Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 11:28 AM EDT

PDB ID	:	9EA0
EMDB ID	:	EMD-47823
Title	:	Structure of the prefusion HKU5-19s Spike trimer (conformation 1)
Authors	:	Park, Y.J.; Gen, R.; Seattle Structural Genomics Center for Infectious Disease (SSGCID); Veesler, D.
Deposited on	:	2024-11-09
Resolution	:	2.00 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:

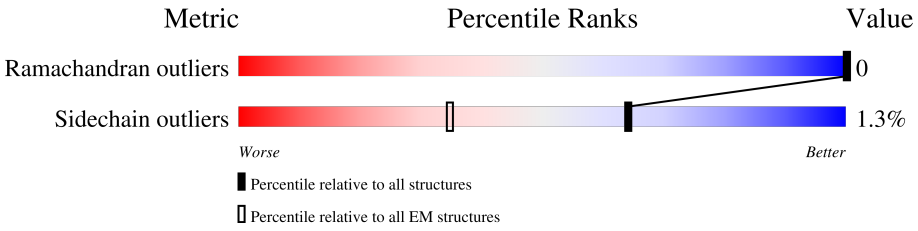
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	207382	16835
Sidechain outliers	206894	16415

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	1365	86% · 13%
1	B	1365	86% · 13%
1	C	1365	86% · 13%
2	D	9	22% 44% 56%
2	R	9	22% 44% 56%
2	f	9	22% 44% 56%
3	E	2	50% 100%
3	F	2	50% 50% 50%
3	G	2	50% 50% 50%

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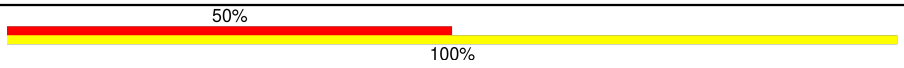
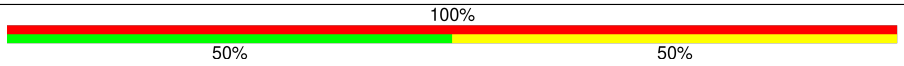
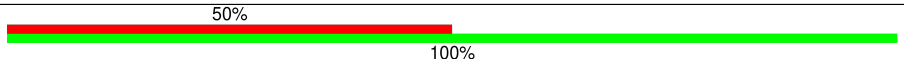
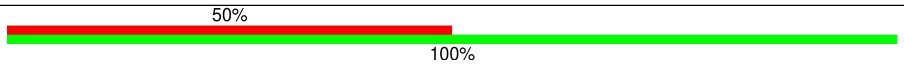
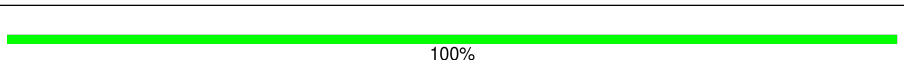
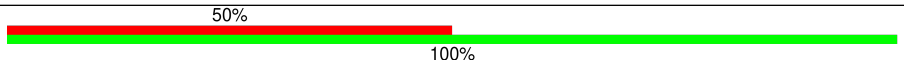
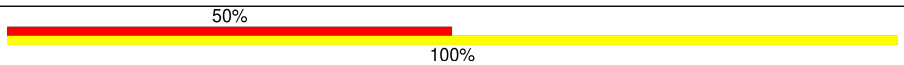
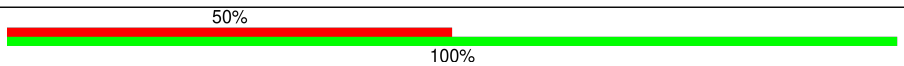
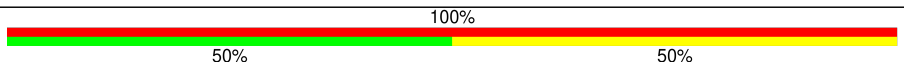
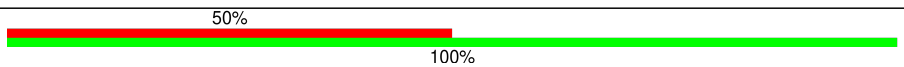
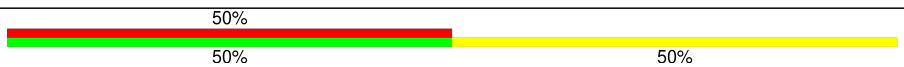
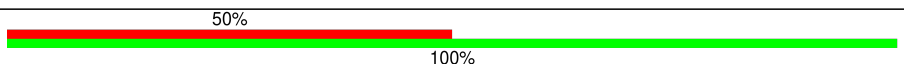
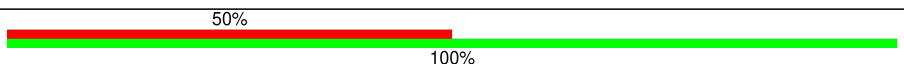
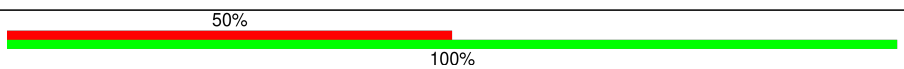
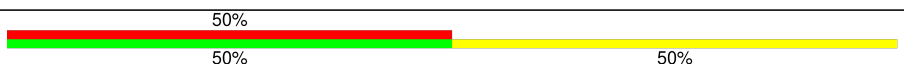
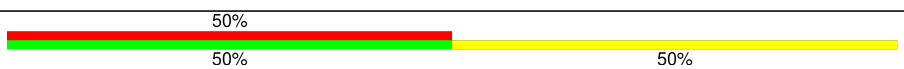
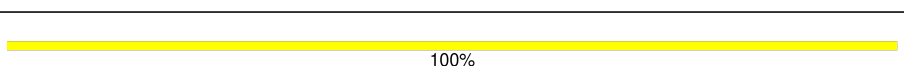
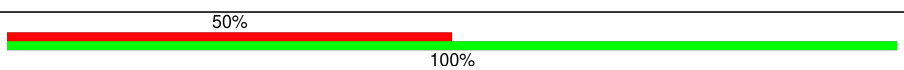
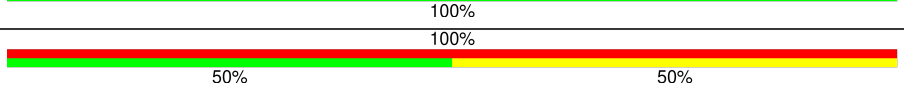
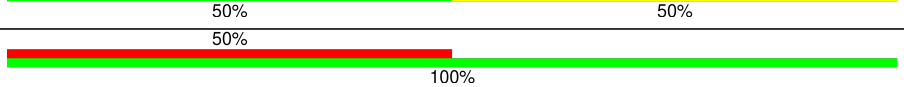
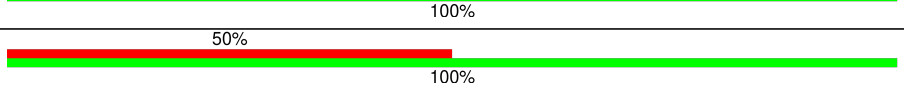
Mol	Chain	Length	Quality of chain
3	H	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	S	2	
3	T	2	
3	U	2	
3	V	2	
3	Y	2	
3	Z	2	
3	a	2	
3	b	2	
3	c	2	
3	d	2	
3	g	2	
3	h	2	
3	i	2	
3	j	2	
3	m	2	
3	n	2	
3	o	2	
3	p	2	

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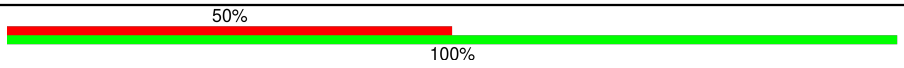
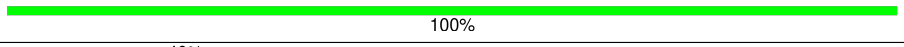
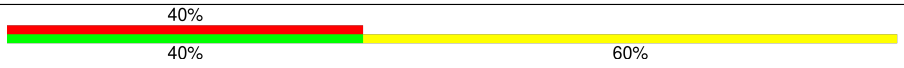
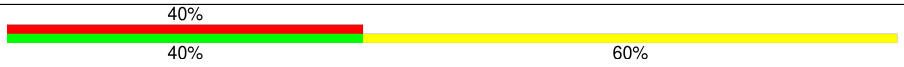
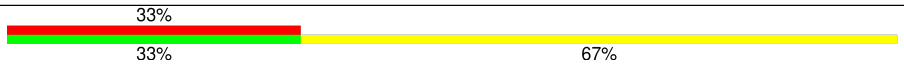
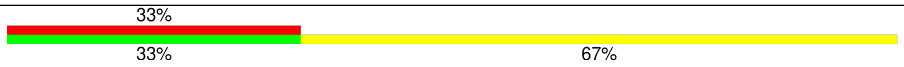
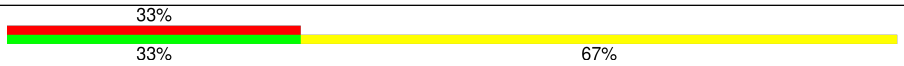
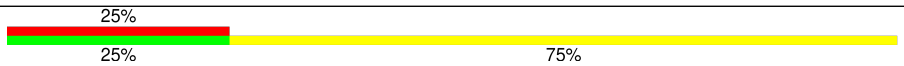
Mol	Chain	Length	Quality of chain
3	q	2	
3	r	2	
4	I	5	
4	W	5	
4	k	5	
5	J	3	
5	X	3	
5	l	3	
6	Q	4	
6	e	4	
6	s	4	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 30002 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	1185	Total	C	N	O	S	0	0
			8972	5739	1499	1681	53		
1	B	1185	Total	C	N	O	S	0	0
			8972	5739	1499	1681	53		
1	C	1185	Total	C	N	O	S	0	0
			8972	5739	1499	1681	53		

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP S4WWR5
A	-9	GLY	-	expression tag	UNP S4WWR5
A	-8	ILE	-	expression tag	UNP S4WWR5
A	-7	LEU	-	expression tag	UNP S4WWR5
A	-6	PRO	-	expression tag	UNP S4WWR5
A	-5	SER	-	expression tag	UNP S4WWR5
A	-4	PRO	-	expression tag	UNP S4WWR5
A	-3	GLY	-	expression tag	UNP S4WWR5
A	-2	MET	-	expression tag	UNP S4WWR5
A	-1	PRO	-	expression tag	UNP S4WWR5
A	0	ALA	-	expression tag	UNP S4WWR5
A	1	LEU	-	expression tag	UNP S4WWR5
A	2	LEU	-	expression tag	UNP S4WWR5
A	3	SER	-	expression tag	UNP S4WWR5
A	4	LEU	-	expression tag	UNP S4WWR5
A	5	VAL	-	expression tag	UNP S4WWR5
A	6	SER	-	expression tag	UNP S4WWR5
A	7	LEU	-	expression tag	UNP S4WWR5
A	8	LEU	-	expression tag	UNP S4WWR5
A	9	SER	-	expression tag	UNP S4WWR5
A	10	VAL	-	expression tag	UNP S4WWR5
A	11	LEU	-	expression tag	UNP S4WWR5
A	12	LEU	-	expression tag	UNP S4WWR5
A	13	MET	-	expression tag	UNP S4WWR5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLY	-	expression tag	UNP S4WWR5
A	15	CYS	-	expression tag	UNP S4WWR5
A	16	VAL	-	expression tag	UNP S4WWR5
A	17	ALA	-	expression tag	UNP S4WWR5
A	18	GLU	-	expression tag	UNP S4WWR5
A	19	THR	-	expression tag	UNP S4WWR5
A	20	GLY	-	expression tag	UNP S4WWR5
A	21	THR	-	expression tag	UNP S4WWR5
A	1058	PRO	THR	conflict	UNP S4WWR5
A	1059	PRO	VAL	conflict	UNP S4WWR5
A	1297	GLY	-	expression tag	UNP S4WWR5
A	1298	SER	-	expression tag	UNP S4WWR5
A	1299	GLY	-	expression tag	UNP S4WWR5
A	1300	TYR	-	expression tag	UNP S4WWR5
A	1301	ILE	-	expression tag	UNP S4WWR5
A	1302	PRO	-	expression tag	UNP S4WWR5
A	1303	GLU	-	expression tag	UNP S4WWR5
A	1304	ALA	-	expression tag	UNP S4WWR5
A	1305	PRO	-	expression tag	UNP S4WWR5
A	1306	ARG	-	expression tag	UNP S4WWR5
A	1307	ASP	-	expression tag	UNP S4WWR5
A	1308	GLY	-	expression tag	UNP S4WWR5
A	1309	GLN	-	expression tag	UNP S4WWR5
A	1310	ALA	-	expression tag	UNP S4WWR5
A	1311	TYR	-	expression tag	UNP S4WWR5
A	1312	VAL	-	expression tag	UNP S4WWR5
A	1313	ARG	-	expression tag	UNP S4WWR5
A	1314	LYS	-	expression tag	UNP S4WWR5
A	1315	ASP	-	expression tag	UNP S4WWR5
A	1316	GLY	-	expression tag	UNP S4WWR5
A	1317	GLU	-	expression tag	UNP S4WWR5
A	1318	TRP	-	expression tag	UNP S4WWR5
A	1319	VAL	-	expression tag	UNP S4WWR5
A	1320	LEU	-	expression tag	UNP S4WWR5
A	1321	LEU	-	expression tag	UNP S4WWR5
A	1322	SER	-	expression tag	UNP S4WWR5
A	1323	THR	-	expression tag	UNP S4WWR5
A	1324	PHE	-	expression tag	UNP S4WWR5
A	1325	LEU	-	expression tag	UNP S4WWR5
A	1326	GLY	-	expression tag	UNP S4WWR5
A	1327	GLY	-	expression tag	UNP S4WWR5
A	1328	SER	-	expression tag	UNP S4WWR5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1329	GLY	-	expression tag	UNP S4WWR5
A	1330	LEU	-	expression tag	UNP S4WWR5
A	1331	ASN	-	expression tag	UNP S4WWR5
A	1332	ASP	-	expression tag	UNP S4WWR5
A	1333	ILE	-	expression tag	UNP S4WWR5
A	1334	PHE	-	expression tag	UNP S4WWR5
A	1335	GLU	-	expression tag	UNP S4WWR5
A	1336	ALA	-	expression tag	UNP S4WWR5
A	1337	GLN	-	expression tag	UNP S4WWR5
A	1338	LYS	-	expression tag	UNP S4WWR5
A	1339	ILE	-	expression tag	UNP S4WWR5
A	1340	GLU	-	expression tag	UNP S4WWR5
A	1341	TRP	-	expression tag	UNP S4WWR5
A	1342	HIS	-	expression tag	UNP S4WWR5
A	1343	GLU	-	expression tag	UNP S4WWR5
A	1344	GLY	-	expression tag	UNP S4WWR5
A	1345	GLY	-	expression tag	UNP S4WWR5
A	1346	SER	-	expression tag	UNP S4WWR5
A	1347	HIS	-	expression tag	UNP S4WWR5
A	1348	HIS	-	expression tag	UNP S4WWR5
A	1349	HIS	-	expression tag	UNP S4WWR5
A	1350	HIS	-	expression tag	UNP S4WWR5
A	1351	HIS	-	expression tag	UNP S4WWR5
A	1352	HIS	-	expression tag	UNP S4WWR5
A	1353	HIS	-	expression tag	UNP S4WWR5
A	1354	HIS	-	expression tag	UNP S4WWR5
B	-10	MET	-	initiating methionine	UNP S4WWR5
B	-9	GLY	-	expression tag	UNP S4WWR5
B	-8	ILE	-	expression tag	UNP S4WWR5
B	-7	LEU	-	expression tag	UNP S4WWR5
B	-6	PRO	-	expression tag	UNP S4WWR5
B	-5	SER	-	expression tag	UNP S4WWR5
B	-4	PRO	-	expression tag	UNP S4WWR5
B	-3	GLY	-	expression tag	UNP S4WWR5
B	-2	MET	-	expression tag	UNP S4WWR5
B	-1	PRO	-	expression tag	UNP S4WWR5
B	0	ALA	-	expression tag	UNP S4WWR5
B	1	LEU	-	expression tag	UNP S4WWR5
B	2	LEU	-	expression tag	UNP S4WWR5
B	3	SER	-	expression tag	UNP S4WWR5
B	4	LEU	-	expression tag	UNP S4WWR5
B	5	VAL	-	expression tag	UNP S4WWR5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	SER	-	expression tag	UNP S4WWR5
B	7	LEU	-	expression tag	UNP S4WWR5
B	8	LEU	-	expression tag	UNP S4WWR5
B	9	SER	-	expression tag	UNP S4WWR5
B	10	VAL	-	expression tag	UNP S4WWR5
B	11	LEU	-	expression tag	UNP S4WWR5
B	12	LEU	-	expression tag	UNP S4WWR5
B	13	MET	-	expression tag	UNP S4WWR5
B	14	GLY	-	expression tag	UNP S4WWR5
B	15	CYS	-	expression tag	UNP S4WWR5
B	16	VAL	-	expression tag	UNP S4WWR5
B	17	ALA	-	expression tag	UNP S4WWR5
B	18	GLU	-	expression tag	UNP S4WWR5
B	19	THR	-	expression tag	UNP S4WWR5
B	20	GLY	-	expression tag	UNP S4WWR5
B	21	THR	-	expression tag	UNP S4WWR5
B	1058	PRO	THR	conflict	UNP S4WWR5
B	1059	PRO	VAL	conflict	UNP S4WWR5
B	1297	GLY	-	expression tag	UNP S4WWR5
B	1298	SER	-	expression tag	UNP S4WWR5
B	1299	GLY	-	expression tag	UNP S4WWR5
B	1300	TYR	-	expression tag	UNP S4WWR5
B	1301	ILE	-	expression tag	UNP S4WWR5
B	1302	PRO	-	expression tag	UNP S4WWR5
B	1303	GLU	-	expression tag	UNP S4WWR5
B	1304	ALA	-	expression tag	UNP S4WWR5
B	1305	PRO	-	expression tag	UNP S4WWR5
B	1306	ARG	-	expression tag	UNP S4WWR5
B	1307	ASP	-	expression tag	UNP S4WWR5
B	1308	GLY	-	expression tag	UNP S4WWR5
B	1309	GLN	-	expression tag	UNP S4WWR5
B	1310	ALA	-	expression tag	UNP S4WWR5
B	1311	TYR	-	expression tag	UNP S4WWR5
B	1312	VAL	-	expression tag	UNP S4WWR5
B	1313	ARG	-	expression tag	UNP S4WWR5
B	1314	LYS	-	expression tag	UNP S4WWR5
B	1315	ASP	-	expression tag	UNP S4WWR5
B	1316	GLY	-	expression tag	UNP S4WWR5
B	1317	GLU	-	expression tag	UNP S4WWR5
B	1318	TRP	-	expression tag	UNP S4WWR5
B	1319	VAL	-	expression tag	UNP S4WWR5
B	1320	LEU	-	expression tag	UNP S4WWR5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1321	LEU	-	expression tag	UNP S4WWR5
B	1322	SER	-	expression tag	UNP S4WWR5
B	1323	THR	-	expression tag	UNP S4WWR5
B	1324	PHE	-	expression tag	UNP S4WWR5
B	1325	LEU	-	expression tag	UNP S4WWR5
B	1326	GLY	-	expression tag	UNP S4WWR5
B	1327	GLY	-	expression tag	UNP S4WWR5
B	1328	SER	-	expression tag	UNP S4WWR5
B	1329	GLY	-	expression tag	UNP S4WWR5
B	1330	LEU	-	expression tag	UNP S4WWR5
B	1331	ASN	-	expression tag	UNP S4WWR5
B	1332	ASP	-	expression tag	UNP S4WWR5
B	1333	ILE	-	expression tag	UNP S4WWR5
B	1334	PHE	-	expression tag	UNP S4WWR5
B	1335	GLU	-	expression tag	UNP S4WWR5
B	1336	ALA	-	expression tag	UNP S4WWR5
B	1337	GLN	-	expression tag	UNP S4WWR5
B	1338	LYS	-	expression tag	UNP S4WWR5
B	1339	ILE	-	expression tag	UNP S4WWR5
B	1340	GLU	-	expression tag	UNP S4WWR5
B	1341	TRP	-	expression tag	UNP S4WWR5
B	1342	HIS	-	expression tag	UNP S4WWR5
B	1343	GLU	-	expression tag	UNP S4WWR5
B	1344	GLY	-	expression tag	UNP S4WWR5
B	1345	GLY	-	expression tag	UNP S4WWR5
B	1346	SER	-	expression tag	UNP S4WWR5
B	1347	HIS	-	expression tag	UNP S4WWR5
B	1348	HIS	-	expression tag	UNP S4WWR5
B	1349	HIS	-	expression tag	UNP S4WWR5
B	1350	HIS	-	expression tag	UNP S4WWR5
B	1351	HIS	-	expression tag	UNP S4WWR5
B	1352	HIS	-	expression tag	UNP S4WWR5
B	1353	HIS	-	expression tag	UNP S4WWR5
B	1354	HIS	-	expression tag	UNP S4WWR5
C	-10	MET	-	initiating methionine	UNP S4WWR5
C	-9	GLY	-	expression tag	UNP S4WWR5
C	-8	ILE	-	expression tag	UNP S4WWR5
C	-7	LEU	-	expression tag	UNP S4WWR5
C	-6	PRO	-	expression tag	UNP S4WWR5
C	-5	SER	-	expression tag	UNP S4WWR5
C	-4	PRO	-	expression tag	UNP S4WWR5
C	-3	GLY	-	expression tag	UNP S4WWR5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	MET	-	expression tag	UNP S4WWR5
C	-1	PRO	-	expression tag	UNP S4WWR5
C	0	ALA	-	expression tag	UNP S4WWR5
C	1	LEU	-	expression tag	UNP S4WWR5
C	2	LEU	-	expression tag	UNP S4WWR5
C	3	SER	-	expression tag	UNP S4WWR5
C	4	LEU	-	expression tag	UNP S4WWR5
C	5	VAL	-	expression tag	UNP S4WWR5
C	6	SER	-	expression tag	UNP S4WWR5
C	7	LEU	-	expression tag	UNP S4WWR5
C	8	LEU	-	expression tag	UNP S4WWR5
C	9	SER	-	expression tag	UNP S4WWR5
C	10	VAL	-	expression tag	UNP S4WWR5
C	11	LEU	-	expression tag	UNP S4WWR5
C	12	LEU	-	expression tag	UNP S4WWR5
C	13	MET	-	expression tag	UNP S4WWR5
C	14	GLY	-	expression tag	UNP S4WWR5
C	15	CYS	-	expression tag	UNP S4WWR5
C	16	VAL	-	expression tag	UNP S4WWR5
C	17	ALA	-	expression tag	UNP S4WWR5
C	18	GLU	-	expression tag	UNP S4WWR5
C	19	THR	-	expression tag	UNP S4WWR5
C	20	GLY	-	expression tag	UNP S4WWR5
C	21	THR	-	expression tag	UNP S4WWR5
C	1058	PRO	THR	conflict	UNP S4WWR5
C	1059	PRO	VAL	conflict	UNP S4WWR5
C	1297	GLY	-	expression tag	UNP S4WWR5
C	1298	SER	-	expression tag	UNP S4WWR5
C	1299	GLY	-	expression tag	UNP S4WWR5
C	1300	TYR	-	expression tag	UNP S4WWR5
C	1301	ILE	-	expression tag	UNP S4WWR5
C	1302	PRO	-	expression tag	UNP S4WWR5
C	1303	GLU	-	expression tag	UNP S4WWR5
C	1304	ALA	-	expression tag	UNP S4WWR5
C	1305	PRO	-	expression tag	UNP S4WWR5
C	1306	ARG	-	expression tag	UNP S4WWR5
C	1307	ASP	-	expression tag	UNP S4WWR5
C	1308	GLY	-	expression tag	UNP S4WWR5
C	1309	GLN	-	expression tag	UNP S4WWR5
C	1310	ALA	-	expression tag	UNP S4WWR5
C	1311	TYR	-	expression tag	UNP S4WWR5
C	1312	VAL	-	expression tag	UNP S4WWR5

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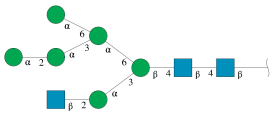
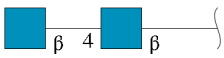
Chain	Residue	Modelled	Actual	Comment	Reference
C	1313	ARG	-	expression tag	UNP S4WWR5
C	1314	LYS	-	expression tag	UNP S4WWR5
C	1315	ASP	-	expression tag	UNP S4WWR5
C	1316	GLY	-	expression tag	UNP S4WWR5
C	1317	GLU	-	expression tag	UNP S4WWR5
C	1318	TRP	-	expression tag	UNP S4WWR5
C	1319	VAL	-	expression tag	UNP S4WWR5
C	1320	LEU	-	expression tag	UNP S4WWR5
C	1321	LEU	-	expression tag	UNP S4WWR5
C	1322	SER	-	expression tag	UNP S4WWR5
C	1323	THR	-	expression tag	UNP S4WWR5
C	1324	PHE	-	expression tag	UNP S4WWR5
C	1325	LEU	-	expression tag	UNP S4WWR5
C	1326	GLY	-	expression tag	UNP S4WWR5
C	1327	GLY	-	expression tag	UNP S4WWR5
C	1328	SER	-	expression tag	UNP S4WWR5
C	1329	GLY	-	expression tag	UNP S4WWR5
C	1330	LEU	-	expression tag	UNP S4WWR5
C	1331	ASN	-	expression tag	UNP S4WWR5
C	1332	ASP	-	expression tag	UNP S4WWR5
C	1333	ILE	-	expression tag	UNP S4WWR5
C	1334	PHE	-	expression tag	UNP S4WWR5
C	1335	GLU	-	expression tag	UNP S4WWR5
C	1336	ALA	-	expression tag	UNP S4WWR5
C	1337	GLN	-	expression tag	UNP S4WWR5
C	1338	LYS	-	expression tag	UNP S4WWR5
C	1339	ILE	-	expression tag	UNP S4WWR5
C	1340	GLU	-	expression tag	UNP S4WWR5
C	1341	TRP	-	expression tag	UNP S4WWR5
C	1342	HIS	-	expression tag	UNP S4WWR5
C	1343	GLU	-	expression tag	UNP S4WWR5
C	1344	GLY	-	expression tag	UNP S4WWR5
C	1345	GLY	-	expression tag	UNP S4WWR5
C	1346	SER	-	expression tag	UNP S4WWR5
C	1347	HIS	-	expression tag	UNP S4WWR5
C	1348	HIS	-	expression tag	UNP S4WWR5
C	1349	HIS	-	expression tag	UNP S4WWR5
C	1350	HIS	-	expression tag	UNP S4WWR5
C	1351	HIS	-	expression tag	UNP S4WWR5
C	1352	HIS	-	expression tag	UNP S4WWR5
C	1353	HIS	-	expression tag	UNP S4WWR5
C	1354	HIS	-	expression tag	UNP S4WWR5

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	9	Total	C	N	O	0	0
			108	60	3	45		
2	R	9	Total	C	N	O	0	0
			108	60	3	45		
2	f	9	Total	C	N	O	0	0
			108	60	3	45		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		

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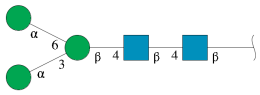
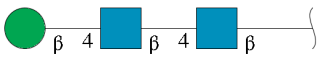
Mol	Chain	Residues	Atoms				AltConf	Trace
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		
3	b	2	Total	C	N	O	0	0
			28	16	2	10		
3	c	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	2	Total	C	N	O	0	0
			28	16	2	10		
3	g	2	Total	C	N	O	0	0
			28	16	2	10		
3	h	2	Total	C	N	O	0	0
			28	16	2	10		
3	i	2	Total	C	N	O	0	0
			28	16	2	10		
3	j	2	Total	C	N	O	0	0
			28	16	2	10		
3	m	2	Total	C	N	O	0	0
			28	16	2	10		
3	n	2	Total	C	N	O	0	0
			28	16	2	10		
3	o	2	Total	C	N	O	0	0
			28	16	2	10		
3	p	2	Total	C	N	O	0	0
			28	16	2	10		
3	q	2	Total	C	N	O	0	0
			28	16	2	10		
3	r	2	Total	C	N	O	0	0
			28	16	2	10		

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



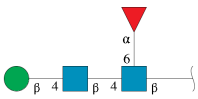
Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	5	Total	C	N	O	0	0
			61	34	2	25		
4	W	5	Total	C	N	O	0	0
			61	34	2	25		
4	k	5	Total	C	N	O	0	0
			61	34	2	25		

- 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	J	3	Total	C	N	O	0	0
			39	22	2	15		
5	X	3	Total	C	N	O	0	0
			39	22	2	15		
5	l	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 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
6	Q	4	Total	C	N	O	0	0
			49	28	2	19		
6	e	4	Total	C	N	O	0	0
			49	28	2	19		

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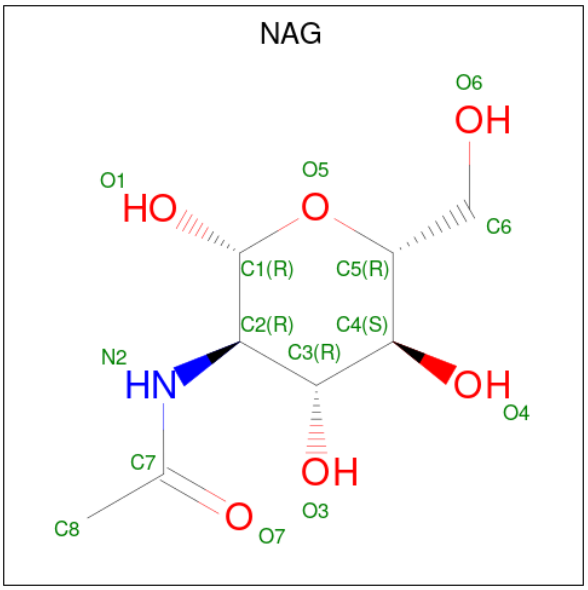
Mol	Chain	Residues	Atoms				AltConf	Trace
6	s	4	Total 49	C 28	N 2	O 19	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

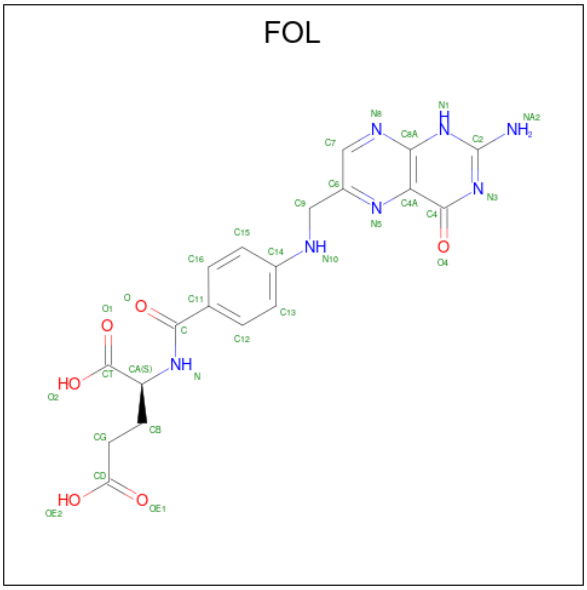


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 14	C 8	N 1	O 5	0
7	A	1	Total 14	C 8	N 1	O 5	0
7	A	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	B	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

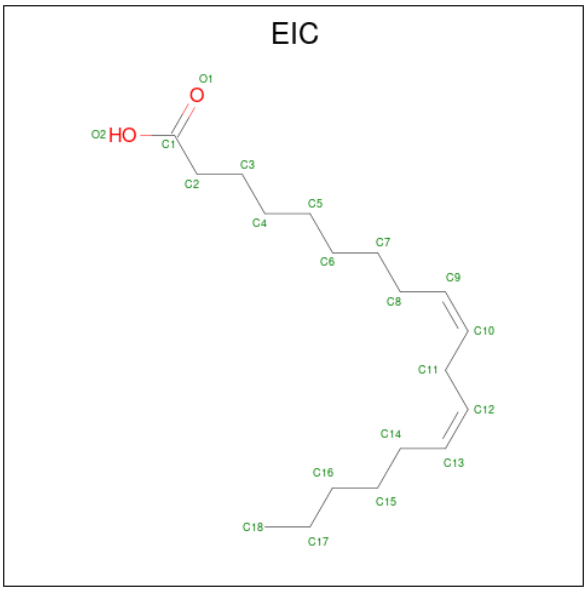
Mol	Chain	Residues	Atoms	AltConf
8	A	2	Total Zn 2 2	0
8	B	2	Total Zn 2 2	0
8	C	2	Total Zn 2 2	0

- Molecule 9 is FOLIC ACID (three-letter code: FOL) (formula: $C_{19}H_{19}N_7O_6$).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C N O 23 14 7 2	0
9	B	1	Total C N O 23 14 7 2	0
9	C	1	Total C N O 23 14 7 2	0

- Molecule 10 is LINOLEIC ACID (three-letter code: EIC) (formula: $C_{18}H_{32}O_2$).



Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O 20 18 2	0
10	B	1	Total C O 20 18 2	0
10	C	1	Total C O 20 18 2	0

- Molecule 11 is water.

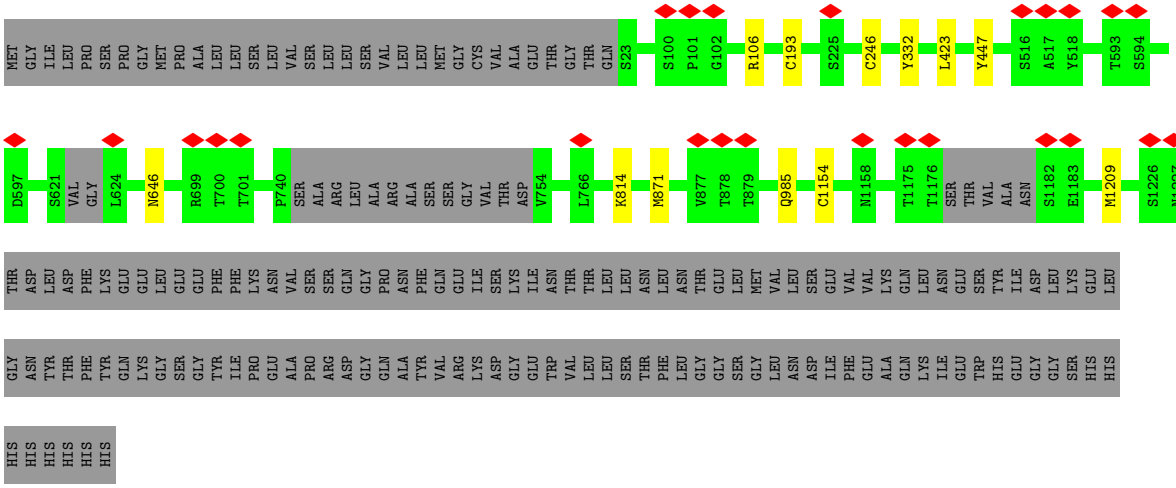
Mol	Chain	Residues	Atoms	AltConf
11	A	405	Total O 405 405	0
11	B	405	Total O 405 405	0
11	C	404	Total O 404 404	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

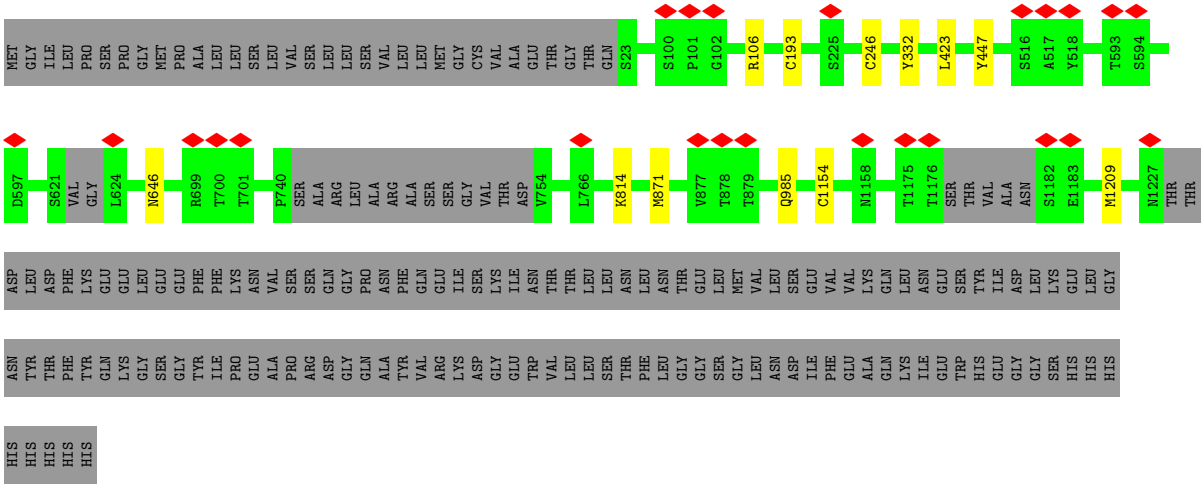
• Molecule 1: Spike glycoprotein

Chain A:



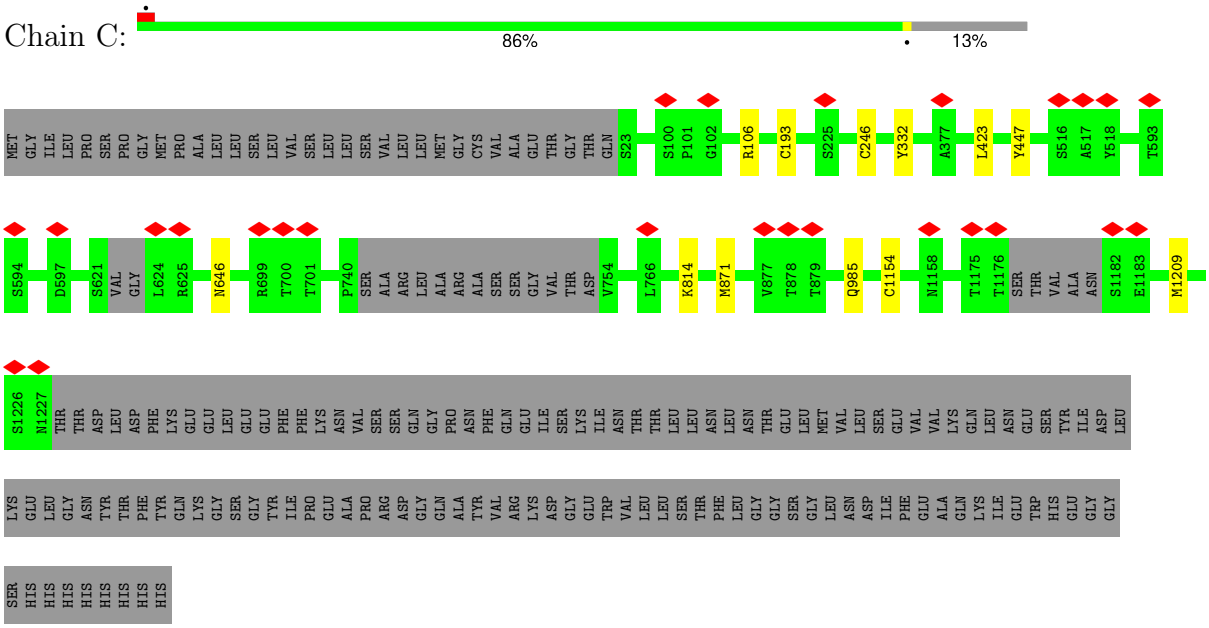
• Molecule 1: Spike glycoprotein

Chain B:



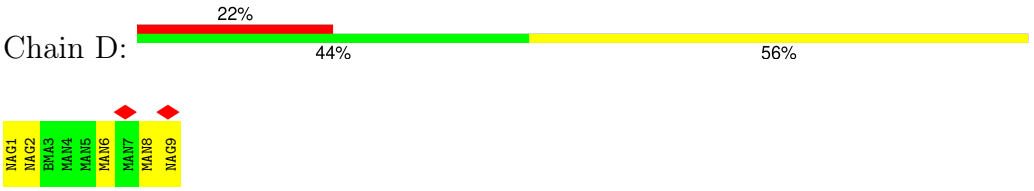
• Molecule 1: Spike glycoprotein

Chain C:



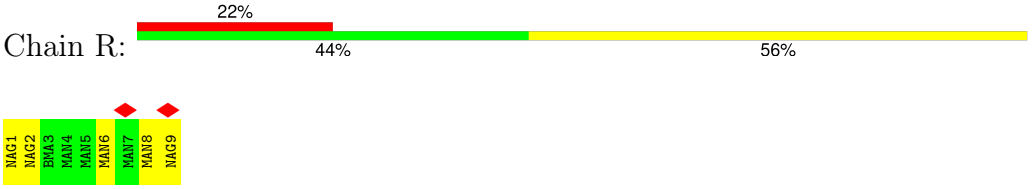
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



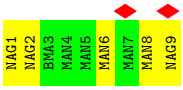
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



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

Chain f:



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

Chain E:

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

Chain F:

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

Chain G:

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

Chain H:

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

Chain K:

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

Chain L:

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

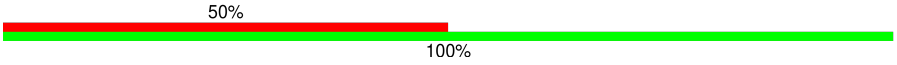
Chain M:

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

Chain N:

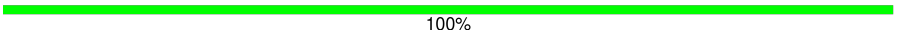
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



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

Chain P:



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

Chain S:

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

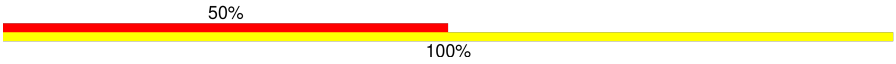
Chain T:

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

Chain U:

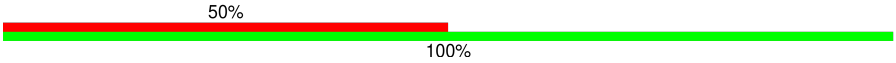
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



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

Chain Y:

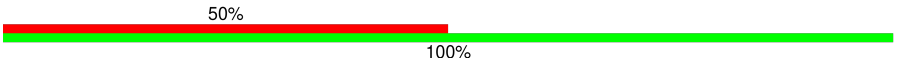


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

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

Chain a:

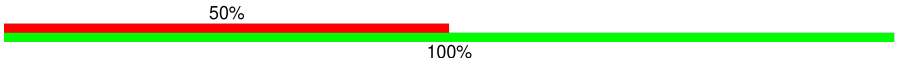


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

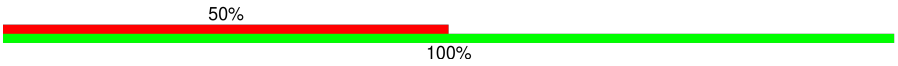
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



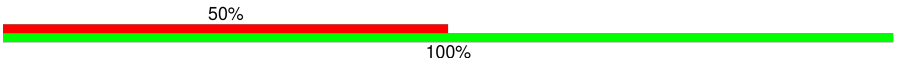
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



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

Chain g:



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

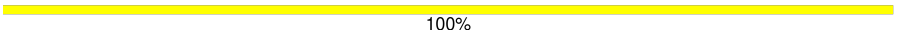
Chain h:

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

Chain i:

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

Chain j:



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

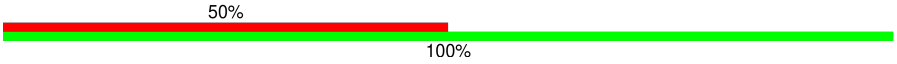
Chain m:

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

Chain n:

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

Chain o:

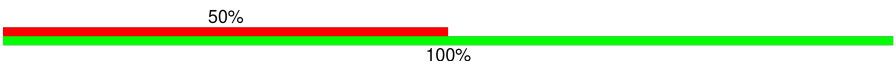


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

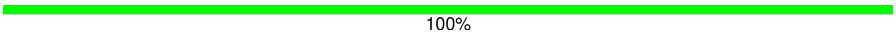
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:



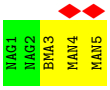
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



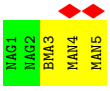
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



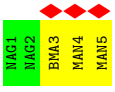
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



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

Chain k:



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

Chain J:

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

Chain X:

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

Chain l:

• Molecule 6: 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 Q:

• Molecule 6: 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 e:

• Molecule 6: 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 s:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	790848, 790848, 790848, 790848	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60.00	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.915	Depositor
Minimum map value	-1.945	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	512.544, 512.544, 512.544	wwPDB
Map dimensions	608, 608, 608	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.843, 0.843, 0.843	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/9193	0.46	0/12541
1	B	0.26	0/9193	0.46	0/12541
1	C	0.26	0/9193	0.46	0/12541
All	All	0.26	0/27579	0.46	0/37623

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	1177/1365 (86%)	1154 (98%)	23 (2%)	0	100	100
1	B	1177/1365 (86%)	1154 (98%)	23 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1177/1365 (86%)	1154 (98%)	23 (2%)	0	100	100
All	All	3531/4095 (86%)	3462 (98%)	69 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	933/1178 (79%)	921 (99%)	12 (1%)	65	71
1	B	933/1178 (79%)	921 (99%)	12 (1%)	65	71
1	C	933/1178 (79%)	921 (99%)	12 (1%)	65	71
All	All	2799/3534 (79%)	2763 (99%)	36 (1%)	64	71

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ARG
1	A	193	CYS
1	A	246	CYS
1	A	332	TYR
1	A	423	LEU
1	A	447	TYR
1	A	646	ASN
1	A	814	LYS
1	A	871	MET
1	A	985	GLN
1	A	1154	CYS
1	A	1209	MET
1	B	106	ARG
1	B	193	CYS
1	B	246	CYS
1	B	332	TYR
1	B	423	LEU

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Mol	Chain	Res	Type
1	B	447	TYR
1	B	646	ASN
1	B	814	LYS
1	B	871	MET
1	B	985	GLN
1	B	1154	CYS
1	B	1209	MET
1	C	106	ARG
1	C	193	CYS
1	C	246	CYS
1	C	332	TYR
1	C	423	LEU
1	C	447	TYR
1	C	646	ASN
1	C	814	LYS
1	C	871	MET
1	C	985	GLN
1	C	1154	CYS
1	C	1209	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	A	386	GLN
1	A	834	HIS
1	A	854	GLN
1	A	992	GLN
1	A	1098	GLN
1	A	1174	GLN
1	A	1185	GLN
1	B	297	GLN
1	B	386	GLN
1	B	834	HIS
1	B	854	GLN
1	B	992	GLN
1	B	1098	GLN
1	B	1174	GLN
1	B	1185	GLN
1	C	297	GLN
1	C	386	GLN
1	C	834	HIS

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Mol	Chain	Res	Type
1	C	854	GLN
1	C	992	GLN
1	C	1098	GLN
1	C	1174	GLN
1	C	1185	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)

123 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	0.73	0	17,19,21	1.01	1 (5%)
2	NAG	D	2	2	14,14,15	0.75	0	17,19,21	0.93	1 (5%)
2	BMA	D	3	2	11,11,12	0.56	0	15,15,17	0.60	0
2	MAN	D	4	2	11,11,12	0.45	0	15,15,17	0.82	0
2	MAN	D	5	2	11,11,12	0.53	0	15,15,17	0.68	0
2	MAN	D	6	2	11,11,12	0.71	0	15,15,17	0.96	1 (6%)
2	MAN	D	7	2	11,11,12	0.36	0	15,15,17	0.51	0
2	MAN	D	8	2	11,11,12	0.74	0	15,15,17	1.05	1 (6%)
2	NAG	D	9	2	14,14,15	0.73	0	17,19,21	0.99	1 (5%)
3	NAG	E	1	3,1	14,14,15	0.72	0	17,19,21	0.86	0
3	NAG	E	2	3	14,14,15	0.71	0	17,19,21	0.81	0
3	NAG	F	1	3,1	14,14,15	0.70	0	17,19,21	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	F	2	3	14,14,15	0.72	0	17,19,21	0.80	0
3	NAG	G	1	3,1	14,14,15	0.74	0	17,19,21	0.84	0
3	NAG	G	2	3	14,14,15	0.77	0	17,19,21	1.12	1 (5%)
3	NAG	H	1	3,1	14,14,15	0.76	0	17,19,21	1.03	2 (11%)
3	NAG	H	2	3	14,14,15	0.72	0	17,19,21	1.00	1 (5%)
4	NAG	I	1	4,1	14,14,15	0.69	0	17,19,21	0.85	0
4	NAG	I	2	4	14,14,15	0.72	0	17,19,21	0.98	0
4	BMA	I	3	4	11,11,12	0.81	0	15,15,17	1.65	1 (6%)
4	MAN	I	4	4	11,11,12	0.68	0	15,15,17	1.17	1 (6%)
4	MAN	I	5	4	11,11,12	0.73	0	15,15,17	1.04	1 (6%)
5	NAG	J	1	5,1	14,14,15	0.70	0	17,19,21	1.13	2 (11%)
5	NAG	J	2	5	14,14,15	0.69	0	17,19,21	0.99	0
5	BMA	J	3	5	11,11,12	0.88	0	15,15,17	1.65	1 (6%)
3	NAG	K	1	3,1	14,14,15	0.73	0	17,19,21	0.89	1 (5%)
3	NAG	K	2	3	14,14,15	0.71	0	17,19,21	0.81	0
3	NAG	L	1	3,1	14,14,15	0.68	0	17,19,21	0.94	1 (5%)
3	NAG	L	2	3	14,14,15	0.70	0	17,19,21	0.97	0
3	NAG	M	1	3,1	14,14,15	0.69	0	17,19,21	0.87	0
3	NAG	M	2	3	14,14,15	0.72	0	17,19,21	0.88	0
3	NAG	N	1	3,1	14,14,15	0.74	0	17,19,21	0.81	0
3	NAG	N	2	3	14,14,15	0.72	0	17,19,21	0.87	1 (5%)
3	NAG	O	1	3,1	14,14,15	0.73	0	17,19,21	0.85	0
3	NAG	O	2	3	14,14,15	0.72	0	17,19,21	0.81	0
3	NAG	P	1	3,1	14,14,15	0.70	0	17,19,21	0.78	0
3	NAG	P	2	3	14,14,15	0.75	0	17,19,21	0.89	0
6	NAG	Q	1	6,1	14,14,15	0.74	0	17,19,21	1.21	2 (11%)
6	NAG	Q	2	6	14,14,15	0.66	0	17,19,21	1.14	0
6	BMA	Q	3	6	11,11,12	0.84	0	15,15,17	1.78	1 (6%)
6	FUC	Q	4	6	10,10,11	0.75	0	14,14,16	1.04	1 (7%)
2	NAG	R	1	2,1	14,14,15	0.73	0	17,19,21	1.01	1 (5%)
2	NAG	R	2	2	14,14,15	0.76	0	17,19,21	0.93	1 (5%)
2	BMA	R	3	2	11,11,12	0.56	0	15,15,17	0.60	0
2	MAN	R	4	2	11,11,12	0.46	0	15,15,17	0.82	0
2	MAN	R	5	2	11,11,12	0.54	0	15,15,17	0.68	0
2	MAN	R	6	2	11,11,12	0.71	0	15,15,17	0.97	1 (6%)
2	MAN	R	7	2	11,11,12	0.36	0	15,15,17	0.51	0
2	MAN	R	8	2	11,11,12	0.74	0	15,15,17	1.04	1 (6%)
2	NAG	R	9	2	14,14,15	0.72	0	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	S	1	3,1	14,14,15	0.71	0	17,19,21	0.87	0
3	NAG	S	2	3	14,14,15	0.71	0	17,19,21	0.80	0
3	NAG	T	1	3,1	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
3	NAG	T	2	3	14,14,15	0.70	0	17,19,21	0.80	0
3	NAG	U	1	3,1	14,14,15	0.76	0	17,19,21	0.83	0
3	NAG	U	2	3	14,14,15	0.76	0	17,19,21	1.12	1 (5%)
3	NAG	V	1	3,1	14,14,15	0.75	0	17,19,21	1.02	2 (11%)
3	NAG	V	2	3	14,14,15	0.74	0	17,19,21	1.00	1 (5%)
4	NAG	W	1	4,1	14,14,15	0.69	0	17,19,21	0.86	0
4	NAG	W	2	4	14,14,15	0.70	0	17,19,21	0.98	0
4	BMA	W	3	4	11,11,12	0.80	0	15,15,17	1.64	1 (6%)
4	MAN	W	4	4	11,11,12	0.67	0	15,15,17	1.17	1 (6%)
4	MAN	W	5	4	11,11,12	0.72	0	15,15,17	1.03	1 (6%)
5	NAG	X	1	5,1	14,14,15	0.70	0	17,19,21	1.13	2 (11%)
5	NAG	X	2	5	14,14,15	0.68	0	17,19,21	0.99	0
5	BMA	X	3	5	11,11,12	0.87	0	15,15,17	1.65	1 (6%)
3	NAG	Y	1	3,1	14,14,15	0.71	0	17,19,21	0.89	0
3	NAG	Y	2	3	14,14,15	0.71	0	17,19,21	0.81	0
3	NAG	Z	1	3,1	14,14,15	0.69	0	17,19,21	0.94	1 (5%)
3	NAG	Z	2	3	14,14,15	0.70	0	17,19,21	0.97	0
3	NAG	a	1	3,1	14,14,15	0.70	0	17,19,21	0.87	0
3	NAG	a	2	3	14,14,15	0.72	0	17,19,21	0.88	0
3	NAG	b	1	3,1	14,14,15	0.74	0	17,19,21	0.81	0
3	NAG	b	2	3	14,14,15	0.72	0	17,19,21	0.87	1 (5%)
3	NAG	c	1	3,1	14,14,15	0.73	0	17,19,21	0.85	0
3	NAG	c	2	3	14,14,15	0.71	0	17,19,21	0.80	0
3	NAG	d	1	3,1	14,14,15	0.71	0	17,19,21	0.78	0
3	NAG	d	2	3	14,14,15	0.74	0	17,19,21	0.89	0
6	NAG	e	1	6,1	14,14,15	0.74	0	17,19,21	1.21	2 (11%)
6	NAG	e	2	6	14,14,15	0.67	0	17,19,21	1.14	0
6	BMA	e	3	6	11,11,12	0.83	0	15,15,17	1.77	1 (6%)
6	FUC	e	4	6	10,10,11	0.75	0	14,14,16	1.04	1 (7%)
2	NAG	f	1	2,1	14,14,15	0.73	0	17,19,21	1.01	1 (5%)
2	NAG	f	2	2	14,14,15	0.75	0	17,19,21	0.93	1 (5%)
2	BMA	f	3	2	11,11,12	0.56	0	15,15,17	0.60	0
2	MAN	f	4	2	11,11,12	0.45	0	15,15,17	0.83	0
2	MAN	f	5	2	11,11,12	0.53	0	15,15,17	0.67	0
2	MAN	f	6	2	11,11,12	0.71	0	15,15,17	0.97	1 (6%)
2	MAN	f	7	2	11,11,12	0.36	0	15,15,17	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	f	8	2	11,11,12	0.75	0	15,15,17	1.05	1 (6%)
2	NAG	f	9	2	14,14,15	0.72	0	17,19,21	0.99	1 (5%)
3	NAG	g	1	3,1	14,14,15	0.73	0	17,19,21	0.88	0
3	NAG	g	2	3	14,14,15	0.71	0	17,19,21	0.80	0
3	NAG	h	1	3,1	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
3	NAG	h	2	3	14,14,15	0.72	0	17,19,21	0.81	0
3	NAG	i	1	3,1	14,14,15	0.73	0	17,19,21	0.84	0
3	NAG	i	2	3	14,14,15	0.76	0	17,19,21	1.11	1 (5%)
3	NAG	j	1	3,1	14,14,15	0.76	0	17,19,21	1.02	2 (11%)
3	NAG	j	2	3	14,14,15	0.73	0	17,19,21	1.00	1 (5%)
4	NAG	k	1	4,1	14,14,15	0.69	0	17,19,21	0.85	0
4	NAG	k	2	4	14,14,15	0.72	0	17,19,21	0.98	0
4	BMA	k	3	4	11,11,12	0.79	0	15,15,17	1.64	1 (6%)
4	MAN	k	4	4	11,11,12	0.67	0	15,15,17	1.17	1 (6%)
4	MAN	k	5	4	11,11,12	0.71	0	15,15,17	1.03	1 (6%)
5	NAG	l	1	5,1	14,14,15	0.69	0	17,19,21	1.12	2 (11%)
5	NAG	l	2	5	14,14,15	0.69	0	17,19,21	0.99	0
5	BMA	l	3	5	11,11,12	0.86	0	15,15,17	1.65	1 (6%)
3	NAG	m	1	3,1	14,14,15	0.71	0	17,19,21	0.88	0
3	NAG	m	2	3	14,14,15	0.70	0	17,19,21	0.81	0
3	NAG	n	1	3,1	14,14,15	0.69	0	17,19,21	0.94	1 (5%)
3	NAG	n	2	3	14,14,15	0.70	0	17,19,21	0.97	0
3	NAG	o	1	3,1	14,14,15	0.69	0	17,19,21	0.86	0
3	NAG	o	2	3	14,14,15	0.72	0	17,19,21	0.88	0
3	NAG	p	1	3,1	14,14,15	0.74	0	17,19,21	0.81	0
3	NAG	p	2	3	14,14,15	0.71	0	17,19,21	0.86	0
3	NAG	q	1	3,1	14,14,15	0.73	0	17,19,21	0.85	0
3	NAG	q	2	3	14,14,15	0.71	0	17,19,21	0.80	0
3	NAG	r	1	3,1	14,14,15	0.70	0	17,19,21	0.79	0
3	NAG	r	2	3	14,14,15	0.74	0	17,19,21	0.89	0
6	NAG	s	1	6,1	14,14,15	0.74	0	17,19,21	1.20	2 (11%)
6	NAG	s	2	6	14,14,15	0.66	0	17,19,21	1.14	0
6	BMA	s	3	6	11,11,12	0.82	0	15,15,17	1.78	1 (6%)
6	FUC	s	4	6	10,10,11	0.73	0	14,14,16	1.04	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	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	0/2/19/22	0/1/1/1
2	MAN	D	6	2	-	0/2/19/22	0/1/1/1
2	MAN	D	7	2	-	0/2/19/22	0/1/1/1
2	MAN	D	8	2	-	0/2/19/22	0/1/1/1
2	NAG	D	9	2	-	0/6/23/26	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	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
4	MAN	I	4	4	-	1/2/19/22	0/1/1/1
4	MAN	I	5	4	-	0/2/19/22	0/1/1/1
5	NAG	J	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	BMA	J	3	5	-	1/2/19/22	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
6	NAG	Q	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FUC	Q	4	6	-	-	0/1/1/1
2	NAG	R	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	BMA	R	3	2	-	0/2/19/22	0/1/1/1
2	MAN	R	4	2	-	0/2/19/22	0/1/1/1
2	MAN	R	5	2	-	0/2/19/22	0/1/1/1
2	MAN	R	6	2	-	0/2/19/22	0/1/1/1
2	MAN	R	7	2	-	0/2/19/22	0/1/1/1
2	MAN	R	8	2	-	0/2/19/22	0/1/1/1
2	NAG	R	9	2	-	0/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1
4	BMA	W	3	4	-	2/2/19/22	0/1/1/1
4	MAN	W	4	4	-	1/2/19/22	0/1/1/1
4	MAN	W	5	4	-	0/2/19/22	0/1/1/1
5	NAG	X	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	X	2	5	-	0/6/23/26	0/1/1/1
5	BMA	X	3	5	-	1/2/19/22	0/1/1/1
3	NAG	Y	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Z	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
3	NAG	a	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1
3	NAG	c	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	c	2	3	-	0/6/23/26	0/1/1/1
3	NAG	d	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	d	2	3	-	0/6/23/26	0/1/1/1
6	NAG	e	1	6,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	e	2	6	-	2/6/23/26	0/1/1/1
6	BMA	e	3	6	-	1/2/19/22	0/1/1/1
6	FUC	e	4	6	-	-	0/1/1/1
2	NAG	f	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	f	2	2	-	2/6/23/26	0/1/1/1
2	BMA	f	3	2	-	0/2/19/22	0/1/1/1
2	MAN	f	4	2	-	0/2/19/22	0/1/1/1
2	MAN	f	5	2	-	0/2/19/22	0/1/1/1
2	MAN	f	6	2	-	0/2/19/22	0/1/1/1
2	MAN	f	7	2	-	0/2/19/22	0/1/1/1
2	MAN	f	8	2	-	0/2/19/22	0/1/1/1
2	NAG	f	9	2	-	0/6/23/26	0/1/1/1
3	NAG	g	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	g	2	3	-	0/6/23/26	0/1/1/1
3	NAG	h	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	h	2	3	-	0/6/23/26	0/1/1/1
3	NAG	i	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	i	2	3	-	0/6/23/26	0/1/1/1
3	NAG	j	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	j	2	3	-	0/6/23/26	0/1/1/1
4	NAG	k	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	k	2	4	-	0/6/23/26	0/1/1/1
4	BMA	k	3	4	-	2/2/19/22	0/1/1/1
4	MAN	k	4	4	-	1/2/19/22	0/1/1/1
4	MAN	k	5	4	-	0/2/19/22	0/1/1/1
5	NAG	l	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	l	2	5	-	0/6/23/26	0/1/1/1
5	BMA	l	3	5	-	1/2/19/22	0/1/1/1
3	NAG	m	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	m	2	3	-	0/6/23/26	0/1/1/1
3	NAG	n	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	n	2	3	-	0/6/23/26	0/1/1/1
3	NAG	o	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	o	2	3	-	2/6/23/26	0/1/1/1
3	NAG	p	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	p	2	3	-	2/6/23/26	0/1/1/1
3	NAG	q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	r	1	3,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	r	2	3	-	0/6/23/26	0/1/1/1
6	NAG	s	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	s	2	6	-	2/6/23/26	0/1/1/1
6	BMA	s	3	6	-	1/2/19/22	0/1/1/1
6	FUC	s	4	6	-	-	0/1/1/1

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	s	3	BMA	C1-O5-C5	5.53	119.60	112.19
6	Q	3	BMA	C1-O5-C5	5.53	119.59	112.19
6	e	3	BMA	C1-O5-C5	5.49	119.54	112.19
5	J	3	BMA	C1-O5-C5	5.12	119.05	112.19
5	l	3	BMA	C1-O5-C5	5.10	119.03	112.19
5	X	3	BMA	C1-O5-C5	5.09	119.01	112.19
4	I	3	BMA	C1-O5-C5	4.86	118.70	112.19
4	W	3	BMA	C1-O5-C5	4.84	118.67	112.19
4	k	3	BMA	C1-O5-C5	4.81	118.63	112.19
4	W	4	MAN	C1-O5-C5	3.38	116.72	112.19
4	k	4	MAN	C1-O5-C5	3.37	116.71	112.19
4	I	4	MAN	C1-O5-C5	3.36	116.69	112.19
6	e	1	NAG	C1-O5-C5	3.22	116.50	112.19
6	Q	1	NAG	C1-O5-C5	3.21	116.49	112.19
6	s	1	NAG	C1-O5-C5	3.20	116.47	112.19
4	I	5	MAN	C1-O5-C5	2.88	116.05	112.19
4	W	5	MAN	C1-O5-C5	2.87	116.03	112.19
4	k	5	MAN	C1-O5-C5	2.86	116.01	112.19
5	X	1	NAG	C1-O5-C5	2.74	115.86	112.19
5	J	1	NAG	C1-O5-C5	2.74	115.85	112.19
5	l	1	NAG	C1-O5-C5	2.71	115.81	112.19
2	R	6	MAN	C1-O5-C5	2.60	115.68	112.19
2	f	6	MAN	C1-O5-C5	2.60	115.68	112.19
2	D	6	MAN	C1-O5-C5	2.59	115.66	112.19
6	s	4	FUC	C1-O5-C5	2.35	118.50	112.97
6	Q	4	FUC	C1-O5-C5	2.34	118.50	112.97
6	e	4	FUC	C1-O5-C5	2.33	118.46	112.97
2	R	1	NAG	O5-C1-C2	-2.32	107.69	111.29
2	f	1	NAG	O5-C1-C2	-2.32	107.70	111.29
2	D	1	NAG	O5-C1-C2	-2.31	107.72	111.29
3	Z	1	NAG	C1-O5-C5	2.30	115.26	112.19
3	n	1	NAG	C1-O5-C5	2.30	115.26	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	1	NAG	C1-O5-C5	2.28	115.24	112.19
2	f	9	NAG	O5-C1-C2	-2.21	107.87	111.29
2	D	9	NAG	O5-C1-C2	-2.20	107.89	111.29
2	R	9	NAG	O5-C1-C2	-2.19	107.90	111.29
3	G	2	NAG	C2-N2-C7	2.19	125.84	122.90
3	i	2	NAG	C2-N2-C7	2.16	125.80	122.90
3	H	1	NAG	C2-N2-C7	2.16	125.80	122.90
5	l	1	NAG	O4-C4-C3	-2.16	105.28	110.38
3	V	1	NAG	C2-N2-C7	2.16	125.79	122.90
5	J	1	NAG	O4-C4-C3	-2.15	105.31	110.38
3	j	1	NAG	C2-N2-C7	2.15	125.78	122.90
3	H	1	NAG	C4-C3-C2	2.15	114.16	111.02
5	X	1	NAG	O4-C4-C3	-2.14	105.32	110.38
3	V	1	NAG	C4-C3-C2	2.14	114.15	111.02
3	j	1	NAG	C4-C3-C2	2.13	114.14	111.02
3	V	2	NAG	C2-N2-C7	2.13	125.75	122.90
3	j	2	NAG	C2-N2-C7	2.13	125.75	122.90
3	U	2	NAG	C2-N2-C7	2.12	125.74	122.90
3	H	2	NAG	C2-N2-C7	2.12	125.74	122.90
3	h	1	NAG	C1-O5-C5	2.10	115.00	112.19
3	T	1	NAG	C1-O5-C5	2.10	115.00	112.19
3	F	1	NAG	C1-O5-C5	2.08	114.98	112.19
2	R	2	NAG	C2-N2-C7	2.07	125.68	122.90
2	D	2	NAG	C2-N2-C7	2.07	125.68	122.90
2	f	2	NAG	C2-N2-C7	2.07	125.67	122.90
3	K	1	NAG	C2-N2-C7	2.04	125.64	122.90
3	b	2	NAG	C2-N2-C7	2.03	125.62	122.90
3	N	2	NAG	C2-N2-C7	2.03	125.62	122.90
2	D	8	MAN	C1-O5-C5	2.02	114.89	112.19
2	R	8	MAN	C1-O5-C5	2.01	114.88	112.19
6	Q	1	NAG	O4-C4-C3	-2.01	105.64	110.38
2	f	8	MAN	C1-O5-C5	2.01	114.88	112.19
6	e	1	NAG	O4-C4-C3	-2.01	105.65	110.38
6	s	1	NAG	O4-C4-C3	-2.00	105.66	110.38

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Q	2	NAG	O5-C5-C6-O6
6	e	2	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	d	1	NAG	O5-C5-C6-O6
3	r	1	NAG	O5-C5-C6-O6
6	s	2	NAG	O5-C5-C6-O6
4	I	3	BMA	C4-C5-C6-O6
4	W	3	BMA	C4-C5-C6-O6
4	k	3	BMA	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	d	1	NAG	C4-C5-C6-O6
3	r	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	R	2	NAG	C8-C7-N2-C2
2	R	2	NAG	O7-C7-N2-C2
2	f	2	NAG	C8-C7-N2-C2
2	f	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	L	1	NAG	C8-C7-N2-C2
3	L	1	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
3	O	1	NAG	C8-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	V	1	NAG	O7-C7-N2-C2
3	Y	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	O7-C7-N2-C2
3	Z	1	NAG	C8-C7-N2-C2
3	Z	1	NAG	O7-C7-N2-C2
3	a	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	a	1	NAG	O7-C7-N2-C2
3	a	2	NAG	C8-C7-N2-C2
3	a	2	NAG	O7-C7-N2-C2
3	b	2	NAG	C8-C7-N2-C2
3	b	2	NAG	O7-C7-N2-C2
3	c	1	NAG	C8-C7-N2-C2
3	c	1	NAG	O7-C7-N2-C2
3	d	1	NAG	C8-C7-N2-C2
3	d	1	NAG	O7-C7-N2-C2
3	g	1	NAG	C8-C7-N2-C2
3	g	1	NAG	O7-C7-N2-C2
3	j	1	NAG	C8-C7-N2-C2
3	j	1	NAG	O7-C7-N2-C2
3	m	1	NAG	C8-C7-N2-C2
3	m	1	NAG	O7-C7-N2-C2
3	n	1	NAG	C8-C7-N2-C2
3	n	1	NAG	O7-C7-N2-C2
3	o	1	NAG	C8-C7-N2-C2
3	o	1	NAG	O7-C7-N2-C2
3	o	2	NAG	C8-C7-N2-C2
3	o	2	NAG	O7-C7-N2-C2
3	p	2	NAG	C8-C7-N2-C2
3	p	2	NAG	O7-C7-N2-C2
3	q	1	NAG	C8-C7-N2-C2
3	q	1	NAG	O7-C7-N2-C2
3	r	1	NAG	C8-C7-N2-C2
3	r	1	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	W	1	NAG	C8-C7-N2-C2
4	W	1	NAG	O7-C7-N2-C2
4	k	1	NAG	C8-C7-N2-C2
4	k	1	NAG	O7-C7-N2-C2
4	I	3	BMA	O5-C5-C6-O6
4	W	3	BMA	O5-C5-C6-O6
4	k	3	BMA	O5-C5-C6-O6
6	Q	3	BMA	O5-C5-C6-O6
6	e	3	BMA	O5-C5-C6-O6
6	s	3	BMA	O5-C5-C6-O6
4	I	4	MAN	O5-C5-C6-O6
4	W	4	MAN	O5-C5-C6-O6
4	k	4	MAN	O5-C5-C6-O6

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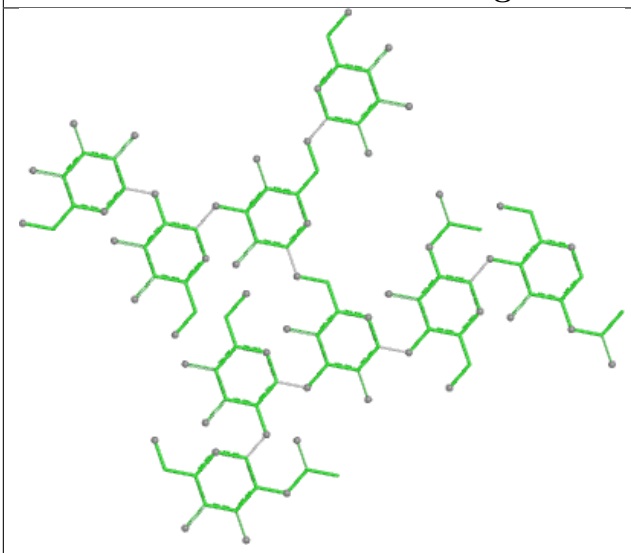
Mol	Chain	Res	Type	Atoms
5	J	3	BMA	O5-C5-C6-O6
5	X	3	BMA	O5-C5-C6-O6
5	l	3	BMA	O5-C5-C6-O6
6	e	2	NAG	C4-C5-C6-O6
6	s	2	NAG	C4-C5-C6-O6
6	Q	2	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	i	1	NAG	C4-C5-C6-O6
2	f	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	i	1	NAG	O5-C5-C6-O6

There are no ring outliers.

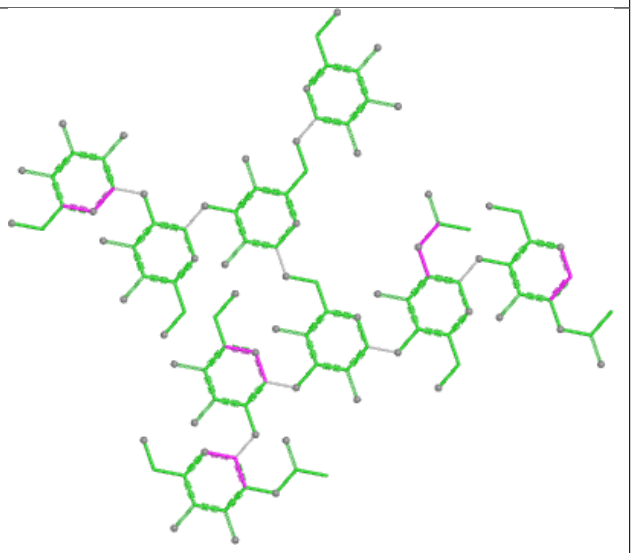
No monomer is involved in short contacts.

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

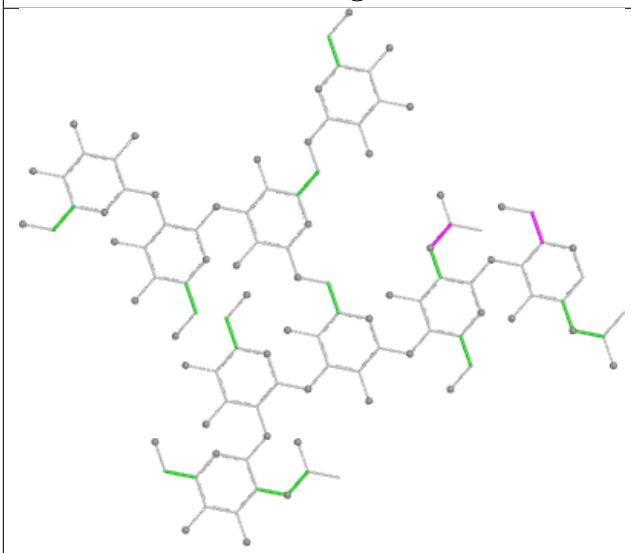
Oligosaccharide Chain D



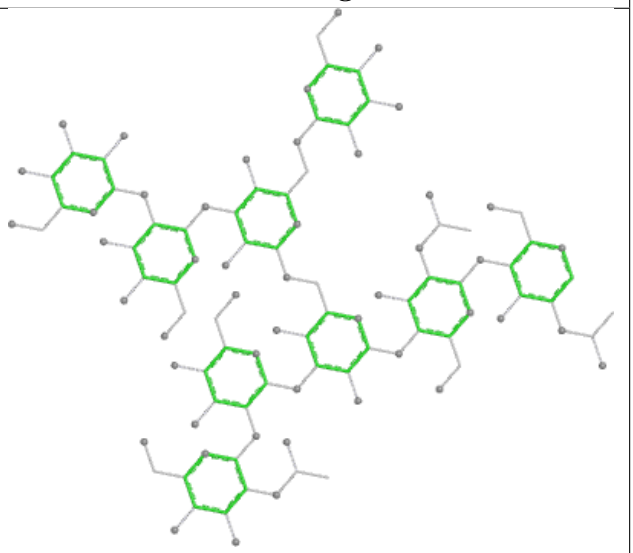
Bond lengths



Bond angles

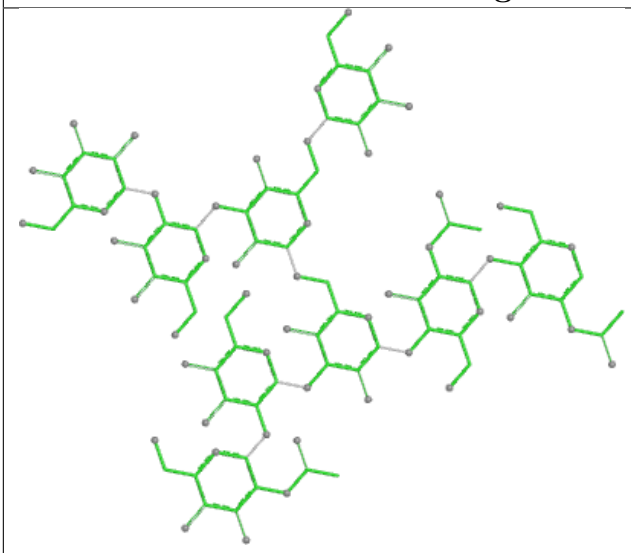


Torsions

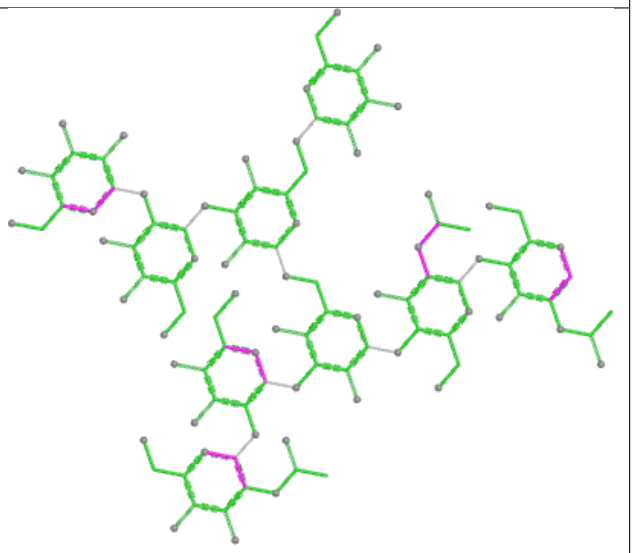


Rings

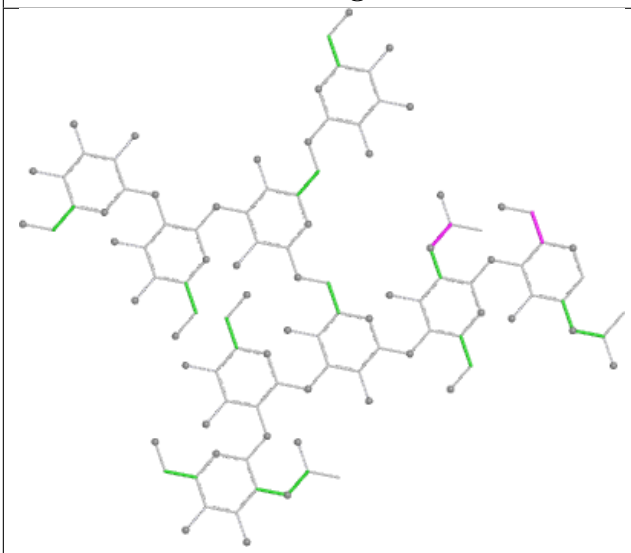
Oligosaccharide Chain R



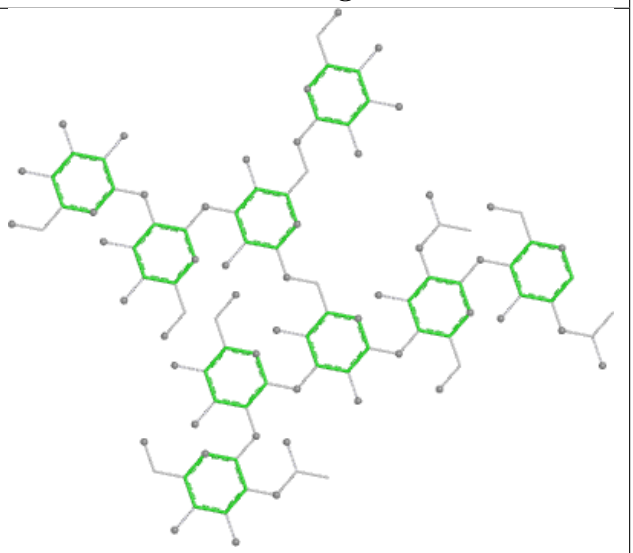
Bond lengths



Bond angles

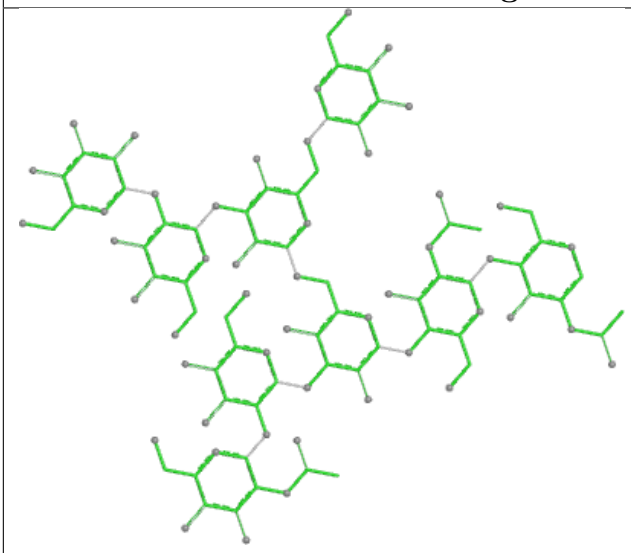


Torsions

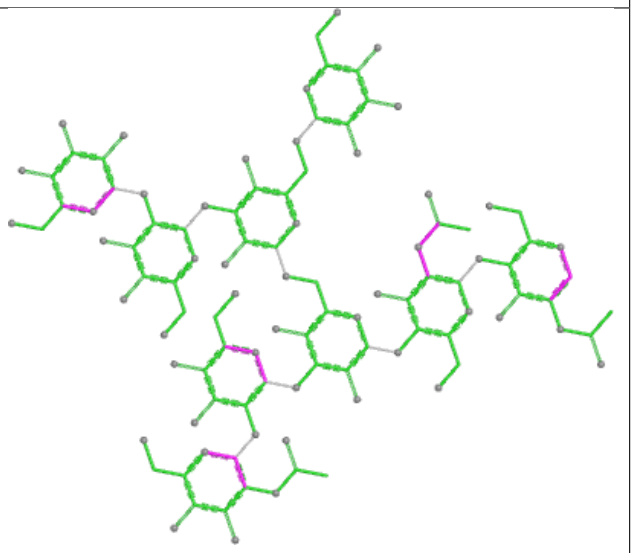


Rings

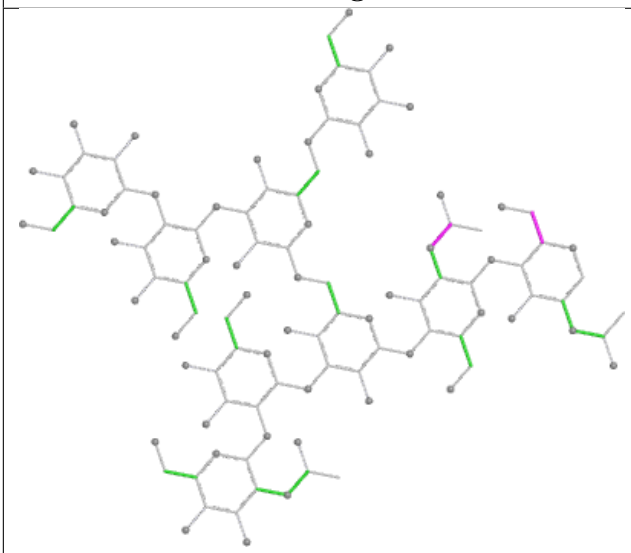
Oligosaccharide Chain f



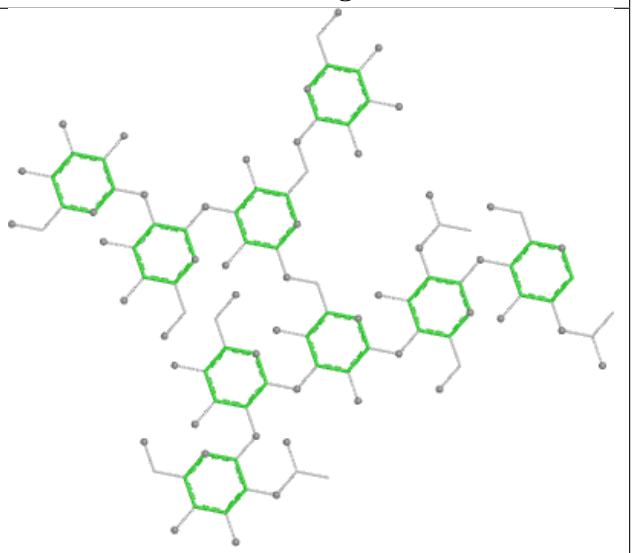
Bond lengths



Bond angles

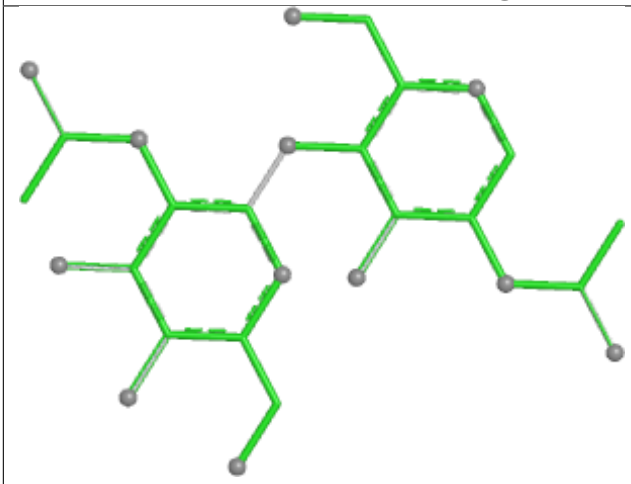


Torsions

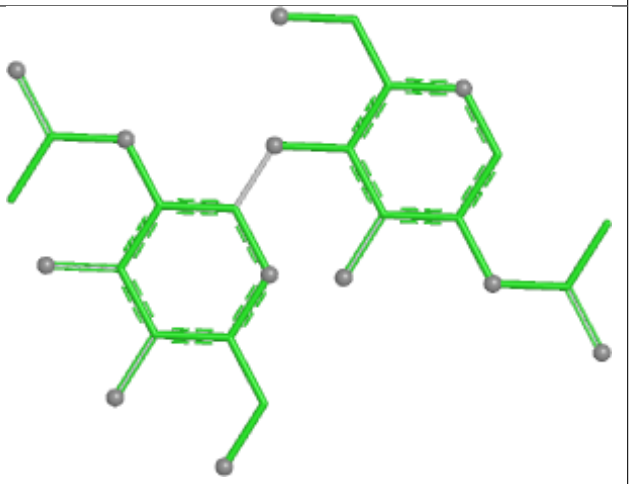


Rings

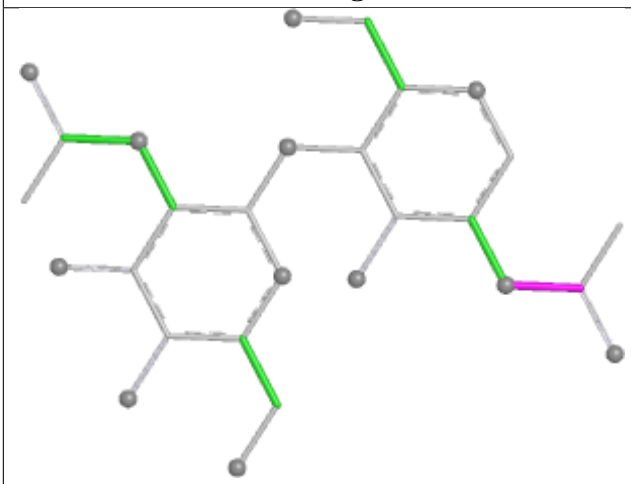
Oligosaccharide Chain E



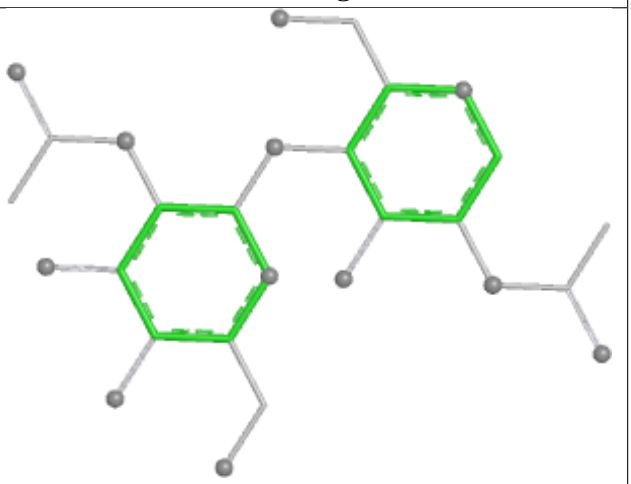
Bond lengths



Bond angles

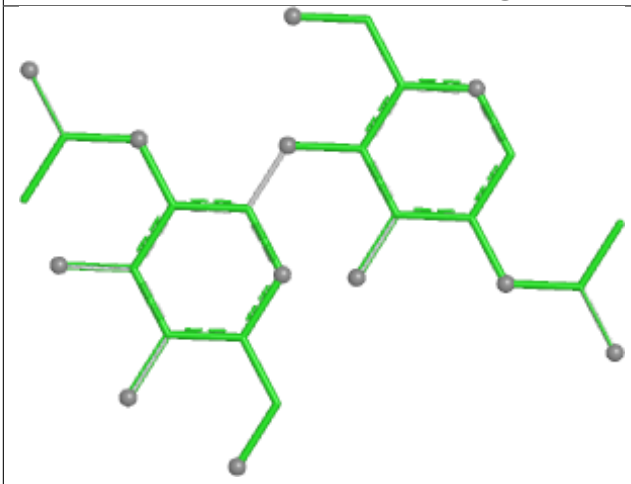


Torsions

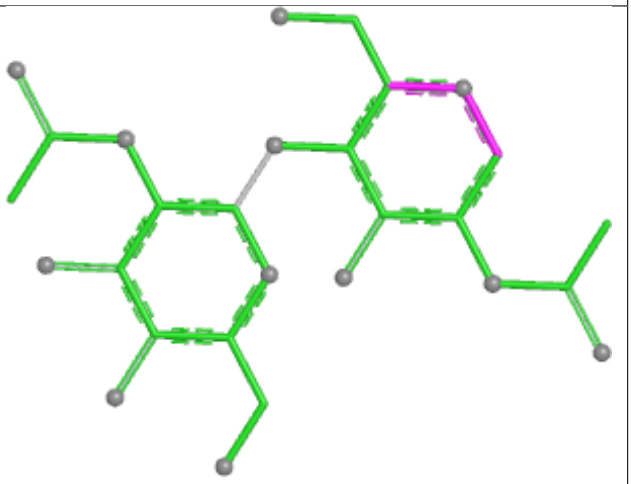


Rings

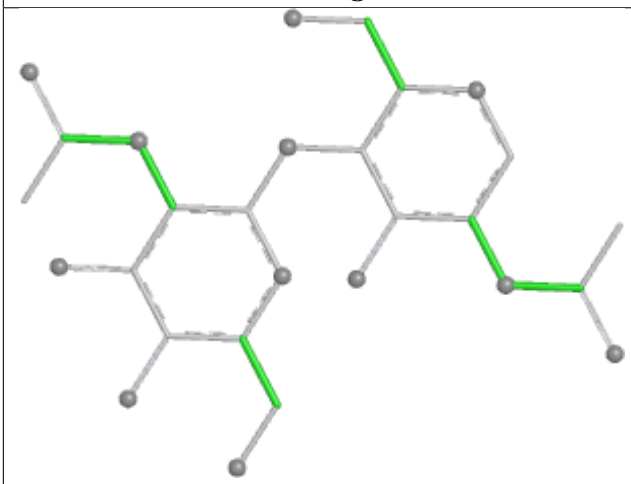
Oligosaccharide Chain F



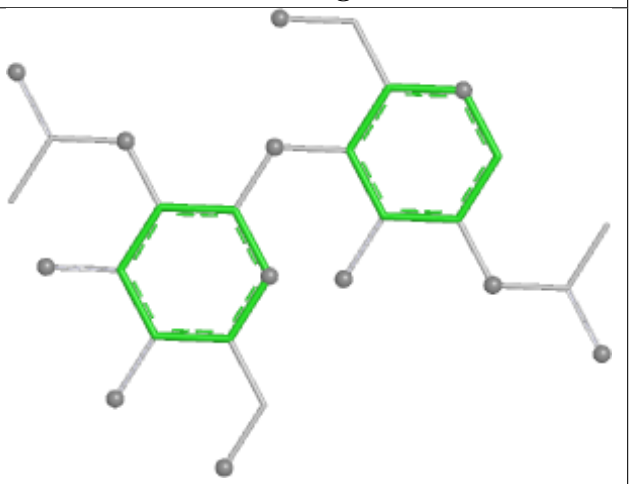
Bond lengths



Bond angles

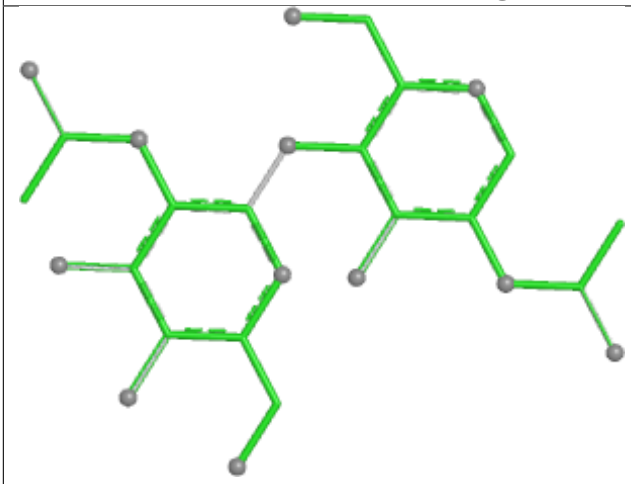


Torsions

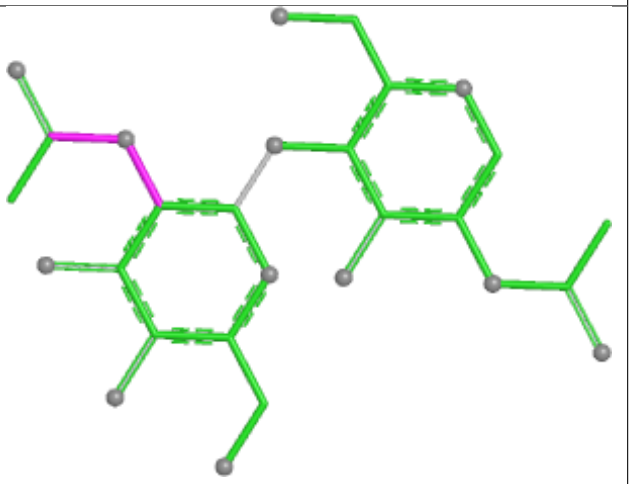


Rings

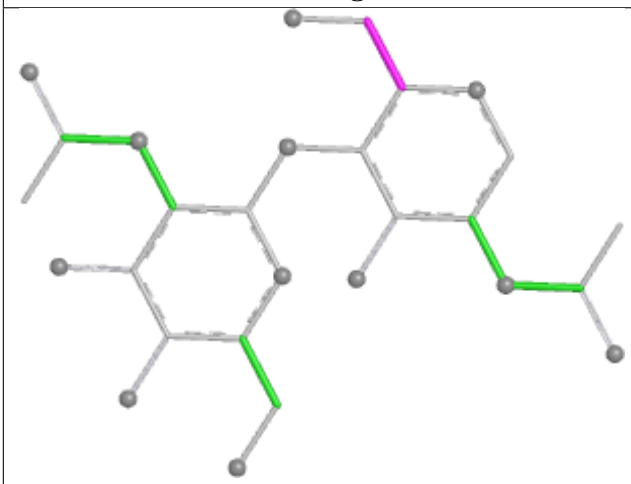
Oligosaccharide Chain G



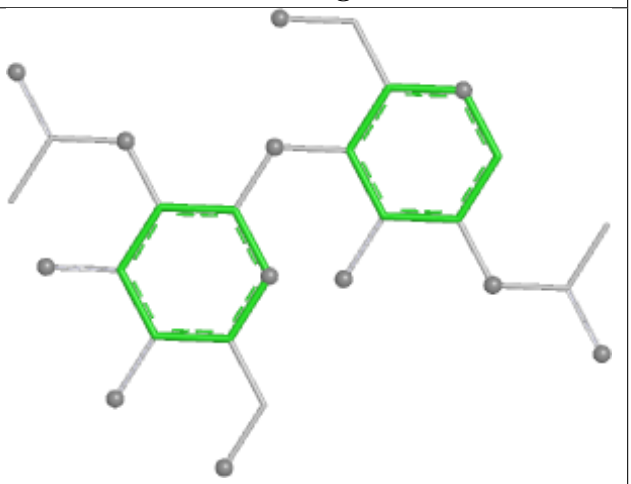
Bond lengths



Bond angles

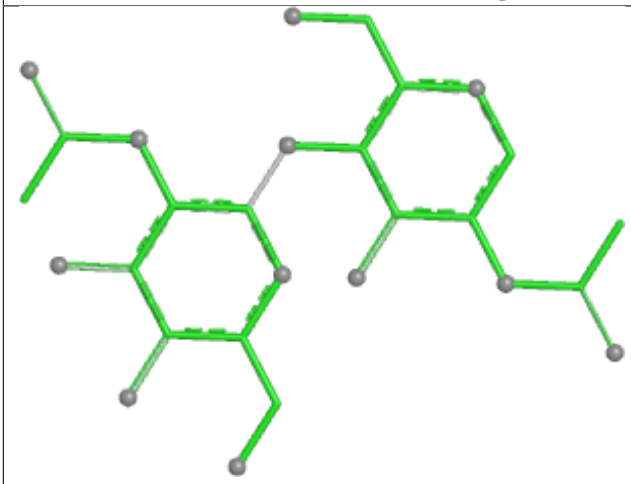


Torsions

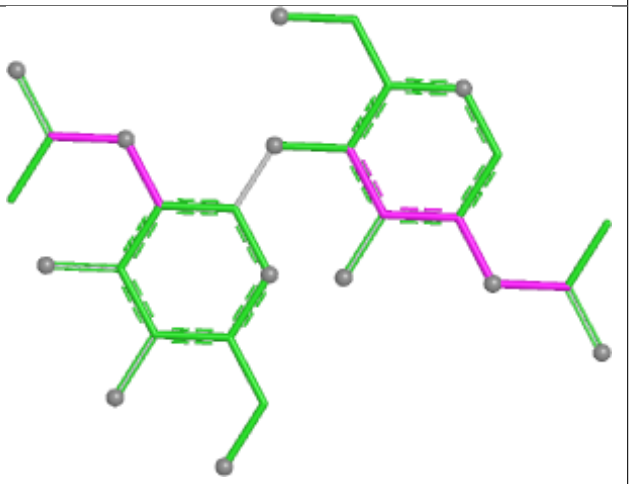


Rings

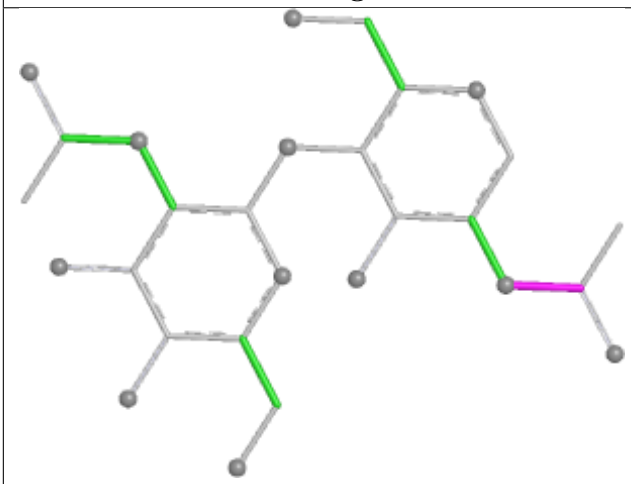
Oligosaccharide Chain H



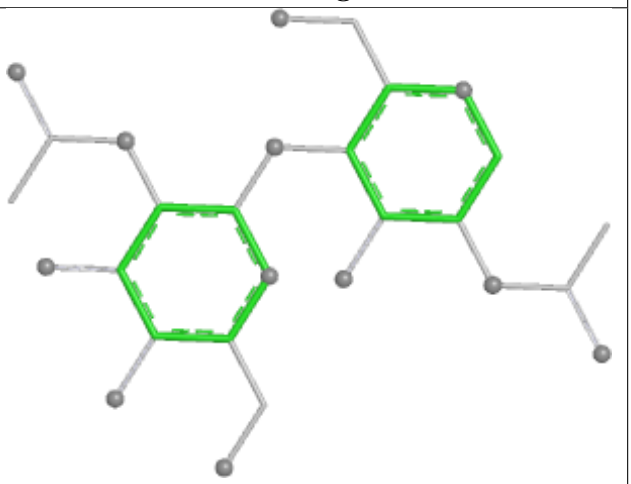
Bond lengths



Bond angles

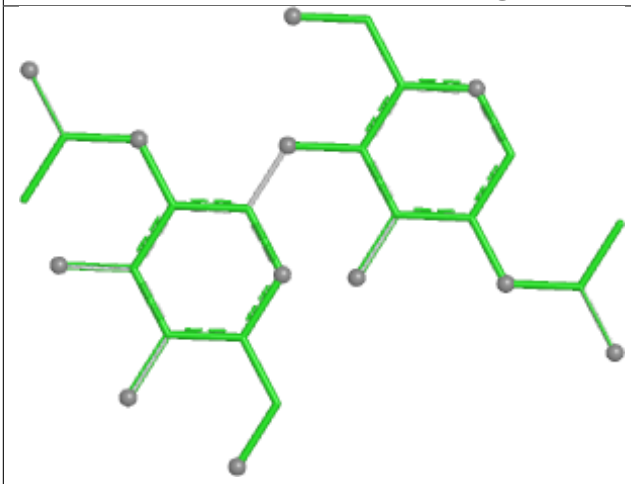


Torsions

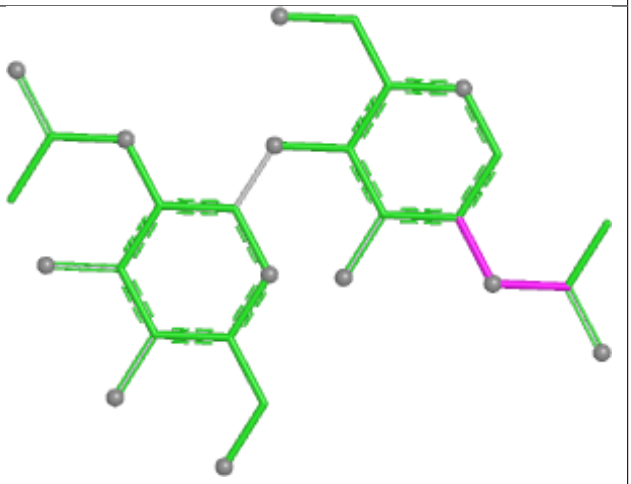


Rings

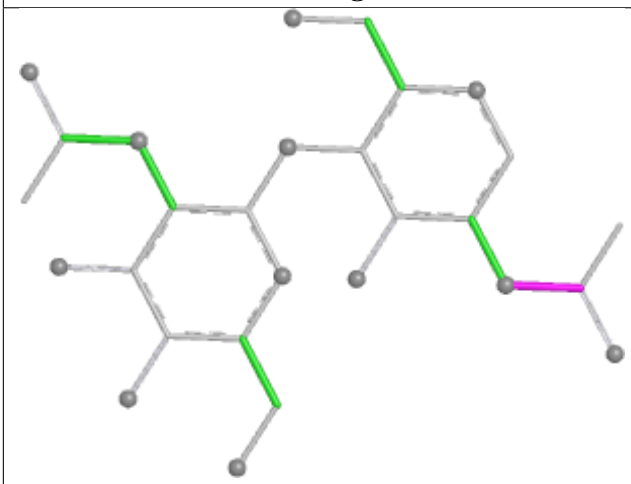
Oligosaccharide Chain K



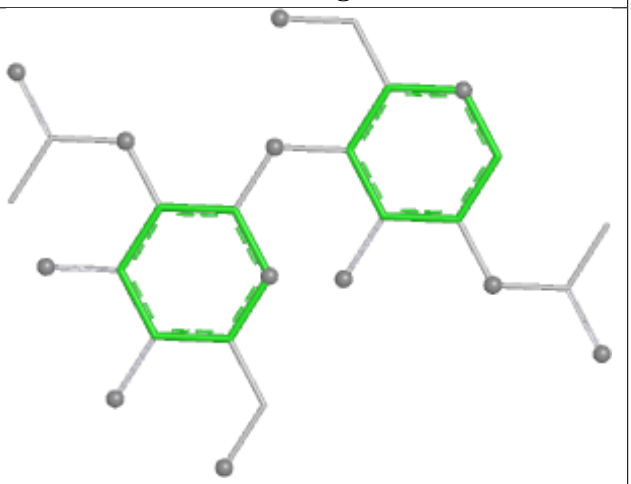
Bond lengths



Bond angles

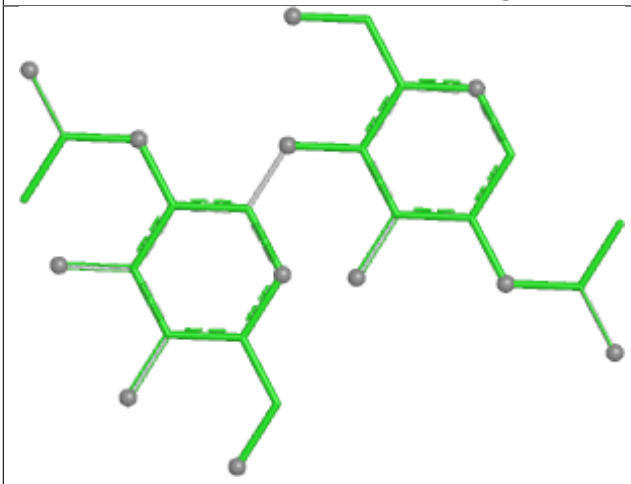


Torsions



Rings

Oligosaccharide Chain L



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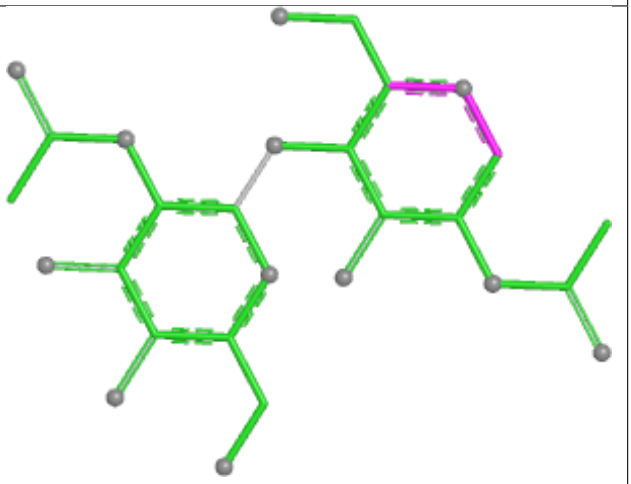
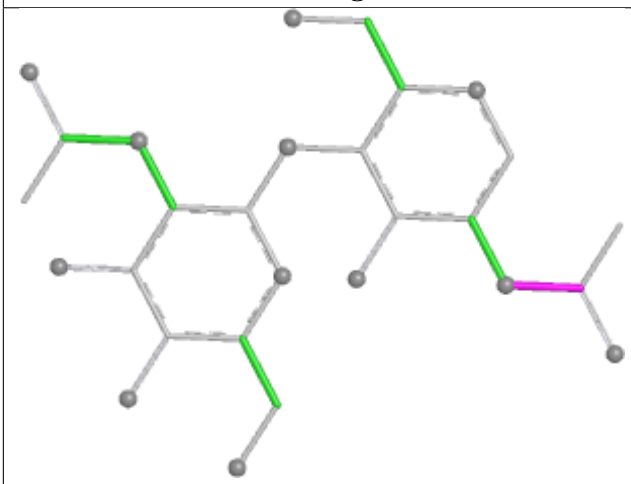


Bond angles



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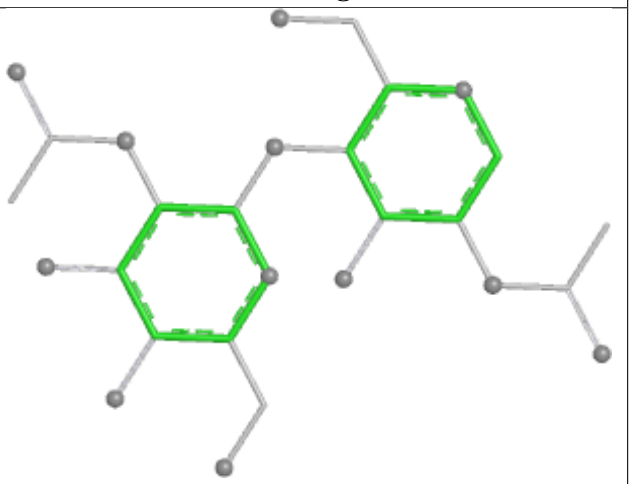
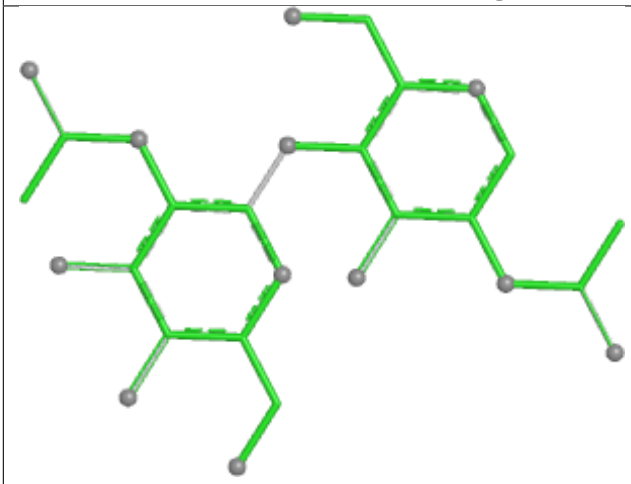
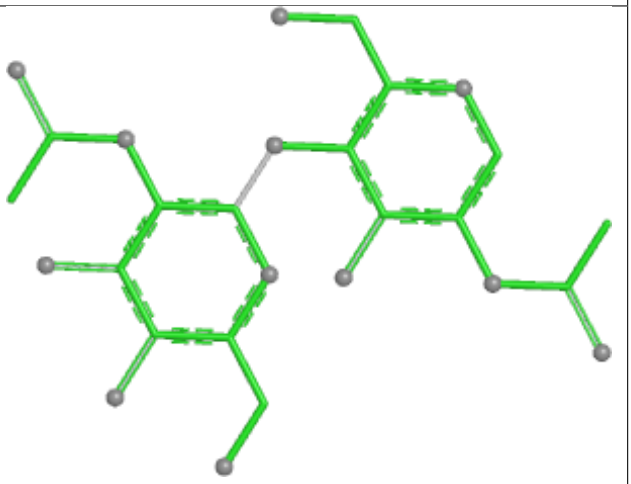


Rings

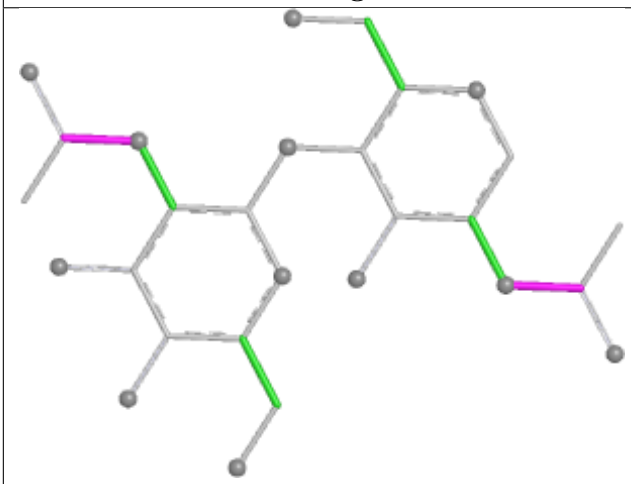
Oligosaccharide Chain M



Bond lengths



Bond angles



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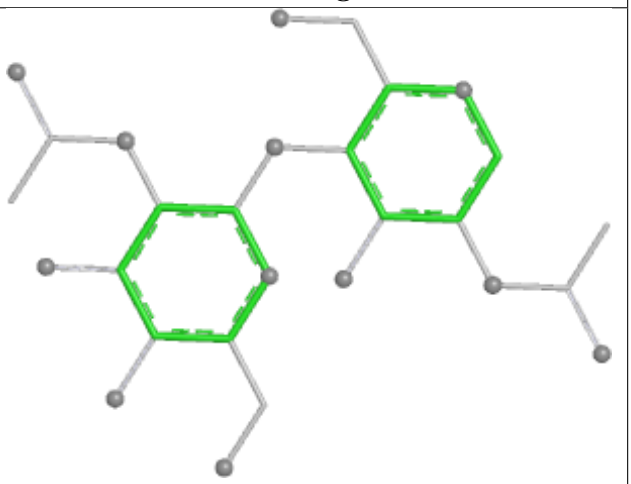
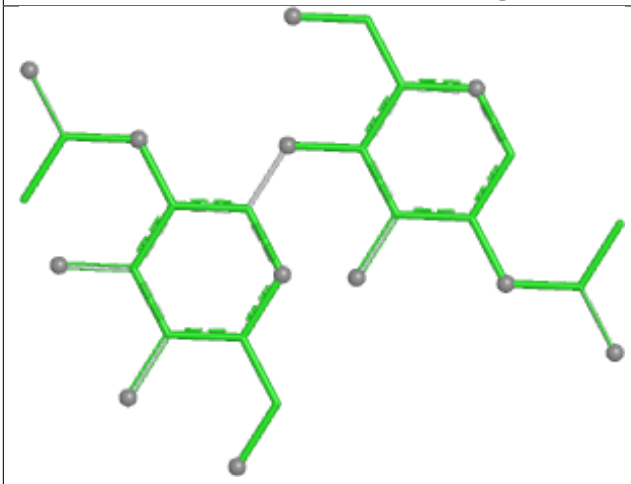


Rings

Oligosaccharide Chain N



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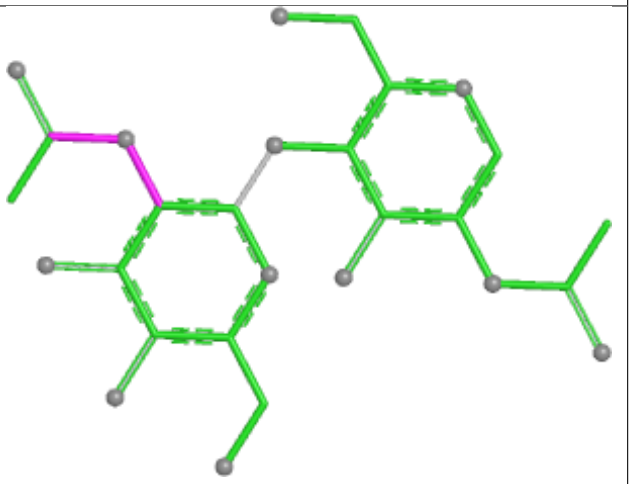
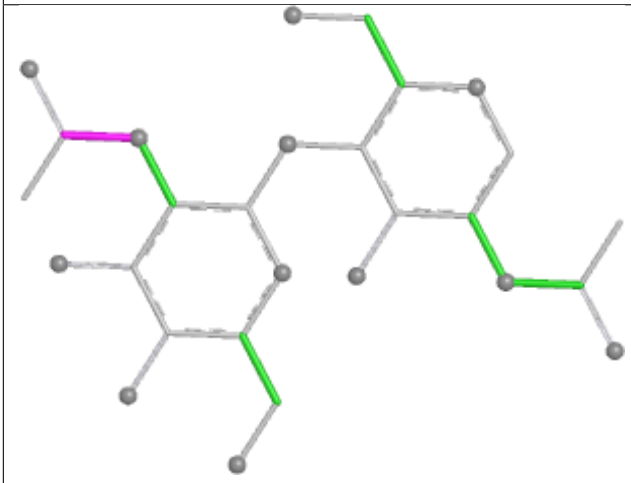
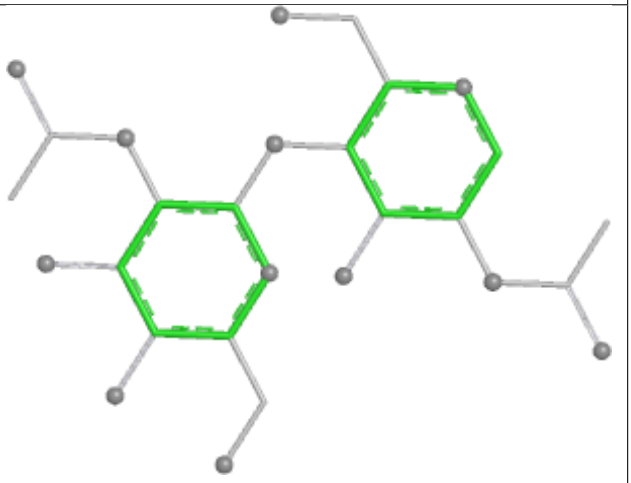


Bond angles

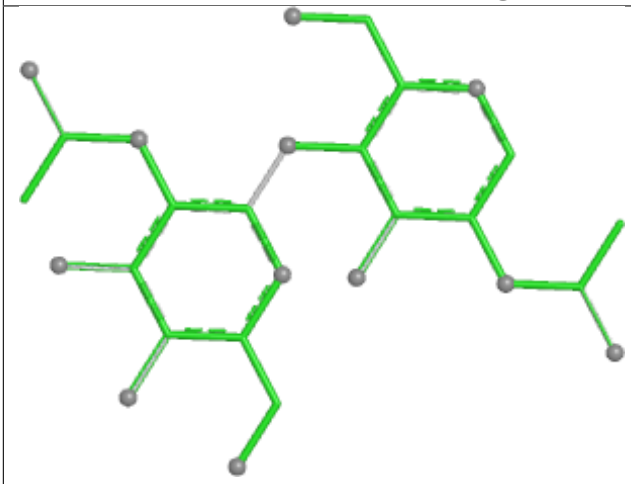


Torsions

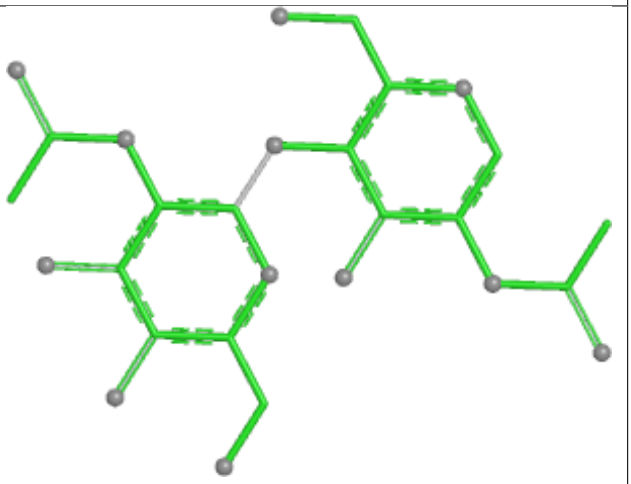


Rings

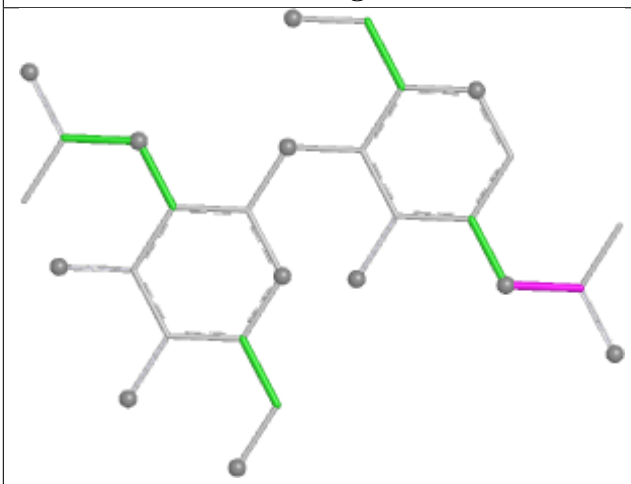
Oligosaccharide Chain O



Bond lengths



Bond angles



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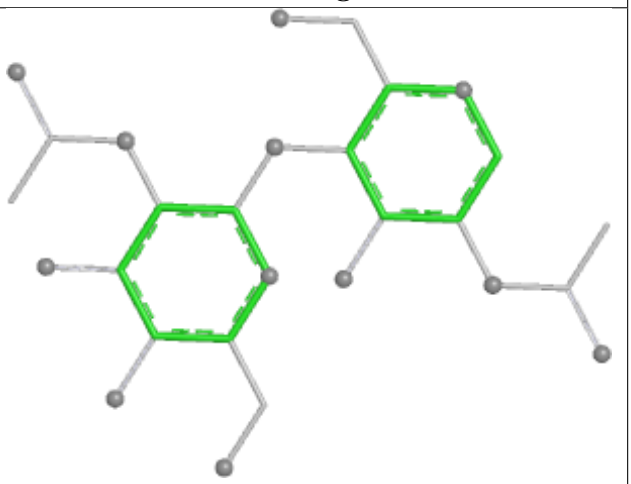
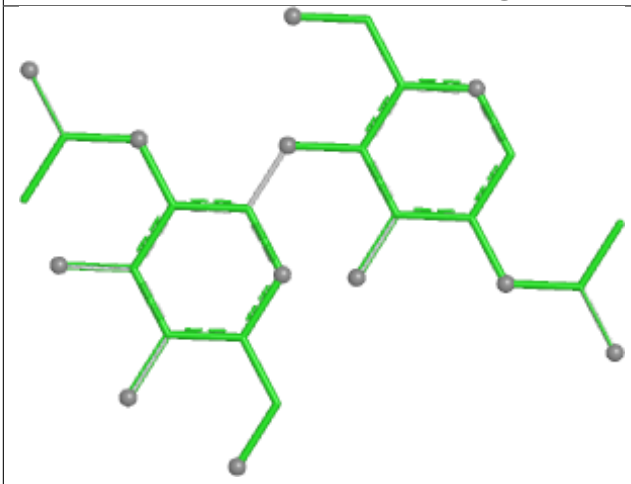


Rings

Oligosaccharide Chain P



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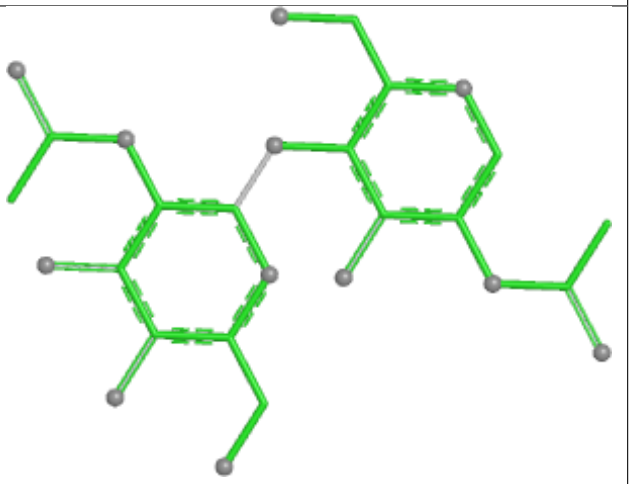
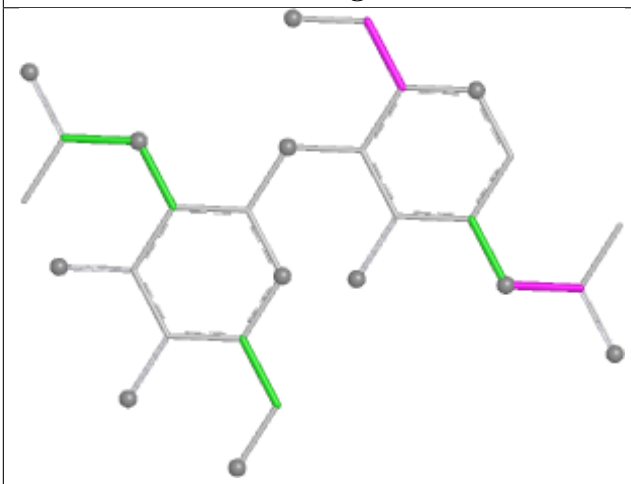


Bond angles



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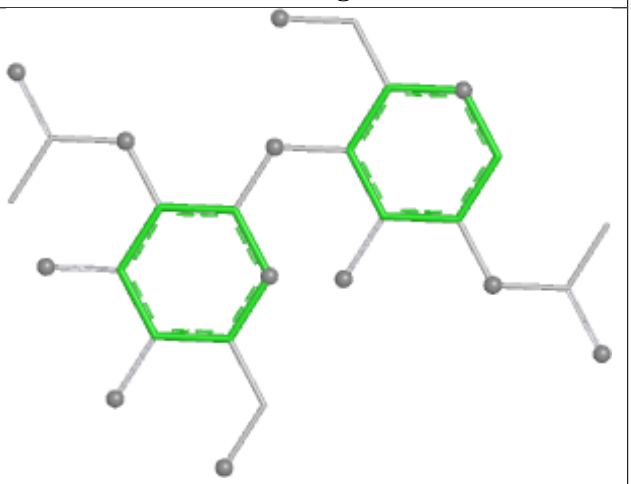
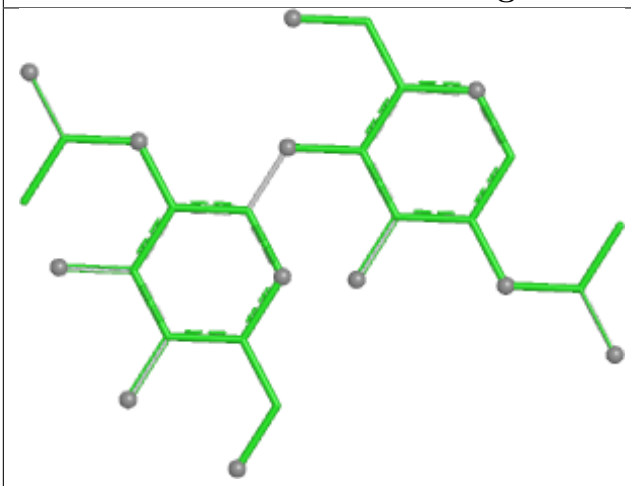


Rings

Oligosaccharide Chain S



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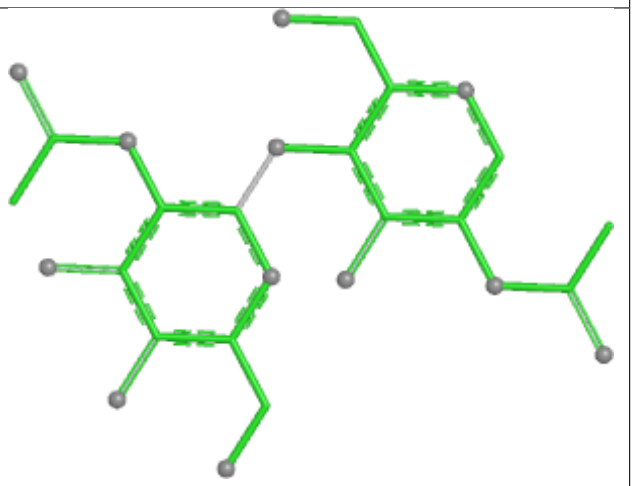
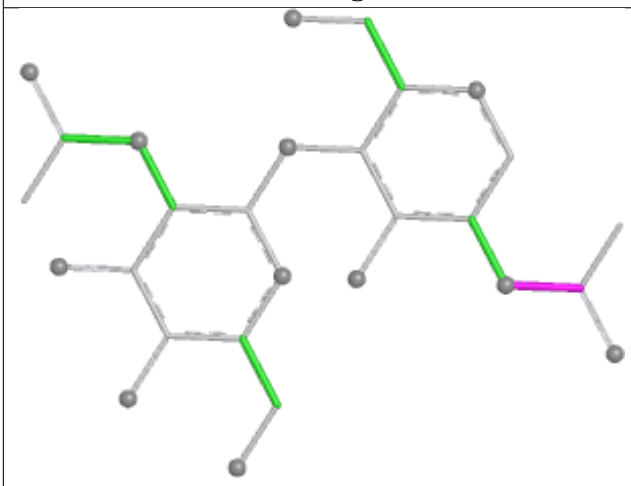
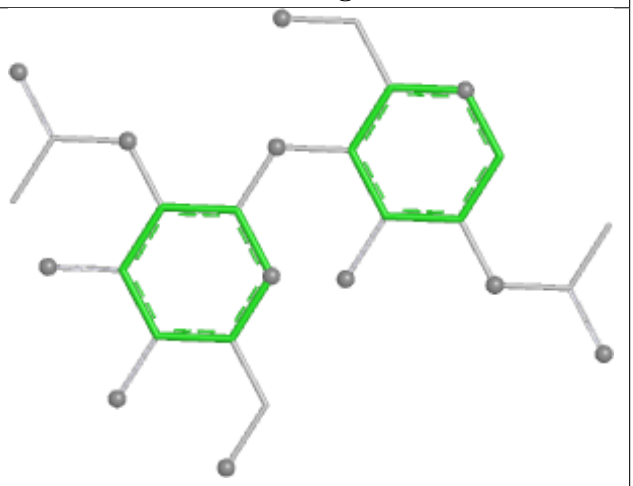


Bond angles

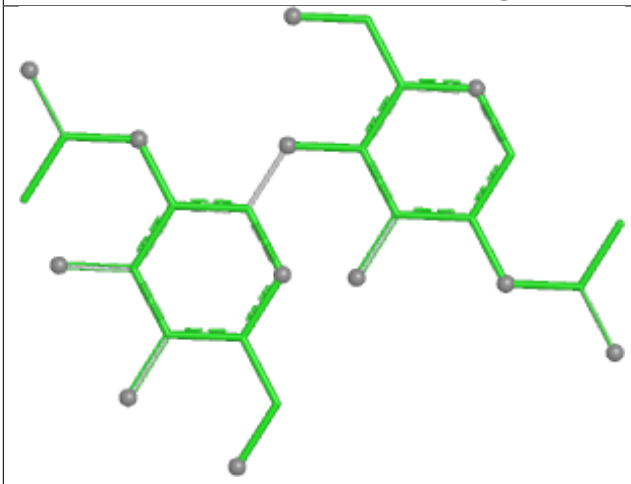


Torsions



Rings

Oligosaccharide Chain T



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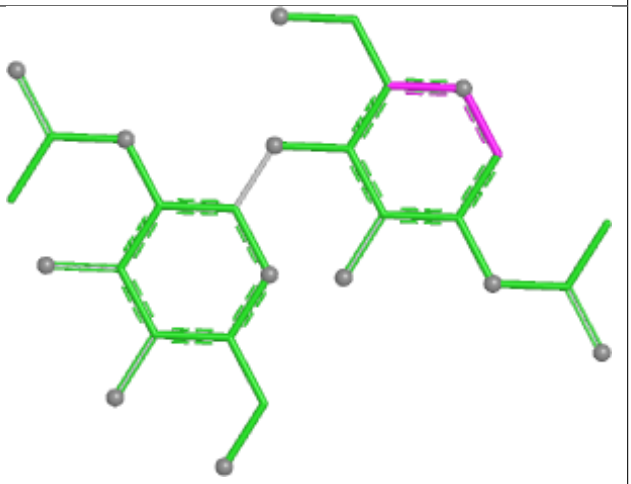
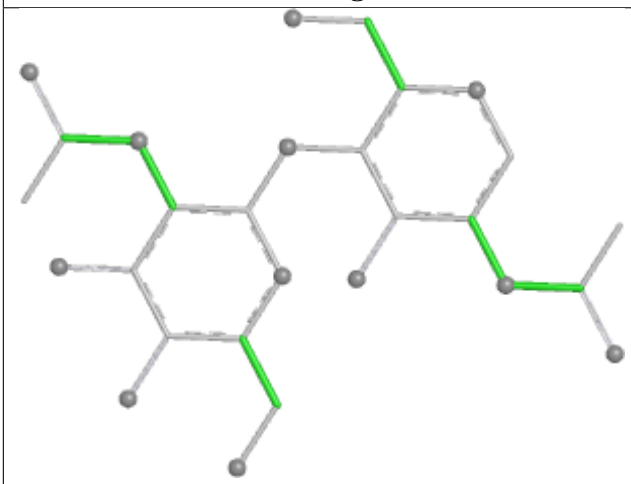


Bond angles



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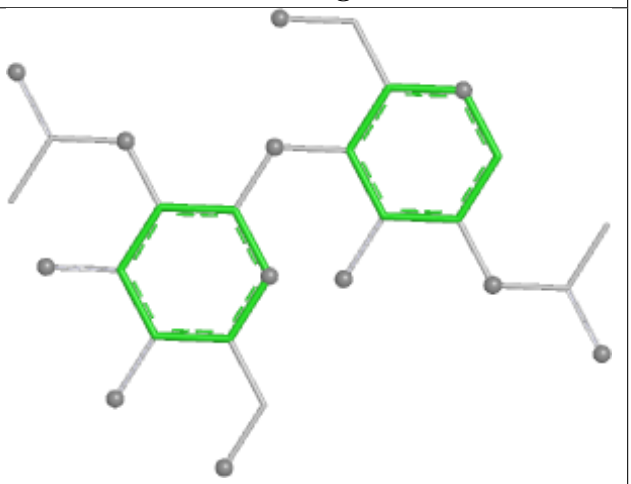
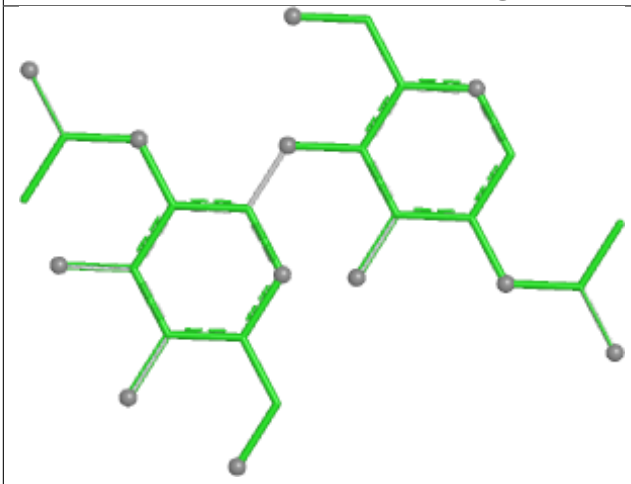


Rings

Oligosaccharide Chain U



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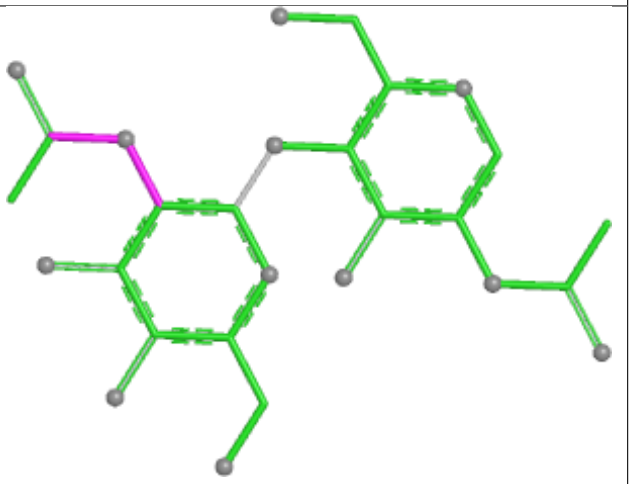
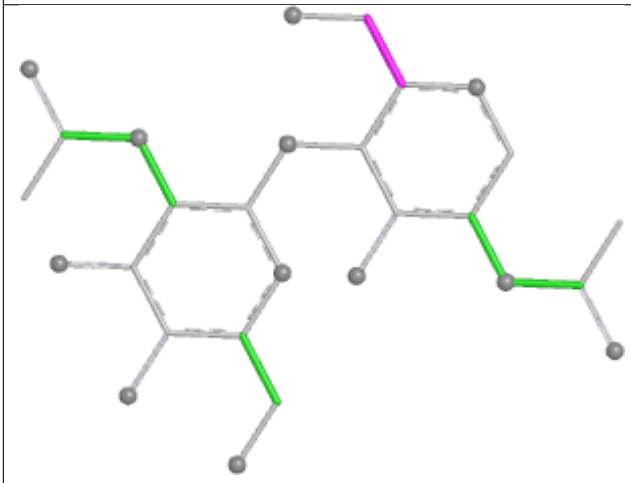
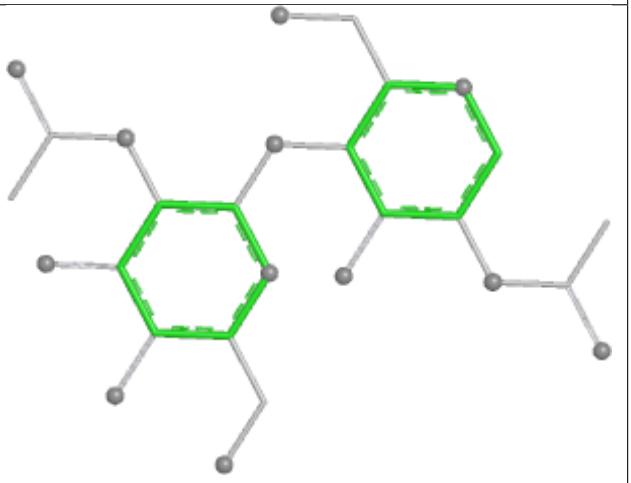


Bond angles

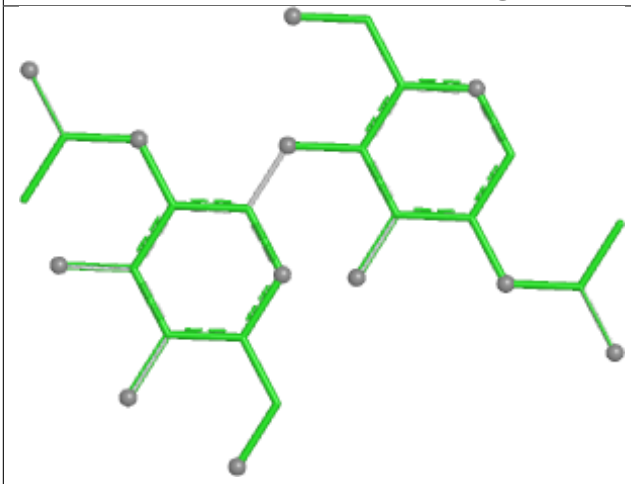


Torsions



Rings

Oligosaccharide Chain V



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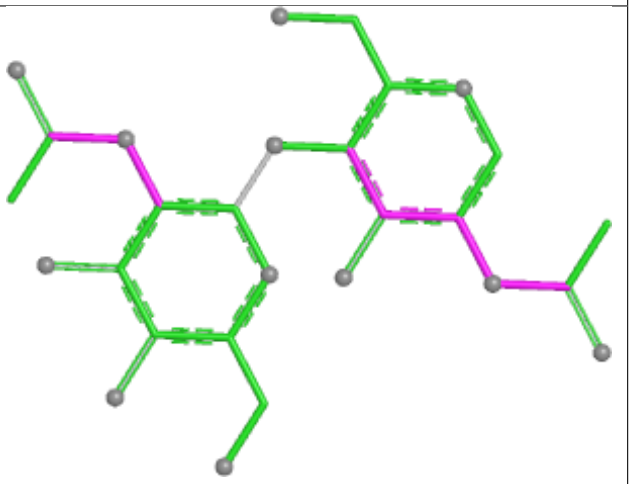
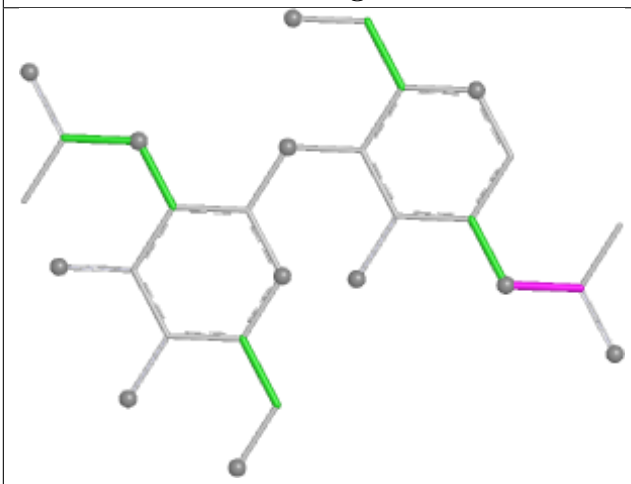


Bond angles



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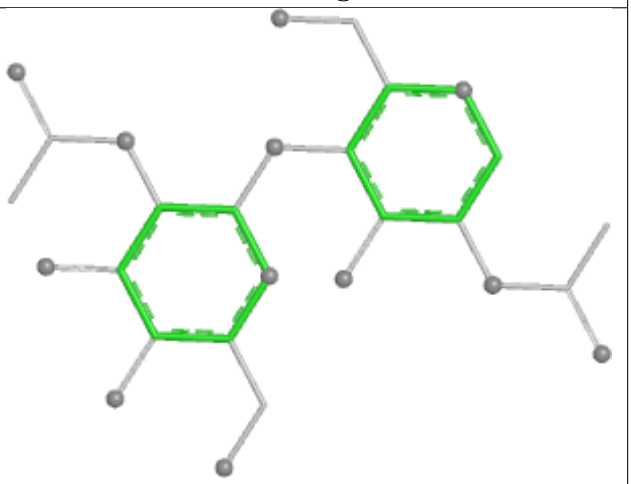
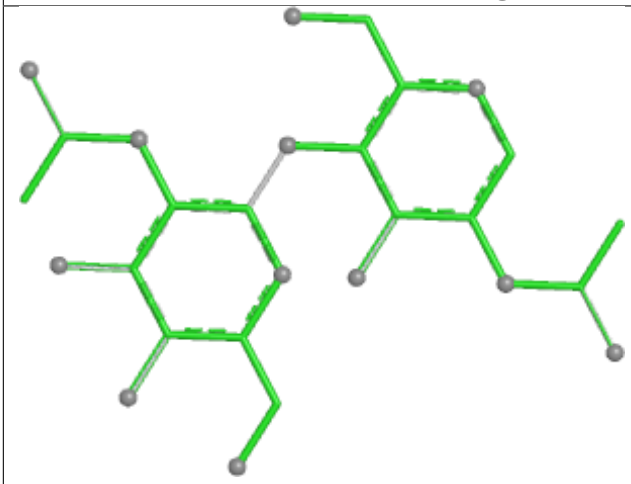


Rings

Oligosaccharide Chain Y



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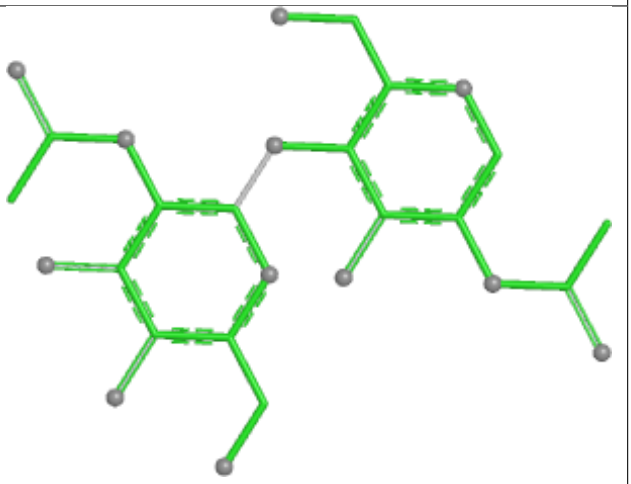
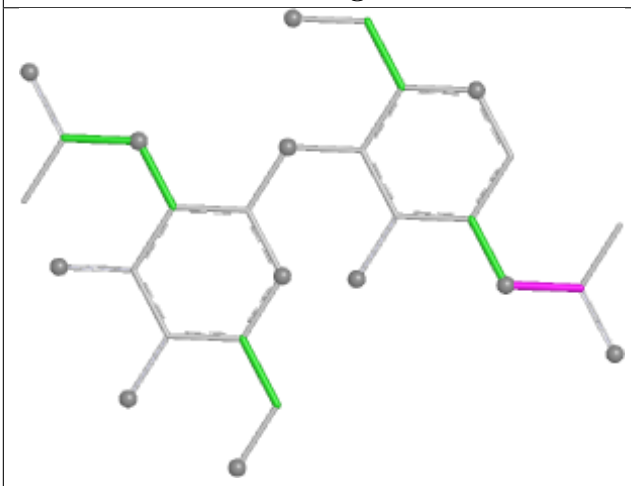


Bond angles



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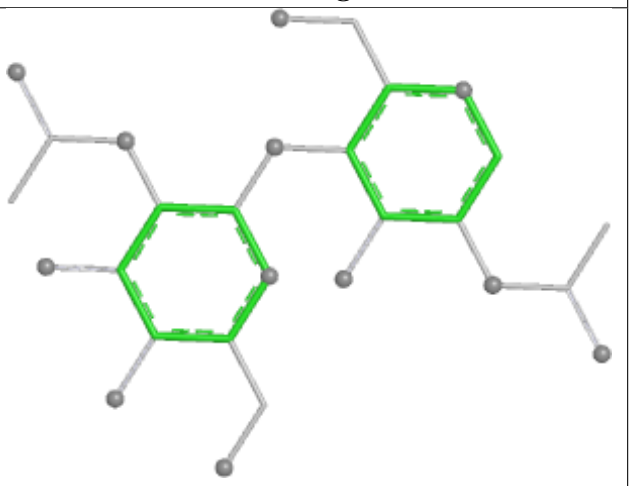
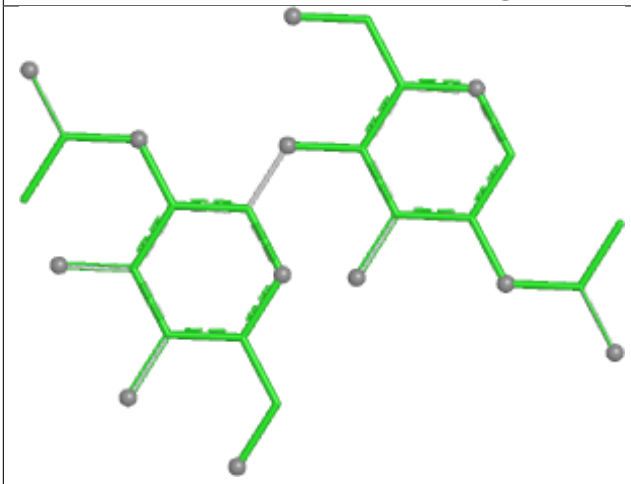


Rings

Oligosaccharide Chain Z



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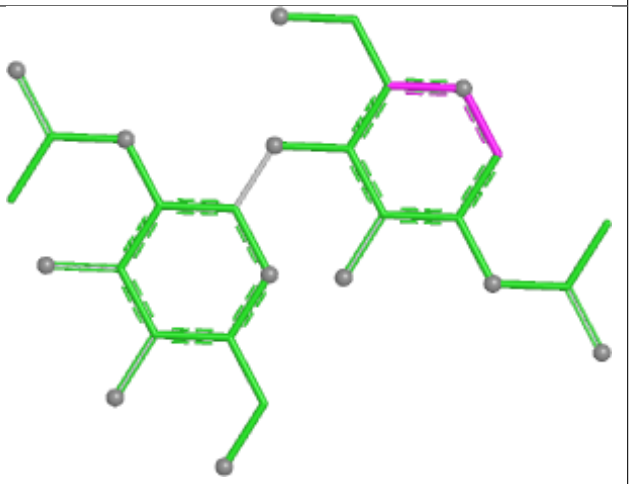
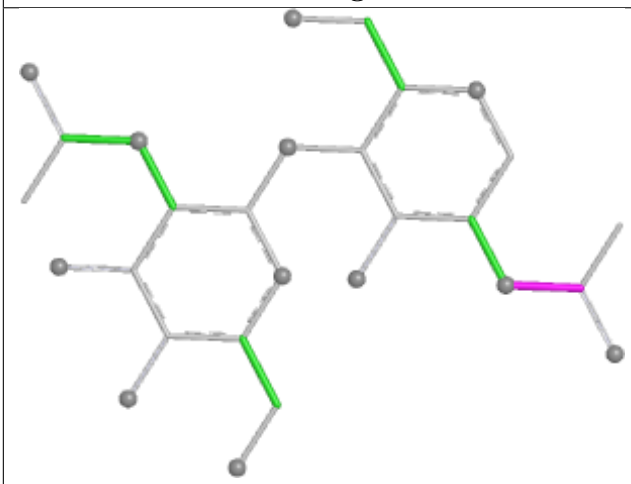
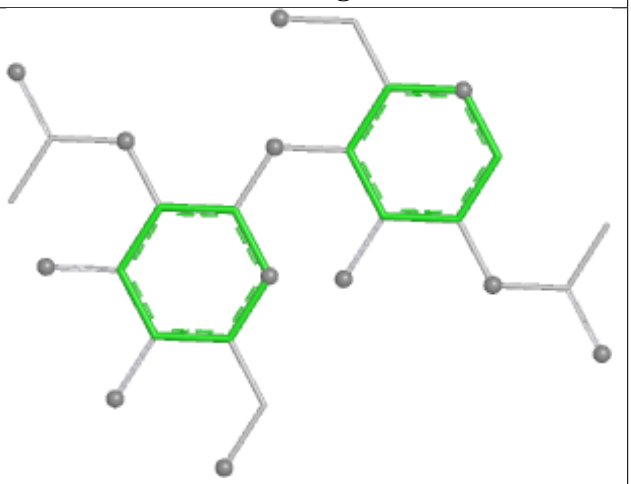


Bond angles

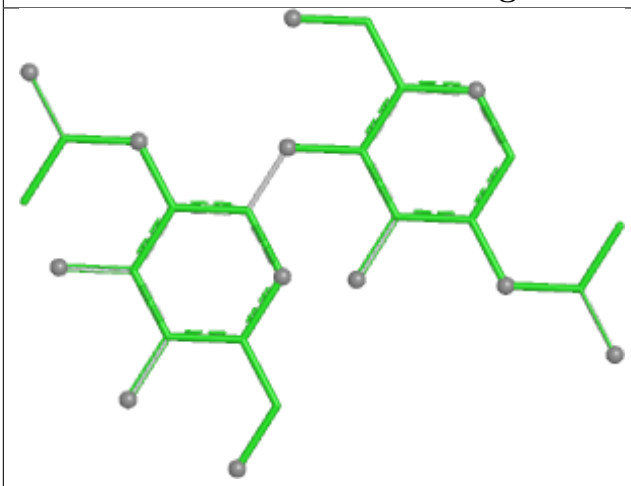


Torsions



Rings

Oligosaccharide Chain a



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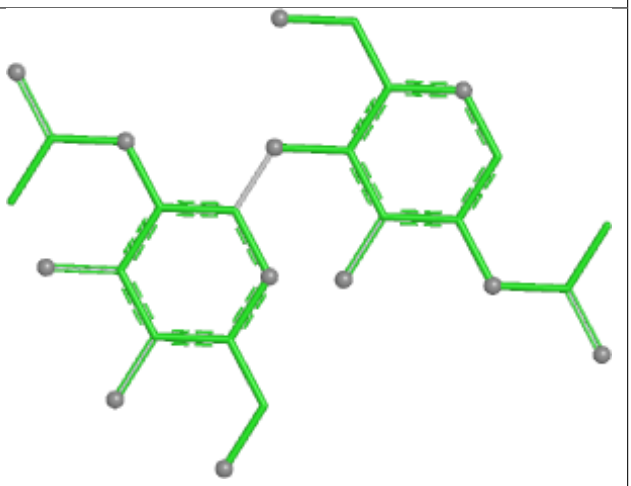
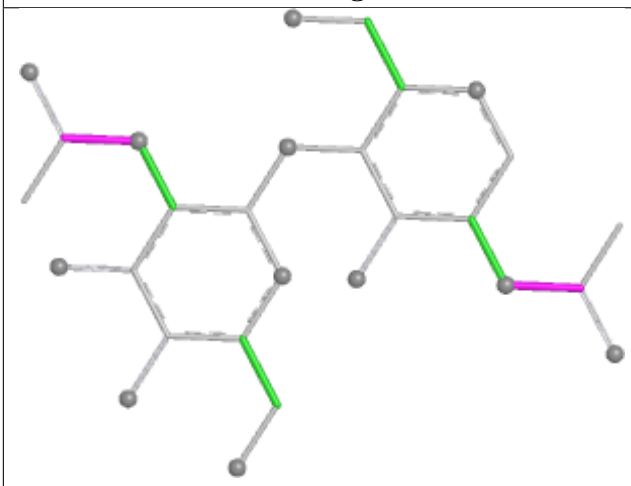
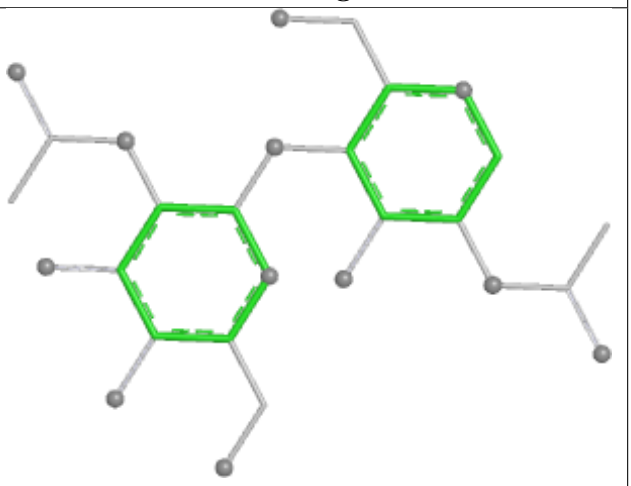


Bond angles

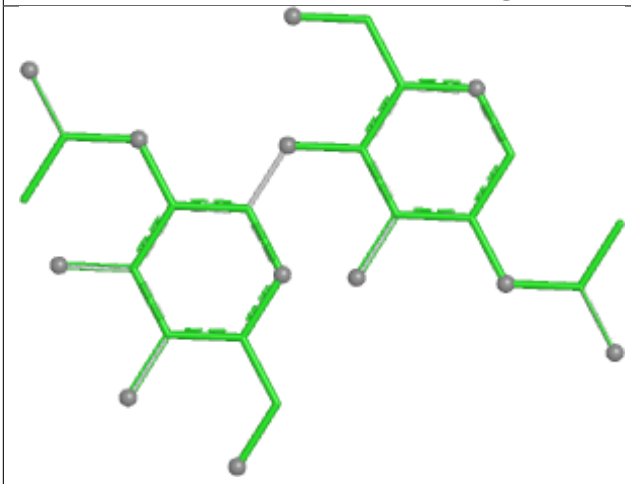


Torsions

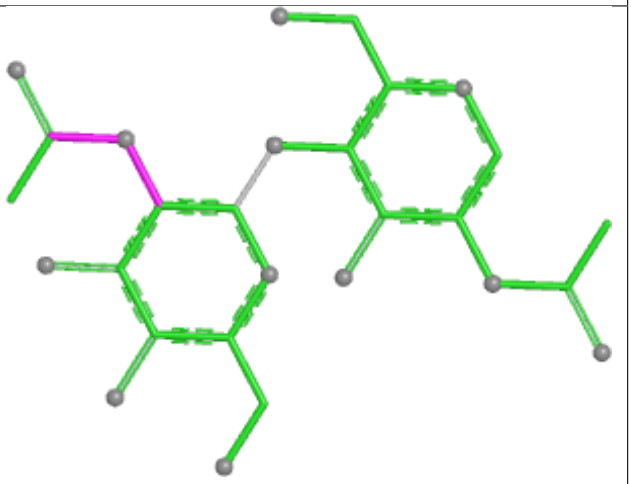


Rings

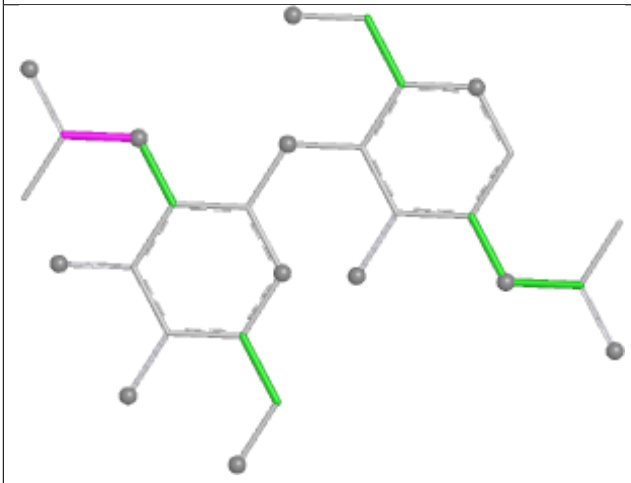
Oligosaccharide Chain b



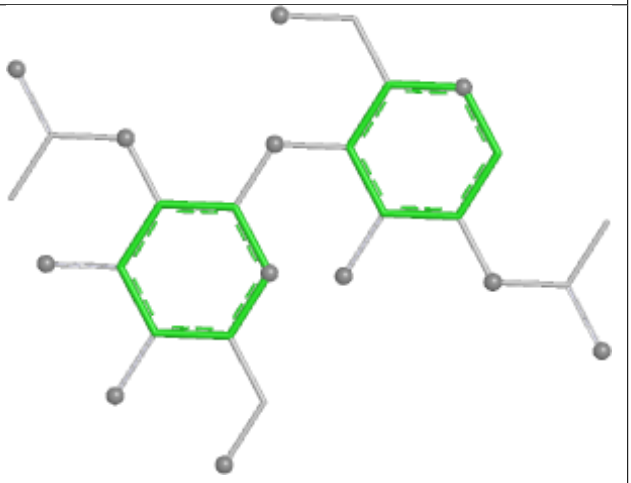
Bond lengths



Bond angles

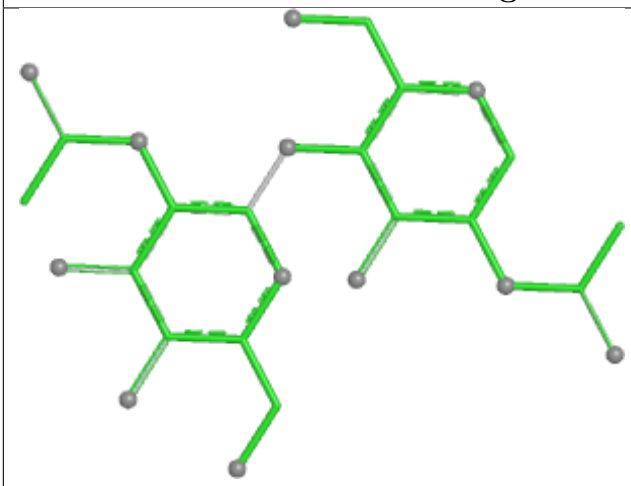


Torsions

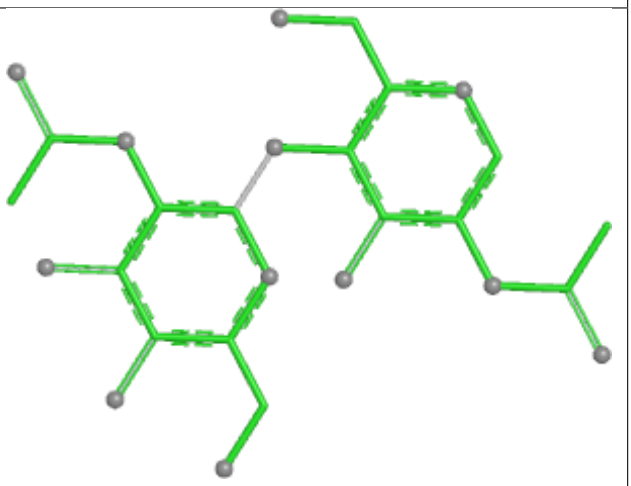


Rings

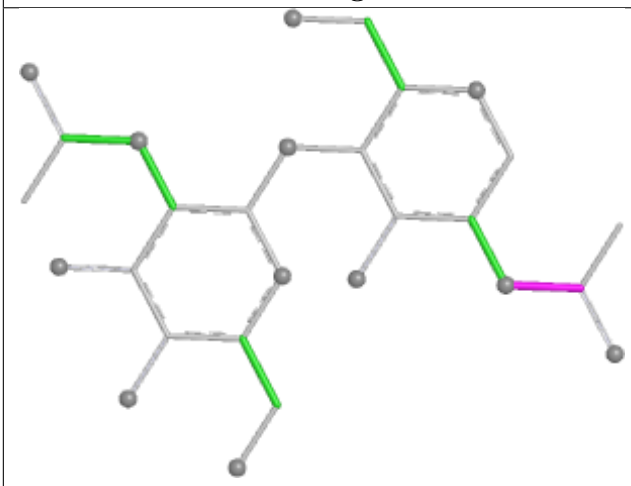
Oligosaccharide Chain c



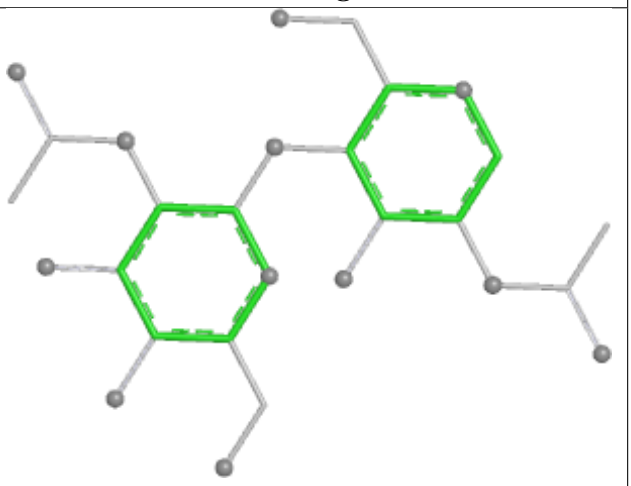
Bond lengths



Bond angles

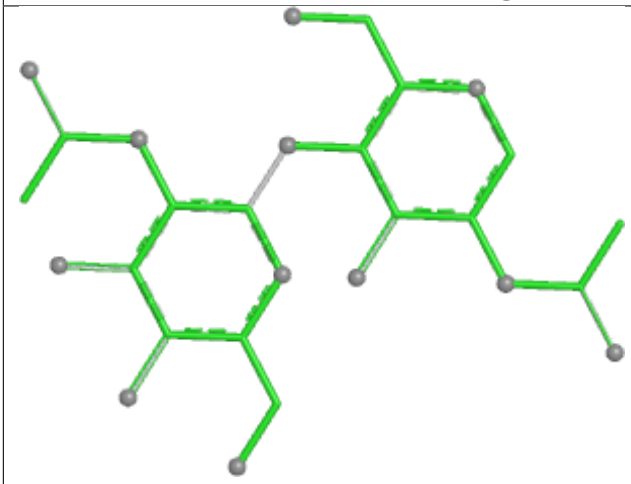


Torsions



Rings

Oligosaccharide Chain d



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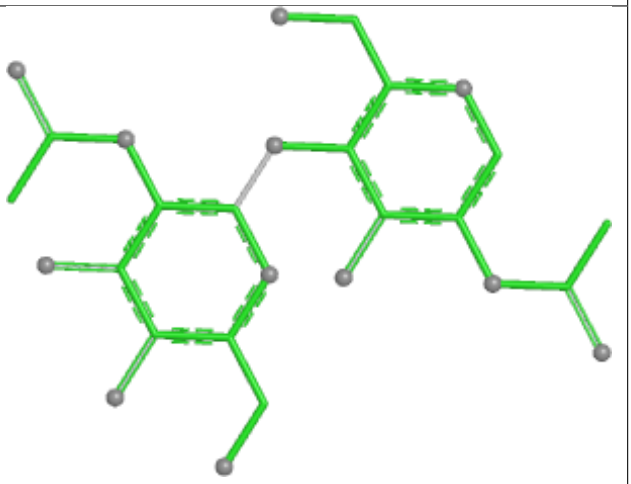
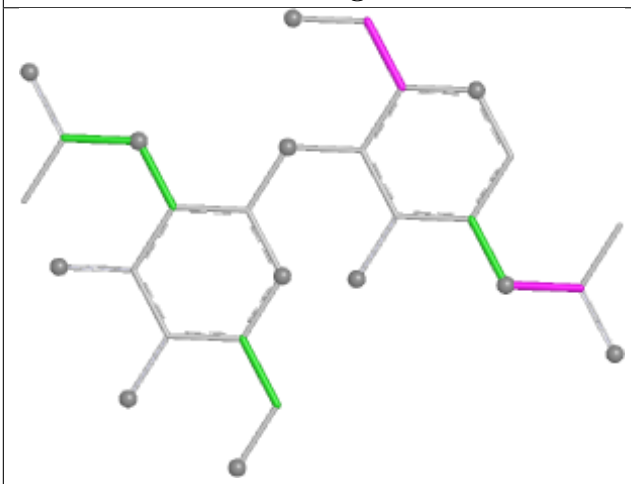


Bond angles



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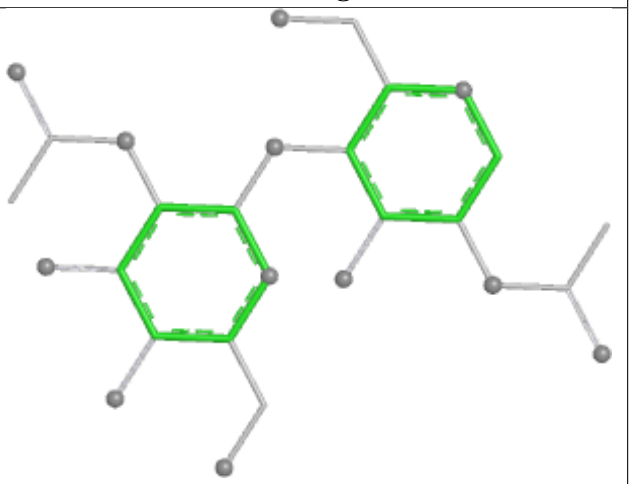
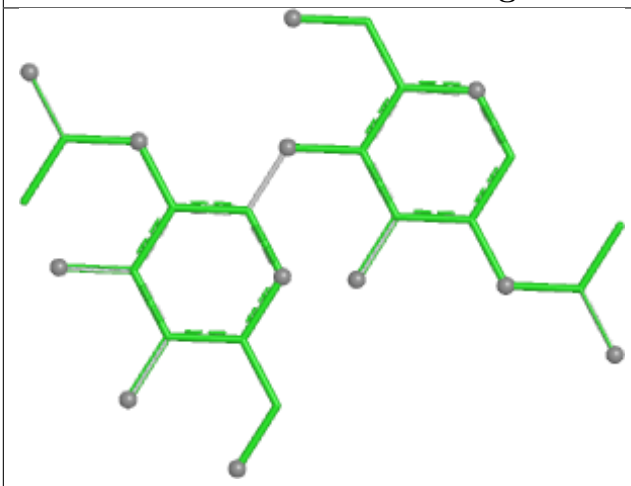


Rings

Oligosaccharide Chain g



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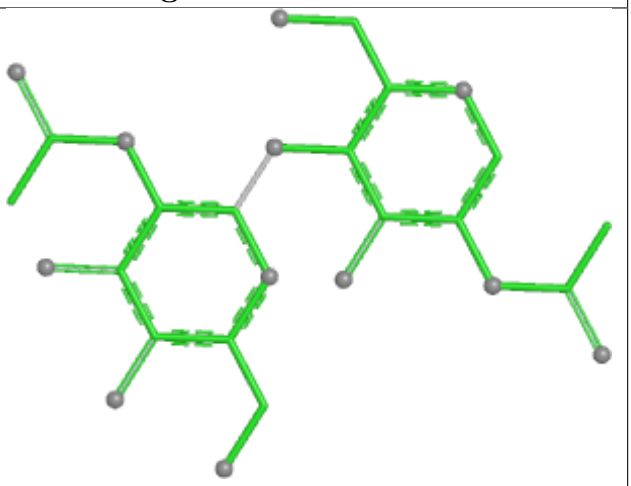
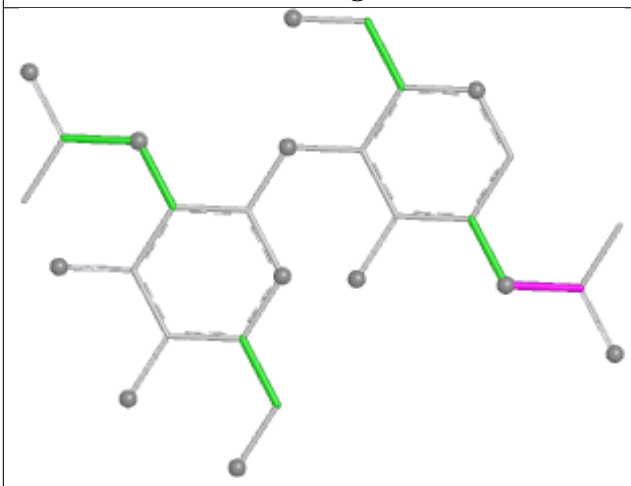


Bond angles



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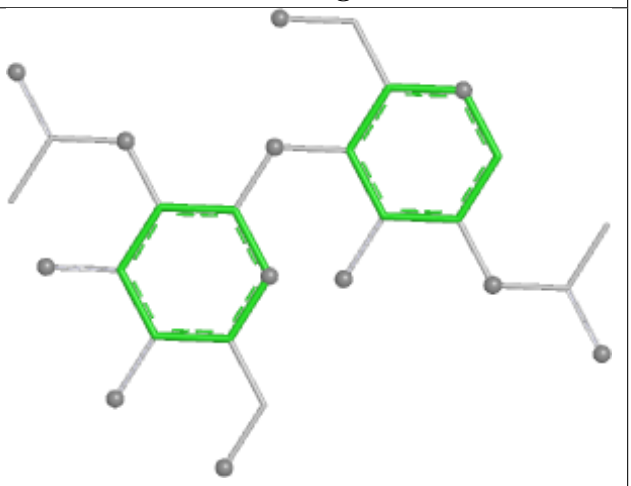
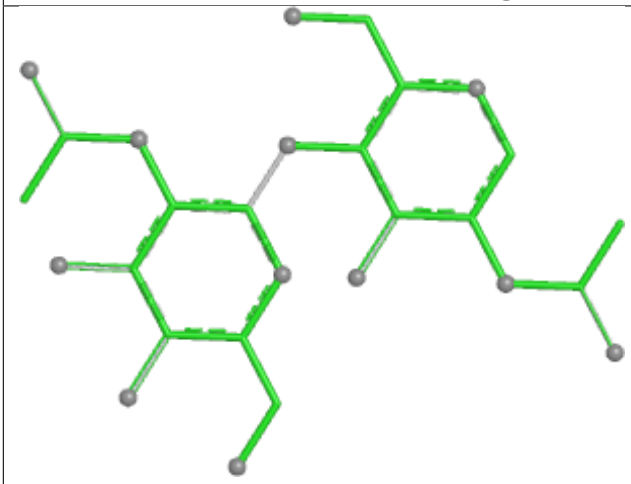


Rings

Oligosaccharide Chain h



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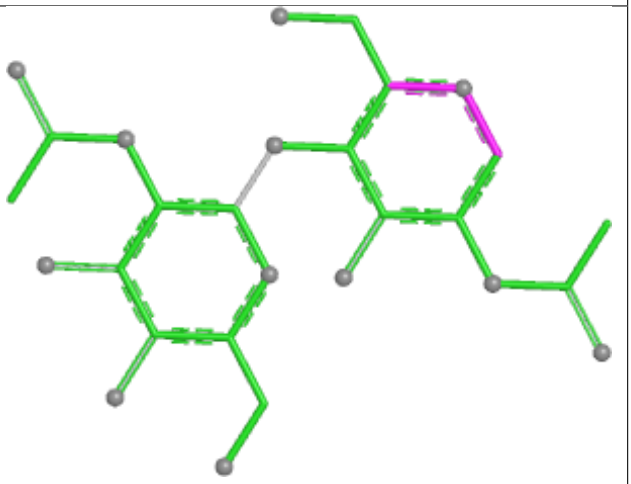
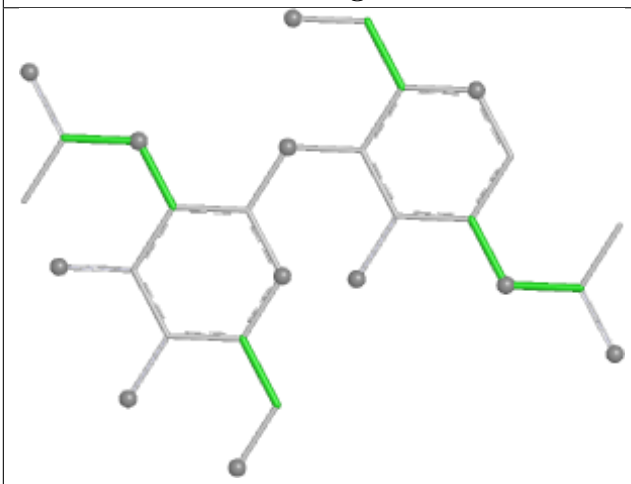


Bond angles



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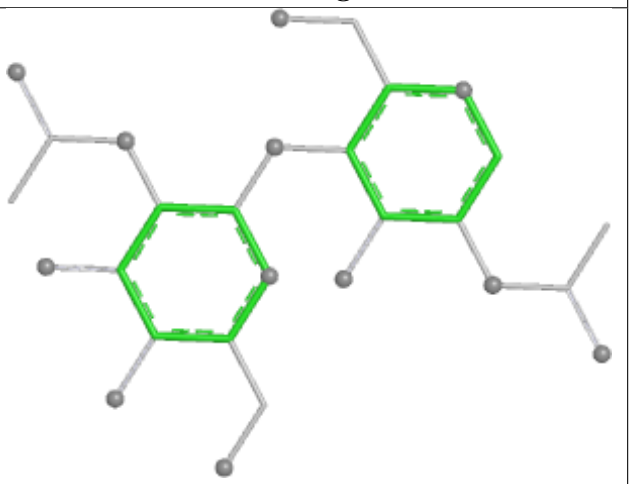
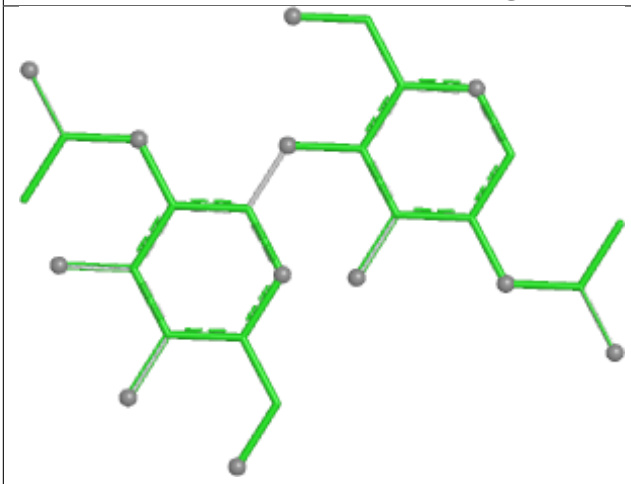


Rings

Oligosaccharide Chain i



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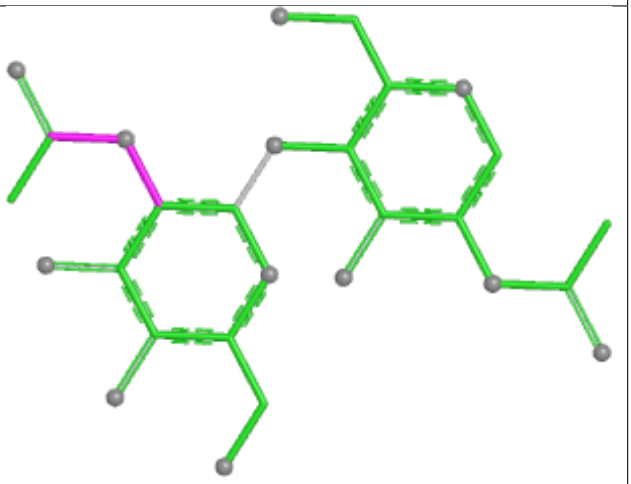

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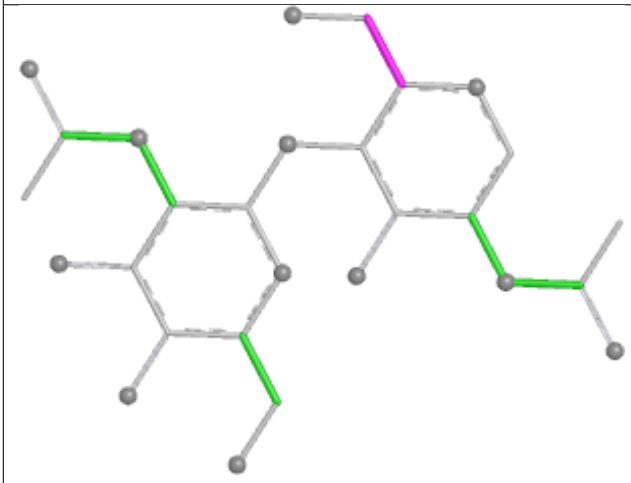
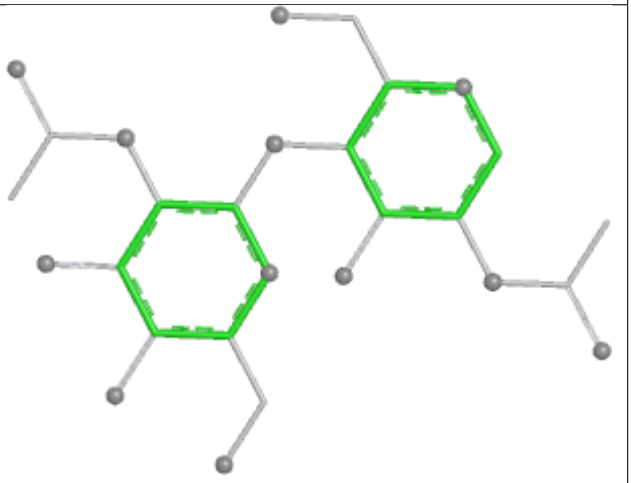
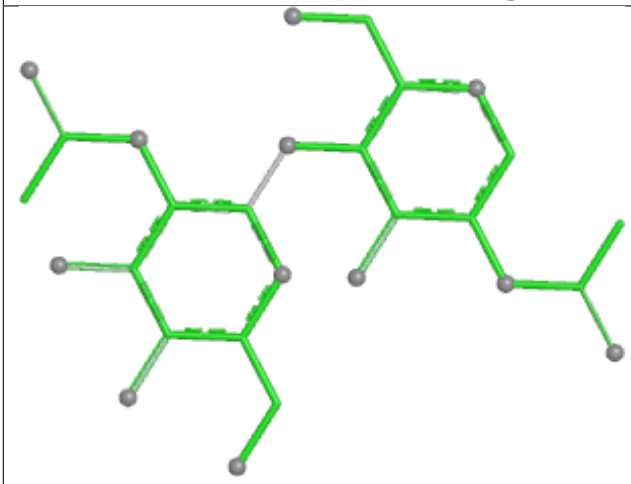


Torsions



Rings

Oligosaccharide Chain j



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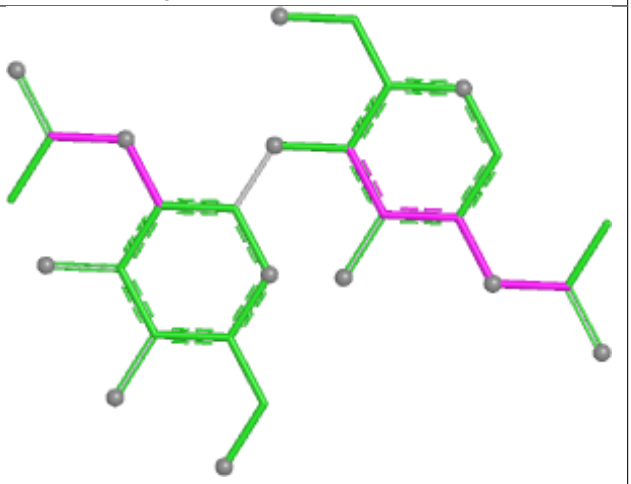
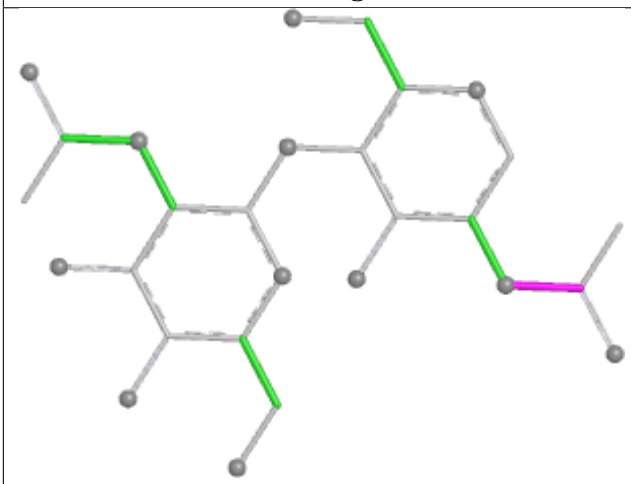


Bond angles



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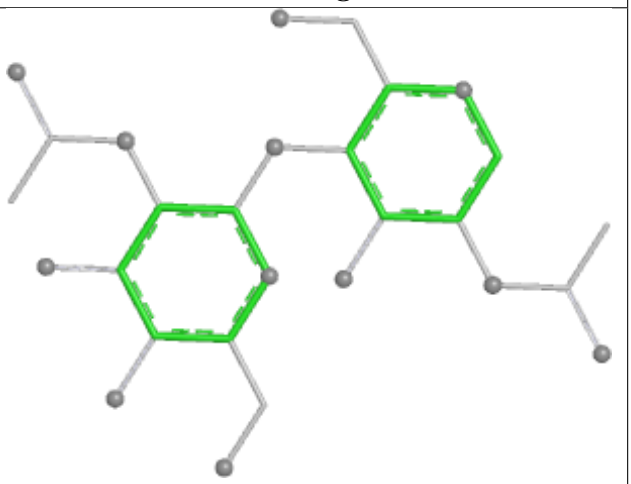
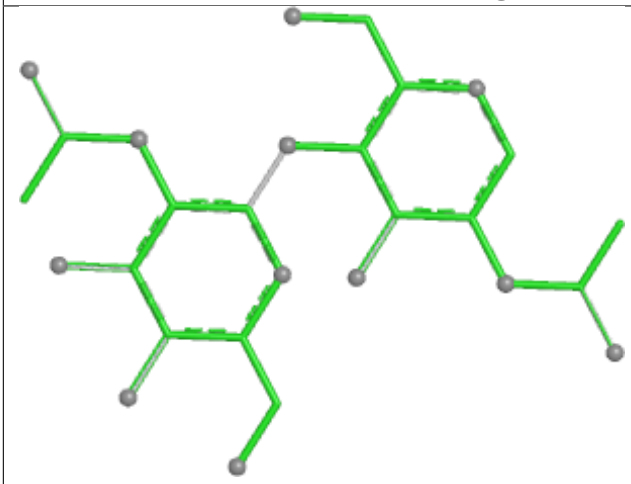


Rings

Oligosaccharide Chain m



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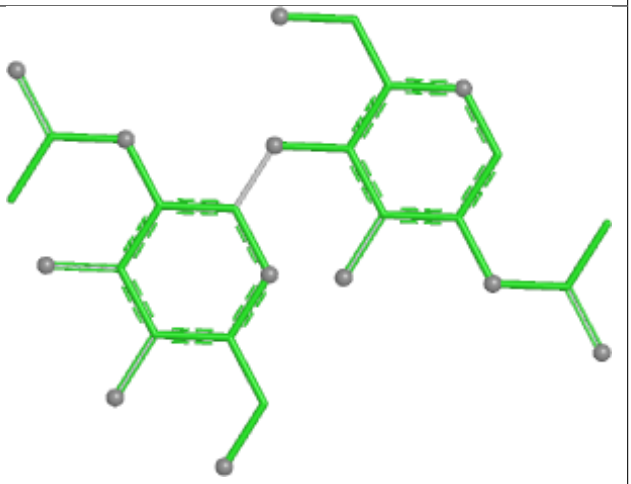
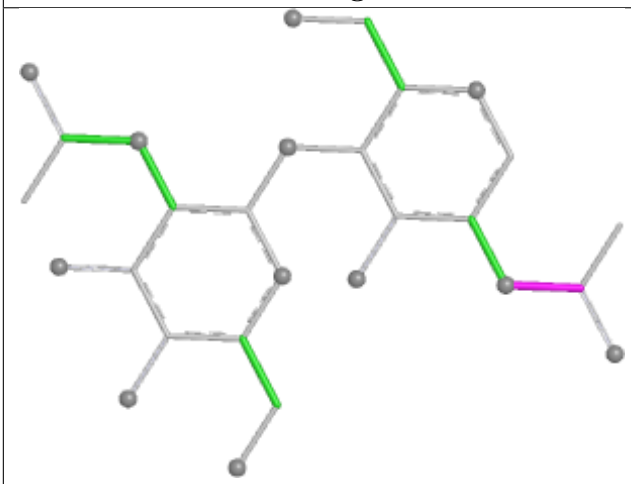


Bond angles



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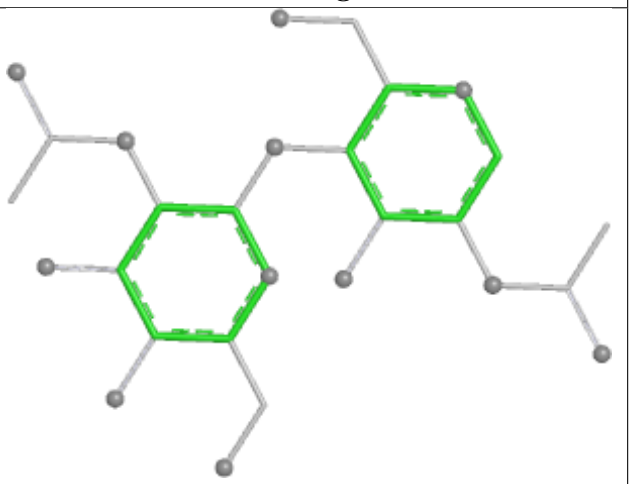
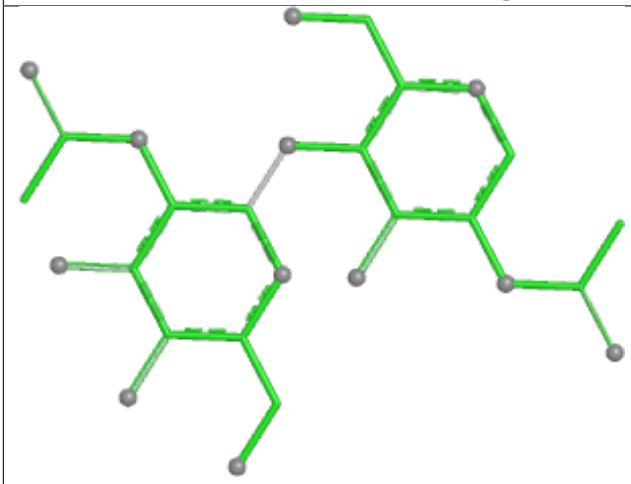


Rings

Oligosaccharide Chain n



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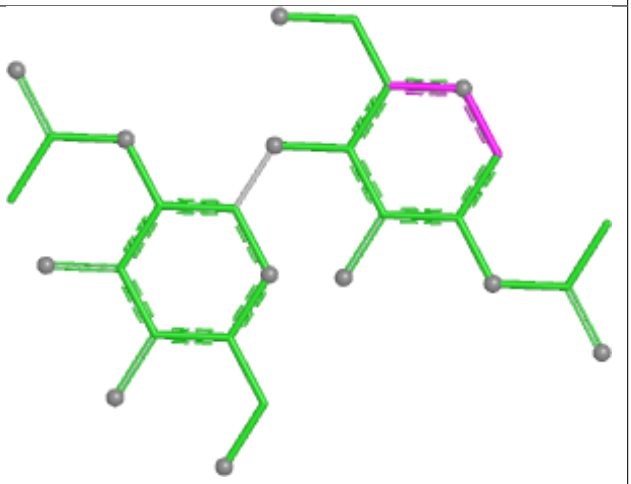
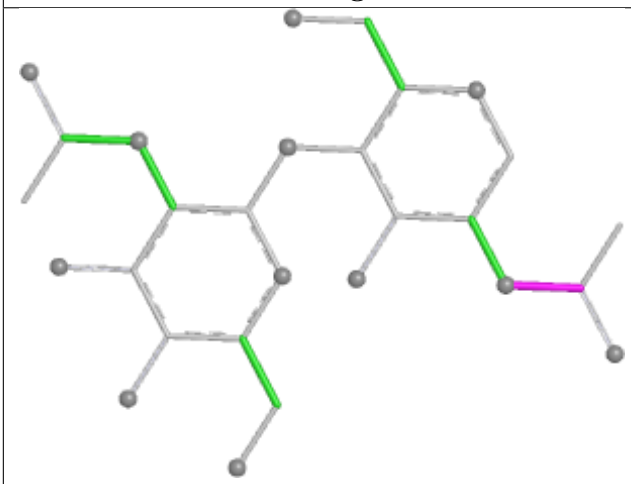


Bond angles



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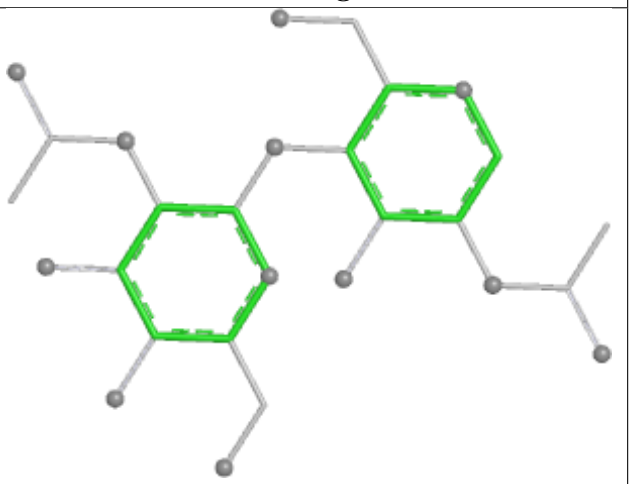
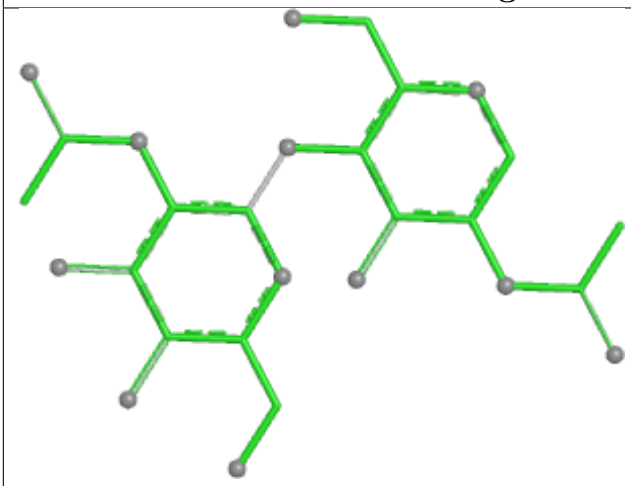


Rings

Oligosaccharide Chain o



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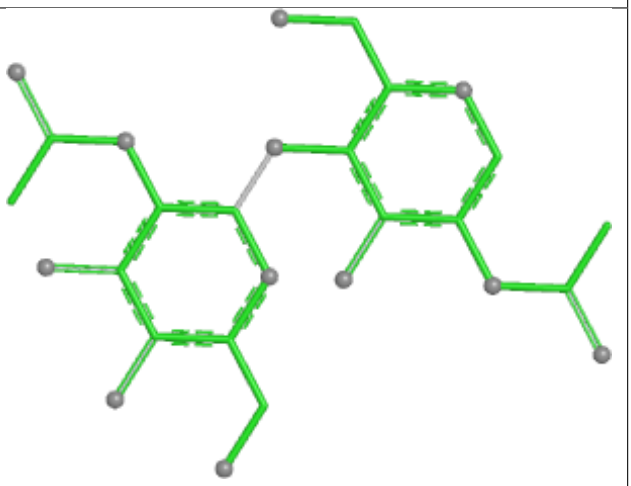
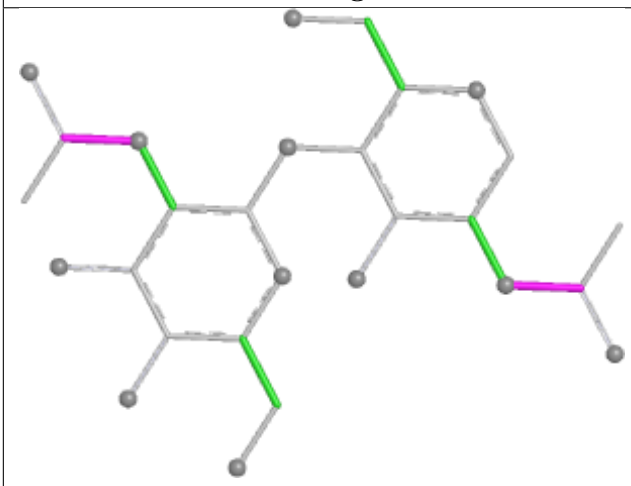


Bond angles



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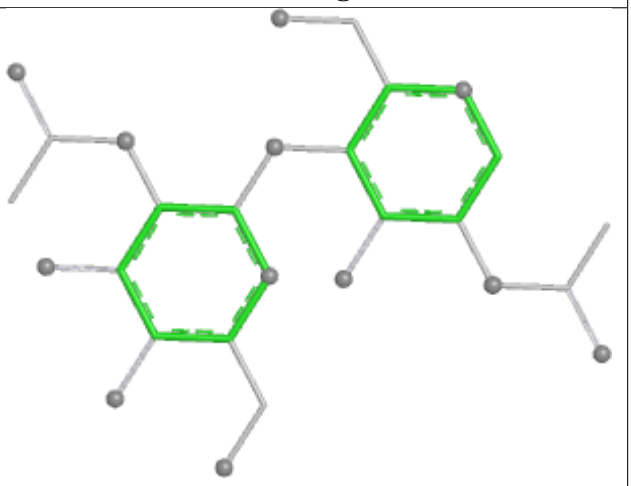
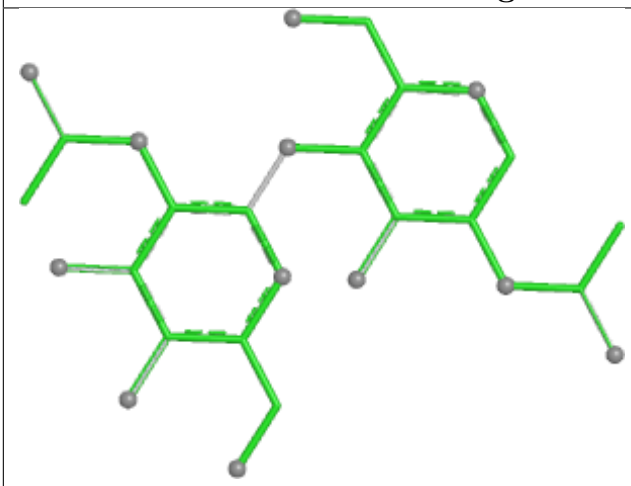


Rings

Oligosaccharide Chain p



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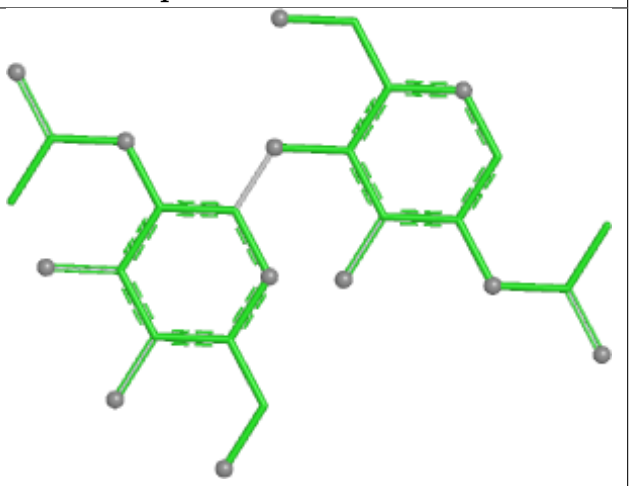
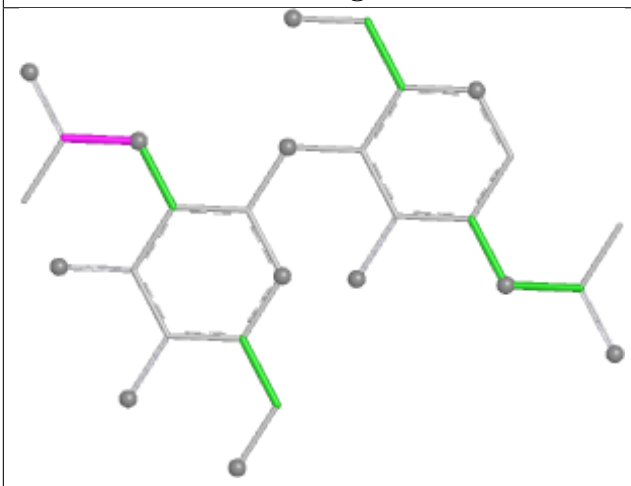


Bond angles



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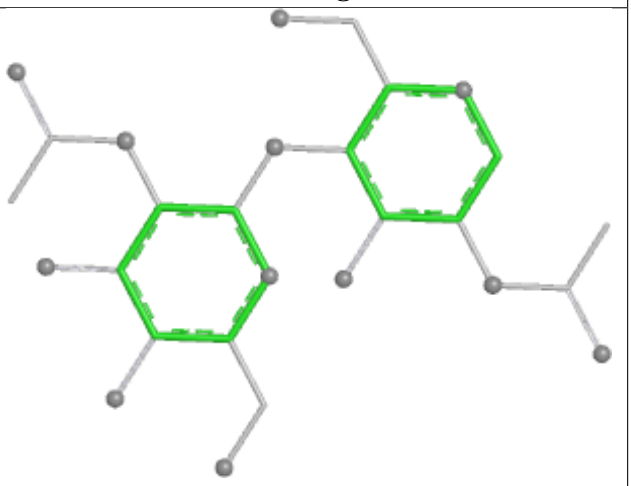
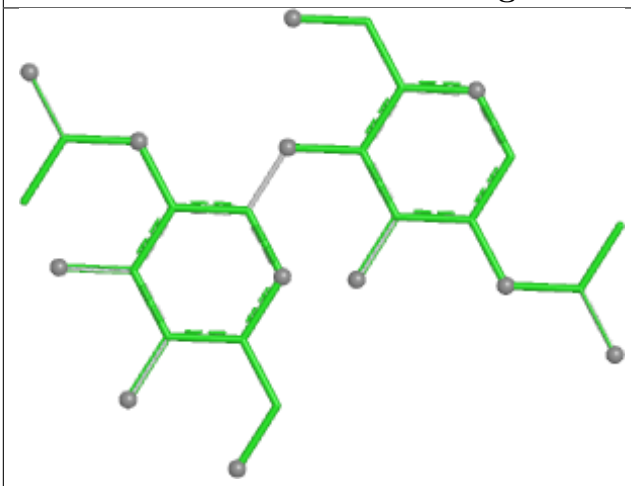


Rings

Oligosaccharide Chain q



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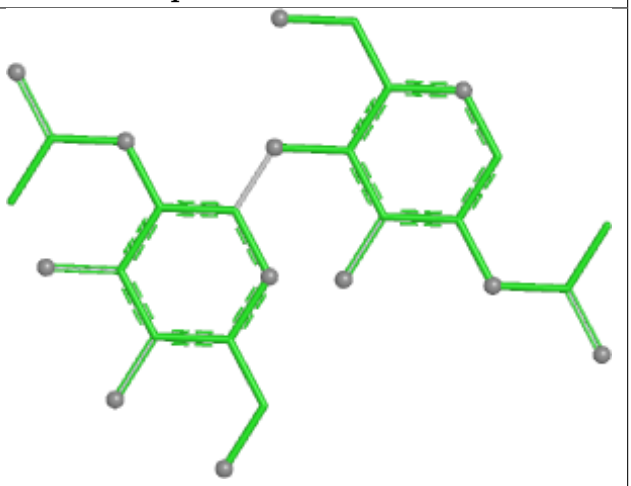
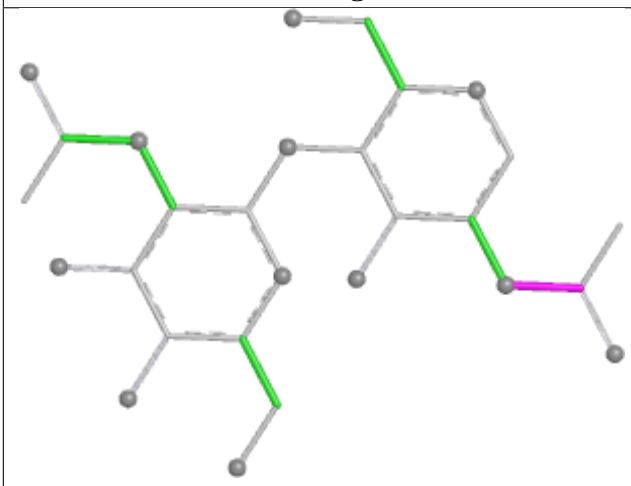


Bond angles



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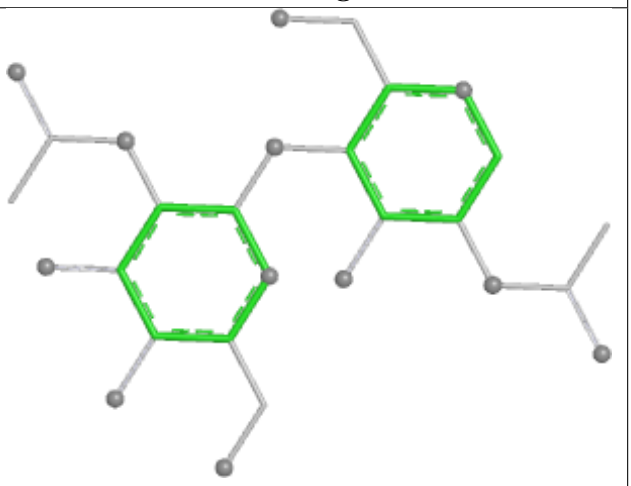
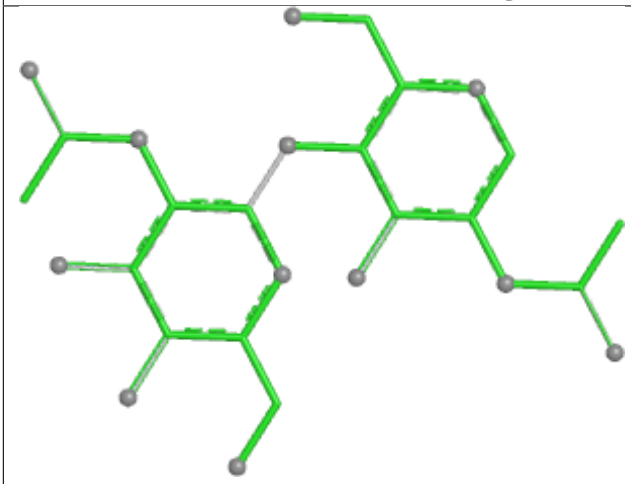


Rings

Oligosaccharide Chain r



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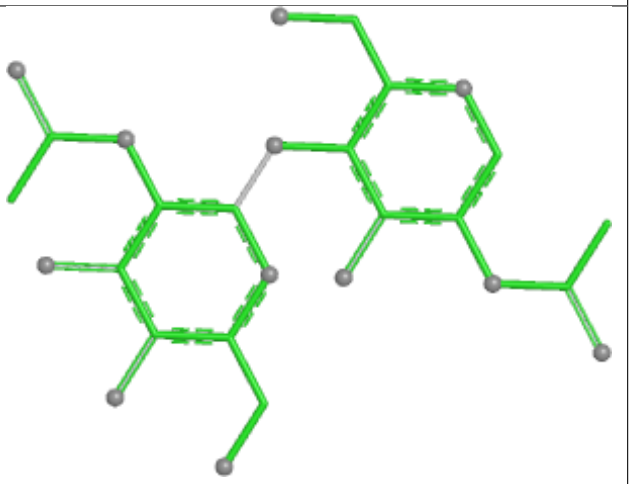
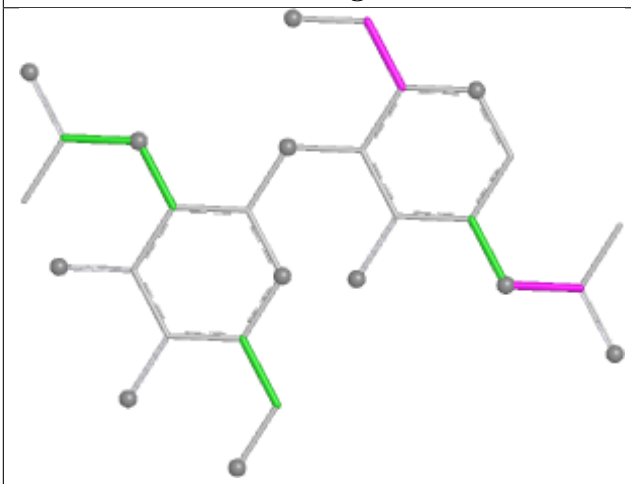


Bond angles



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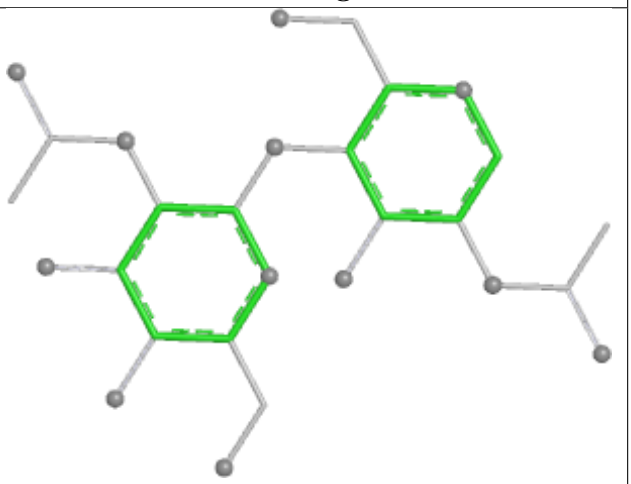
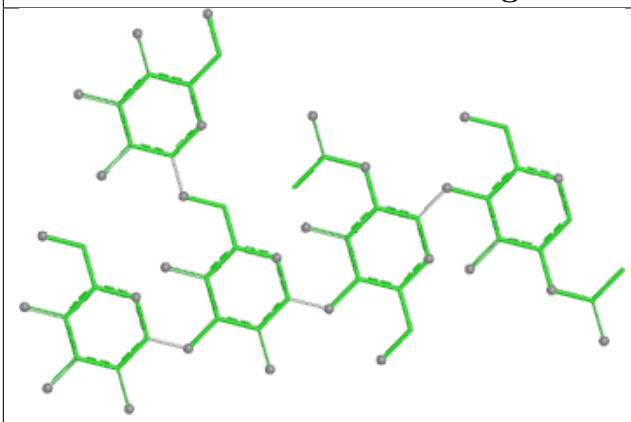


Rings

Oligosaccharide Chain I



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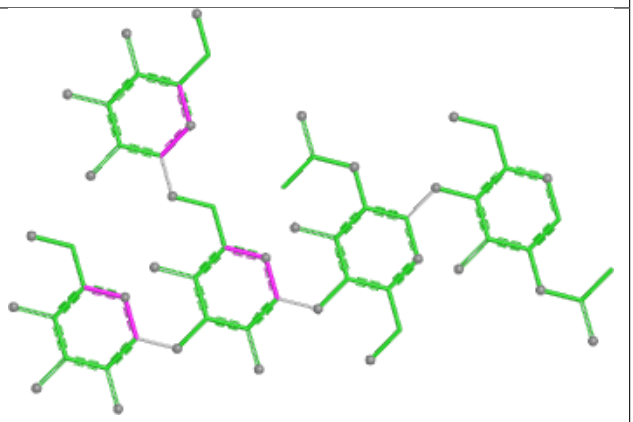
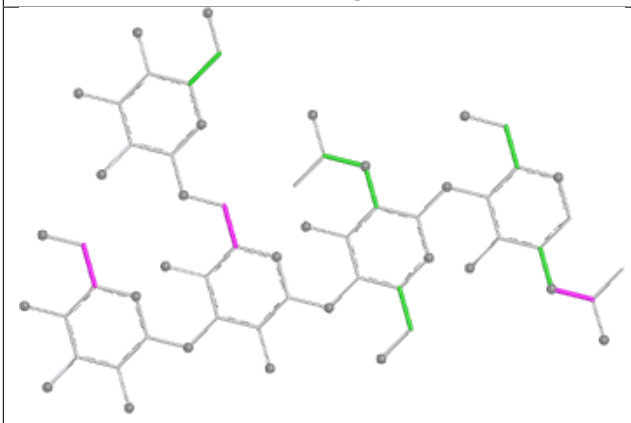


Bond angles



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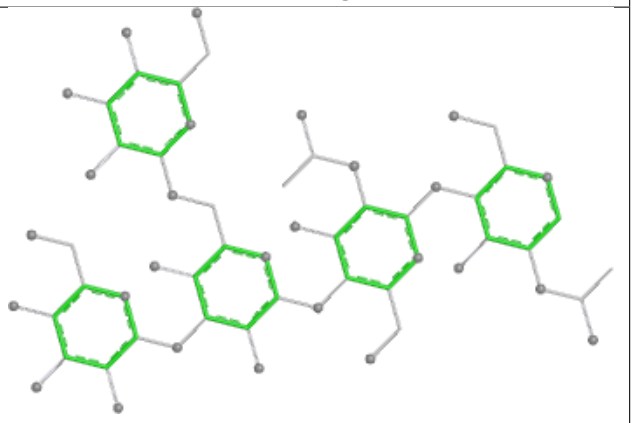
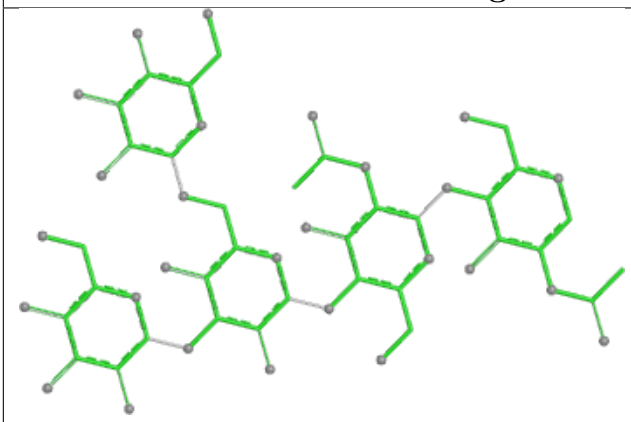
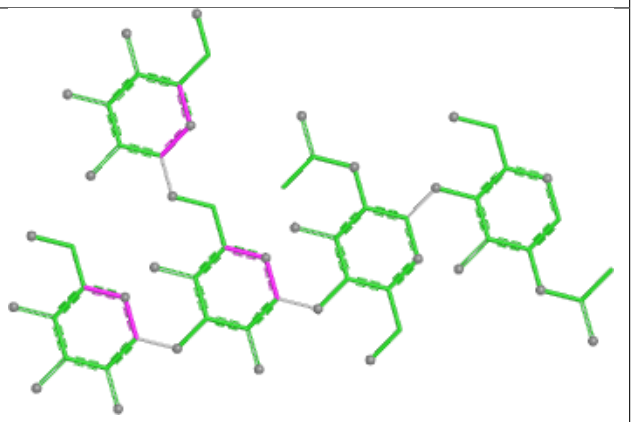


Rings

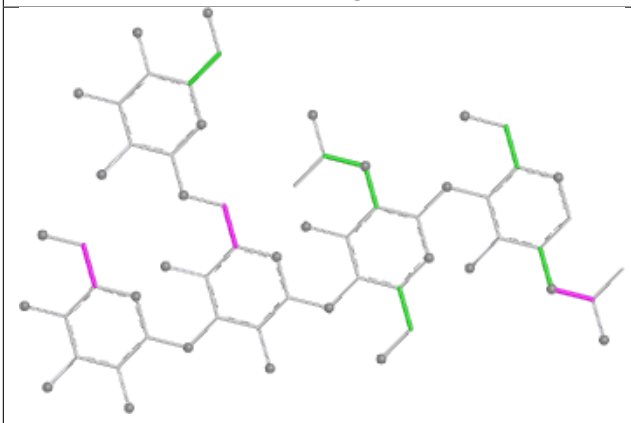
Oligosaccharide Chain W



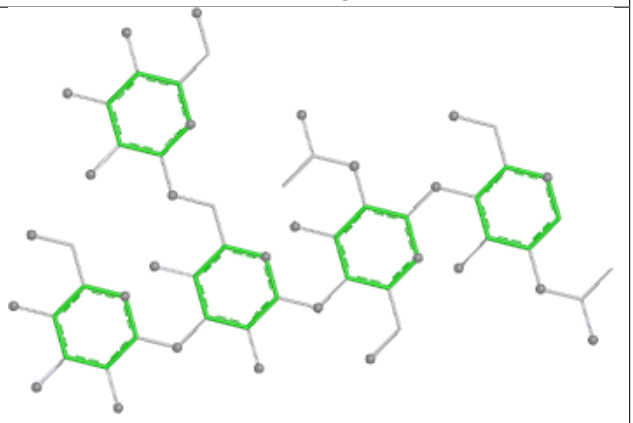
Bond lengths



Bond angles

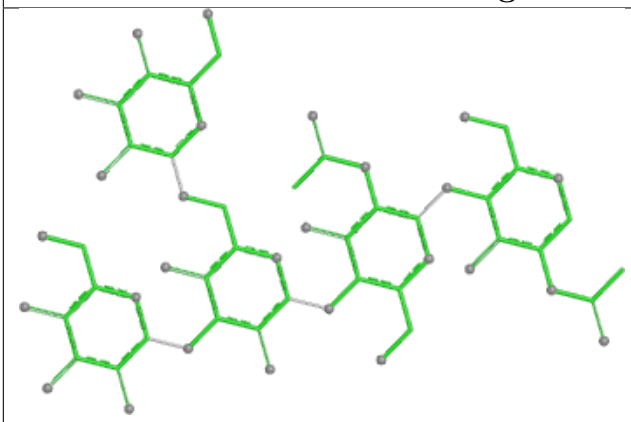


Torsions

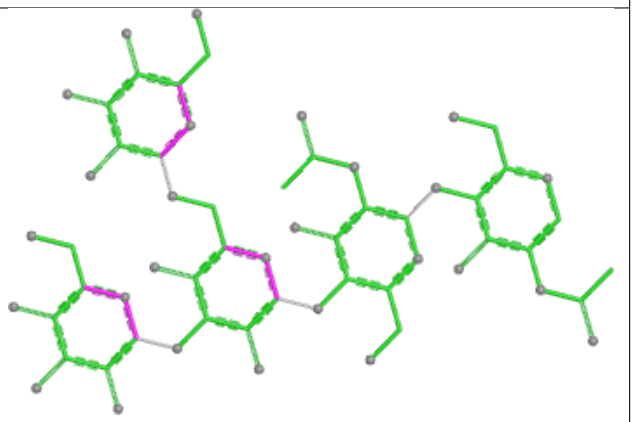


Rings

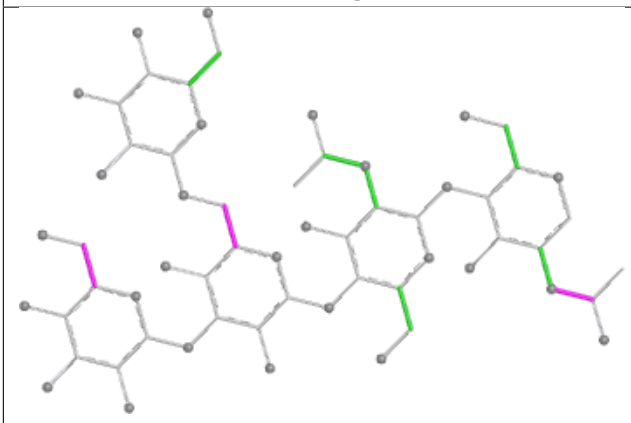
Oligosaccharide Chain k



Bond lengths



Bond angles



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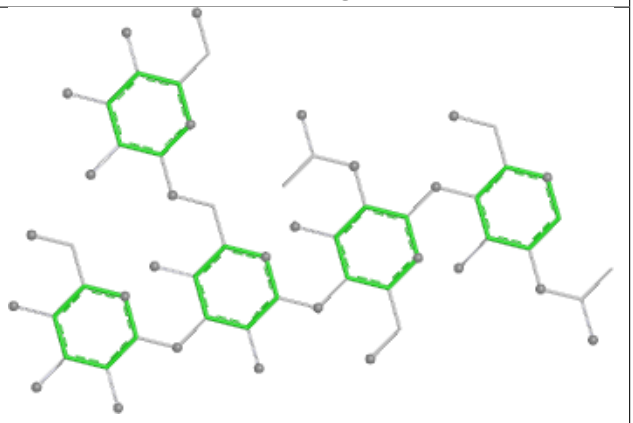
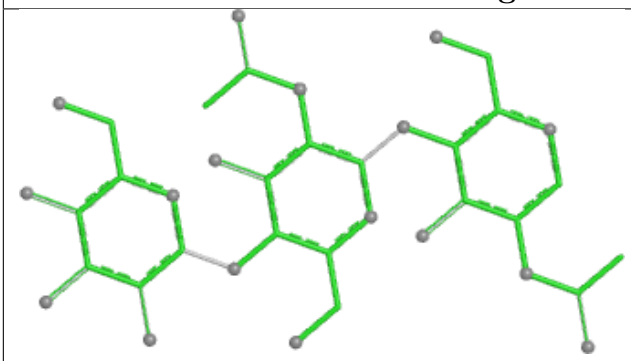
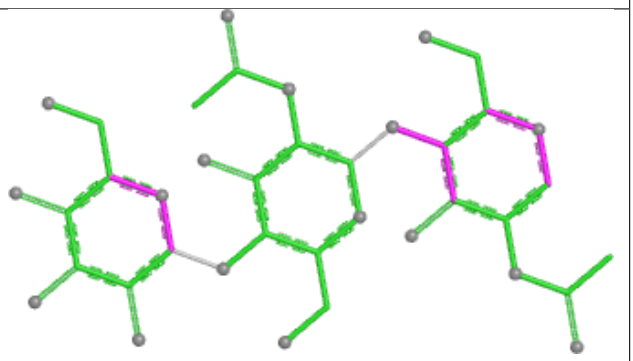


Rings

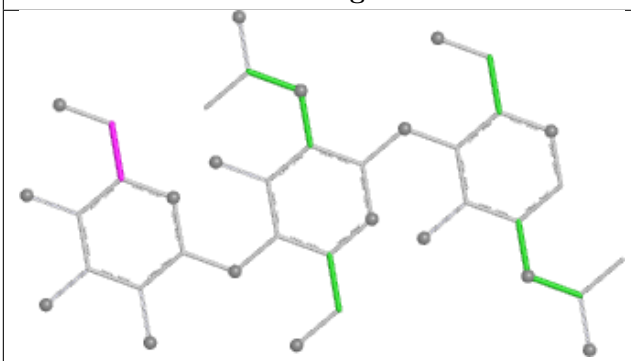
Oligosaccharide Chain J



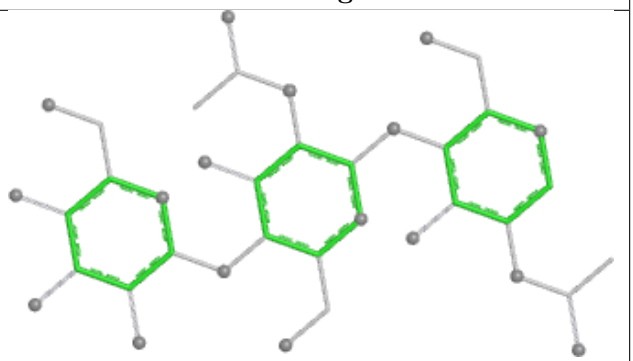
Bond lengths



Bond angles

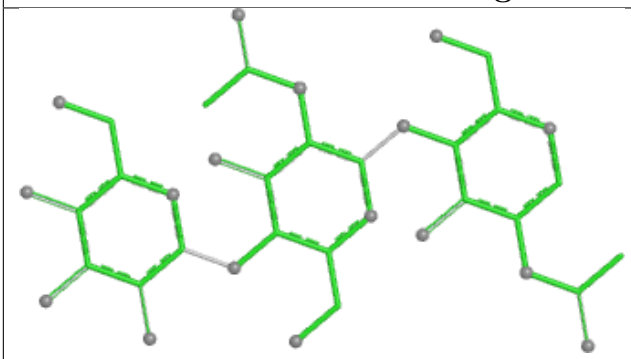


Torsions

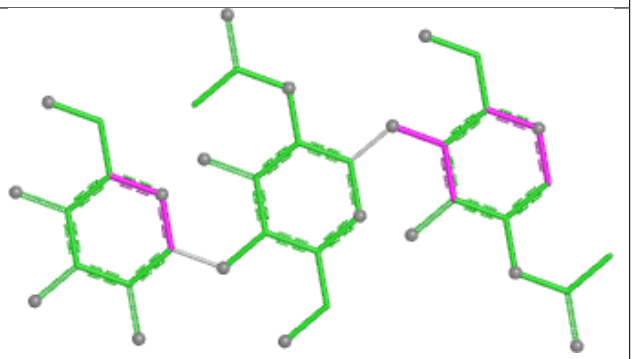


Rings

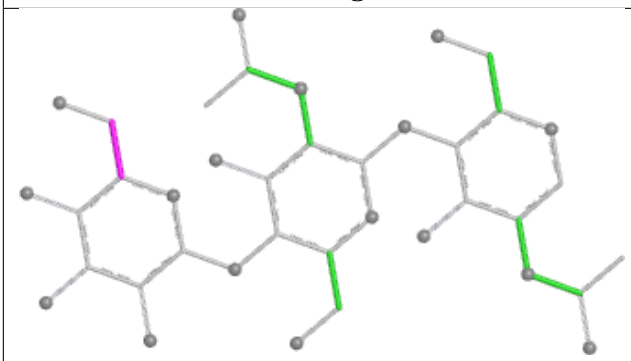
Oligosaccharide Chain X



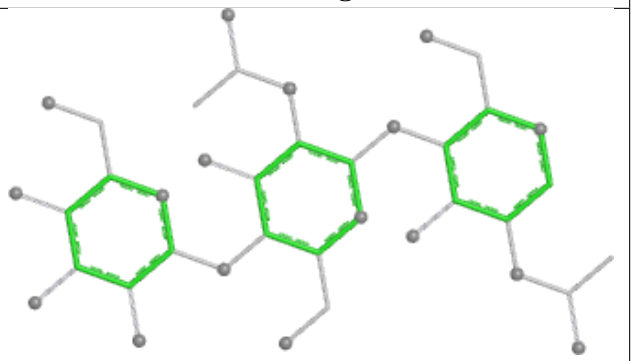
Bond lengths



Bond angles

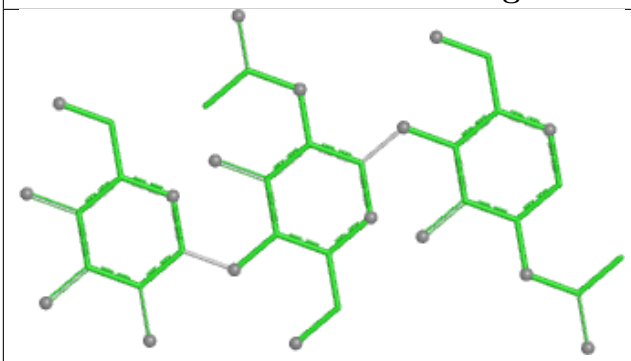


Torsions

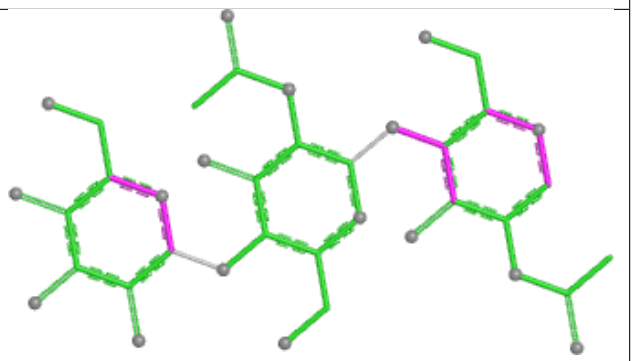


Rings

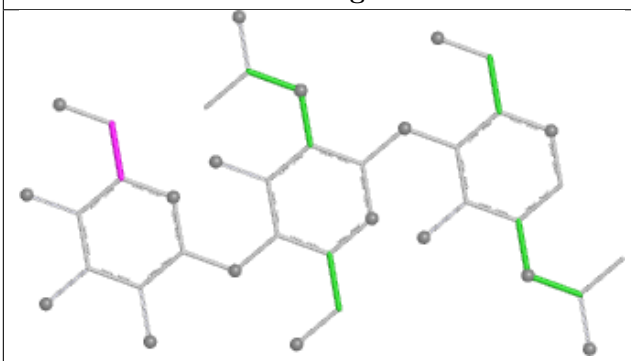
Oligosaccharide Chain l



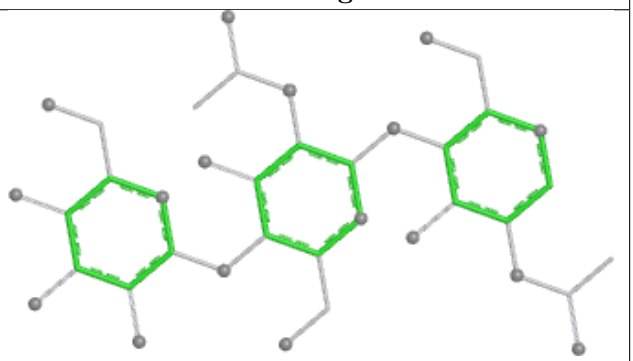
Bond lengths



Bond angles

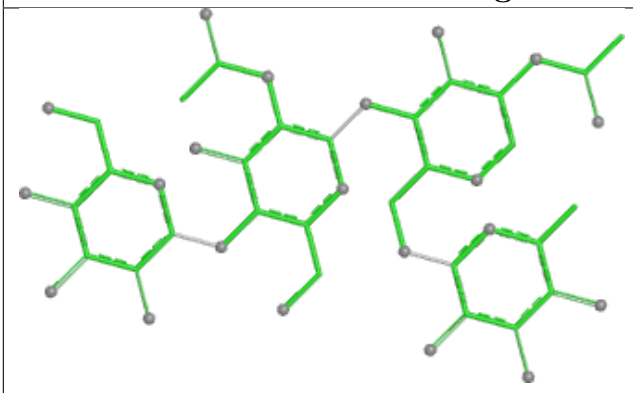


Torsions

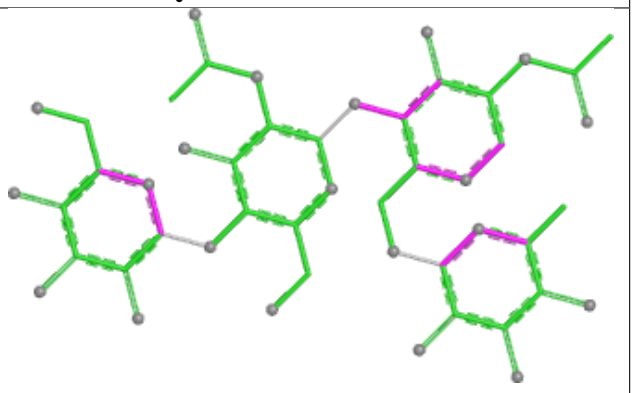


Rings

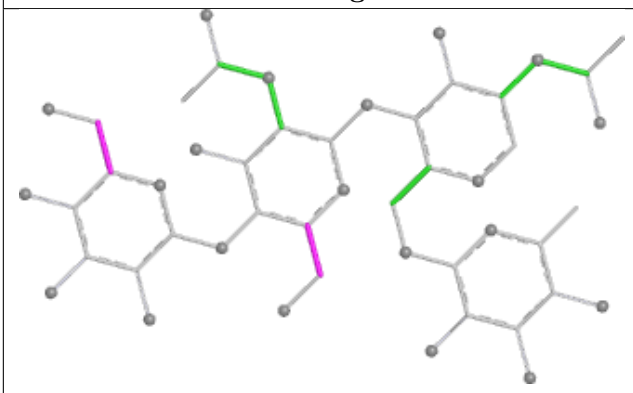
Oligosaccharide Chain Q



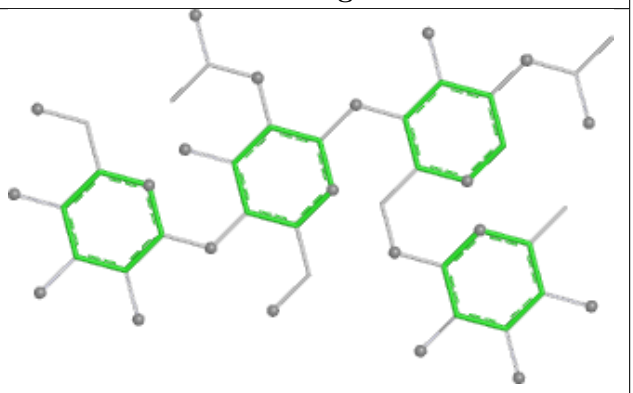
Bond lengths



Bond angles

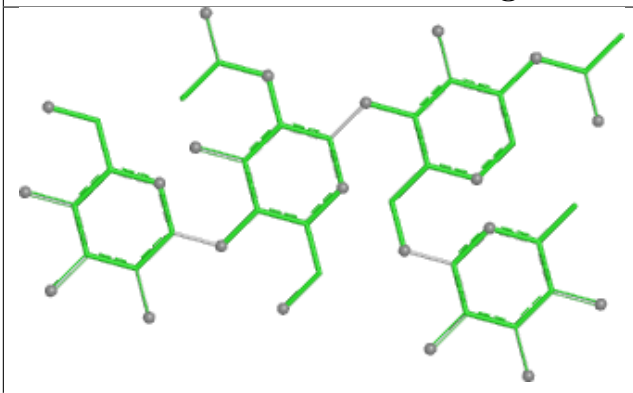


Torsions

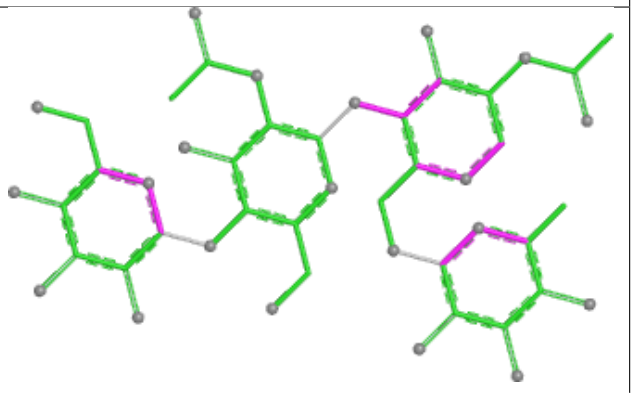


Rings

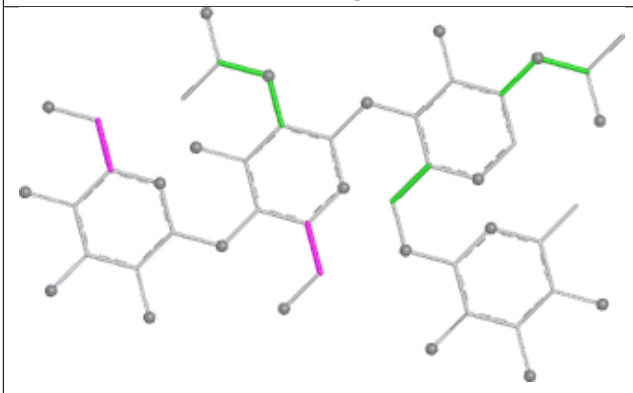
Oligosaccharide Chain e



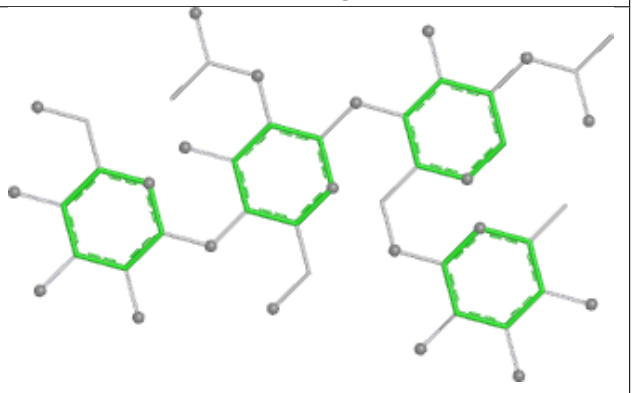
Bond lengths



Bond angles

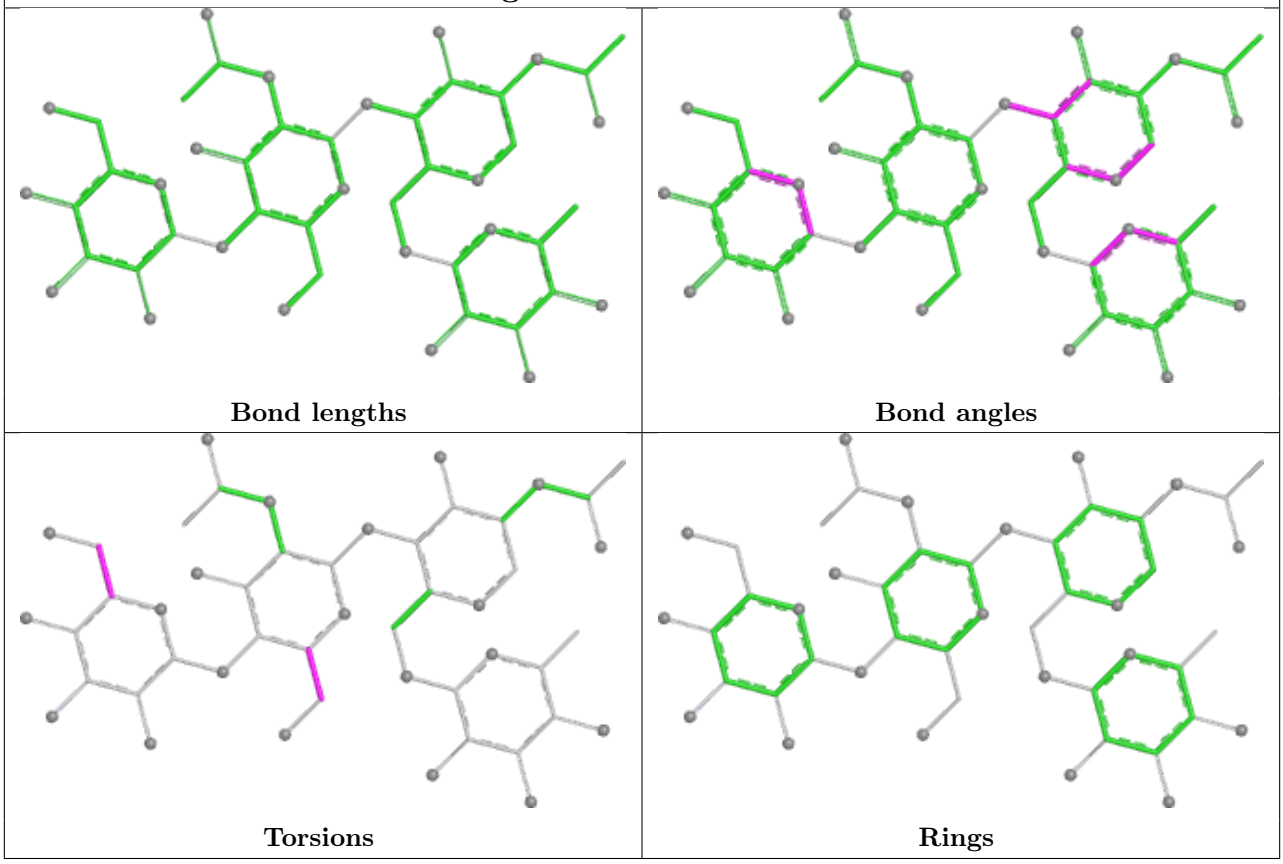


Torsions



Rings

Oligosaccharide Chain s



5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 6 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	EIC	B	1407	-	19,19,19	0.61	0	19,19,19	0.58	0
7	NAG	A	1402	1	14,14,15	0.70	0	17,19,21	0.80	0
7	NAG	B	1401	1	14,14,15	0.72	0	17,19,21	0.80	0
10	EIC	C	1401	-	19,19,19	0.61	0	19,19,19	0.58	0
7	NAG	B	1402	1	14,14,15	0.71	0	17,19,21	0.80	0
7	NAG	C	1403	1	14,14,15	0.70	0	17,19,21	0.80	0
9	FOL	C	1407	-	25,25,34	1.48	2 (8%)	31,35,47	2.33	8 (25%)
7	NAG	A	1401	1	14,14,15	0.72	0	17,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	C	1404	1	14,14,15	0.71	0	17,19,21	0.82	0
9	FOL	B	1406	-	25,25,34	1.47	2 (8%)	31,35,47	2.32	8 (25%)
10	EIC	A	1407	-	19,19,19	0.61	0	19,19,19	0.58	0
9	FOL	A	1406	-	25,25,34	1.48	2 (8%)	31,35,47	2.33	8 (25%)
7	NAG	A	1403	1	14,14,15	0.72	0	17,19,21	0.83	0
7	NAG	C	1402	1	14,14,15	0.73	0	17,19,21	0.80	0
7	NAG	B	1403	1	14,14,15	0.72	0	17,19,21	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	EIC	B	1407	-	-	4/17/17/17	-
7	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
10	EIC	C	1401	-	-	4/17/17/17	-
7	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
9	FOL	C	1407	-	-	0/9/9/22	0/3/3/3
7	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
9	FOL	B	1406	-	-	0/9/9/22	0/3/3/3
10	EIC	A	1407	-	-	4/17/17/17	-
9	FOL	A	1406	-	-	0/9/9/22	0/3/3/3
7	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1403	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1406	FOL	C4A-C4	4.38	1.49	1.41
9	C	1407	FOL	C4A-C4	4.38	1.49	1.41
9	B	1406	FOL	C4A-C4	4.37	1.49	1.41
9	A	1406	FOL	C4A-C8A	4.24	1.48	1.40
9	C	1407	FOL	C4A-C8A	4.24	1.48	1.40
9	B	1406	FOL	C4A-C8A	4.23	1.48	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	1407	FOL	N8-C8A-N1	5.91	122.21	115.77
9	A	1406	FOL	N8-C8A-N1	5.90	122.19	115.77
9	B	1406	FOL	N8-C8A-N1	5.86	122.16	115.77
9	C	1407	FOL	C2-N1-C8A	5.51	121.43	115.48
9	A	1406	FOL	C2-N1-C8A	5.50	121.41	115.48
9	B	1406	FOL	C2-N1-C8A	5.45	121.36	115.48
9	B	1406	FOL	C8A-C4A-C4	-4.60	117.11	119.96
9	C	1407	FOL	C8A-C4A-C4	-4.57	117.13	119.96
9	A	1406	FOL	C8A-C4A-C4	-4.56	117.14	119.96
9	A	1406	FOL	C4A-C4-N3	-4.54	117.34	123.42
9	C	1407	FOL	C4A-C4-N3	-4.54	117.35	123.42
9	B	1406	FOL	C4A-C4-N3	-4.51	117.39	123.42
9	C	1407	FOL	C2-N3-C4	4.44	122.14	115.96
9	A	1406	FOL	C2-N3-C4	4.44	122.14	115.96
9	B	1406	FOL	C2-N3-C4	4.43	122.12	115.96
9	C	1407	FOL	N1-C2-N3	-3.36	122.93	127.21
9	A	1406	FOL	N1-C2-N3	-3.36	122.94	127.21
9	B	1406	FOL	N1-C2-N3	-3.34	122.97	127.21
9	A	1406	FOL	C8A-C4A-N5	-2.61	119.51	122.30
9	B	1406	FOL	C8A-C4A-N5	-2.61	119.52	122.30
9	C	1407	FOL	C8A-C4A-N5	-2.60	119.53	122.30
9	C	1407	FOL	C6-C9-N10	-2.09	108.53	113.13
9	B	1406	FOL	C6-C9-N10	-2.09	108.55	113.13
9	A	1406	FOL	C6-C9-N10	-2.08	108.55	113.13

There are no chirality outliers.

All (12) torsion outliers are listed below:

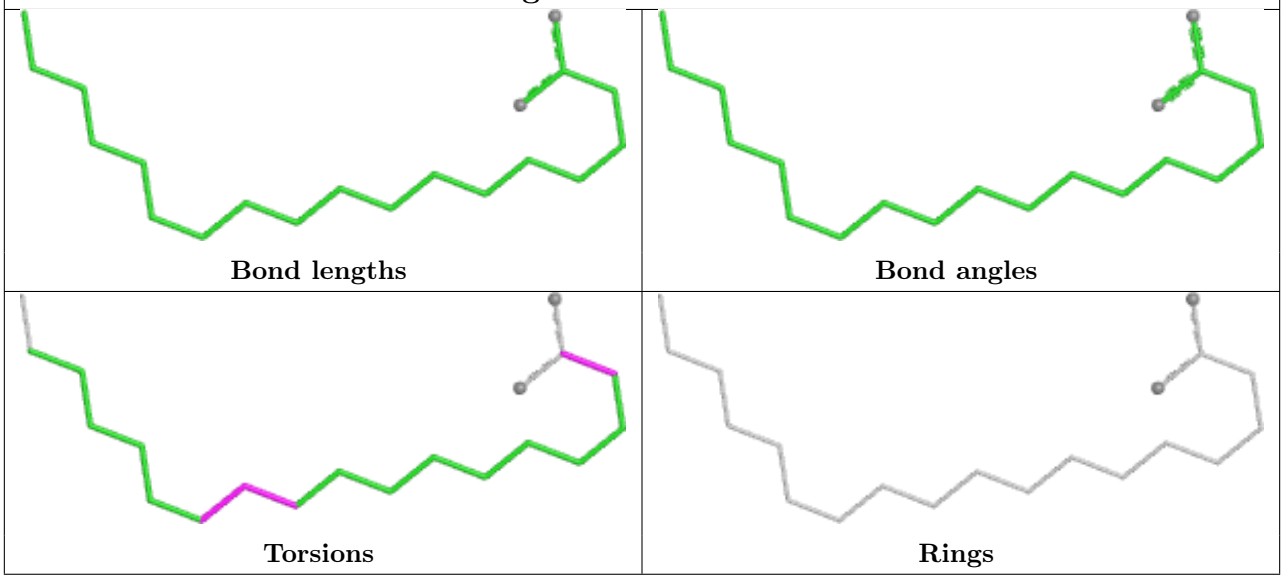
Mol	Chain	Res	Type	Atoms
10	A	1407	EIC	C9-C10-C11-C12
10	A	1407	EIC	C10-C11-C12-C13
10	B	1407	EIC	C9-C10-C11-C12
10	B	1407	EIC	C10-C11-C12-C13
10	C	1401	EIC	C9-C10-C11-C12
10	C	1401	EIC	C10-C11-C12-C13
10	A	1407	EIC	O1-C1-C2-C3
10	B	1407	EIC	O1-C1-C2-C3
10	C	1401	EIC	O1-C1-C2-C3
10	A	1407	EIC	O2-C1-C2-C3
10	B	1407	EIC	O2-C1-C2-C3
10	C	1401	EIC	O2-C1-C2-C3

There are no ring outliers.

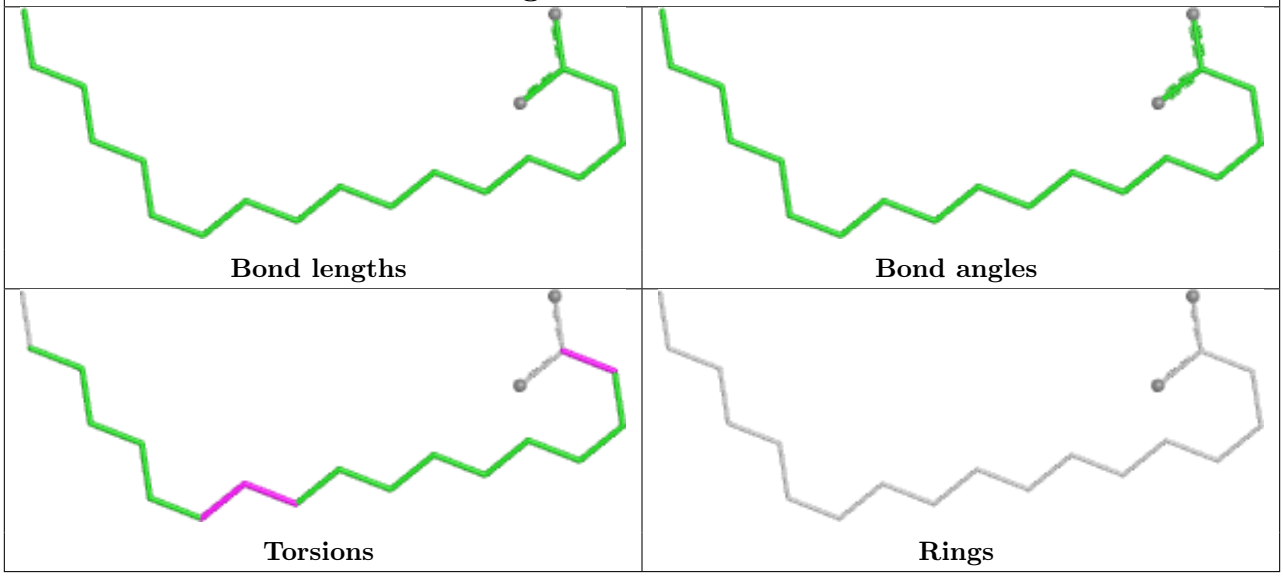
No monomer is involved in short contacts.

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

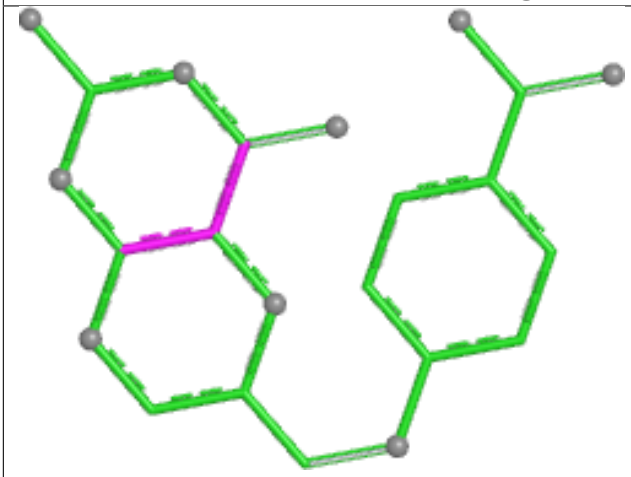
Ligand EIC B 1407



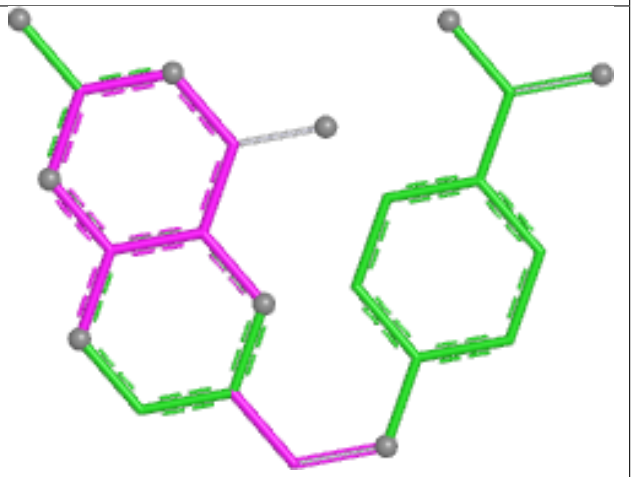
Ligand EIC C 1401



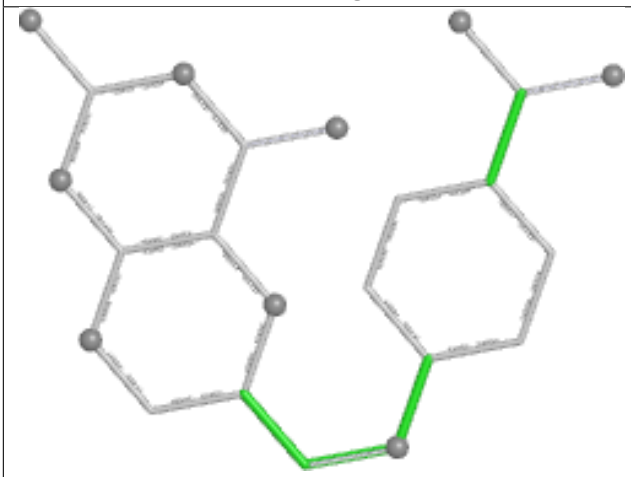
Ligand FOL C 1407



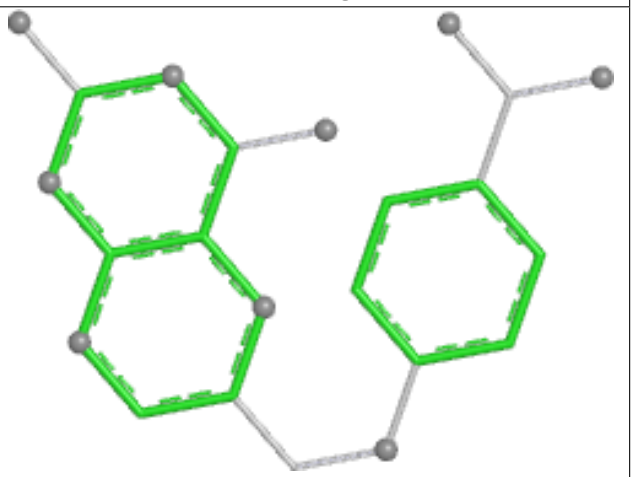
Bond lengths



Bond angles

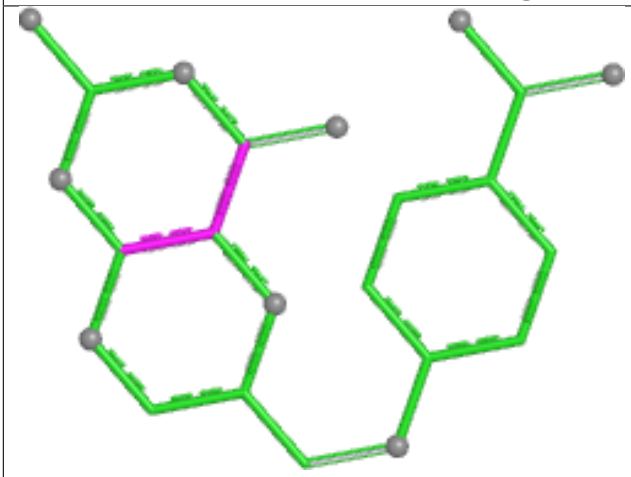


Torsions

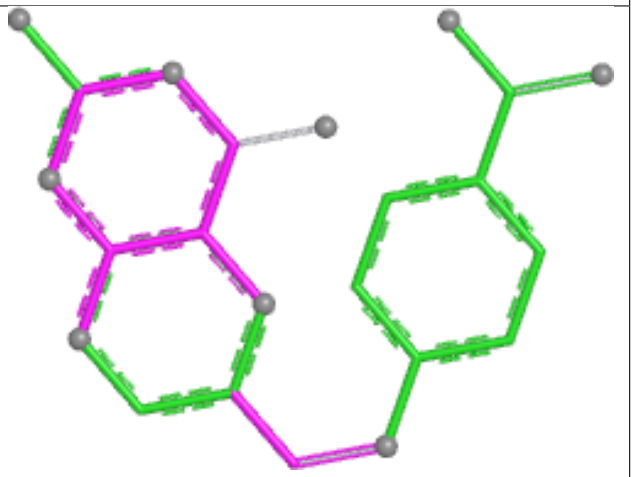


Rings

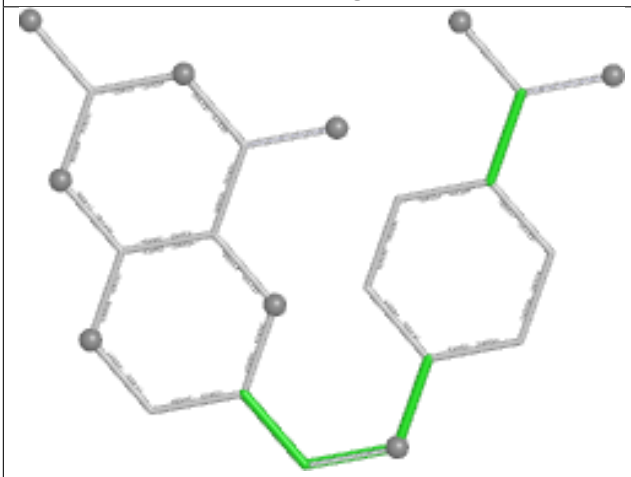
Ligand FOL B 1406



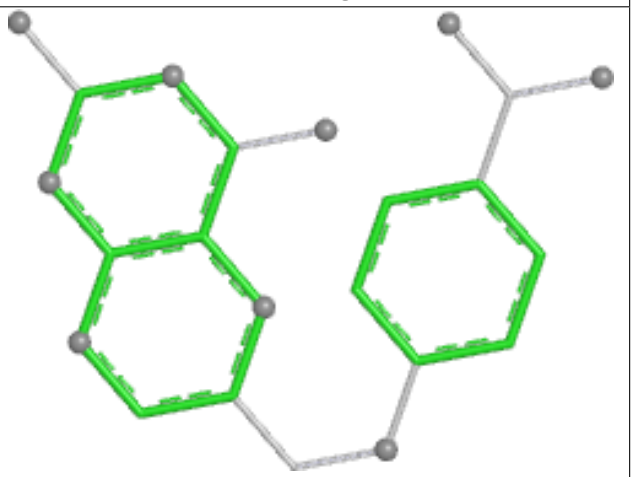
Bond lengths



Bond angles

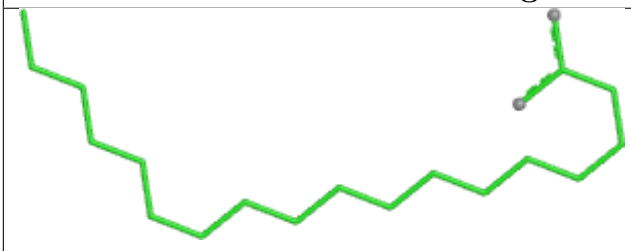


Torsions

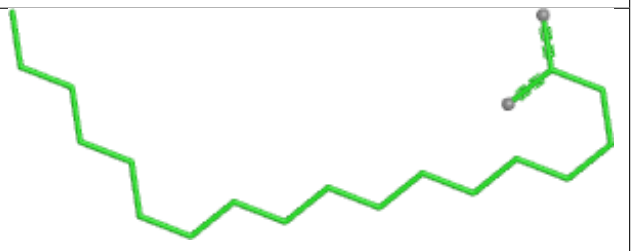


Rings

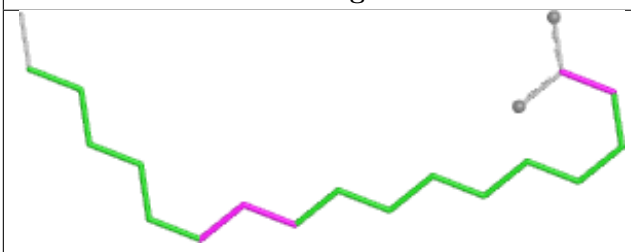
Ligand EIC A 1407



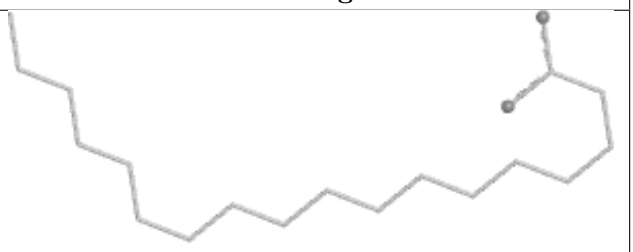
Bond lengths



Bond angles

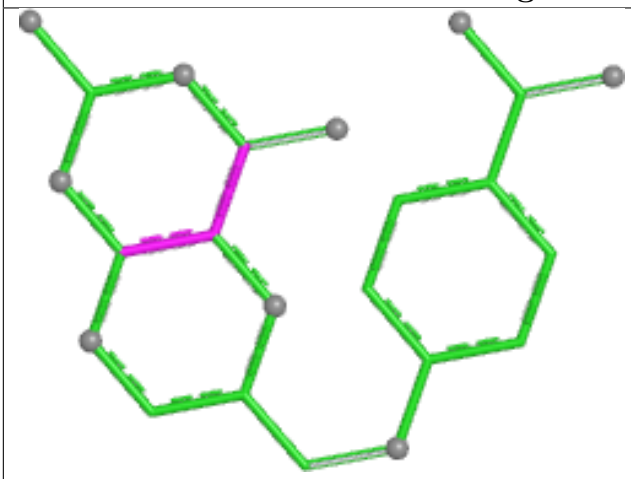


Torsions

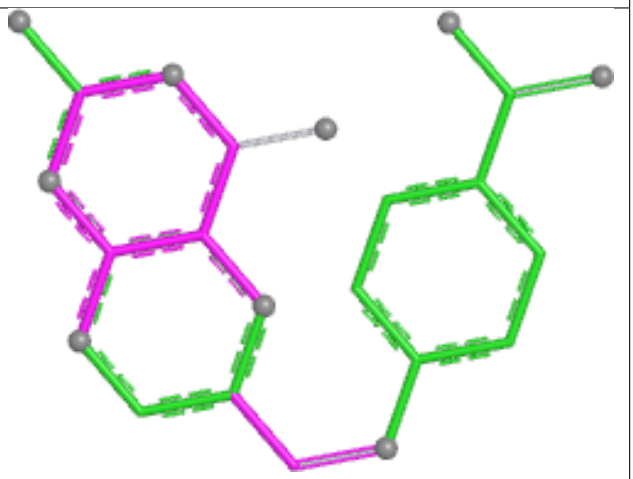


Rings

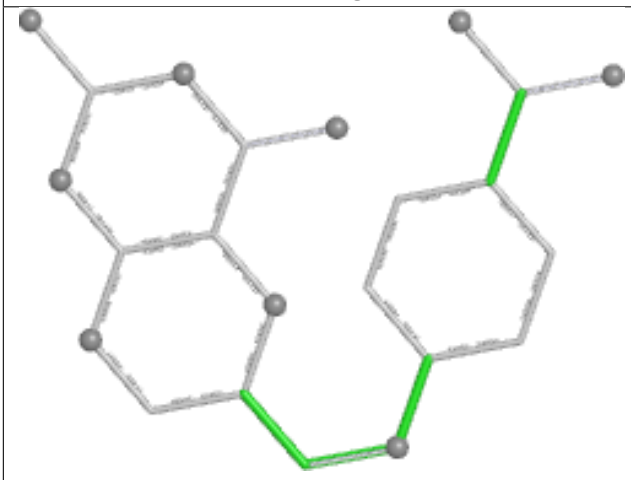
Ligand FOL A 1406



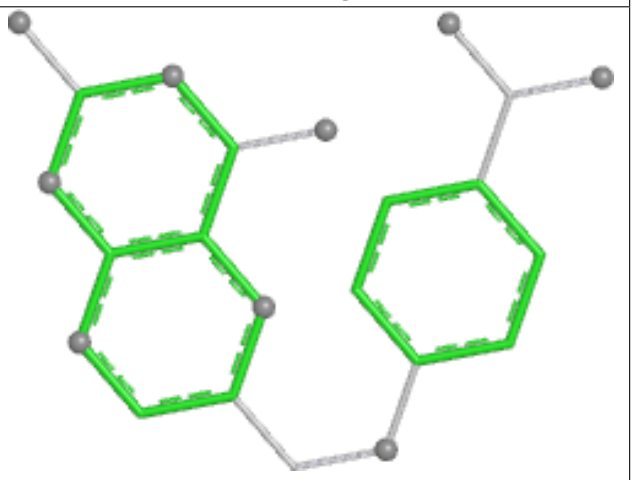
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

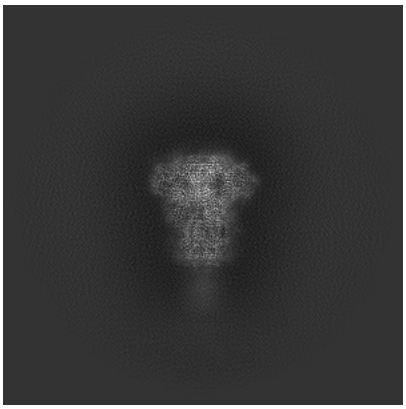
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47823. These allow visual inspection of the internal detail of the map and identification of artifacts.

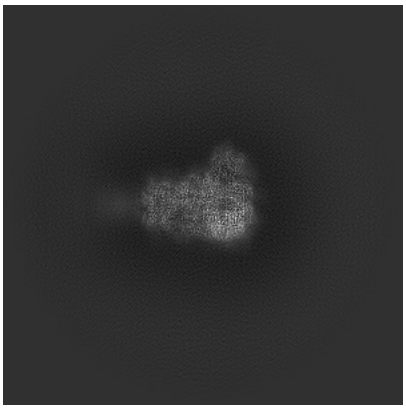
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

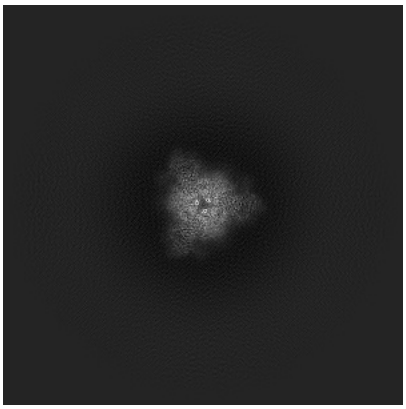
6.1.1 Primary map



X

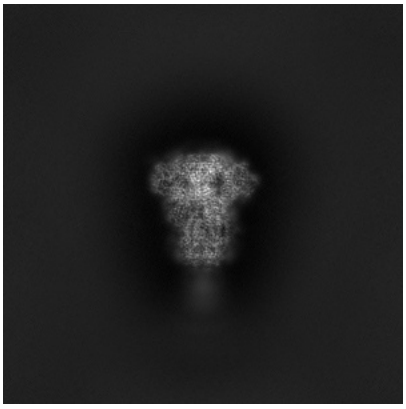


Y

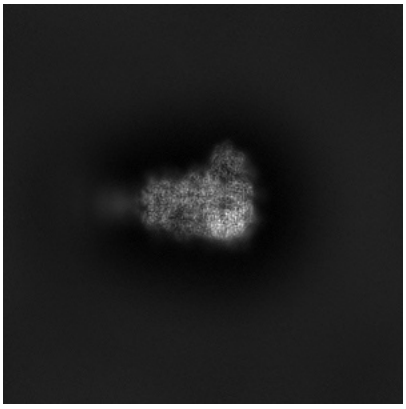


Z

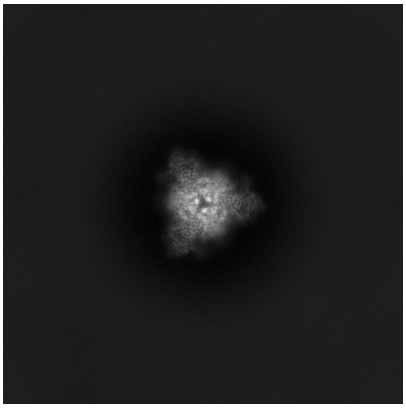
6.1.2 Raw map



X



Y

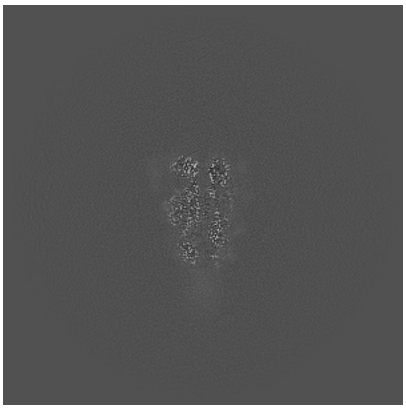


Z

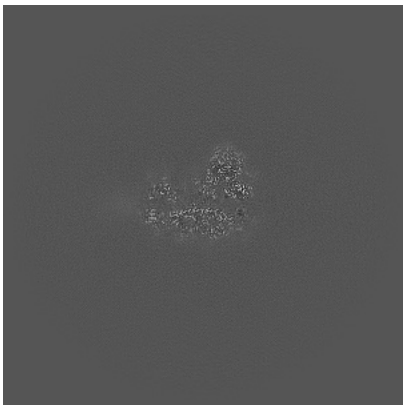
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

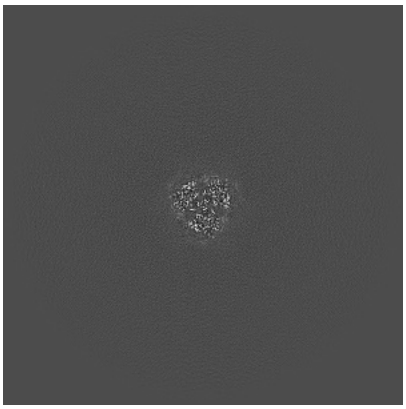
6.2.1 Primary map



X Index: 304

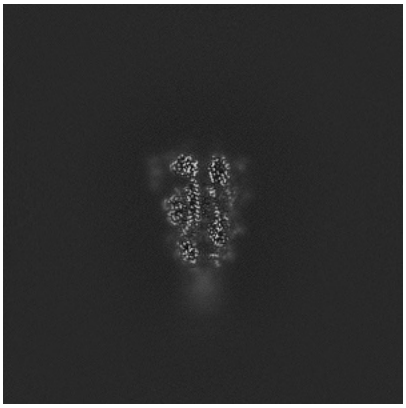


Y Index: 304



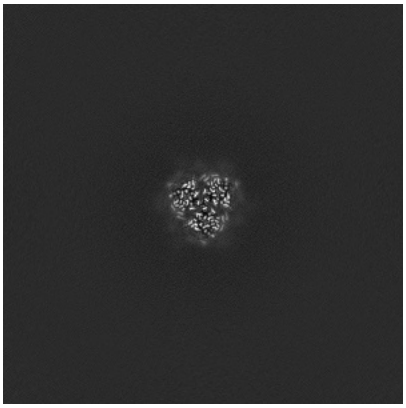
Z Index: 304

6.2.2 Raw map



X Index: 304

Y Index: 304



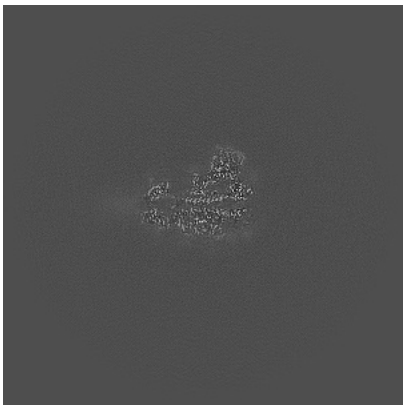
Z Index: 304

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

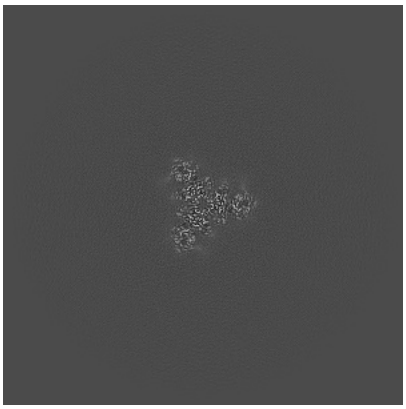
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 284

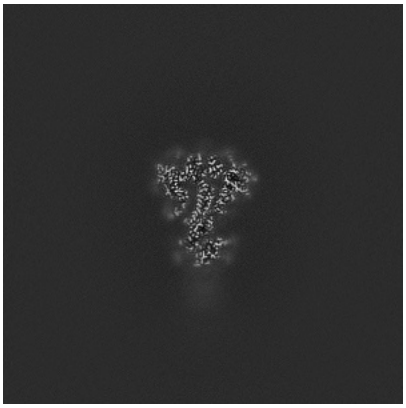


Y Index: 309

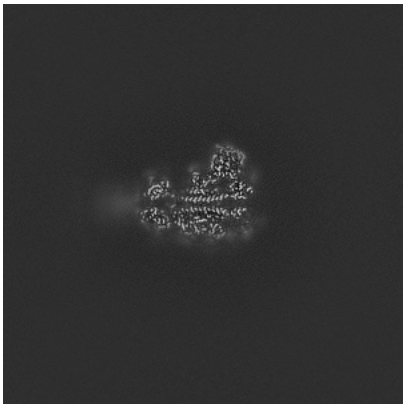


Z Index: 353

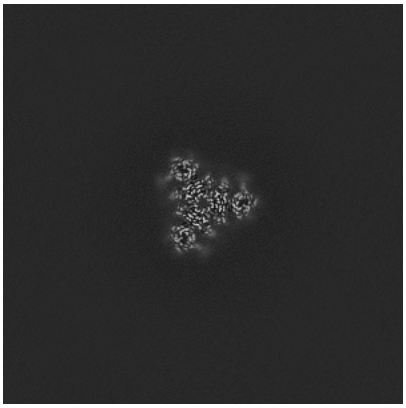
6.3.2 Raw map



X Index: 284



Y Index: 309

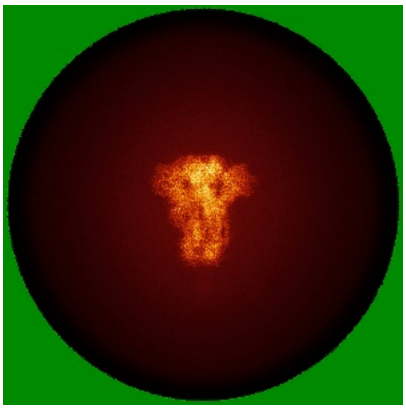


Z Index: 353

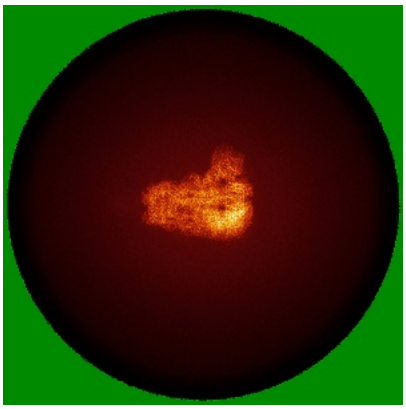
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

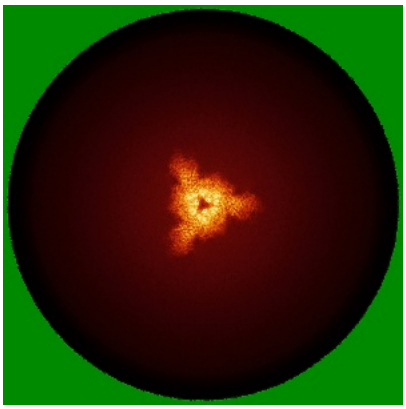
6.4.1 Primary map



X

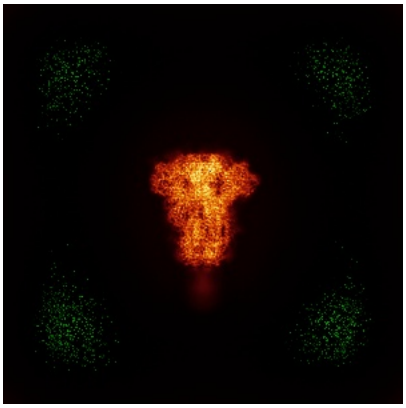


Y

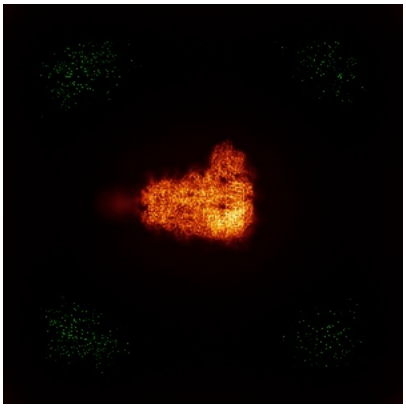


Z

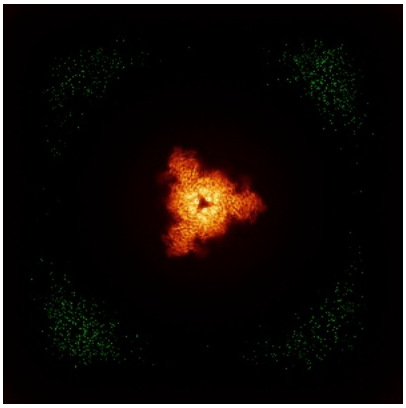
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

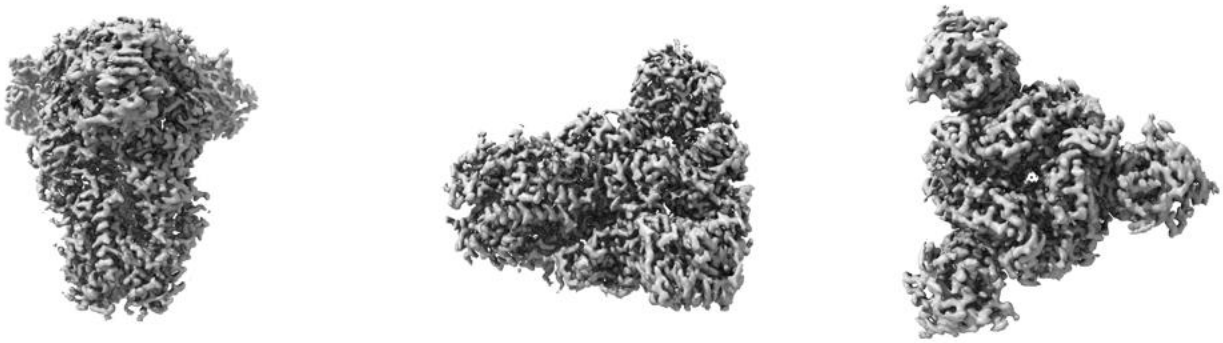
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

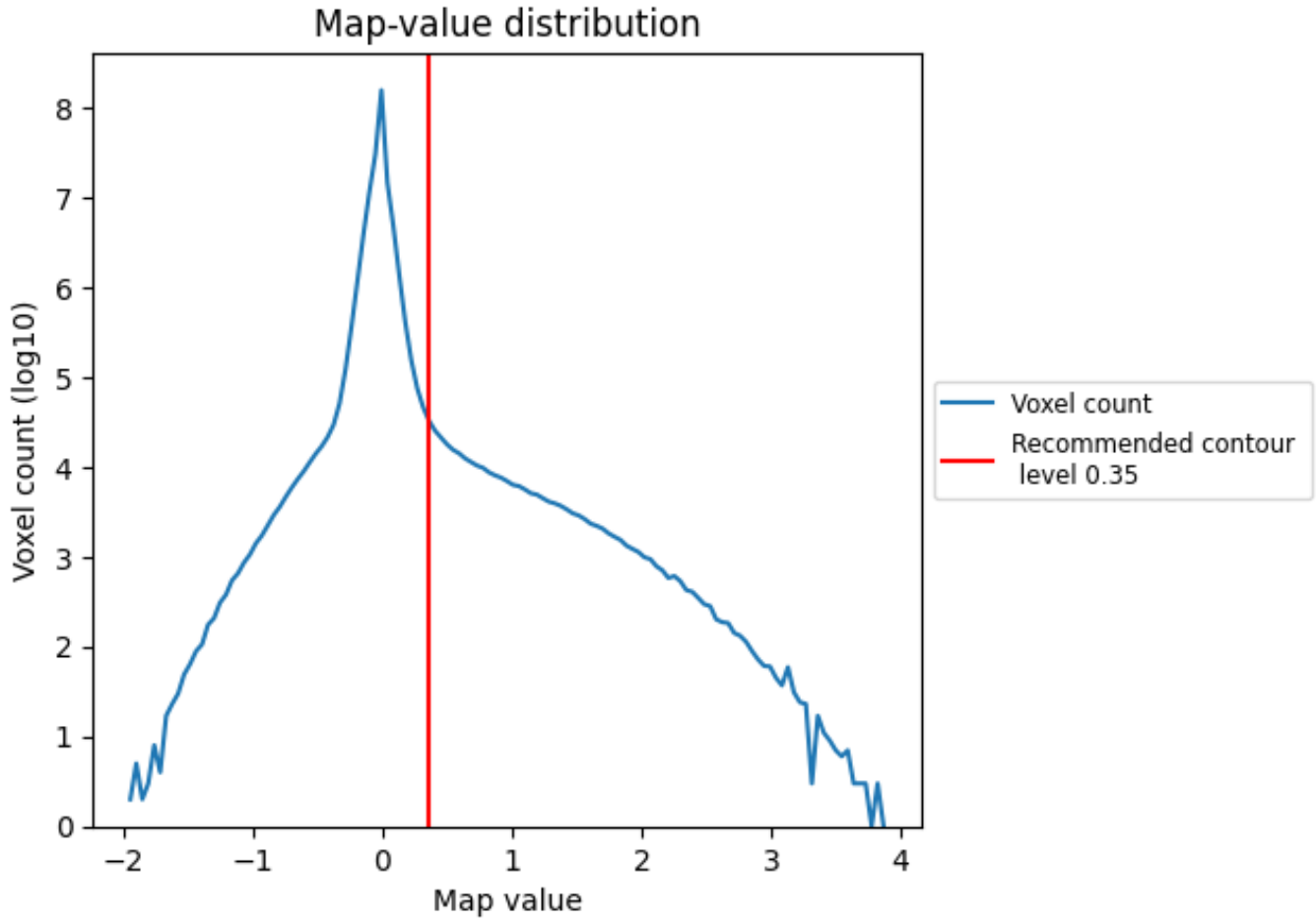
6.6 Mask visualisation (i)

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

7 Map analysis

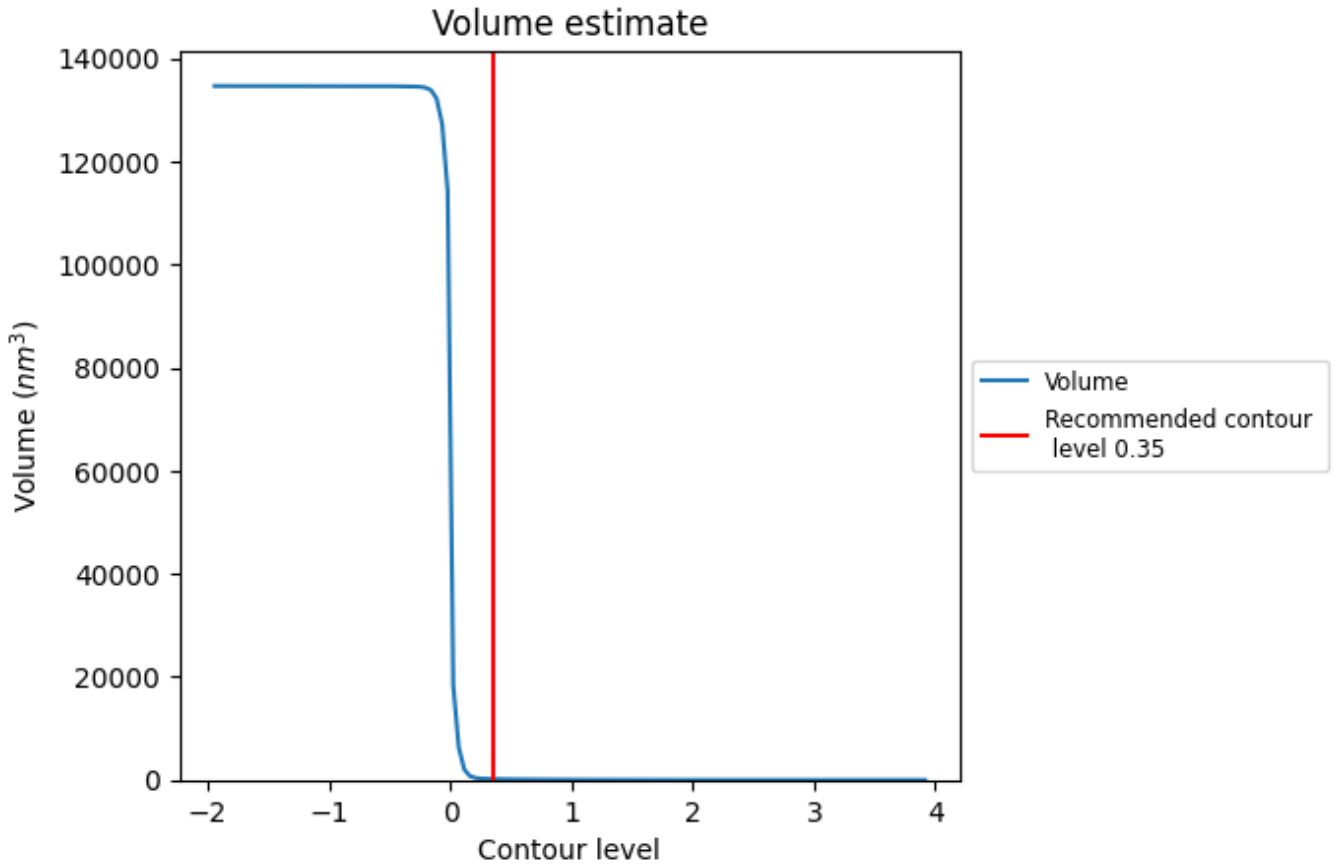
This section contains the results of statistical analysis of the map.

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.

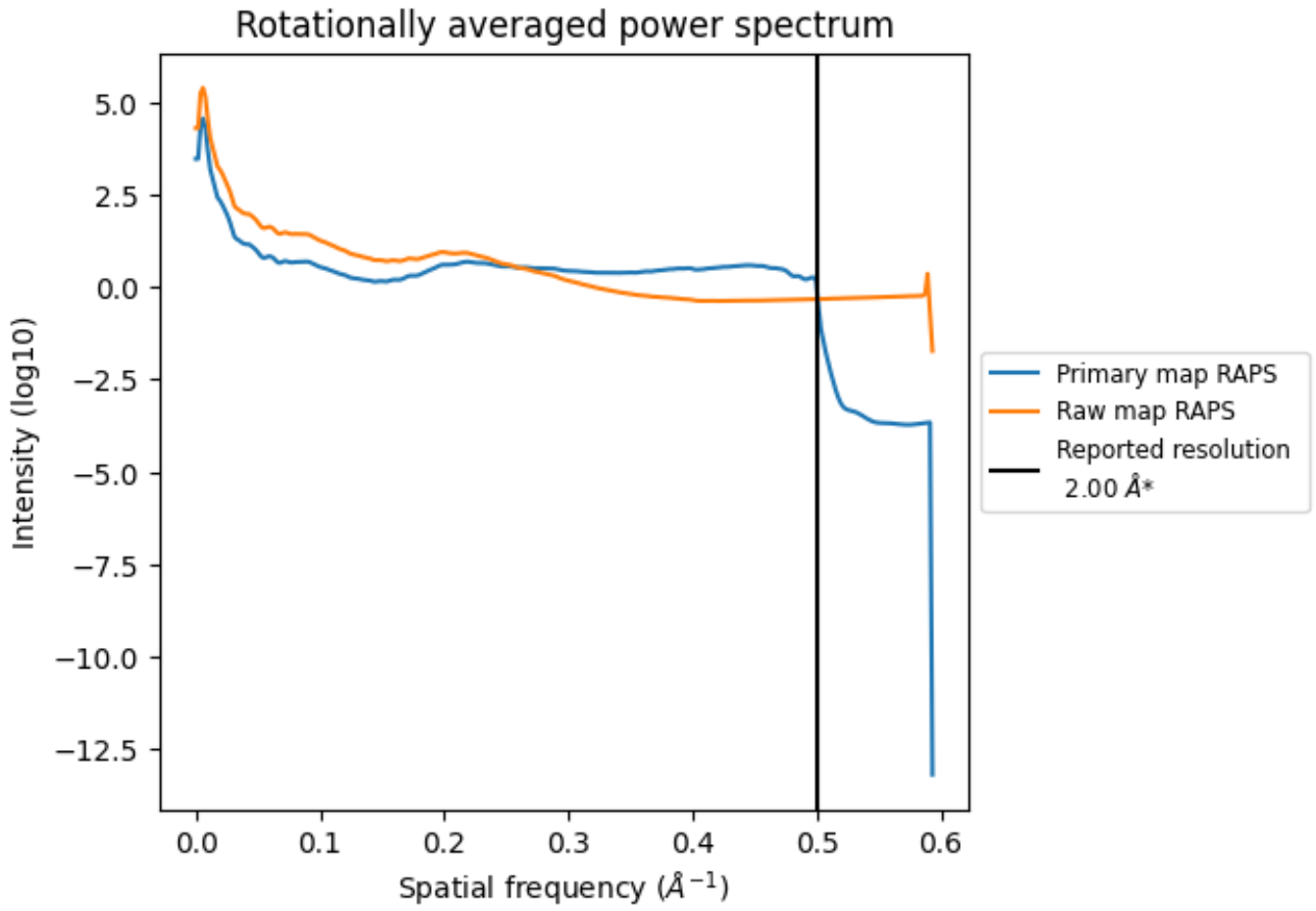
7.2 Volume estimate



The volume at the recommended contour level is 175 nm^3; this corresponds to an approximate mass of 158 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)

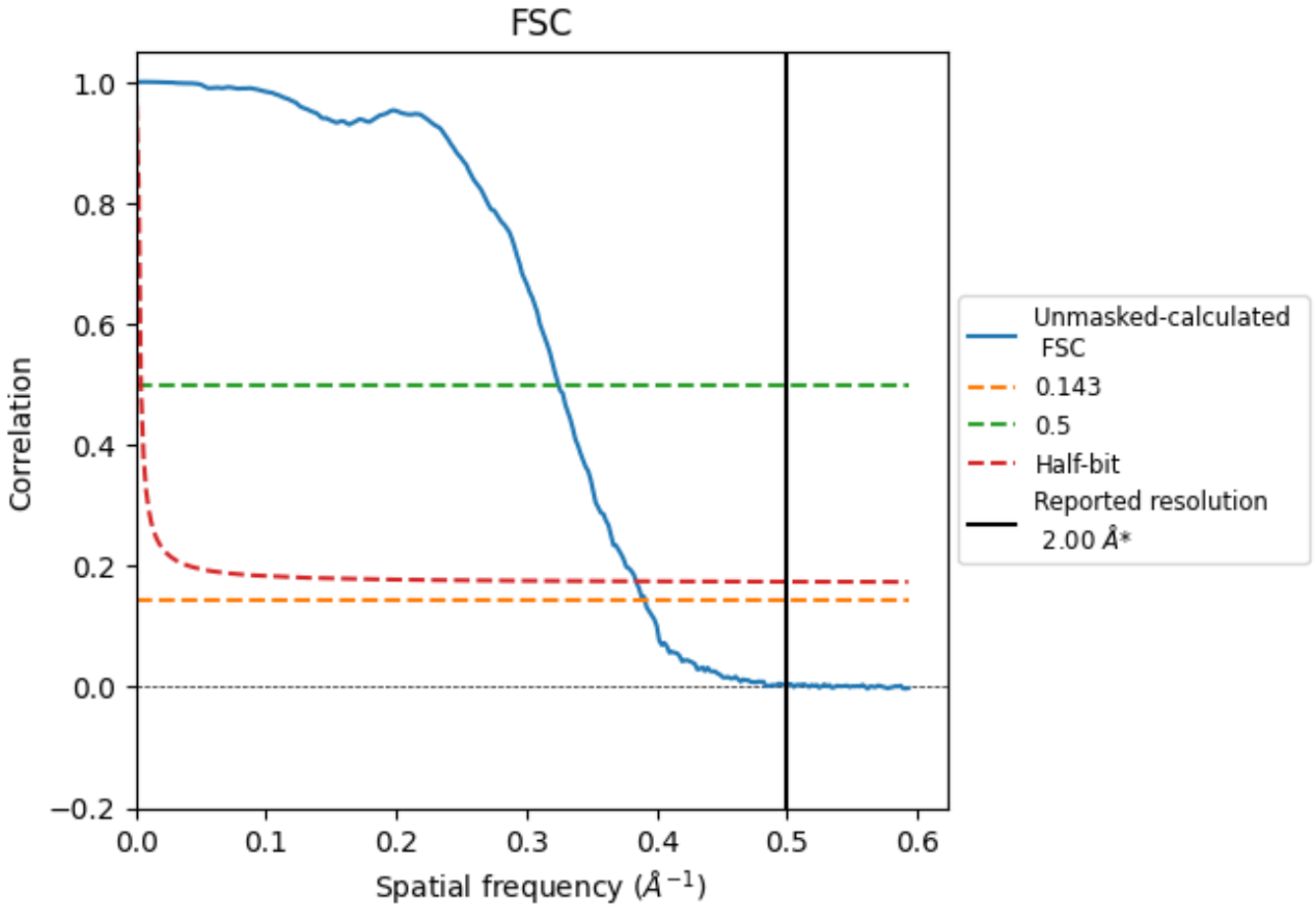


*Reported resolution corresponds to spatial frequency of 0.500 $Å^{-1}$

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 0.500 Å^{-1}

8.2 Resolution estimates (i)

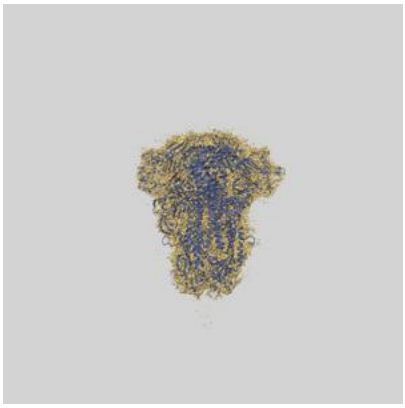
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.56	3.08	2.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

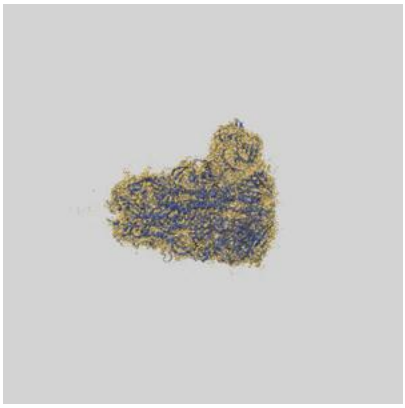
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47823 and PDB model 9EA0. Per-residue inclusion information can be found in section 3 on page 18.

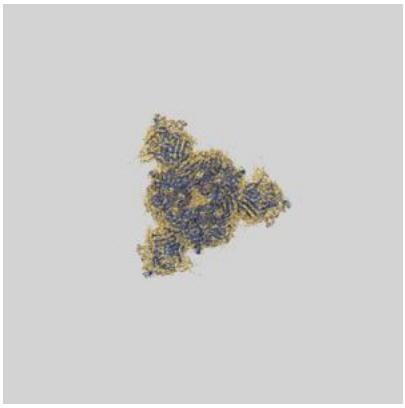
9.1 Map-model overlay



X



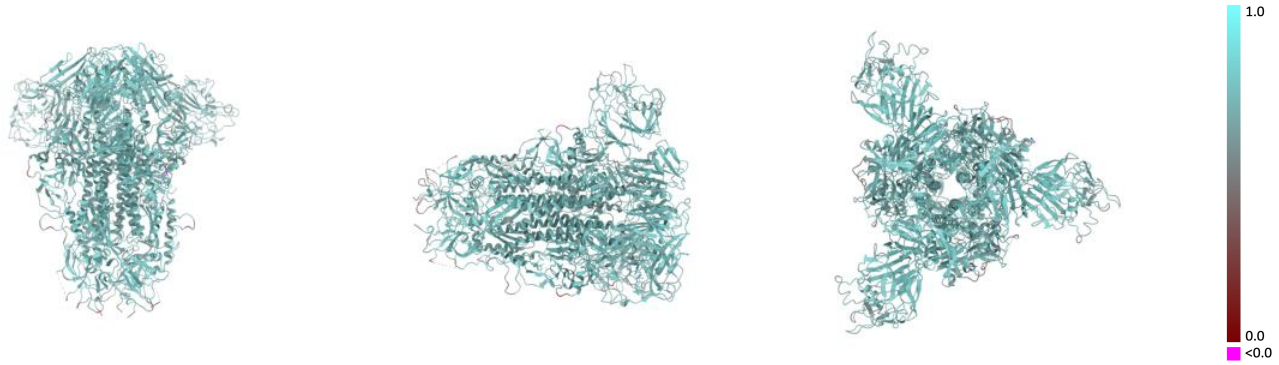
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

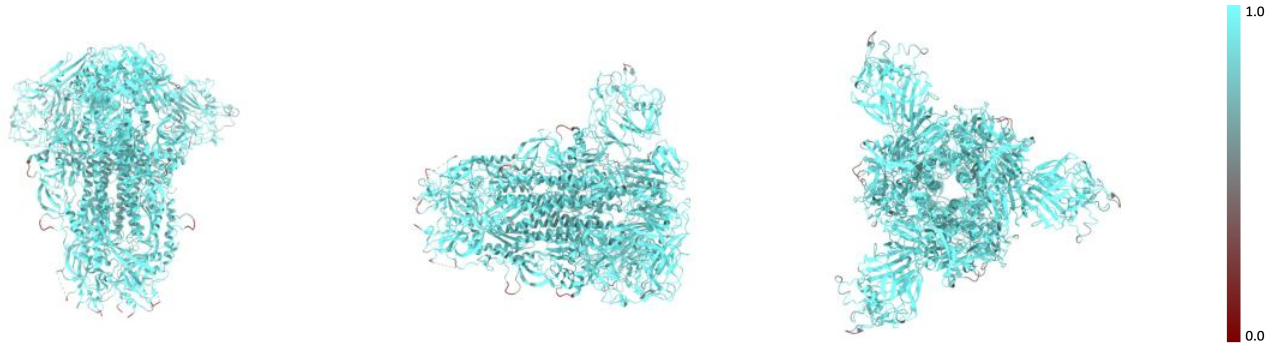
9.2 Q-score mapped to coordinate model (i)



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.

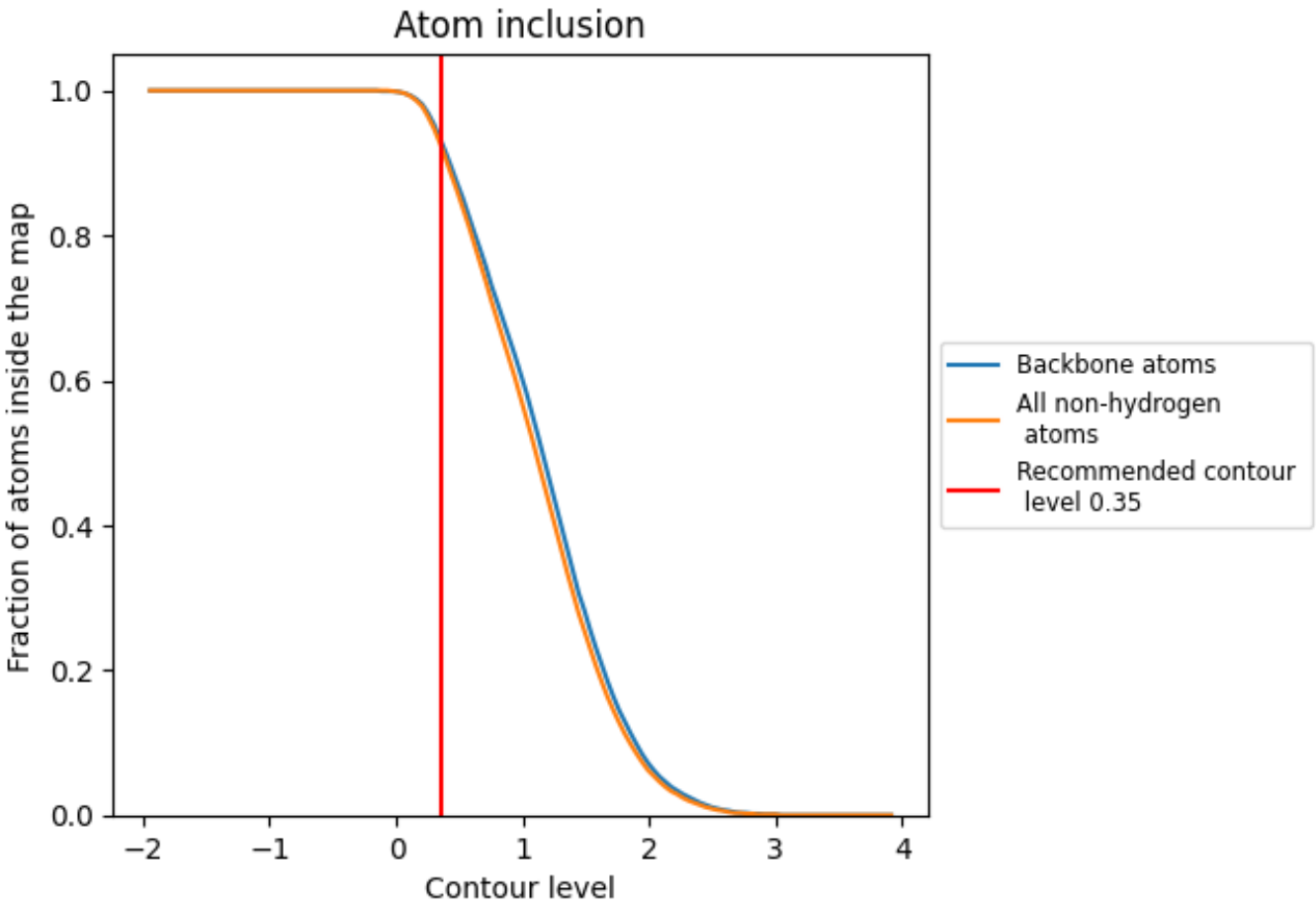
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9260	0.7020
A	0.9490	0.7140
B	0.9490	0.7130
C	0.9500	0.7130
D	0.6850	0.5710
E	0.6070	0.5500
F	0.3210	0.4930
G	0.5710	0.4160
H	0.5710	0.5550
I	0.5570	0.4580
J	0.6410	0.5000
K	0.5710	0.6050
L	0.1790	0.3190
M	0.3570	0.4300
N	0.5360	0.5000
O	0.4640	0.4940
P	0.6430	0.5120
Q	0.5510	0.5400
R	0.6850	0.5710
S	0.5710	0.5450
T	0.3210	0.4930
U	0.5710	0.4310
V	0.5710	0.5450
W	0.5410	0.4470
X	0.6410	0.4880
Y	0.5000	0.5940
Z	0.2140	0.3140
a	0.3210	0.4210
b	0.5360	0.5000
c	0.5000	0.4920
d	0.5710	0.5330
e	0.5710	0.5340
f	0.7040	0.5710
g	0.6070	0.5450
h	0.3210	0.4860

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.6070	0.4380
j	0.6430	0.5590
k	0.5410	0.4490
l	0.6410	0.4850
m	0.5000	0.5910
n	0.1790	0.2890
o	0.3210	0.4200
p	0.5360	0.4890
q	0.4640	0.4870
r	0.6070	0.5100
s	0.5510	0.5350