Full wwPDB EM Validation Report ⓘ

Nov 30, 2022 – 05:13 AM JST

PDB ID	:	7Y6S
EMDB ID	:	EMD-33646
Title	:	Cryo-EM map of IPEC-J2 cell-derived PEDV PT52 S protein with three D0-up
Authors	:	Hsu, S.T.D.; Draczkowski, P.; Wang, Y.S.
Deposited on	:	2022-06-21
Resolution	:	3.10 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:

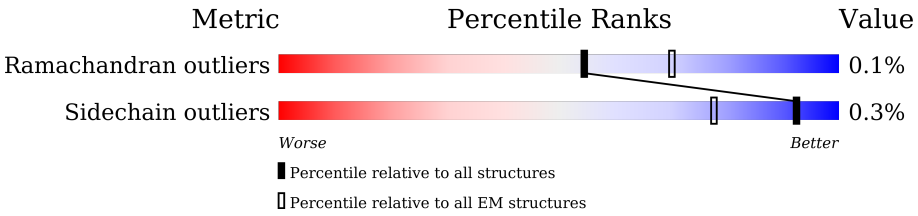
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.10 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	1384	72% 27%
1	B	1384	72% 27%
1	C	1384	72% 27%
2	D	4	100%
2	P	4	100%
2	b	4	100%
3	E	7	43% 57%
3	Q	7	29% 71%
3	c	7	43% 57%

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Mol	Chain	Length	Quality of chain
4	F	2	50% 50%
4	R	2	100%
4	d	2	100%
5	G	3	100%
5	I	3	67% 33%
5	K	3	67% 33%
5	M	3	67% 33%
5	S	3	67% 33%
5	U	3	67% 33%
5	W	3	67% 33%
5	Y	3	67% 33%
5	e	3	100%
5	g	3	67% 33%
5	i	3	100%
5	k	3	67% 33%
6	H	2	100%
6	J	2	50% 50%
6	L	2	100%
6	N	2	100%
6	T	2	100%
6	V	2	100%
6	X	2	100%
6	Z	2	100%
6	f	2	100%
6	h	2	50% 50%

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Mol	Chain	Length	Quality of chain
6	j	2	100%
6	l	2	100%
7	O	3	67% 33%
7	a	3	100%
7	m	3	67% 33%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 24852 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	1004	Total	C	N	O	S	0	0
			7766	4954	1284	1493	35		
1	B	1004	Total	C	N	O	S	0	0
			7766	4954	1284	1493	35		
1	C	1004	Total	C	N	O	S	0	0
			7766	4954	1284	1493	35		

There are 231 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1076	PRO	ILE	engineered mutation	UNP A0A1Y0DD46
A	1077	PRO	LEU	engineered mutation	UNP A0A1Y0DD46
A	1328	GLU	-	expression tag	UNP A0A1Y0DD46
A	1329	PHE	-	expression tag	UNP A0A1Y0DD46
A	1330	GLY	-	expression tag	UNP A0A1Y0DD46
A	1331	SER	-	expression tag	UNP A0A1Y0DD46
A	1332	GLY	-	expression tag	UNP A0A1Y0DD46
A	1333	GLY	-	expression tag	UNP A0A1Y0DD46
A	1334	TYR	-	expression tag	UNP A0A1Y0DD46
A	1335	ILE	-	expression tag	UNP A0A1Y0DD46
A	1336	PRO	-	expression tag	UNP A0A1Y0DD46
A	1337	GLU	-	expression tag	UNP A0A1Y0DD46
A	1338	ALA	-	expression tag	UNP A0A1Y0DD46
A	1339	PRO	-	expression tag	UNP A0A1Y0DD46
A	1340	ARG	-	expression tag	UNP A0A1Y0DD46
A	1341	ASP	-	expression tag	UNP A0A1Y0DD46
A	1342	GLY	-	expression tag	UNP A0A1Y0DD46
A	1343	GLN	-	expression tag	UNP A0A1Y0DD46
A	1344	ALA	-	expression tag	UNP A0A1Y0DD46
A	1345	TYR	-	expression tag	UNP A0A1Y0DD46
A	1346	VAL	-	expression tag	UNP A0A1Y0DD46
A	1347	ARG	-	expression tag	UNP A0A1Y0DD46
A	1348	LYS	-	expression tag	UNP A0A1Y0DD46
A	1349	ASP	-	expression tag	UNP A0A1Y0DD46

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1350	GLY	-	expression tag	UNP A0A1Y0DD46
A	1351	GLU	-	expression tag	UNP A0A1Y0DD46
A	1352	TRP	-	expression tag	UNP A0A1Y0DD46
A	1353	VAL	-	expression tag	UNP A0A1Y0DD46
A	1354	LEU	-	expression tag	UNP A0A1Y0DD46
A	1355	LEU	-	expression tag	UNP A0A1Y0DD46
A	1356	SER	-	expression tag	UNP A0A1Y0DD46
A	1357	THR	-	expression tag	UNP A0A1Y0DD46
A	1358	PHE	-	expression tag	UNP A0A1Y0DD46
A	1359	LEU	-	expression tag	UNP A0A1Y0DD46
A	1360	LYS	-	expression tag	UNP A0A1Y0DD46
A	1361	GLY	-	expression tag	UNP A0A1Y0DD46
A	1362	GLN	-	expression tag	UNP A0A1Y0DD46
A	1363	ASP	-	expression tag	UNP A0A1Y0DD46
A	1364	ASN	-	expression tag	UNP A0A1Y0DD46
A	1365	SER	-	expression tag	UNP A0A1Y0DD46
A	1366	ALA	-	expression tag	UNP A0A1Y0DD46
A	1367	ASP	-	expression tag	UNP A0A1Y0DD46
A	1368	ILE	-	expression tag	UNP A0A1Y0DD46
A	1369	GLN	-	expression tag	UNP A0A1Y0DD46
A	1370	HIS	-	expression tag	UNP A0A1Y0DD46
A	1371	SER	-	expression tag	UNP A0A1Y0DD46
A	1372	GLY	-	expression tag	UNP A0A1Y0DD46
A	1373	ARG	-	expression tag	UNP A0A1Y0DD46
A	1374	PRO	-	expression tag	UNP A0A1Y0DD46
A	1375	LEU	-	expression tag	UNP A0A1Y0DD46
A	1376	GLU	-	expression tag	UNP A0A1Y0DD46
A	1377	SER	-	expression tag	UNP A0A1Y0DD46
A	1378	ARG	-	expression tag	UNP A0A1Y0DD46
A	1379	GLY	-	expression tag	UNP A0A1Y0DD46
A	1380	PRO	-	expression tag	UNP A0A1Y0DD46
A	1381	PHE	-	expression tag	UNP A0A1Y0DD46
A	1382	GLU	-	expression tag	UNP A0A1Y0DD46
A	1383	GLN	-	expression tag	UNP A0A1Y0DD46
A	1384	LYS	-	expression tag	UNP A0A1Y0DD46
A	1385	LEU	-	expression tag	UNP A0A1Y0DD46
A	1386	ILE	-	expression tag	UNP A0A1Y0DD46
A	1387	SER	-	expression tag	UNP A0A1Y0DD46
A	1388	GLU	-	expression tag	UNP A0A1Y0DD46
A	1389	GLU	-	expression tag	UNP A0A1Y0DD46
A	1390	ASP	-	expression tag	UNP A0A1Y0DD46
A	1391	LEU	-	expression tag	UNP A0A1Y0DD46

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1392	ASN	-	expression tag	UNP A0A1Y0DD46
A	1393	MET	-	expression tag	UNP A0A1Y0DD46
A	1394	HIS	-	expression tag	UNP A0A1Y0DD46
A	1395	THR	-	expression tag	UNP A0A1Y0DD46
A	1396	GLY	-	expression tag	UNP A0A1Y0DD46
A	1397	HIS	-	expression tag	UNP A0A1Y0DD46
A	1398	HIS	-	expression tag	UNP A0A1Y0DD46
A	1399	HIS	-	expression tag	UNP A0A1Y0DD46
A	1400	HIS	-	expression tag	UNP A0A1Y0DD46
A	1401	HIS	-	expression tag	UNP A0A1Y0DD46
A	1402	HIS	-	expression tag	UNP A0A1Y0DD46
B	1076	PRO	ILE	engineered mutation	UNP A0A1Y0DD46
B	1077	PRO	LEU	engineered mutation	UNP A0A1Y0DD46
B	1328	GLU	-	expression tag	UNP A0A1Y0DD46
B	1329	PHE	-	expression tag	UNP A0A1Y0DD46
B	1330	GLY	-	expression tag	UNP A0A1Y0DD46
B	1331	SER	-	expression tag	UNP A0A1Y0DD46
B	1332	GLY	-	expression tag	UNP A0A1Y0DD46
B	1333	GLY	-	expression tag	UNP A0A1Y0DD46
B	1334	TYR	-	expression tag	UNP A0A1Y0DD46
B	1335	ILE	-	expression tag	UNP A0A1Y0DD46
B	1336	PRO	-	expression tag	UNP A0A1Y0DD46
B	1337	GLU	-	expression tag	UNP A0A1Y0DD46
B	1338	ALA	-	expression tag	UNP A0A1Y0DD46
B	1339	PRO	-	expression tag	UNP A0A1Y0DD46
B	1340	ARG	-	expression tag	UNP A0A1Y0DD46
B	1341	ASP	-	expression tag	UNP A0A1Y0DD46
B	1342	GLY	-	expression tag	UNP A0A1Y0DD46
B	1343	GLN	-	expression tag	UNP A0A1Y0DD46
B	1344	ALA	-	expression tag	UNP A0A1Y0DD46
B	1345	TYR	-	expression tag	UNP A0A1Y0DD46
B	1346	VAL	-	expression tag	UNP A0A1Y0DD46
B	1347	ARG	-	expression tag	UNP A0A1Y0DD46
B	1348	LYS	-	expression tag	UNP A0A1Y0DD46
B	1349	ASP	-	expression tag	UNP A0A1Y0DD46
B	1350	GLY	-	expression tag	UNP A0A1Y0DD46
B	1351	GLU	-	expression tag	UNP A0A1Y0DD46
B	1352	TRP	-	expression tag	UNP A0A1Y0DD46
B	1353	VAL	-	expression tag	UNP A0A1Y0DD46
B	1354	LEU	-	expression tag	UNP A0A1Y0DD46
B	1355	LEU	-	expression tag	UNP A0A1Y0DD46
B	1356	SER	-	expression tag	UNP A0A1Y0DD46

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1357	THR	-	expression tag	UNP A0A1Y0DD46
B	1358	PHE	-	expression tag	UNP A0A1Y0DD46
B	1359	LEU	-	expression tag	UNP A0A1Y0DD46
B	1360	LYS	-	expression tag	UNP A0A1Y0DD46
B	1361	GLY	-	expression tag	UNP A0A1Y0DD46
B	1362	GLN	-	expression tag	UNP A0A1Y0DD46
B	1363	ASP	-	expression tag	UNP A0A1Y0DD46
B	1364	ASN	-	expression tag	UNP A0A1Y0DD46
B	1365	SER	-	expression tag	UNP A0A1Y0DD46
B	1366	ALA	-	expression tag	UNP A0A1Y0DD46
B	1367	ASP	-	expression tag	UNP A0A1Y0DD46
B	1368	ILE	-	expression tag	UNP A0A1Y0DD46
B	1369	GLN	-	expression tag	UNP A0A1Y0DD46
B	1370	HIS	-	expression tag	UNP A0A1Y0DD46
B	1371	SER	-	expression tag	UNP A0A1Y0DD46
B	1372	GLY	-	expression tag	UNP A0A1Y0DD46
B	1373	ARG	-	expression tag	UNP A0A1Y0DD46
B	1374	PRO	-	expression tag	UNP A0A1Y0DD46
B	1375	LEU	-	expression tag	UNP A0A1Y0DD46
B	1376	GLU	-	expression tag	UNP A0A1Y0DD46
B	1377	SER	-	expression tag	UNP A0A1Y0DD46
B	1378	ARG	-	expression tag	UNP A0A1Y0DD46
B	1379	GLY	-	expression tag	UNP A0A1Y0DD46
B	1380	PRO	-	expression tag	UNP A0A1Y0DD46
B	1381	PHE	-	expression tag	UNP A0A1Y0DD46
B	1382	GLU	-	expression tag	UNP A0A1Y0DD46
B	1383	GLN	-	expression tag	UNP A0A1Y0DD46
B	1384	LYS	-	expression tag	UNP A0A1Y0DD46
B	1385	LEU	-	expression tag	UNP A0A1Y0DD46
B	1386	ILE	-	expression tag	UNP A0A1Y0DD46
B	1387	SER	-	expression tag	UNP A0A1Y0DD46
B	1388	GLU	-	expression tag	UNP A0A1Y0DD46
B	1389	GLU	-	expression tag	UNP A0A1Y0DD46
B	1390	ASP	-	expression tag	UNP A0A1Y0DD46
B	1391	LEU	-	expression tag	UNP A0A1Y0DD46
B	1392	ASN	-	expression tag	UNP A0A1Y0DD46
B	1393	MET	-	expression tag	UNP A0A1Y0DD46
B	1394	HIS	-	expression tag	UNP A0A1Y0DD46
B	1395	THR	-	expression tag	UNP A0A1Y0DD46
B	1396	GLY	-	expression tag	UNP A0A1Y0DD46
B	1397	HIS	-	expression tag	UNP A0A1Y0DD46
B	1398	HIS	-	expression tag	UNP A0A1Y0DD46

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1399	HIS	-	expression tag	UNP A0A1Y0DD46
B	1400	HIS	-	expression tag	UNP A0A1Y0DD46
B	1401	HIS	-	expression tag	UNP A0A1Y0DD46
B	1402	HIS	-	expression tag	UNP A0A1Y0DD46
C	1076	PRO	ILE	engineered mutation	UNP A0A1Y0DD46
C	1077	PRO	LEU	engineered mutation	UNP A0A1Y0DD46
C	1328	GLU	-	expression tag	UNP A0A1Y0DD46
C	1329	PHE	-	expression tag	UNP A0A1Y0DD46
C	1330	GLY	-	expression tag	UNP A0A1Y0DD46
C	1331	SER	-	expression tag	UNP A0A1Y0DD46
C	1332	GLY	-	expression tag	UNP A0A1Y0DD46
C	1333	GLY	-	expression tag	UNP A0A1Y0DD46
C	1334	TYR	-	expression tag	UNP A0A1Y0DD46
C	1335	ILE	-	expression tag	UNP A0A1Y0DD46
C	1336	PRO	-	expression tag	UNP A0A1Y0DD46
C	1337	GLU	-	expression tag	UNP A0A1Y0DD46
C	1338	ALA	-	expression tag	UNP A0A1Y0DD46
C	1339	PRO	-	expression tag	UNP A0A1Y0DD46
C	1340	ARG	-	expression tag	UNP A0A1Y0DD46
C	1341	ASP	-	expression tag	UNP A0A1Y0DD46
C	1342	GLY	-	expression tag	UNP A0A1Y0DD46
C	1343	GLN	-	expression tag	UNP A0A1Y0DD46
C	1344	ALA	-	expression tag	UNP A0A1Y0DD46
C	1345	TYR	-	expression tag	UNP A0A1Y0DD46
C	1346	VAL	-	expression tag	UNP A0A1Y0DD46
C	1347	ARG	-	expression tag	UNP A0A1Y0DD46
C	1348	LYS	-	expression tag	UNP A0A1Y0DD46
C	1349	ASP	-	expression tag	UNP A0A1Y0DD46
C	1350	GLY	-	expression tag	UNP A0A1Y0DD46
C	1351	GLU	-	expression tag	UNP A0A1Y0DD46
C	1352	TRP	-	expression tag	UNP A0A1Y0DD46
C	1353	VAL	-	expression tag	UNP A0A1Y0DD46
C	1354	LEU	-	expression tag	UNP A0A1Y0DD46
C	1355	LEU	-	expression tag	UNP A0A1Y0DD46
C	1356	SER	-	expression tag	UNP A0A1Y0DD46
C	1357	THR	-	expression tag	UNP A0A1Y0DD46
C	1358	PHE	-	expression tag	UNP A0A1Y0DD46
C	1359	LEU	-	expression tag	UNP A0A1Y0DD46
C	1360	LYS	-	expression tag	UNP A0A1Y0DD46
C	1361	GLY	-	expression tag	UNP A0A1Y0DD46
C	1362	GLN	-	expression tag	UNP A0A1Y0DD46
C	1363	ASP	-	expression tag	UNP A0A1Y0DD46

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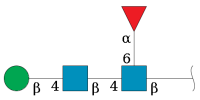
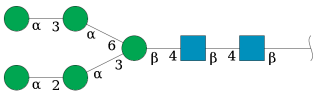
Chain	Residue	Modelled	Actual	Comment	Reference
C	1364	ASN	-	expression tag	UNP A0A1Y0DD46
C	1365	SER	-	expression tag	UNP A0A1Y0DD46
C	1366	ALA	-	expression tag	UNP A0A1Y0DD46
C	1367	ASP	-	expression tag	UNP A0A1Y0DD46
C	1368	ILE	-	expression tag	UNP A0A1Y0DD46
C	1369	GLN	-	expression tag	UNP A0A1Y0DD46
C	1370	HIS	-	expression tag	UNP A0A1Y0DD46
C	1371	SER	-	expression tag	UNP A0A1Y0DD46
C	1372	GLY	-	expression tag	UNP A0A1Y0DD46
C	1373	ARG	-	expression tag	UNP A0A1Y0DD46
C	1374	PRO	-	expression tag	UNP A0A1Y0DD46
C	1375	LEU	-	expression tag	UNP A0A1Y0DD46
C	1376	GLU	-	expression tag	UNP A0A1Y0DD46
C	1377	SER	-	expression tag	UNP A0A1Y0DD46
C	1378	ARG	-	expression tag	UNP A0A1Y0DD46
C	1379	GLY	-	expression tag	UNP A0A1Y0DD46
C	1380	PRO	-	expression tag	UNP A0A1Y0DD46
C	1381	PHE	-	expression tag	UNP A0A1Y0DD46
C	1382	GLU	-	expression tag	UNP A0A1Y0DD46
C	1383	GLN	-	expression tag	UNP A0A1Y0DD46
C	1384	LYS	-	expression tag	UNP A0A1Y0DD46
C	1385	LEU	-	expression tag	UNP A0A1Y0DD46
C	1386	ILE	-	expression tag	UNP A0A1Y0DD46
C	1387	SER	-	expression tag	UNP A0A1Y0DD46
C	1388	GLU	-	expression tag	UNP A0A1Y0DD46
C	1389	GLU	-	expression tag	UNP A0A1Y0DD46
C	1390	ASP	-	expression tag	UNP A0A1Y0DD46
C	1391	LEU	-	expression tag	UNP A0A1Y0DD46
C	1392	ASN	-	expression tag	UNP A0A1Y0DD46
C	1393	MET	-	expression tag	UNP A0A1Y0DD46
C	1394	HIS	-	expression tag	UNP A0A1Y0DD46
C	1395	THR	-	expression tag	UNP A0A1Y0DD46
C	1396	GLY	-	expression tag	UNP A0A1Y0DD46
C	1397	HIS	-	expression tag	UNP A0A1Y0DD46
C	1398	HIS	-	expression tag	UNP A0A1Y0DD46
C	1399	HIS	-	expression tag	UNP A0A1Y0DD46
C	1400	HIS	-	expression tag	UNP A0A1Y0DD46
C	1401	HIS	-	expression tag	UNP A0A1Y0DD46
C	1402	HIS	-	expression tag	UNP A0A1Y0DD46

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	4	Total	C	N	O	0	0
			49	28	2	19		
2	P	4	Total	C	N	O	0	0
			49	28	2	19		
2	b	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 3 is an oligosaccharide called 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.

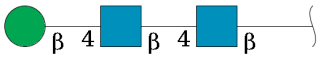


Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	7	Total	C	N	O	0	0
			83	46	2	35		
3	Q	7	Total	C	N	O	0	0
			83	46	2	35		
3	c	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			24	14	1	9		
4	R	2	Total	C	N	O	0	0
			24	14	1	9		
4	d	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 5 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
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	I	3	Total	C	N	O	0	0
			39	22	2	15		
5	K	3	Total	C	N	O	0	0
			39	22	2	15		
5	M	3	Total	C	N	O	0	0
			39	22	2	15		
5	S	3	Total	C	N	O	0	0
			39	22	2	15		
5	U	3	Total	C	N	O	0	0
			39	22	2	15		
5	W	3	Total	C	N	O	0	0
			39	22	2	15		
5	Y	3	Total	C	N	O	0	0
			39	22	2	15		
5	e	3	Total	C	N	O	0	0
			39	22	2	15		
5	g	3	Total	C	N	O	0	0
			39	22	2	15		
5	i	3	Total	C	N	O	0	0
			39	22	2	15		
5	k	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 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
6	H	2	Total	C	N	O	0	0
			28	16	2	10		

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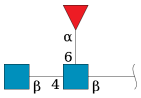
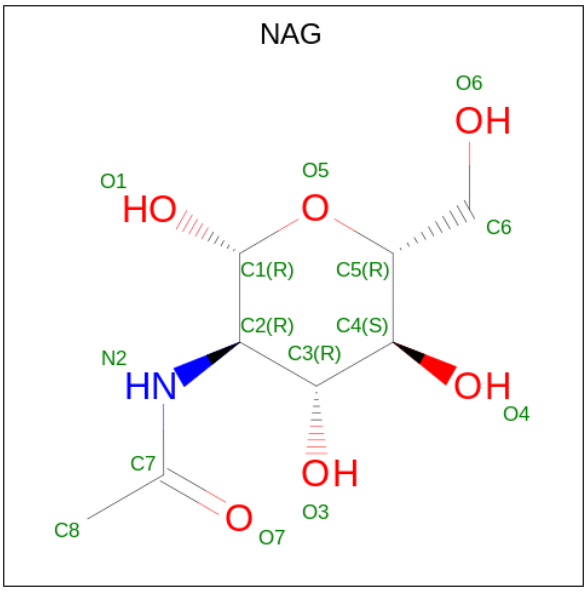
Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	2	Total	C	N	O	0	0
			28	16	2	10		
6	L	2	Total	C	N	O	0	0
			28	16	2	10		
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		
6	V	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		
6	Z	2	Total	C	N	O	0	0
			28	16	2	10		
6	f	2	Total	C	N	O	0	0
			28	16	2	10		
6	h	2	Total	C	N	O	0	0
			28	16	2	10		
6	j	2	Total	C	N	O	0	0
			28	16	2	10		
6	l	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	3	Total	C	N	O	0	0
			38	22	2	14		
7	a	3	Total	C	N	O	0	0
			38	22	2	14		
7	m	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



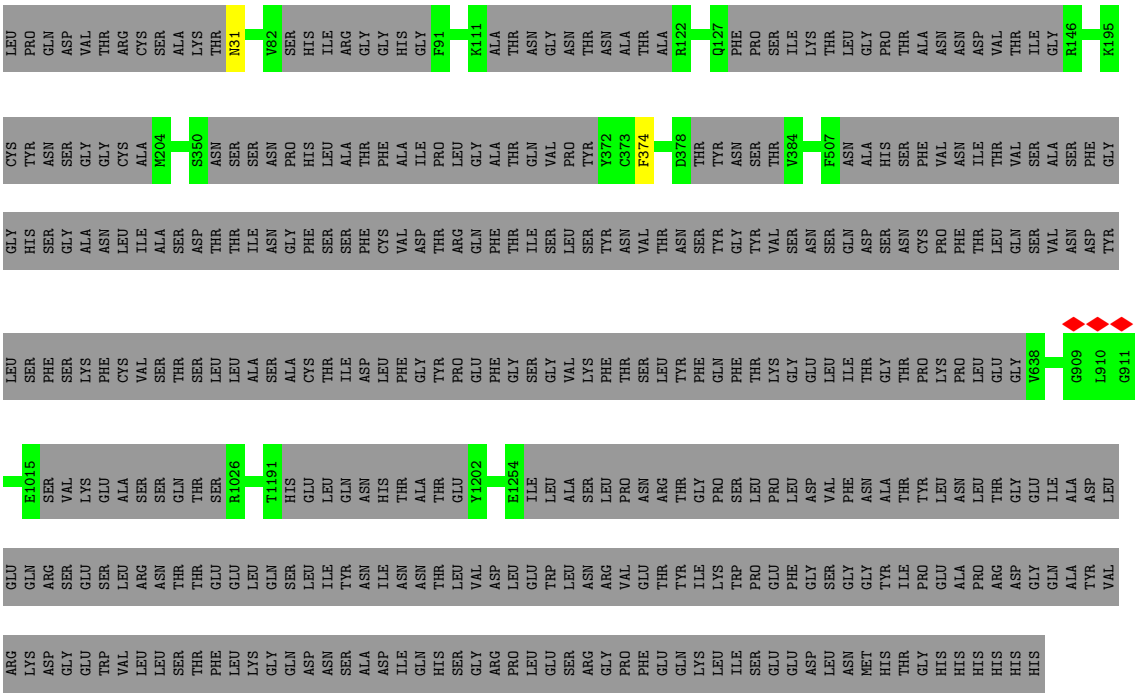
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			56	32	4	20	
8	A	1	Total	C	N	O	0
			56	32	4	20	
8	A	1	Total	C	N	O	0
			56	32	4	20	
8	A	1	Total	C	N	O	0
			56	32	4	20	
8	B	1	Total	C	N	O	0
			56	32	4	20	
8	B	1	Total	C	N	O	0
			56	32	4	20	
8	B	1	Total	C	N	O	0
			56	32	4	20	
8	B	1	Total	C	N	O	0
			56	32	4	20	
8	C	1	Total	C	N	O	0
			56	32	4	20	
8	C	1	Total	C	N	O	0
			56	32	4	20	
8	C	1	Total	C	N	O	0
			56	32	4	20	
8	C	1	Total	C	N	O	0
			56	32	4	20	

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.

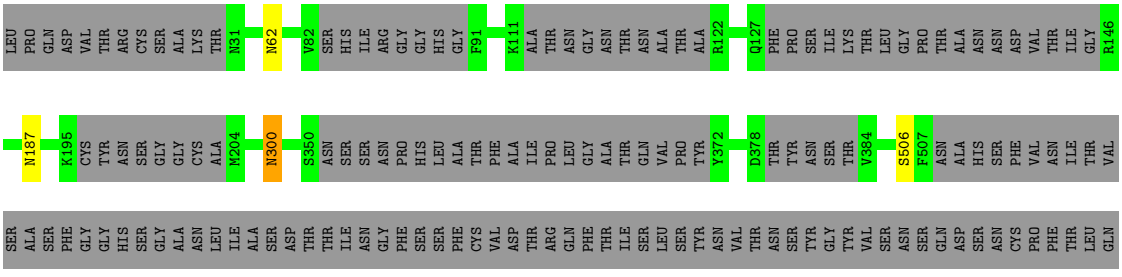
• Molecule 1: Spike glycoprotein

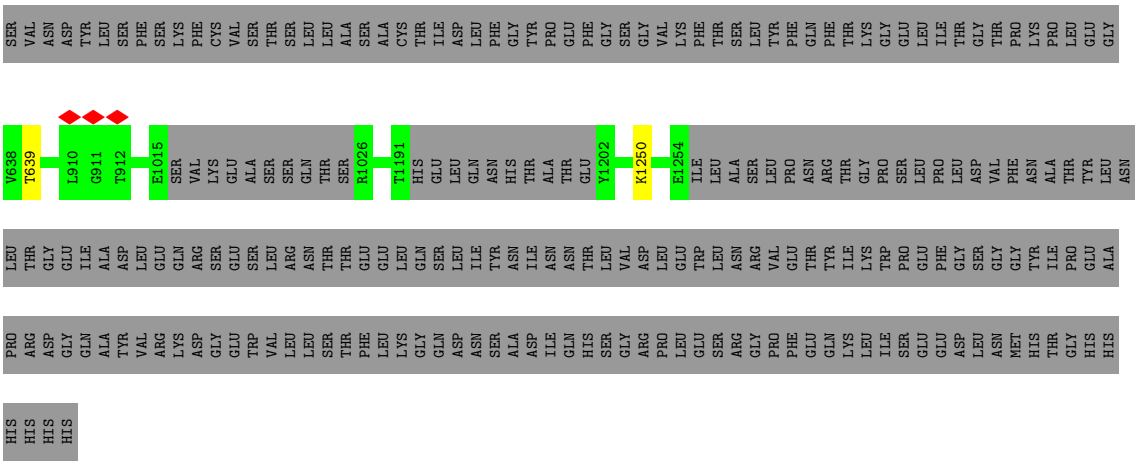
Chain A:



• Molecule 1: Spike glycoprotein

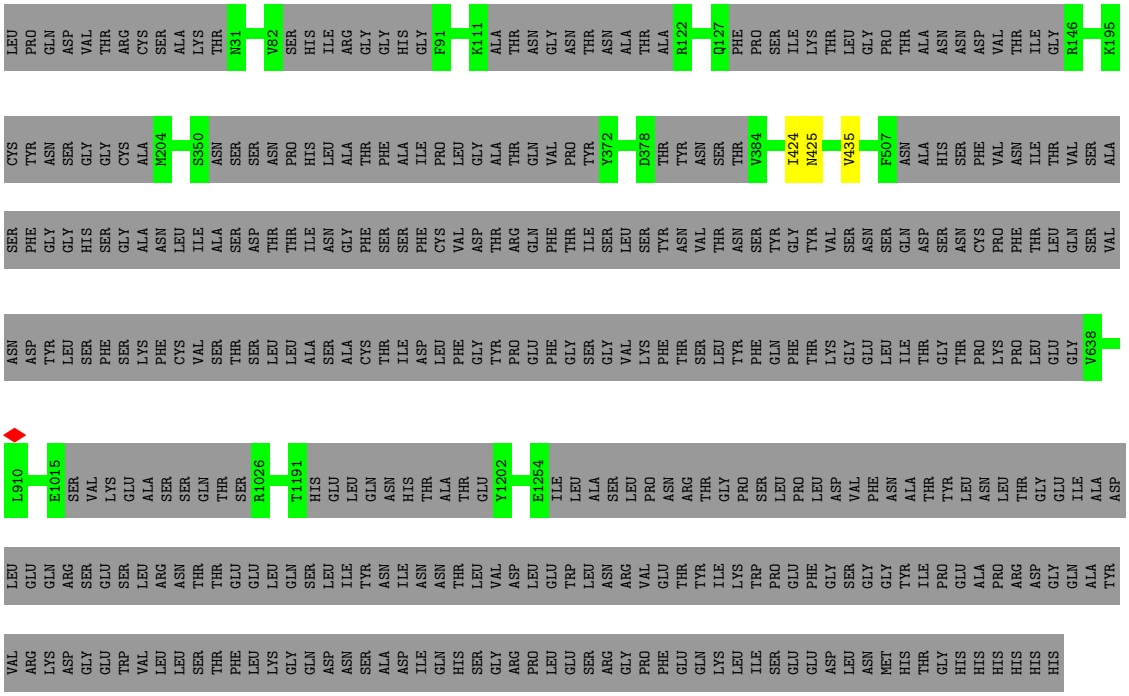
Chain B:





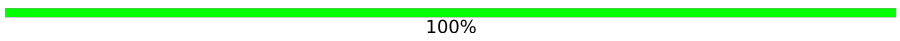
• Molecule 1: Spike glycoprotein

Chain C:



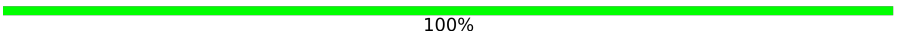
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



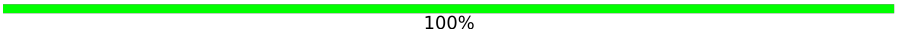
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



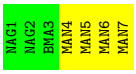
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



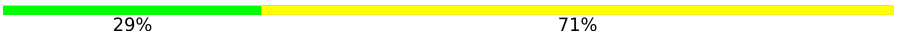
• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

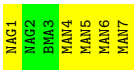
Chain E:



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

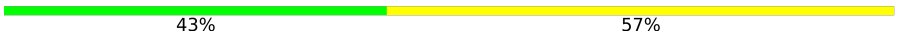
Chain Q:

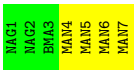




• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



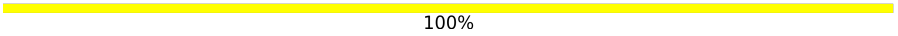


• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

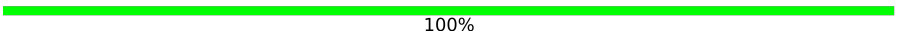
Chain F:

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

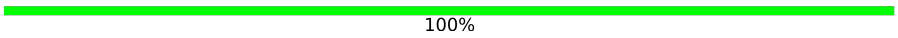
Chain R:



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

Chain d: 

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

Chain G: 

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

Chain I:

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

Chain K:

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

Chain M:

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

Chain S:

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

Chain U:

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

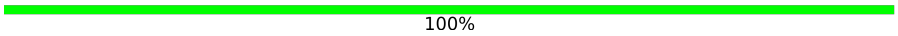
Chain W:

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

Chain Y:

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

Chain e:



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

Chain g:

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

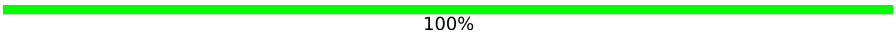
Chain i:

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

Chain H:

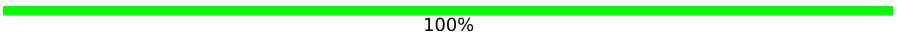


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

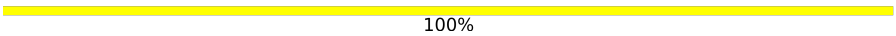
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



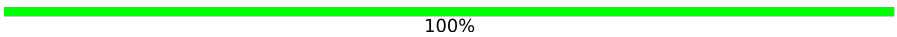
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



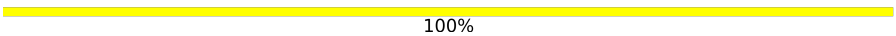
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



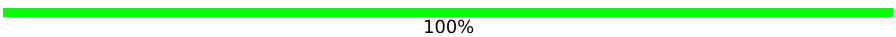
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



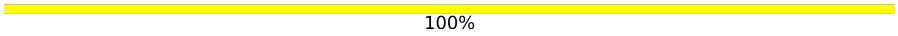
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



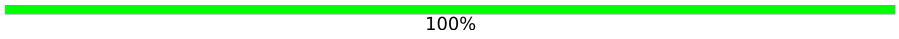
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



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

Chain f:

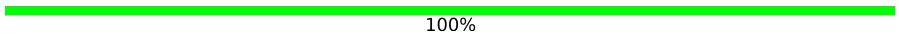


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

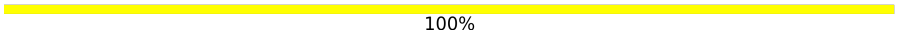
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



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

Chain l:

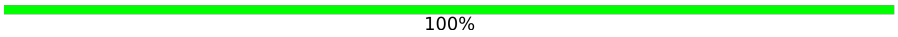


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	298195	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 ($e^-/Å^2$)	55.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.128	Depositor
Minimum map value	-0.325	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	385.83997, 385.83997, 385.83997	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/7929	0.50	0/10788
1	B	0.27	0/7929	0.49	0/10788
1	C	0.27	0/7929	0.50	0/10788
All	All	0.27	0/23787	0.50	0/32364

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	984/1384 (71%)	940 (96%)	44 (4%)	0	100	100
1	B	984/1384 (71%)	940 (96%)	42 (4%)	2 (0%)	47	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	984/1384 (71%)	940 (96%)	42 (4%)	2 (0%)	47 79
All	All	2952/4152 (71%)	2820 (96%)	128 (4%)	4 (0%)	54 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	425	ASN
1	B	300	ASN
1	B	62	ASN
1	C	435	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	865/1191 (73%)	863 (100%)	2 (0%)	93 97
1	B	865/1191 (73%)	860 (99%)	5 (1%)	86 94
1	C	865/1191 (73%)	864 (100%)	1 (0%)	93 98
All	All	2595/3573 (73%)	2587 (100%)	8 (0%)	92 96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	374	PHE
1	B	187	ASN
1	B	300	ASN
1	B	506	SER
1	B	639	THR
1	B	1250	LYS
1	C	424	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1051	GLN
1	A	1126	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

108 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	2,1	14,14,15	0.20	0	17,19,21	0.55	0
2	NAG	D	2	2	14,14,15	0.23	0	17,19,21	0.59	0
2	BMA	D	3	2	11,11,12	0.62	0	15,15,17	0.74	0
2	FUC	D	4	2	10,10,11	0.72	0	14,14,16	0.84	0
3	NAG	E	1	3,1	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.19	0	17,19,21	0.45	0
3	BMA	E	3	3	11,11,12	0.51	0	15,15,17	0.91	0
3	MAN	E	4	3	11,11,12	0.79	0	15,15,17	1.15	2 (13%)
3	MAN	E	5	3	11,11,12	0.72	0	15,15,17	1.12	2 (13%)
3	MAN	E	6	3	11,11,12	0.89	0	15,15,17	0.96	1 (6%)
3	MAN	E	7	3	11,11,12	0.84	1 (9%)	15,15,17	1.10	2 (13%)
4	NAG	F	1	4,1	14,14,15	0.25	0	17,19,21	0.32	0
4	FUC	F	2	4	10,10,11	0.69	0	14,14,16	0.97	1 (7%)
5	NAG	G	1	5,1	14,14,15	0.55	0	17,19,21	0.39	0
5	NAG	G	2	5	14,14,15	0.24	0	17,19,21	0.60	0
5	BMA	G	3	5	11,11,12	0.68	0	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	H	1	6,1	14,14,15	0.33	0	17,19,21	0.45	0
6	NAG	H	2	6	14,14,15	0.28	0	17,19,21	0.48	0
5	NAG	I	1	5,1	14,14,15	0.71	0	17,19,21	1.18	1 (5%)
5	NAG	I	2	5	14,14,15	0.34	0	17,19,21	0.40	0
5	BMA	I	3	5	11,11,12	0.59	0	15,15,17	0.74	0
6	NAG	J	1	6,1	14,14,15	0.58	0	17,19,21	1.48	3 (17%)
6	NAG	J	2	6	14,14,15	0.26	0	17,19,21	0.53	0
5	NAG	K	1	5,1	14,14,15	0.48	0	17,19,21	1.28	2 (11%)
5	NAG	K	2	5	14,14,15	0.19	0	17,19,21	0.49	0
5	BMA	K	3	5	11,11,12	0.66	0	15,15,17	0.77	0
6	NAG	L	1	6,1	14,14,15	0.26	0	17,19,21	0.62	0
6	NAG	L	2	6	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	M	1	5,1	14,14,15	0.52	0	17,19,21	0.52	0
5	NAG	M	2	5	14,14,15	0.25	0	17,19,21	0.47	0
5	BMA	M	3	5	11,11,12	0.95	0	15,15,17	0.99	1 (6%)
6	NAG	N	1	6,1	14,14,15	0.48	0	17,19,21	1.24	1 (5%)
6	NAG	N	2	6	14,14,15	0.39	0	17,19,21	1.24	1 (5%)
7	NAG	O	1	7,1	14,14,15	0.47	0	17,19,21	0.76	0
7	NAG	O	2	7	14,14,15	0.20	0	17,19,21	0.47	0
7	FUC	O	3	7	10,10,11	0.68	0	14,14,16	0.94	1 (7%)
2	NAG	P	1	2,1	14,14,15	0.17	0	17,19,21	0.63	0
2	NAG	P	2	2	14,14,15	0.32	0	17,19,21	0.47	0
2	BMA	P	3	2	11,11,12	0.59	0	15,15,17	0.72	0
2	FUC	P	4	2	10,10,11	0.76	0	14,14,16	0.76	0
3	NAG	Q	1	3,1	14,14,15	0.38	0	17,19,21	0.70	1 (5%)
3	NAG	Q	2	3	14,14,15	0.16	0	17,19,21	0.41	0
3	BMA	Q	3	3	11,11,12	0.64	0	15,15,17	0.79	0
3	MAN	Q	4	3	11,11,12	0.66	0	15,15,17	0.93	2 (13%)
3	MAN	Q	5	3	11,11,12	0.93	1 (9%)	15,15,17	1.59	4 (26%)
3	MAN	Q	6	3	11,11,12	0.76	0	15,15,17	0.89	1 (6%)
3	MAN	Q	7	3	11,11,12	0.77	0	15,15,17	1.06	2 (13%)
4	NAG	R	1	4,1	14,14,15	0.55	0	17,19,21	1.13	1 (5%)
4	FUC	R	2	4	10,10,11	0.92	1 (10%)	14,14,16	1.12	2 (14%)
5	NAG	S	1	5,1	14,14,15	0.60	1 (7%)	17,19,21	0.40	0
5	NAG	S	2	5	14,14,15	0.23	0	17,19,21	0.54	0
5	BMA	S	3	5	11,11,12	0.67	0	15,15,17	0.73	0
6	NAG	T	1	6,1	14,14,15	0.27	0	17,19,21	0.40	0
6	NAG	T	2	6	14,14,15	0.25	0	17,19,21	0.51	0
5	NAG	U	1	5,1	14,14,15	0.84	1 (7%)	17,19,21	1.33	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	U	2	5	14,14,15	0.54	0	17,19,21	0.54	0
5	BMA	U	3	5	11,11,12	0.63	0	15,15,17	0.83	0
6	NAG	V	1	6,1	14,14,15	1.00	1 (7%)	17,19,21	1.52	2 (11%)
6	NAG	V	2	6	14,14,15	0.41	0	17,19,21	1.26	1 (5%)
5	NAG	W	1	5,1	14,14,15	0.47	0	17,19,21	1.33	2 (11%)
5	NAG	W	2	5	14,14,15	0.17	0	17,19,21	0.55	0
5	BMA	W	3	5	11,11,12	0.64	0	15,15,17	0.69	0
6	NAG	X	1	6,1	14,14,15	0.44	0	17,19,21	0.60	0
6	NAG	X	2	6	14,14,15	0.26	0	17,19,21	0.42	0
5	NAG	Y	1	5,1	14,14,15	0.75	1 (7%)	17,19,21	0.59	0
5	NAG	Y	2	5	14,14,15	0.19	0	17,19,21	0.54	0
5	BMA	Y	3	5	11,11,12	0.89	0	15,15,17	0.93	0
6	NAG	Z	1	6,1	14,14,15	0.50	0	17,19,21	1.25	1 (5%)
6	NAG	Z	2	6	14,14,15	0.39	0	17,19,21	1.24	1 (5%)
7	NAG	a	1	7,1	14,14,15	0.27	0	17,19,21	0.50	0
7	NAG	a	2	7	14,14,15	0.20	0	17,19,21	0.45	0
7	FUC	a	3	7	10,10,11	0.63	0	14,14,16	0.80	0
2	NAG	b	1	2,1	14,14,15	0.27	0	17,19,21	0.66	0
2	NAG	b	2	2	14,14,15	0.26	0	17,19,21	0.54	0
2	BMA	b	3	2	11,11,12	0.56	0	15,15,17	0.76	0
2	FUC	b	4	2	10,10,11	0.66	0	14,14,16	0.82	0
3	NAG	c	1	3,1	14,14,15	0.31	0	17,19,21	0.47	0
3	NAG	c	2	3	14,14,15	0.23	0	17,19,21	0.41	0
3	BMA	c	3	3	11,11,12	0.52	0	15,15,17	0.85	0
3	MAN	c	4	3	11,11,12	0.65	0	15,15,17	0.95	1 (6%)
3	MAN	c	5	3	11,11,12	0.76	0	15,15,17	1.08	2 (13%)
3	MAN	c	6	3	11,11,12	0.85	0	15,15,17	0.88	1 (6%)
3	MAN	c	7	3	11,11,12	0.83	1 (9%)	15,15,17	1.05	2 (13%)
4	NAG	d	1	4,1	14,14,15	0.25	0	17,19,21	0.45	0
4	FUC	d	2	4	10,10,11	0.71	0	14,14,16	0.94	0
5	NAG	e	1	5,1	14,14,15	0.48	0	17,19,21	0.47	0
5	NAG	e	2	5	14,14,15	0.27	0	17,19,21	0.58	0
5	BMA	e	3	5	11,11,12	0.69	0	15,15,17	0.75	0
6	NAG	f	1	6,1	14,14,15	0.29	0	17,19,21	0.45	0
6	NAG	f	2	6	14,14,15	0.31	0	17,19,21	0.49	0
5	NAG	g	1	5,1	14,14,15	0.41	0	17,19,21	0.74	1 (5%)
5	NAG	g	2	5	14,14,15	0.33	0	17,19,21	0.47	0
5	BMA	g	3	5	11,11,12	0.50	0	15,15,17	0.77	0
6	NAG	h	1	6,1	14,14,15	0.60	0	17,19,21	1.32	1 (5%)
6	NAG	h	2	6	14,14,15	0.33	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	i	1	5,1	14,14,15	0.28	0	17,19,21	0.41	0
5	NAG	i	2	5	14,14,15	0.20	0	17,19,21	0.45	0
5	BMA	i	3	5	11,11,12	0.60	0	15,15,17	0.75	0
6	NAG	j	1	6,1	14,14,15	0.20	0	17,19,21	0.53	0
6	NAG	j	2	6	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	k	1	5,1	14,14,15	0.79	1 (7%)	17,19,21	0.82	0
5	NAG	k	2	5	14,14,15	0.25	0	17,19,21	0.56	0
5	BMA	k	3	5	11,11,12	0.97	0	15,15,17	0.90	0
6	NAG	l	1	6,1	14,14,15	0.37	0	17,19,21	1.29	1 (5%)
6	NAG	l	2	6	14,14,15	0.40	0	17,19,21	1.23	1 (5%)
7	NAG	m	1	7,1	14,14,15	0.46	0	17,19,21	0.69	0
7	NAG	m	2	7	14,14,15	0.24	0	17,19,21	0.38	0
7	FUC	m	3	7	10,10,11	0.62	0	14,14,16	0.91	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	FUC	D	4	2	-	-	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	MAN	E	5	3	-	1/2/19/22	1/1/1/1
3	MAN	E	6	3	-	2/2/19/22	0/1/1/1
3	MAN	E	7	3	-	0/2/19/22	1/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	FUC	F	2	4	-	-	0/1/1/1
5	NAG	G	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	4/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
6	NAG	H	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	4/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	J	2	6	-	3/6/23/26	0/1/1/1
5	NAG	K	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	2/2/19/22	0/1/1/1
6	NAG	L	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	L	2	6	-	1/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	1/2/19/22	0/1/1/1
6	NAG	N	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	N	2	6	-	4/6/23/26	0/1/1/1
7	NAG	O	1	7,1	-	3/6/23/26	0/1/1/1
7	NAG	O	2	7	-	4/6/23/26	0/1/1/1
7	FUC	O	3	7	-	-	0/1/1/1
2	NAG	P	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	P	2	2	-	3/6/23/26	0/1/1/1
2	BMA	P	3	2	-	0/2/19/22	0/1/1/1
2	FUC	P	4	2	-	-	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
3	MAN	Q	4	3	-	2/2/19/22	0/1/1/1
3	MAN	Q	5	3	-	1/2/19/22	0/1/1/1
3	MAN	Q	6	3	-	1/2/19/22	0/1/1/1
3	MAN	Q	7	3	-	2/2/19/22	1/1/1/1
4	NAG	R	1	4,1	-	1/6/23/26	0/1/1/1
4	FUC	R	2	4	-	-	0/1/1/1
5	NAG	S	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
5	BMA	S	3	5	-	1/2/19/22	0/1/1/1
6	NAG	T	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
5	NAG	U	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	U	3	5	-	2/2/19/22	0/1/1/1
6	NAG	V	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	V	2	6	-	5/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	W	2	5	-	4/6/23/26	0/1/1/1
5	BMA	W	3	5	-	0/2/19/22	0/1/1/1
6	NAG	X	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	X	2	6	-	1/6/23/26	0/1/1/1
5	NAG	Y	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	4/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	0/2/19/22	0/1/1/1
6	NAG	Z	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	5/6/23/26	0/1/1/1
7	NAG	a	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	a	2	7	-	3/6/23/26	0/1/1/1
7	FUC	a	3	7	-	-	0/1/1/1
2	NAG	b	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	b	2	2	-	3/6/23/26	0/1/1/1
2	BMA	b	3	2	-	2/2/19/22	0/1/1/1
2	FUC	b	4	2	-	-	0/1/1/1
3	NAG	c	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	c	2	3	-	0/6/23/26	0/1/1/1
3	BMA	c	3	3	-	2/2/19/22	0/1/1/1
3	MAN	c	4	3	-	0/2/19/22	0/1/1/1
3	MAN	c	5	3	-	1/2/19/22	1/1/1/1
3	MAN	c	6	3	-	1/2/19/22	0/1/1/1
3	MAN	c	7	3	-	2/2/19/22	1/1/1/1
4	NAG	d	1	4,1	-	0/6/23/26	0/1/1/1
4	FUC	d	2	4	-	-	0/1/1/1
5	NAG	e	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	2/6/23/26	0/1/1/1
5	BMA	e	3	5	-	1/2/19/22	0/1/1/1
6	NAG	f	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	f	2	6	-	3/6/23/26	0/1/1/1
5	NAG	g	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	g	2	5	-	2/6/23/26	0/1/1/1
5	BMA	g	3	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	h	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	h	2	6	-	2/6/23/26	0/1/1/1
5	NAG	i	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	i	2	5	-	4/6/23/26	0/1/1/1
5	BMA	i	3	5	-	0/2/19/22	0/1/1/1
6	NAG	j	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	j	2	6	-	2/6/23/26	0/1/1/1
5	NAG	k	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	k	2	5	-	0/6/23/26	0/1/1/1
5	BMA	k	3	5	-	1/2/19/22	0/1/1/1
6	NAG	l	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	l	2	6	-	4/6/23/26	0/1/1/1
7	NAG	m	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	m	2	7	-	4/6/23/26	0/1/1/1
7	FUC	m	3	7	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	1	NAG	O5-C1	-3.55	1.38	1.43
5	U	1	NAG	O5-C1	2.92	1.48	1.43
5	k	1	NAG	O5-C1	-2.83	1.39	1.43
5	Y	1	NAG	O5-C1	-2.70	1.39	1.43
3	Q	5	MAN	C1-C2	2.46	1.57	1.52
5	S	1	NAG	O5-C1	-2.05	1.40	1.43
3	E	7	MAN	C1-C2	2.03	1.56	1.52
4	R	2	FUC	C1-C2	2.03	1.56	1.52
3	c	7	MAN	C1-C2	2.01	1.56	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	U	1	NAG	C1-O5-C5	5.26	119.31	112.19
6	J	1	NAG	C2-N2-C7	4.66	129.53	122.90
6	V	1	NAG	C2-N2-C7	4.52	129.34	122.90
4	R	1	NAG	C1-O5-C5	4.42	118.18	112.19
6	V	2	NAG	C2-N2-C7	4.40	129.16	122.90
5	I	1	NAG	C1-O5-C5	4.38	118.12	112.19
6	h	1	NAG	C2-N2-C7	4.36	129.12	122.90
3	Q	5	MAN	C1-O5-C5	4.32	118.04	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	l	2	NAG	C2-N2-C7	4.32	129.05	122.90
6	Z	2	NAG	C2-N2-C7	4.31	129.04	122.90
5	K	1	NAG	C2-N2-C7	4.30	129.02	122.90
6	l	1	NAG	C2-N2-C7	4.29	129.01	122.90
6	N	2	NAG	C2-N2-C7	4.29	129.01	122.90
6	Z	1	NAG	C2-N2-C7	4.28	129.00	122.90
5	W	1	NAG	C2-N2-C7	4.28	129.00	122.90
6	N	1	NAG	C2-N2-C7	4.23	128.93	122.90
3	E	5	MAN	C1-O5-C5	3.20	116.53	112.19
3	E	7	MAN	C1-O5-C5	3.07	116.35	112.19
3	c	5	MAN	C1-O5-C5	3.07	116.35	112.19
3	Q	7	MAN	C1-O5-C5	2.87	116.09	112.19
3	c	7	MAN	C1-O5-C5	2.84	116.04	112.19
5	g	1	NAG	C1-O5-C5	2.59	115.70	112.19
6	J	1	NAG	C1-C2-N2	2.49	114.75	110.49
6	V	1	NAG	C3-C4-C5	2.42	114.56	110.24
3	E	6	MAN	O2-C2-C3	-2.42	105.30	110.14
3	c	6	MAN	O2-C2-C3	-2.40	105.33	110.14
3	Q	6	MAN	O2-C2-C3	-2.37	105.39	110.14
3	Q	5	MAN	O2-C2-C3	-2.27	105.59	110.14
3	Q	7	MAN	O2-C2-C3	-2.26	105.62	110.14
3	E	5	MAN	O2-C2-C3	-2.22	105.70	110.14
3	E	7	MAN	O2-C2-C3	-2.21	105.71	110.14
3	Q	5	MAN	C1-C2-C3	2.19	112.36	109.67
3	Q	4	MAN	C1-O5-C5	2.19	115.17	112.19
3	c	7	MAN	O2-C2-C3	-2.16	105.80	110.14
3	c	5	MAN	O2-C2-C3	-2.13	105.87	110.14
5	W	1	NAG	C1-C2-N2	2.12	114.11	110.49
4	R	2	FUC	C1-C2-C3	2.12	112.27	109.67
5	K	1	NAG	C1-C2-N2	2.11	114.09	110.49
7	O	3	FUC	C1-O5-C5	2.10	117.55	112.78
4	R	2	FUC	O5-C5-C4	2.10	113.28	109.52
3	Q	4	MAN	O2-C2-C3	-2.09	105.95	110.14
7	m	3	FUC	C1-O5-C5	2.08	117.50	112.78
6	J	1	NAG	C3-C4-C5	2.08	113.96	110.24
5	M	3	BMA	C2-C3-C4	2.08	114.50	110.89
3	c	4	MAN	C1-O5-C5	2.07	114.99	112.19
3	Q	1	NAG	C1-O5-C5	2.06	114.99	112.19
3	Q	5	MAN	O5-C1-C2	2.05	113.93	110.77
3	E	4	MAN	C1-C2-C3	2.00	112.13	109.67
4	F	2	FUC	C1-O5-C5	2.00	117.31	112.78
3	E	4	MAN	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (207) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	3	BMA	C4-C5-C6-O6
6	j	2	NAG	C4-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	S	1	NAG	O5-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
6	j	2	NAG	O5-C5-C6-O6
7	a	1	NAG	C4-C5-C6-O6
6	h	2	NAG	C4-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
3	c	3	BMA	O5-C5-C6-O6
7	a	1	NAG	O5-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
2	b	2	NAG	O5-C5-C6-O6
3	c	7	MAN	O5-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
5	e	1	NAG	O5-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6
6	Z	1	NAG	O5-C5-C6-O6
6	l	1	NAG	O5-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
3	E	6	MAN	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	h	2	NAG	O5-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
5	S	1	NAG	C4-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	b	2	NAG	C4-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
6	f	1	NAG	C4-C5-C6-O6
3	Q	3	BMA	O5-C5-C6-O6
3	E	6	MAN	C4-C5-C6-O6
7	m	1	NAG	C4-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	S	2	NAG	C8-C7-N2-C2
5	S	2	NAG	O7-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
5	W	1	NAG	O7-C7-N2-C2
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
5	Y	2	NAG	C8-C7-N2-C2
5	Y	2	NAG	O7-C7-N2-C2
5	e	2	NAG	C8-C7-N2-C2
5	e	2	NAG	O7-C7-N2-C2
5	i	2	NAG	C8-C7-N2-C2
5	i	2	NAG	O7-C7-N2-C2
6	J	1	NAG	C8-C7-N2-C2
6	J	1	NAG	O7-C7-N2-C2
6	N	1	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
6	V	1	NAG	C8-C7-N2-C2
6	V	1	NAG	O7-C7-N2-C2
6	V	2	NAG	C8-C7-N2-C2
6	V	2	NAG	O7-C7-N2-C2
6	Z	1	NAG	C8-C7-N2-C2
6	Z	1	NAG	O7-C7-N2-C2
6	Z	2	NAG	C8-C7-N2-C2
6	Z	2	NAG	O7-C7-N2-C2
6	h	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	h	1	NAG	O7-C7-N2-C2
6	l	1	NAG	C8-C7-N2-C2
6	l	1	NAG	O7-C7-N2-C2
6	l	2	NAG	C8-C7-N2-C2
6	l	2	NAG	O7-C7-N2-C2
7	O	2	NAG	C8-C7-N2-C2
7	O	2	NAG	O7-C7-N2-C2
7	a	2	NAG	C8-C7-N2-C2
7	a	2	NAG	O7-C7-N2-C2
7	m	2	NAG	C8-C7-N2-C2
7	m	2	NAG	O7-C7-N2-C2
5	i	1	NAG	O5-C5-C6-O6
5	e	1	NAG	C4-C5-C6-O6
7	O	2	NAG	C4-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
2	b	3	BMA	O5-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
7	m	2	NAG	O5-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	U	3	BMA	C4-C5-C6-O6
5	i	1	NAG	C4-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
6	f	1	NAG	O5-C5-C6-O6
6	l	1	NAG	C4-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
2	b	3	BMA	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	c	3	BMA	C4-C5-C6-O6
6	l	2	NAG	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
5	U	3	BMA	O5-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
3	c	7	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	Q	4	MAN	O5-C5-C6-O6
7	m	1	NAG	O5-C5-C6-O6
5	Y	2	NAG	C4-C5-C6-O6
3	Q	5	MAN	O5-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
3	c	6	MAN	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
6	f	2	NAG	O5-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6
5	e	3	BMA	O5-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6
3	Q	7	MAN	C4-C5-C6-O6
5	k	3	BMA	O5-C5-C6-O6
3	E	5	MAN	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
3	Q	6	MAN	O5-C5-C6-O6
5	S	3	BMA	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
3	c	5	MAN	O5-C5-C6-O6
7	O	1	NAG	C3-C2-N2-C7
3	Q	7	MAN	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
5	g	3	BMA	C4-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	b	1	NAG	C4-C5-C6-O6
6	h	1	NAG	C4-C5-C6-O6
6	h	1	NAG	O5-C5-C6-O6
6	H	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C3-C2-N2-C7
2	P	1	NAG	C3-C2-N2-C7
2	P	2	NAG	C3-C2-N2-C7
2	b	2	NAG	C3-C2-N2-C7
5	M	1	NAG	C3-C2-N2-C7
6	J	2	NAG	C3-C2-N2-C7
6	L	1	NAG	C3-C2-N2-C7
6	N	2	NAG	C3-C2-N2-C7
6	X	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	Z	1	NAG	C3-C2-N2-C7
6	Z	2	NAG	C3-C2-N2-C7
5	i	2	NAG	C4-C5-C6-O6
5	g	3	BMA	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
6	j	1	NAG	C4-C5-C6-O6
3	Q	4	MAN	C4-C5-C6-O6
2	P	1	NAG	C1-C2-N2-C7
5	I	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
3	Q	3	BMA	C4-C5-C6-O6
7	m	2	NAG	C4-C5-C6-O6
5	i	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7
2	b	1	NAG	C3-C2-N2-C7
5	K	1	NAG	C3-C2-N2-C7
5	W	1	NAG	C3-C2-N2-C7
6	H	2	NAG	C3-C2-N2-C7
6	J	1	NAG	C3-C2-N2-C7
6	N	1	NAG	C3-C2-N2-C7
6	T	2	NAG	C3-C2-N2-C7
6	V	1	NAG	C3-C2-N2-C7
6	V	2	NAG	C3-C2-N2-C7
6	f	2	NAG	C3-C2-N2-C7
6	h	1	NAG	C3-C2-N2-C7
6	j	1	NAG	C3-C2-N2-C7
6	l	1	NAG	C3-C2-N2-C7
6	l	2	NAG	C3-C2-N2-C7
7	a	1	NAG	C3-C2-N2-C7
7	m	1	NAG	C3-C2-N2-C7
6	j	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
5	Y	1	NAG	C1-C2-N2-C7
6	H	2	NAG	C1-C2-N2-C7
6	J	1	NAG	C1-C2-N2-C7
6	f	2	NAG	C1-C2-N2-C7
7	a	1	NAG	C1-C2-N2-C7
7	m	1	NAG	C1-C2-N2-C7

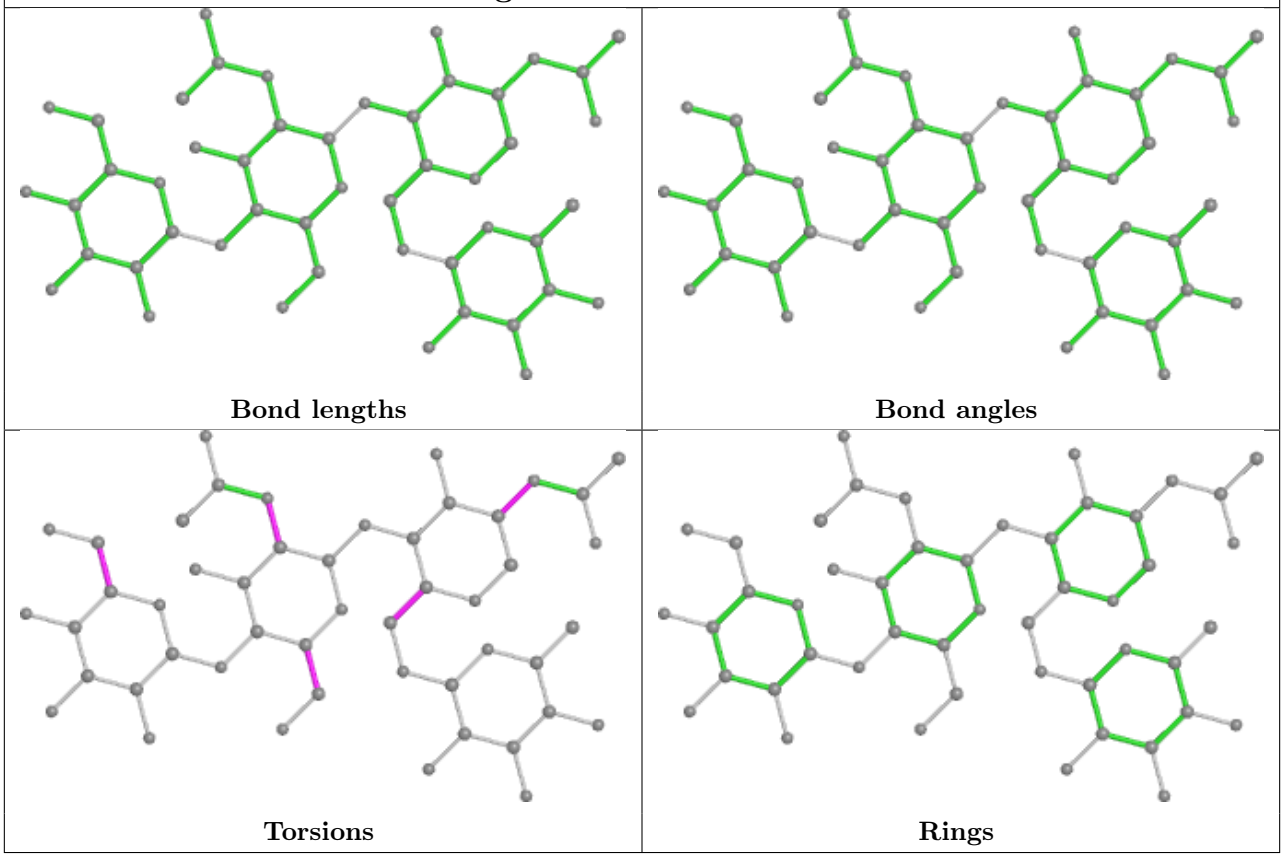
All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	c	5	MAN	C1-C2-C3-C4-C5-O5
3	c	7	MAN	C1-C2-C3-C4-C5-O5
3	E	5	MAN	C1-C2-C3-C4-C5-O5
3	Q	7	MAN	C1-C2-C3-C4-C5-O5
3	E	7	MAN	C1-C2-C3-C4-C5-O5

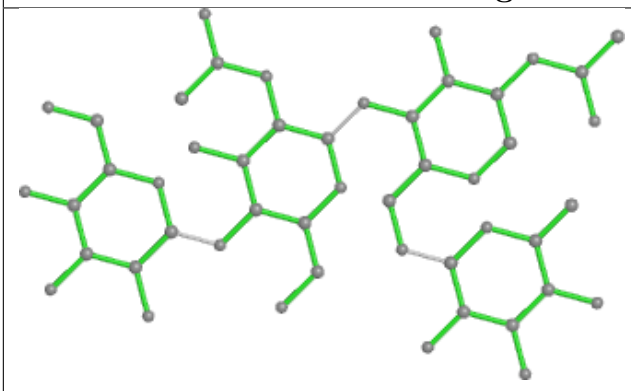
No monomer is involved in short contacts.

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

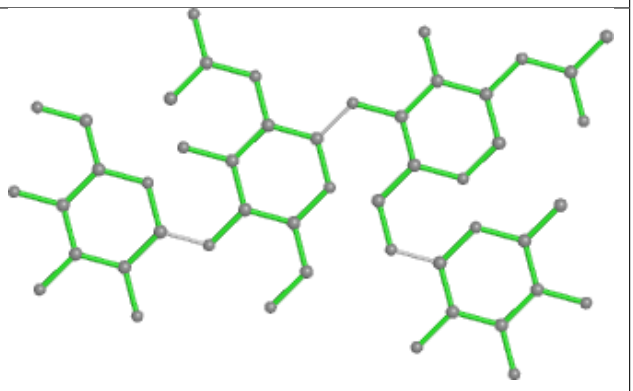
Oligosaccharide Chain D



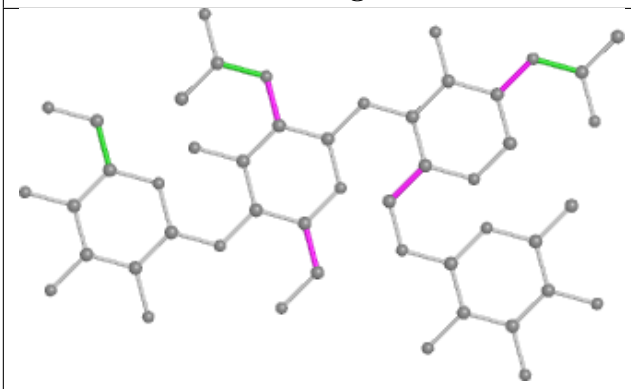
Oligosaccharide Chain P



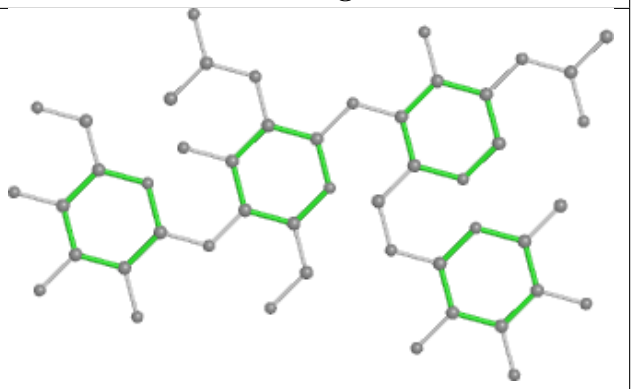
Bond lengths



Bond angles

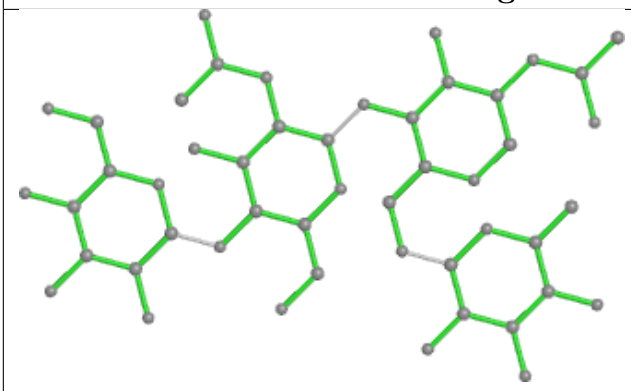


Torsions

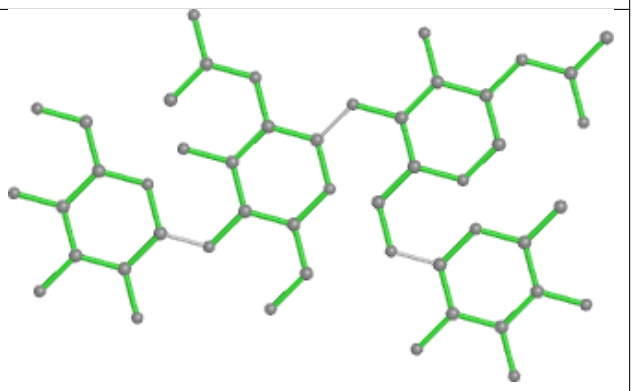


Rings

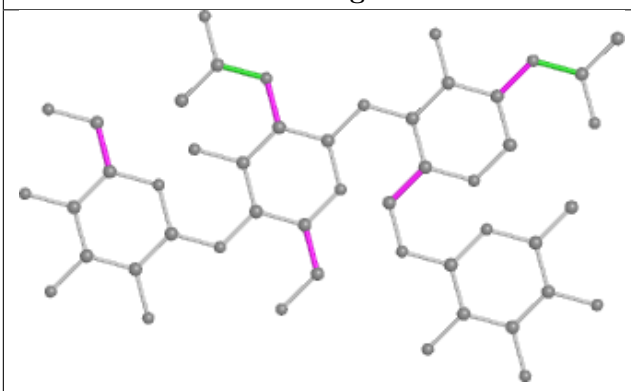
Oligosaccharide Chain b



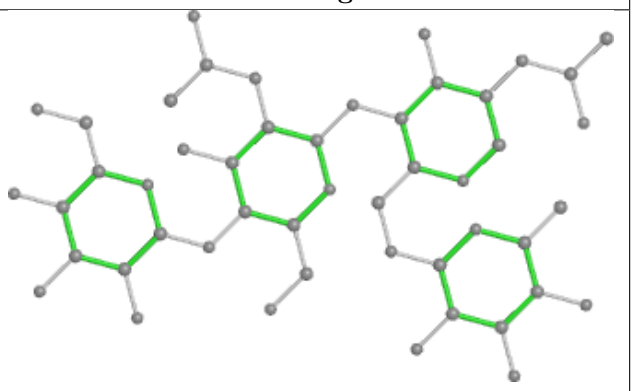
Bond lengths



Bond angles

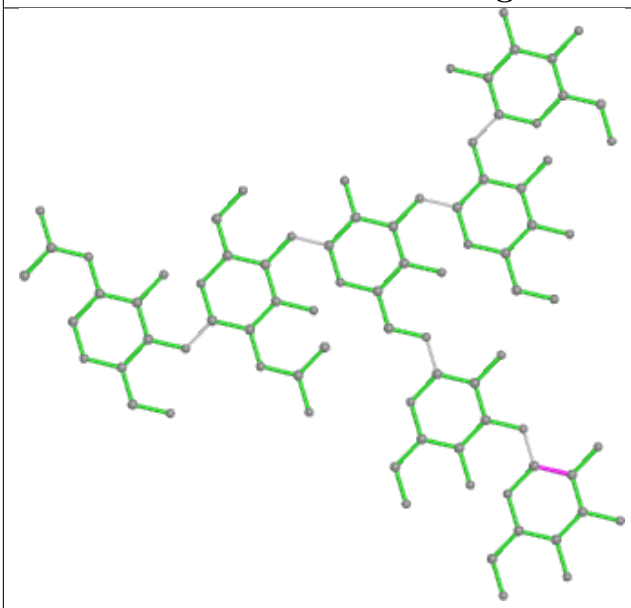


Torsions

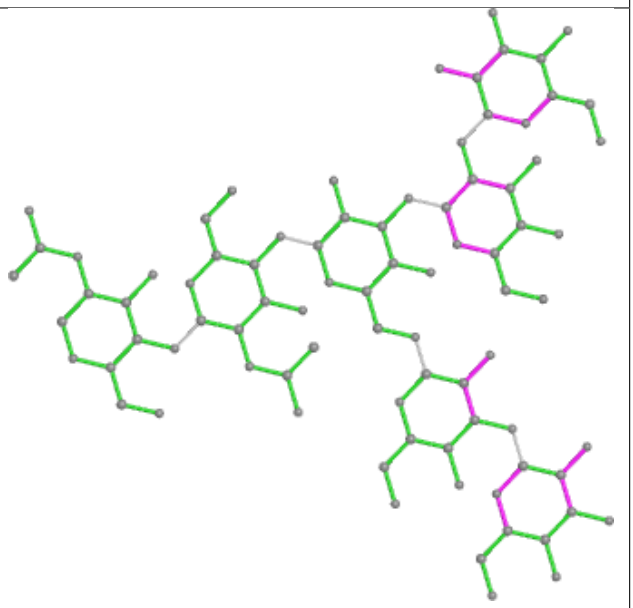


Rings

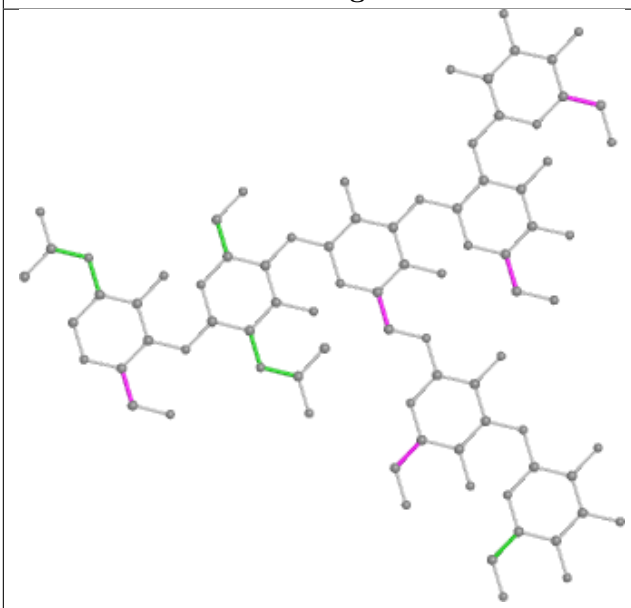
Oligosaccharide Chain E



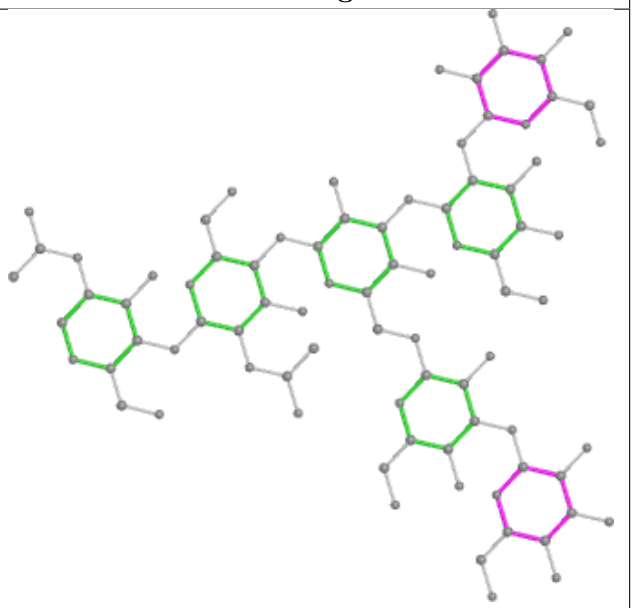
Bond lengths



Bond angles

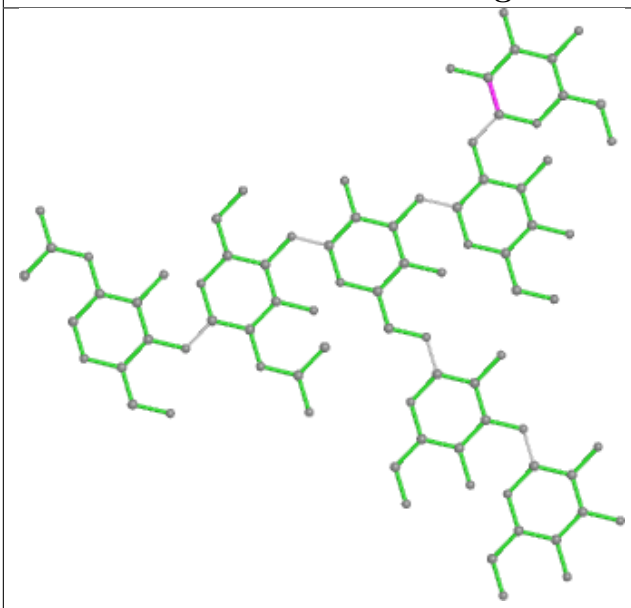


Torsions

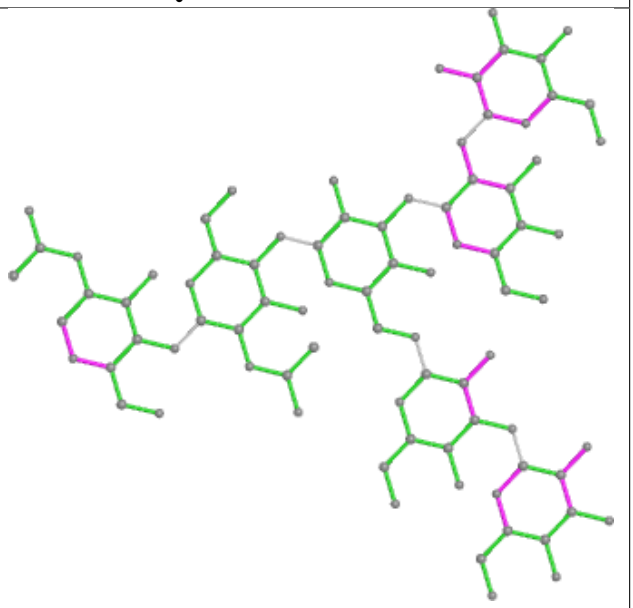


Rings

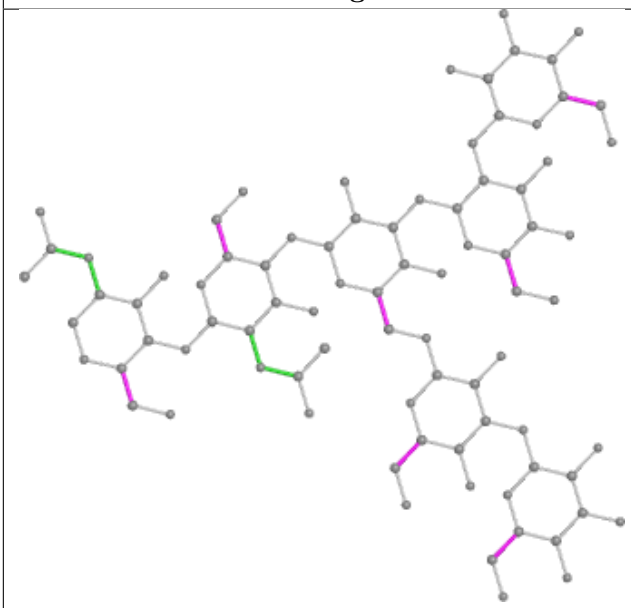
Oligosaccharide Chain Q



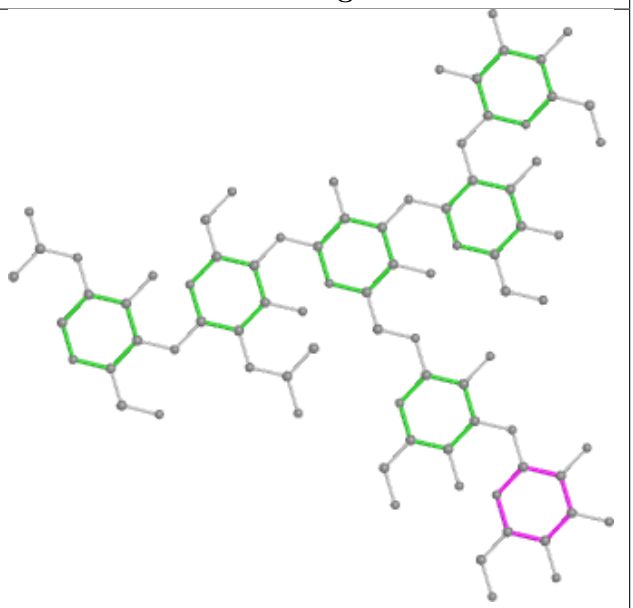
Bond lengths



Bond angles

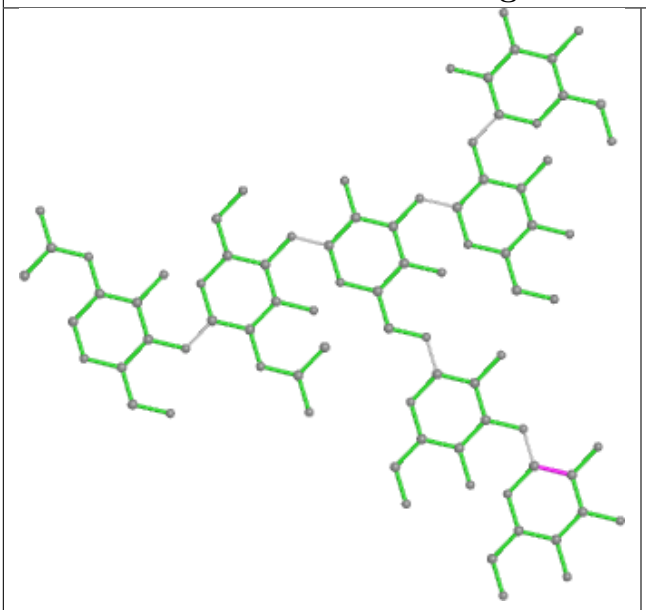


Torsions

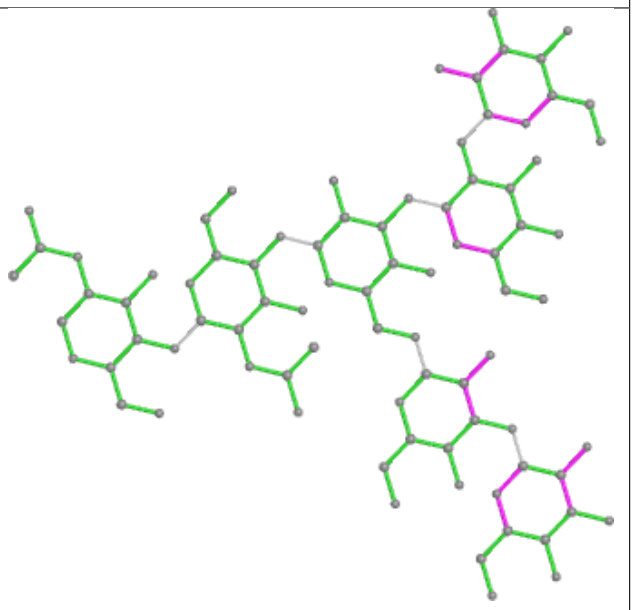


Rings

Oligosaccharide Chain c



Bond lengths



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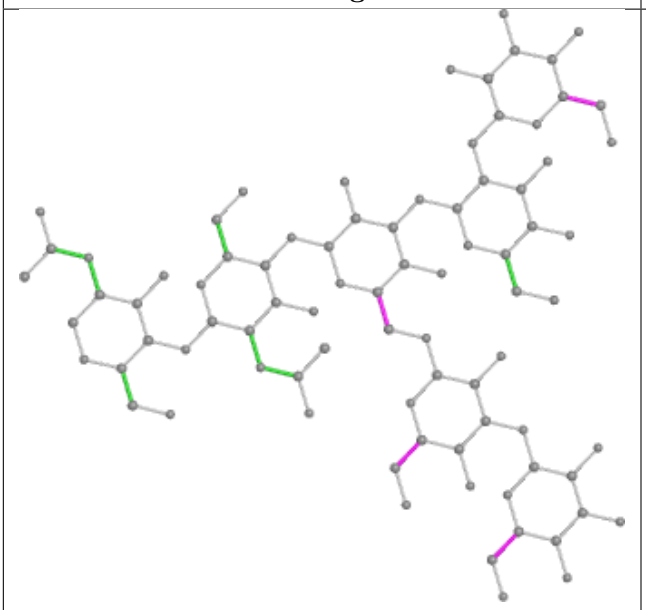

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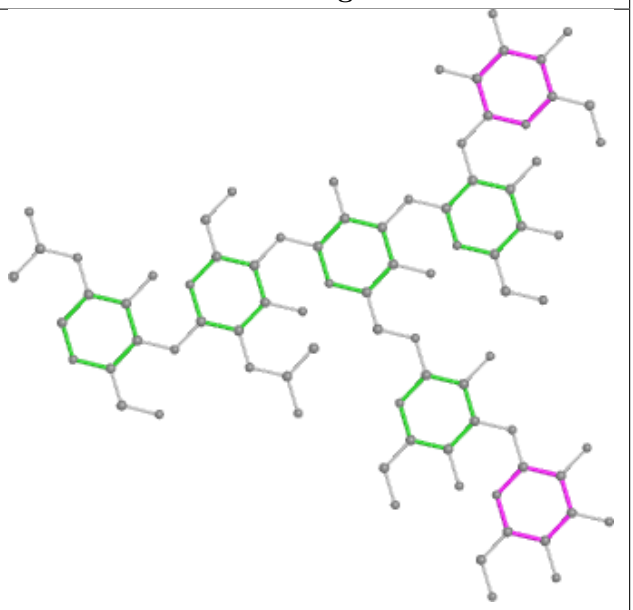
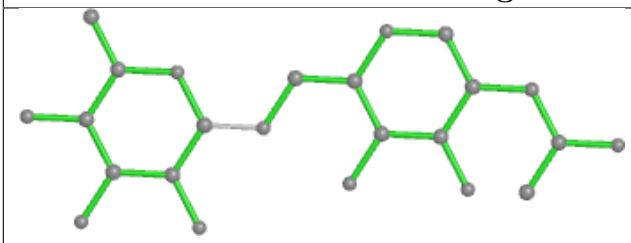
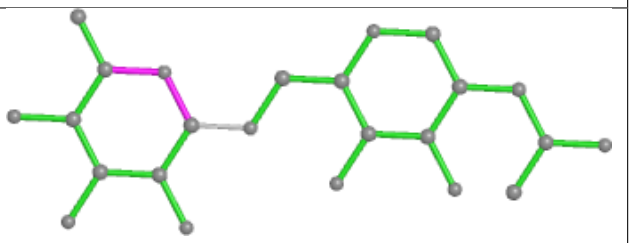
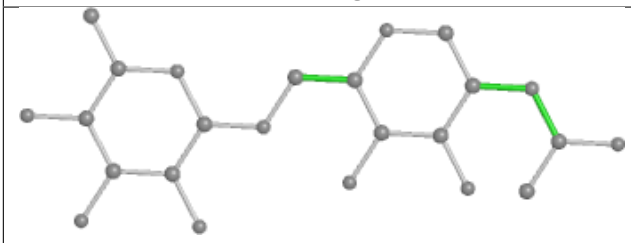
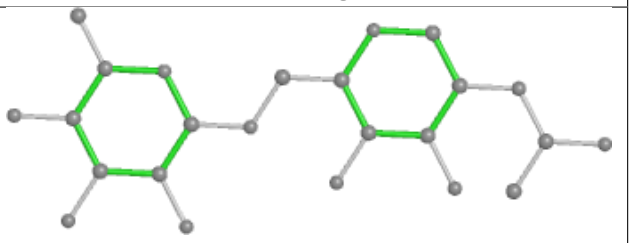
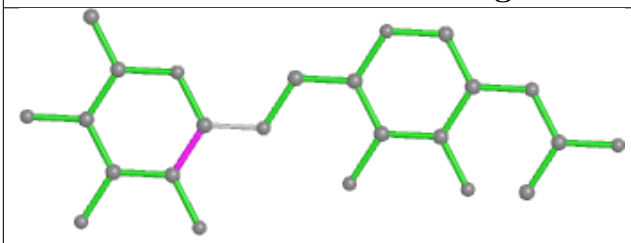
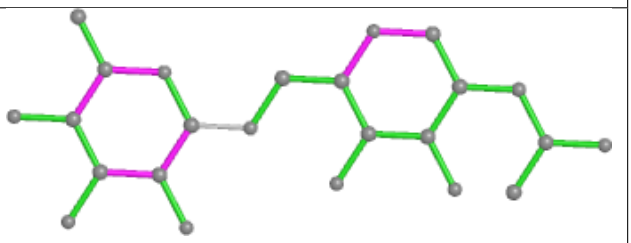
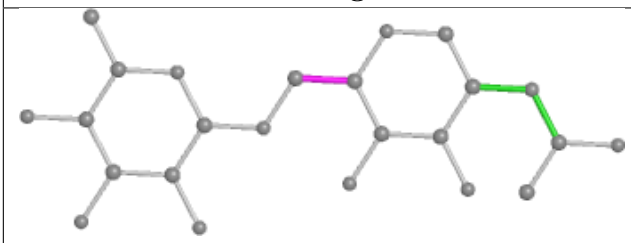
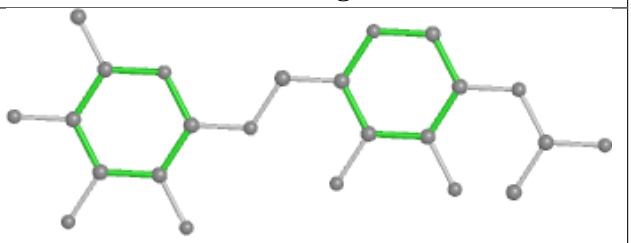
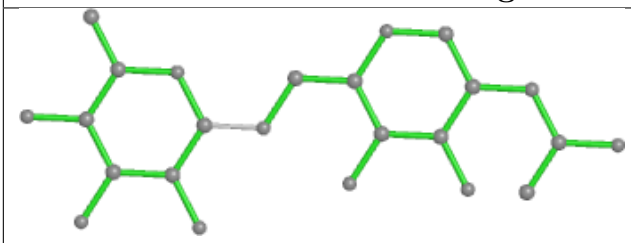


Rings

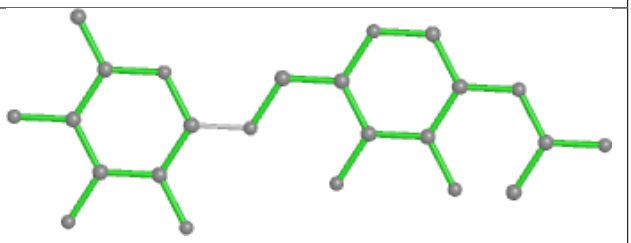
Oligosaccharide Chain F	
	
Bond lengths	Bond angles
	
Torsions	Rings

Oligosaccharide Chain R	
	
Bond lengths	Bond angles
	
Torsions	Rings

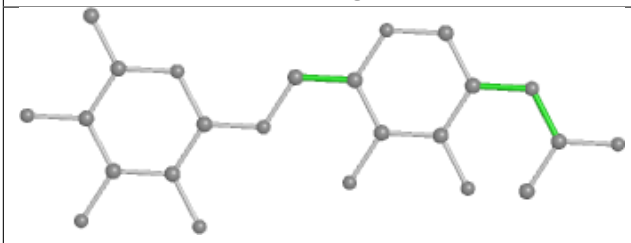
Oligosaccharide Chain d



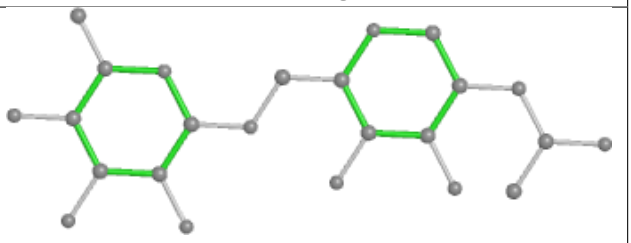
Bond lengths



Bond angles

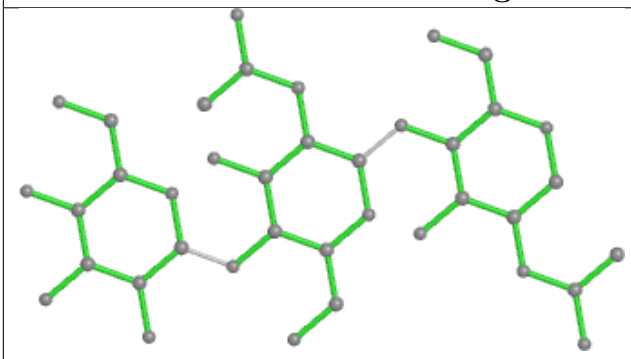


Torsions

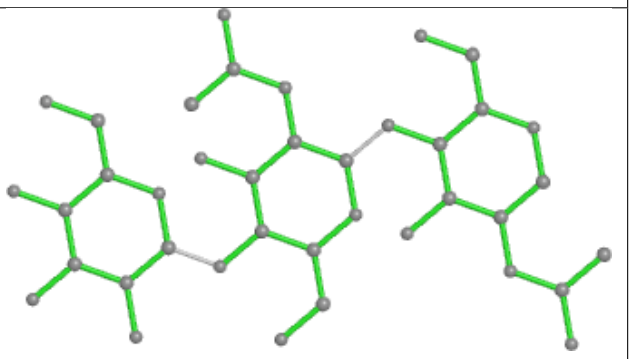


Rings

Oligosaccharide Chain G



Bond lengths



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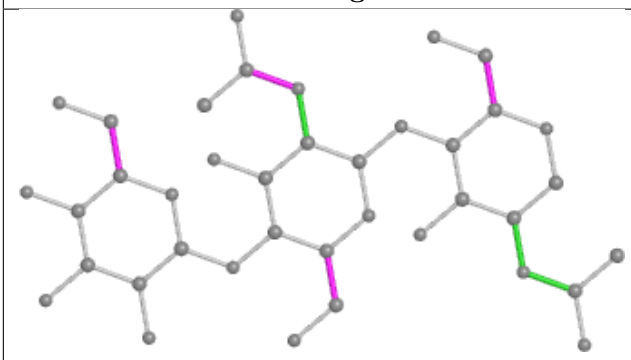
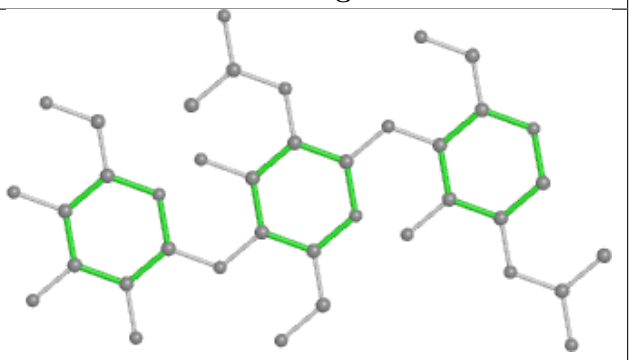
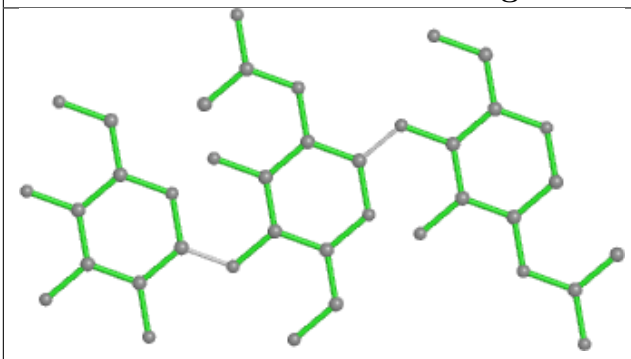


Torsions

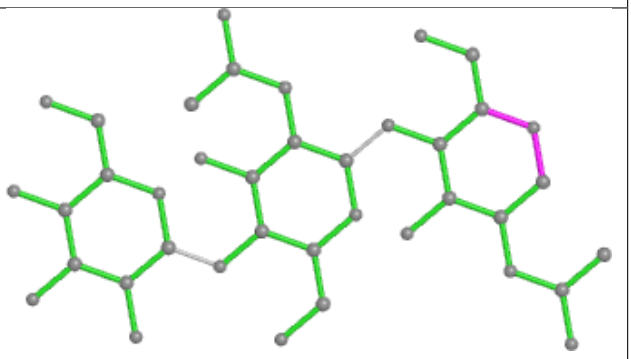


Rings

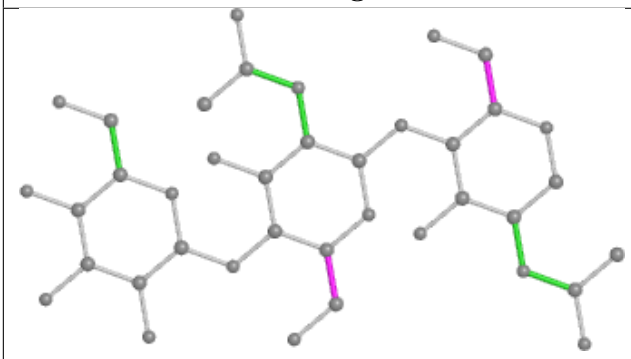
Oligosaccharide Chain I



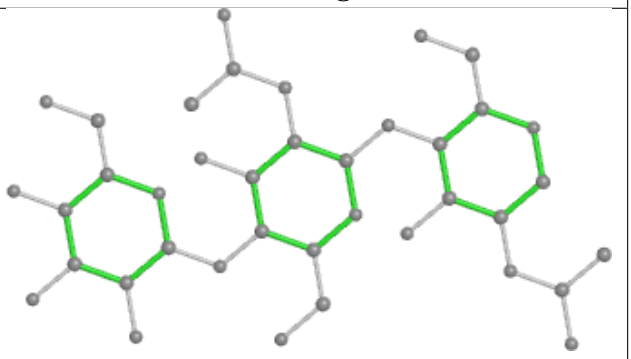
Bond lengths



Bond angles

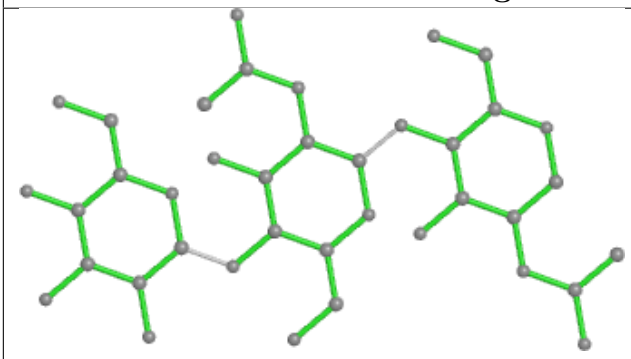


Torsions

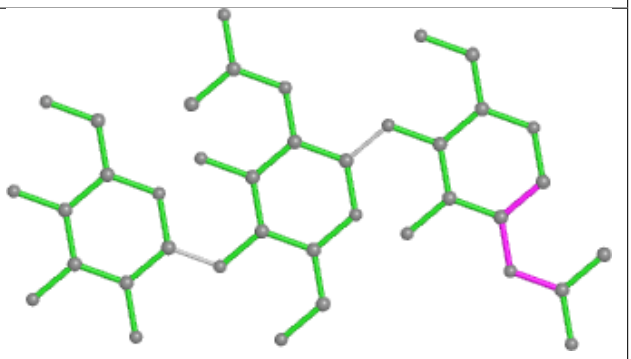


Rings

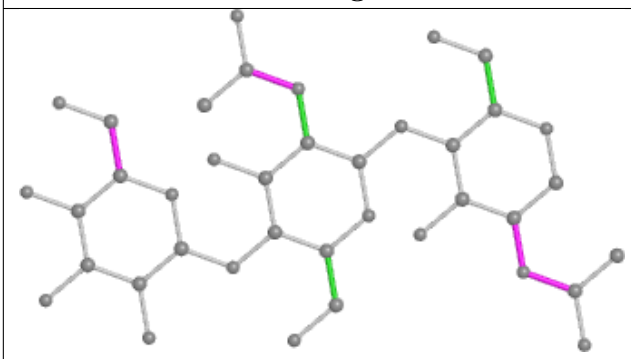
Oligosaccharide Chain K



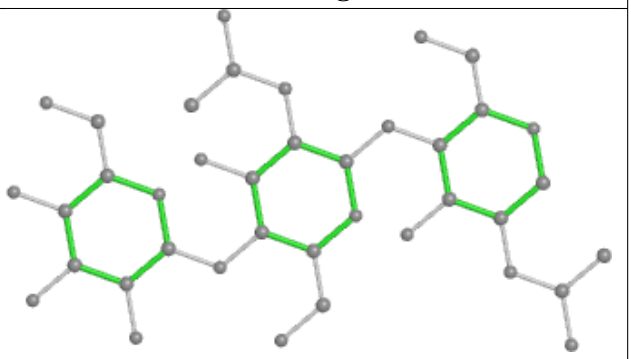
Bond lengths



Bond angles

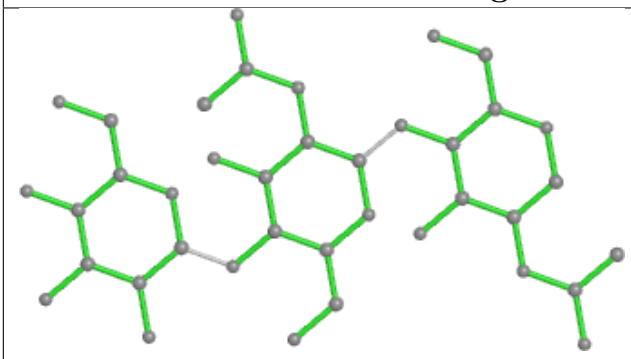


Torsions

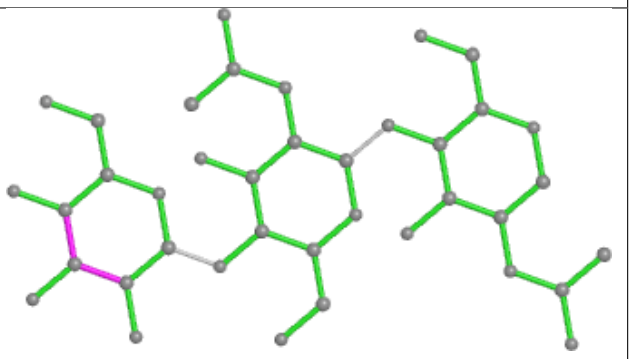


Rings

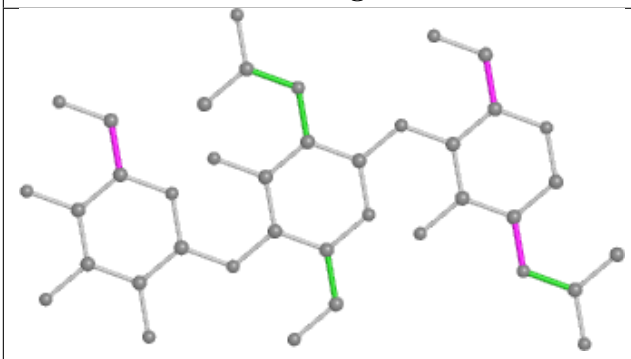
Oligosaccharide Chain M



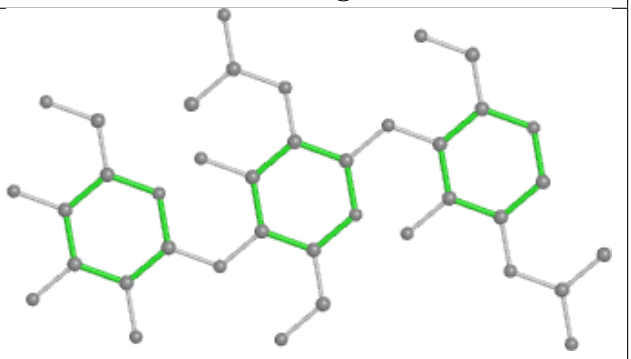
Bond lengths



Bond angles

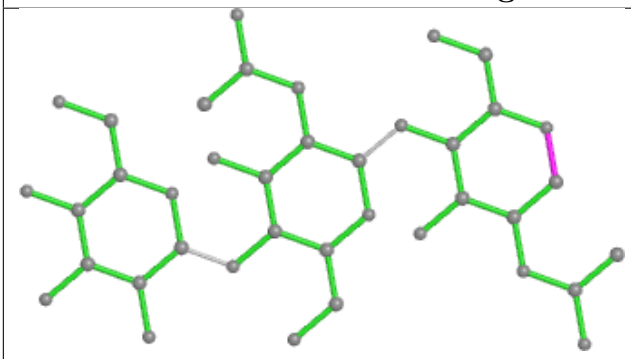


Torsions

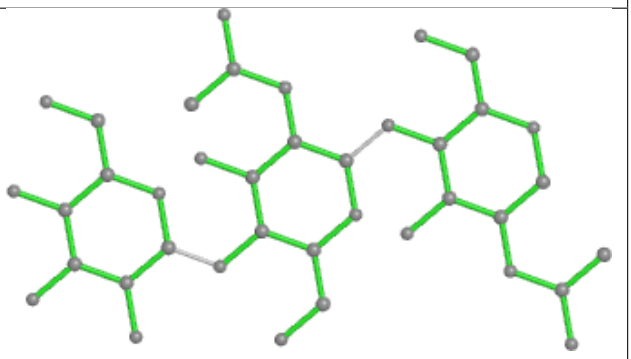


Rings

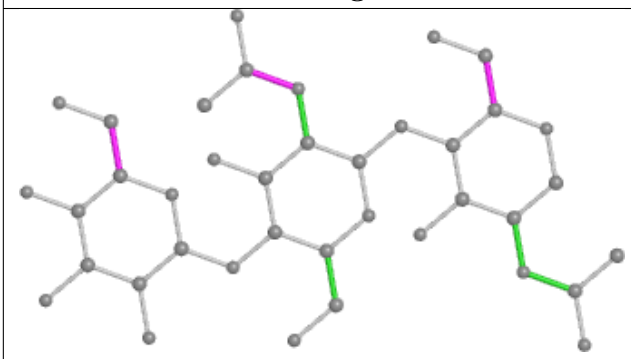
Oligosaccharide Chain S



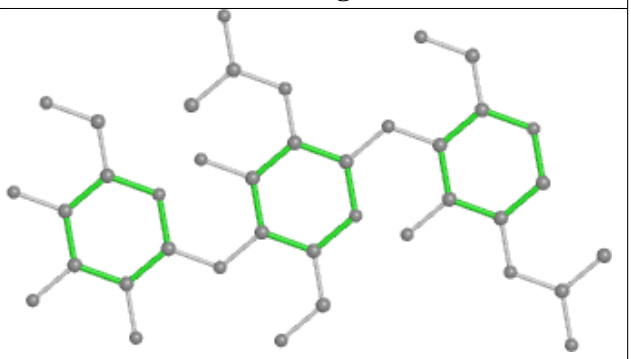
Bond lengths



Bond angles

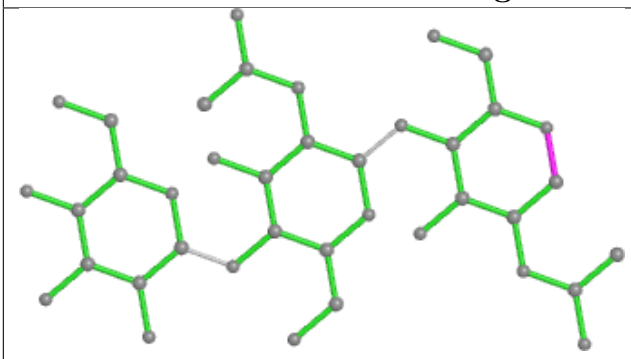


Torsions

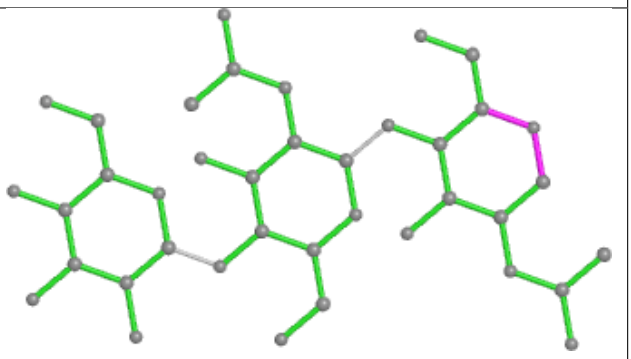


Rings

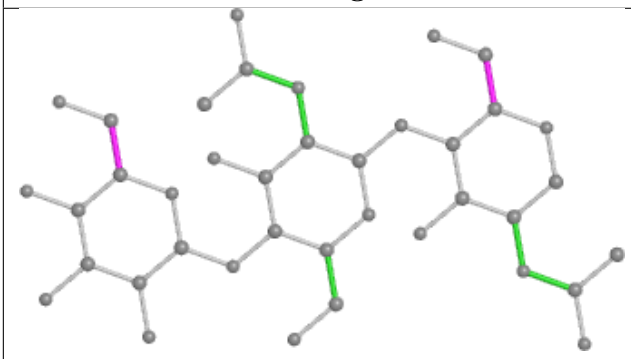
Oligosaccharide Chain U



Bond lengths



Bond angles



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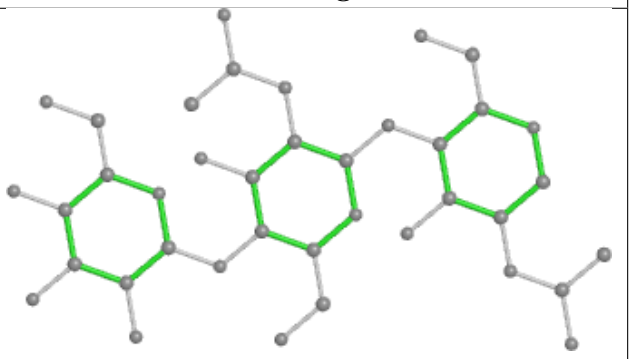
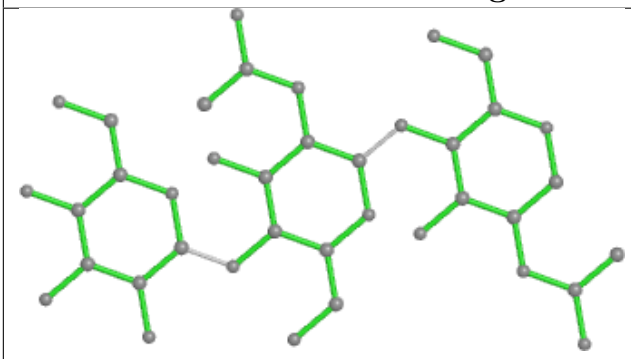


Rings

Oligosaccharide Chain W



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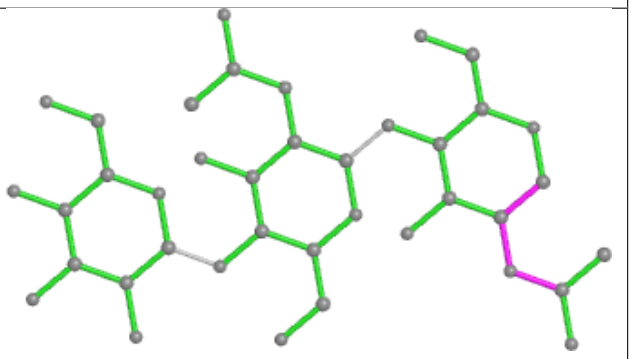
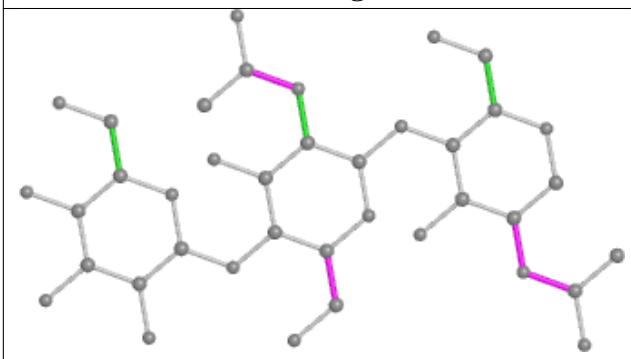


Bond angles



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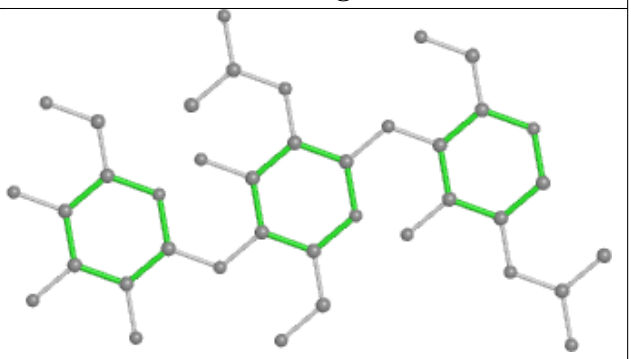
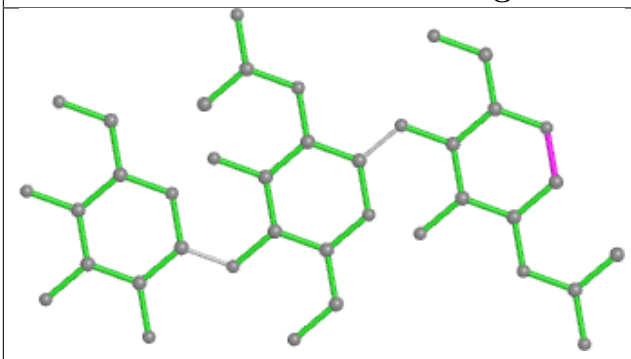


Rings

Oligosaccharide Chain Y



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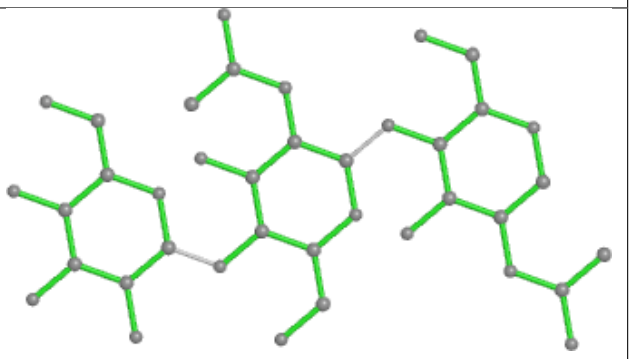

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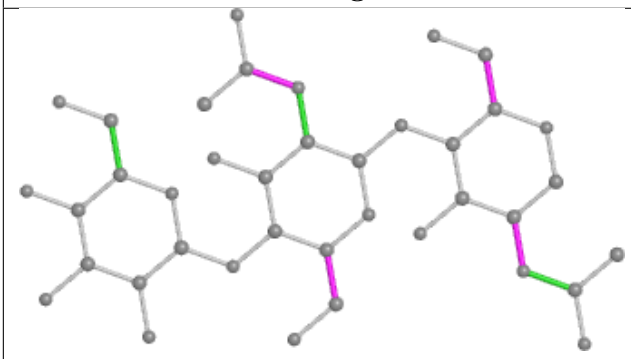

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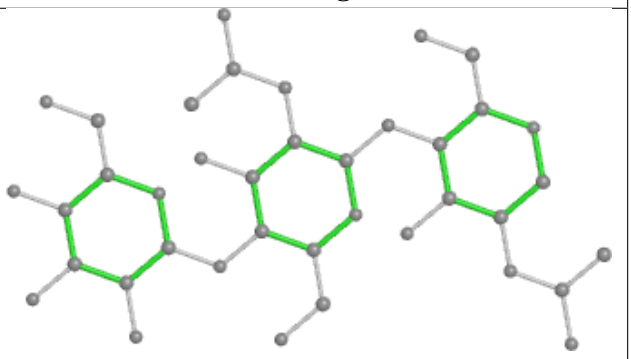
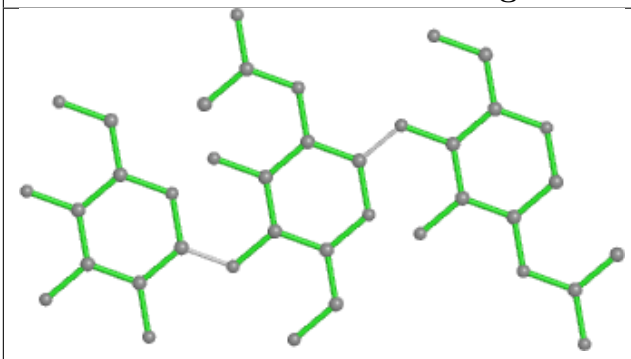


Rings

Oligosaccharide Chain e



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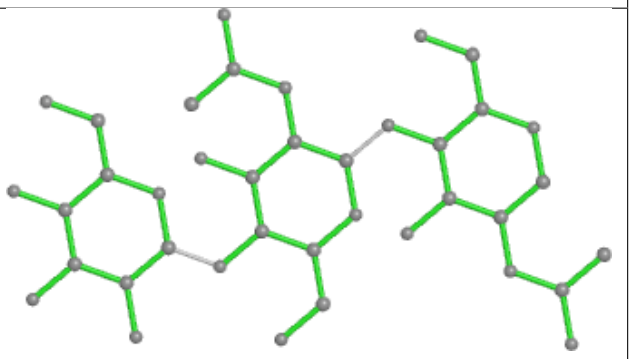
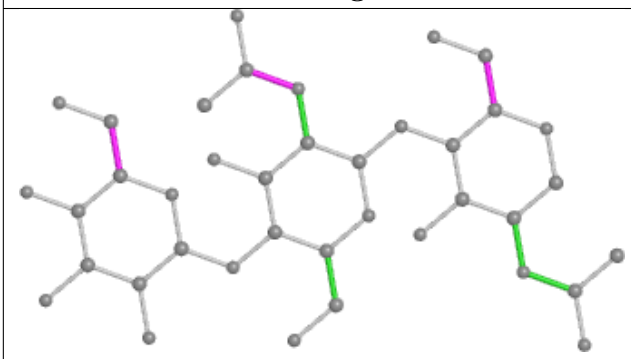


Bond angles



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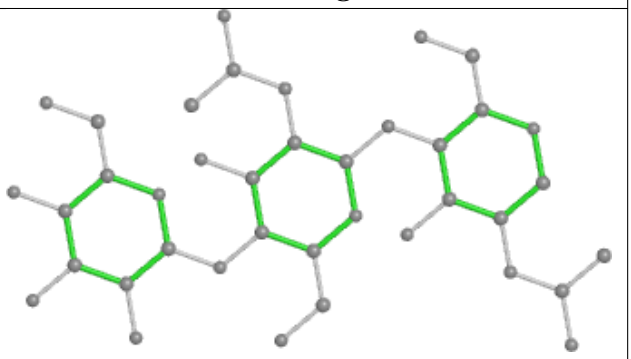
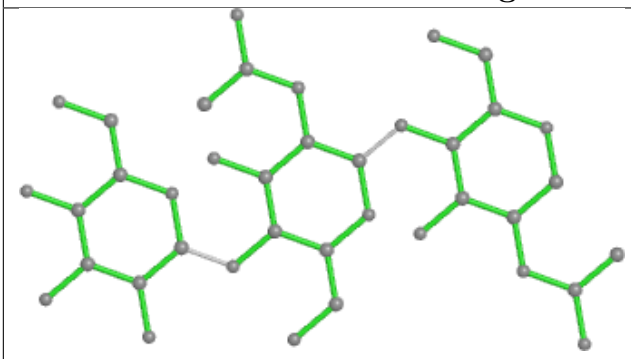


Rings

Oligosaccharide Chain g



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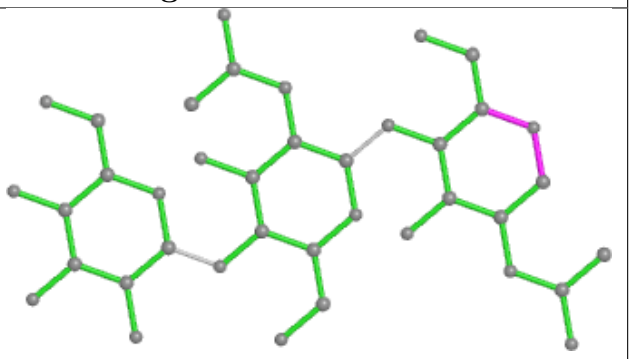

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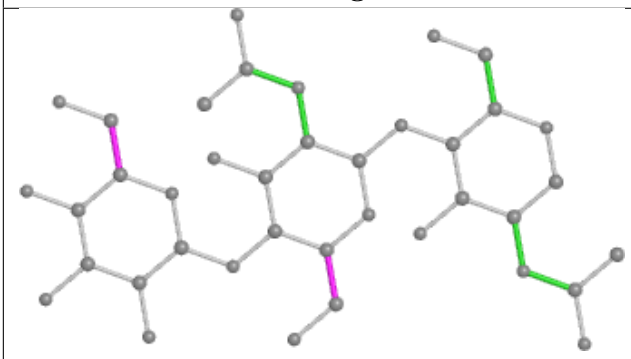

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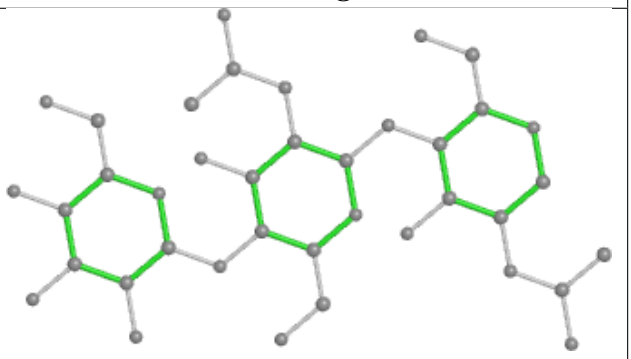
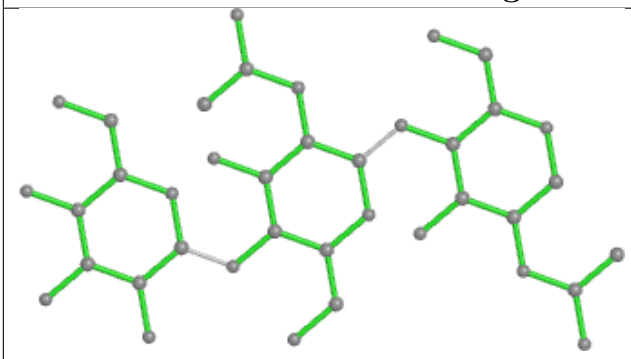


Rings

Oligosaccharide Chain i



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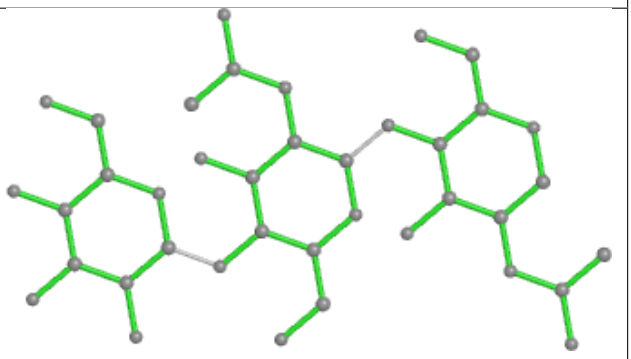

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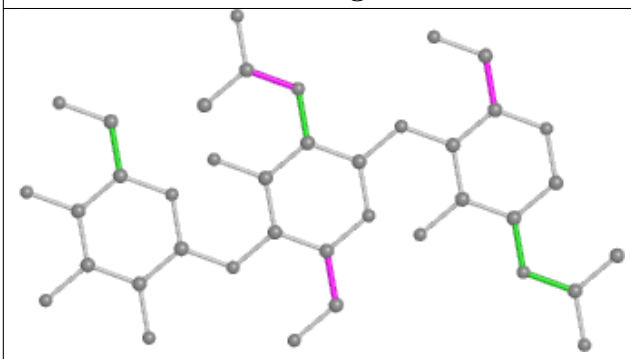

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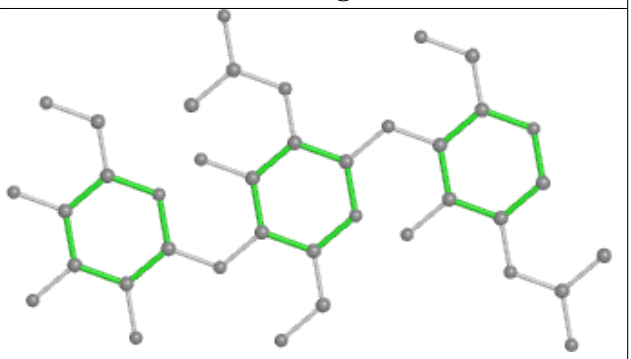
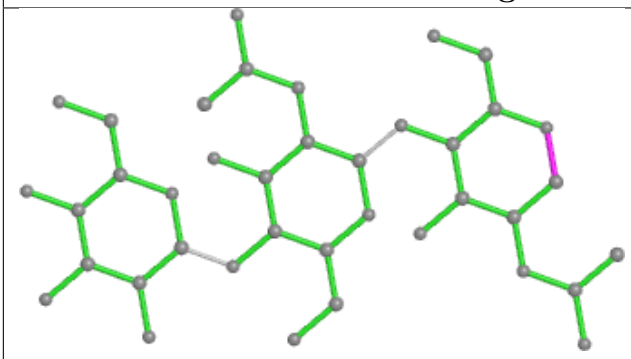


Rings

Oligosaccharide Chain k



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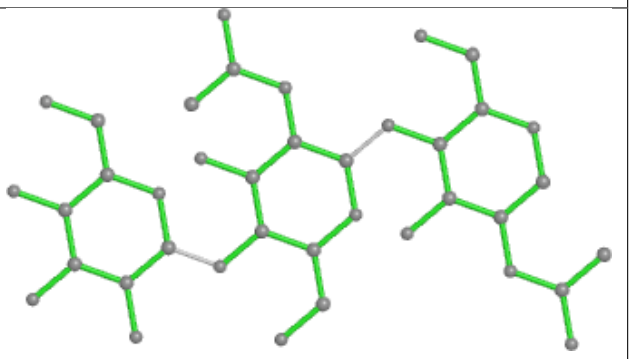

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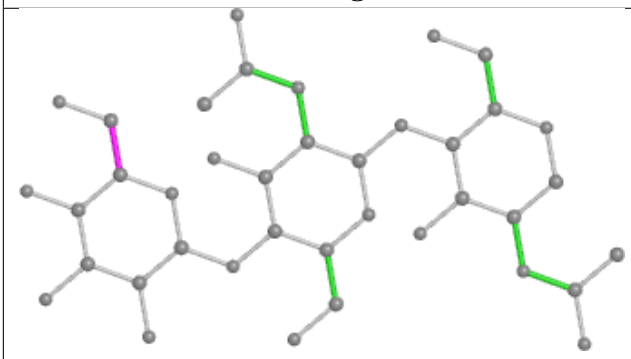

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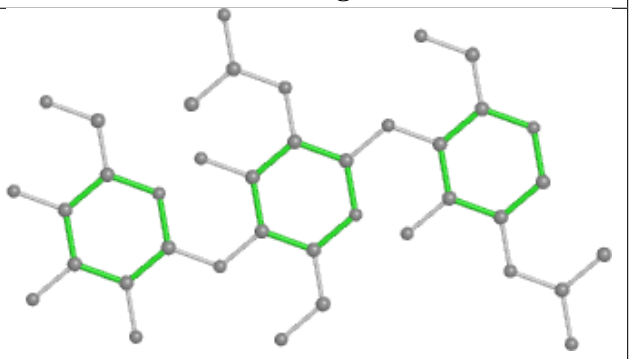
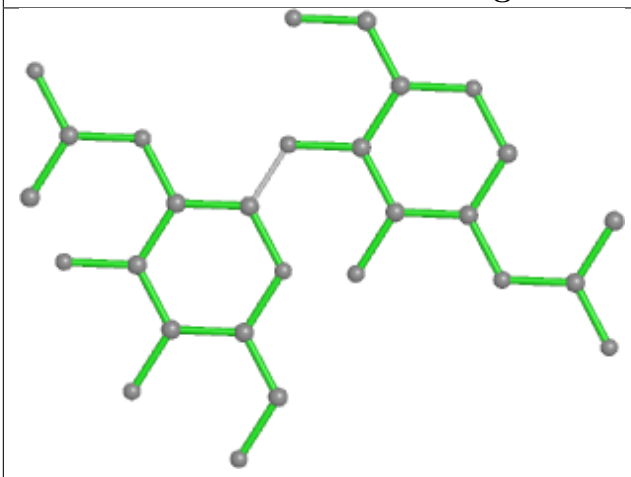


Rings

Oligosaccharide Chain H



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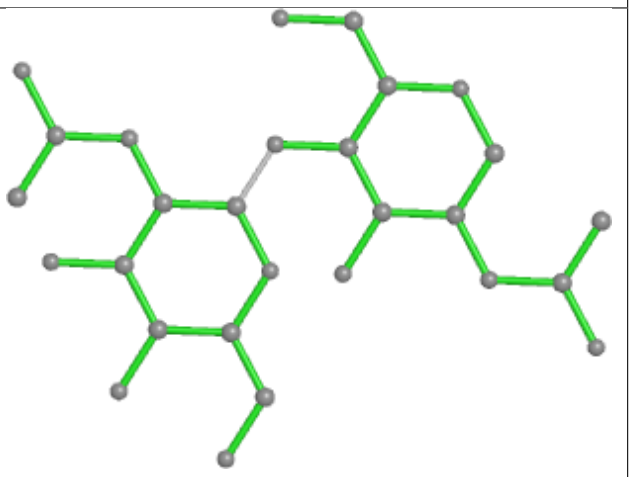

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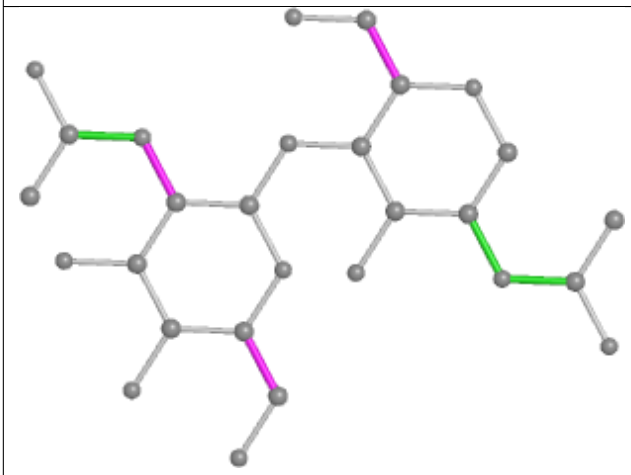

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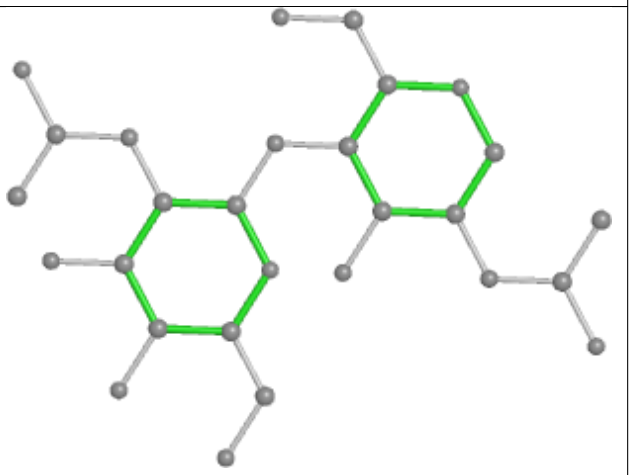
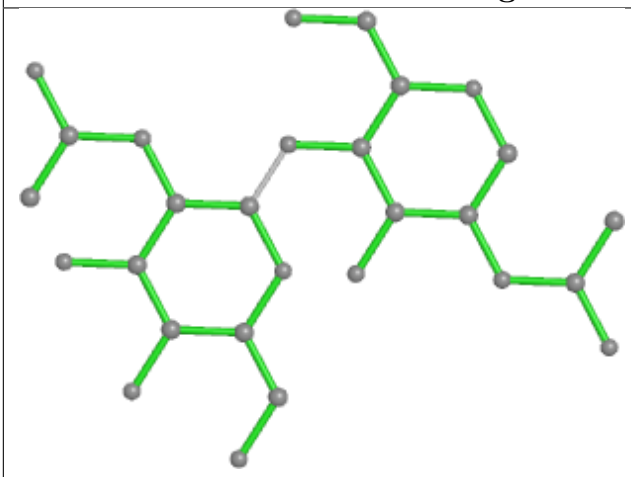


Rings

Oligosaccharide Chain J



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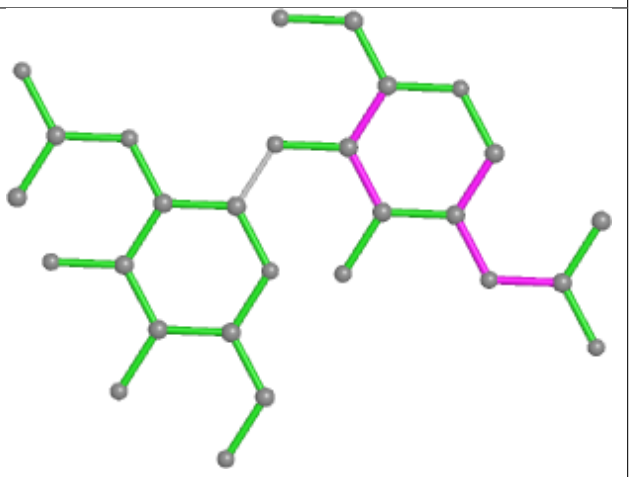

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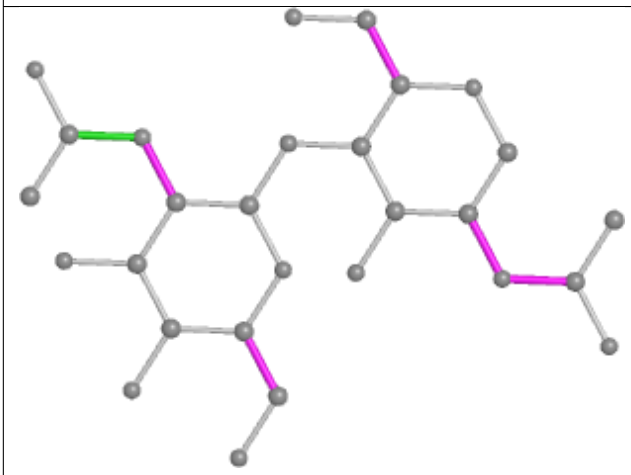

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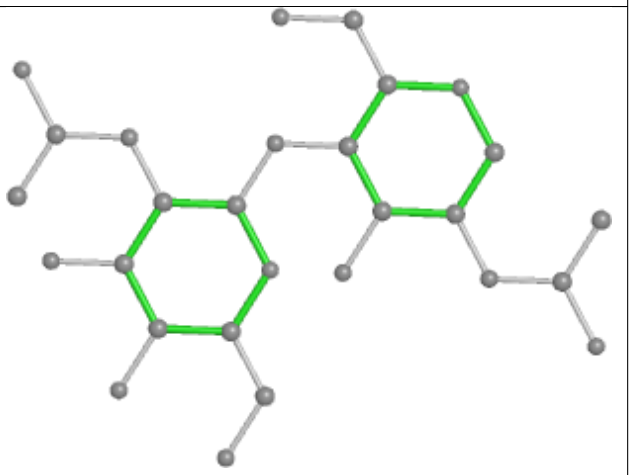
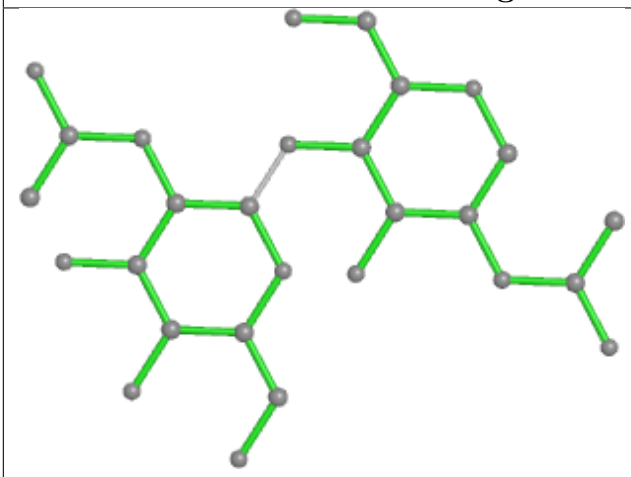


Rings

Oligosaccharide Chain L



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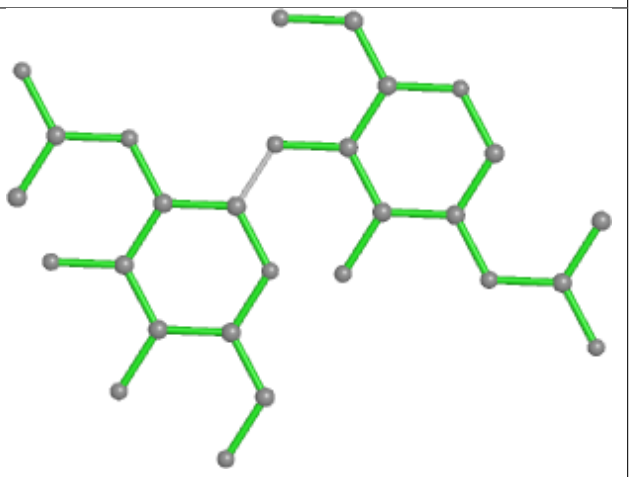
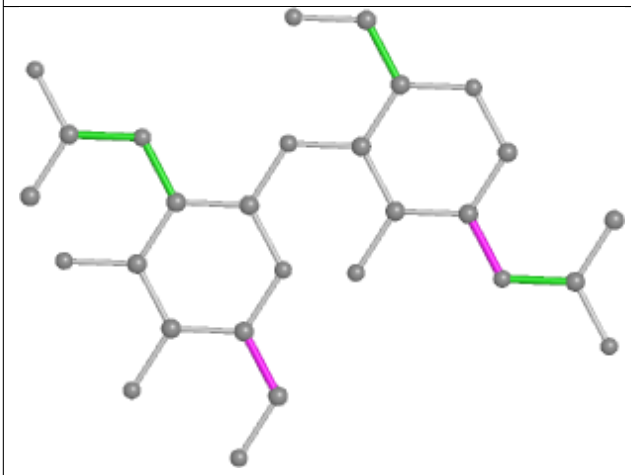


Bond angles



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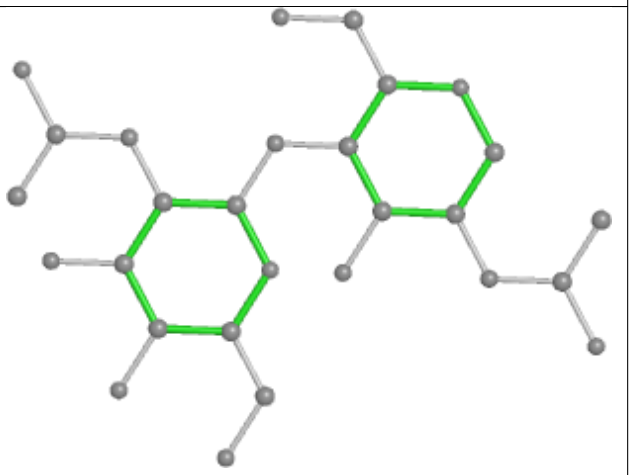
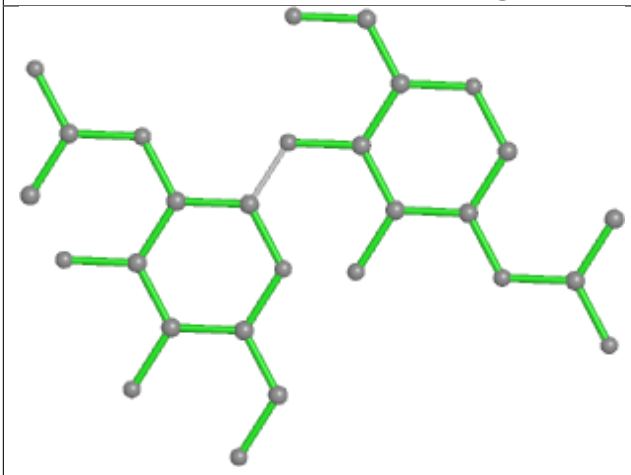


Rings

Oligosaccharide Chain N



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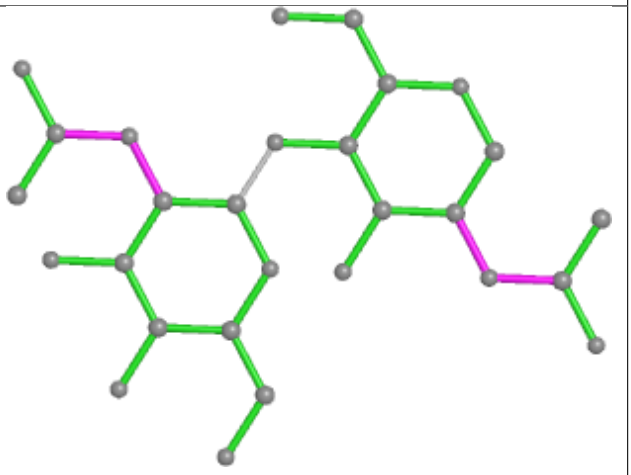
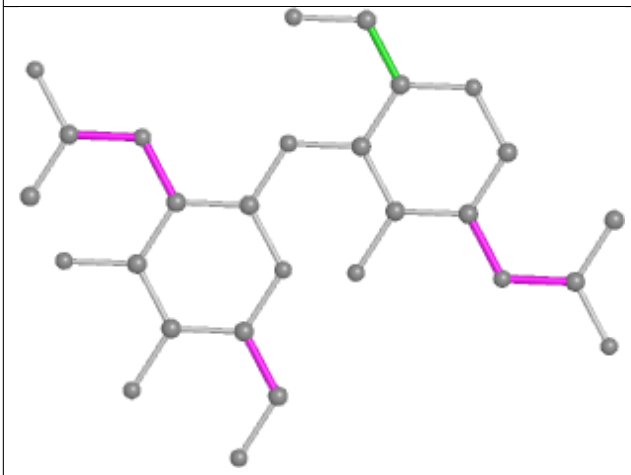


Bond angles



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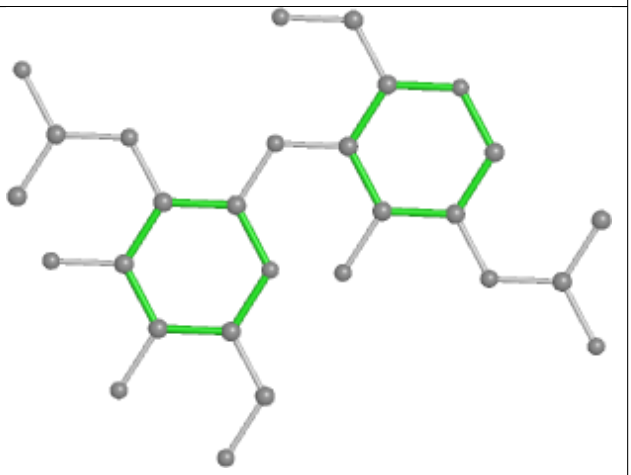
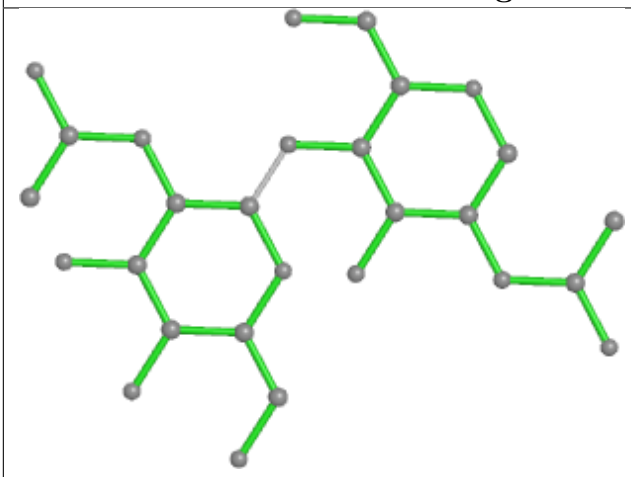


Rings

Oligosaccharide Chain T



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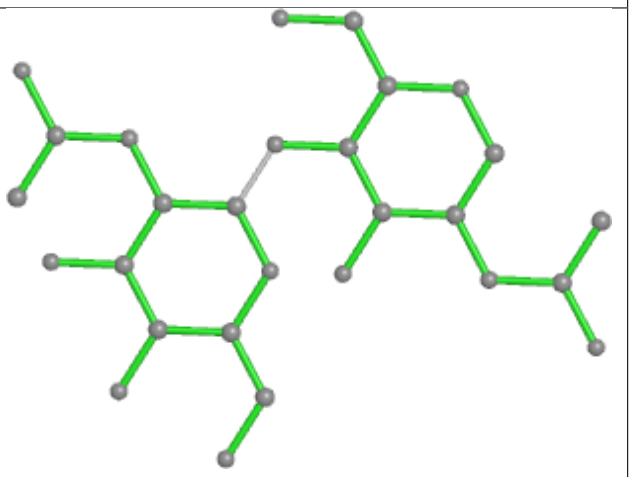
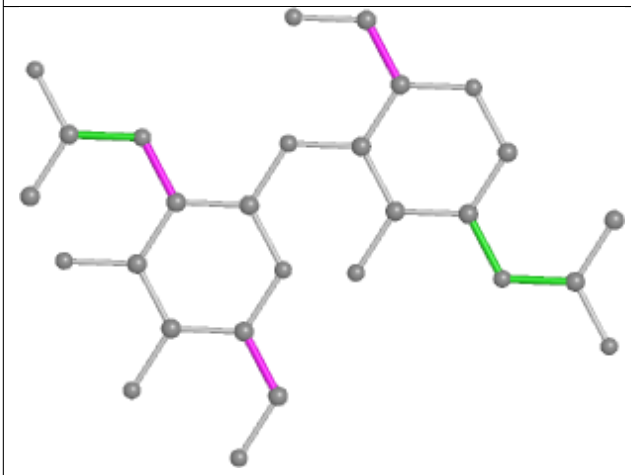


Bond angles



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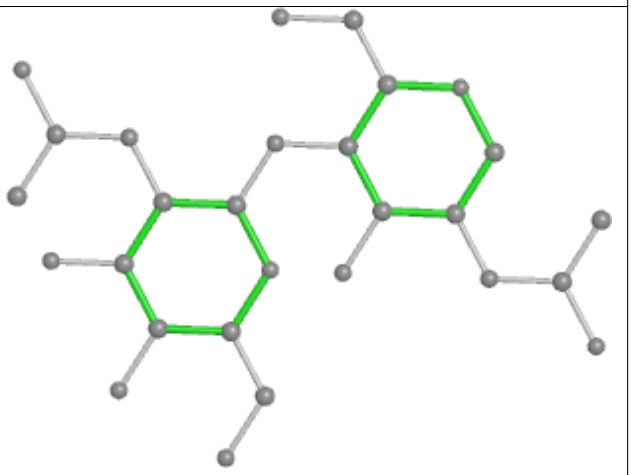
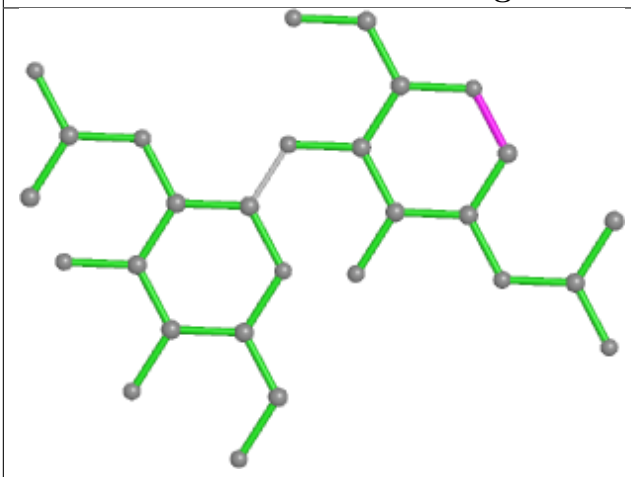


Rings

Oligosaccharide Chain V



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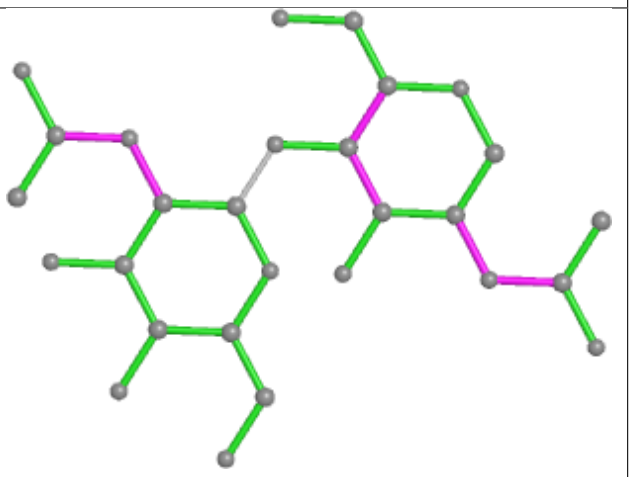
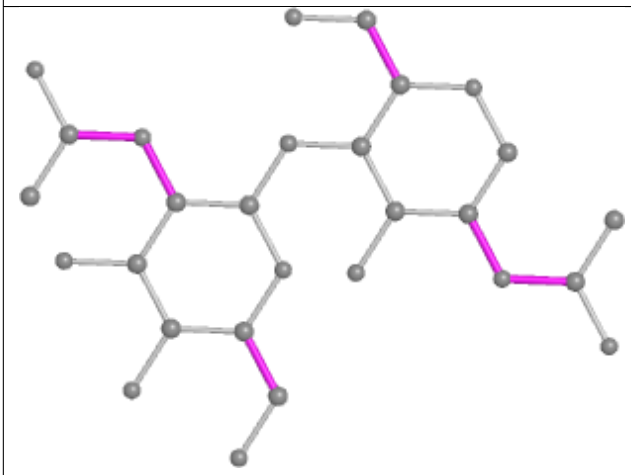


Bond angles



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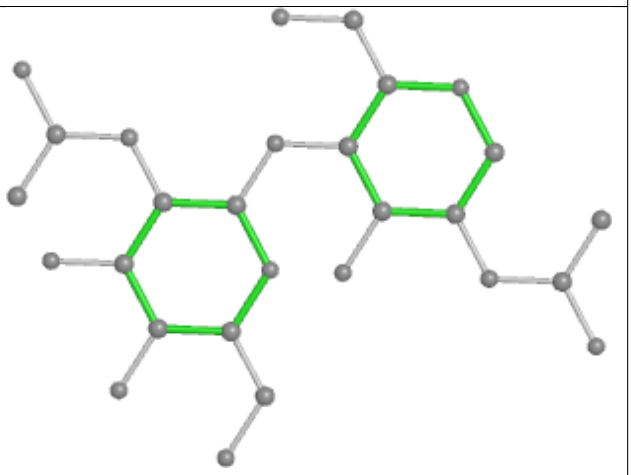
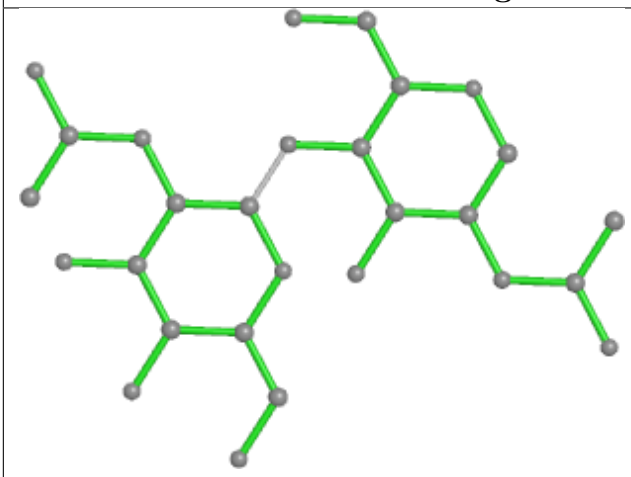
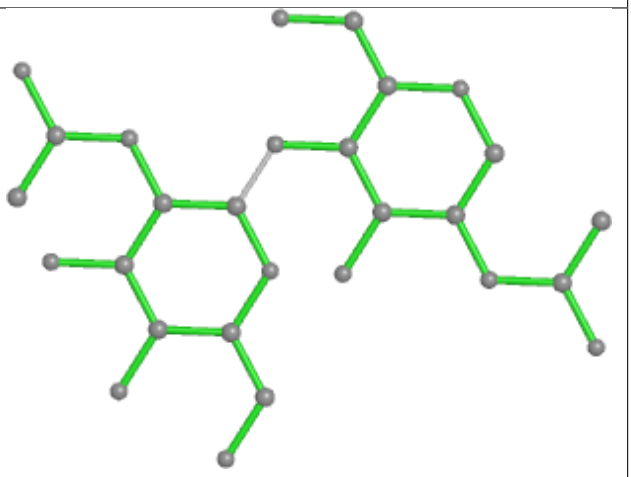


Rings

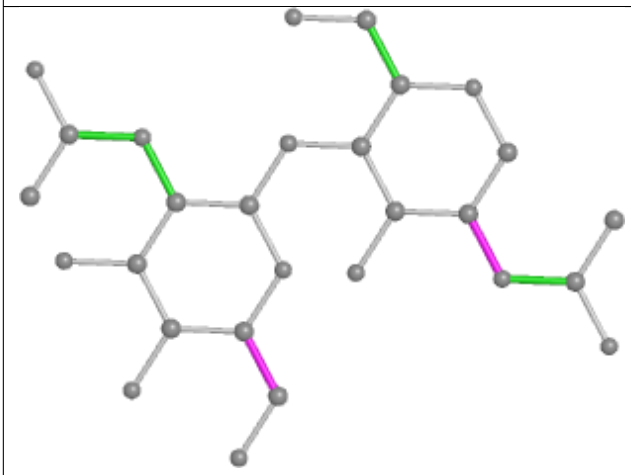
Oligosaccharide Chain X



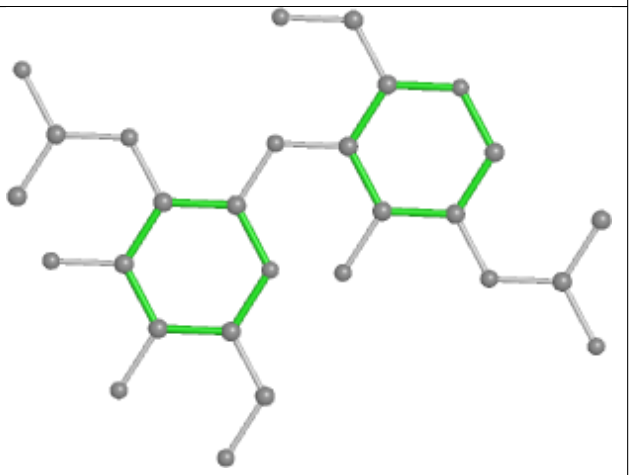
Bond lengths



Bond angles

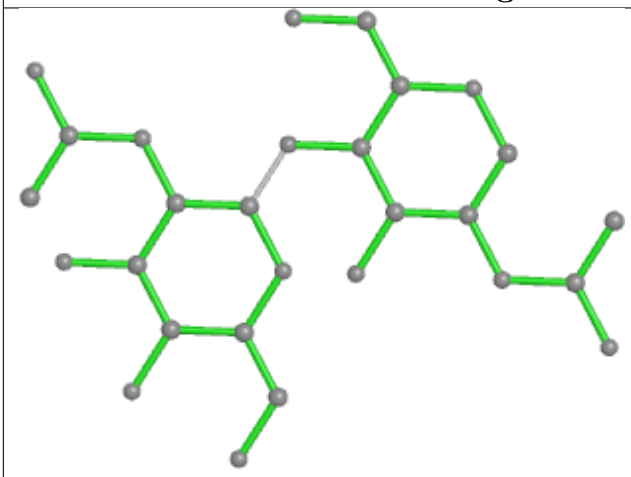


Torsions

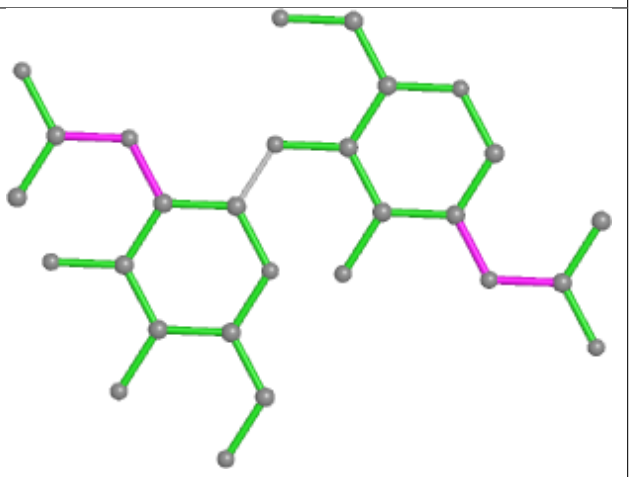


Rings

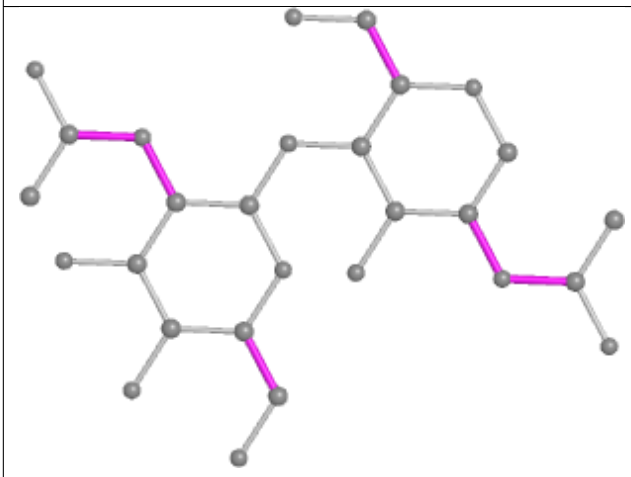
Oligosaccharide Chain Z



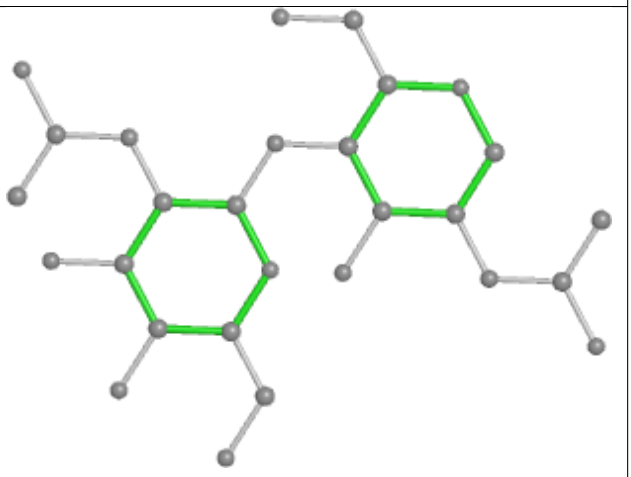
Bond lengths



Bond angles

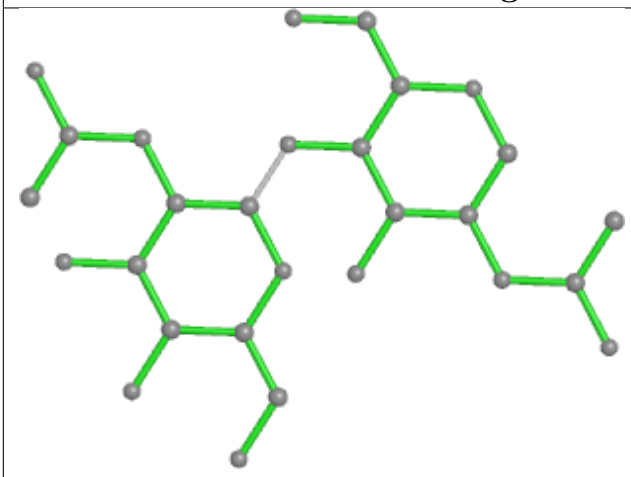


Torsions

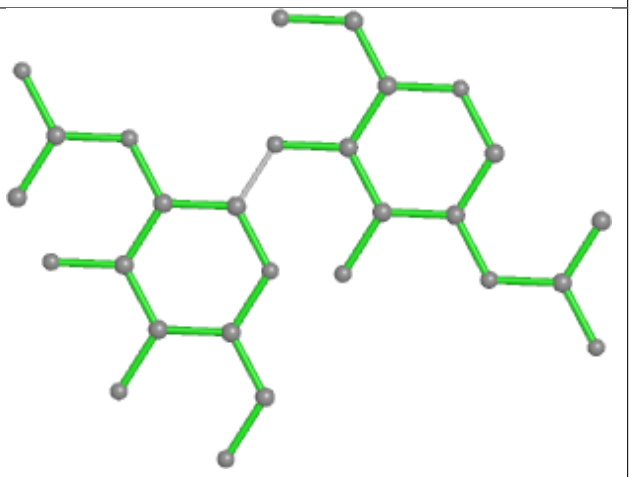


Rings

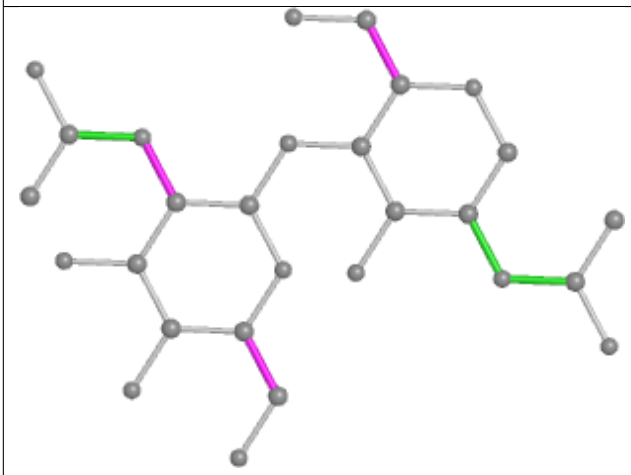
Oligosaccharide Chain f



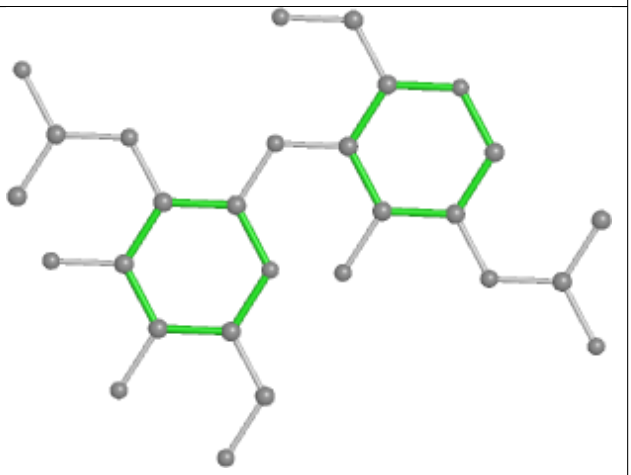
Bond lengths



Bond angles

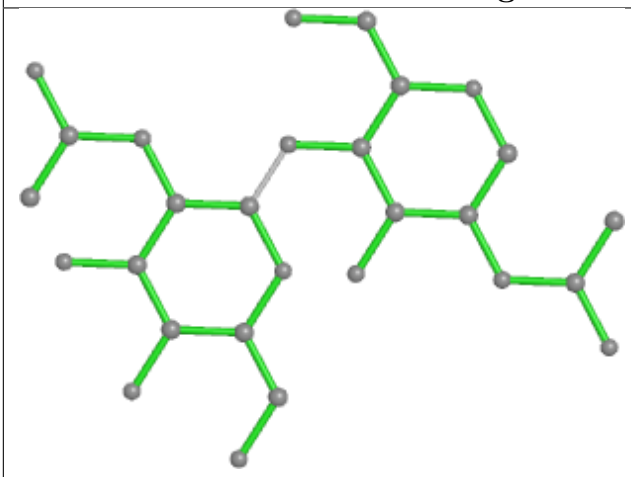


Torsions

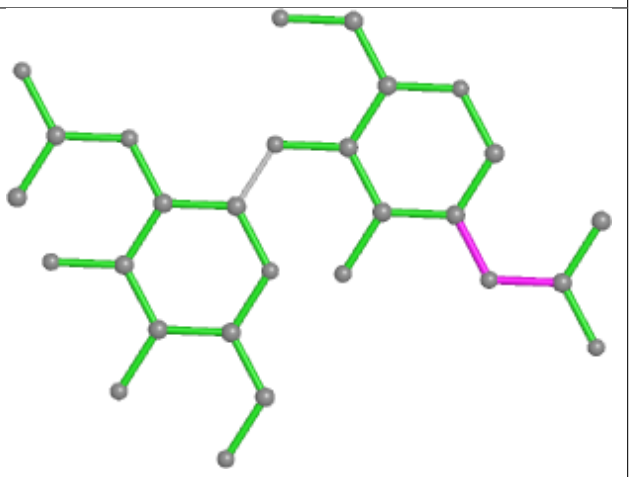


Rings

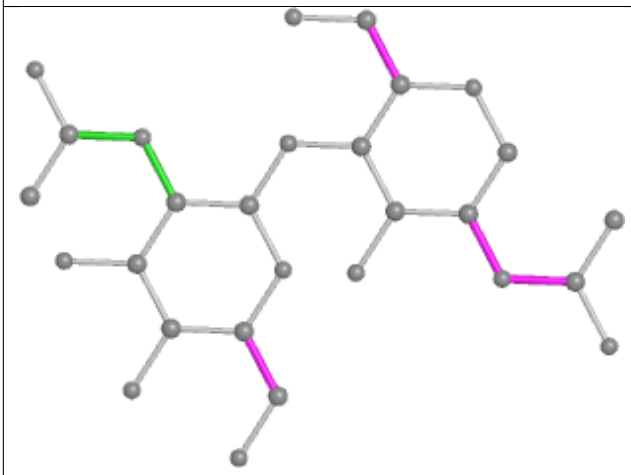
Oligosaccharide Chain h



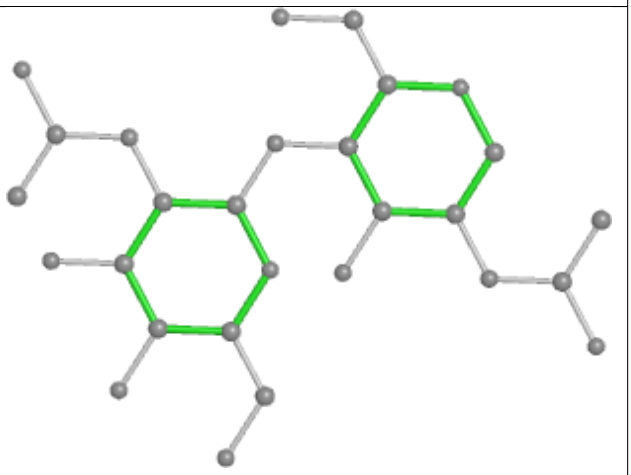
Bond lengths



Bond angles

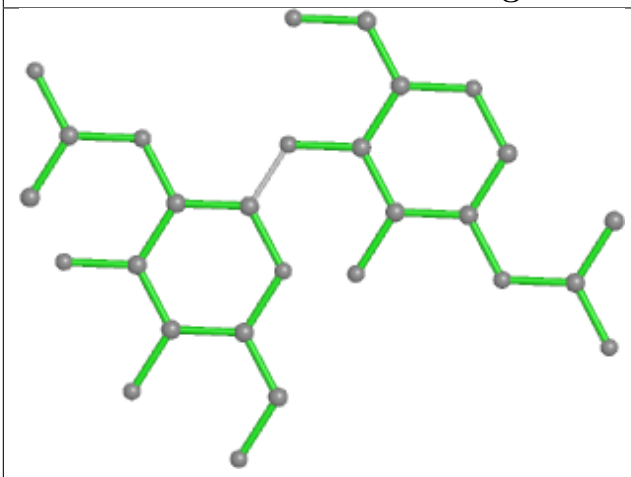


Torsions

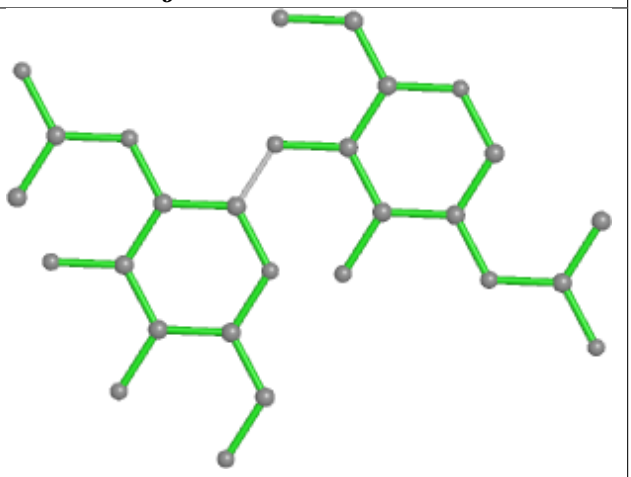


Rings

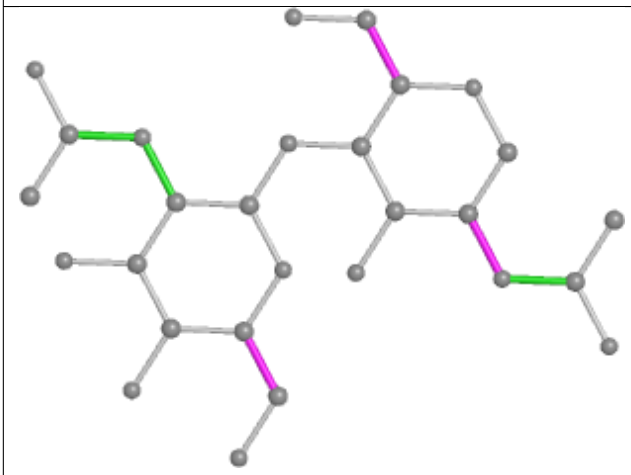
Oligosaccharide Chain j



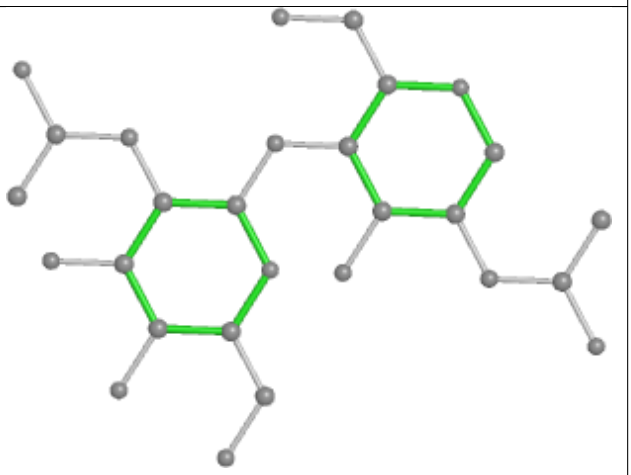
Bond lengths



Bond angles

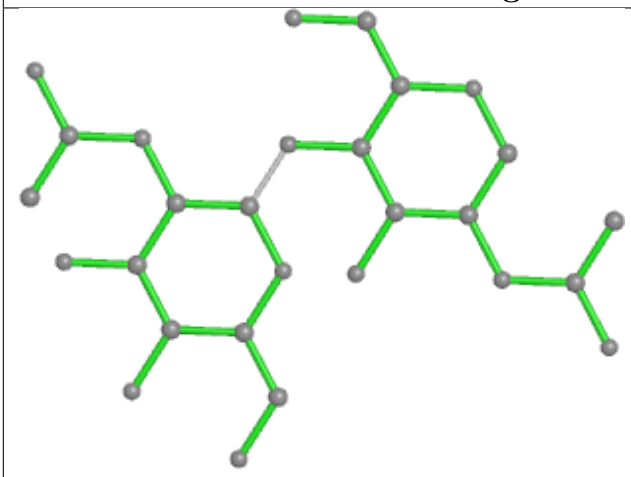


Torsions

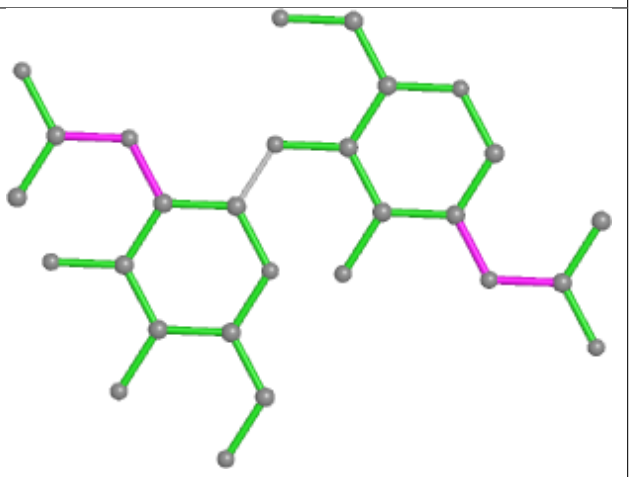


Rings

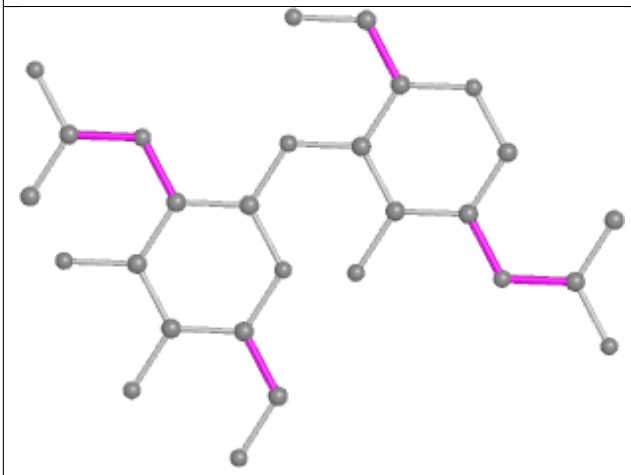
Oligosaccharide Chain l



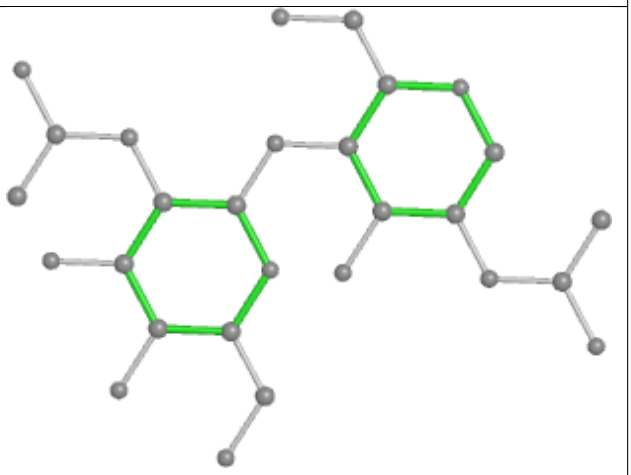
Bond lengths



Bond angles

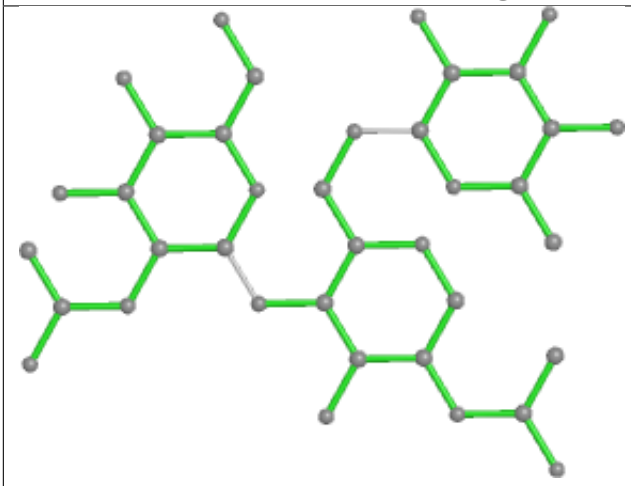


Torsions

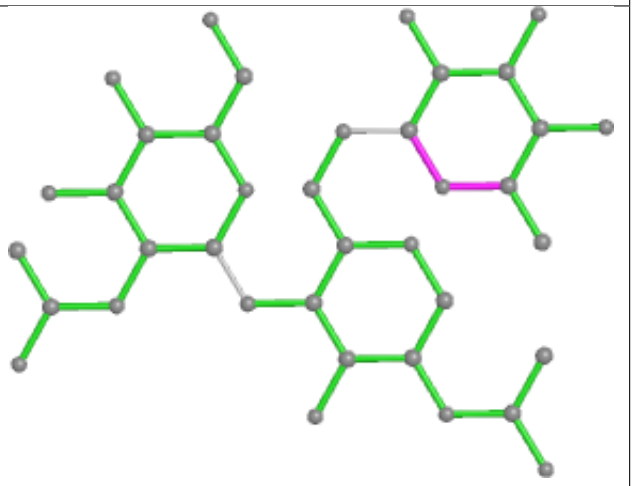


Rings

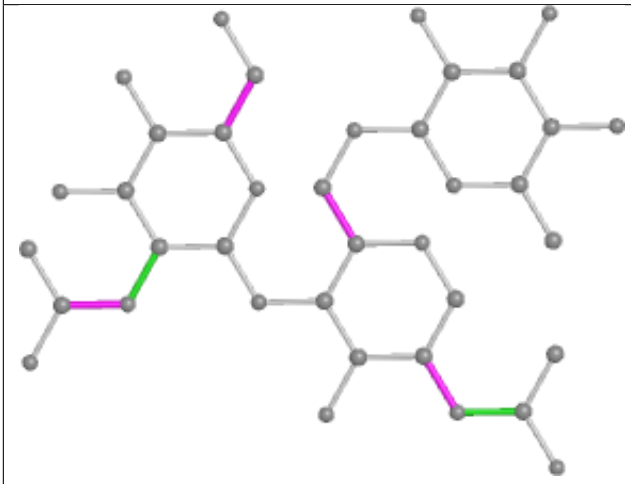
Oligosaccharide Chain O



Bond lengths



Bond angles



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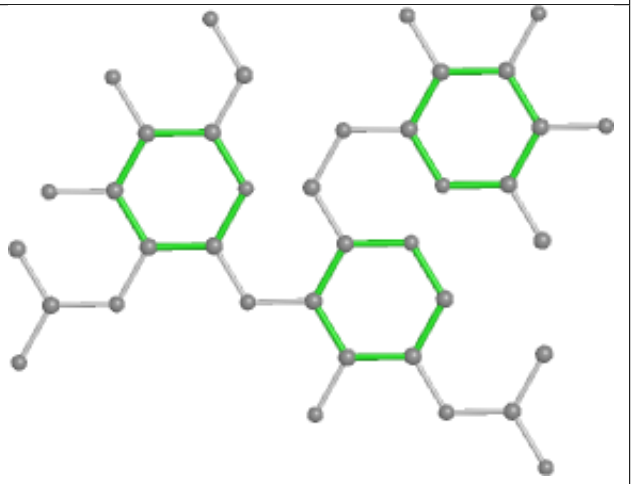
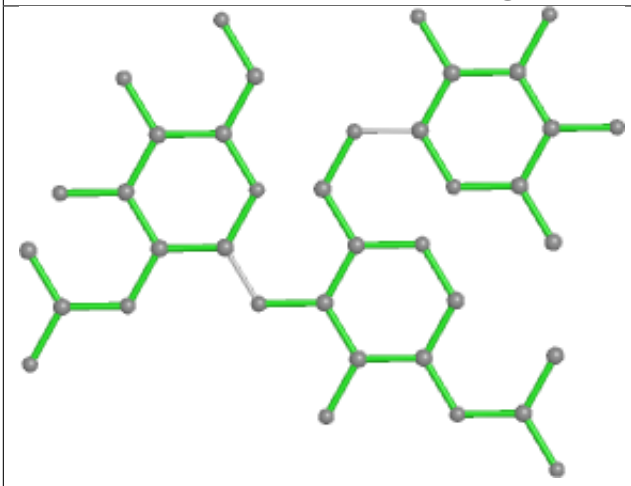
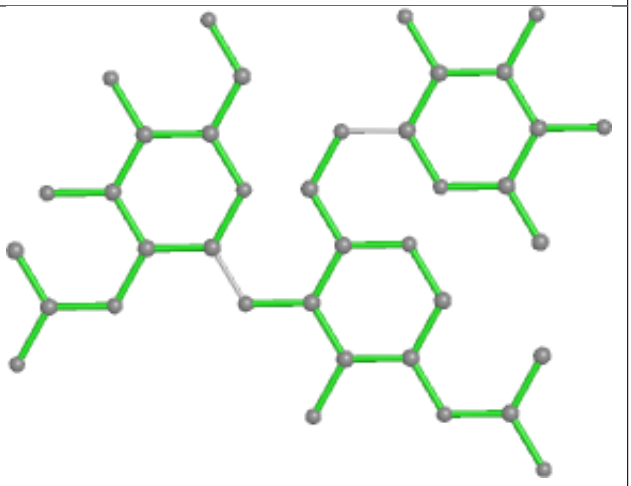


Rings

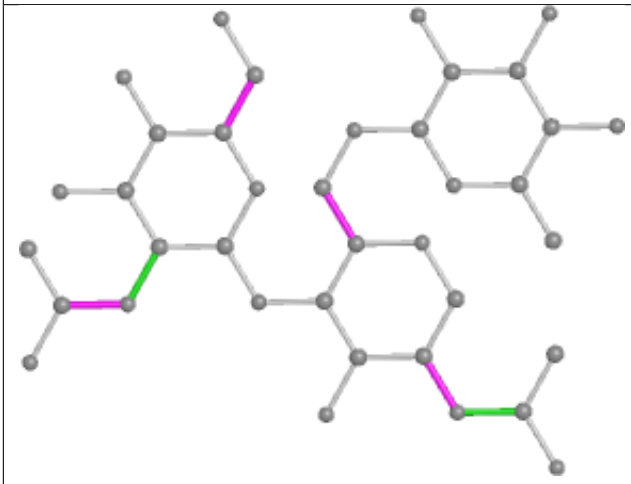
Oligosaccharide Chain a



Bond lengths



Bond angles



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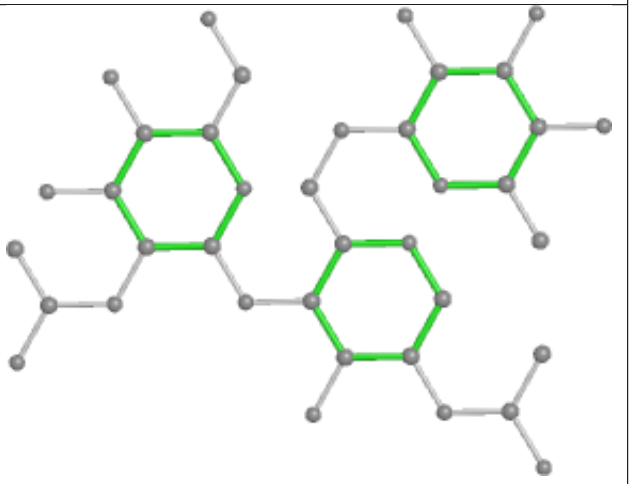
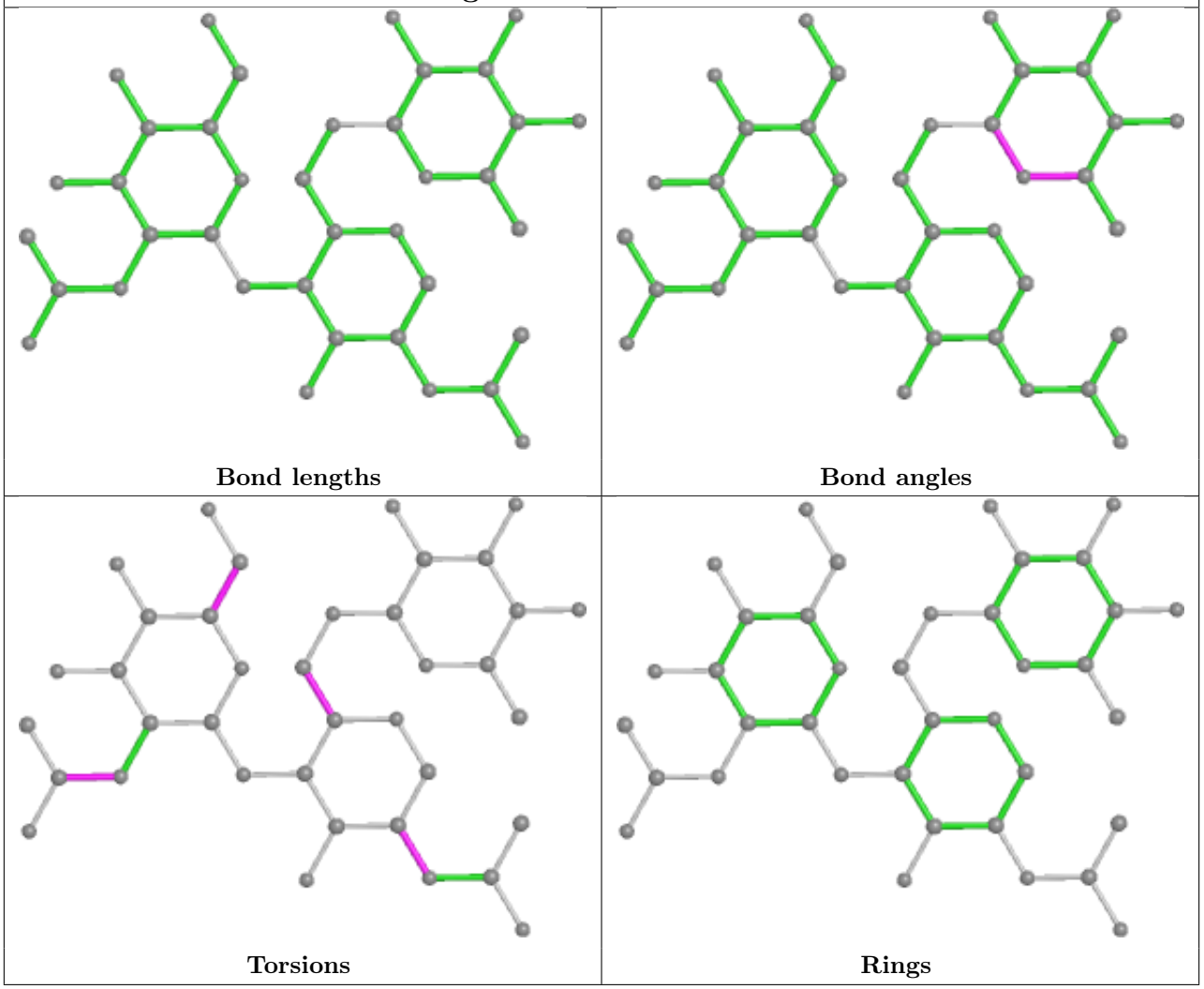


Rings

Oligosaccharide Chain m



5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
8	NAG	B	1504	1	14,14,15	0.26	0	17,19,21	0.35	0
8	NAG	B	1502	1	14,14,15	0.33	0	17,19,21	0.38	0
8	NAG	A	1502	1	14,14,15	0.50	0	17,19,21	0.73	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	C	1503	1	14,14,15	0.31	0	17,19,21	0.39	0
8	NAG	A	1503	1	14,14,15	0.46	0	17,19,21	0.45	0
8	NAG	C	1504	1	14,14,15	0.20	0	17,19,21	0.43	0
8	NAG	B	1503	1	14,14,15	0.34	0	17,19,21	0.59	1 (5%)
8	NAG	A	1501	1	14,14,15	0.46	0	17,19,21	0.51	0
8	NAG	C	1502	1	14,14,15	0.22	0	17,19,21	0.34	0
8	NAG	C	1501	1	14,14,15	0.20	0	17,19,21	0.37	0
8	NAG	A	1504	1	14,14,15	0.23	0	17,19,21	0.48	0
8	NAG	B	1501	1	14,14,15	0.67	0	17,19,21	1.36	2 (11%)

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
8	NAG	B	1504	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1502	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1502	1	-	4/6/23/26	0/1/1/1
8	NAG	C	1503	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1503	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1504	1	-	4/6/23/26	0/1/1/1
8	NAG	B	1503	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1501	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1502	1	-	4/6/23/26	0/1/1/1
8	NAG	C	1501	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1504	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1501	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1501	NAG	C2-N2-C7	4.21	128.90	122.90
8	A	1502	NAG	C1-O5-C5	2.63	115.76	112.19
8	B	1501	NAG	C1-O5-C5	2.56	115.66	112.19
8	B	1503	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1502	NAG	O5-C5-C6-O6
8	A	1503	NAG	O5-C5-C6-O6
8	C	1504	NAG	O5-C5-C6-O6
8	C	1502	NAG	C4-C5-C6-O6
8	A	1502	NAG	O5-C5-C6-O6
8	B	1502	NAG	O5-C5-C6-O6
8	A	1502	NAG	C4-C5-C6-O6
8	B	1502	NAG	C4-C5-C6-O6
8	A	1502	NAG	C8-C7-N2-C2
8	A	1502	NAG	O7-C7-N2-C2
8	B	1501	NAG	C8-C7-N2-C2
8	B	1501	NAG	O7-C7-N2-C2
8	B	1502	NAG	C8-C7-N2-C2
8	B	1502	NAG	O7-C7-N2-C2
8	C	1502	NAG	C8-C7-N2-C2
8	C	1502	NAG	O7-C7-N2-C2
8	C	1504	NAG	C8-C7-N2-C2
8	C	1504	NAG	O7-C7-N2-C2
8	C	1503	NAG	O5-C5-C6-O6
8	A	1504	NAG	O5-C5-C6-O6
8	A	1503	NAG	C4-C5-C6-O6
8	C	1504	NAG	C4-C5-C6-O6
8	A	1504	NAG	C4-C5-C6-O6
8	C	1501	NAG	O5-C5-C6-O6
8	C	1503	NAG	C4-C5-C6-O6
8	C	1501	NAG	C4-C5-C6-O6
8	B	1501	NAG	C3-C2-N2-C7

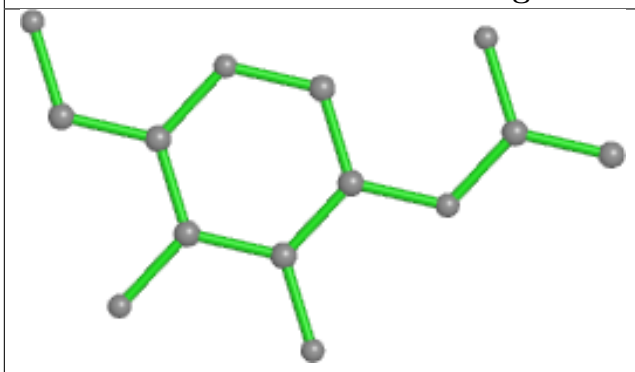
There are no ring outliers.

No monomer is involved in short contacts.

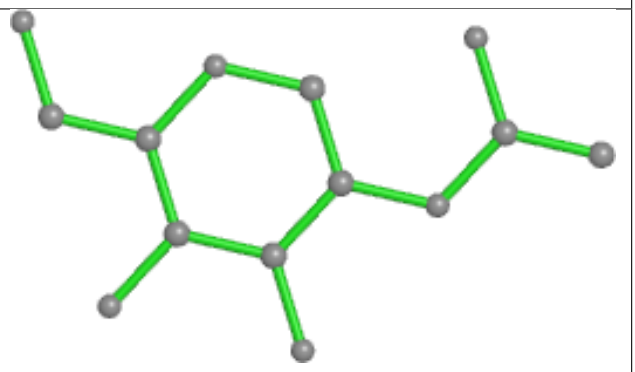
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

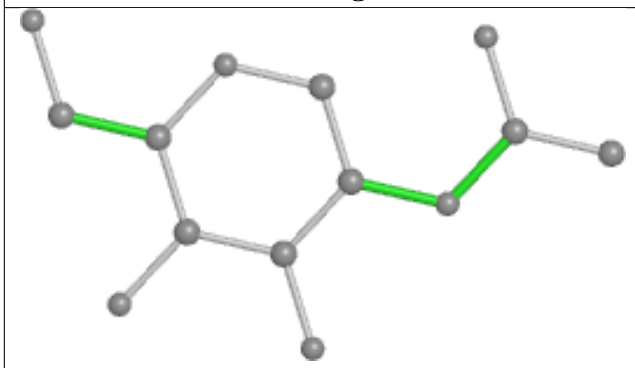
Ligand NAG B 1504



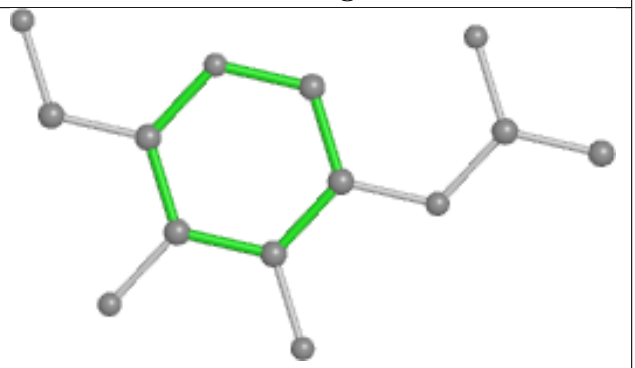
Bond lengths



Bond angles

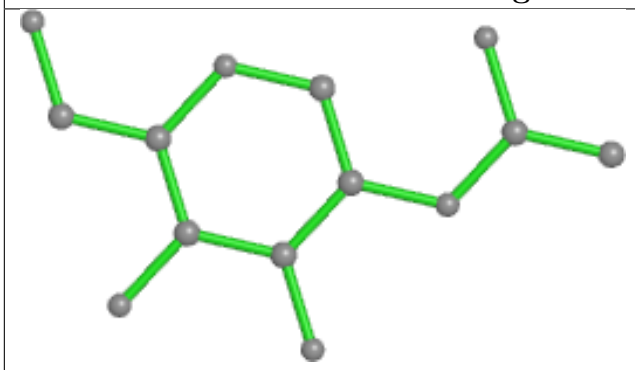


Torsions

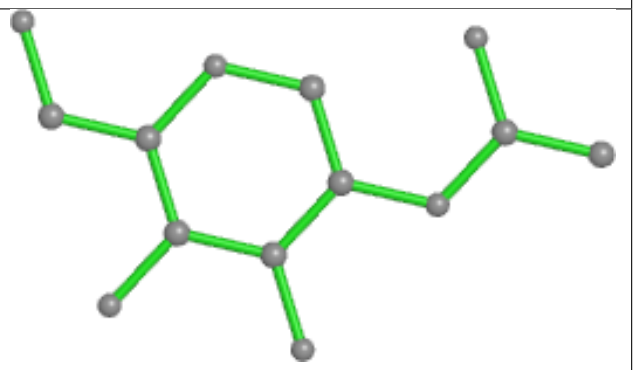


Rings

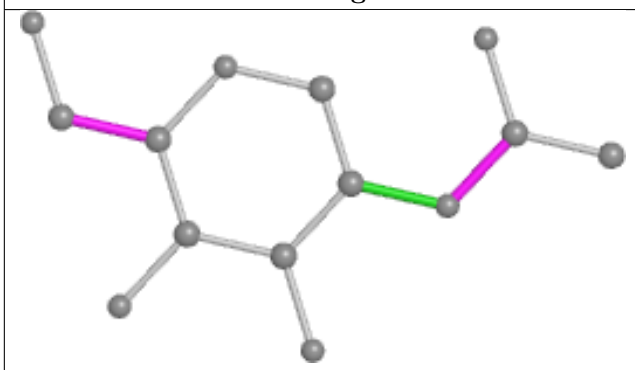
Ligand NAG B 1502



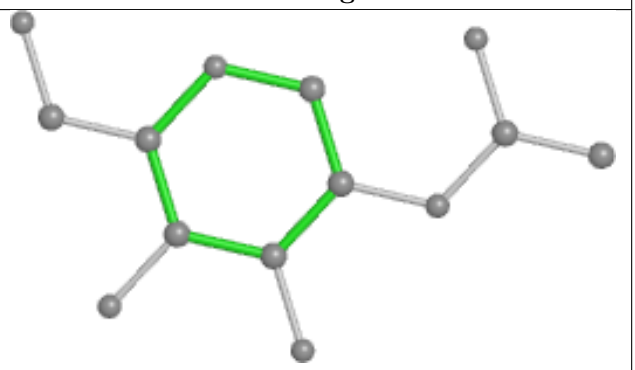
Bond lengths



Bond angles

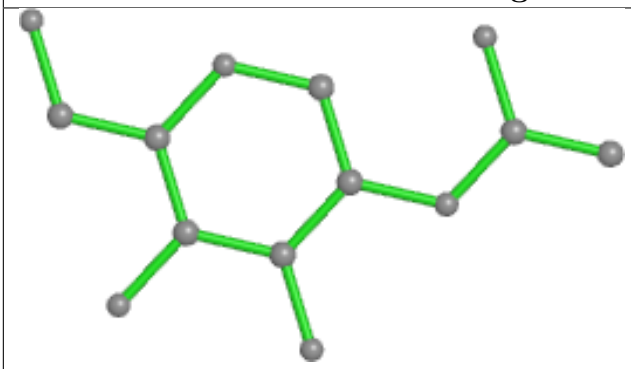


Torsions

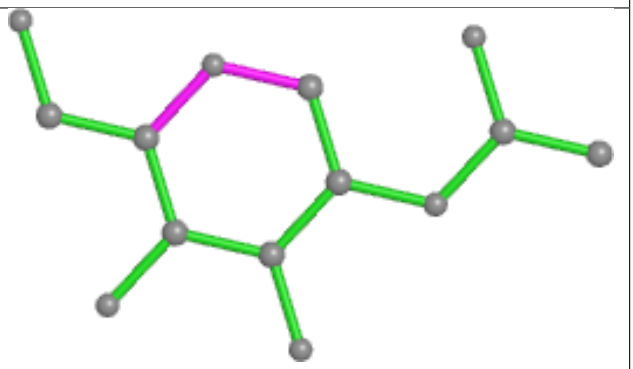


Rings

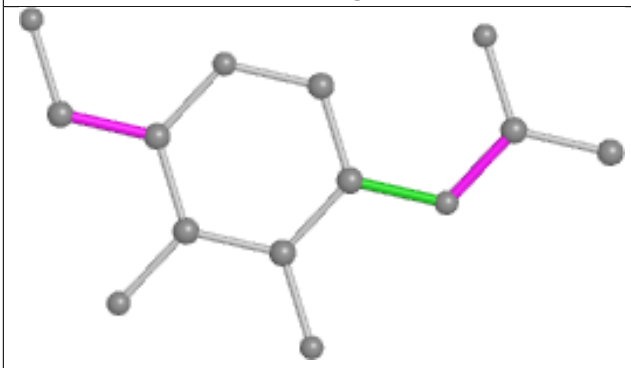
Ligand NAG A 1502



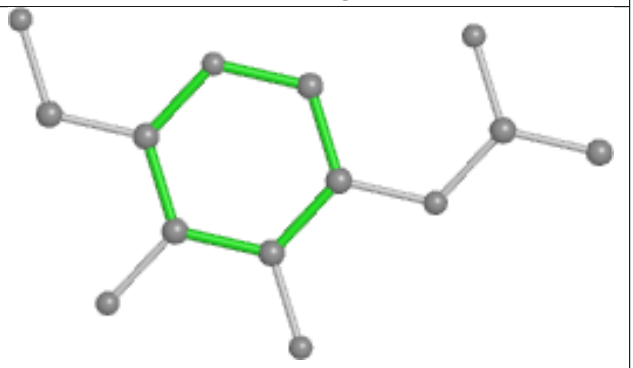
Bond lengths



Bond angles

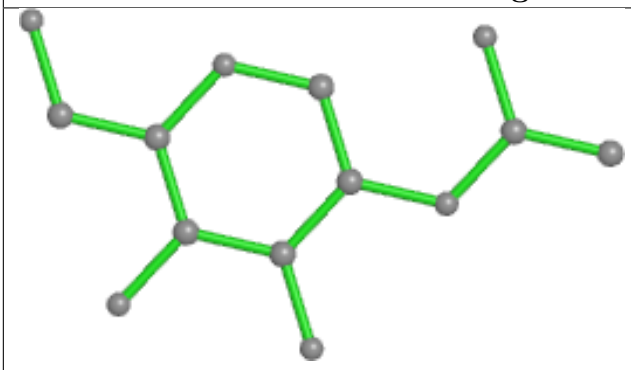


Torsions

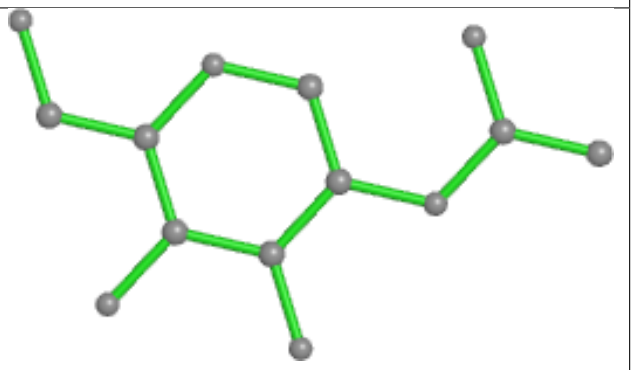


Rings

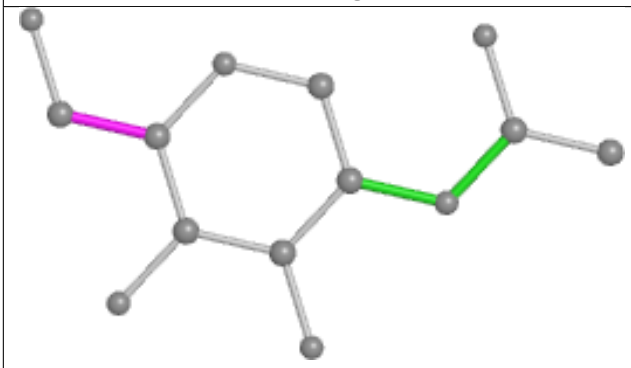
Ligand NAG C 1503



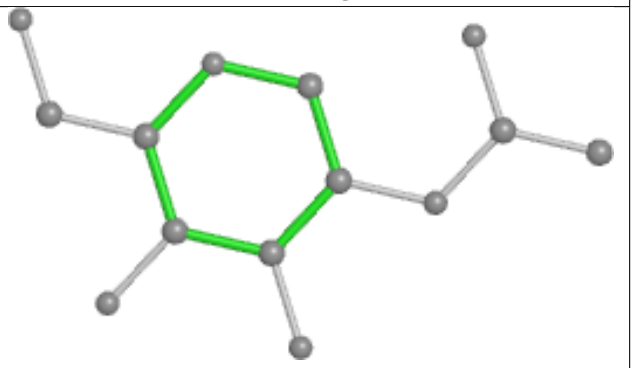
Bond lengths



Bond angles

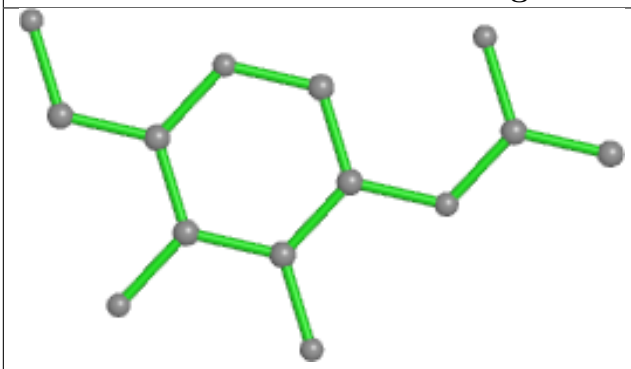


Torsions

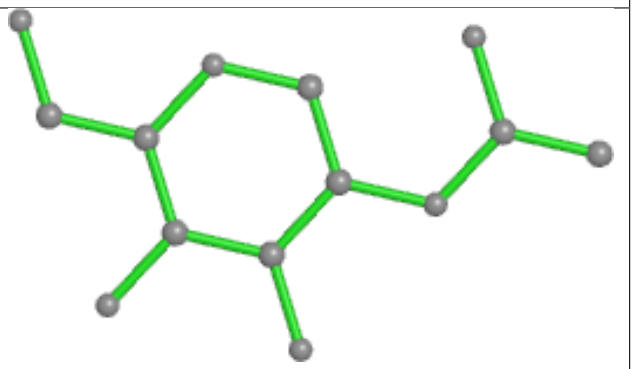


Rings

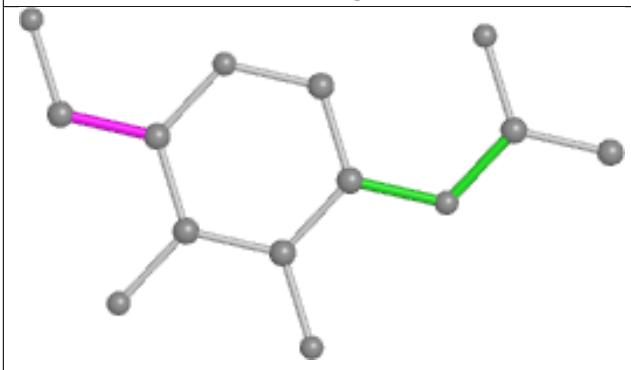
Ligand NAG A 1503



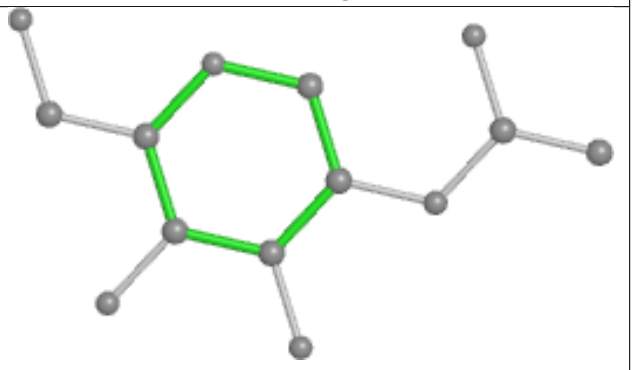
Bond lengths



Bond angles

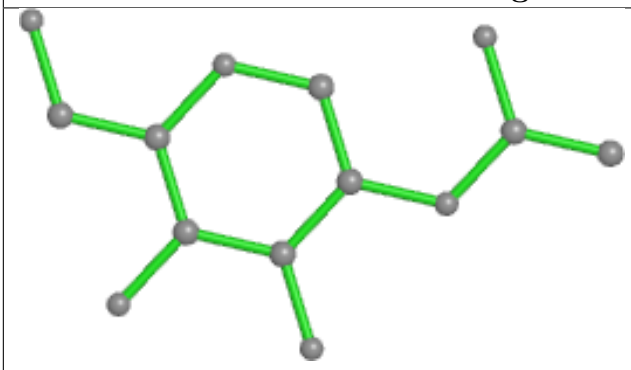


Torsions

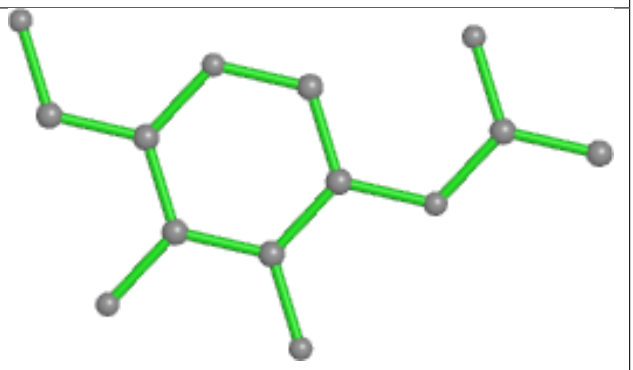


Rings

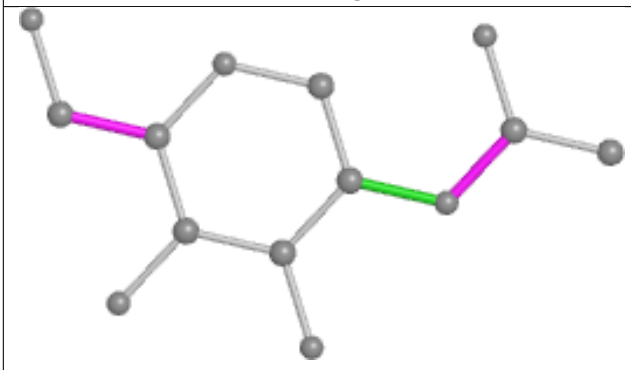
Ligand NAG C 1504



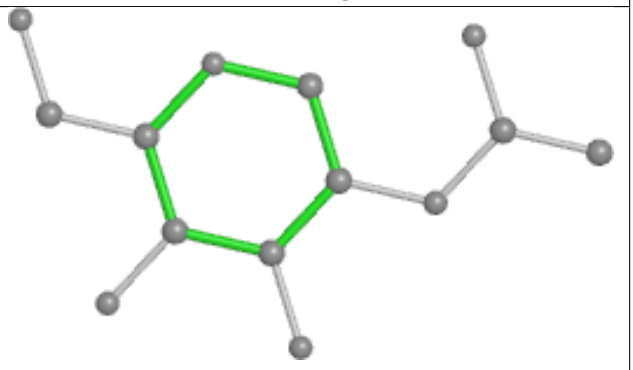
Bond lengths



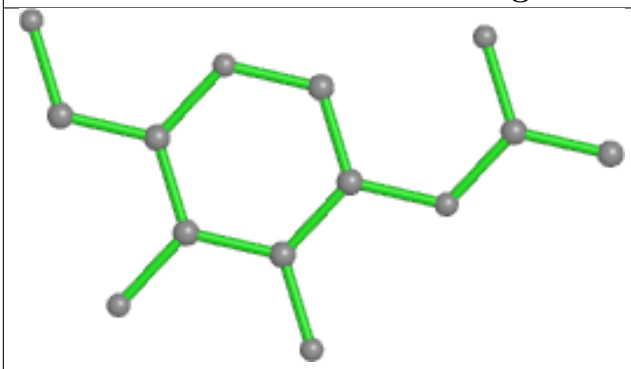
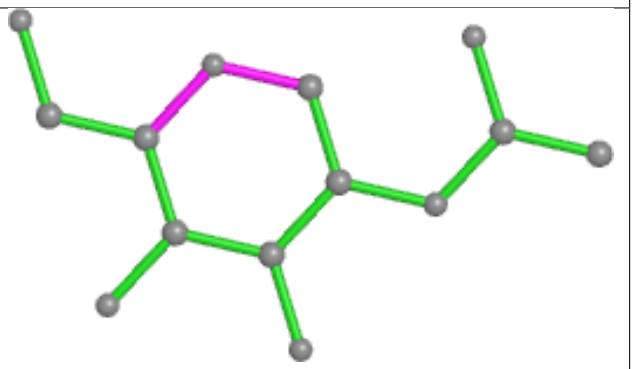
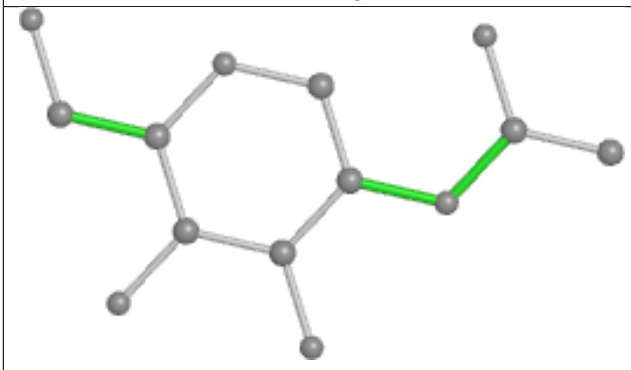
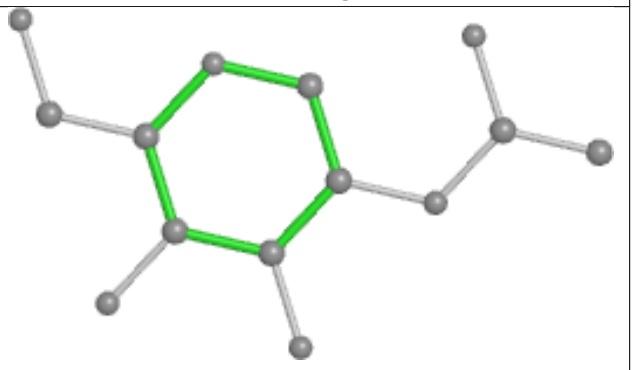
Bond angles

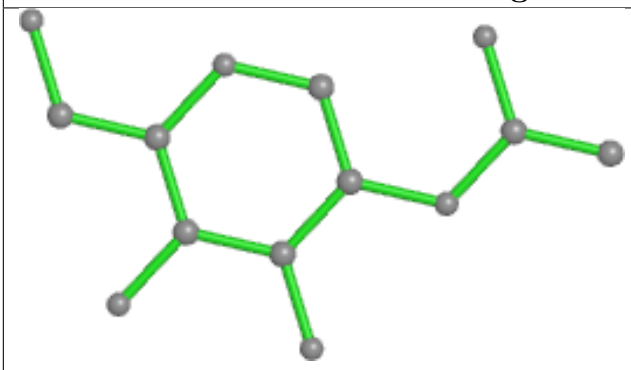
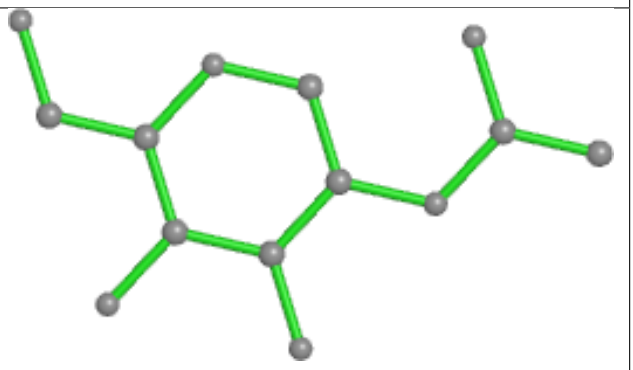
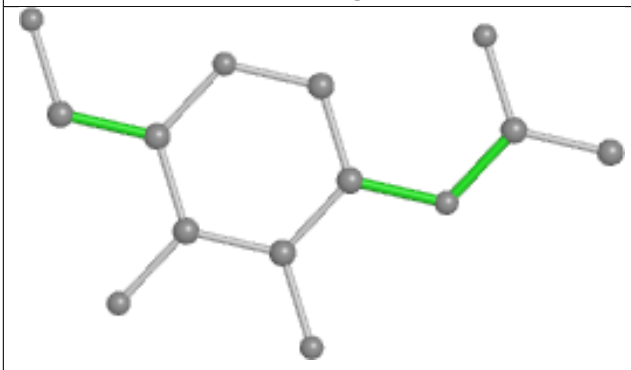
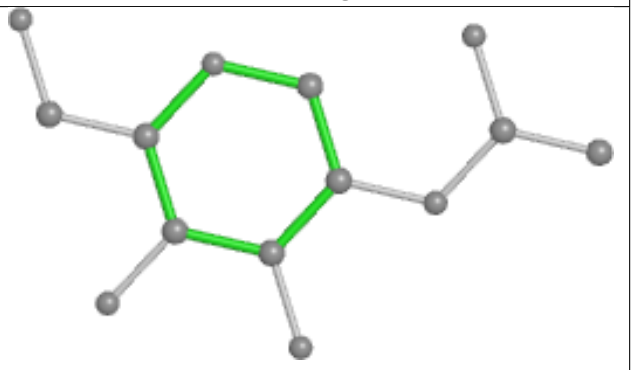


Torsions

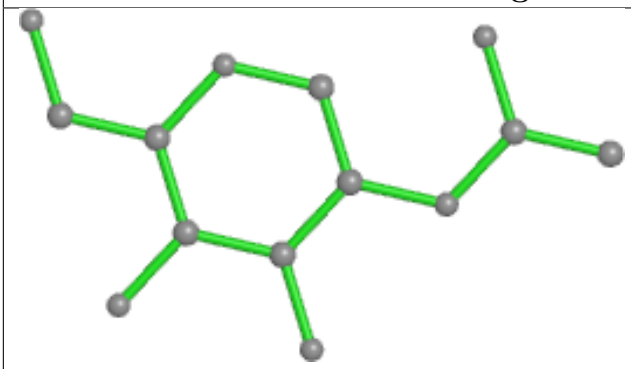


Rings

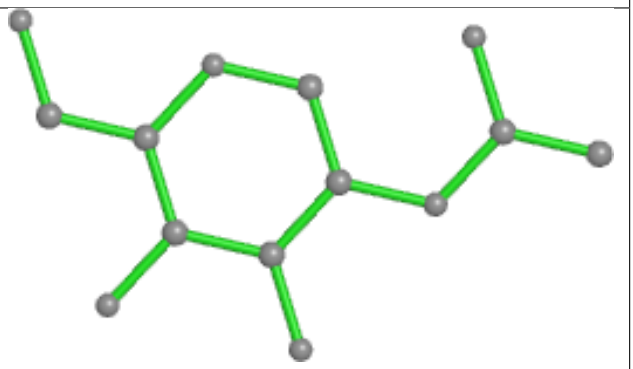
Ligand NAG B 1503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1501	
 Bond lengths	 Bond angles
 Torsions	 Rings

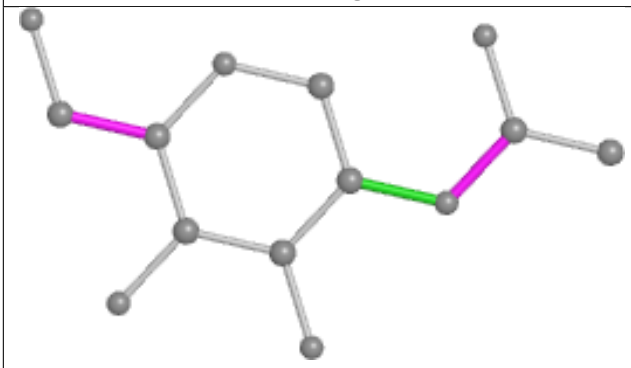
Ligand NAG C 1502



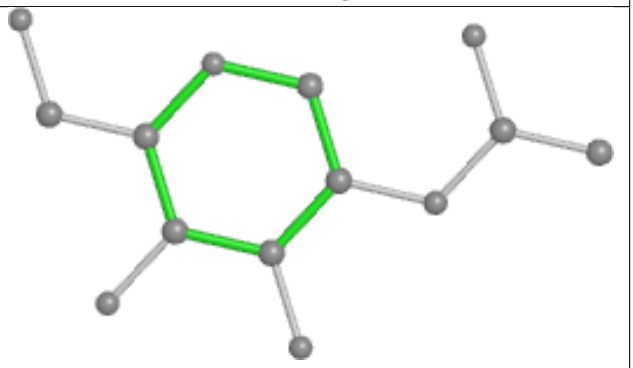
Bond lengths



Bond angles

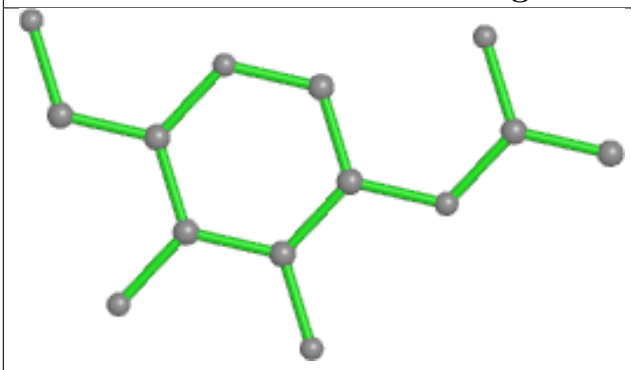


Torsions

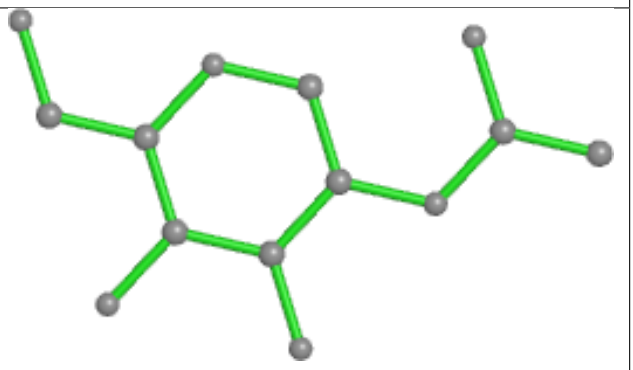


Rings

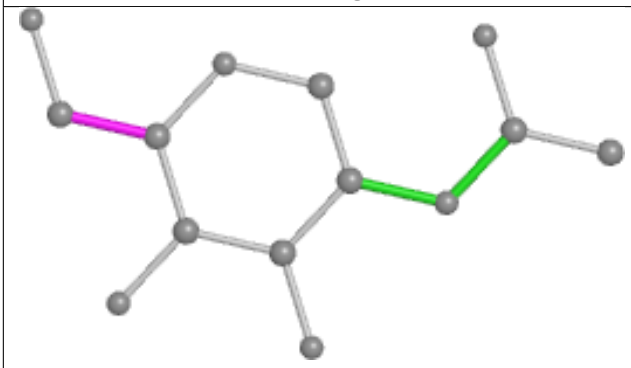
Ligand NAG C 1501



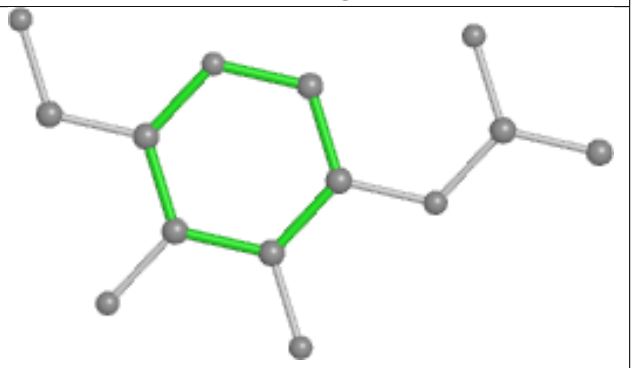
Bond lengths



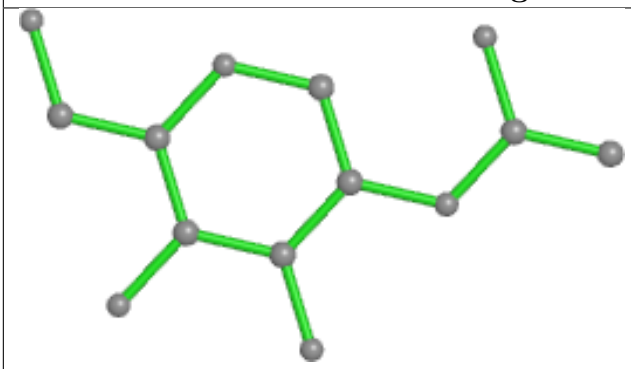
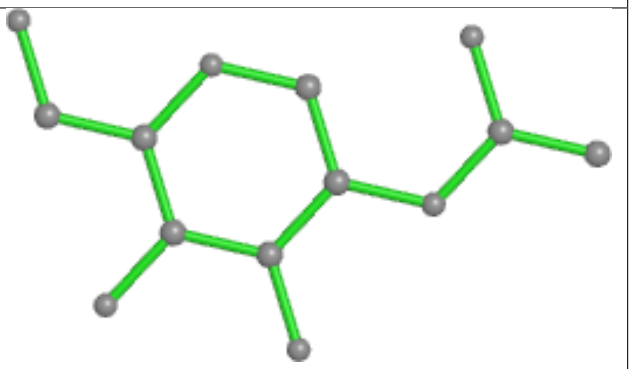
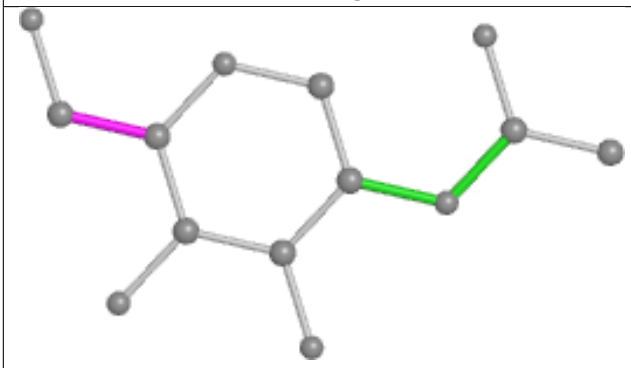
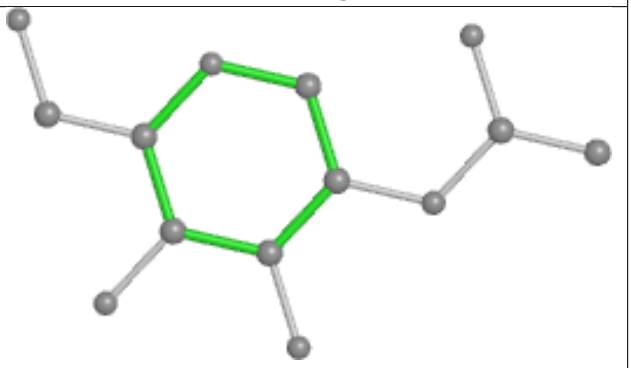
Bond angles

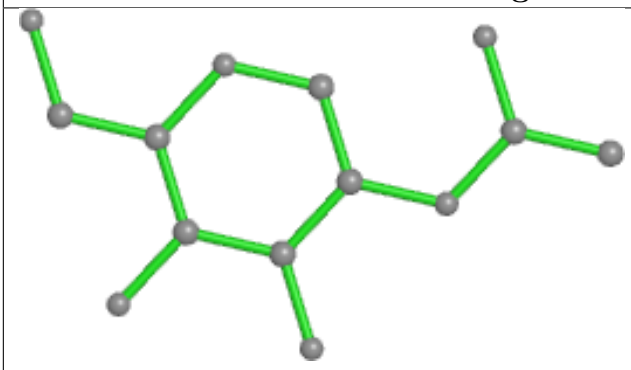
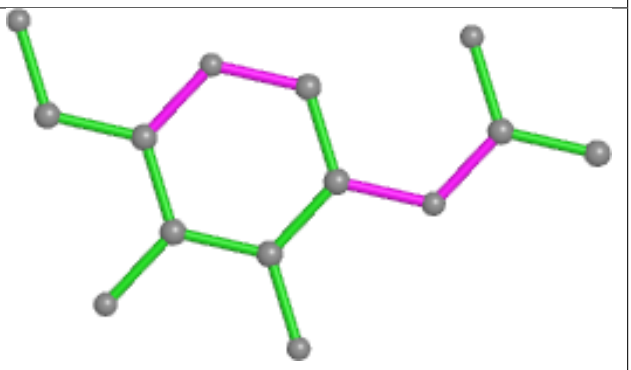
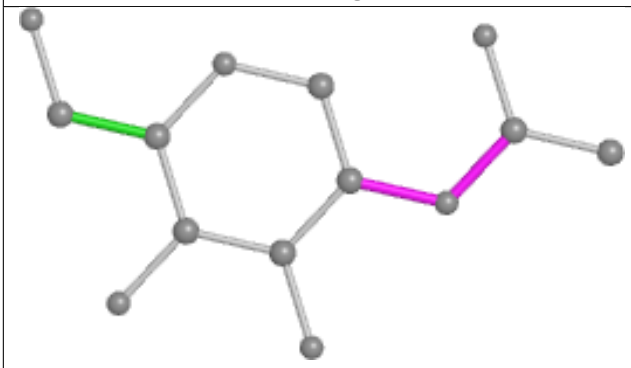
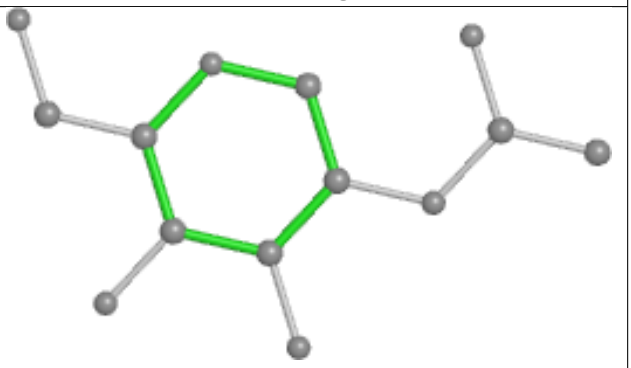


Torsions



Rings

Ligand NAG A 1504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

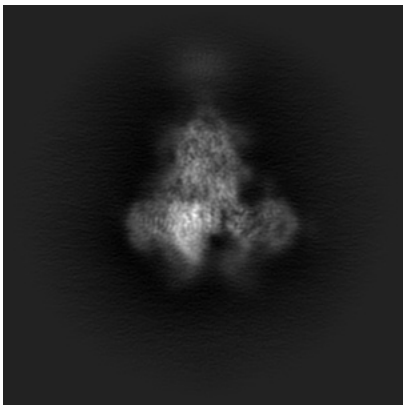
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33646. These allow visual inspection of the internal detail of the map and identification of artifacts.

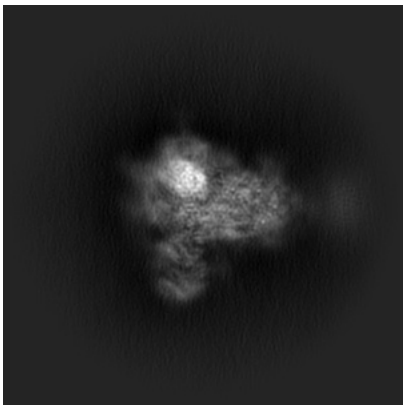
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

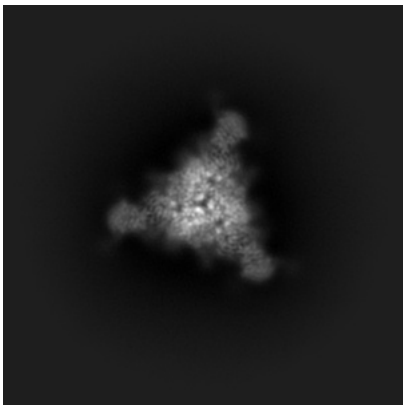
6.1.1 Primary map



X

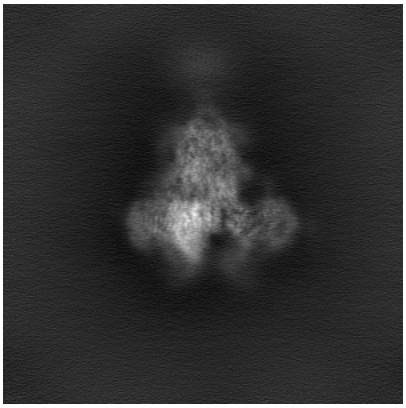


Y

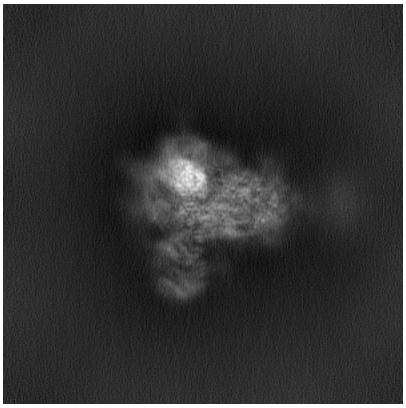


Z

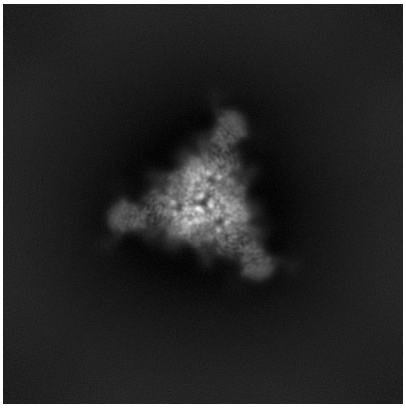
6.1.2 Raw map



X



Y

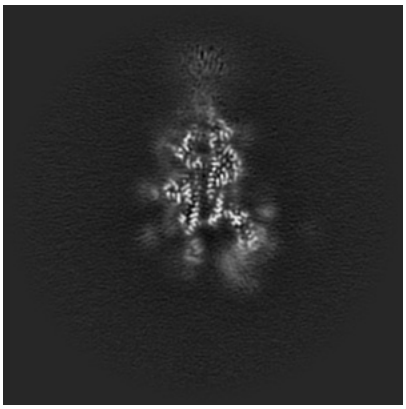


Z

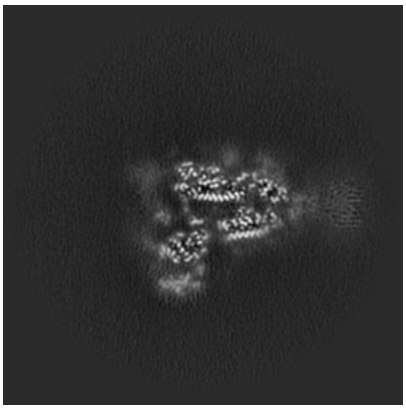
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

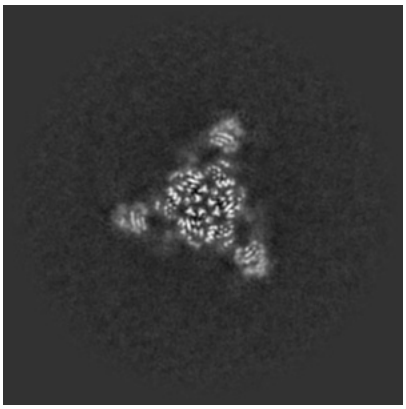
6.2.1 Primary map



X Index: 182

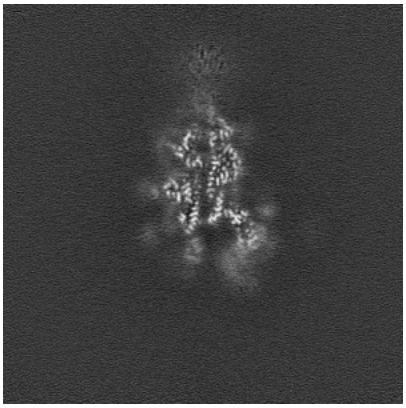


Y Index: 182

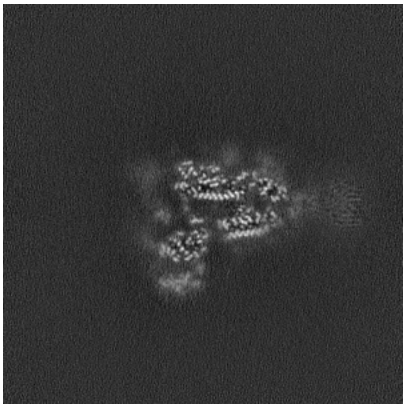


Z Index: 182

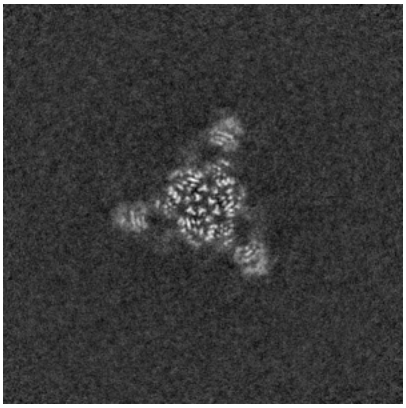
6.2.2 Raw map



X Index: 182



Y Index: 182

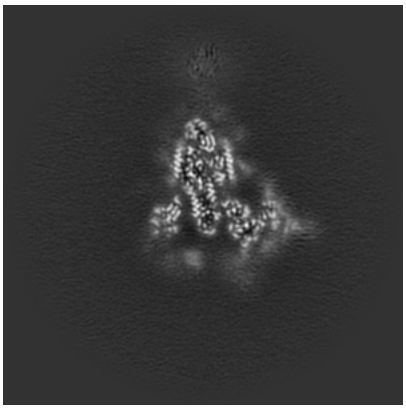


Z Index: 182

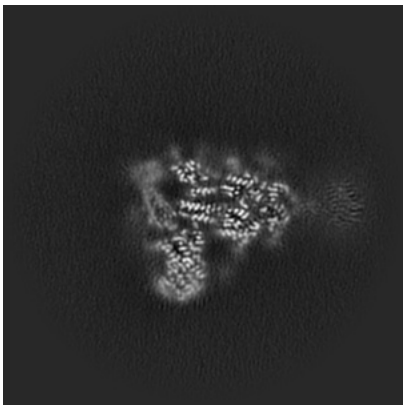
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

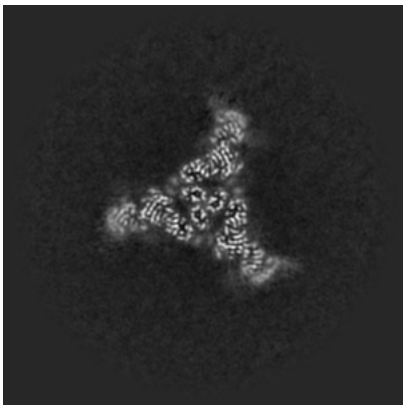
6.3.1 Primary map



X Index: 195

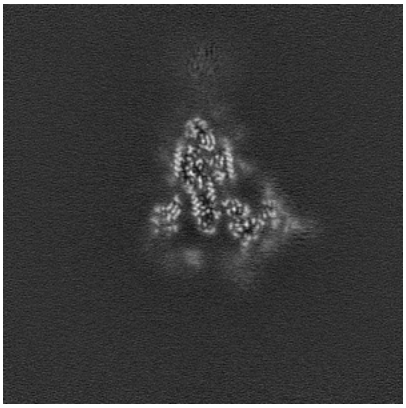


Y Index: 174

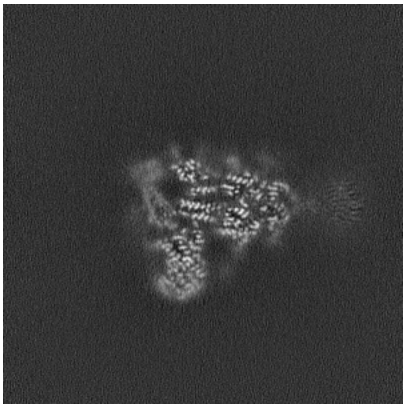


Z Index: 167

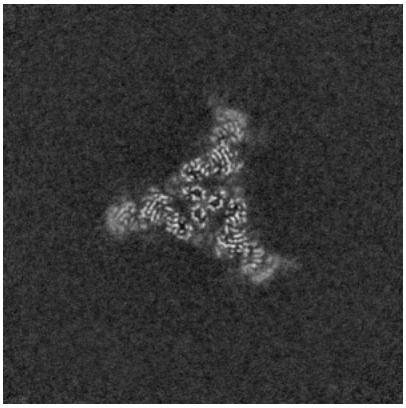
6.3.2 Raw map



X Index: 195



Y Index: 174



Z Index: 167

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

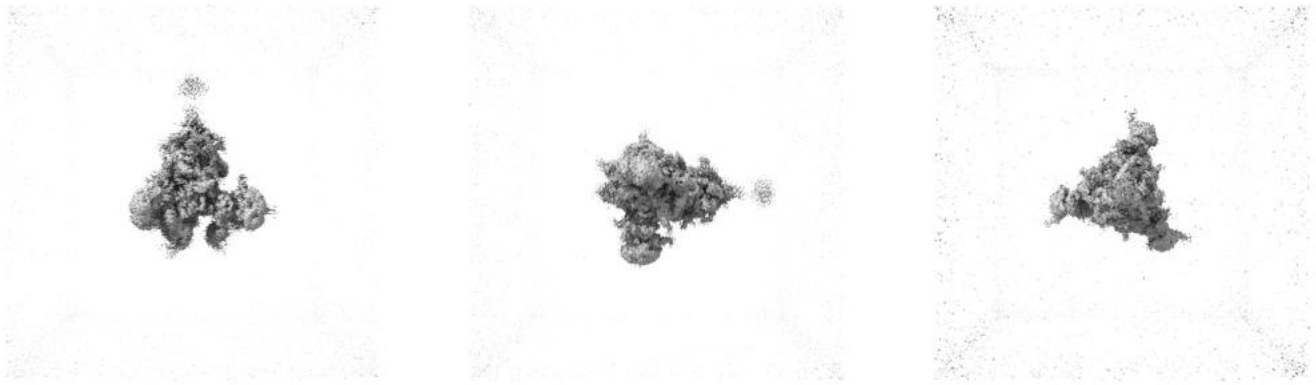
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

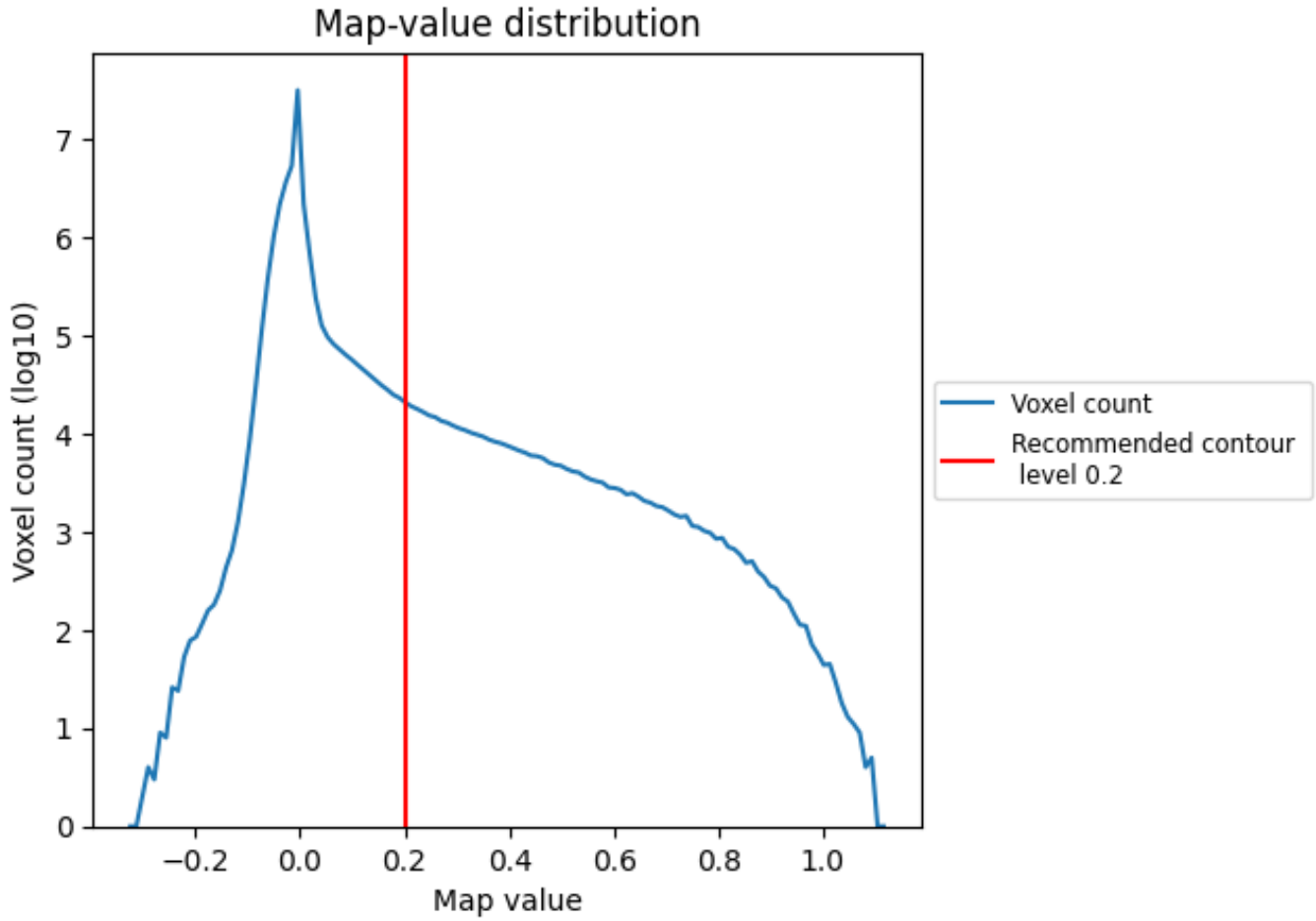
6.5 Mask visualisation (i)

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

7 Map analysis

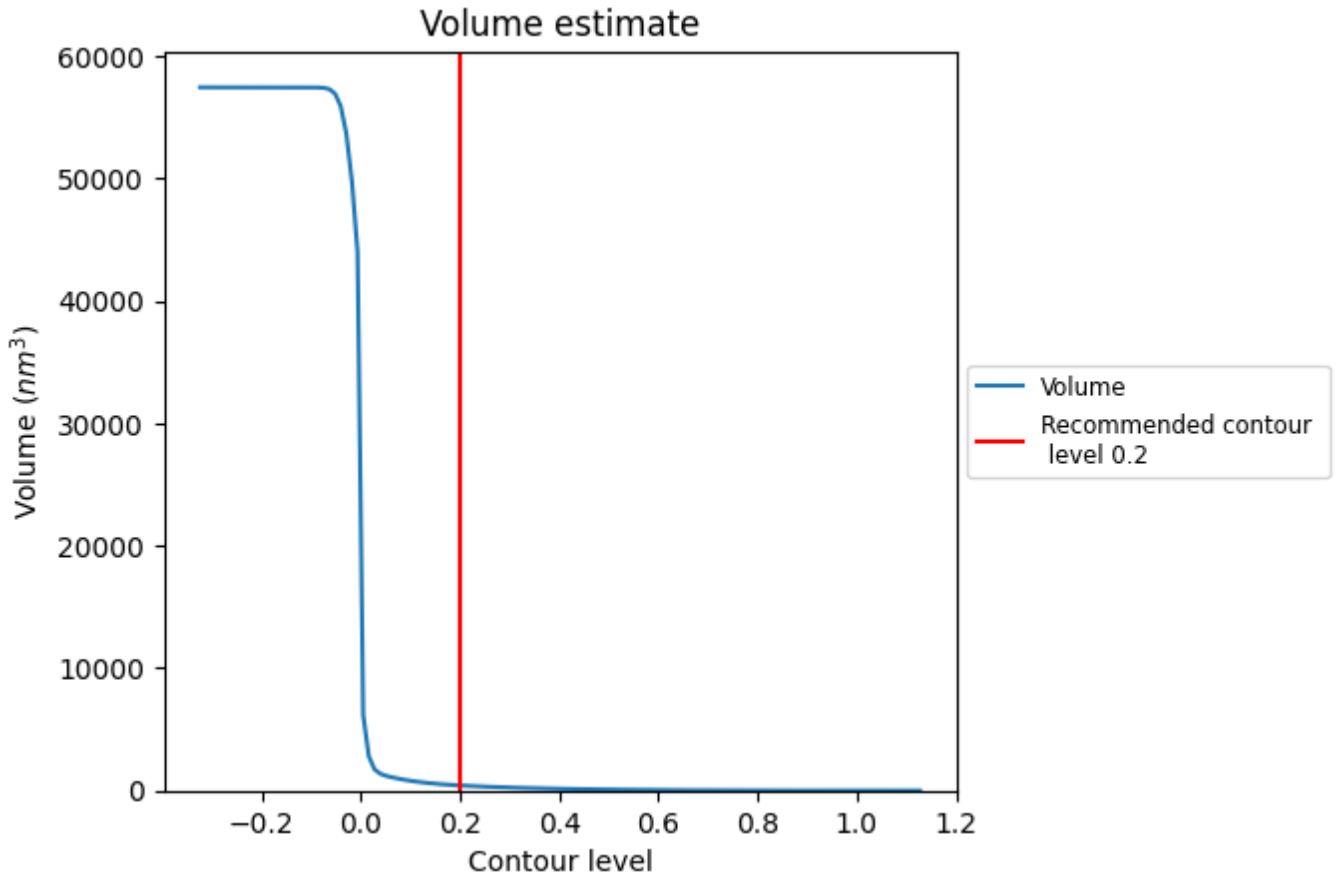
This section contains the results of statistical analysis of the map.

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.

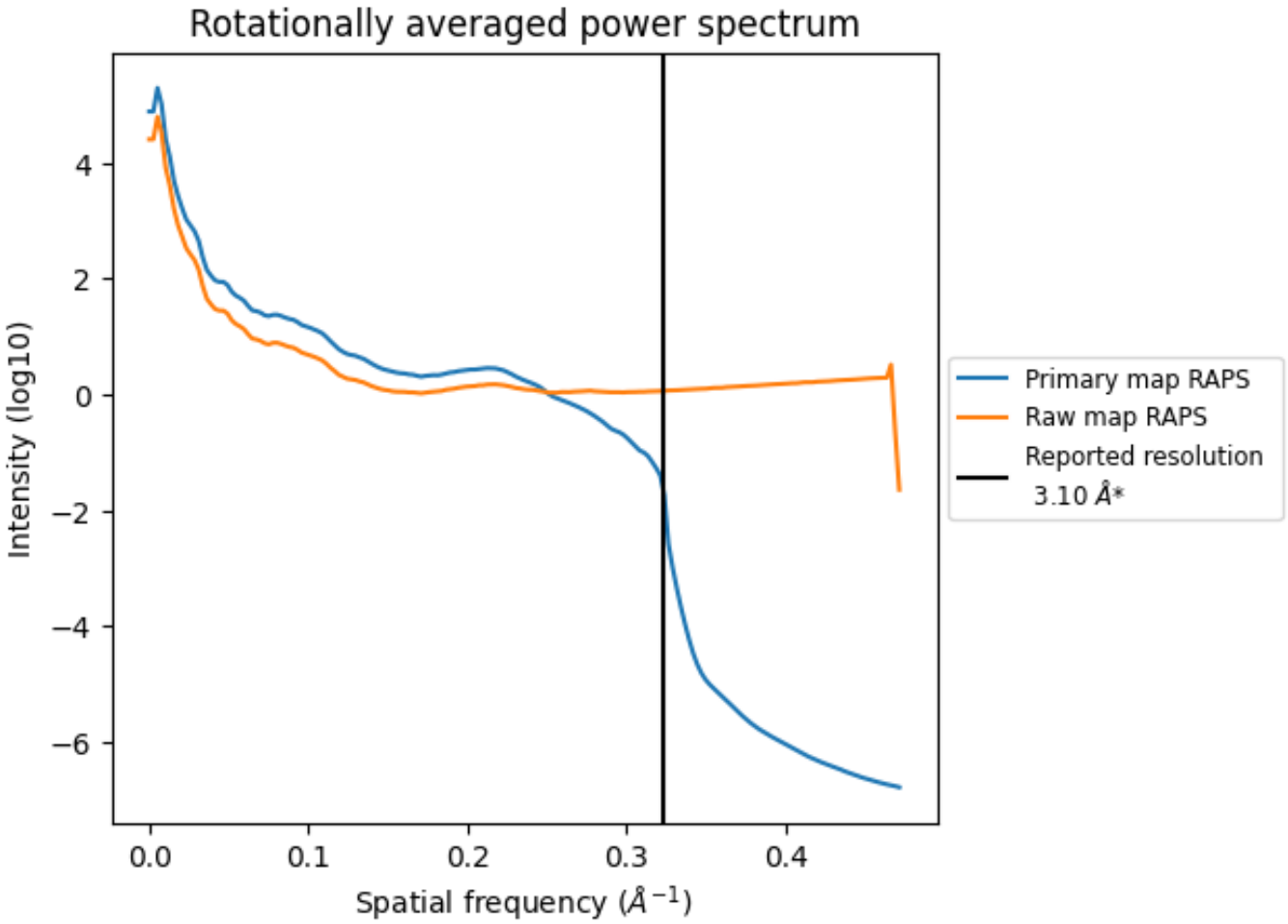
7.2 Volume estimate



The volume at the recommended contour level is 414 nm^3; this corresponds to an approximate mass of 374 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)

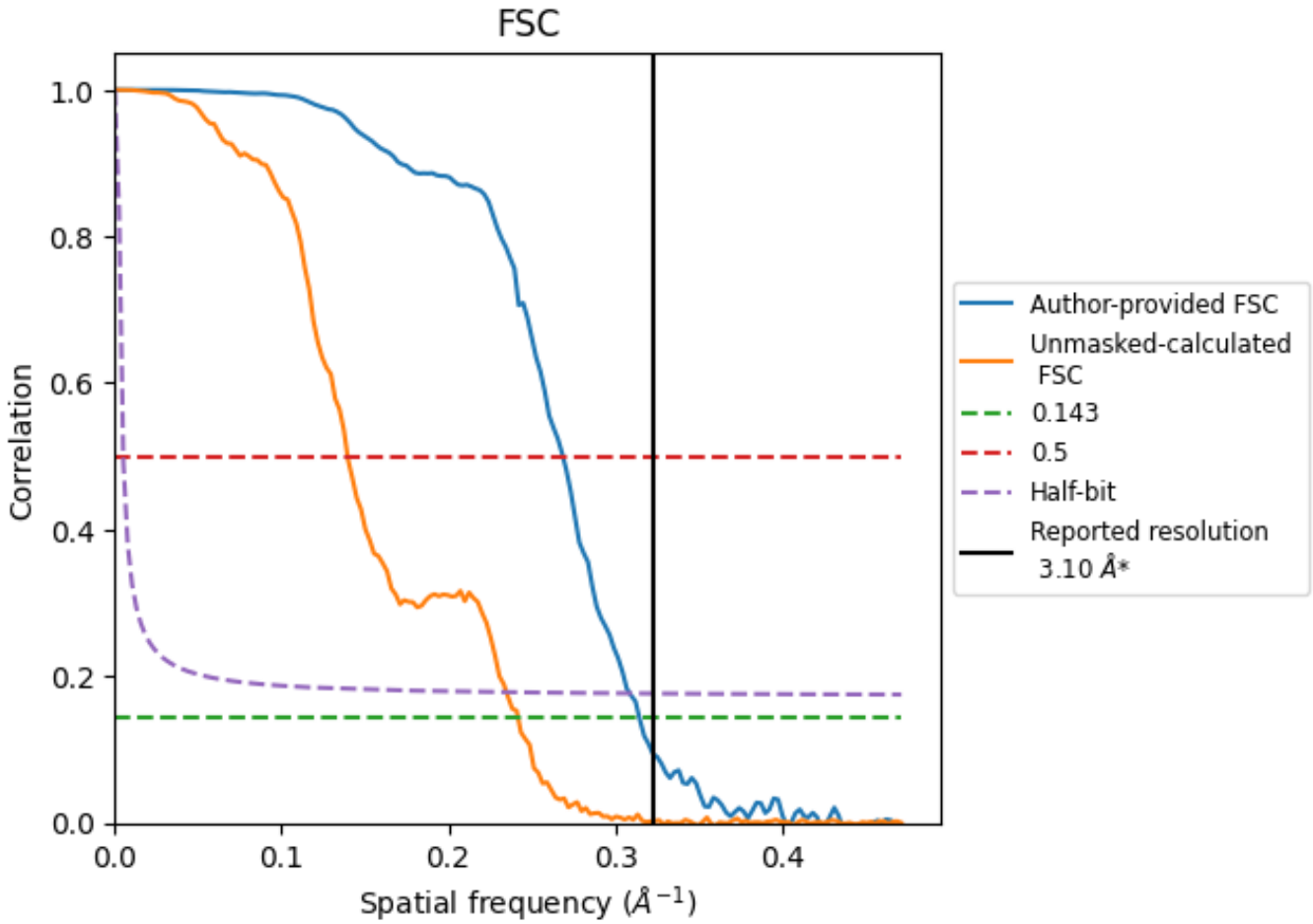


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

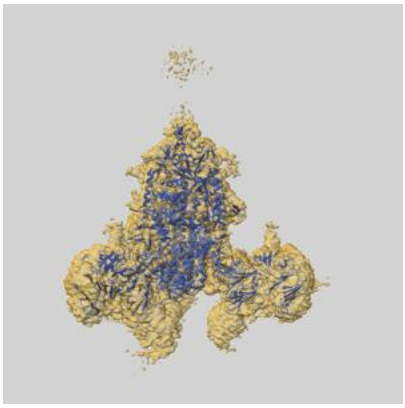
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.18	3.72	3.24
Unmasked-calculated*	4.13	7.16	4.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.13 differs from the reported value 3.1 by more than 10 %

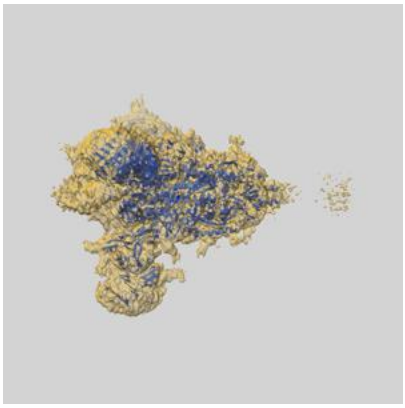
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33646 and PDB model 7Y6S. Per-residue inclusion information can be found in section 3 on page 15.

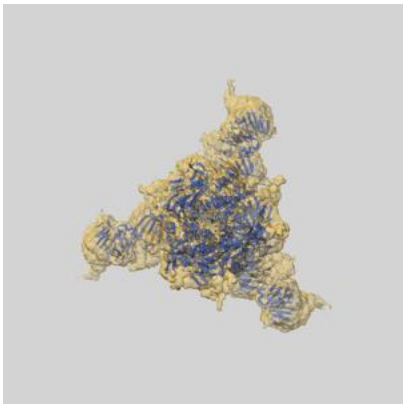
9.1 Map-model overlay



X



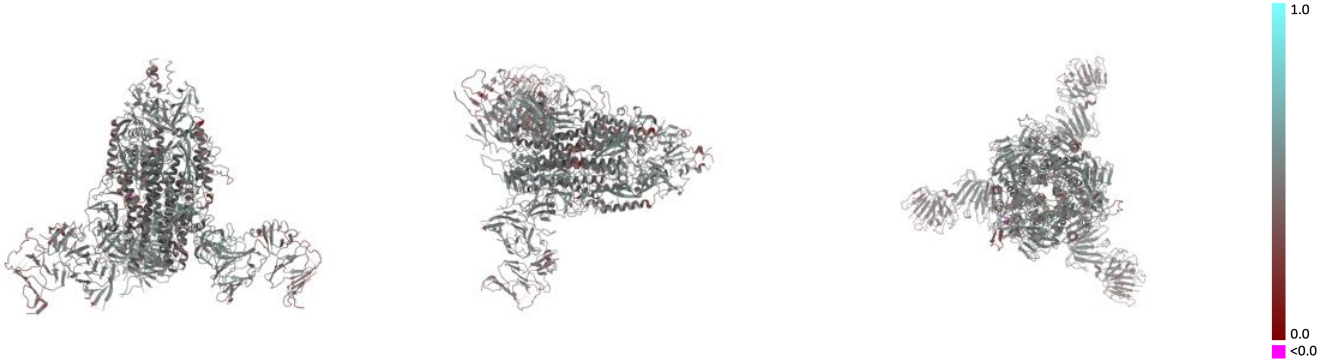
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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

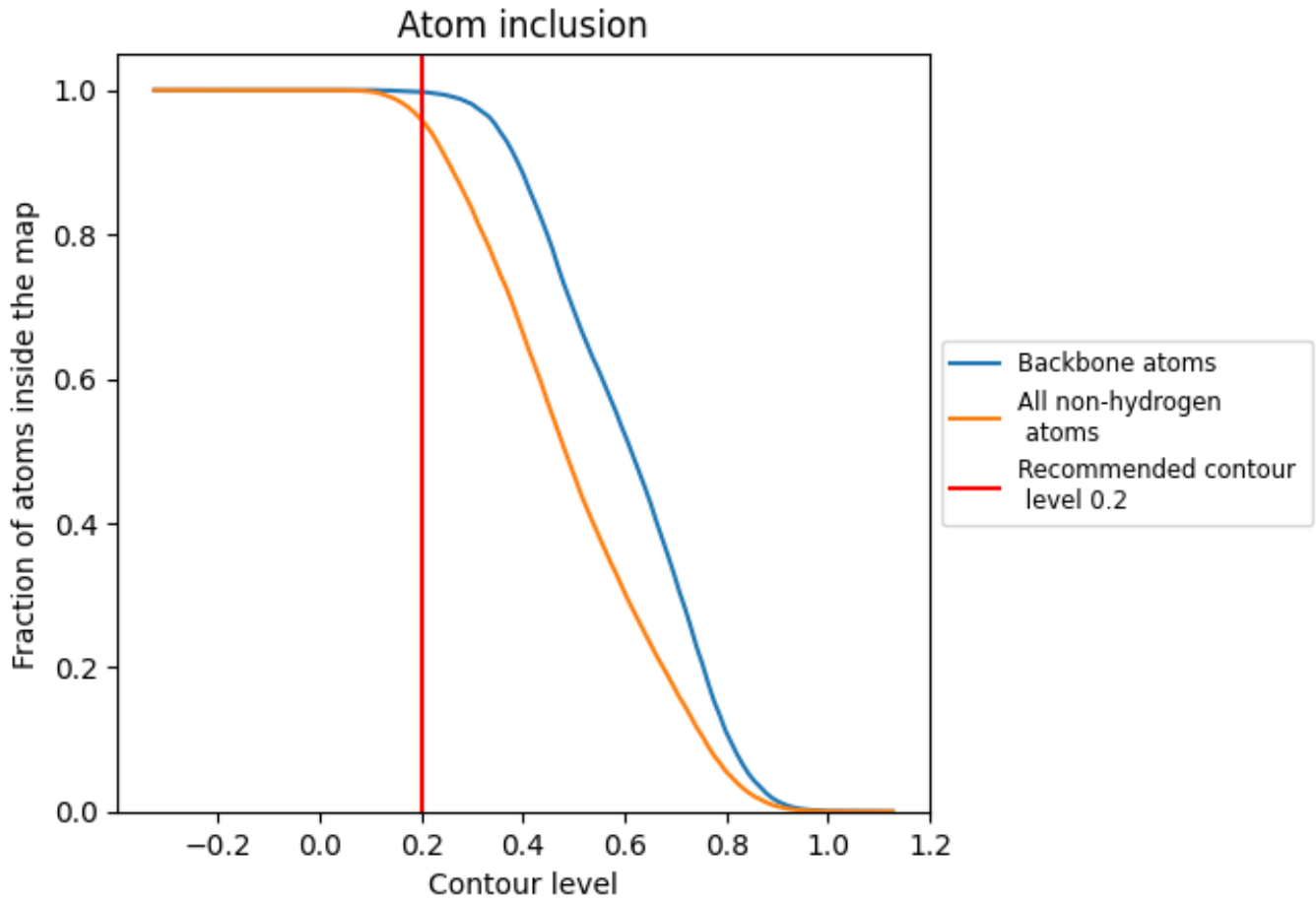
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 96% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9591	0.4600
A	0.9600	0.4650
B	0.9623	0.4630
C	0.9616	0.4640
D	0.9184	0.3510
E	0.9880	0.4620
F	0.9167	0.3690
G	0.9487	0.3530
H	0.9286	0.3670
I	0.9487	0.4150
J	0.9643	0.3370
K	0.9487	0.4060
L	0.9643	0.4000
M	0.9487	0.3760
N	0.9643	0.3880
O	0.8684	0.4020
P	0.9184	0.3430
Q	0.9398	0.4320
R	0.8750	0.2970
S	0.9487	0.3240
T	0.8929	0.4220
U	0.8974	0.3570
V	0.8929	0.4090
W	0.9231	0.4250
X	0.8571	0.3050
Y	0.9487	0.3820
Z	0.8929	0.3620
a	0.9211	0.4120
b	0.9388	0.3800
c	0.9277	0.4380
d	0.7917	0.3330
e	0.9231	0.2950
f	0.8929	0.4090
g	0.9231	0.4560
h	0.7857	0.3460

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Chain	Atom inclusion	Q-score
i	0.9744	0.4500
j	0.9286	0.3280
k	0.9231	0.4370
l	0.9286	0.3490
m	0.8158	0.3480