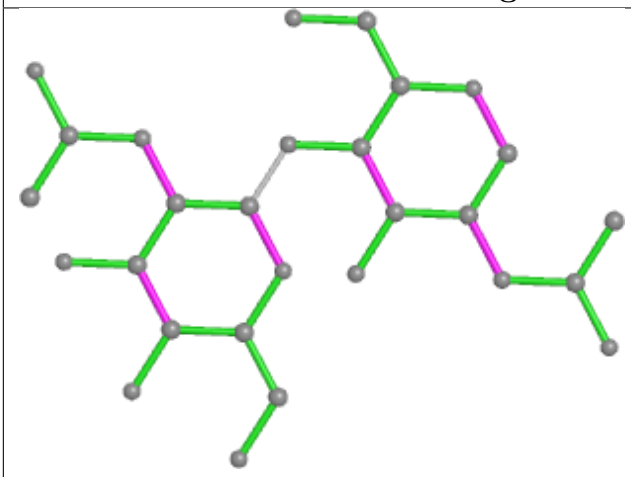


Rings

Oligosaccharide Chain e



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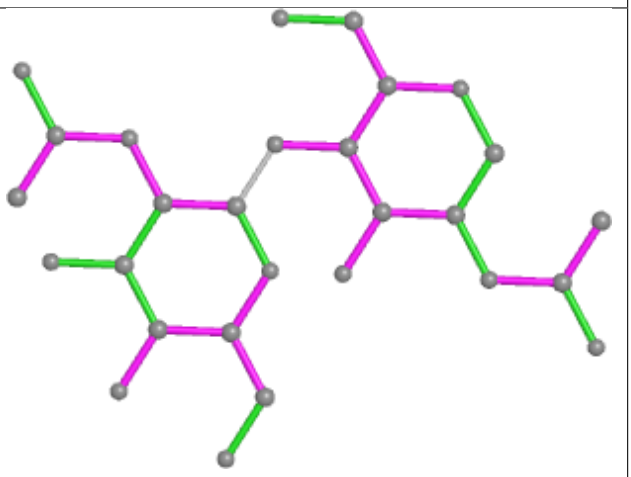

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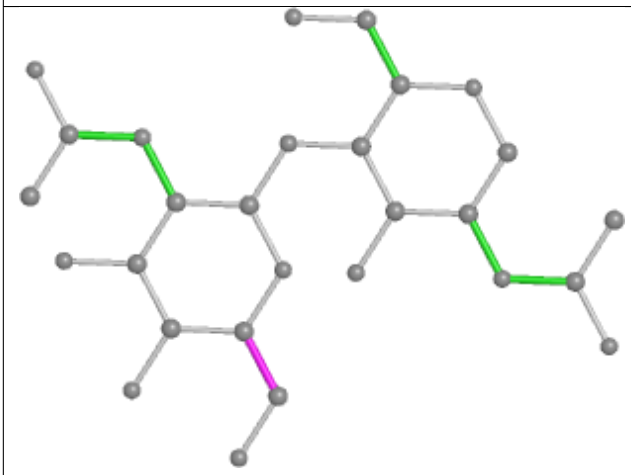

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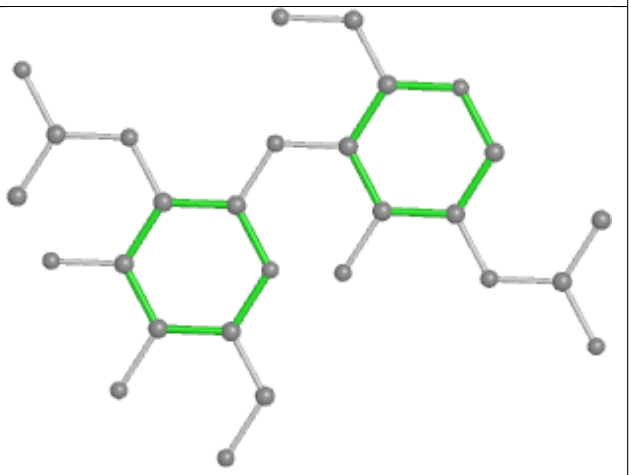
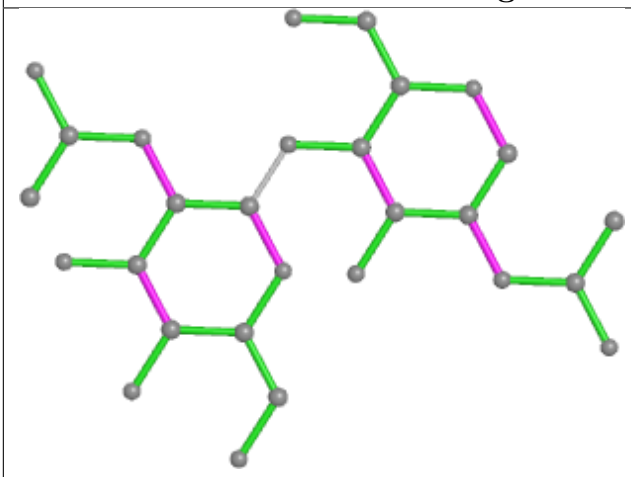


Rings

Oligosaccharide Chain h



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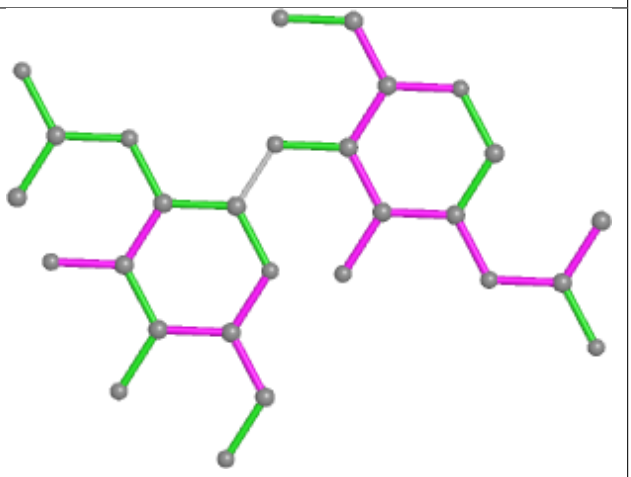

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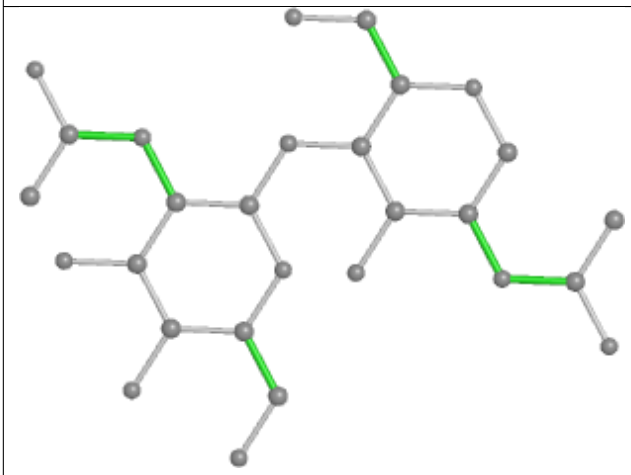

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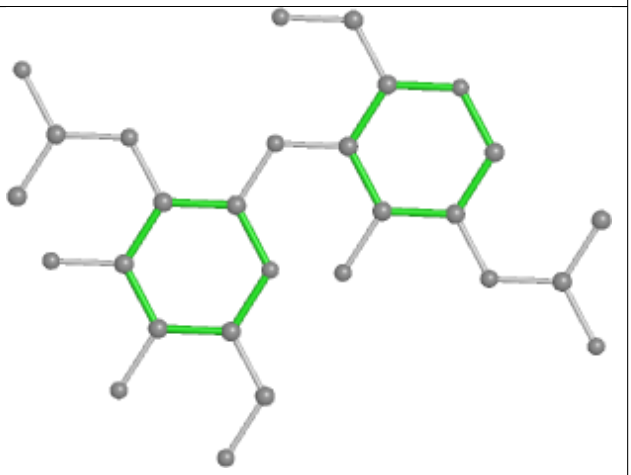
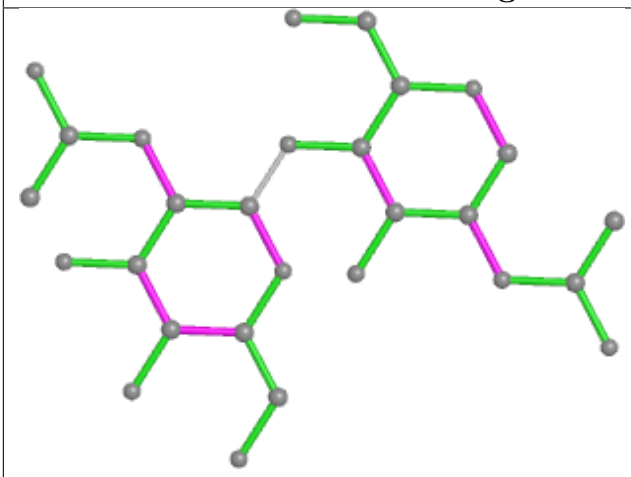


Rings

Oligosaccharide Chain k



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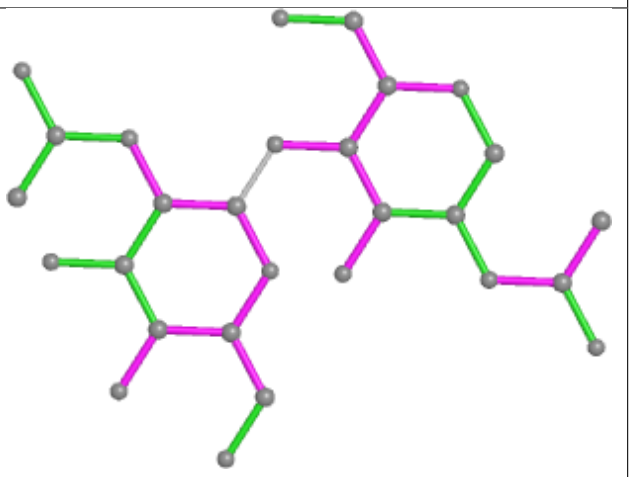
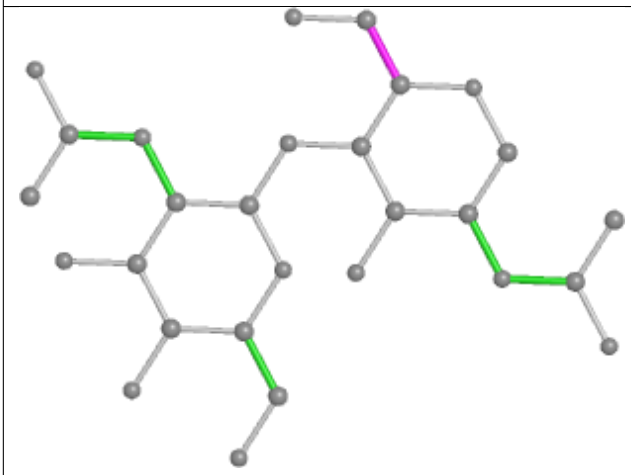


Bond angles



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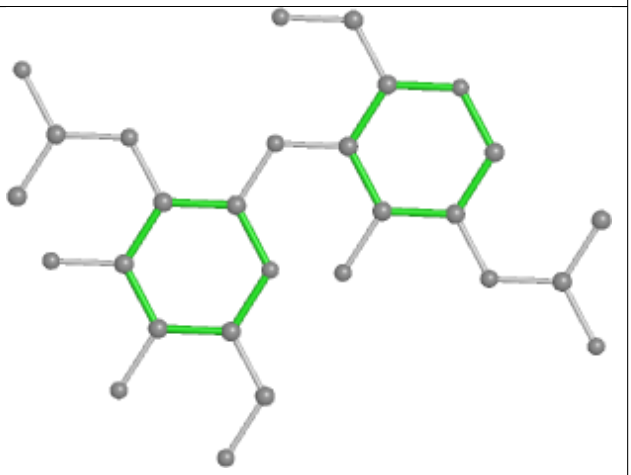
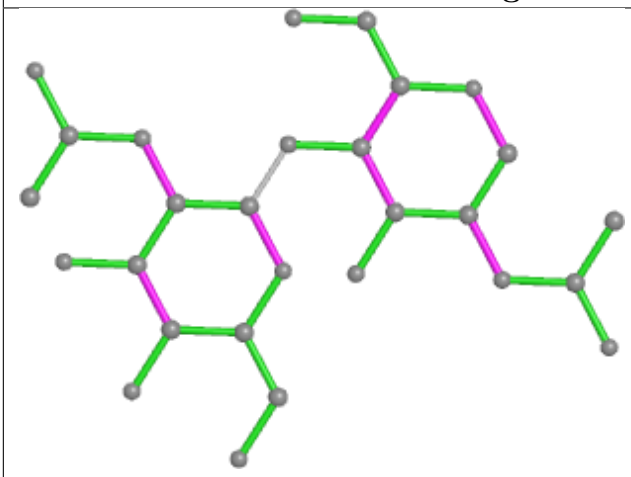


Rings

Oligosaccharide Chain l



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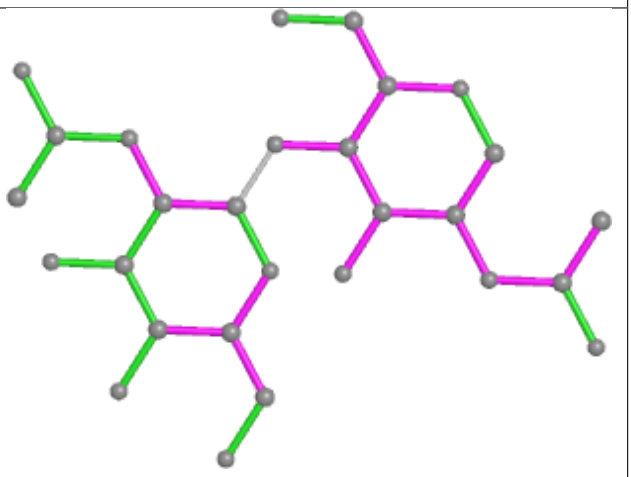

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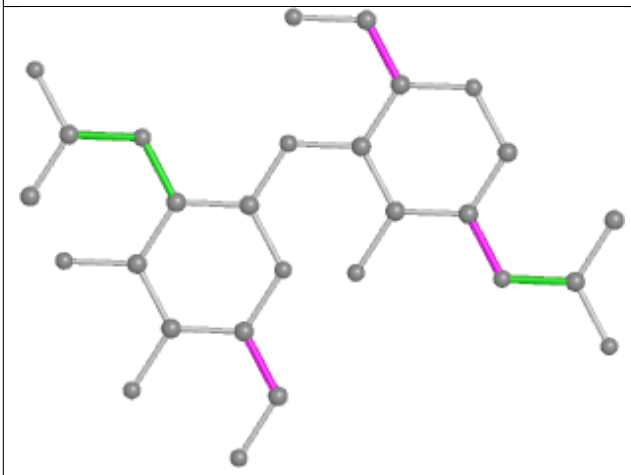

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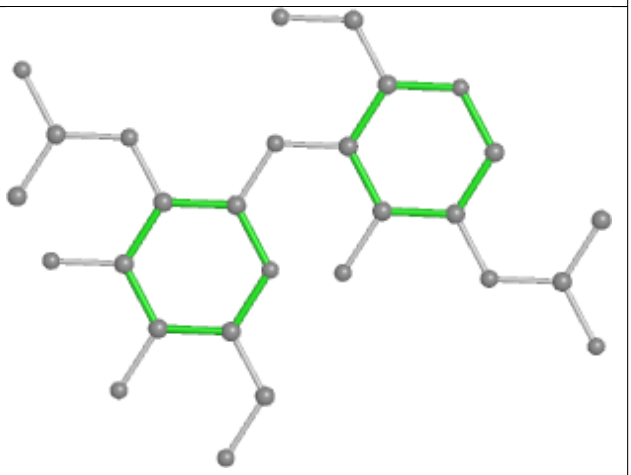
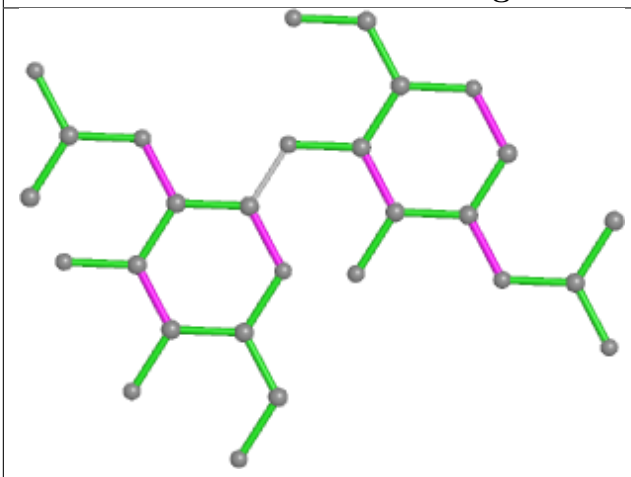


Rings

Oligosaccharide Chain m



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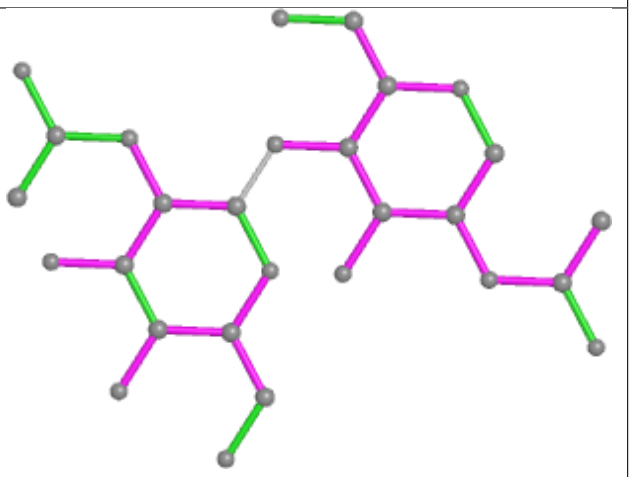
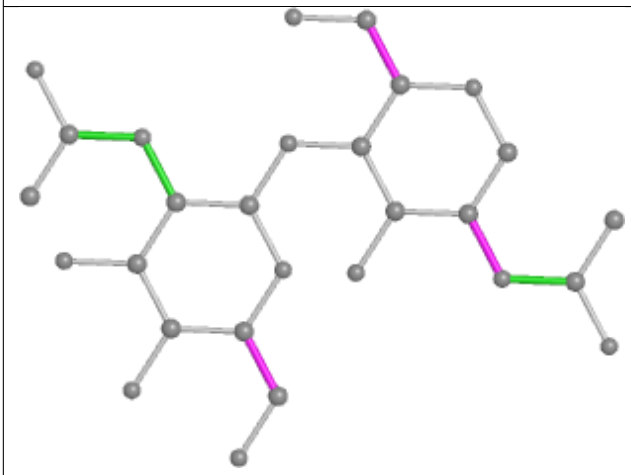


Bond angles



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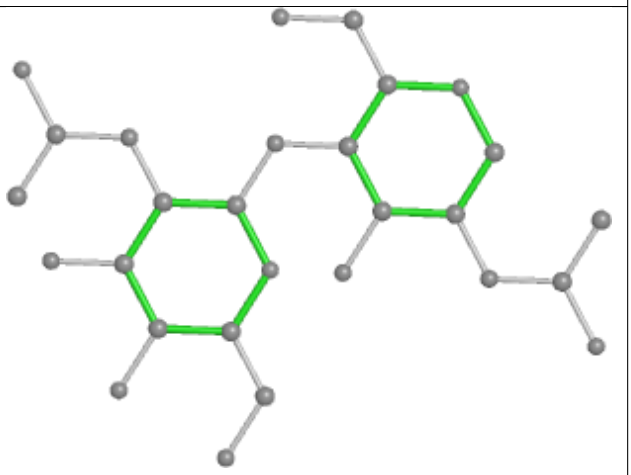
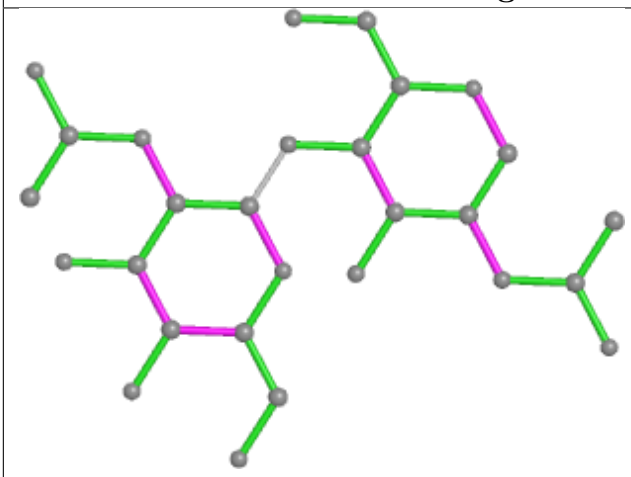
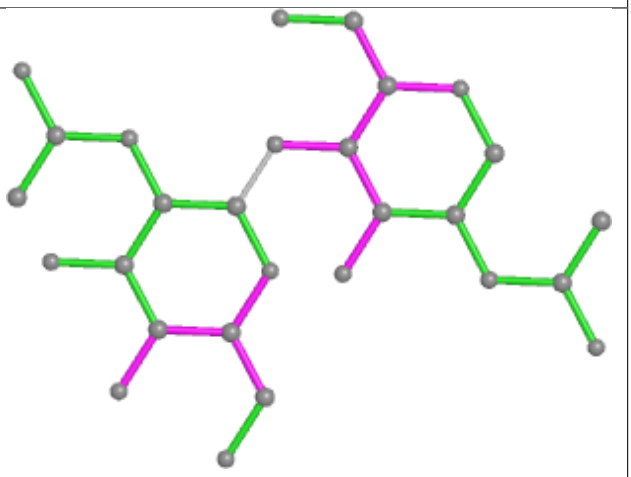
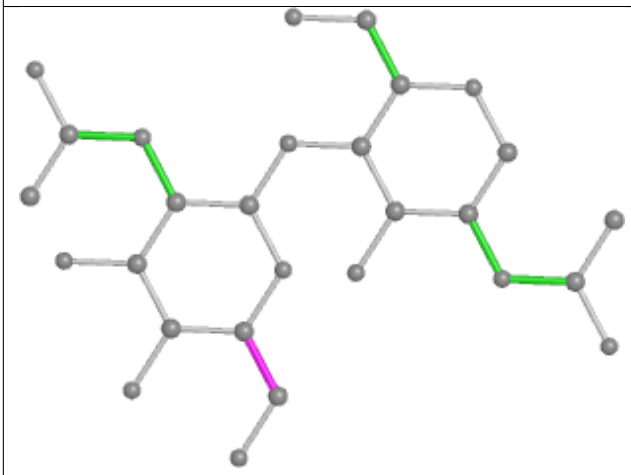
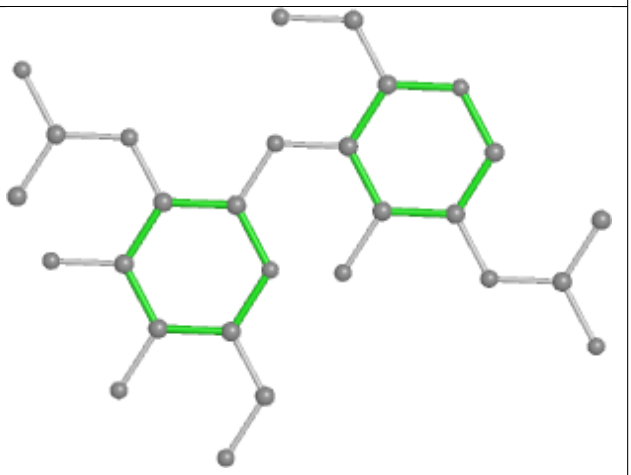
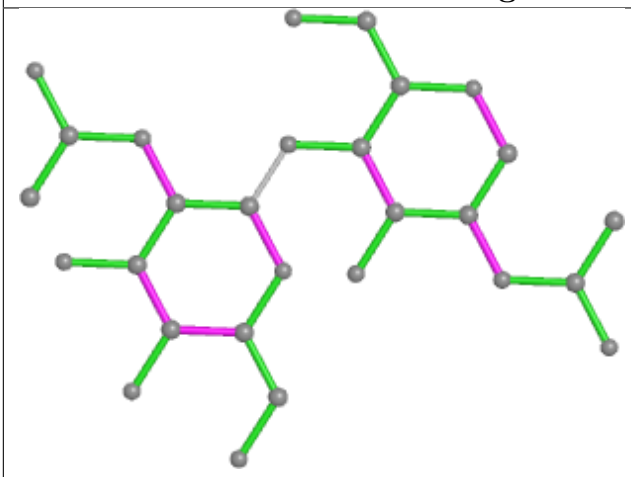


Rings

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

Oligosaccharide Chain o



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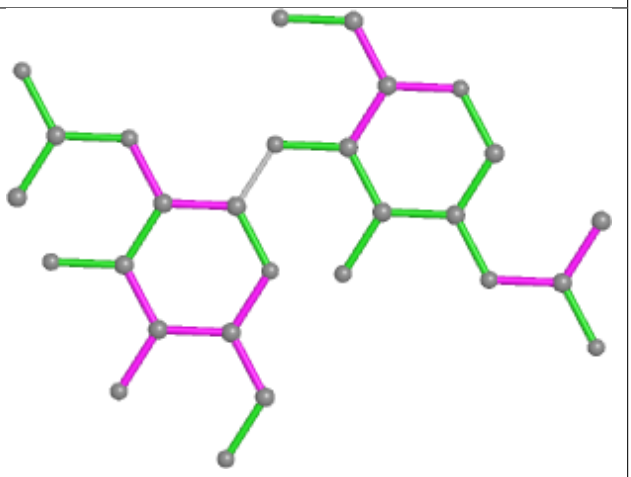
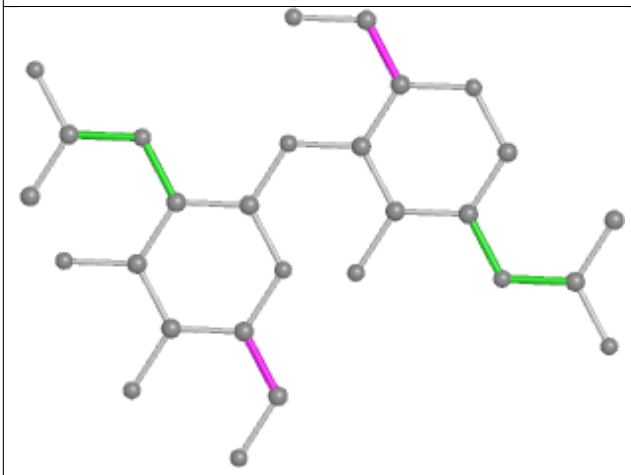
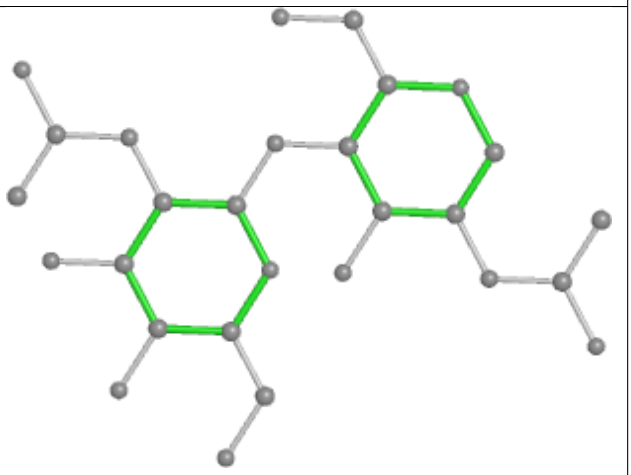


Bond angles

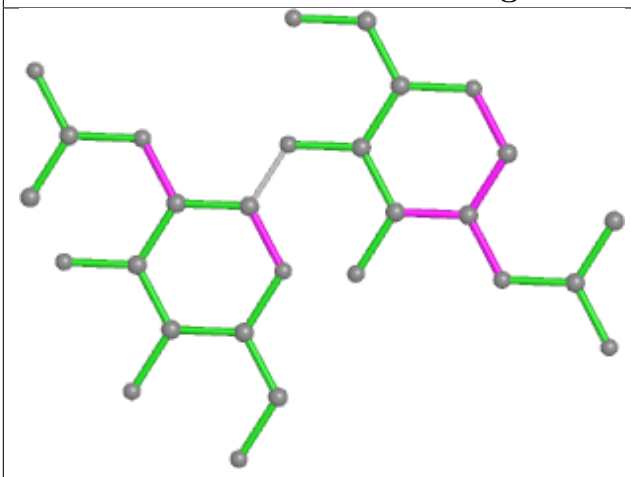


Torsions



Rings

Oligosaccharide Chain r



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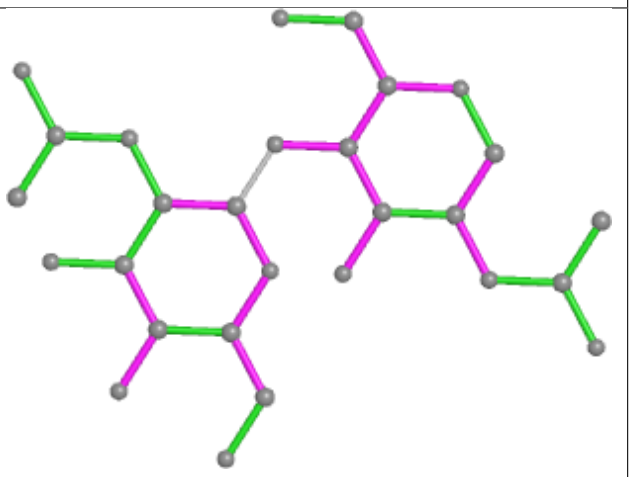
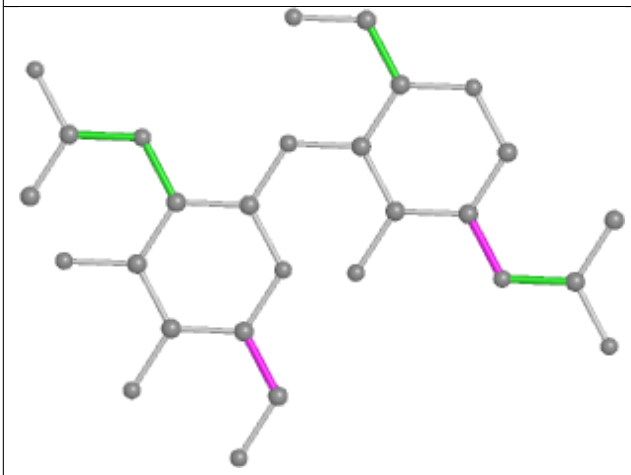


Bond angles



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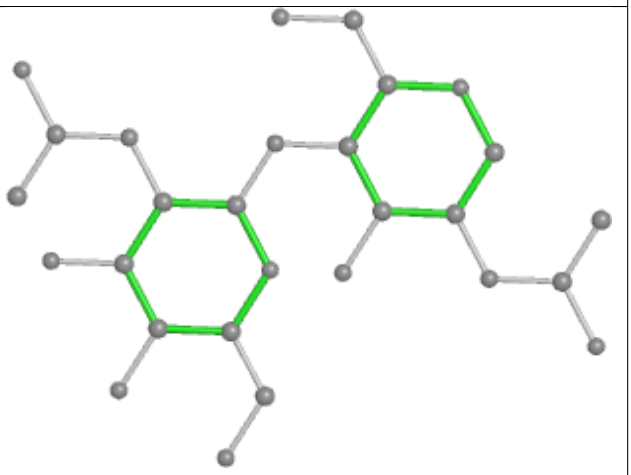
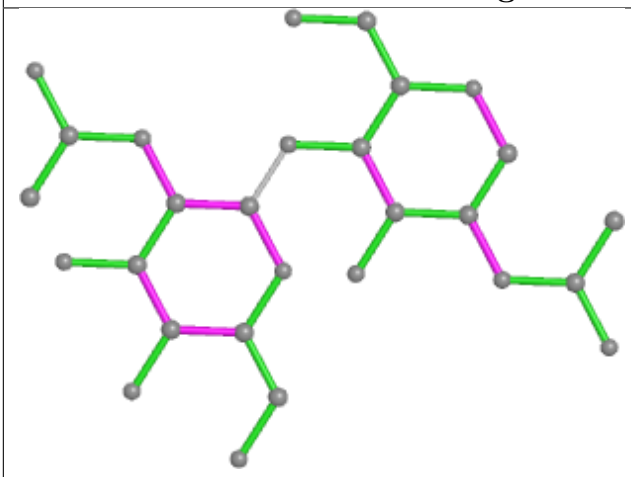


Rings

Oligosaccharide Chain u



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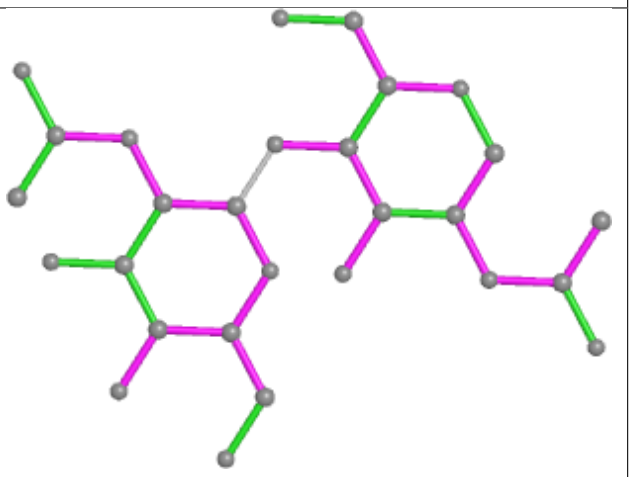
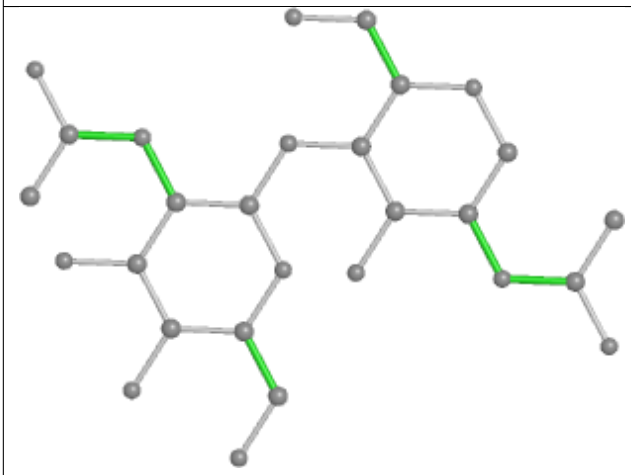


Bond angles



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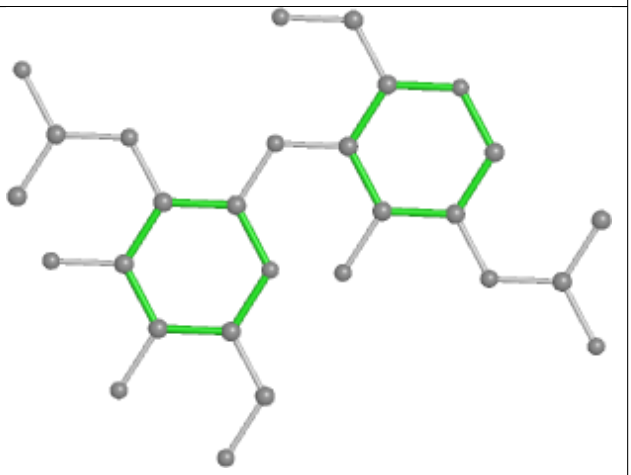
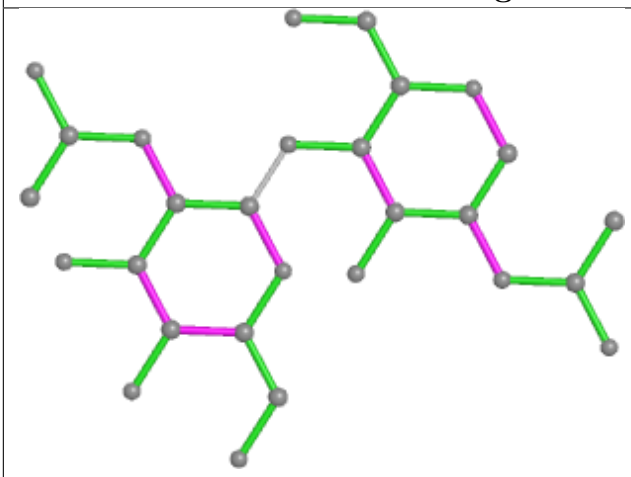
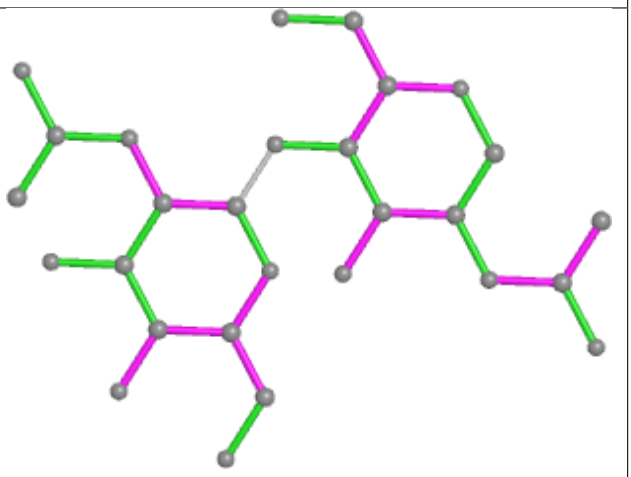
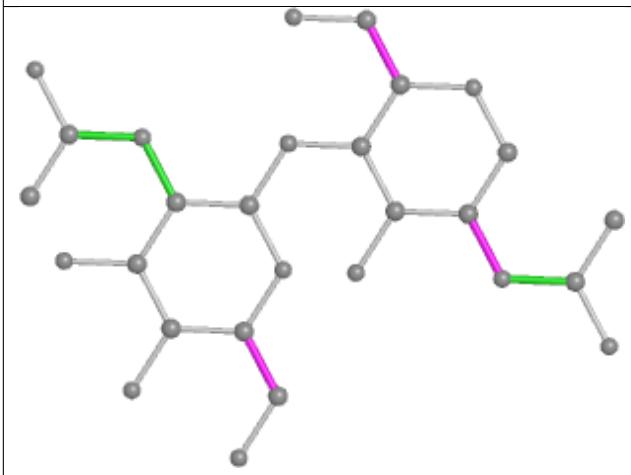
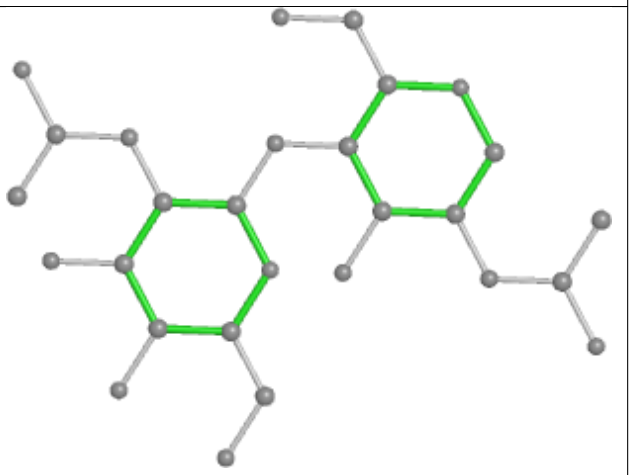
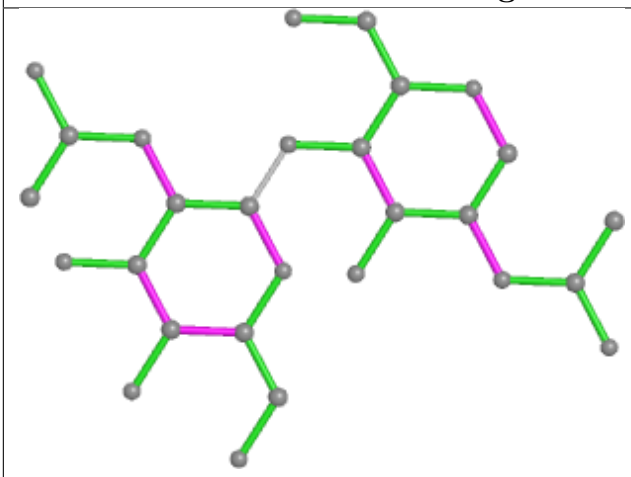


Rings

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

Oligosaccharide Chain y



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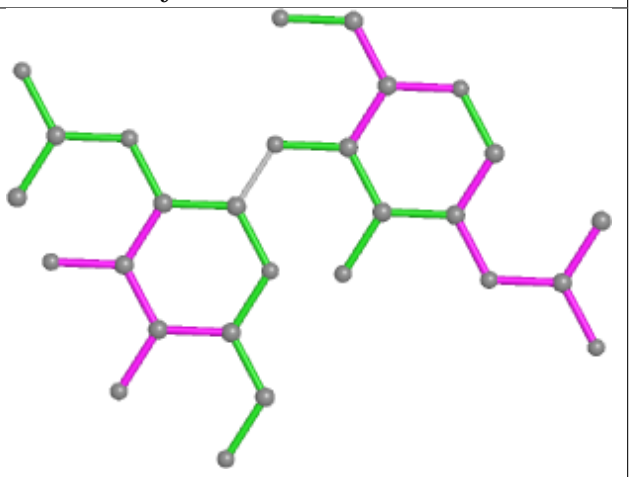
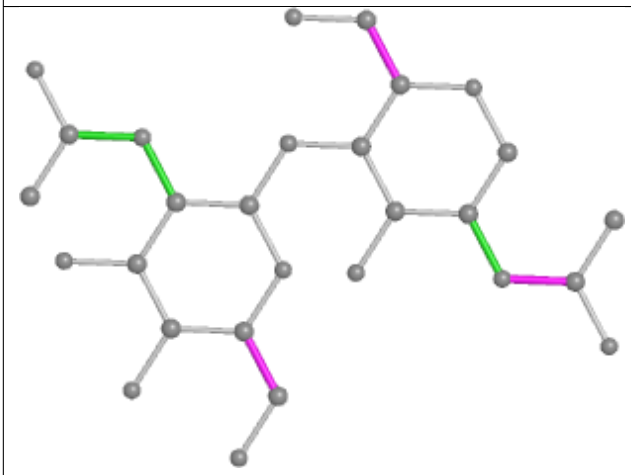
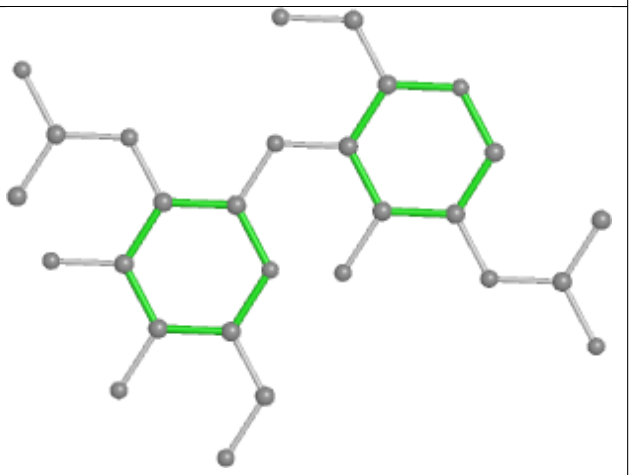


Bond angles

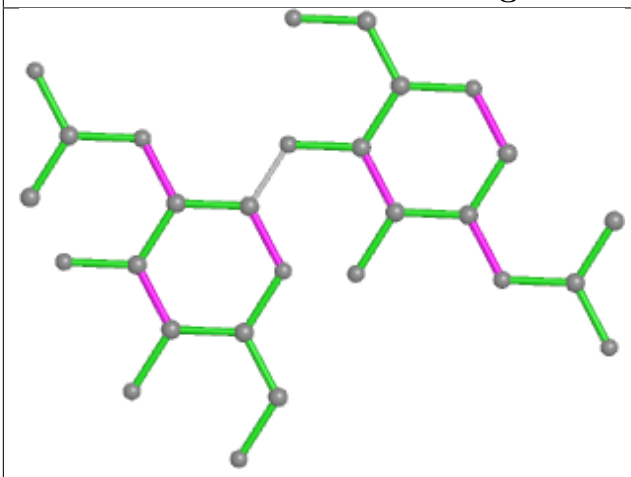


Torsions



Rings

Oligosaccharide Chain z



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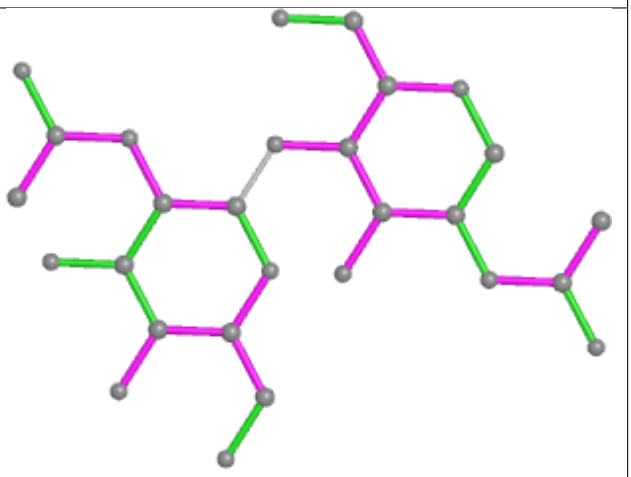
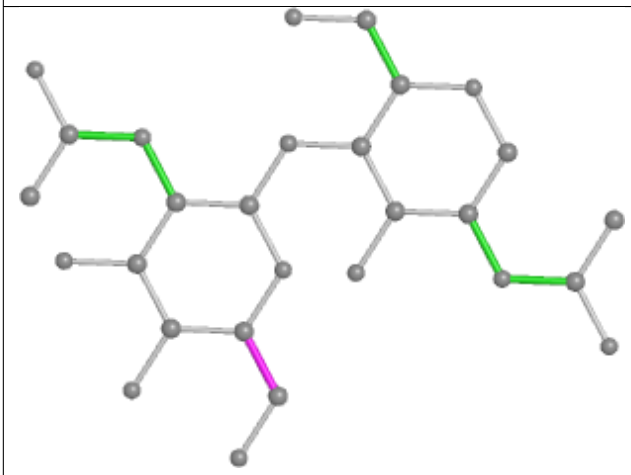
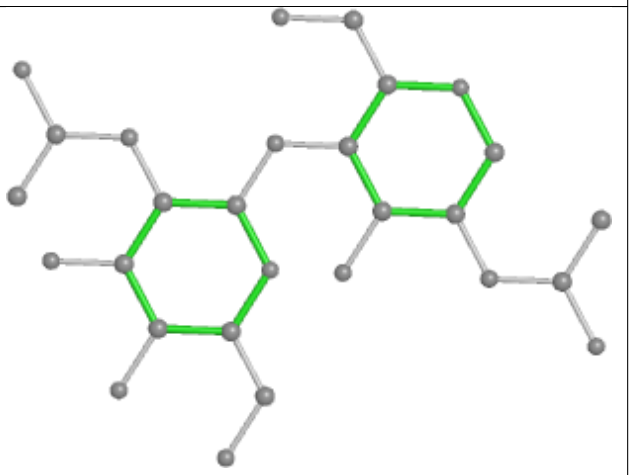


Bond angles

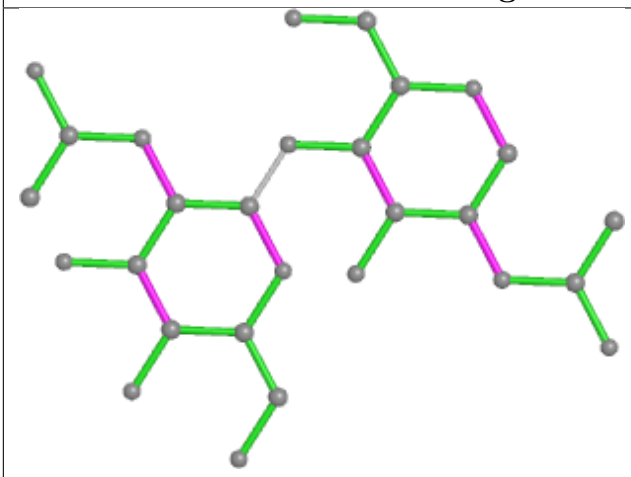


Torsions



Rings

Oligosaccharide Chain 2



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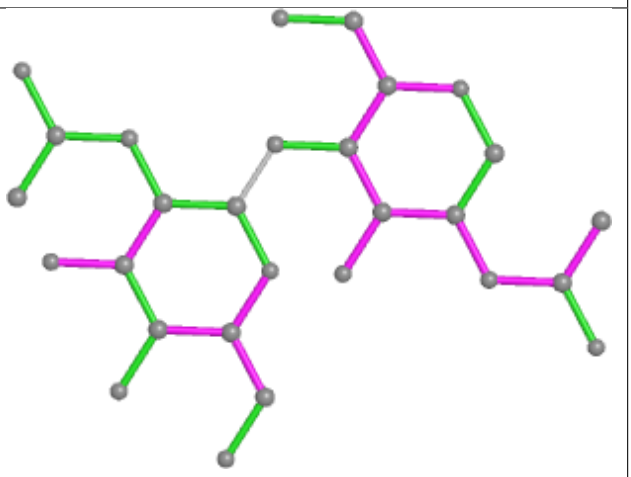

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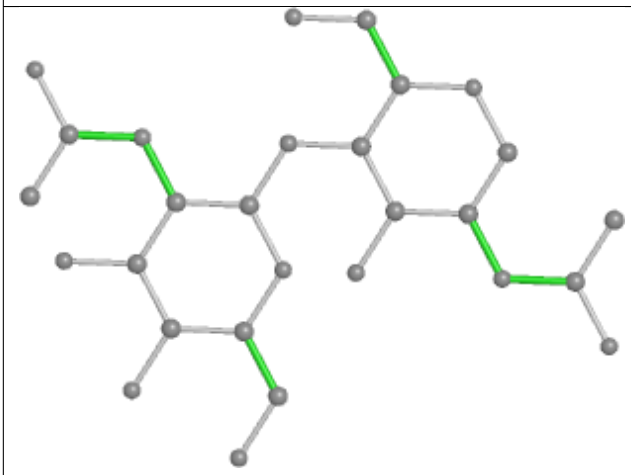

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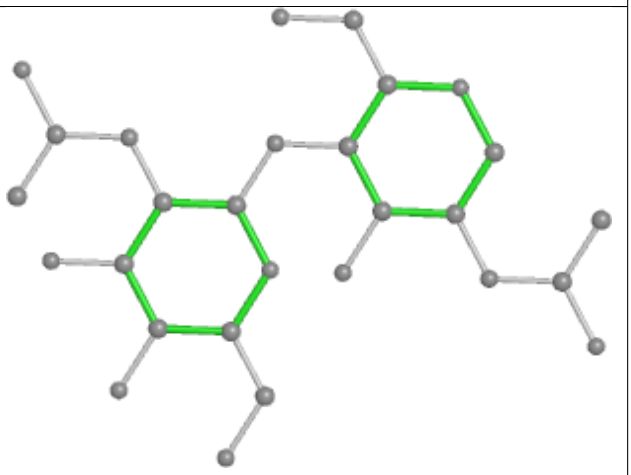
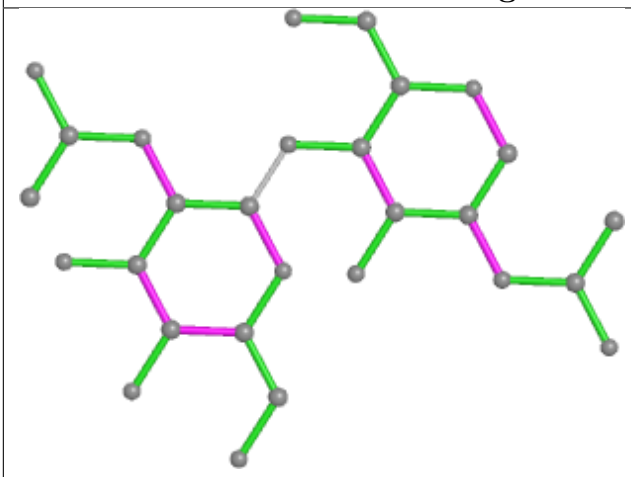
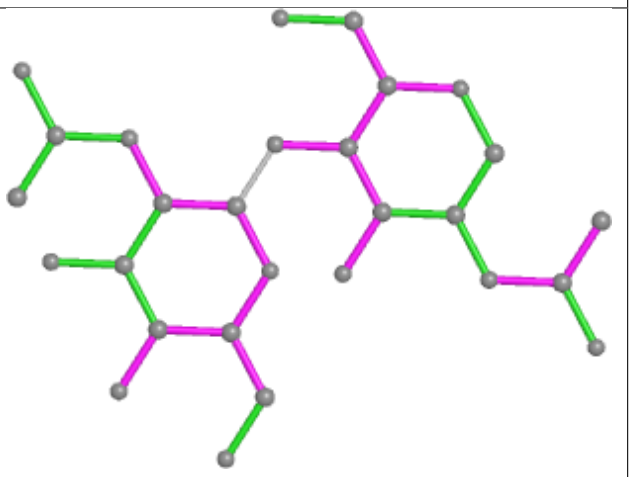


Rings

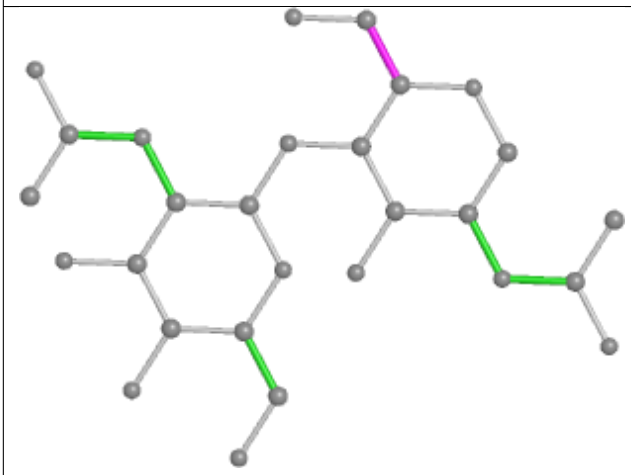
Oligosaccharide Chain 5



Bond lengths



Bond angles



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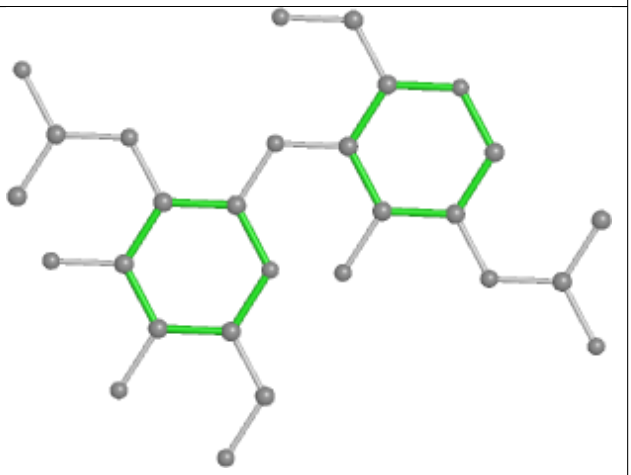
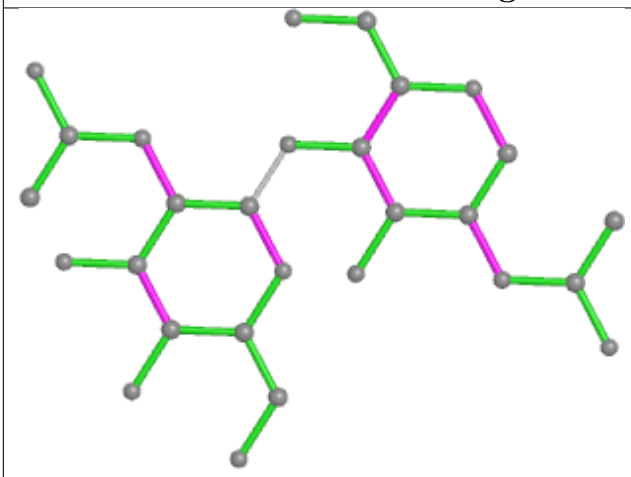


Rings

Oligosaccharide Chain 6



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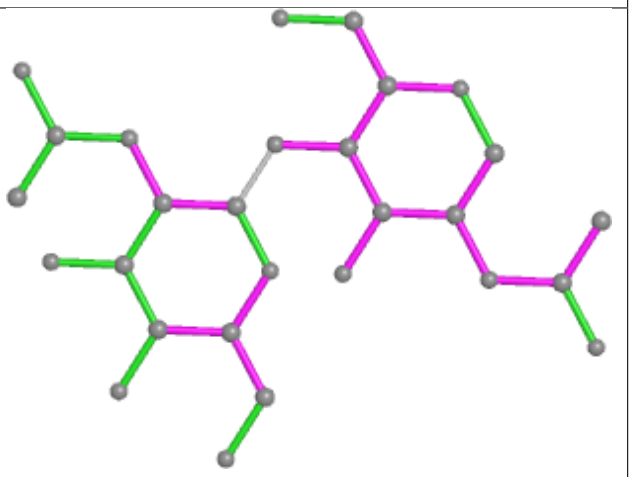
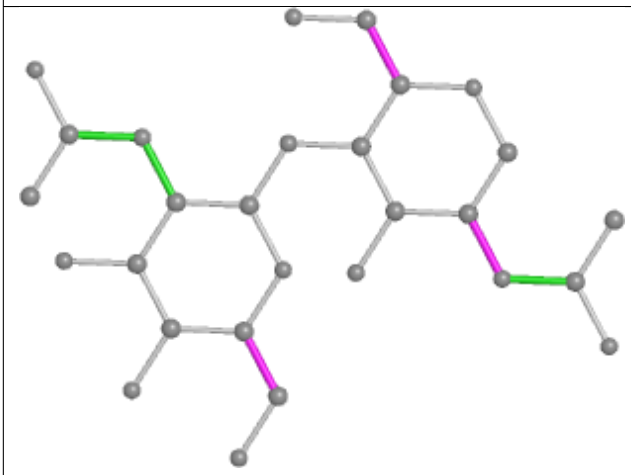


Bond angles



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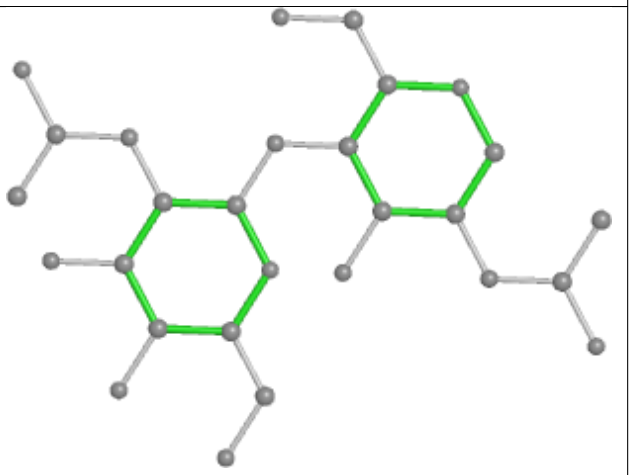
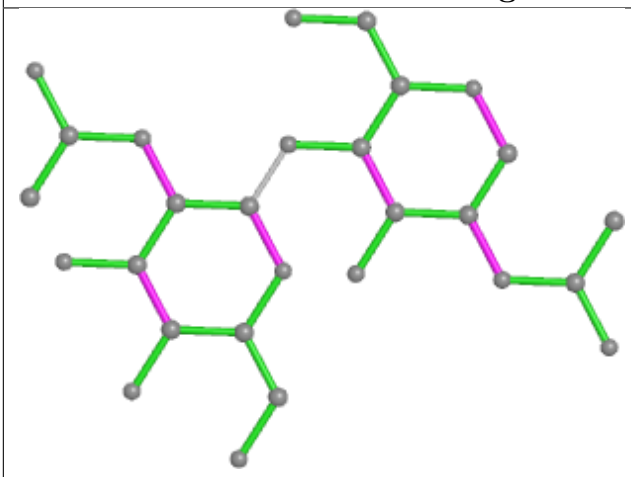


Rings

Oligosaccharide Chain 7



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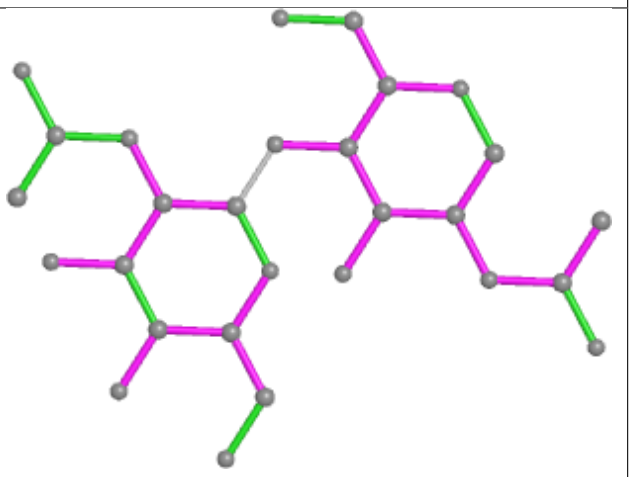
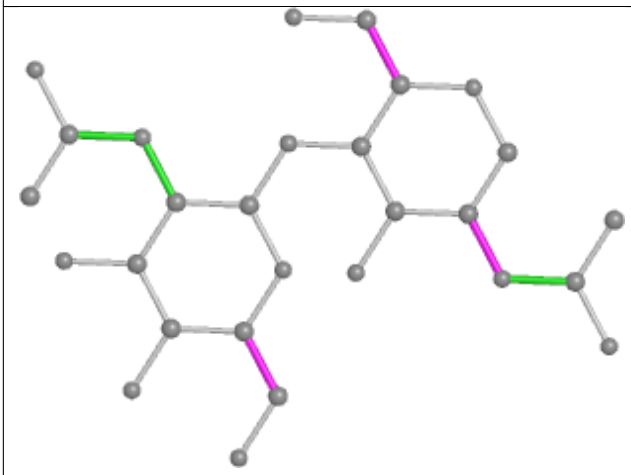


Bond angles



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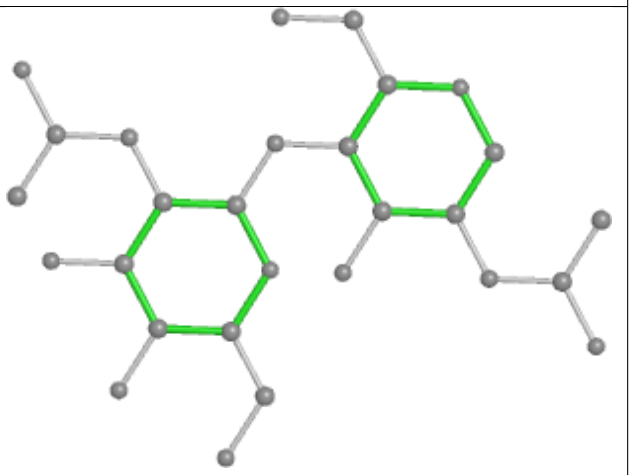
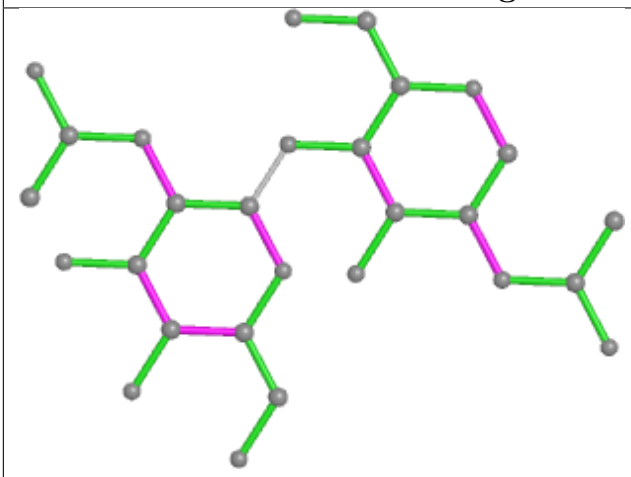


Rings

Oligosaccharide Chain 8



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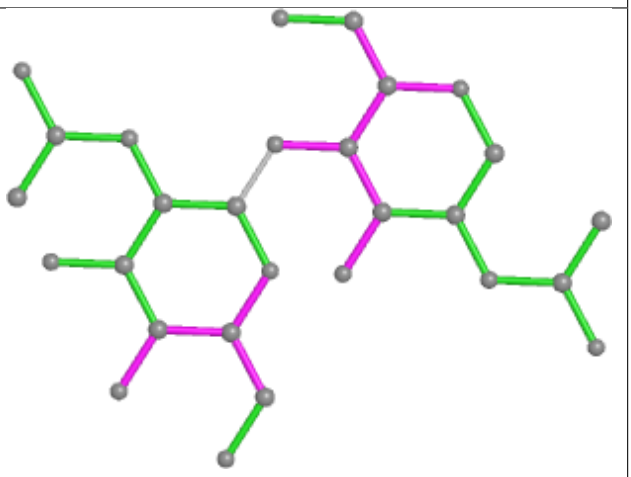
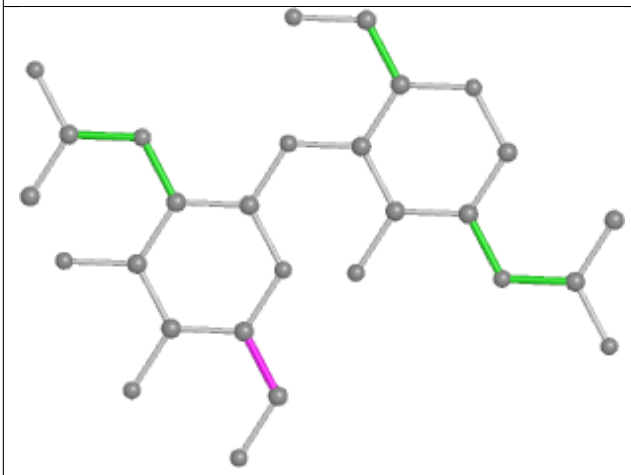


Bond angles



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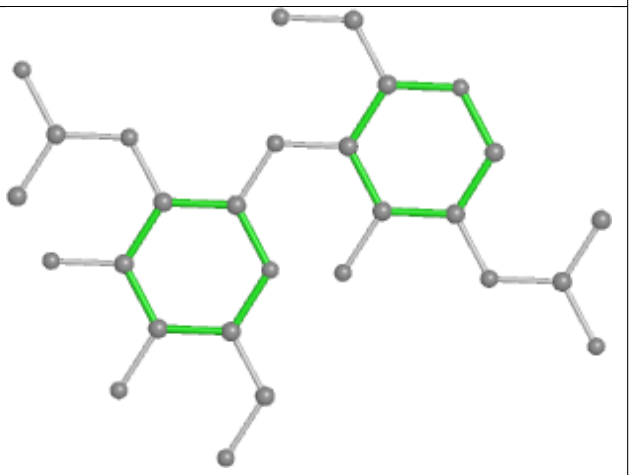
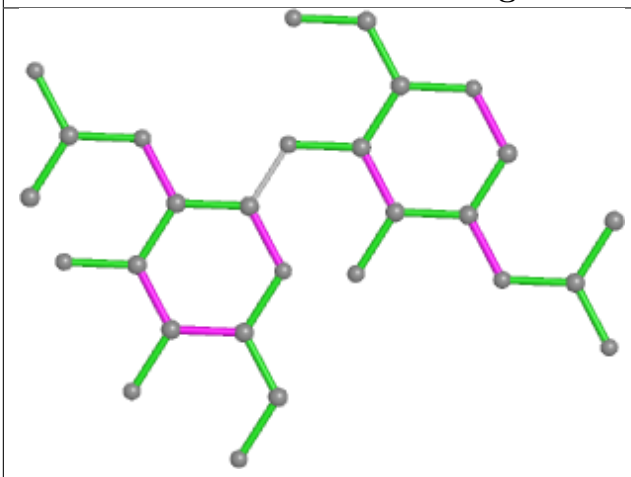


Rings

Oligosaccharide Chain 9



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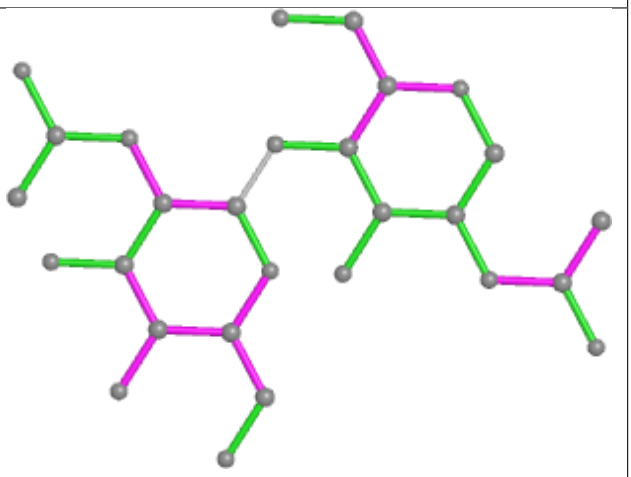

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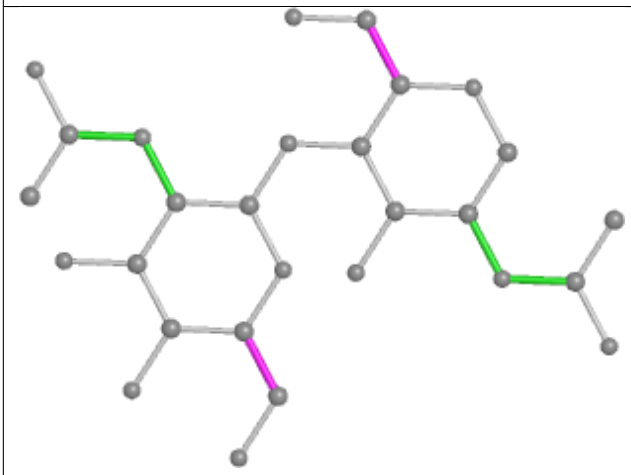

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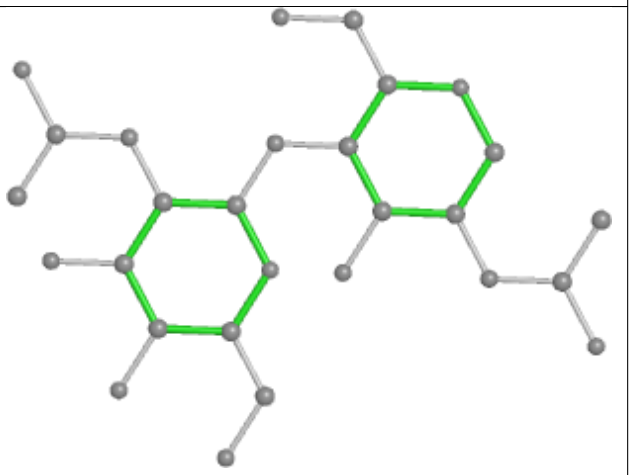
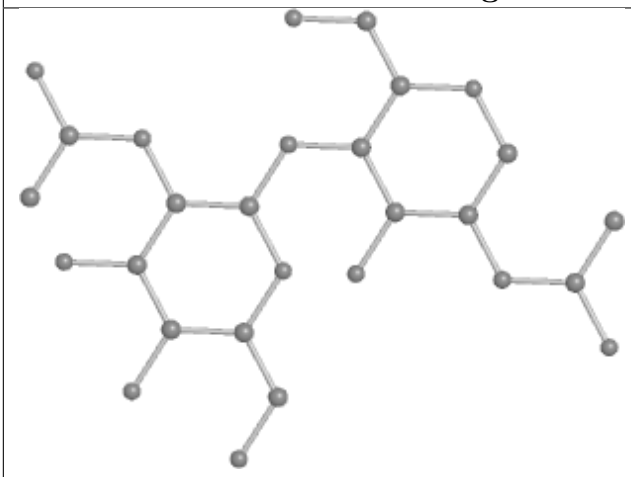


Rings

Oligosaccharide Chain CA



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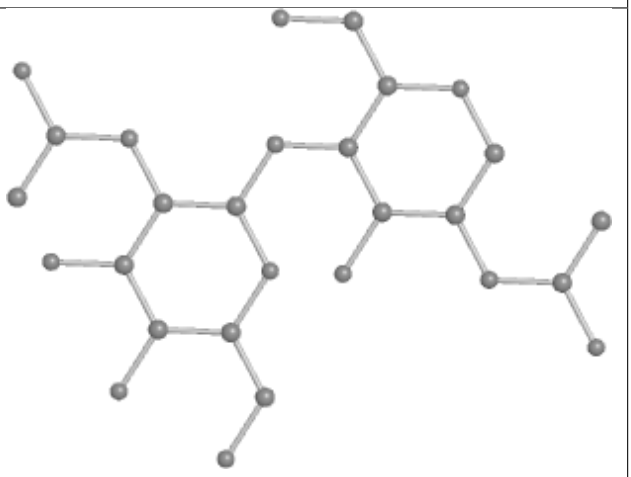

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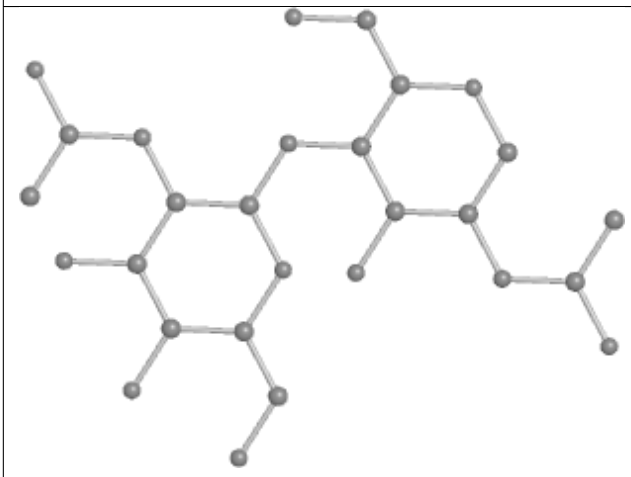

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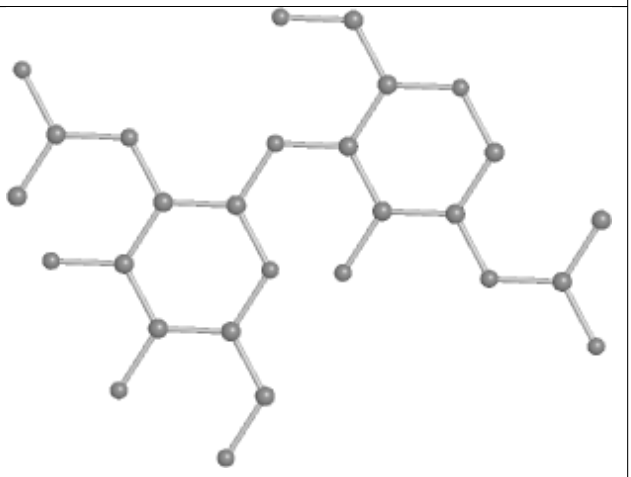
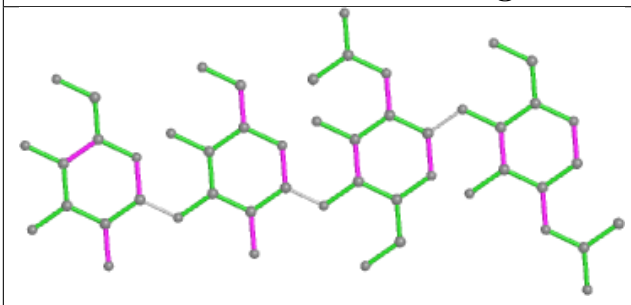


Rings

Oligosaccharide Chain F



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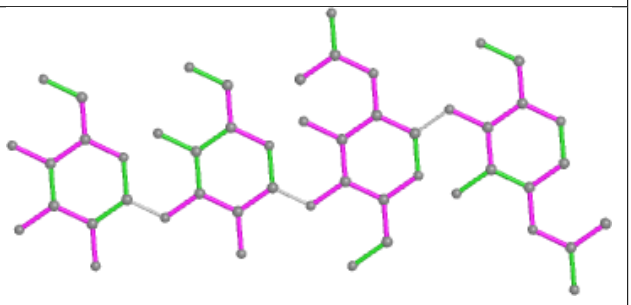
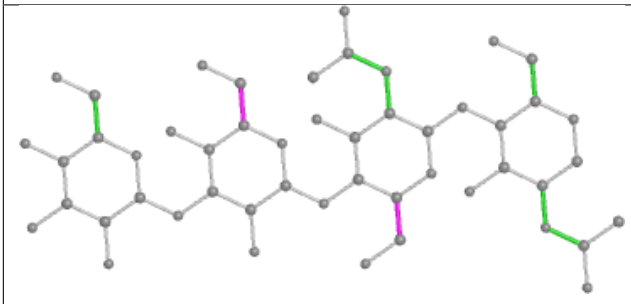


Bond angles



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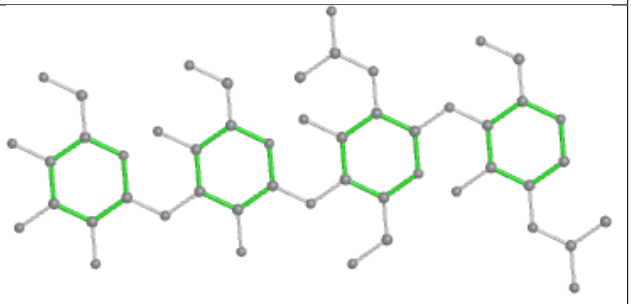
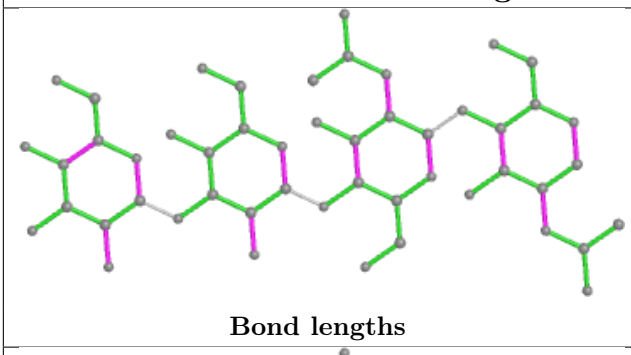


Rings

Oligosaccharide Chain U



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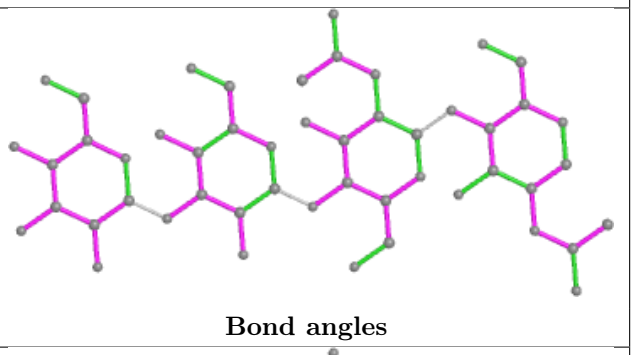

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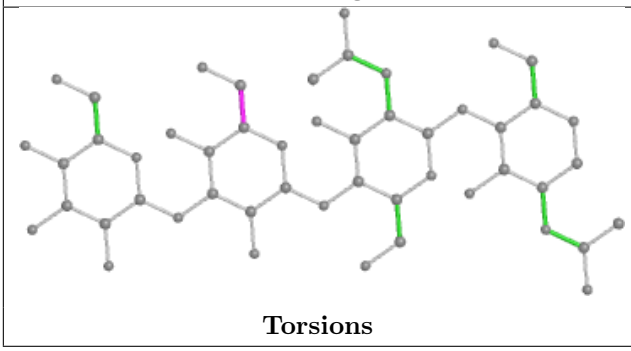

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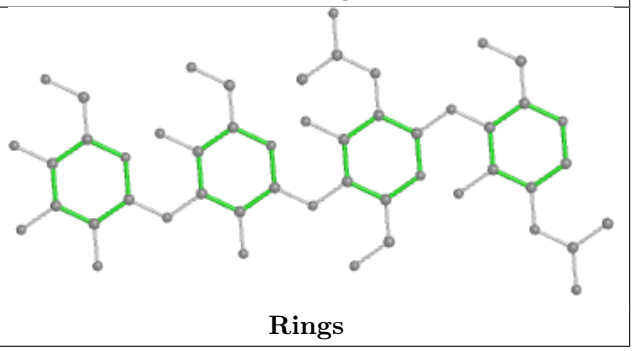
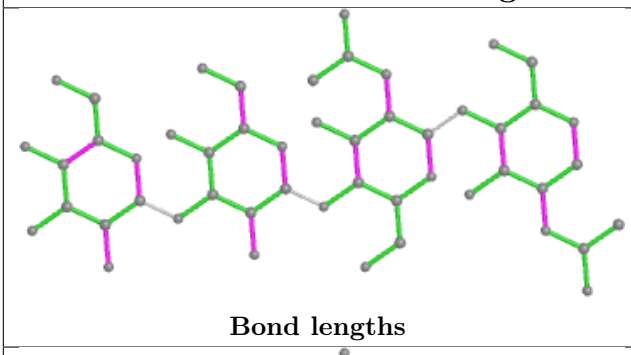


Rings

Oligosaccharide Chain a



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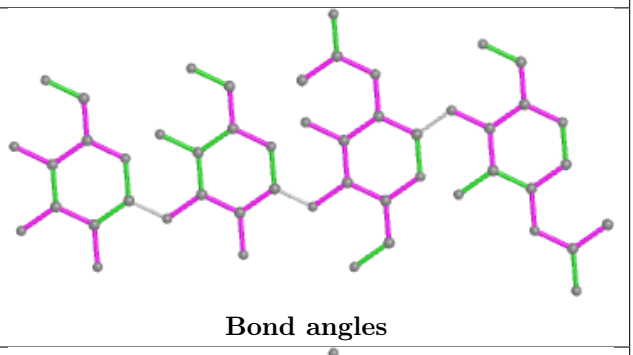
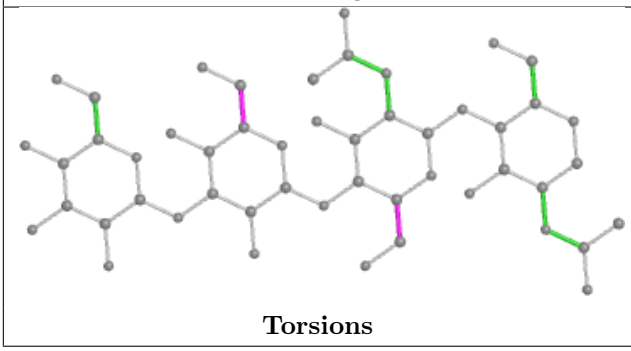
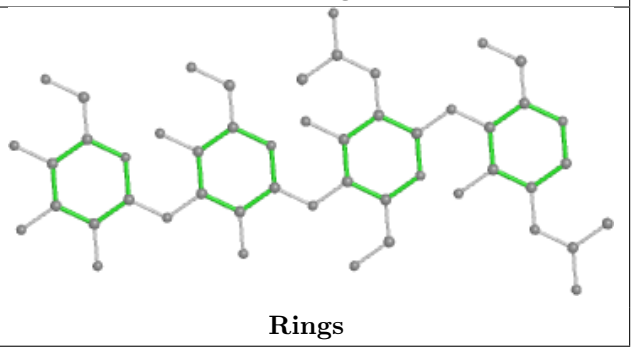


Bond angles

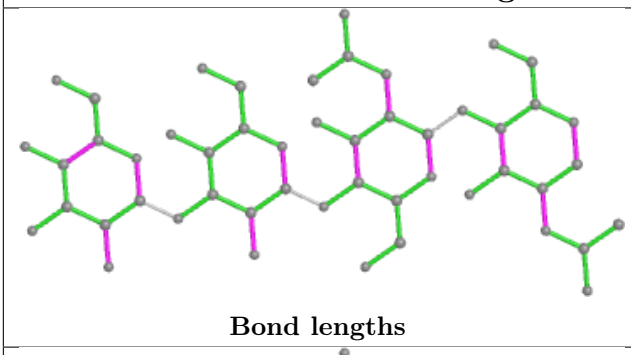


Torsions

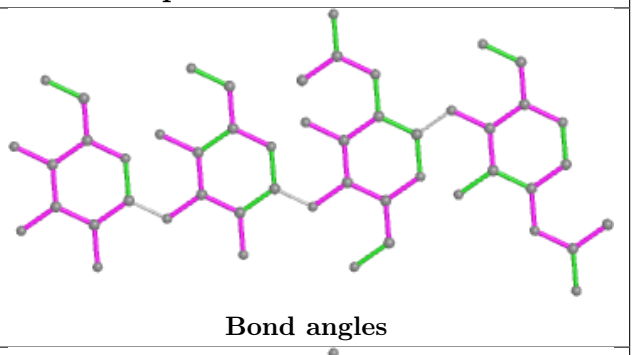


Rings

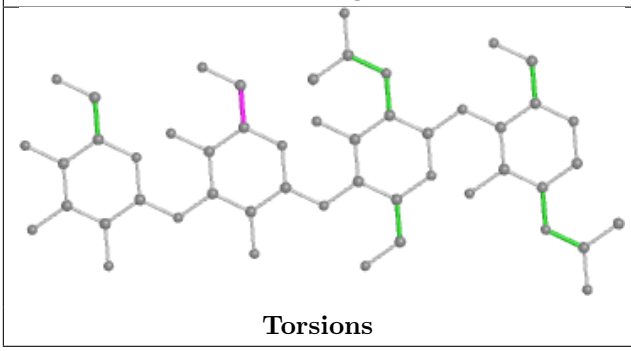
Oligosaccharide Chain p



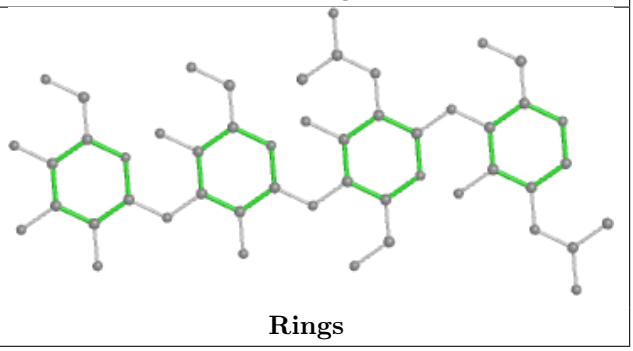
Bond lengths



Bond angles

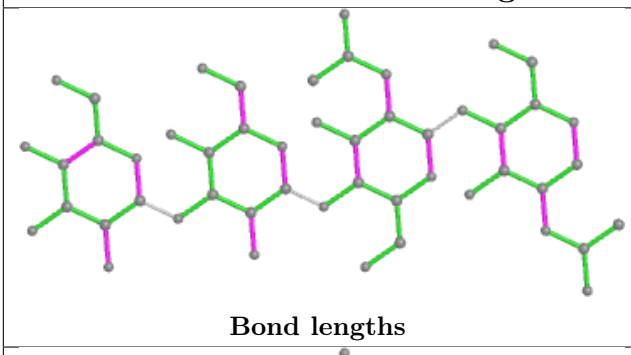


Torsions

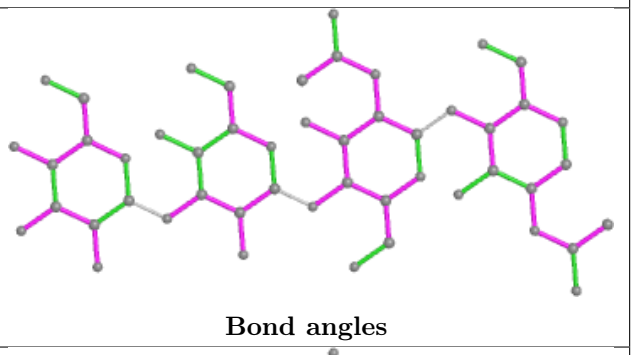


Rings

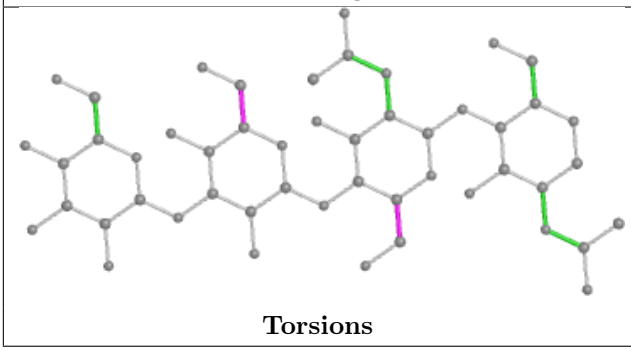
Oligosaccharide Chain v



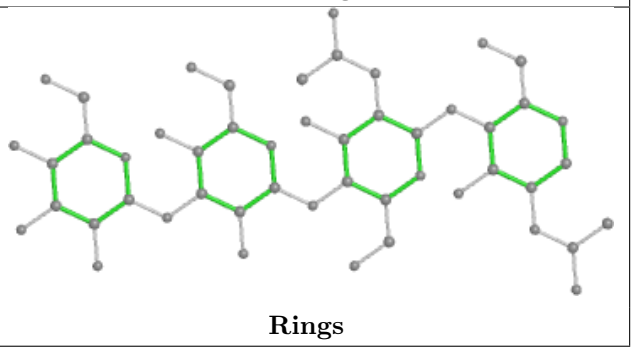
Bond lengths



Bond angles

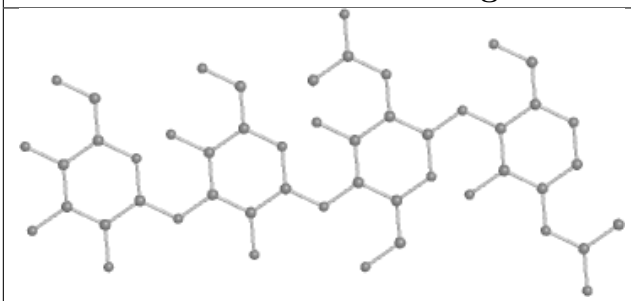


Torsions

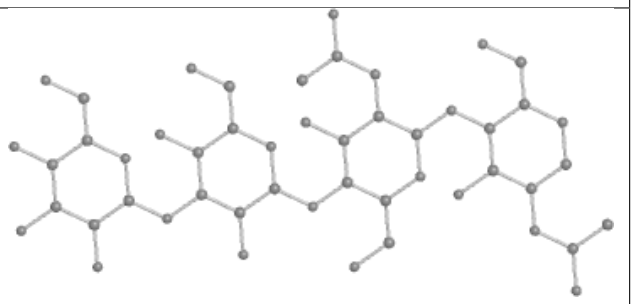


Rings

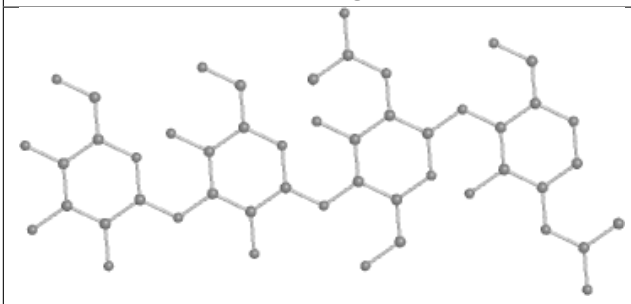
Oligosaccharide Chain AA



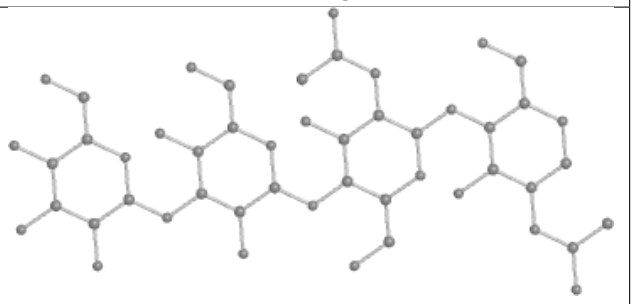
Bond lengths



Bond angles

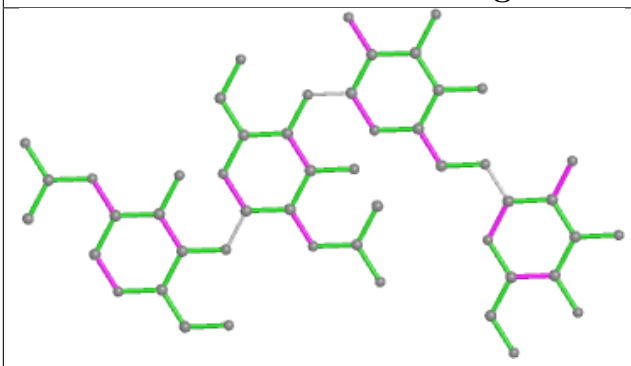


Torsions



Rings

Oligosaccharide Chain H



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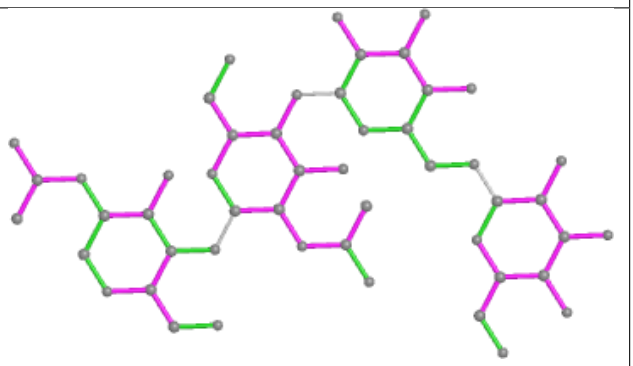

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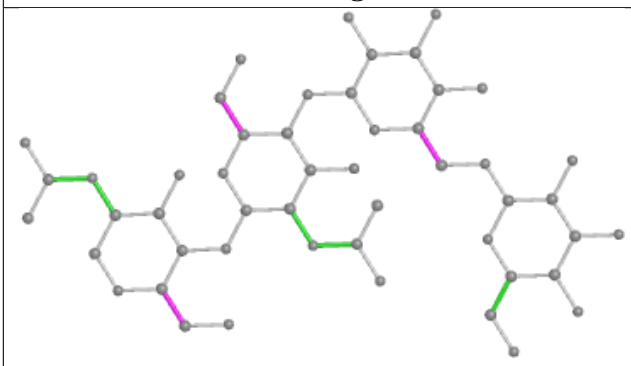

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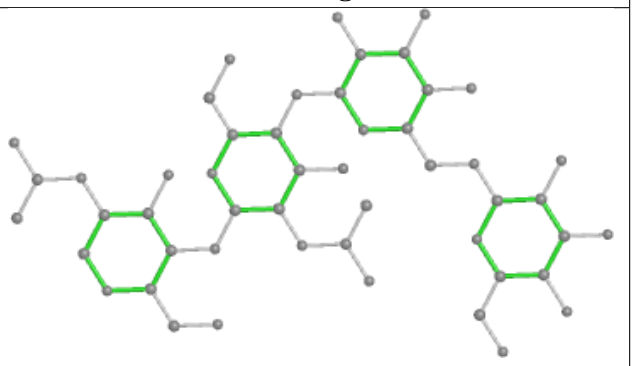
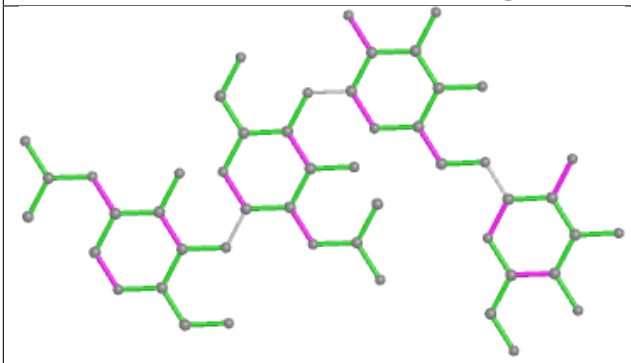


Rings

Oligosaccharide Chain c



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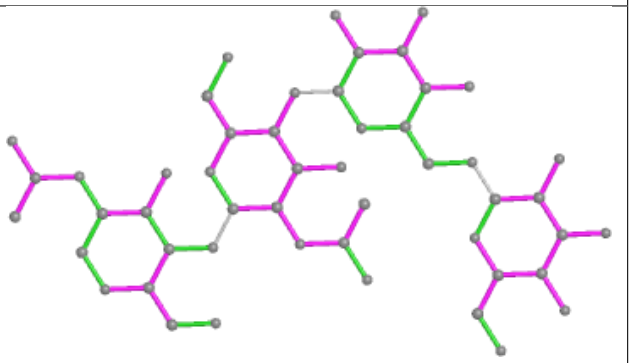

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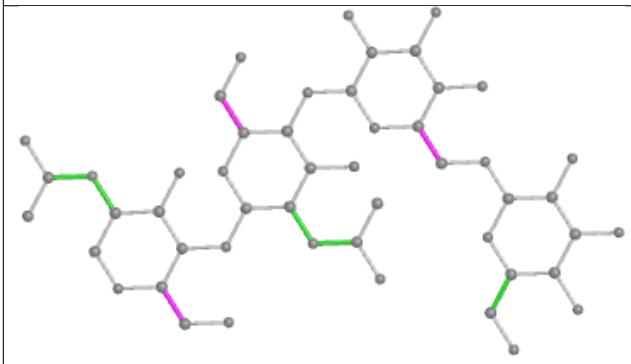

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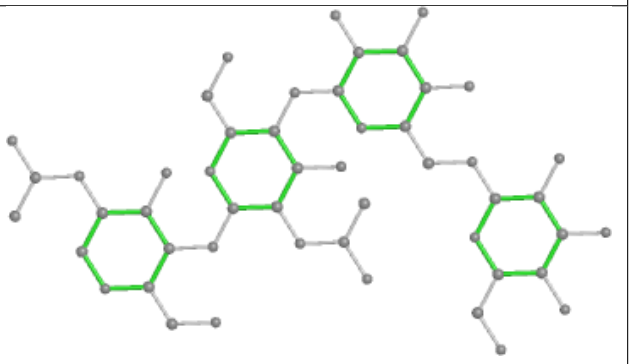
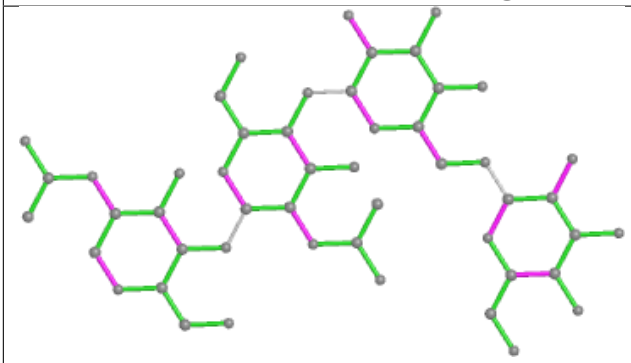


Rings

Oligosaccharide Chain x



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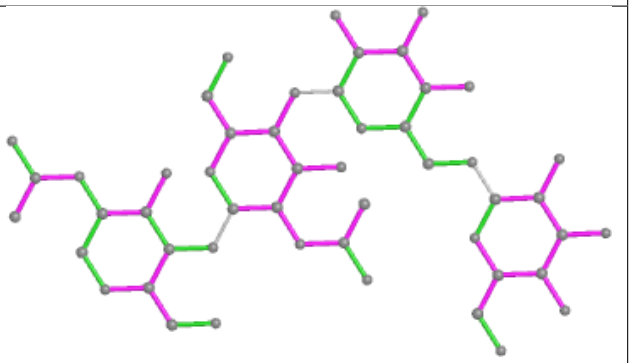
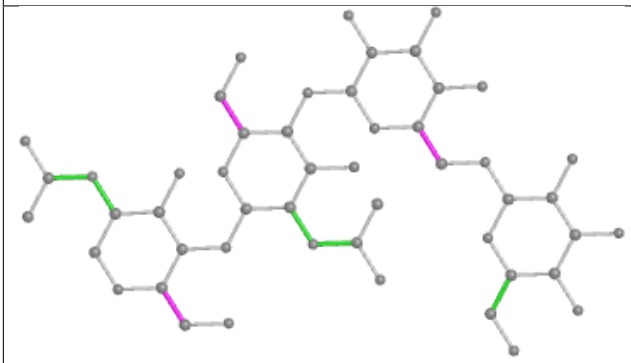
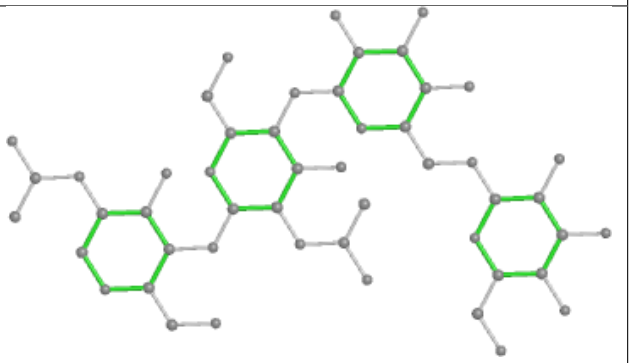


Bond angles

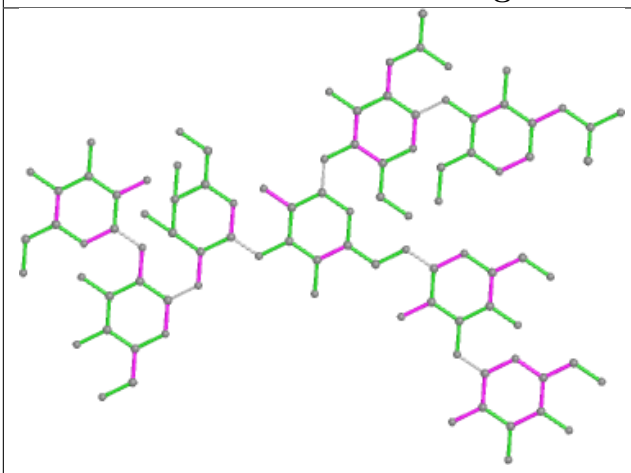


Torsions



Rings

Oligosaccharide Chain K



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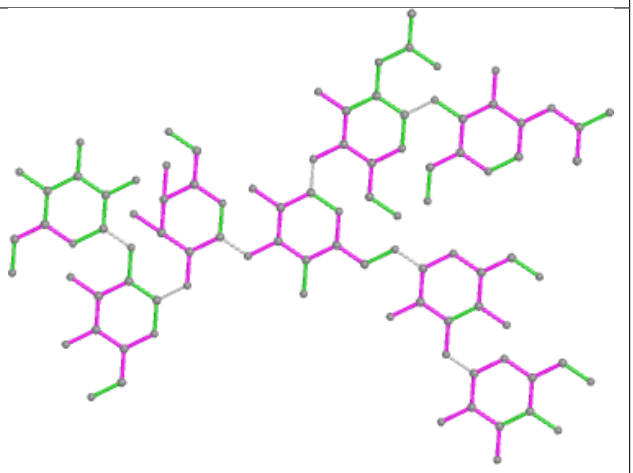

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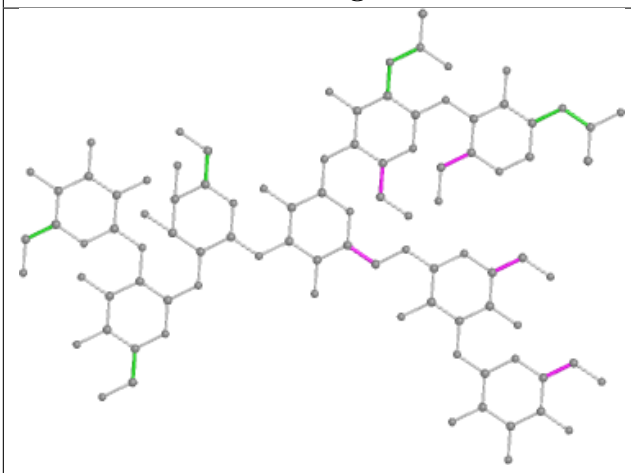

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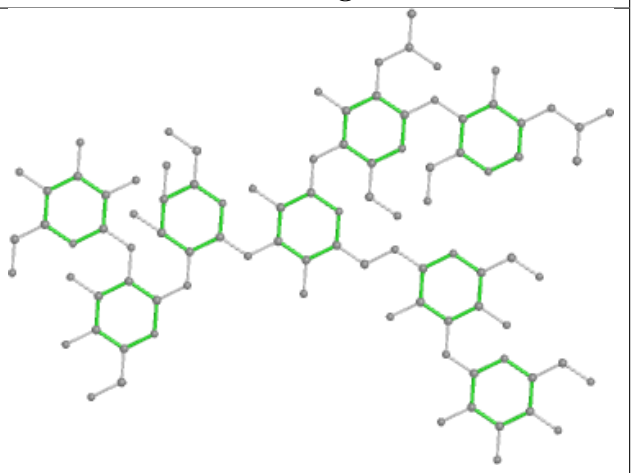
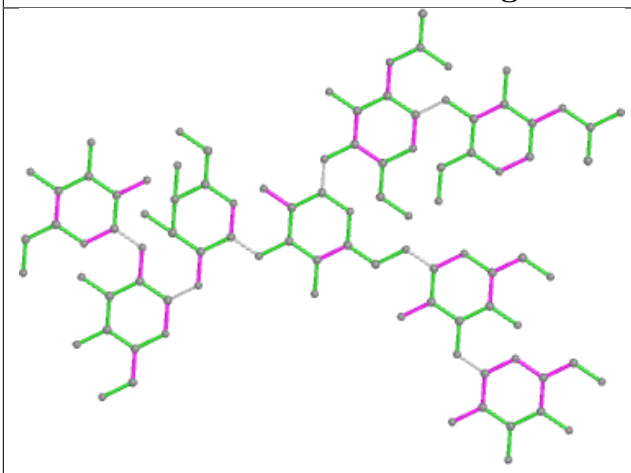


Rings

Oligosaccharide Chain f



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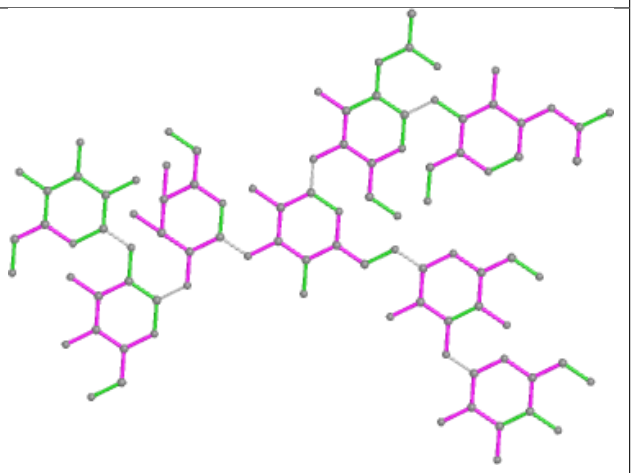

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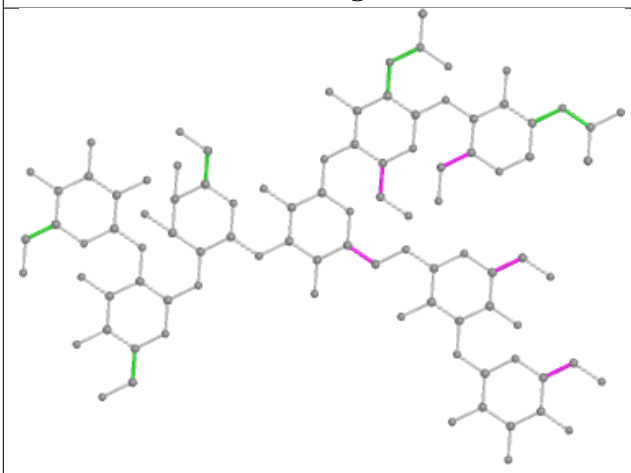

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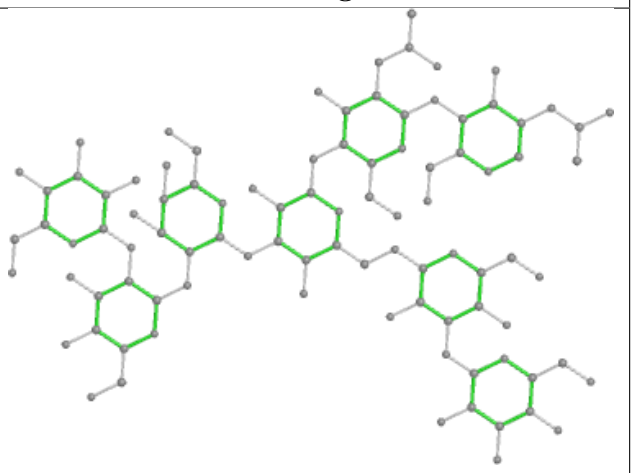
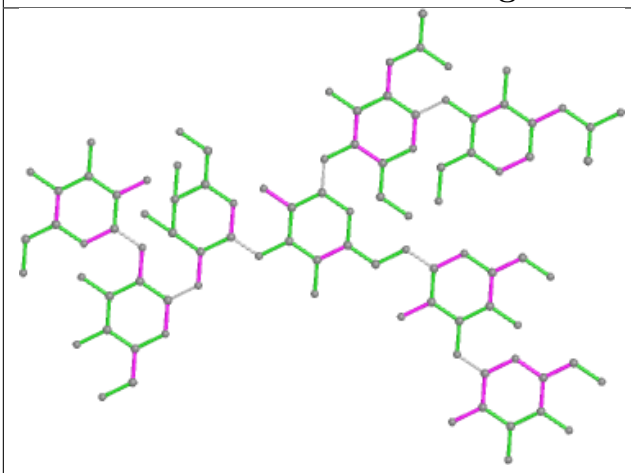


Rings

Oligosaccharide Chain 0



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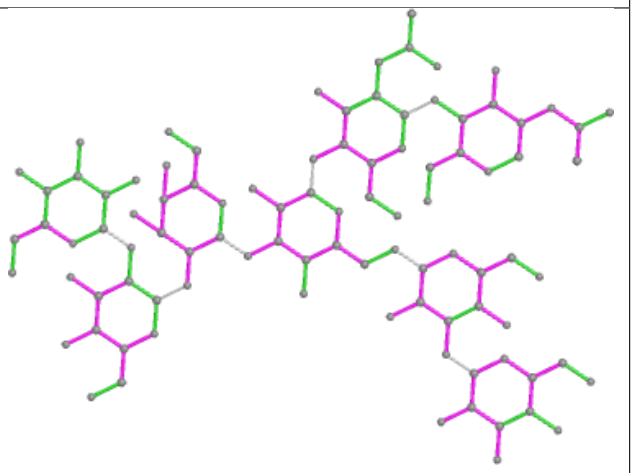

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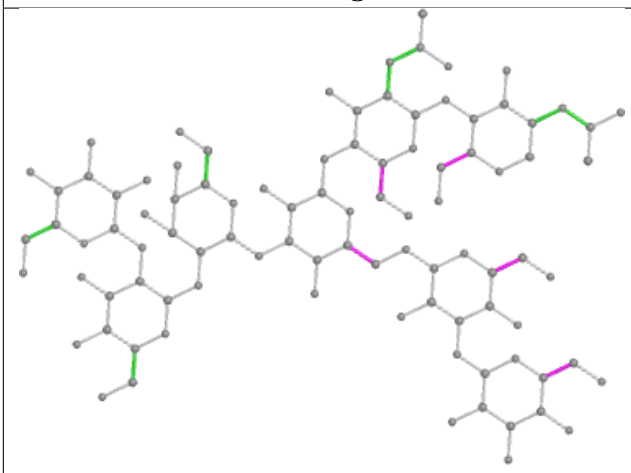

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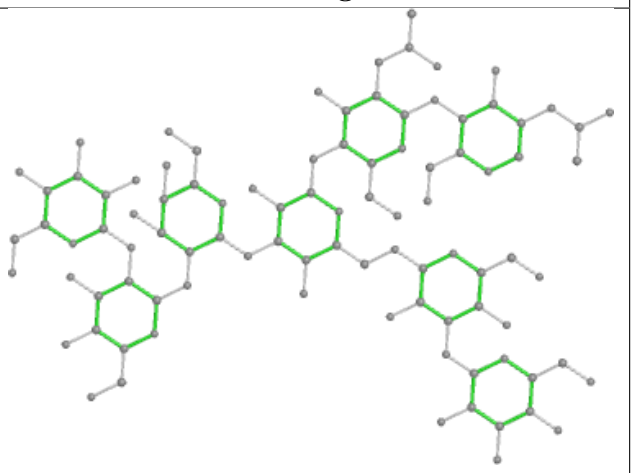
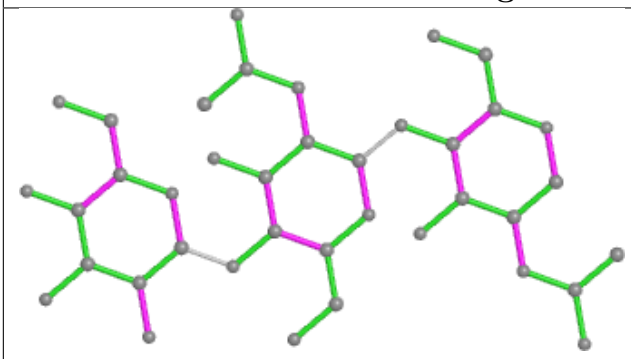


Rings

Oligosaccharide Chain L



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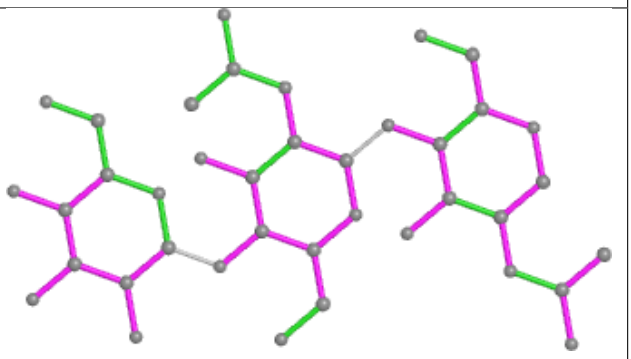

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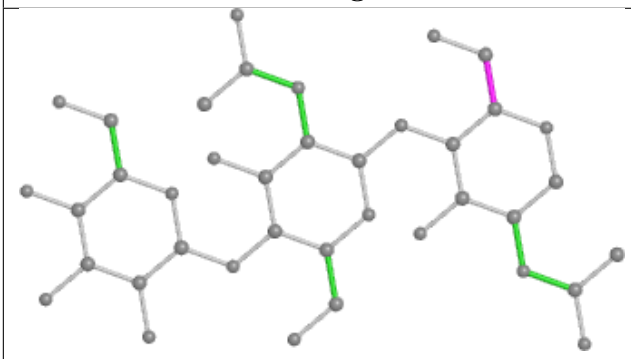

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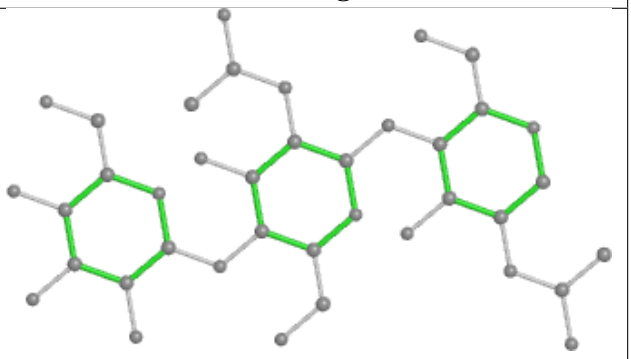
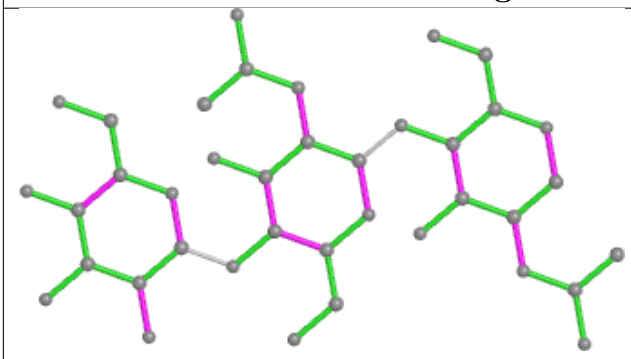


Rings

Oligosaccharide Chain O



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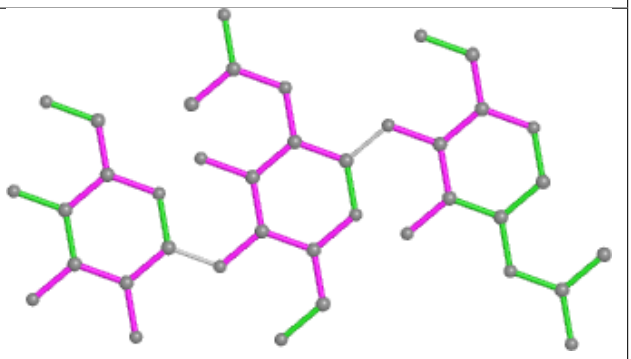
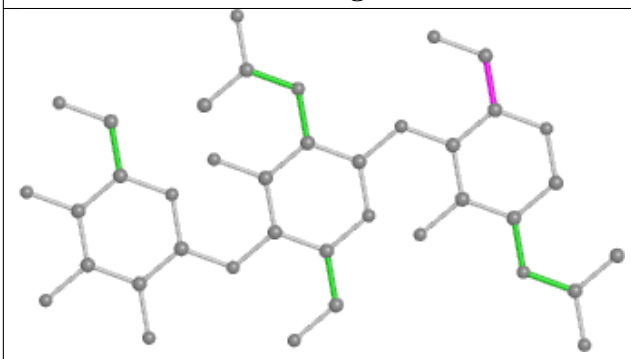


Bond angles



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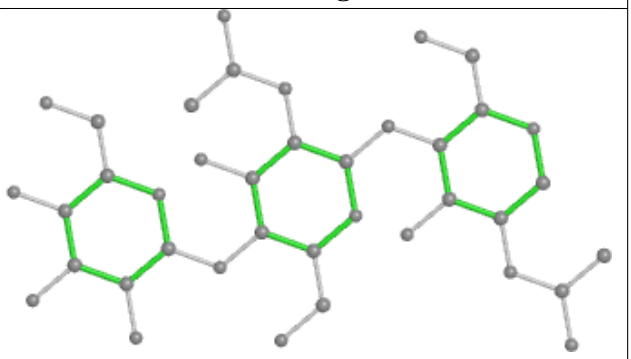
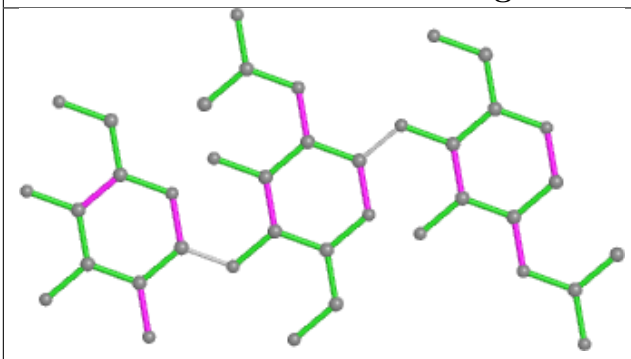


Rings

Oligosaccharide Chain X



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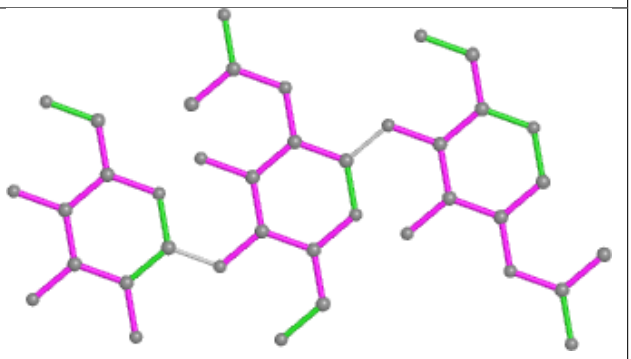

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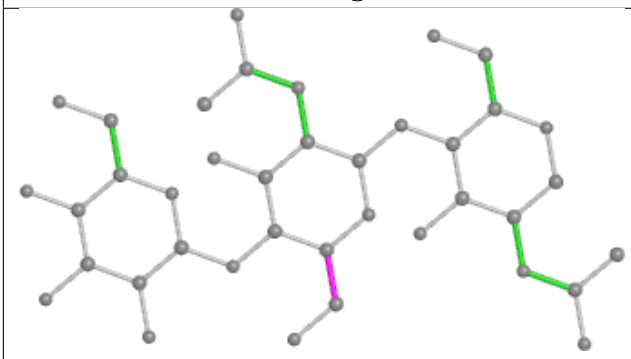

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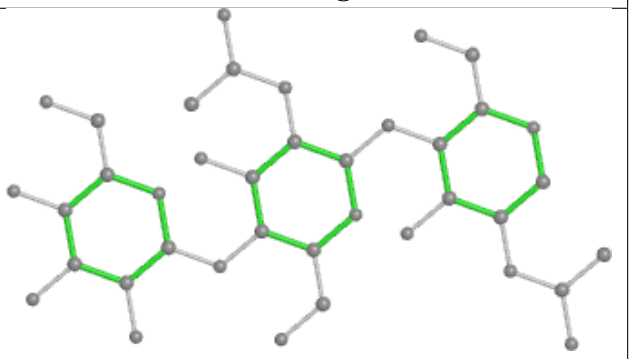
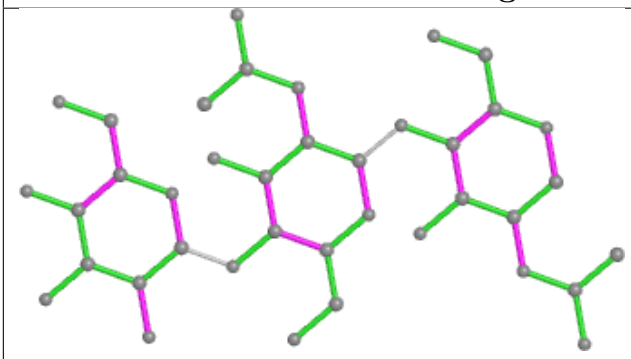


Rings

Oligosaccharide Chain g



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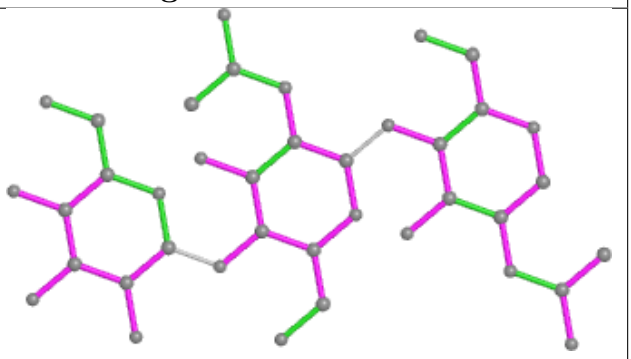
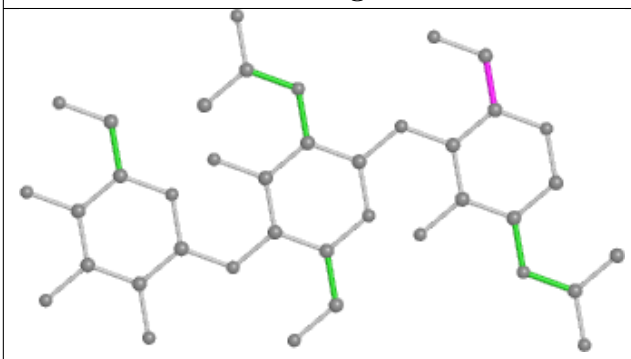


Bond angles



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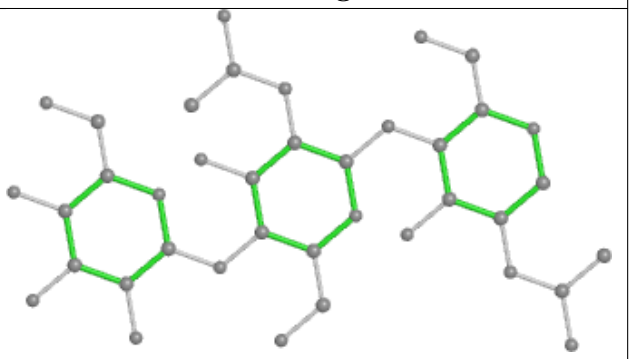
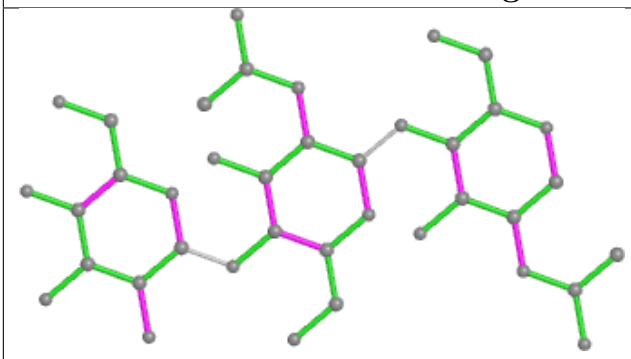


Rings

Oligosaccharide Chain j



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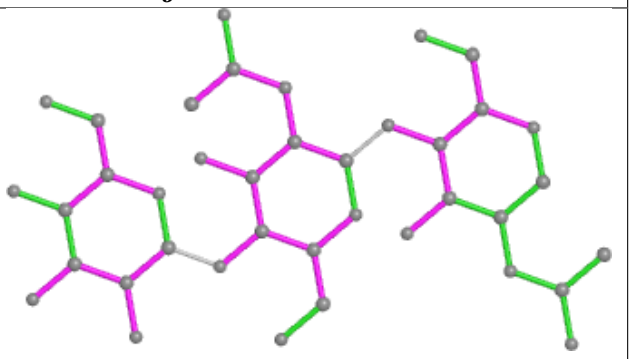
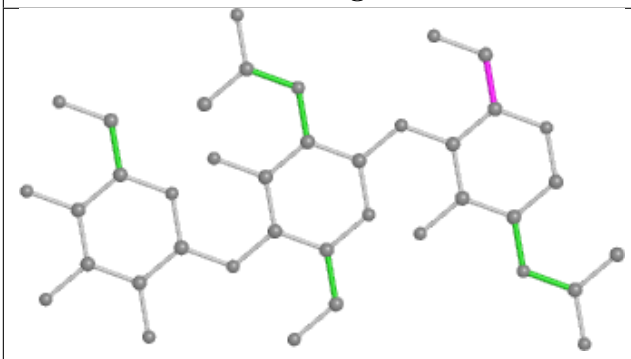


Bond angles



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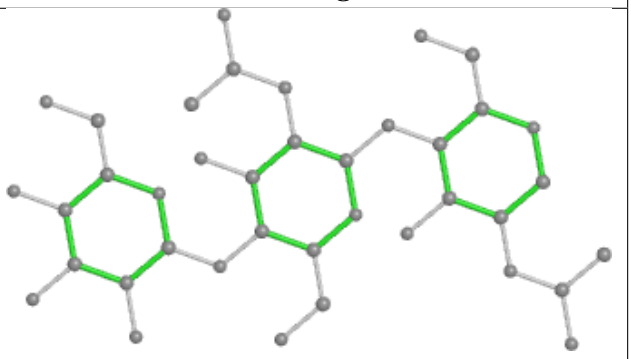
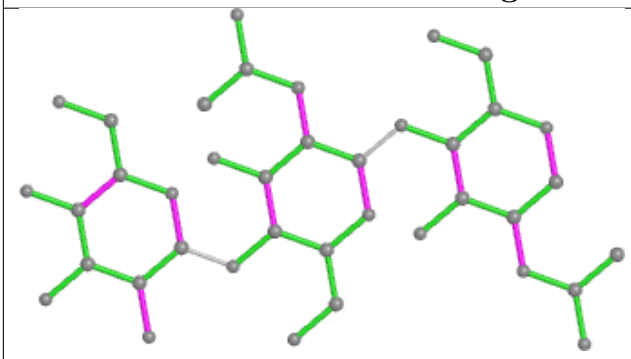


Rings

Oligosaccharide Chain s



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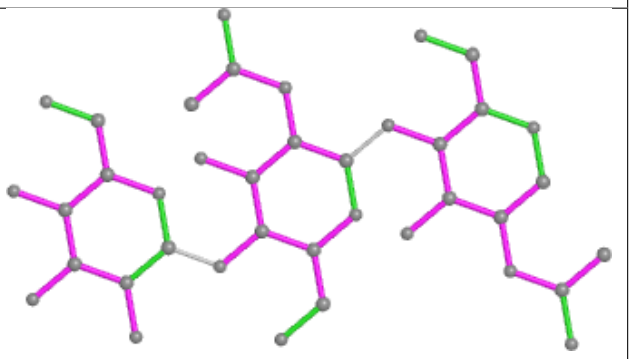
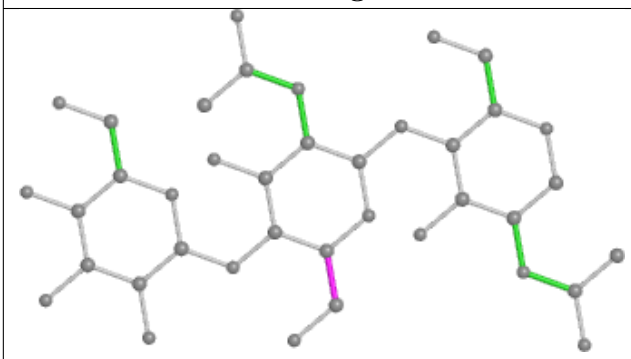


Bond angles



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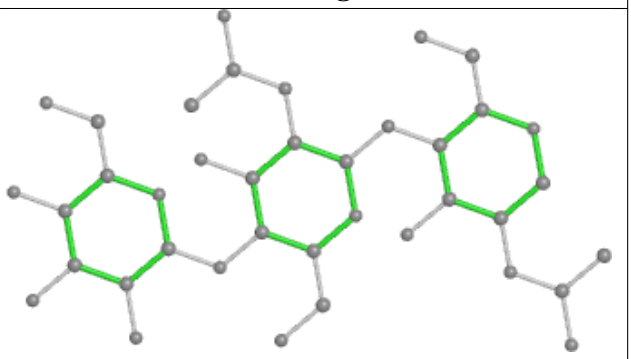
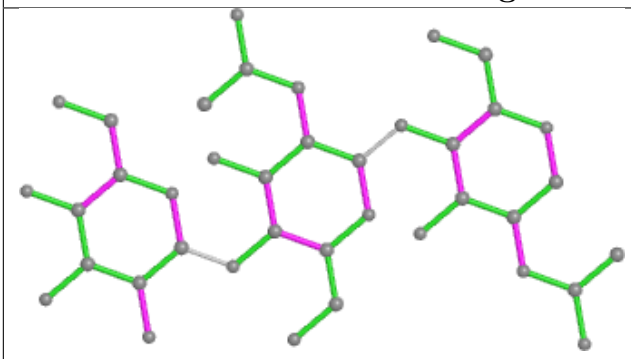
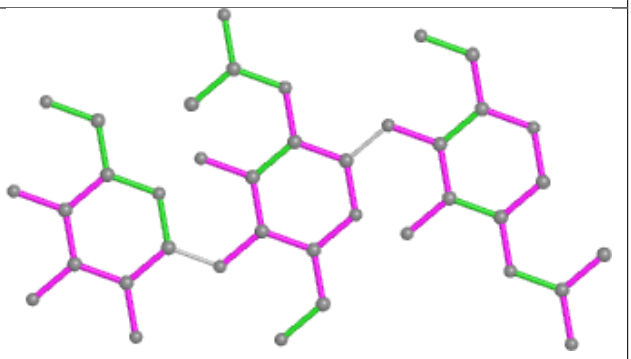


Rings

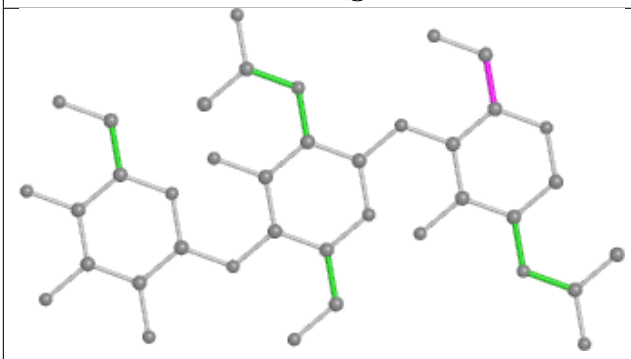
Oligosaccharide Chain 1



Bond lengths



Bond angles



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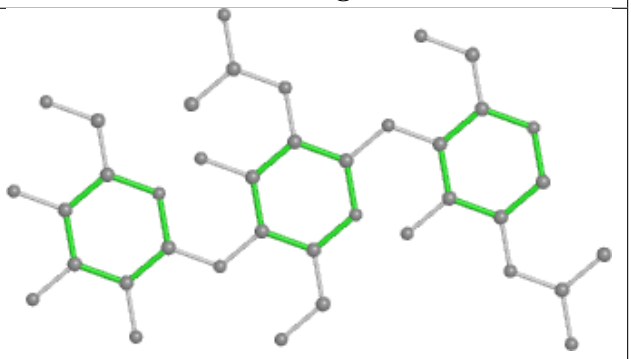
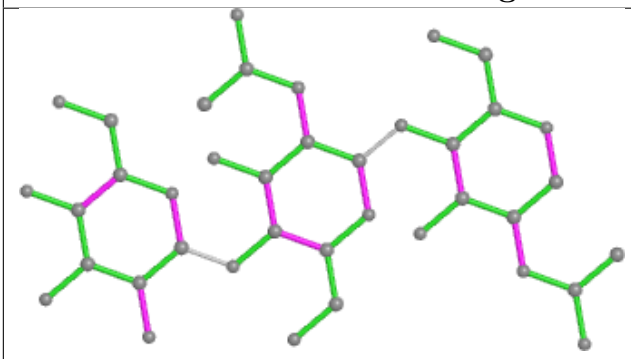
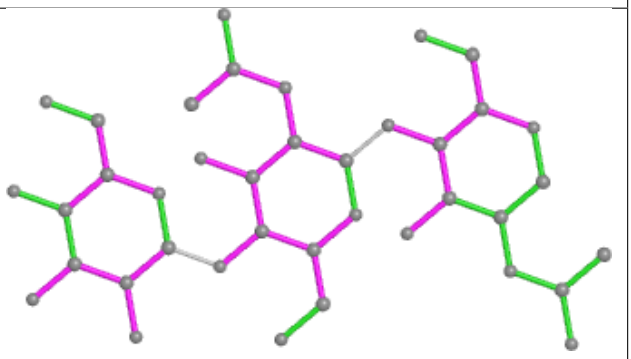


Rings

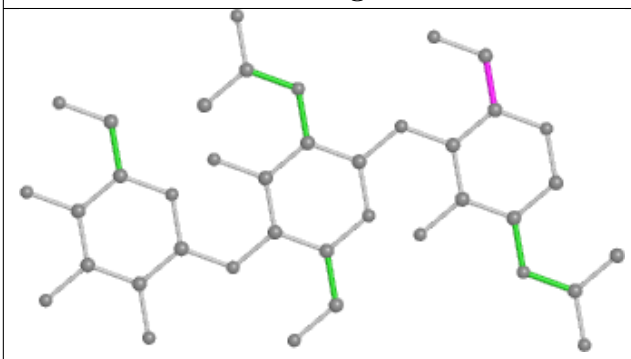
Oligosaccharide Chain 4



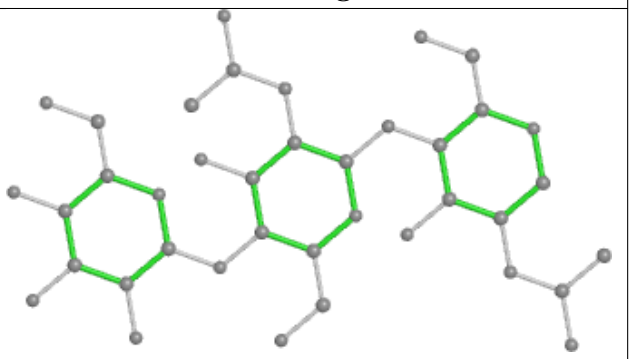
Bond lengths



Bond angles

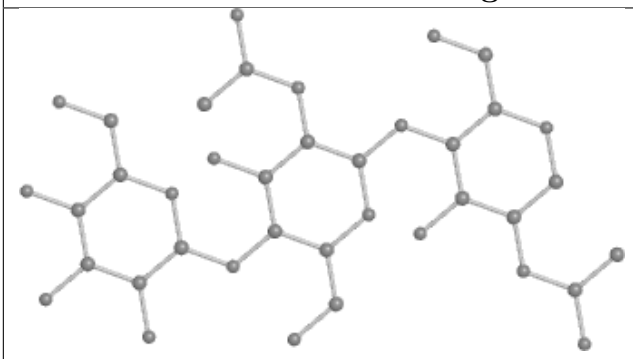


Torsions

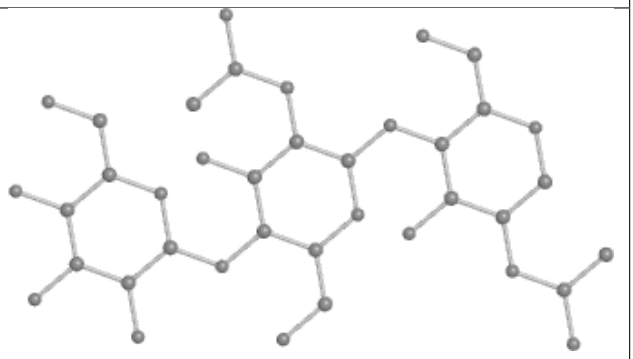


Rings

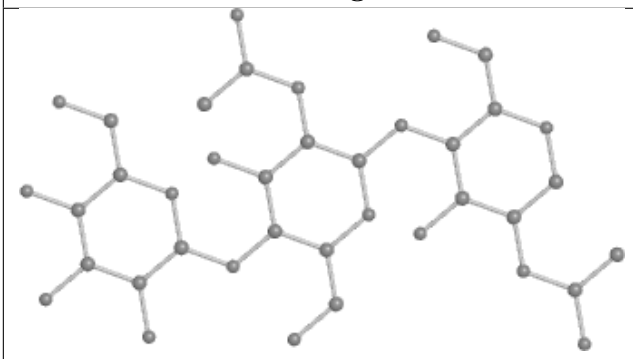
Oligosaccharide Chain DA



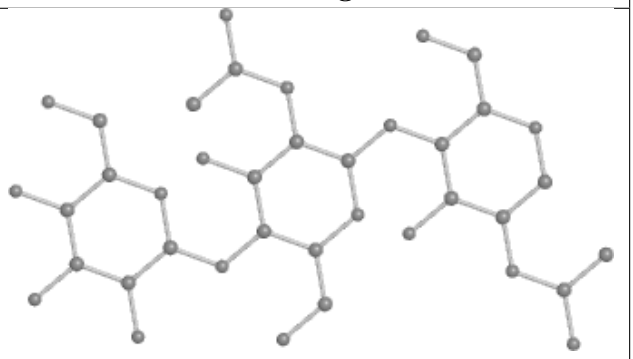
Bond lengths



Bond angles

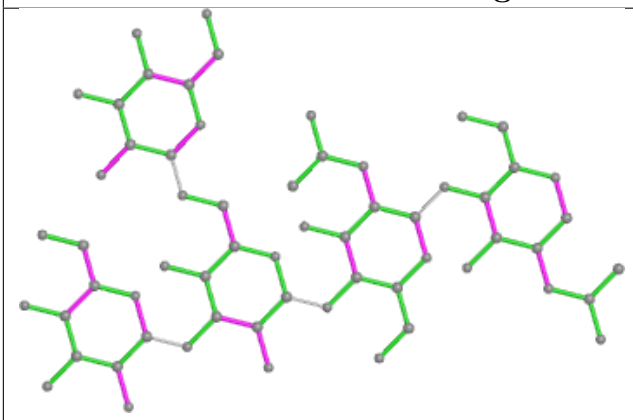


Torsions

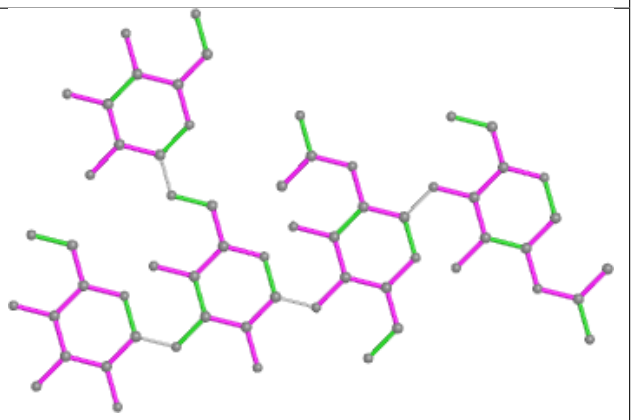


Rings

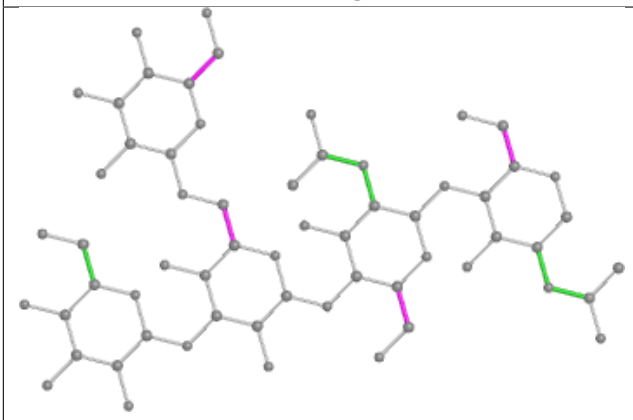
Oligosaccharide Chain N



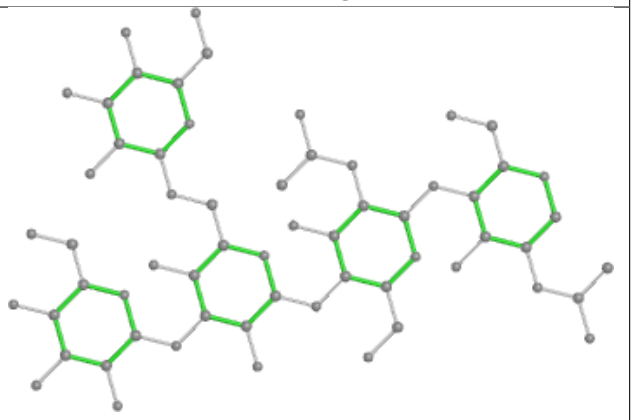
Bond lengths



Bond angles

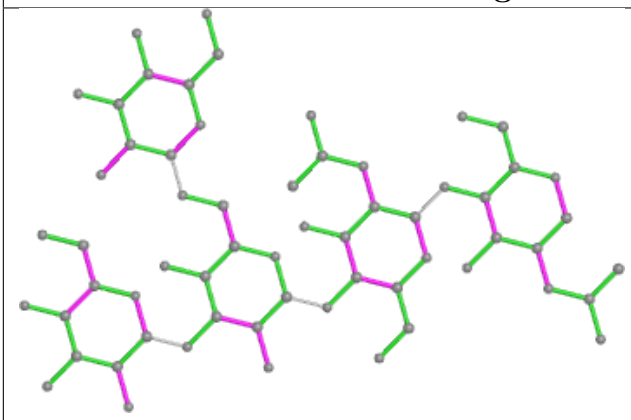


Torsions

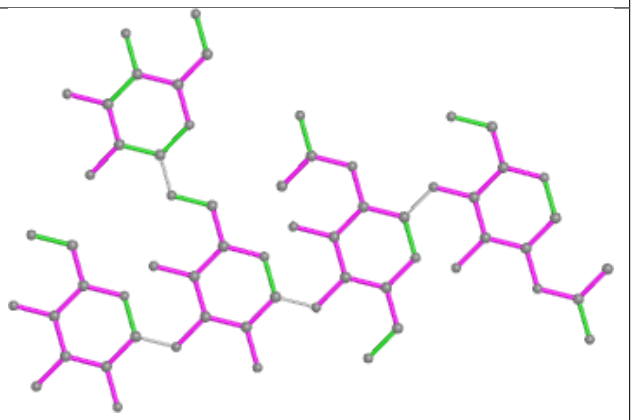


Rings

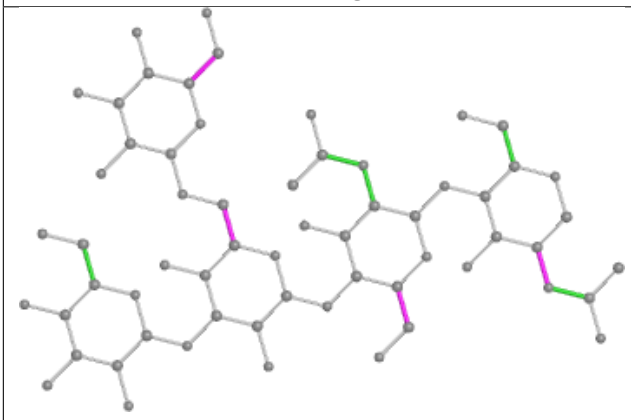
Oligosaccharide Chain V



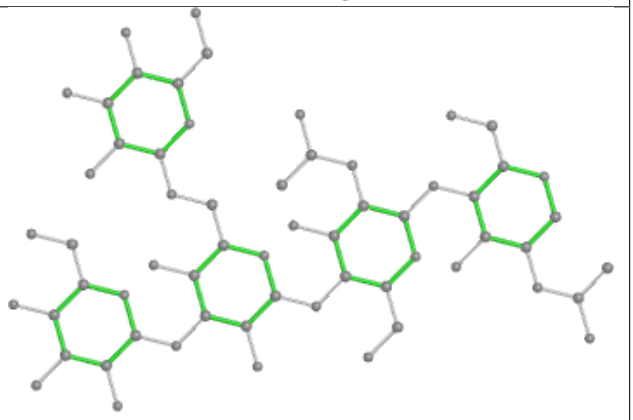
Bond lengths



Bond angles

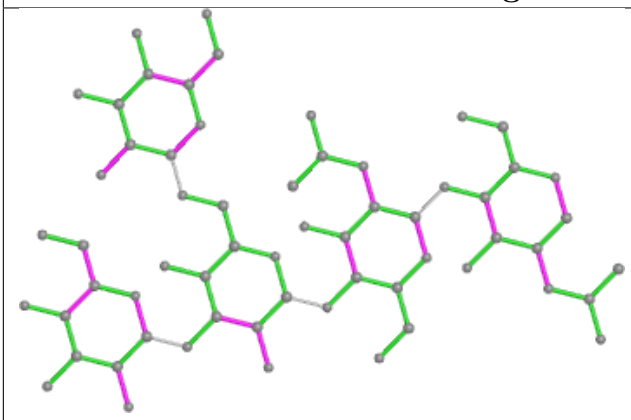


Torsions

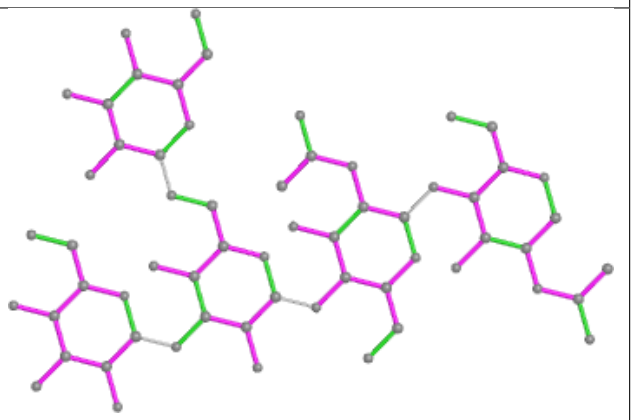


Rings

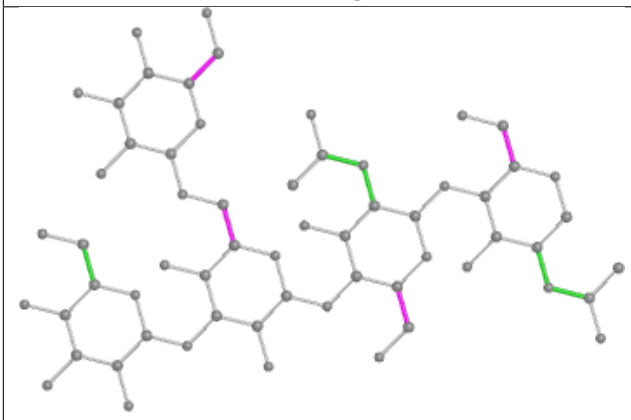
Oligosaccharide Chain i



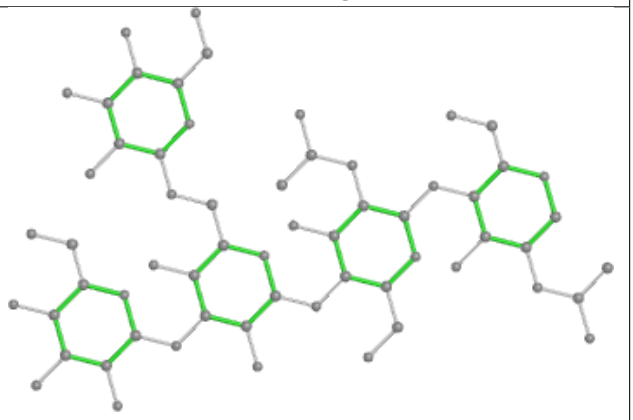
Bond lengths



Bond angles

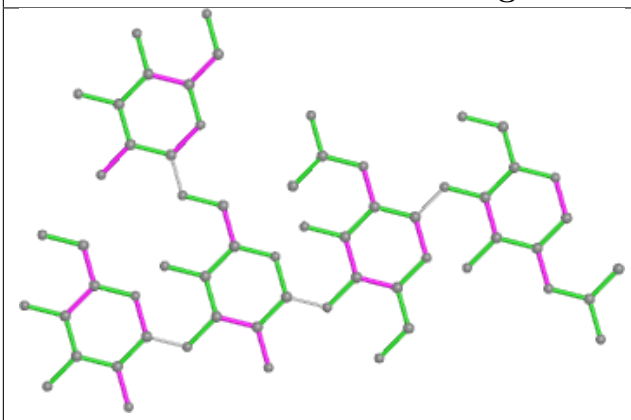


Torsions

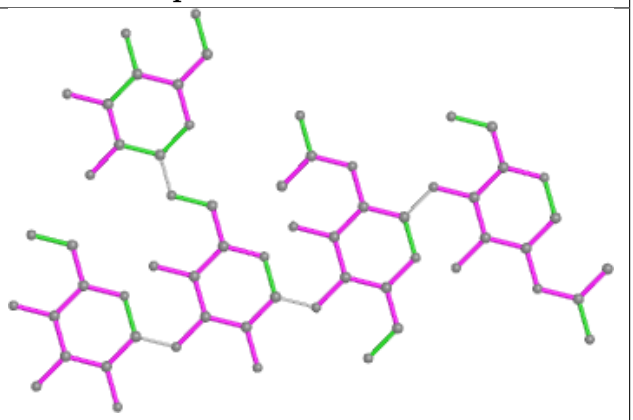


Rings

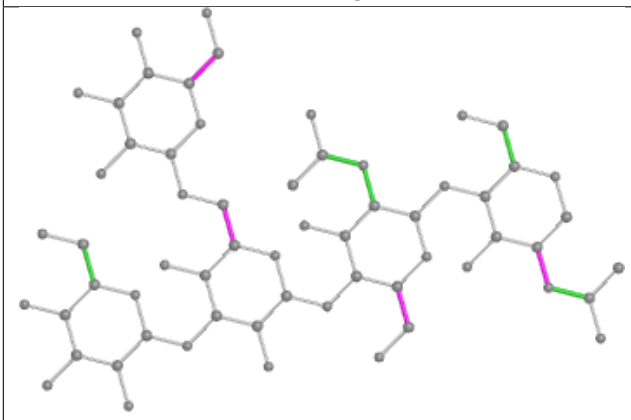
Oligosaccharide Chain q



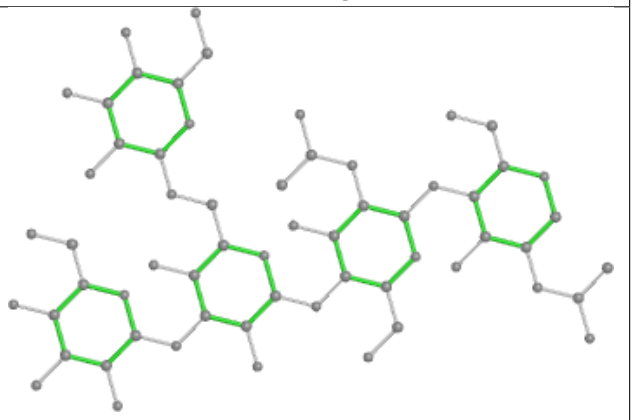
Bond lengths



Bond angles

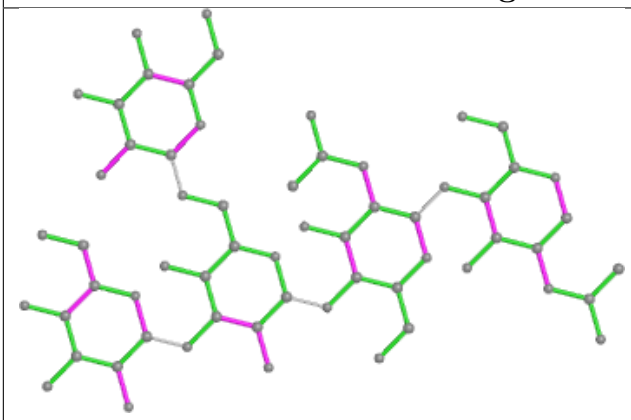


Torsions

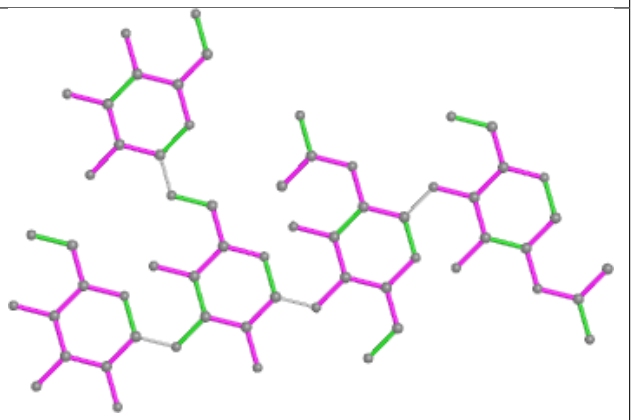


Rings

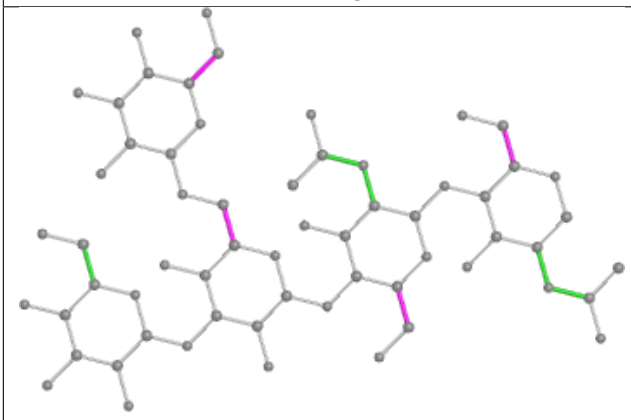
Oligosaccharide Chain 3



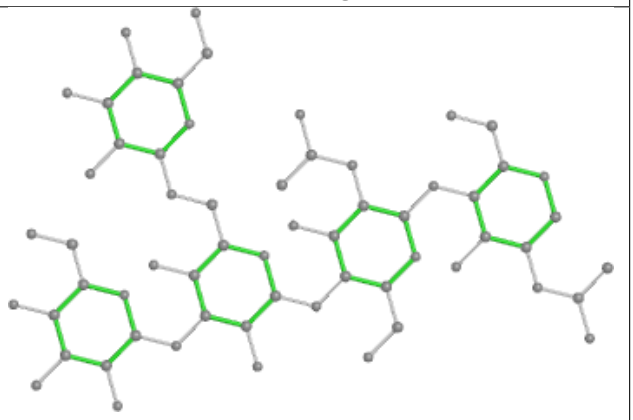
Bond lengths



Bond angles

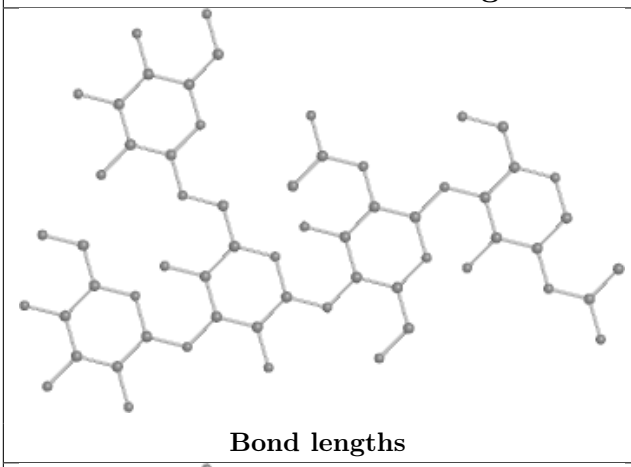


Torsions

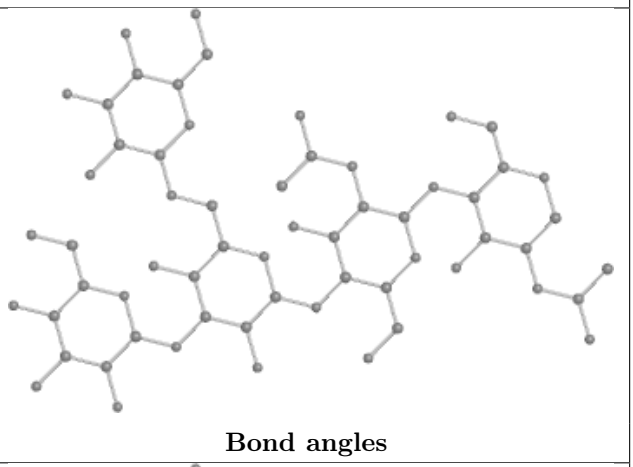


Rings

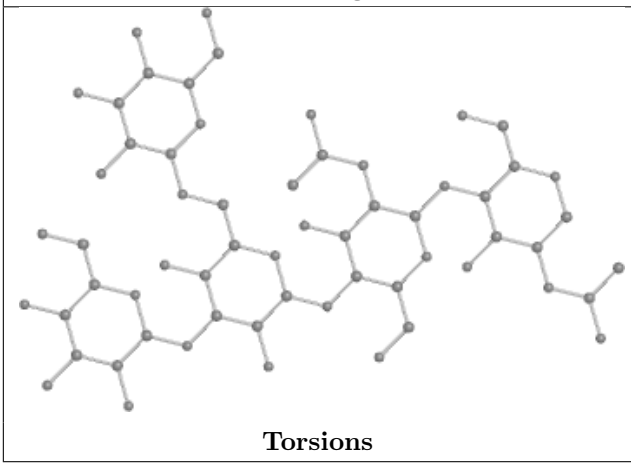
Oligosaccharide Chain BA



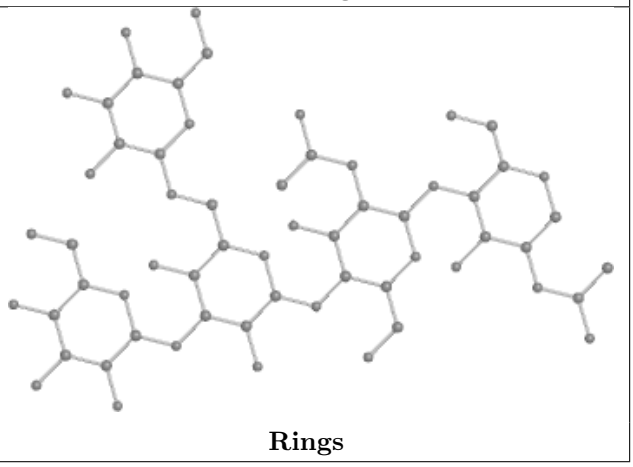
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	B	1439	1	14,14,15	2.50	3 (21%)	17,19,21	3.70	3 (17%)
9	NAG	B	1440	1	14,14,15	3.60	6 (42%)	17,19,21	3.73	8 (47%)
9	NAG	A	1440	1	14,14,15	3.60	6 (42%)	17,19,21	3.73	8 (47%)
9	NAG	B	1474	1	14,14,15	2.82	3 (21%)	17,19,21	3.48	4 (23%)
9	NAG	A	1402	1	14,14,15	2.74	4 (28%)	17,19,21	4.14	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	C	1401	1	14,14,15	2.87	4 (28%)	17,19,21	2.23	3 (17%)
9	NAG	A	1474	1	14,14,15	2.83	3 (21%)	17,19,21	3.48	4 (23%)
9	NAG	A	1403	1	14,14,15	2.67	3 (21%)	17,19,21	4.69	6 (35%)
9	NAG	B	1402	1	14,14,15	2.74	4 (28%)	17,19,21	4.14	6 (35%)
9	NAG	C	1402	1	14,14,15	2.74	4 (28%)	17,19,21	4.14	6 (35%)
9	NAG	B	1441	1	14,14,15	3.05	4 (28%)	17,19,21	4.78	4 (23%)
9	NAG	C	1440	1	14,14,15	3.60	6 (42%)	17,19,21	3.74	8 (47%)
9	NAG	C	1439	1	14,14,15	2.51	3 (21%)	17,19,21	3.70	3 (17%)
9	NAG	B	1403	1	14,14,15	2.67	3 (21%)	17,19,21	4.70	6 (35%)
9	NAG	A	1439	1	14,14,15	2.51	3 (21%)	17,19,21	3.70	3 (17%)
9	NAG	C	1441	1	14,14,15	3.04	4 (28%)	17,19,21	4.79	4 (23%)
9	NAG	A	1441	1	14,14,15	3.05	4 (28%)	17,19,21	4.79	4 (23%)
9	NAG	A	1401	1	14,14,15	2.87	4 (28%)	17,19,21	2.23	3 (17%)
9	NAG	C	1403	1	14,14,15	2.66	3 (21%)	17,19,21	4.69	6 (35%)
9	NAG	B	1401	1	14,14,15	2.87	4 (28%)	17,19,21	2.23	3 (17%)
9	NAG	C	1474	1	14,14,15	2.82	3 (21%)	17,19,21	3.48	4 (23%)

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
9	NAG	B	1439	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1440	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1440	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1474	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1402	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1474	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1402	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1402	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1441	1	-	2/6/23/26	0/1/1/1
9	NAG	C	1440	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1439	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1439	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1441	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	1441	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
9	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
9	NAG	C	1474	1	-	0/6/23/26	0/1/1/1

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1440	NAG	O5-C1	8.98	1.58	1.43
9	A	1440	NAG	O5-C1	8.97	1.58	1.43
9	B	1440	NAG	O5-C1	8.97	1.58	1.43
9	A	1441	NAG	O5-C1	8.06	1.56	1.43
9	C	1441	NAG	O5-C1	8.05	1.56	1.43
9	B	1441	NAG	O5-C1	8.05	1.56	1.43
9	C	1401	NAG	O5-C1	7.70	1.56	1.43
9	B	1401	NAG	O5-C1	7.70	1.56	1.43
9	A	1401	NAG	O5-C1	7.70	1.56	1.43
9	C	1402	NAG	O5-C1	7.53	1.55	1.43
9	A	1402	NAG	O5-C1	7.53	1.55	1.43
9	B	1402	NAG	O5-C1	7.52	1.55	1.43
9	A	1474	NAG	O5-C1	7.35	1.55	1.43
9	C	1474	NAG	O5-C1	7.34	1.55	1.43
9	B	1474	NAG	O5-C1	7.28	1.55	1.43
9	B	1403	NAG	O5-C1	7.19	1.55	1.43
9	A	1403	NAG	O5-C1	7.16	1.55	1.43
9	C	1403	NAG	O5-C1	7.14	1.55	1.43
9	A	1439	NAG	O5-C1	6.79	1.54	1.43
9	B	1439	NAG	O5-C1	6.79	1.54	1.43
9	C	1439	NAG	O5-C1	6.78	1.54	1.43
9	B	1441	NAG	C2-N2	-6.66	1.35	1.46
9	A	1441	NAG	C2-N2	-6.66	1.35	1.46
9	C	1441	NAG	C2-N2	-6.60	1.35	1.46
9	B	1474	NAG	C2-N2	-6.33	1.35	1.46
9	A	1474	NAG	C2-N2	-6.32	1.35	1.46
9	C	1474	NAG	C2-N2	-6.28	1.35	1.46
9	A	1401	NAG	C2-N2	-6.16	1.35	1.46
9	C	1401	NAG	C2-N2	-6.16	1.35	1.46
9	B	1401	NAG	C2-N2	-6.13	1.35	1.46
9	B	1440	NAG	C2-N2	-5.84	1.36	1.46
9	A	1440	NAG	C2-N2	-5.83	1.36	1.46
9	C	1440	NAG	C2-N2	-5.82	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1402	NAG	C2-N2	-5.51	1.36	1.46
9	A	1402	NAG	C2-N2	-5.49	1.37	1.46
9	C	1402	NAG	C2-N2	-5.48	1.37	1.46
9	B	1403	NAG	C2-N2	-5.32	1.37	1.46
9	A	1403	NAG	C2-N2	-5.31	1.37	1.46
9	C	1403	NAG	C2-N2	-5.30	1.37	1.46
9	C	1439	NAG	C2-N2	-5.07	1.37	1.46
9	A	1439	NAG	C2-N2	-5.03	1.37	1.46
9	B	1439	NAG	C2-N2	-5.01	1.37	1.46
9	B	1440	NAG	C4-C3	4.58	1.64	1.52
9	A	1440	NAG	C4-C3	4.58	1.64	1.52
9	C	1440	NAG	C4-C3	4.58	1.64	1.52
9	A	1440	NAG	C4-C5	4.23	1.61	1.53
9	C	1440	NAG	C4-C5	4.22	1.61	1.53
9	B	1440	NAG	C4-C5	4.22	1.61	1.53
9	B	1440	NAG	C1-C2	3.47	1.57	1.52
9	A	1440	NAG	C1-C2	3.43	1.57	1.52
9	C	1440	NAG	C1-C2	3.42	1.57	1.52
9	A	1441	NAG	C4-C3	2.99	1.59	1.52
9	B	1441	NAG	C4-C3	2.99	1.59	1.52
9	C	1441	NAG	C4-C3	2.98	1.59	1.52
9	C	1440	NAG	O5-C5	2.61	1.48	1.43
9	A	1440	NAG	O5-C5	2.61	1.48	1.43
9	B	1440	NAG	O5-C5	2.61	1.48	1.43
9	A	1439	NAG	C4-C3	2.46	1.58	1.52
9	B	1439	NAG	C4-C3	2.45	1.58	1.52
9	C	1439	NAG	C4-C3	2.45	1.58	1.52
9	B	1441	NAG	C4-C5	2.40	1.58	1.53
9	A	1401	NAG	C4-C3	2.38	1.58	1.52
9	B	1401	NAG	C4-C3	2.38	1.58	1.52
9	C	1401	NAG	C4-C3	2.36	1.58	1.52
9	A	1441	NAG	C4-C5	2.36	1.58	1.53
9	C	1441	NAG	C4-C5	2.35	1.58	1.53
9	C	1403	NAG	C4-C3	2.35	1.58	1.52
9	A	1403	NAG	C4-C3	2.33	1.58	1.52
9	B	1403	NAG	C4-C3	2.32	1.58	1.52
9	A	1402	NAG	C1-C2	2.31	1.55	1.52
9	B	1402	NAG	C1-C2	2.30	1.55	1.52
9	C	1402	NAG	C1-C2	2.30	1.55	1.52
9	A	1474	NAG	C4-C3	2.28	1.58	1.52
9	C	1474	NAG	C4-C3	2.28	1.58	1.52
9	B	1474	NAG	C4-C3	2.25	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1402	NAG	C4-C3	2.21	1.58	1.52
9	A	1402	NAG	C4-C3	2.20	1.57	1.52
9	C	1402	NAG	C4-C3	2.19	1.57	1.52
9	A	1401	NAG	C4-C5	2.09	1.57	1.53
9	C	1401	NAG	C4-C5	2.08	1.57	1.53
9	B	1401	NAG	C4-C5	2.07	1.57	1.53

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1403	NAG	O5-C5-C6	-17.17	80.28	107.20
9	A	1403	NAG	O5-C5-C6	-17.17	80.29	107.20
9	C	1403	NAG	O5-C5-C6	-17.16	80.31	107.20
9	A	1402	NAG	O5-C5-C6	-13.88	85.44	107.20
9	C	1402	NAG	O5-C5-C6	-13.88	85.44	107.20
9	B	1402	NAG	O5-C5-C6	-13.87	85.45	107.20
9	C	1441	NAG	O5-C5-C6	-12.76	87.20	107.20
9	A	1441	NAG	O5-C5-C6	-12.75	87.22	107.20
9	B	1441	NAG	O5-C5-C6	-12.72	87.26	107.20
9	C	1439	NAG	O5-C5-C6	-12.72	87.26	107.20
9	B	1439	NAG	O5-C5-C6	-12.71	87.27	107.20
9	A	1439	NAG	O5-C5-C6	-12.71	87.28	107.20
9	A	1474	NAG	O5-C5-C6	-12.59	87.47	107.20
9	C	1474	NAG	O5-C5-C6	-12.58	87.48	107.20
9	B	1474	NAG	O5-C5-C6	-12.58	87.48	107.20
9	A	1440	NAG	O5-C5-C6	-11.21	89.63	107.20
9	B	1440	NAG	O5-C5-C6	-11.21	89.63	107.20
9	C	1440	NAG	O5-C5-C6	-11.21	89.63	107.20
9	C	1441	NAG	C6-C5-C4	10.57	137.76	113.00
9	A	1441	NAG	C6-C5-C4	10.55	137.73	113.00
9	B	1441	NAG	C6-C5-C4	10.55	137.72	113.00
9	C	1441	NAG	C1-C2-N2	9.53	126.77	110.49
9	A	1441	NAG	C1-C2-N2	9.53	126.77	110.49
9	B	1441	NAG	C1-C2-N2	9.53	126.77	110.49
9	A	1401	NAG	O5-C5-C6	-7.68	95.17	107.20
9	B	1401	NAG	O5-C5-C6	-7.67	95.18	107.20
9	C	1401	NAG	O5-C5-C6	-7.66	95.19	107.20
9	B	1403	NAG	O4-C4-C5	-6.59	92.94	109.30
9	A	1403	NAG	O4-C4-C5	-6.58	92.96	109.30
9	C	1403	NAG	O4-C4-C5	-6.58	92.96	109.30
9	C	1402	NAG	O3-C3-C2	6.14	122.17	109.47
9	A	1402	NAG	O3-C3-C2	6.13	122.15	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1402	NAG	O3-C3-C2	6.12	122.13	109.47
9	C	1440	NAG	C1-C2-N2	6.10	120.91	110.49
9	A	1440	NAG	C1-C2-N2	6.09	120.89	110.49
9	B	1440	NAG	C1-C2-N2	6.09	120.88	110.49
9	B	1439	NAG	C1-C2-N2	-5.59	100.93	110.49
9	A	1439	NAG	C1-C2-N2	-5.59	100.95	110.49
9	C	1439	NAG	C1-C2-N2	-5.56	100.99	110.49
9	C	1440	NAG	O3-C3-C2	-5.08	98.95	109.47
9	A	1440	NAG	O3-C3-C2	-5.07	98.97	109.47
9	B	1440	NAG	O3-C3-C2	-5.06	98.99	109.47
9	C	1402	NAG	C6-C5-C4	4.56	123.69	113.00
9	B	1402	NAG	C6-C5-C4	4.56	123.67	113.00
9	A	1402	NAG	C6-C5-C4	4.55	123.67	113.00
9	C	1474	NAG	O4-C4-C3	-4.39	100.19	110.35
9	A	1474	NAG	O4-C4-C3	-4.38	100.23	110.35
9	B	1474	NAG	O4-C4-C3	-4.37	100.24	110.35
9	B	1439	NAG	O3-C3-C2	4.33	118.42	109.47
9	A	1439	NAG	O3-C3-C2	4.32	118.40	109.47
9	C	1439	NAG	O3-C3-C2	4.31	118.37	109.47
9	A	1441	NAG	O3-C3-C2	-3.75	101.71	109.47
9	B	1441	NAG	O3-C3-C2	-3.74	101.72	109.47
9	C	1441	NAG	O3-C3-C2	-3.73	101.74	109.47
9	B	1402	NAG	C1-C2-N2	-3.71	104.14	110.49
9	C	1402	NAG	C1-C2-N2	-3.71	104.14	110.49
9	A	1402	NAG	C1-C2-N2	-3.71	104.15	110.49
9	B	1440	NAG	O4-C4-C3	-3.45	102.36	110.35
9	A	1440	NAG	O4-C4-C3	-3.45	102.37	110.35
9	C	1440	NAG	O4-C4-C3	-3.45	102.37	110.35
9	B	1403	NAG	C6-C5-C4	3.21	120.51	113.00
9	C	1403	NAG	C6-C5-C4	3.20	120.50	113.00
9	A	1403	NAG	C6-C5-C4	3.20	120.49	113.00
9	A	1474	NAG	C6-C5-C4	3.19	120.48	113.00
9	B	1474	NAG	C6-C5-C4	3.19	120.48	113.00
9	C	1474	NAG	C6-C5-C4	3.19	120.47	113.00
9	C	1403	NAG	C1-C2-N2	2.92	115.48	110.49
9	B	1403	NAG	C1-C2-N2	2.90	115.44	110.49
9	A	1403	NAG	C1-C2-N2	2.90	115.44	110.49
9	B	1440	NAG	C2-N2-C7	2.89	127.02	122.90
9	A	1440	NAG	C2-N2-C7	2.88	127.01	122.90
9	C	1440	NAG	C2-N2-C7	2.88	127.00	122.90
9	C	1402	NAG	O5-C1-C2	-2.87	106.75	111.29
9	A	1402	NAG	O5-C1-C2	-2.85	106.78	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1402	NAG	O5-C1-C2	-2.85	106.79	111.29
9	C	1440	NAG	C6-C5-C4	2.55	118.97	113.00
9	A	1440	NAG	C6-C5-C4	2.54	118.94	113.00
9	B	1440	NAG	C6-C5-C4	2.52	118.91	113.00
9	A	1440	NAG	O4-C4-C5	-2.50	103.09	109.30
9	C	1440	NAG	O4-C4-C5	-2.50	103.10	109.30
9	B	1440	NAG	O4-C4-C5	-2.48	103.13	109.30
9	B	1440	NAG	C4-C3-C2	2.46	114.62	111.02
9	A	1440	NAG	C4-C3-C2	2.46	114.62	111.02
9	C	1440	NAG	C4-C3-C2	2.46	114.62	111.02
9	B	1403	NAG	C8-C7-N2	2.45	120.24	116.10
9	A	1403	NAG	C8-C7-N2	2.43	120.22	116.10
9	C	1403	NAG	C8-C7-N2	2.42	120.19	116.10
9	A	1403	NAG	O7-C7-C8	-2.32	117.75	122.06
9	C	1403	NAG	O7-C7-C8	-2.30	117.78	122.06
9	B	1403	NAG	O7-C7-C8	-2.30	117.78	122.06
9	A	1474	NAG	O3-C3-C2	2.30	114.22	109.47
9	C	1401	NAG	C6-C5-C4	2.29	118.37	113.00
9	C	1474	NAG	O3-C3-C2	2.29	114.20	109.47
9	B	1474	NAG	O3-C3-C2	2.29	114.20	109.47
9	A	1401	NAG	C6-C5-C4	2.29	118.36	113.00
9	B	1401	NAG	C6-C5-C4	2.28	118.34	113.00
9	C	1401	NAG	C1-C2-N2	2.21	114.26	110.49
9	A	1401	NAG	C1-C2-N2	2.20	114.25	110.49
9	B	1401	NAG	C1-C2-N2	2.18	114.20	110.49
9	C	1402	NAG	C4-C3-C2	-2.14	107.89	111.02
9	A	1402	NAG	C4-C3-C2	-2.12	107.91	111.02
9	B	1402	NAG	C4-C3-C2	-2.11	107.93	111.02

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1439	NAG	O5-C5-C6-O6
9	A	1439	NAG	O5-C5-C6-O6
9	B	1439	NAG	O5-C5-C6-O6
9	A	1441	NAG	O5-C5-C6-O6
9	B	1441	NAG	O5-C5-C6-O6
9	C	1441	NAG	O5-C5-C6-O6
9	A	1441	NAG	C1-C2-N2-C7
9	B	1441	NAG	C1-C2-N2-C7
9	C	1441	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
9	A	1402	NAG	C1-C2-N2-C7
9	B	1402	NAG	C1-C2-N2-C7
9	C	1402	NAG	C1-C2-N2-C7
9	B	1440	NAG	C1-C2-N2-C7
9	A	1440	NAG	C1-C2-N2-C7
9	C	1440	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

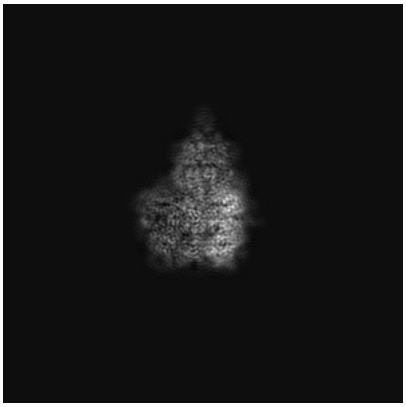
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8331. These allow visual inspection of the internal detail of the map and identification of artifacts.

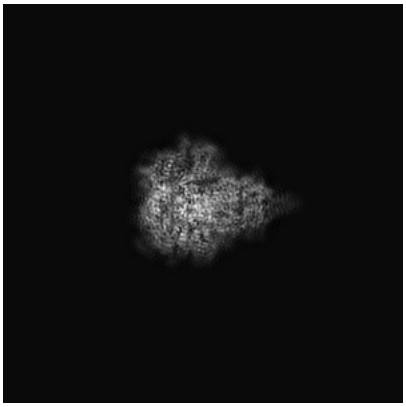
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

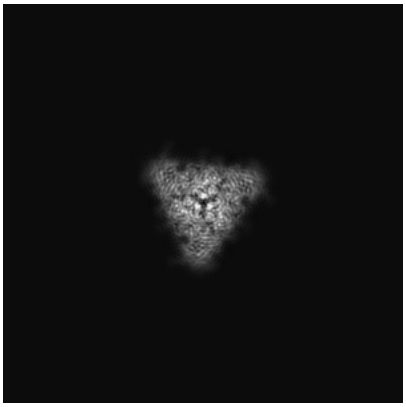
6.1.1 Primary map



X



Y

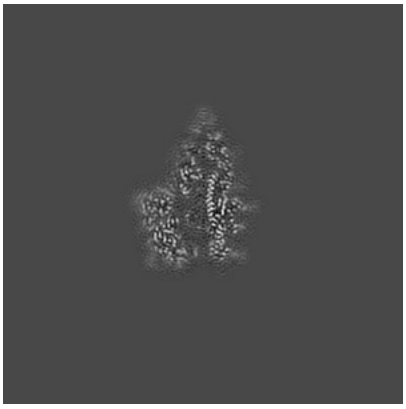


Z

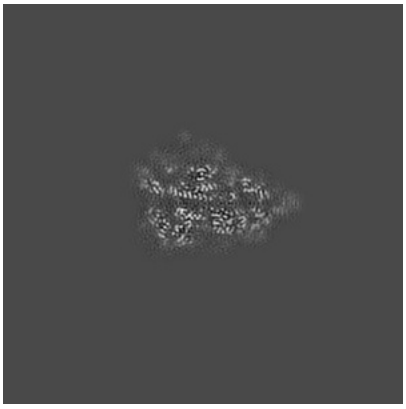
The images above show the map projected in three orthogonal directions.

6.2 Central slices

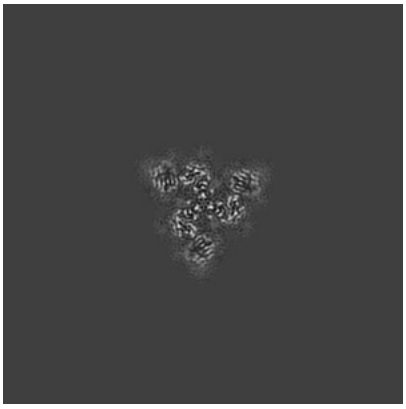
6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

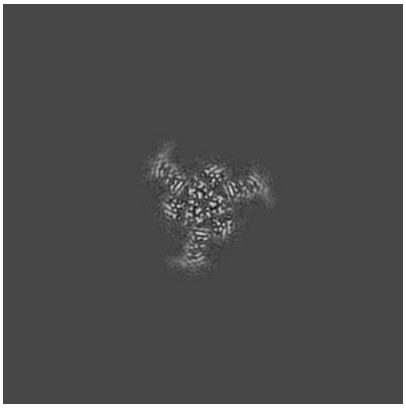
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 165

Y Index: 168

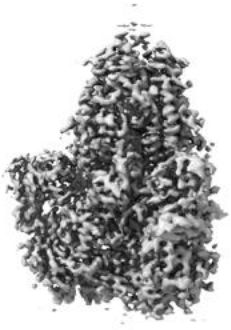


Z Index: 145

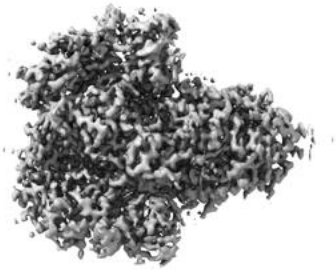
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

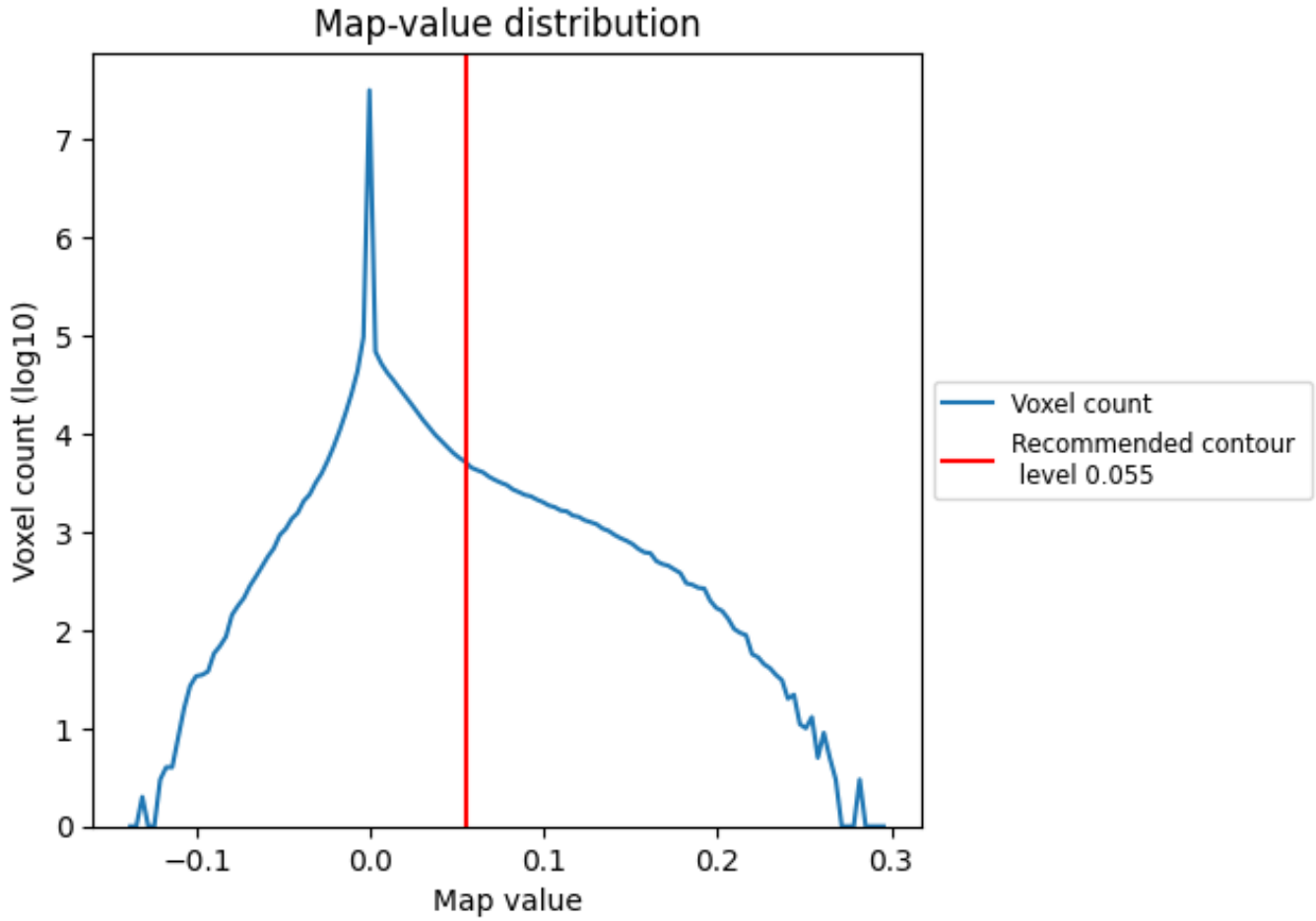
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

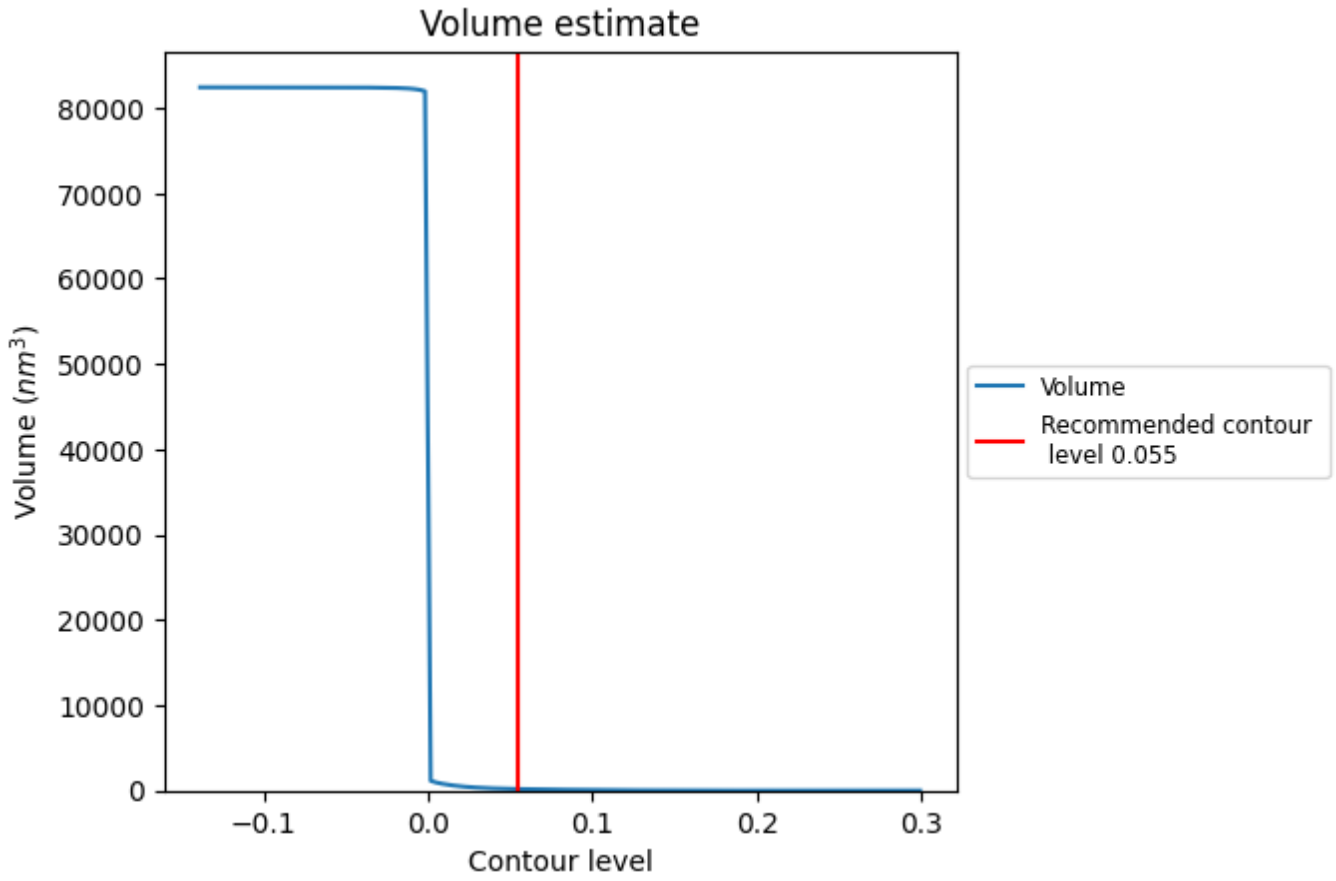
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

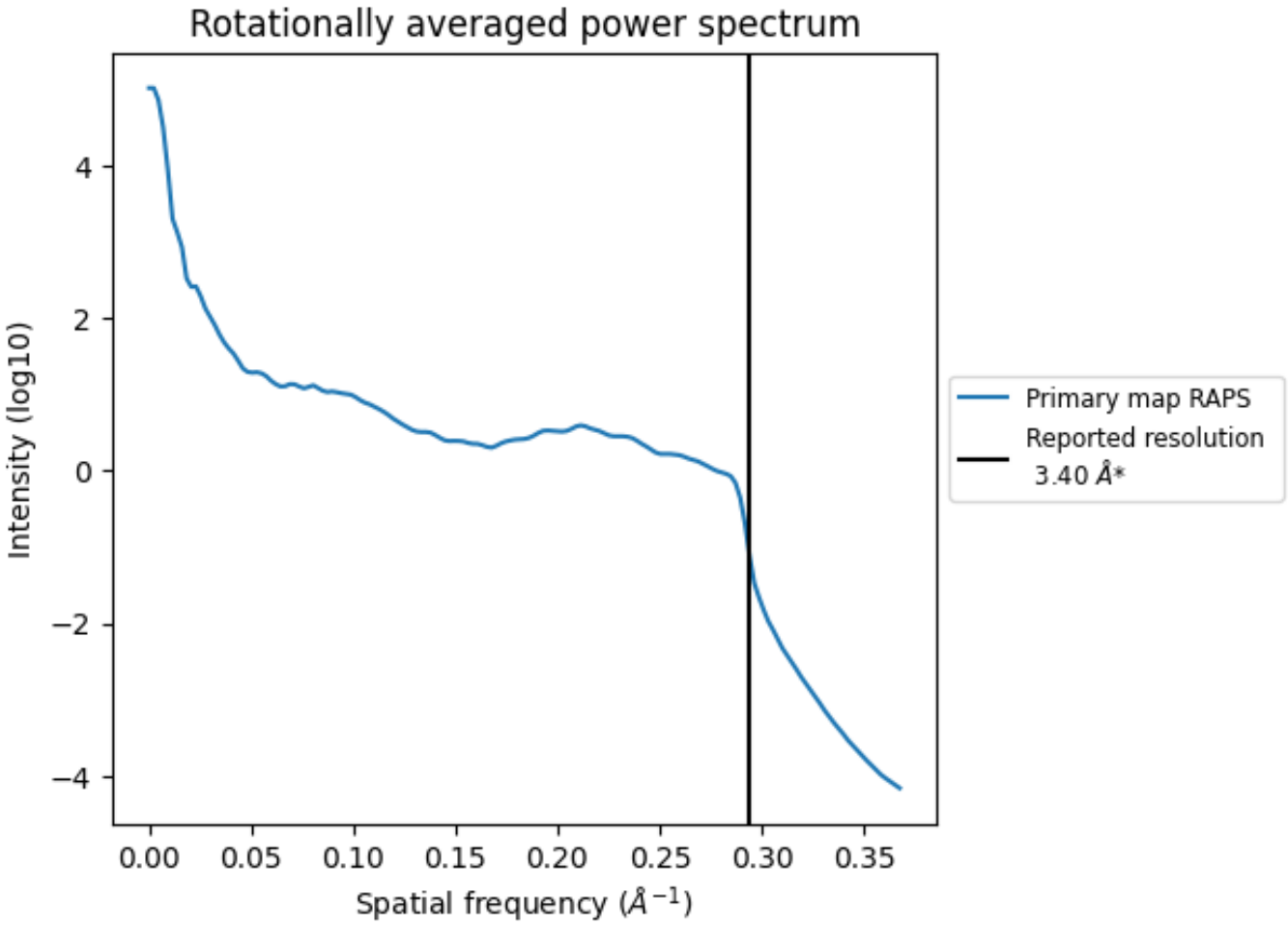
7.2 Volume estimate



The volume at the recommended contour level is 177 nm^3; this corresponds to an approximate mass of 160 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

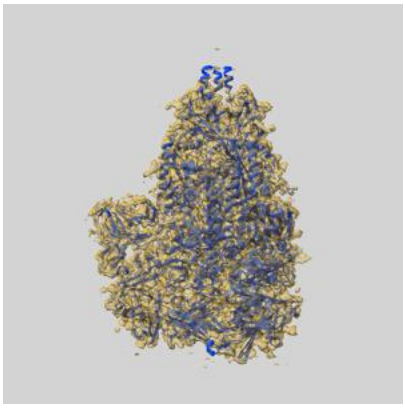
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

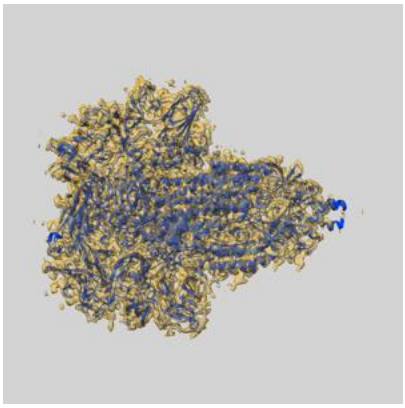
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8331 and PDB model 5SZS. Per-residue inclusion information can be found in section 3 on page 16.

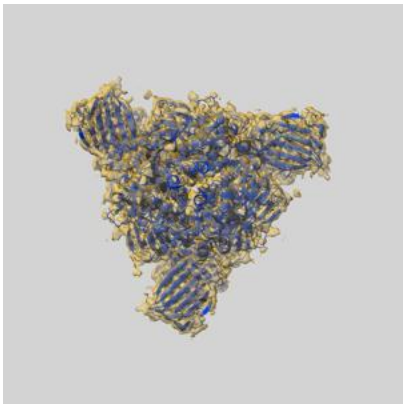
9.1 Map-model overlay



X



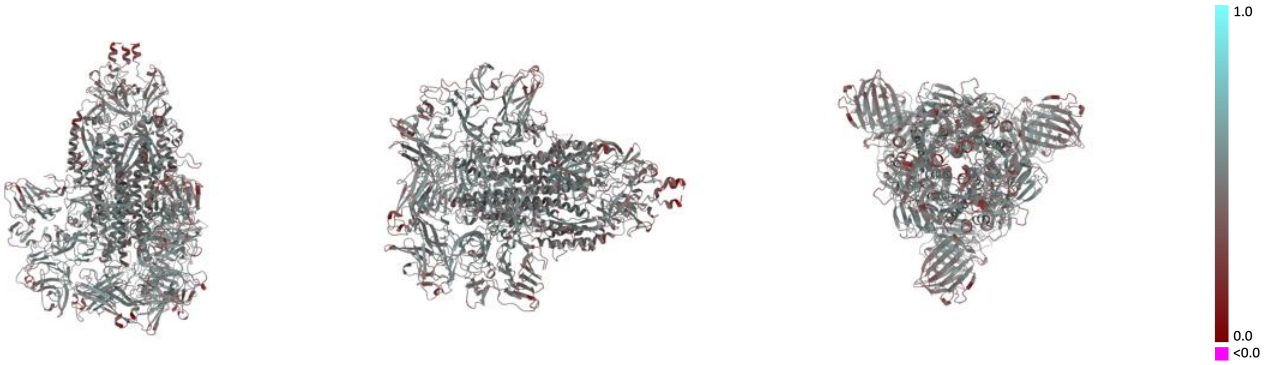
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

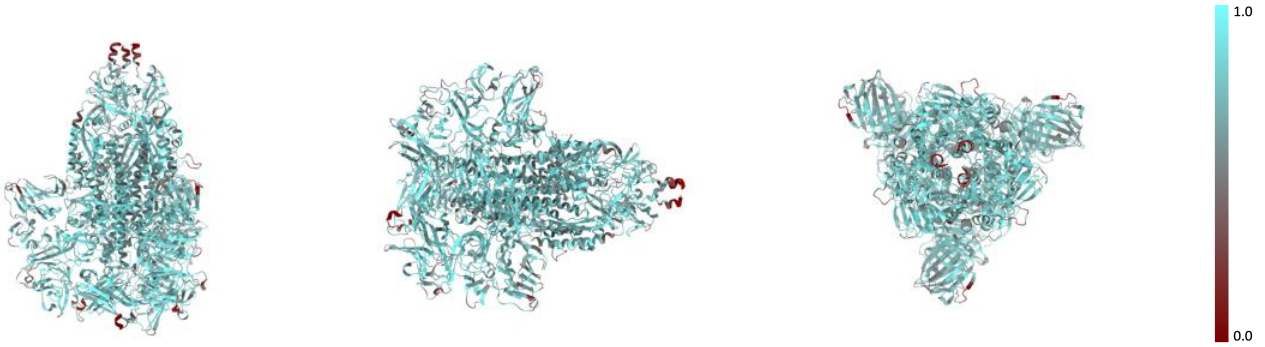
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

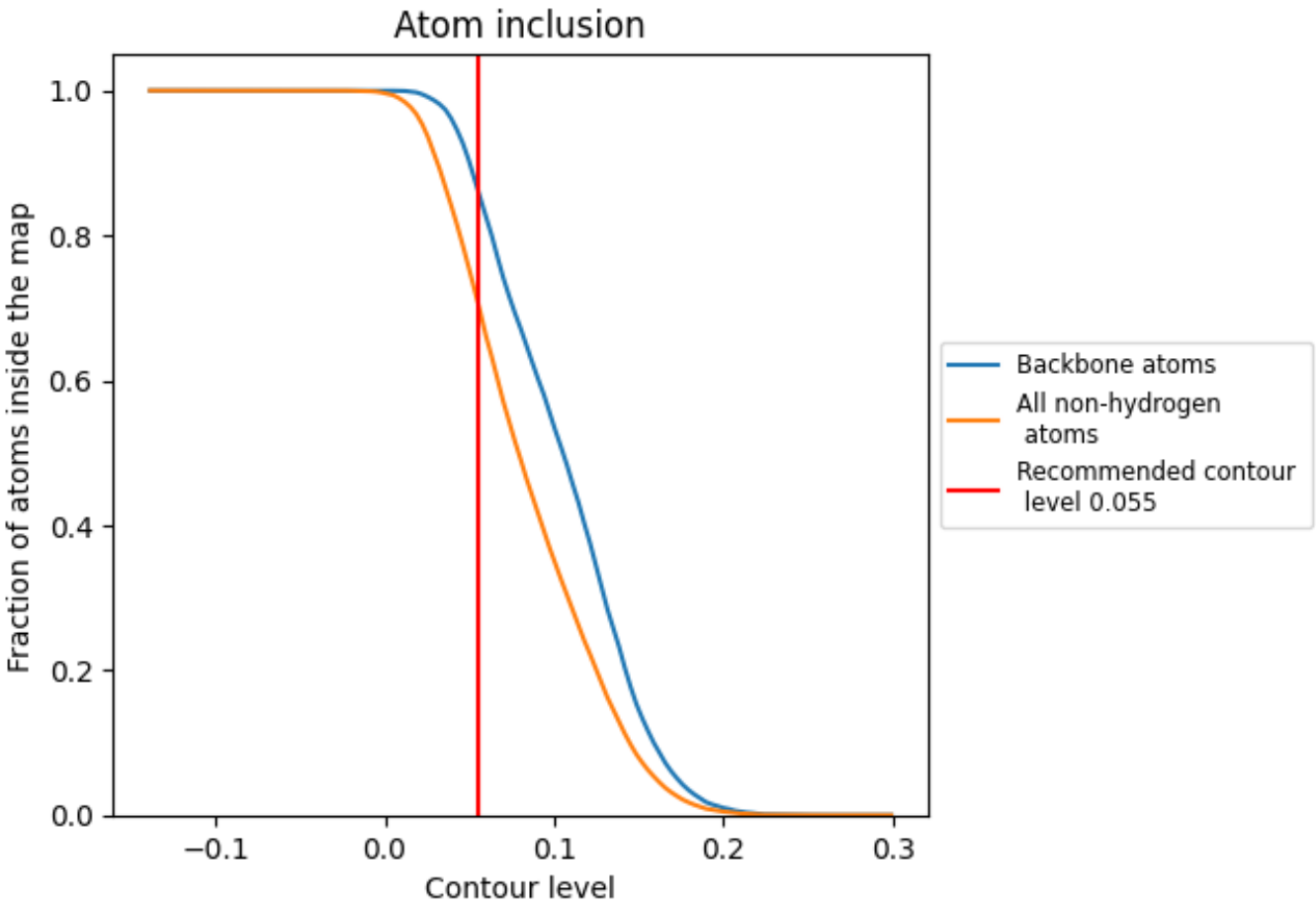
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.055).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7070	0.4500
0	0.4894	0.4000
1	0.2821	0.2840
2	0.2143	0.3660
3	0.1803	0.2190
4	0.2564	0.3880
5	0.1071	0.2770
6	0.2857	0.1090
7	0.2857	0.2640
8	0.2500	0.3110
9	0.1786	0.1990
A	0.7443	0.4630
AA	0.2400	0.2810
B	0.7442	0.4620
BA	0.2295	0.2980
C	0.7448	0.4630
CA	0.5000	0.4620
D	0.5139	0.3610
DA	0.2821	0.3110
E	0.5000	0.3390
F	0.3400	0.3400
G	0.2857	0.3100
H	0.3600	0.3390
I	0.0357	0.1950
J	0.2857	0.3410
K	0.4894	0.4060
L	0.2821	0.2780
M	0.1786	0.3610
N	0.1803	0.2230
O	0.2564	0.3910
P	0.1429	0.2880
Q	0.2500	0.1180
R	0.2857	0.2760
S	0.2500	0.3170
T	0.1786	0.2120

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Chain	Atom inclusion	Q-score
U	0.2800	0.2650
V	0.2459	0.2990
W	0.5000	0.4490
X	0.3077	0.3330
Y	0.5278	0.3640
Z	0.5000	0.3260
a	0.3400	0.3360
b	0.2500	0.3020
c	0.3400	0.3480
d	0.0357	0.1820
e	0.2857	0.2960
f	0.5106	0.4040
g	0.2821	0.2750
h	0.2143	0.3580
i	0.1639	0.2280
j	0.2564	0.3800
k	0.1071	0.2850
l	0.2143	0.1100
m	0.2500	0.2600
n	0.2500	0.3110
o	0.1786	0.1950
p	0.2800	0.2680
q	0.2295	0.3000
r	0.5000	0.4250
s	0.2821	0.3290
t	0.5556	0.3710
u	0.4643	0.3480
v	0.3400	0.3410
w	0.2500	0.3140
x	0.3800	0.3520
y	0.0357	0.1720
z	0.2857	0.3160