Full wwPDB EM Validation Report (i)

Nov 12, 2022 – 05:44 PM EST

PDB ID	:	6ULC
EMDB ID	:	EMD-20813
Title	:	Structure of full-length, fully glycosylated, non-modified HIV-1 gp160 bound to PG16 Fab at a nominal resolution of 4.6 Angstrom
Authors	:	Pan, J.; Chen, B.; Harrison, S.C.
Deposited on	:	2019-10-07
Resolution	:	4.60 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 (i) symbol.

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

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

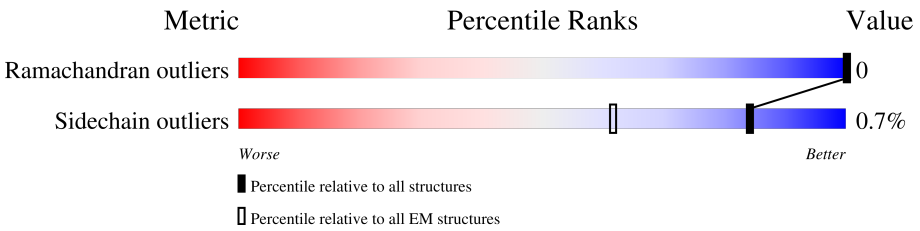
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	505	92% • 7%
1	C	505	91% • 7%
1	E	505	92% • 7%
2	B	353	9% 41% 59%
2	D	353	8% 40% • 59%
2	F	353	8% 41% 59%
3	H	297	7% 81% 19%
4	L	250	85% • 14%
5	G	6	67% 33%

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Mol	Chain	Length	Quality of chain
6	I	5	40% 60%
6	J	5	20% 40% 60%
7	K	3	67% 33%
7	N	3	67% 33%
7	Q	3	100%
7	S	3	67% 33%
7	V	3	100%
7	X	3	100%
7	Y	3	67% 33%
7	c	3	33% 100%
7	d	3	67% 33%
7	e	3	100%
7	f	3	33% 67%
7	g	3	33% 67% 33%
7	i	3	67% 33%
7	j	3	100%
7	k	3	33% 100%
7	n	3	100%
8	M	2	100%
8	O	2	50% 100%
8	P	2	50% 100%
8	R	2	50% 50%
8	U	2	50% 50%
8	W	2	100%
8	Z	2	50% 50%

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Mol	Chain	Length	Quality of chain
8	b	2	100%
8	h	2	100%
8	l	2	100%
9	T	3	100%
10	a	7	29% 71%
11	m	4	50% 50%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 19968 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 envelope glycoprotein gp120,envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	471	3717	2321	658	710	28	0	0
1	C	471	3717	2321	658	710	28	0	0
1	E	471	3717	2321	658	710	28	0	0

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	144	1167	739	203	221	4	0	0
2	D	144	1167	739	203	221	4	0	0
2	F	144	1167	739	203	221	4	0	0

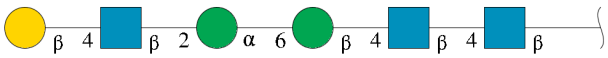
- Molecule 3 is a protein called antibody PG16 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	240	1836	1162	310	354	10	0	0

- Molecule 4 is a protein called antibody PG16 Fab light chain.

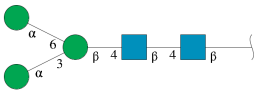
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	216	1593	988	270	329	6	0	0

- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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.



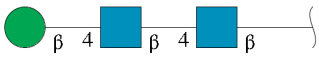
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	6	75	42	3	30	0	0

- Molecule 6 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
			Total	C	N	O		
6	I	5	61	34	2	25	0	0
6	J	5	61	34	2	25	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	K	3	39	22	2	15	0	0
7	N	3	39	22	2	15	0	0
7	Q	3	39	22	2	15	0	0
7	S	3	39	22	2	15	0	0
7	V	3	39	22	2	15	0	0
7	X	3	39	22	2	15	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	Y	3	39	22	2	15	0	0
7	c	3	39	22	2	15	0	0
7	d	3	39	22	2	15	0	0
7	e	3	39	22	2	15	0	0
7	f	3	39	22	2	15	0	0
7	g	3	39	22	2	15	0	0
7	i	3	39	22	2	15	0	0
7	j	3	39	22	2	15	0	0
7	k	3	39	22	2	15	0	0
7	n	3	39	22	2	15	0	0

- Molecule 8 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
			Total	C	N	O		
8	M	2	28	16	2	10	0	0
8	O	2	28	16	2	10	0	0
8	P	2	28	16	2	10	0	0
8	R	2	28	16	2	10	0	0
8	U	2	28	16	2	10	0	0
8	W	2	28	16	2	10	0	0
8	Z	2	28	16	2	10	0	0

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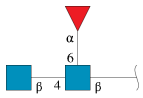
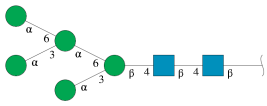
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	b	2	28	16	2	10	0	0
8	h	2	28	16	2	10	0	0
8	l	2	28	16	2	10	0	0

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



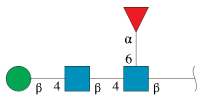
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	T	3	38	22	2	14	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



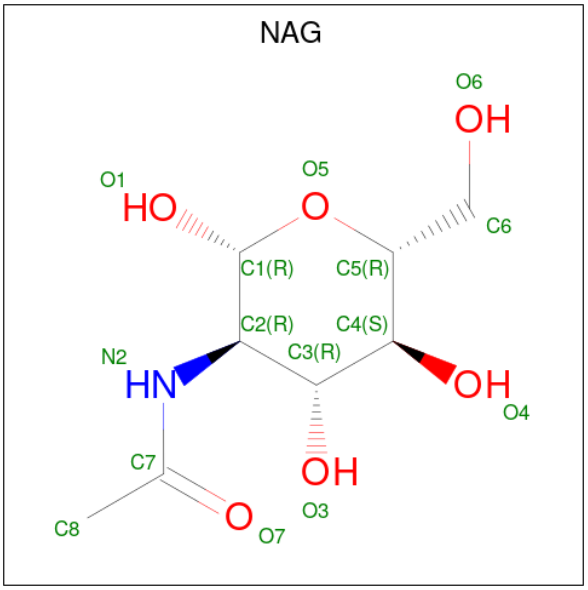
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	a	7	83	46	2	35	0	0

- Molecule 11 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
			Total	C	N	O		
11	m	4	49	28	2	19	0	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	A	1	238	136	17	85	0
12	A	1	238	136	17	85	0
12	A	1	238	136	17	85	0
12	A	1	238	136	17	85	0
12	A	1	238	136	17	85	0
12	A	1	238	136	17	85	0
12	A	1	238	136	17	85	0
12	A	1	238	136	17	85	0
12	A	1	238	136	17	85	0
12	A	1	238	136	17	85	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	A	1	238	136	17	85	0
			Total	C	N	O	
12	A	1	238	136	17	85	0
			Total	C	N	O	
12	A	1	238	136	17	85	0
			Total	C	N	O	
12	A	1	238	136	17	85	0
			Total	C	N	O	
12	A	1	238	136	17	85	0
			Total	C	N	O	
12	A	1	238	136	17	85	0
			Total	C	N	O	
12	A	1	238	136	17	85	0
			Total	C	N	O	
12	B	1	14	8	1	5	0
			Total	C	N	O	
12	C	1	196	112	14	70	0
			Total	C	N	O	
12	C	1	196	112	14	70	0
			Total	C	N	O	
12	C	1	196	112	14	70	0
			Total	C	N	O	
12	C	1	196	112	14	70	0
			Total	C	N	O	
12	C	1	196	112	14	70	0
			Total	C	N	O	
12	C	1	196	112	14	70	0
			Total	C	N	O	
12	C	1	196	112	14	70	0
			Total	C	N	O	
12	C	1	196	112	14	70	0
			Total	C	N	O	
12	C	1	196	112	14	70	0
			Total	C	N	O	
12	C	1	196	112	14	70	0
			Total	C	N	O	
12	C	1	196	112	14	70	0
			Total	C	N	O	
12	C	1	196	112	14	70	0

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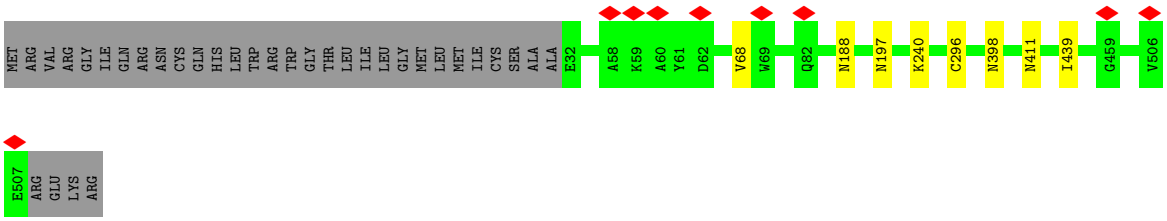
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	C	1	196	112	14	70	0
			Total	C	N	O	
12	D	1	14	8	1	5	0
			Total	C	N	O	
12	E	1	126	72	9	45	0
			Total	C	N	O	
12	E	1	126	72	9	45	0
			Total	C	N	O	
12	E	1	126	72	9	45	0
			Total	C	N	O	
12	E	1	126	72	9	45	0
			Total	C	N	O	
12	E	1	126	72	9	45	0
			Total	C	N	O	
12	E	1	126	72	9	45	0
			Total	C	N	O	
12	E	1	126	72	9	45	0
			Total	C	N	O	
12	E	1	126	72	9	45	0
			Total	C	N	O	
12	E	1	126	72	9	45	0
			Total	C	N	O	
12	F	1	28	16	2	10	0
			Total	C	N	O	
12	F	1	28	16	2	10	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.

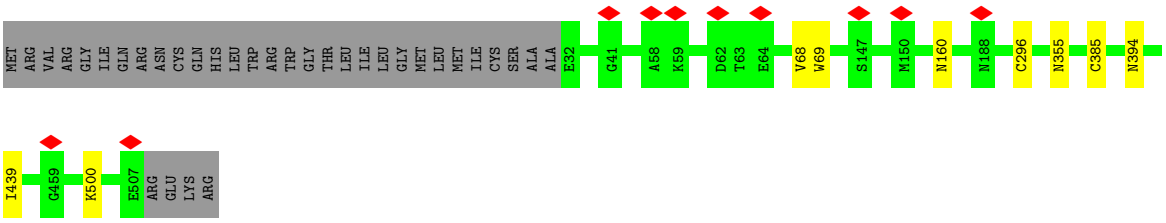
• Molecule 1: envelope glycoprotein gp120,envelope glycoprotein gp120

Chain A:



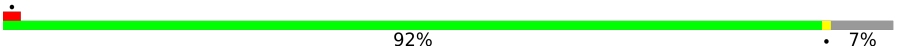
• Molecule 1: envelope glycoprotein gp120,envelope glycoprotein gp120

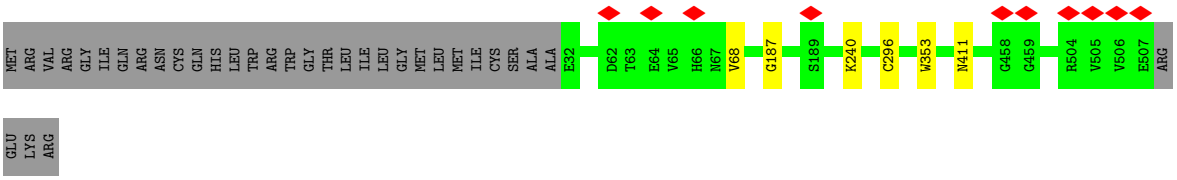
Chain C:



• Molecule 1: envelope glycoprotein gp120,envelope glycoprotein gp120

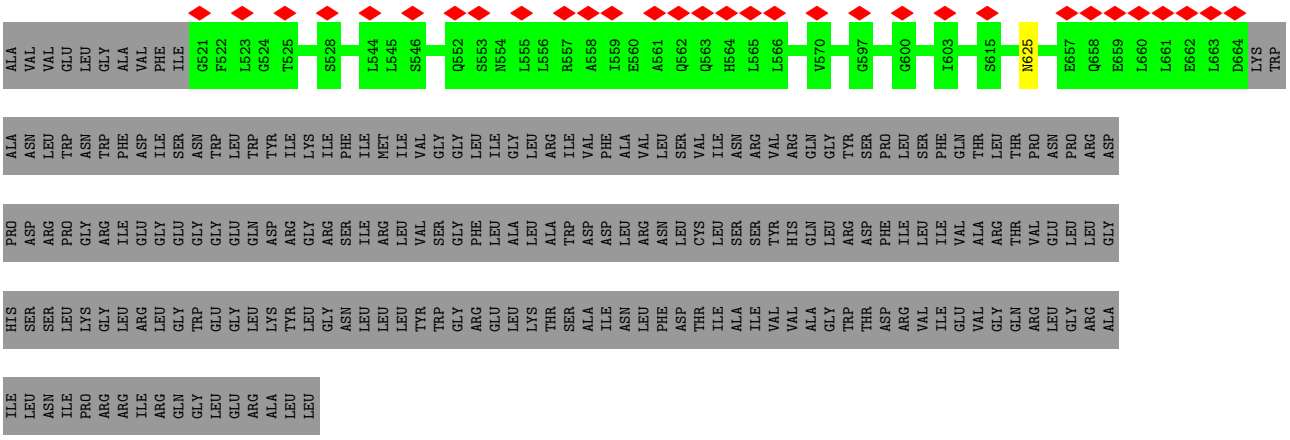
Chain E:





• Molecule 2: Envelope glycoprotein gp41

Chain B:



• Molecule 2: Envelope glycoprotein gp41

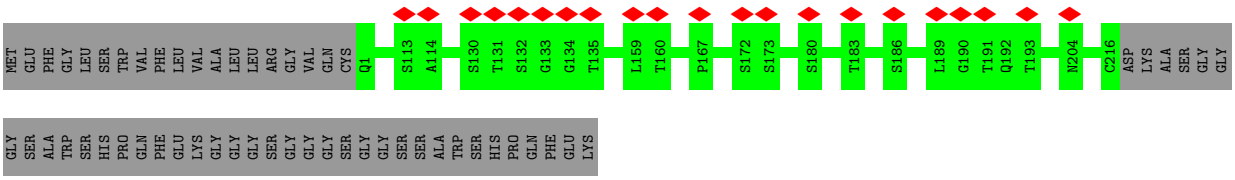
Chain D:

• Molecule 2: Envelope glycoprotein gp41

Chain F:

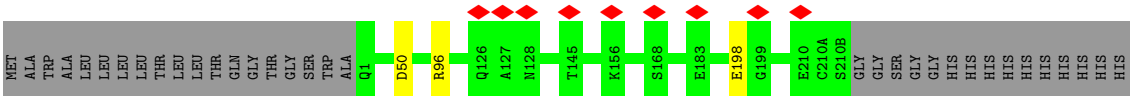
• Molecule 3: antibody PG16 Fab heavy chain

Chain H:



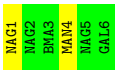
• Molecule 4: antibody PG16 Fab light chain

Chain L:



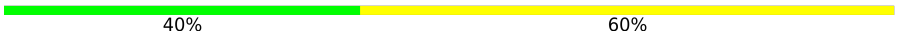
• Molecule 5: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



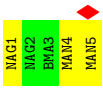
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 6: 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 J:



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

Chain K:

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

Chain N: 67% 33%

NAG1 NAG2 BMA3

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

Chain Q: 100%

NAG1 NAG2 BMA3

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

Chain S: 67% 33%

NAG1 NAG2 BMA3

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

Chain V: 100%

NAG1 NAG2 BMA3

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

Chain X: 100%

NAG1 NAG2 BMA3

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

Chain Y: 67% 33%

NAG1 NAG2 BMA3

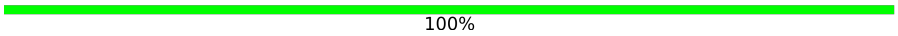
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 33% 100%

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

Chain d:

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

Chain e: 

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

Chain f:

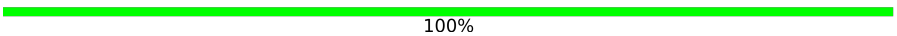
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

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

Chain i:

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

Chain j: 

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

Chain k: 33% 100%

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

Chain n: 100%

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 100%

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 50% 100%

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 50% 100%

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 50% 50%

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 50% 50%

NAG1 NAG2

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 100%

NAG1 NAG2

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 50% 50%

NAG1 NAG2

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 100%

NAG1 NAG2

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h: 100%

NAG1 NAG2

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

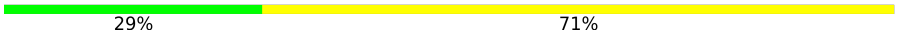
Chain l: 100%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 100%

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

Chain a: 

• Molecule 11: 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 m:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	492995	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	30488	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	314.88, 314.88, 314.88	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.64, 1.64, 1.64	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.32	1/3793 (0.0%)	0.55	0/5161
1	C	0.31	2/3793 (0.1%)	0.55	0/5161
1	E	0.30	1/3793 (0.0%)	0.54	0/5161
2	B	0.27	0/1187	0.56	0/1607
2	D	0.27	0/1187	0.55	0/1607
2	F	0.27	0/1187	0.59	0/1607
3	H	0.26	0/1887	0.52	0/2565
4	L	0.27	0/1630	0.51	0/2219
All	All	0.29	4/18457 (0.0%)	0.54	0/25088

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	3
1	E	0	3
2	D	0	1
4	L	0	2
All	All	0	11

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	296	CYS	CB-SG	6.37	1.93	1.82
1	A	296	CYS	CB-SG	6.20	1.92	1.82
1	E	296	CYS	CB-SG	5.94	1.92	1.82
1	C	385	CYS	CB-SG	5.84	1.92	1.82

There are no bond angle outliers.

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	439	ILE	Peptide
1	A	68	VAL	Peptide
1	C	439	ILE	Peptide
1	C	68	VAL	Peptide
1	C	69	TRP	Peptide
2	D	557	ARG	Peptide
1	E	187	GLY	Peptide
1	E	353	TRP	Peptide
1	E	68	VAL	Peptide
4	L	198	GLU	Peptide
4	L	50	ASP	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/505 (93%)	469 (100%)	0	0	100	100
1	C	469/505 (93%)	469 (100%)	0	0	100	100
1	E	469/505 (93%)	469 (100%)	0	0	100	100
2	B	142/353 (40%)	142 (100%)	0	0	100	100
2	D	142/353 (40%)	142 (100%)	0	0	100	100
2	F	142/353 (40%)	142 (100%)	0	0	100	100
3	H	238/297 (80%)	238 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	214/250 (86%)	214 (100%)	0	0	100	100
All	All	2285/3121 (73%)	2285 (100%)	0	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	422/451 (94%)	417 (99%)	5 (1%)	71	84
1	C	422/451 (94%)	418 (99%)	4 (1%)	78	87
1	E	422/451 (94%)	420 (100%)	2 (0%)	88	93
2	B	128/304 (42%)	127 (99%)	1 (1%)	81	89
2	D	128/304 (42%)	127 (99%)	1 (1%)	81	89
2	F	128/304 (42%)	128 (100%)	0	100	100
3	H	204/244 (84%)	204 (100%)	0	100	100
4	L	183/208 (88%)	182 (100%)	1 (0%)	88	93
All	All	2037/2717 (75%)	2023 (99%)	14 (1%)	84	90

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	A	197	ASN
1	A	240	LYS
1	A	398	ASN
1	A	411	ASN
2	B	625	ASN
1	C	160	ASN
1	C	355	ASN
1	C	394	ASN
1	C	500	LYS

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Mol	Chain	Res	Type
2	D	617	LYS
1	E	240	LYS
1	E	411	ASN
4	L	96	ARG

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

Mol	Chain	Res	Type
2	B	563	GLN
1	C	114	GLN
1	E	377	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

98 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	$\#\|Z\| > 2$
5	NAG	G	1	1,5	14,14,15	0.31	0	17,19,21	0.69	1 (5%)
5	NAG	G	2	5	14,14,15	0.20	0	17,19,21	0.43	0
5	BMA	G	3	5	11,11,12	0.60	0	15,15,17	0.74	0
5	MAN	G	4	5	11,11,12	1.63	4 (36%)	15,15,17	1.44	3 (20%)
5	NAG	G	5	5	14,14,15	0.25	0	17,19,21	0.45	0
5	GAL	G	6	5	11,11,12	0.53	0	15,15,17	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	I	1	1,6	14,14,15	0.30	0	17,19,21	0.38	0
6	NAG	I	2	6	14,14,15	0.21	0	17,19,21	0.42	0
6	BMA	I	3	6	11,11,12	0.94	1 (9%)	15,15,17	1.00	0
6	MAN	I	4	6	11,11,12	1.06	1 (9%)	15,15,17	1.43	3 (20%)
6	MAN	I	5	6	11,11,12	0.84	1 (9%)	15,15,17	1.71	1 (6%)
6	NAG	J	1	1,6	14,14,15	0.41	0	17,19,21	1.62	2 (11%)
6	NAG	J	2	6	14,14,15	0.26	0	17,19,21	0.56	0
6	BMA	J	3	6	11,11,12	0.66	0	15,15,17	0.71	0
6	MAN	J	4	6	11,11,12	0.67	0	15,15,17	1.35	3 (20%)
6	MAN	J	5	6	11,11,12	0.69	0	15,15,17	1.05	2 (13%)
7	NAG	K	1	1,7	14,14,15	0.20	0	17,19,21	0.49	0
7	NAG	K	2	7	14,14,15	0.35	0	17,19,21	1.57	2 (11%)
7	BMA	K	3	7	11,11,12	0.55	0	15,15,17	0.87	0
8	NAG	M	1	1,8	14,14,15	0.45	0	17,19,21	0.44	0
8	NAG	M	2	8	14,14,15	0.18	0	17,19,21	0.44	0
7	NAG	N	1	1,7	14,14,15	0.37	0	17,19,21	0.54	0
7	NAG	N	2	7	14,14,15	0.33	0	17,19,21	0.49	0
7	BMA	N	3	7	11,11,12	0.52	0	15,15,17	0.98	1 (6%)
8	NAG	O	1	2,8	14,14,15	0.38	0	17,19,21	0.49	0
8	NAG	O	2	8	14,14,15	0.21	0	17,19,21	0.47	0
8	NAG	P	1	2,8	14,14,15	0.31	0	17,19,21	0.56	0
8	NAG	P	2	8	14,14,15	0.25	0	17,19,21	0.39	0
7	NAG	Q	1	1,7	14,14,15	0.40	0	17,19,21	0.47	0
7	NAG	Q	2	7	14,14,15	0.40	0	17,19,21	0.42	0
7	BMA	Q	3	7	11,11,12	0.57	0	15,15,17	0.83	0
8	NAG	R	1	1,8	14,14,15	0.59	0	17,19,21	0.60	0
8	NAG	R	2	8	14,14,15	0.28	0	17,19,21	1.56	2 (11%)
7	NAG	S	1	1,7	14,14,15	0.38	0	17,19,21	0.86	1 (5%)
7	NAG	S	2	7	14,14,15	0.23	0	17,19,21	0.41	0
7	BMA	S	3	7	11,11,12	0.63	0	15,15,17	0.74	0
9	NAG	T	1	9,1	14,14,15	0.20	0	17,19,21	0.58	0
9	NAG	T	2	9	14,14,15	0.21	0	17,19,21	0.41	0
9	FUC	T	3	9	10,10,11	0.71	0	14,14,16	0.87	0
8	NAG	U	1	1,8	14,14,15	0.17	0	17,19,21	0.52	0
8	NAG	U	2	8	14,14,15	0.29	0	17,19,21	1.56	2 (11%)
7	NAG	V	1	1,7	14,14,15	0.26	0	17,19,21	0.53	0
7	NAG	V	2	7	14,14,15	0.29	0	17,19,21	0.53	0
7	BMA	V	3	7	11,11,12	0.62	0	15,15,17	0.72	0
8	NAG	W	1	1,8	14,14,15	0.31	0	17,19,21	0.67	1 (5%)
8	NAG	W	2	8	14,14,15	0.26	0	17,19,21	0.80	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	X	1	1,7	14,14,15	0.27	0	17,19,21	0.45	0
7	NAG	X	2	7	14,14,15	0.16	0	17,19,21	0.40	0
7	BMA	X	3	7	11,11,12	0.65	0	15,15,17	0.73	0
7	NAG	Y	1	1,7	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
7	NAG	Y	2	7	14,14,15	0.24	0	17,19,21	0.38	0
7	BMA	Y	3	7	11,11,12	0.63	0	15,15,17	0.71	0
8	NAG	Z	1	1,8	14,14,15	0.34	0	17,19,21	0.66	1 (5%)
8	NAG	Z	2	8	14,14,15	0.21	0	17,19,21	0.39	0
10	NAG	a	1	10,1	14,14,15	0.29	0	17,19,21	0.45	0
10	NAG	a	2	10	14,14,15	0.28	0	17,19,21	0.60	0
10	BMA	a	3	10	11,11,12	1.12	1 (9%)	15,15,17	1.10	1 (6%)
10	MAN	a	4	10	11,11,12	1.10	2 (18%)	15,15,17	1.92	4 (26%)
10	MAN	a	5	10	11,11,12	0.63	0	15,15,17	1.12	2 (13%)
10	MAN	a	6	10	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
10	MAN	a	7	10	11,11,12	0.60	0	15,15,17	1.18	2 (13%)
8	NAG	b	1	1,8	14,14,15	0.36	0	17,19,21	0.38	0
8	NAG	b	2	8	14,14,15	0.21	0	17,19,21	0.40	0
7	NAG	c	1	1,7	14,14,15	0.36	0	17,19,21	0.56	0
7	NAG	c	2	7	14,14,15	0.54	0	17,19,21	0.65	0
7	BMA	c	3	7	11,11,12	0.63	0	15,15,17	0.78	0
7	NAG	d	1	1,7	14,14,15	0.33	0	17,19,21	0.38	0
7	NAG	d	2	7	14,14,15	0.41	0	17,19,21	1.55	2 (11%)
7	BMA	d	3	7	11,11,12	0.55	0	15,15,17	0.78	0
7	NAG	e	1	1,7	14,14,15	0.22	0	17,19,21	0.52	0
7	NAG	e	2	7	14,14,15	0.21	0	17,19,21	0.39	0
7	BMA	e	3	7	11,11,12	0.59	0	15,15,17	0.78	0
7	NAG	f	1	1,7	14,14,15	0.39	0	17,19,21	1.57	2 (11%)
7	NAG	f	2	7	14,14,15	0.27	0	17,19,21	0.62	1 (5%)
7	BMA	f	3	7	11,11,12	0.60	0	15,15,17	0.84	0
7	NAG	g	1	1,7	14,14,15	0.46	0	17,19,21	1.10	2 (11%)
7	NAG	g	2	7	14,14,15	0.27	0	17,19,21	0.46	0
7	BMA	g	3	7	11,11,12	0.56	0	15,15,17	0.88	0
8	NAG	h	1	1,8	14,14,15	0.18	0	17,19,21	0.46	0
8	NAG	h	2	8	14,14,15	0.23	0	17,19,21	0.44	0
7	NAG	i	1	1,7	14,14,15	0.22	0	17,19,21	0.48	0
7	NAG	i	2	7	14,14,15	0.31	0	17,19,21	1.55	2 (11%)
7	BMA	i	3	7	11,11,12	0.64	0	15,15,17	0.79	0
7	NAG	j	1	1,7	14,14,15	0.21	0	17,19,21	0.46	0
7	NAG	j	2	7	14,14,15	0.22	0	17,19,21	0.46	0
7	BMA	j	3	7	11,11,12	0.64	0	15,15,17	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	k	1	1,7	14,14,15	0.27	0	17,19,21	0.60	0
7	NAG	k	2	7	14,14,15	0.27	0	17,19,21	0.58	0
7	BMA	k	3	7	11,11,12	0.55	0	15,15,17	0.79	0
8	NAG	l	1	2,8	14,14,15	0.55	0	17,19,21	1.02	1 (5%)
8	NAG	l	2	8	14,14,15	0.64	1 (7%)	17,19,21	0.75	1 (5%)
11	NAG	m	1	11,1	14,14,15	0.42	0	17,19,21	0.55	0
11	NAG	m	2	11	14,14,15	0.47	0	17,19,21	0.39	0
11	BMA	m	3	11	11,11,12	0.89	0	15,15,17	1.09	1 (6%)
11	FUC	m	4	11	10,10,11	0.84	1 (10%)	14,14,16	0.75	0
7	NAG	n	1	4,7	14,14,15	0.23	0	17,19,21	0.51	0
7	NAG	n	2	7	14,14,15	0.20	0	17,19,21	0.36	0
7	BMA	n	3	7	11,11,12	0.58	0	15,15,17	0.79	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
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	NAG	G	5	5	-	1/6/23/26	0/1/1/1
5	GAL	G	6	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
6	MAN	I	4	6	-	2/2/19/22	0/1/1/1
6	MAN	I	5	6	-	0/2/19/22	1/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	5/6/23/26	0/1/1/1
7	BMA	K	3	7	-	1/2/19/22	0/1/1/1
8	NAG	M	1	1,8	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	M	2	8	-	2/6/23/26	0/1/1/1
7	NAG	N	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
8	NAG	O	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	O	2	8	-	2/6/23/26	0/1/1/1
8	NAG	P	1	2,8	-	1/6/23/26	0/1/1/1
8	NAG	P	2	8	-	1/6/23/26	0/1/1/1
7	NAG	Q	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	2/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	1/2/19/22	0/1/1/1
8	NAG	R	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	R	2	8	-	5/6/23/26	0/1/1/1
7	NAG	S	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1
7	BMA	S	3	7	-	0/2/19/22	0/1/1/1
9	NAG	T	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	T	2	9	-	2/6/23/26	0/1/1/1
9	FUC	T	3	9	-	-	0/1/1/1
8	NAG	U	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	U	2	8	-	4/6/23/26	0/1/1/1
7	NAG	V	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	V	2	7	-	1/6/23/26	0/1/1/1
7	BMA	V	3	7	-	0/2/19/22	0/1/1/1
8	NAG	W	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	W	2	8	-	4/6/23/26	0/1/1/1
7	NAG	X	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	X	2	7	-	2/6/23/26	0/1/1/1
7	BMA	X	3	7	-	0/2/19/22	0/1/1/1
7	NAG	Y	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	0/6/23/26	0/1/1/1
7	BMA	Y	3	7	-	0/2/19/22	0/1/1/1
8	NAG	Z	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	2/6/23/26	0/1/1/1
10	NAG	a	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	a	2	10	-	2/6/23/26	0/1/1/1
10	BMA	a	3	10	-	2/2/19/22	0/1/1/1
10	MAN	a	4	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	a	5	10	-	0/2/19/22	0/1/1/1
10	MAN	a	6	10	-	0/2/19/22	0/1/1/1
10	MAN	a	7	10	-	2/2/19/22	0/1/1/1
8	NAG	b	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
7	NAG	c	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	c	2	7	-	2/6/23/26	0/1/1/1
7	BMA	c	3	7	-	0/2/19/22	0/1/1/1
7	NAG	d	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	d	2	7	-	5/6/23/26	0/1/1/1
7	BMA	d	3	7	-	1/2/19/22	0/1/1/1
7	NAG	e	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	e	2	7	-	1/6/23/26	0/1/1/1
7	BMA	e	3	7	-	0/2/19/22	0/1/1/1
7	NAG	f	1	1,7	-	5/6/23/26	0/1/1/1
7	NAG	f	2	7	-	2/6/23/26	0/1/1/1
7	BMA	f	3	7	-	0/2/19/22	0/1/1/1
7	NAG	g	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	g	2	7	-	2/6/23/26	0/1/1/1
7	BMA	g	3	7	-	0/2/19/22	0/1/1/1
8	NAG	h	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	h	2	8	-	2/6/23/26	0/1/1/1
7	NAG	i	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	i	2	7	-	3/6/23/26	0/1/1/1
7	BMA	i	3	7	-	1/2/19/22	0/1/1/1
7	NAG	j	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	j	2	7	-	2/6/23/26	0/1/1/1
7	BMA	j	3	7	-	0/2/19/22	0/1/1/1
7	NAG	k	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	k	2	7	-	2/6/23/26	0/1/1/1
7	BMA	k	3	7	-	0/2/19/22	0/1/1/1
8	NAG	l	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	l	2	8	-	2/6/23/26	0/1/1/1
11	NAG	m	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	m	2	11	-	4/6/23/26	0/1/1/1
11	BMA	m	3	11	-	1/2/19/22	0/1/1/1
11	FUC	m	4	11	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	n	1	4,7	-	0/6/23/26	0/1/1/1
7	NAG	n	2	7	-	2/6/23/26	0/1/1/1
7	BMA	n	3	7	-	1/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	4	MAN	C2-C3	3.29	1.57	1.52
10	a	4	MAN	C1-C2	2.52	1.57	1.52
5	G	4	MAN	O5-C1	-2.47	1.39	1.43
10	a	3	BMA	O5-C1	-2.45	1.39	1.43
5	G	4	MAN	O2-C2	2.41	1.48	1.43
6	I	5	MAN	O5-C5	2.40	1.48	1.43
6	I	4	MAN	O5-C1	-2.37	1.39	1.43
6	I	3	BMA	O5-C1	-2.33	1.40	1.43
8	l	2	NAG	C1-C2	2.25	1.55	1.52
10	a	4	MAN	C2-C3	2.24	1.55	1.52
11	m	4	FUC	O5-C1	-2.13	1.40	1.43
5	G	4	MAN	C1-C2	2.02	1.56	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	1	NAG	C1-O5-C5	5.97	120.28	112.19
6	I	5	MAN	C1-O5-C5	5.59	119.77	112.19
7	K	2	NAG	C2-N2-C7	5.11	130.17	122.90
8	U	2	NAG	C2-N2-C7	5.10	130.16	122.90
7	i	2	NAG	C2-N2-C7	5.04	130.08	122.90
8	R	2	NAG	C2-N2-C7	5.00	130.02	122.90
7	d	2	NAG	C2-N2-C7	4.91	129.90	122.90
7	f	1	NAG	C2-N2-C7	4.84	129.79	122.90
10	a	4	MAN	C1-C2-C3	4.16	114.78	109.67
10	a	4	MAN	C1-O5-C5	3.83	117.38	112.19
10	a	4	MAN	O5-C1-C2	3.40	116.01	110.77
7	f	1	NAG	C1-C2-N2	3.24	116.03	110.49
7	d	2	NAG	C1-C2-N2	3.15	115.88	110.49
6	J	4	MAN	C1-O5-C5	3.11	116.40	112.19
5	G	4	MAN	C1-C2-C3	3.07	113.44	109.67
8	l	1	NAG	C1-O5-C5	3.03	116.29	112.19
6	I	4	MAN	C1-C2-C3	3.02	113.38	109.67
10	a	7	MAN	C1-O5-C5	2.89	116.11	112.19
7	S	1	NAG	C1-O5-C5	2.84	116.04	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	2	NAG	C1-C2-N2	2.82	115.31	110.49
10	a	5	MAN	C1-O5-C5	2.82	116.01	112.19
7	i	2	NAG	C1-C2-N2	2.78	115.23	110.49
7	K	2	NAG	C1-C2-N2	2.75	115.18	110.49
8	U	2	NAG	C1-C2-N2	2.64	115.00	110.49
8	l	2	NAG	C1-O5-C5	2.64	115.77	112.19
8	W	2	NAG	C2-N2-C7	2.61	126.62	122.90
10	a	6	MAN	C1-O5-C5	2.61	115.73	112.19
10	a	3	BMA	C1-C2-C3	-2.60	106.47	109.67
7	g	1	NAG	C2-N2-C7	2.59	126.59	122.90
7	g	1	NAG	C1-O5-C5	2.57	115.67	112.19
7	N	3	BMA	C1-O5-C5	2.47	115.54	112.19
5	G	4	MAN	C2-C3-C4	2.44	115.12	110.89
6	I	4	MAN	O2-C2-C3	-2.41	105.32	110.14
6	J	4	MAN	O2-C2-C3	-2.40	105.34	110.14
6	J	4	MAN	O5-C1-C2	2.39	114.46	110.77
5	G	4	MAN	O2-C2-C1	2.34	113.95	109.15
6	J	5	MAN	C1-O5-C5	2.28	115.28	112.19
6	J	5	MAN	O2-C2-C3	-2.28	105.57	110.14
10	a	7	MAN	O2-C2-C3	-2.28	105.58	110.14
6	I	4	MAN	O5-C1-C2	2.27	114.28	110.77
7	Y	1	NAG	C1-O5-C5	2.27	115.26	112.19
6	J	1	NAG	C3-C4-C5	2.24	114.24	110.24
10	a	4	MAN	O2-C2-C3	-2.21	105.70	110.14
10	a	5	MAN	O2-C2-C3	-2.18	105.76	110.14
8	Z	1	NAG	C1-O5-C5	2.15	115.10	112.19
5	G	1	NAG	C1-O5-C5	2.14	115.10	112.19
7	f	2	NAG	C1-O5-C5	2.11	115.05	112.19
11	m	3	BMA	C1-C2-C3	2.06	112.20	109.67
8	W	1	NAG	C1-O5-C5	2.04	114.96	112.19
10	a	6	MAN	O2-C2-C3	-2.00	106.12	110.14

There are no chirality outliers.

All (134) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	Z	2	NAG	C4-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
10	a	3	BMA	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
7	e	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	N	2	NAG	O5-C5-C6-O6
8	Z	2	NAG	O5-C5-C6-O6
7	V	1	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
8	b	2	NAG	C4-C5-C6-O6
8	h	2	NAG	C4-C5-C6-O6
7	X	2	NAG	O5-C5-C6-O6
8	M	2	NAG	O5-C5-C6-O6
8	l	1	NAG	O5-C5-C6-O6
11	m	2	NAG	O5-C5-C6-O6
7	V	1	NAG	C4-C5-C6-O6
8	O	2	NAG	O5-C5-C6-O6
10	a	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
10	a	1	NAG	C4-C5-C6-O6
10	a	3	BMA	C4-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
7	K	2	NAG	C4-C5-C6-O6
8	O	2	NAG	C4-C5-C6-O6
8	l	2	NAG	O5-C5-C6-O6
7	N	2	NAG	C4-C5-C6-O6
8	W	2	NAG	C4-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
8	M	2	NAG	C4-C5-C6-O6
11	m	2	NAG	C4-C5-C6-O6
8	b	2	NAG	O5-C5-C6-O6
8	h	2	NAG	O5-C5-C6-O6
6	I	4	MAN	C4-C5-C6-O6
6	I	4	MAN	O5-C5-C6-O6
7	n	2	NAG	O5-C5-C6-O6
8	W	2	NAG	O5-C5-C6-O6
8	R	2	NAG	C4-C5-C6-O6
7	e	1	NAG	C4-C5-C6-O6
7	N	1	NAG	C4-C5-C6-O6
7	k	2	NAG	O5-C5-C6-O6
8	l	1	NAG	C4-C5-C6-O6
8	l	2	NAG	C4-C5-C6-O6
7	K	2	NAG	C8-C7-N2-C2
7	K	2	NAG	O7-C7-N2-C2
7	d	2	NAG	C8-C7-N2-C2
7	d	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	f	1	NAG	C8-C7-N2-C2
7	f	1	NAG	O7-C7-N2-C2
7	g	1	NAG	C8-C7-N2-C2
7	g	1	NAG	O7-C7-N2-C2
7	i	2	NAG	C8-C7-N2-C2
7	i	2	NAG	O7-C7-N2-C2
8	R	2	NAG	C8-C7-N2-C2
8	R	2	NAG	O7-C7-N2-C2
8	U	2	NAG	C8-C7-N2-C2
8	U	2	NAG	O7-C7-N2-C2
8	W	2	NAG	C8-C7-N2-C2
8	W	2	NAG	O7-C7-N2-C2
7	i	1	NAG	O5-C5-C6-O6
8	U	1	NAG	C4-C5-C6-O6
7	c	2	NAG	O5-C5-C6-O6
9	T	2	NAG	O5-C5-C6-O6
7	n	2	NAG	C4-C5-C6-O6
6	J	3	BMA	O5-C5-C6-O6
7	f	1	NAG	O5-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
8	R	2	NAG	O5-C5-C6-O6
7	f	1	NAG	C4-C5-C6-O6
5	G	5	NAG	O5-C5-C6-O6
8	b	1	NAG	O5-C5-C6-O6
7	X	2	NAG	C4-C5-C6-O6
9	T	2	NAG	C4-C5-C6-O6
7	c	2	NAG	C4-C5-C6-O6
10	a	1	NAG	O5-C5-C6-O6
7	k	2	NAG	C4-C5-C6-O6
11	m	1	NAG	C1-C2-N2-C7
7	j	2	NAG	O5-C5-C6-O6
6	J	3	BMA	C4-C5-C6-O6
7	j	2	NAG	C4-C5-C6-O6
8	U	1	NAG	O5-C5-C6-O6
8	M	1	NAG	O5-C5-C6-O6
7	K	3	BMA	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
8	R	1	NAG	O5-C5-C6-O6
7	i	1	NAG	C4-C5-C6-O6
7	N	1	NAG	O5-C5-C6-O6
7	f	2	NAG	O5-C5-C6-O6
7	k	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	Q	2	NAG	C4-C5-C6-O6
7	g	2	NAG	C4-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
8	Z	1	NAG	O5-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
7	d	1	NAG	C1-C2-N2-C7
8	b	1	NAG	C1-C2-N2-C7
11	m	2	NAG	C1-C2-N2-C7
5	G	2	NAG	O5-C5-C6-O6
7	Q	3	BMA	O5-C5-C6-O6
8	P	1	NAG	O5-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
8	W	1	NAG	O5-C5-C6-O6
7	n	3	BMA	O5-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
7	d	3	BMA	O5-C5-C6-O6
7	i	3	BMA	O5-C5-C6-O6
10	a	7	MAN	C4-C5-C6-O6
8	U	2	NAG	O5-C5-C6-O6
7	d	2	NAG	O5-C5-C6-O6
10	a	2	NAG	C4-C5-C6-O6
11	m	3	BMA	C4-C5-C6-O6
7	K	1	NAG	C4-C5-C6-O6
7	e	2	NAG	O5-C5-C6-O6
10	a	7	MAN	O5-C5-C6-O6
7	f	1	NAG	C1-C2-N2-C7
7	K	2	NAG	C3-C2-N2-C7
7	i	2	NAG	C3-C2-N2-C7
8	R	2	NAG	C3-C2-N2-C7
8	U	2	NAG	C3-C2-N2-C7
7	K	1	NAG	O5-C5-C6-O6
9	T	1	NAG	C4-C5-C6-O6
7	f	2	NAG	C4-C5-C6-O6
8	M	1	NAG	C4-C5-C6-O6
8	P	2	NAG	C4-C5-C6-O6
7	d	2	NAG	C1-C2-N2-C7
7	k	1	NAG	C4-C5-C6-O6
7	d	1	NAG	C3-C2-N2-C7
7	d	2	NAG	C3-C2-N2-C7
8	b	1	NAG	C3-C2-N2-C7
11	m	1	NAG	C3-C2-N2-C7

Continued on next page...

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Mol	Chain	Res	Type	Atoms
11	m	2	NAG	C3-C2-N2-C7
7	X	1	NAG	C1-C2-N2-C7

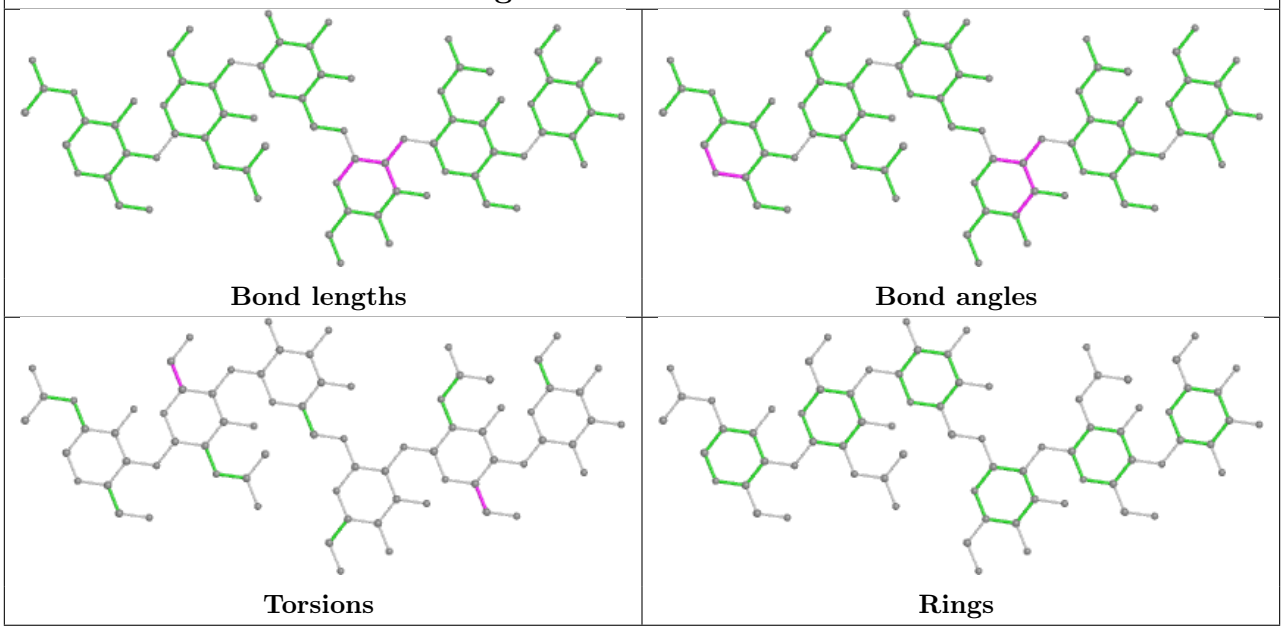
All (1) ring outliers are listed below:

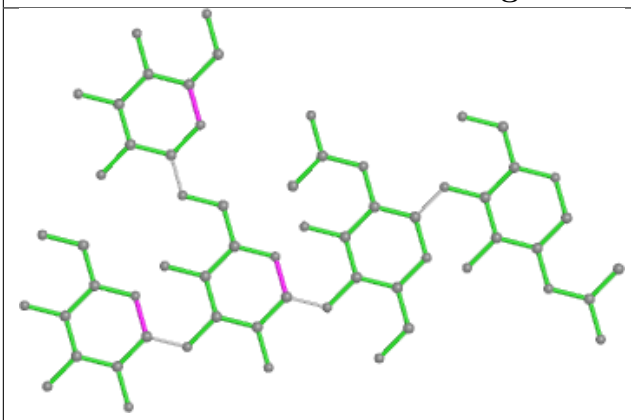
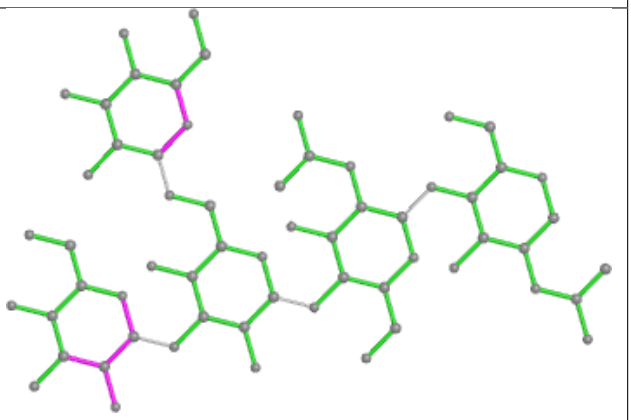
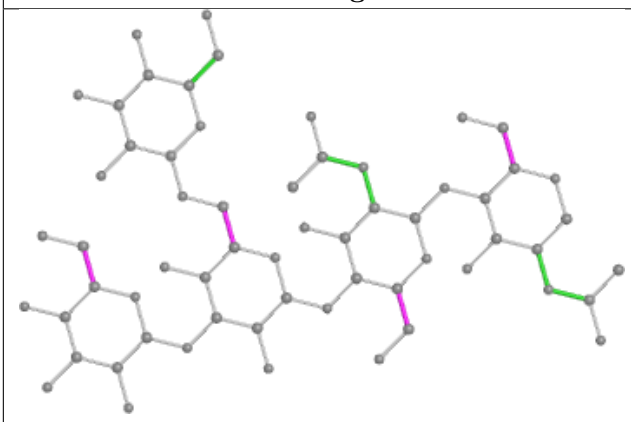
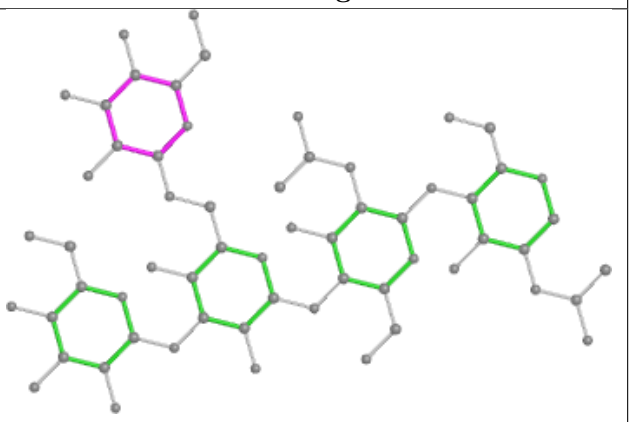
Mol	Chain	Res	Type	Atoms
6	I	5	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

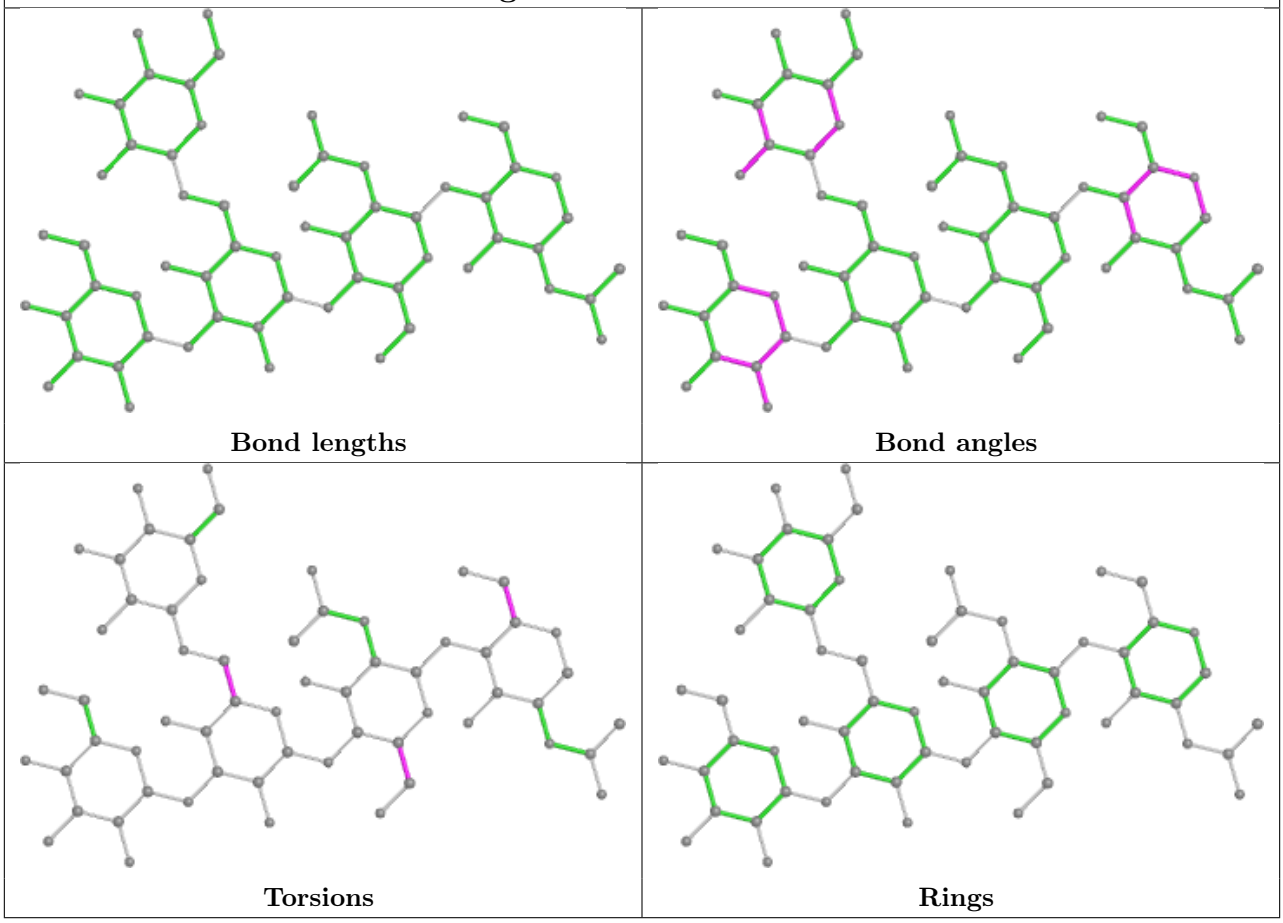
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain G

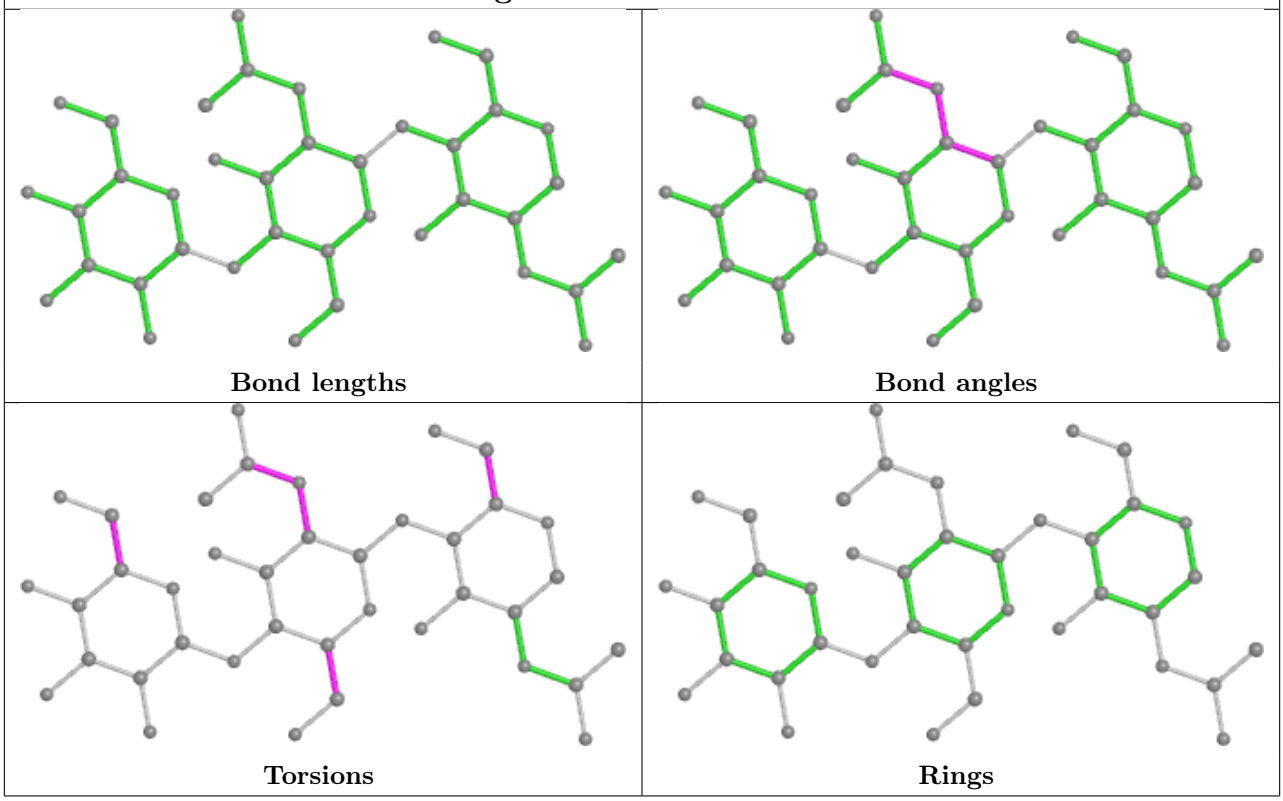


Oligosaccharide Chain I	
 Bond lengths	 Bond angles
 Torsions	 Rings

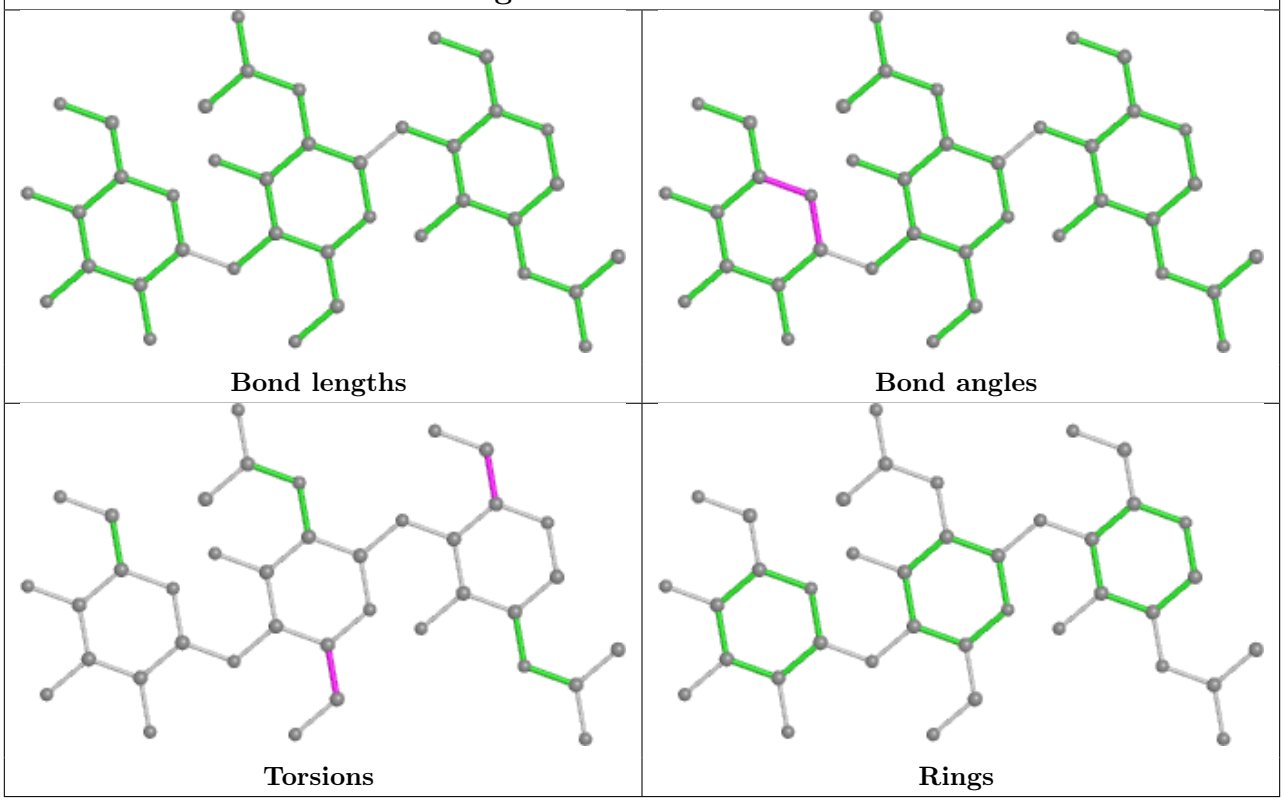
Oligosaccharide Chain J



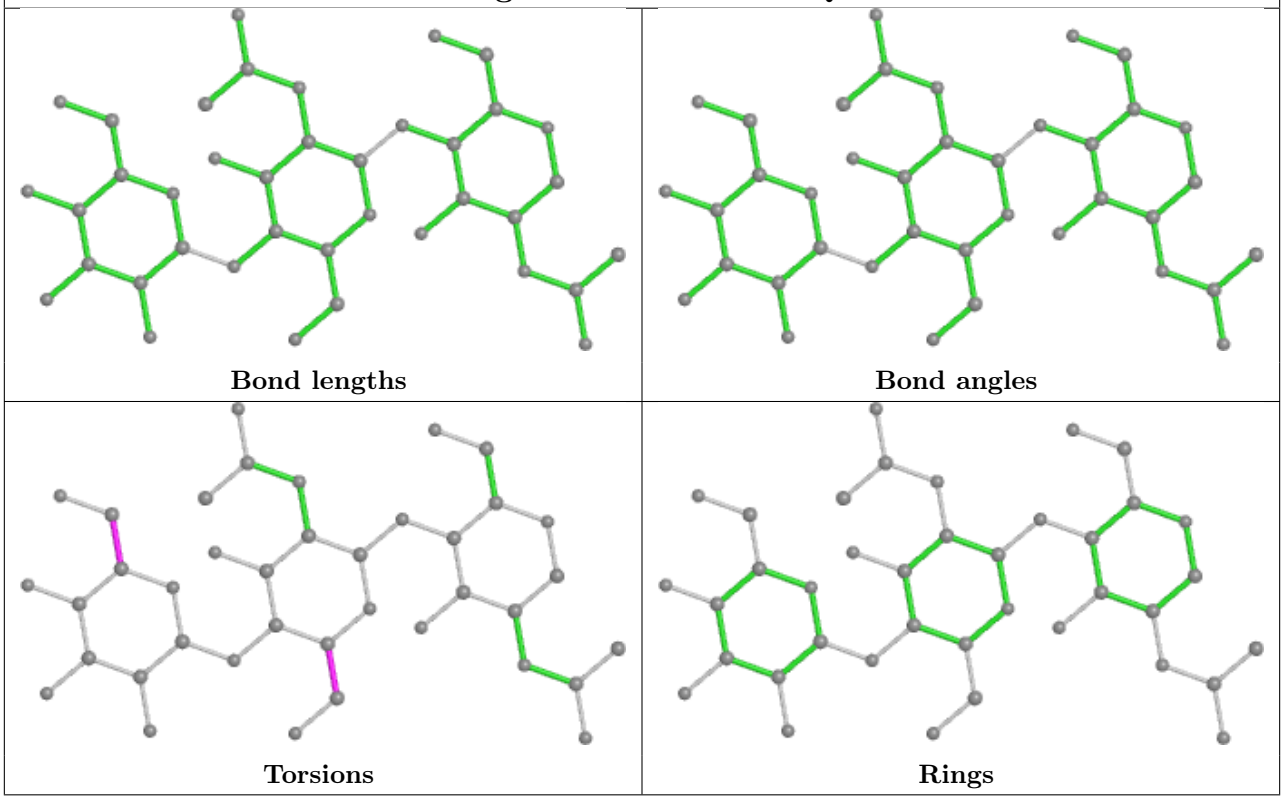
Oligosaccharide Chain K



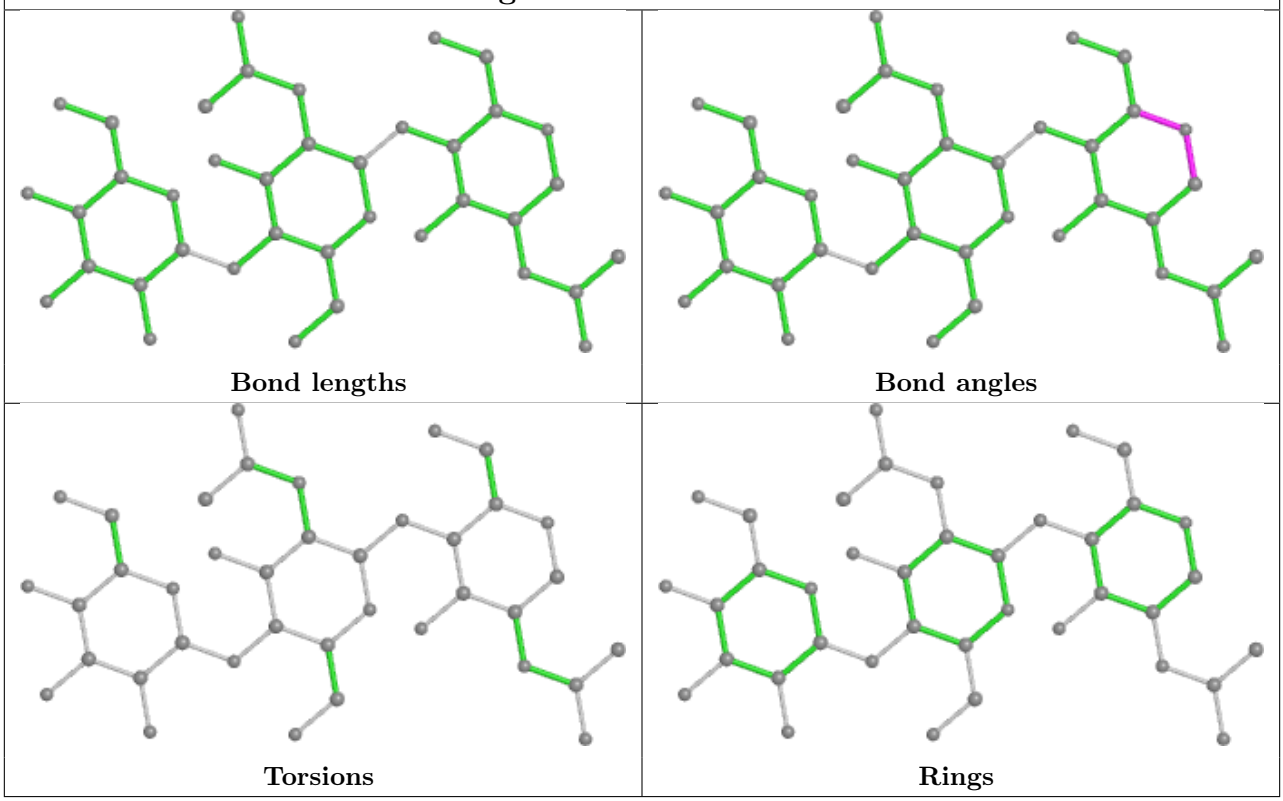
Oligosaccharide Chain N



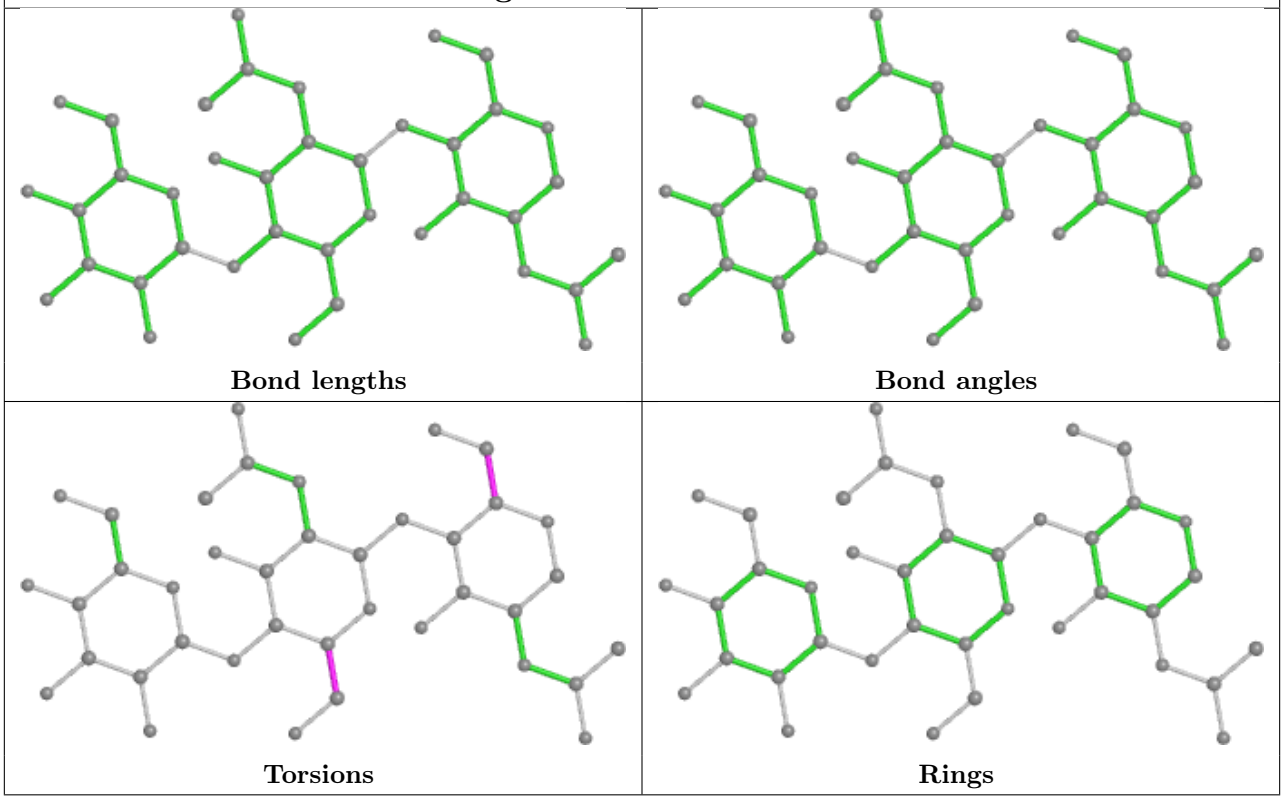
Oligosaccharide Chain Q



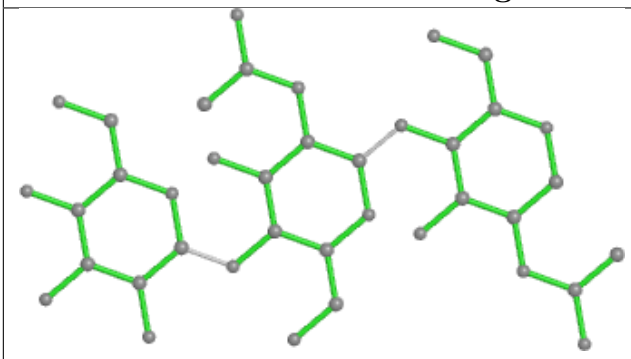
Oligosaccharide Chain S



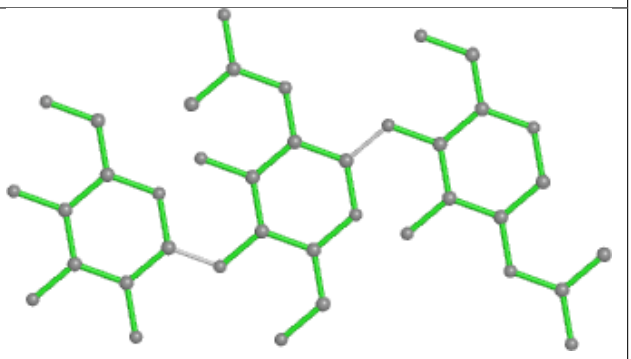
Oligosaccharide Chain V



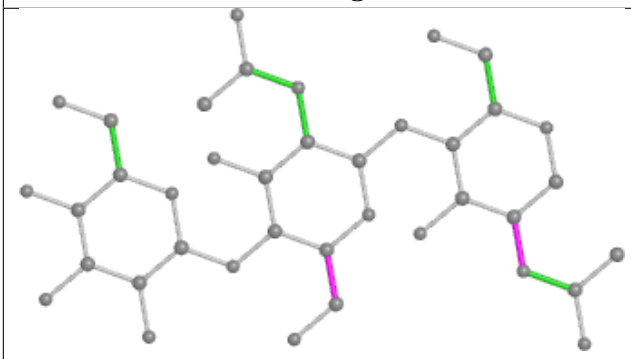
Oligosaccharide Chain X



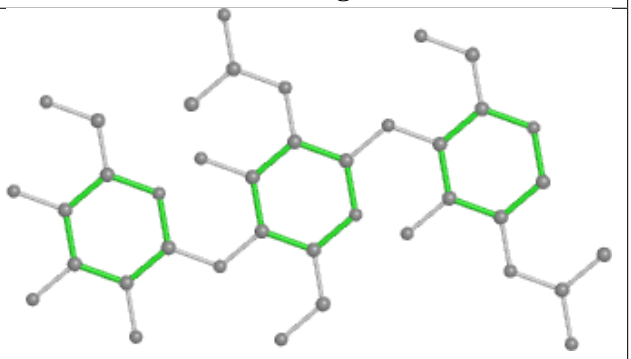
Bond lengths



Bond angles

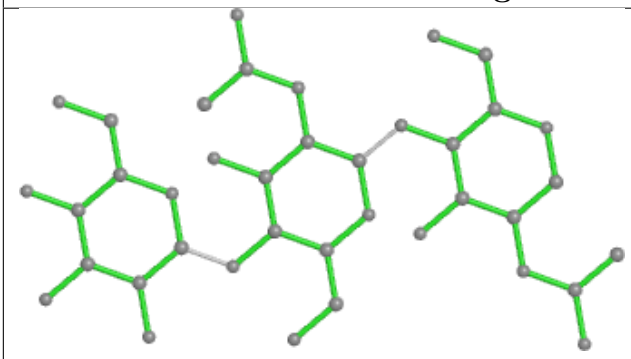


Torsions



Rings

Oligosaccharide Chain Y



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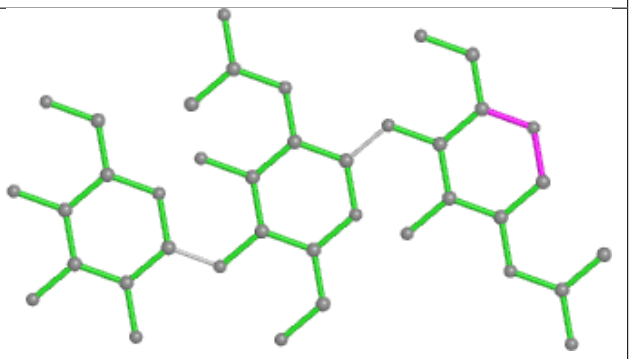
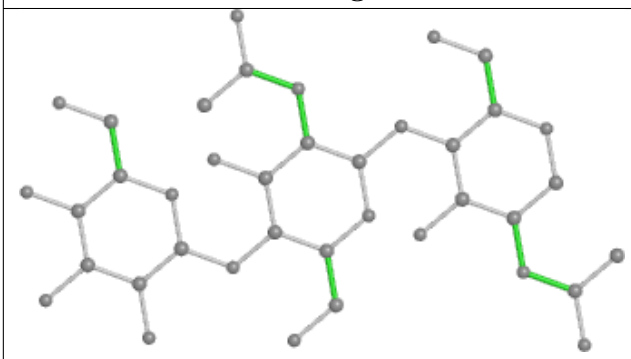


Bond angles



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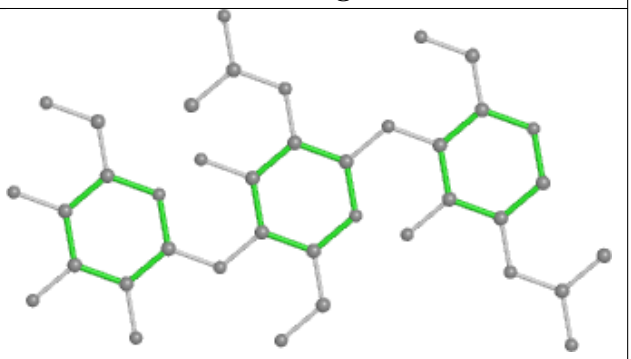
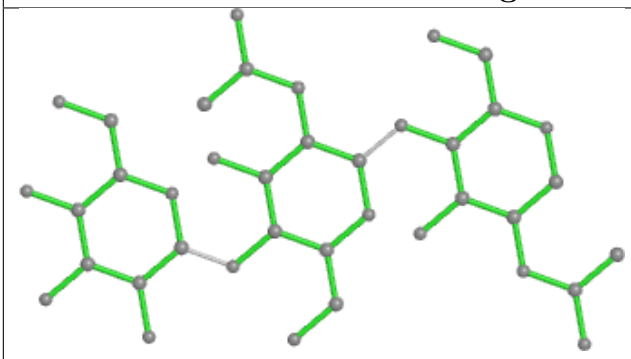


Rings

Oligosaccharide Chain c



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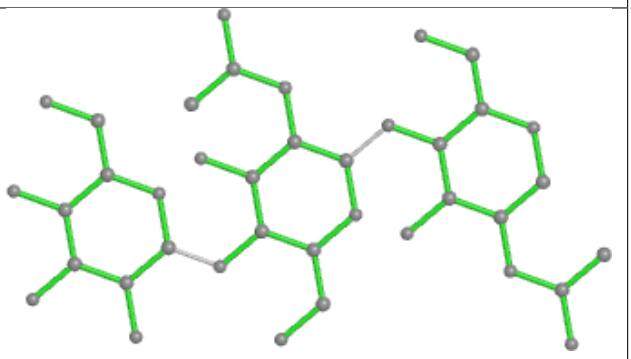
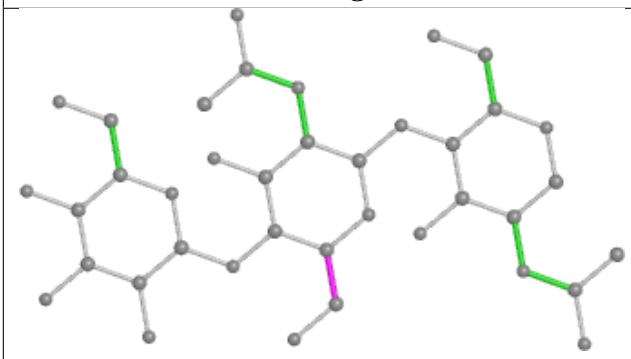


Bond angles



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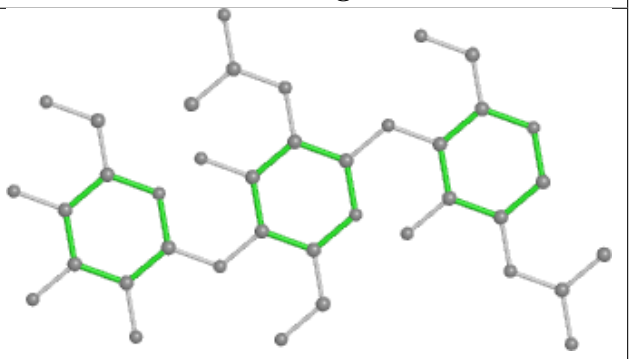
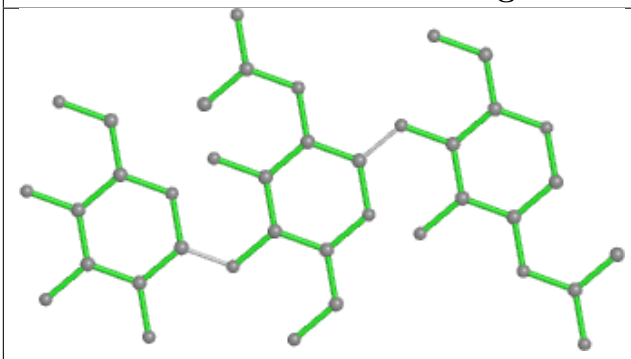


Rings

Oligosaccharide Chain d



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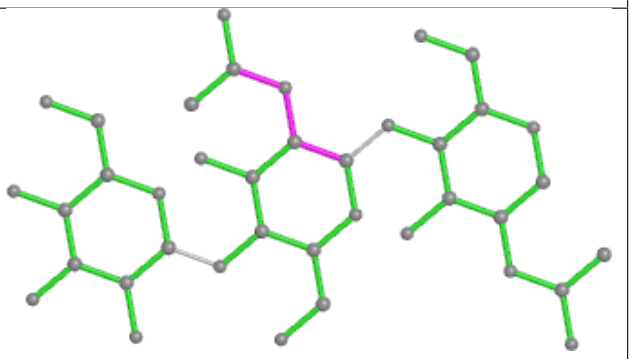

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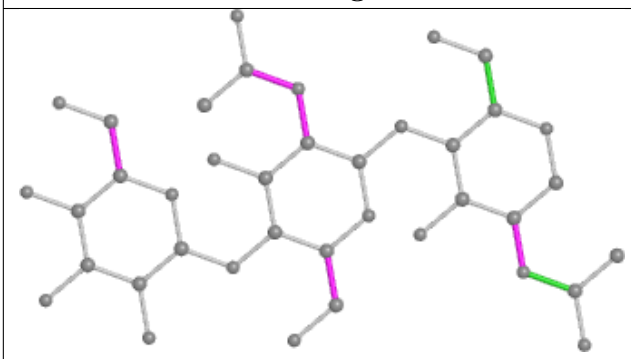

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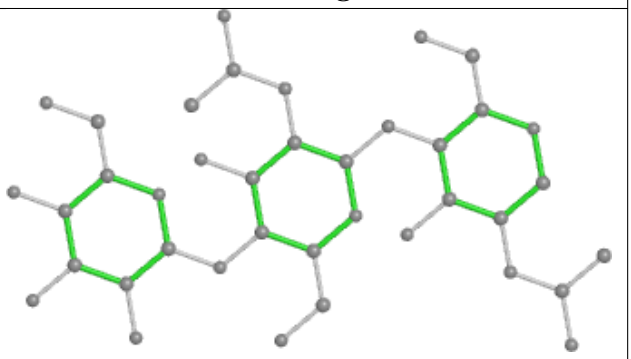
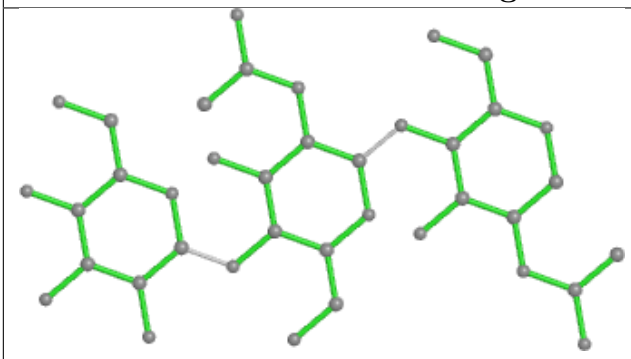


Rings

Oligosaccharide Chain e



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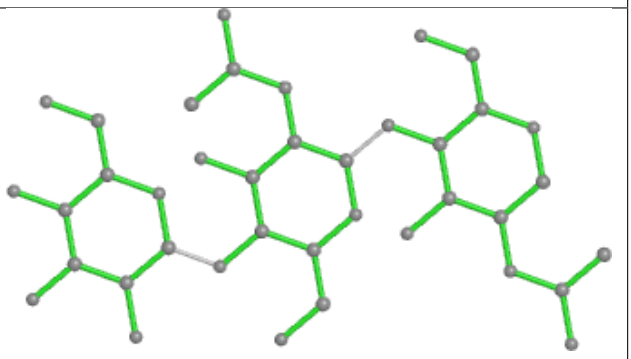
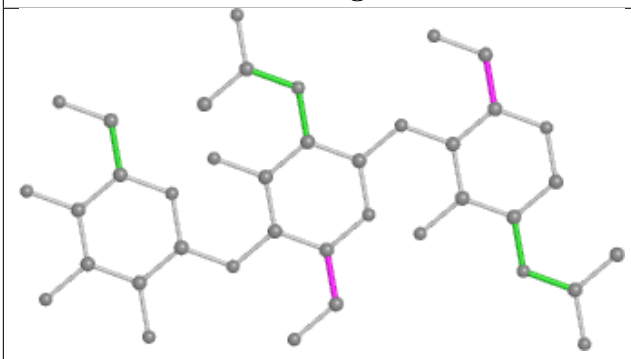


Bond angles



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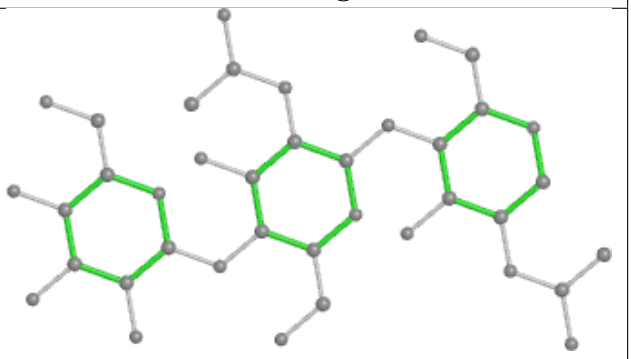
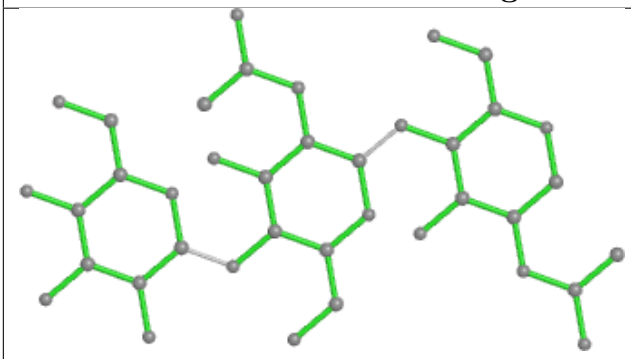


Rings

Oligosaccharide Chain f



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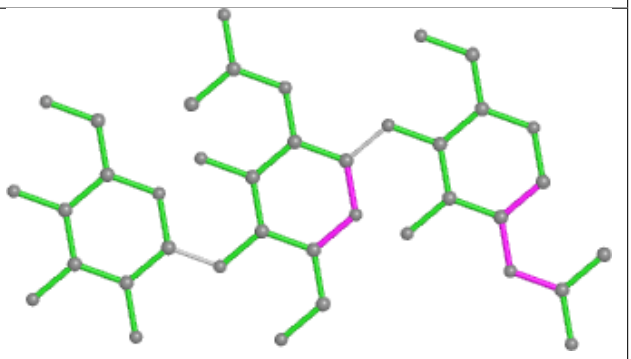
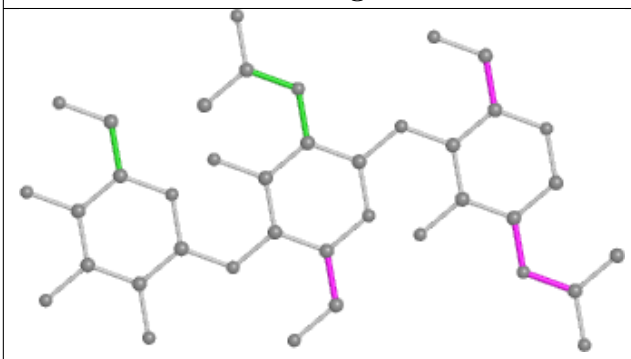


Bond angles



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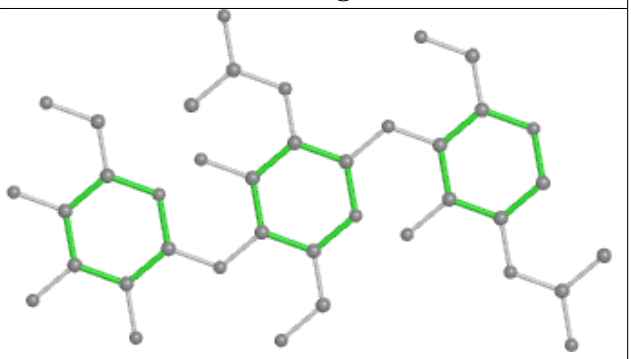
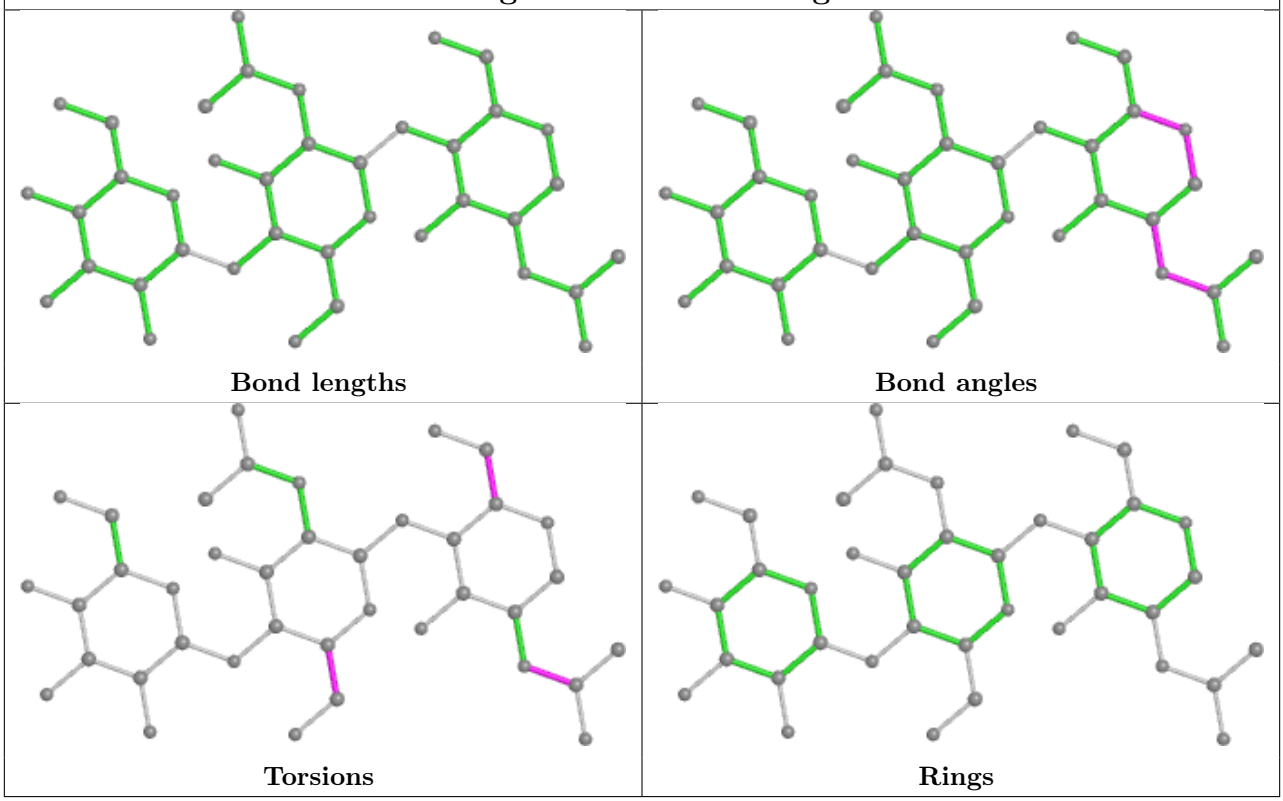
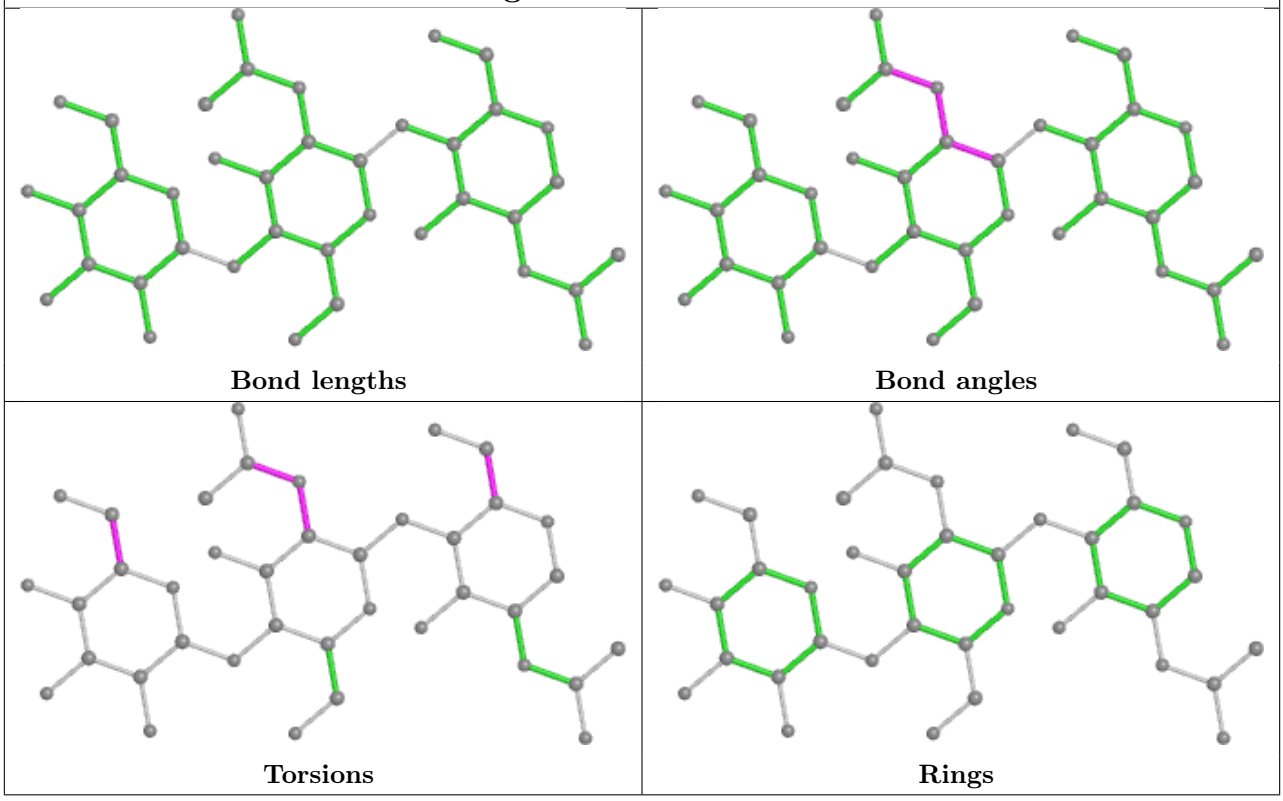


Rings

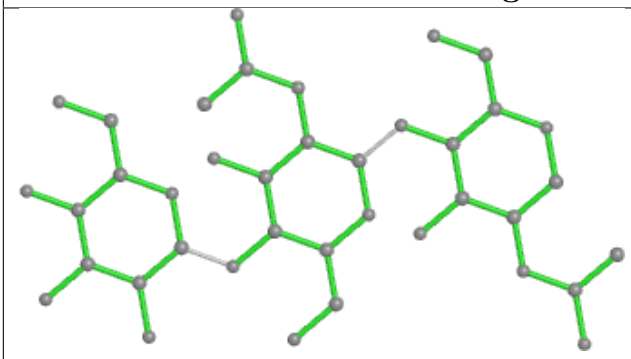
Oligosaccharide Chain g



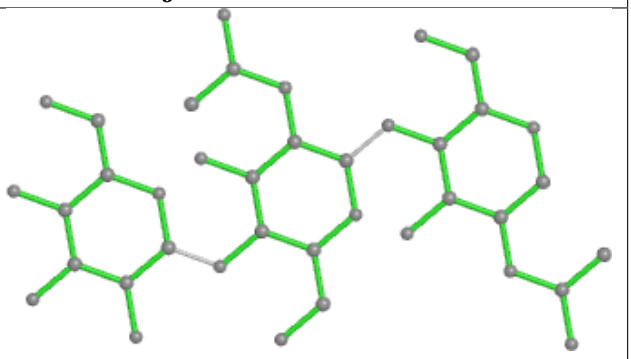
Oligosaccharide Chain i



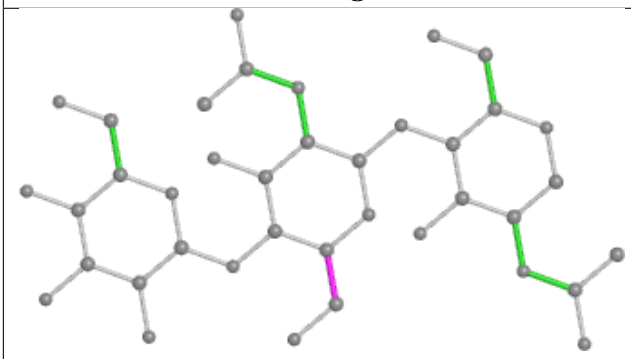
Oligosaccharide Chain j



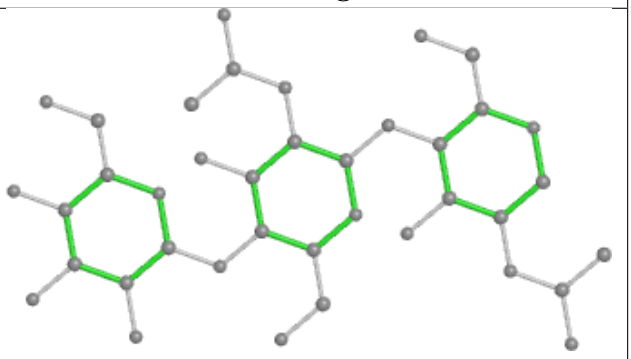
Bond lengths



Bond angles

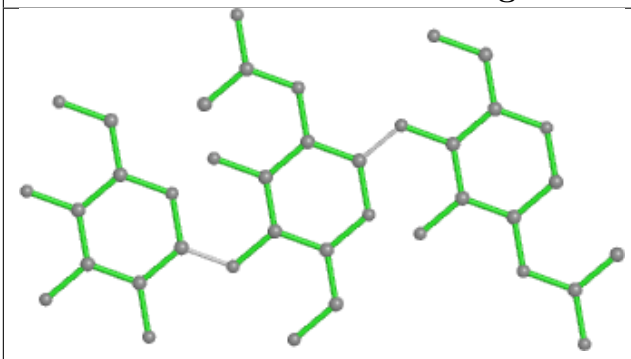


Torsions

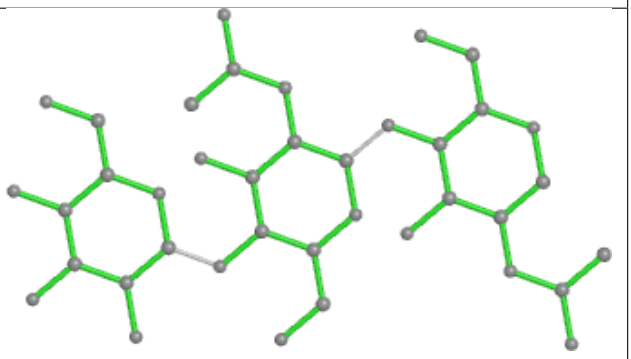


Rings

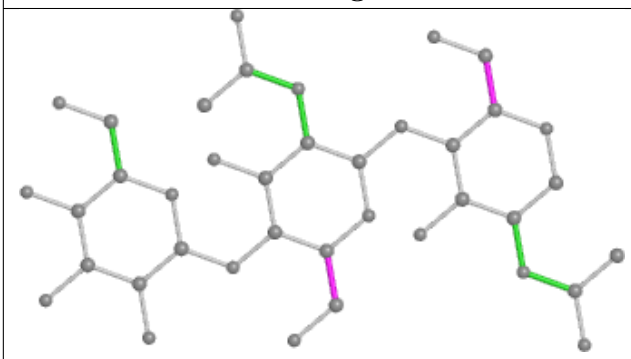
Oligosaccharide Chain k



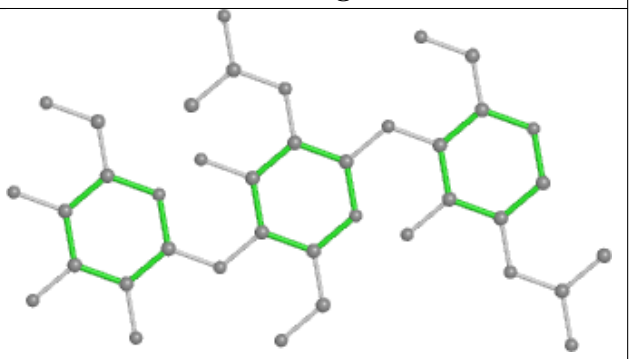
Bond lengths



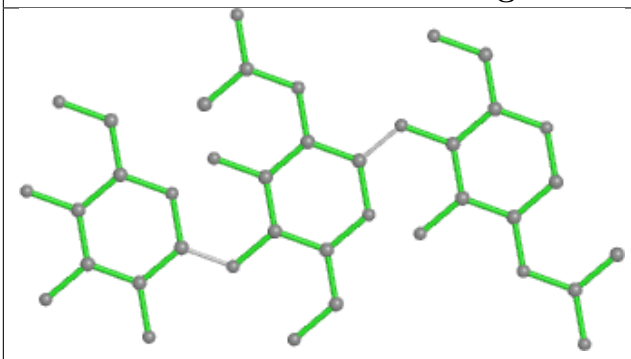
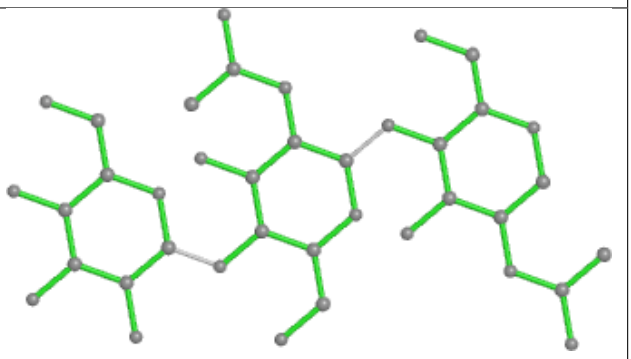
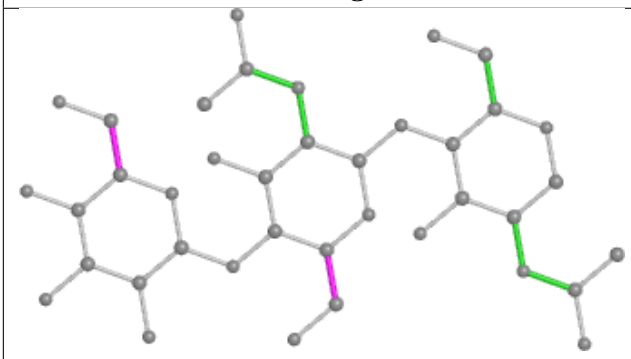
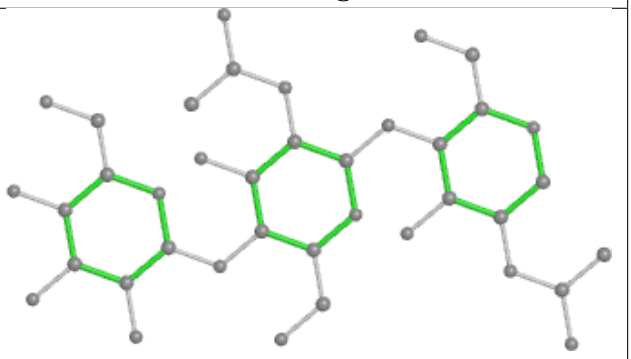
Bond angles

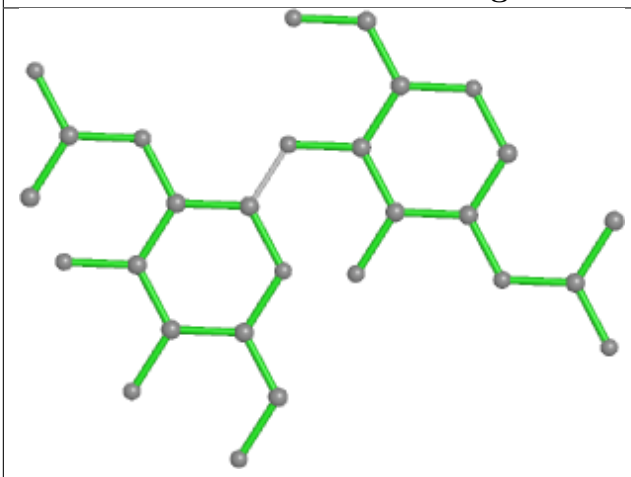
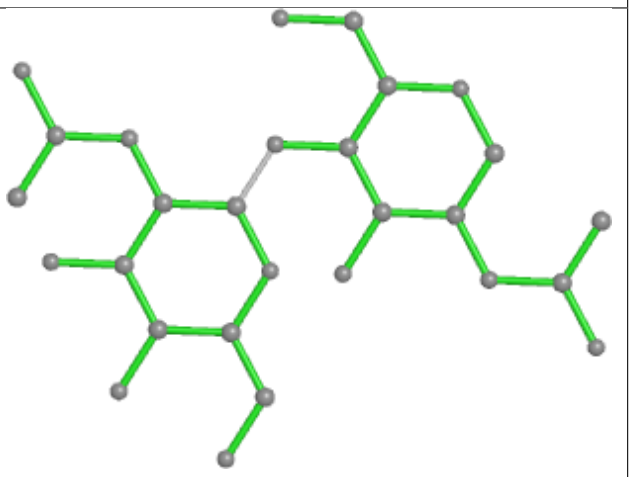
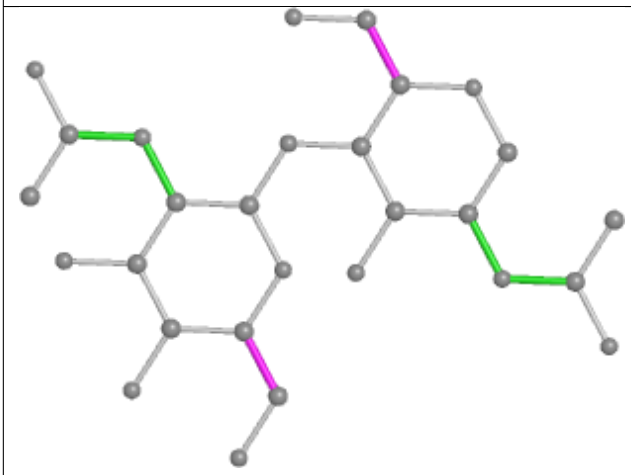
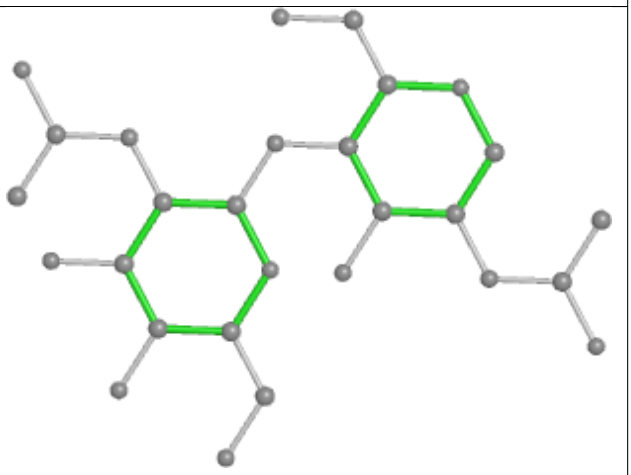


Torsions

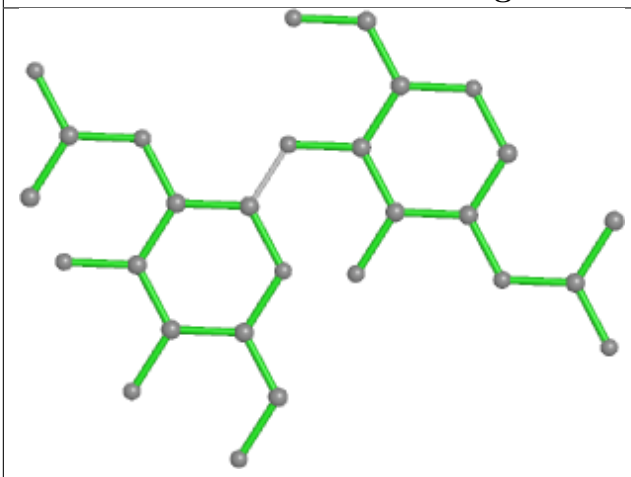


Rings

Oligosaccharide Chain n	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain O



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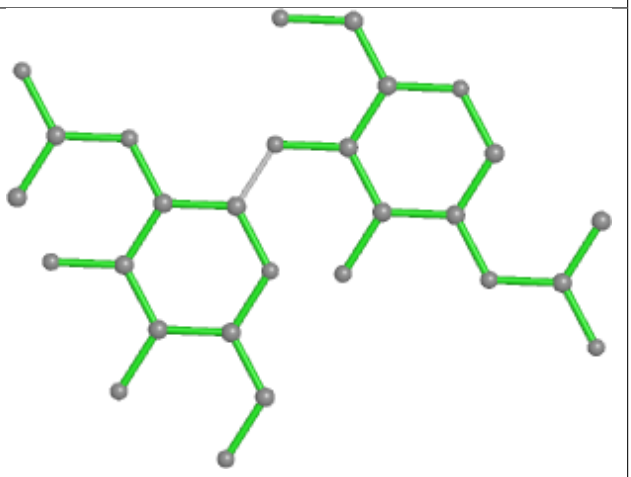
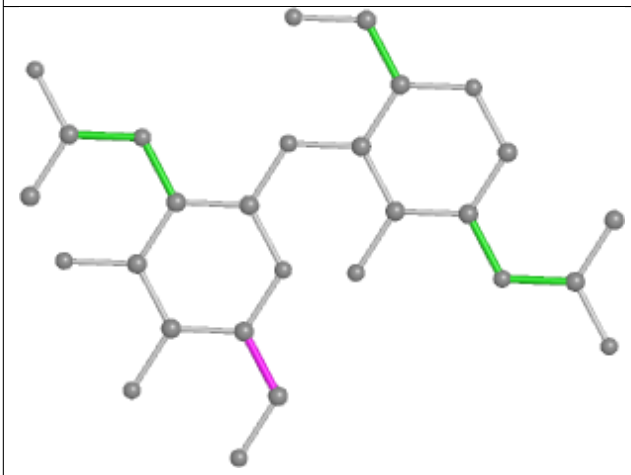


Bond angles



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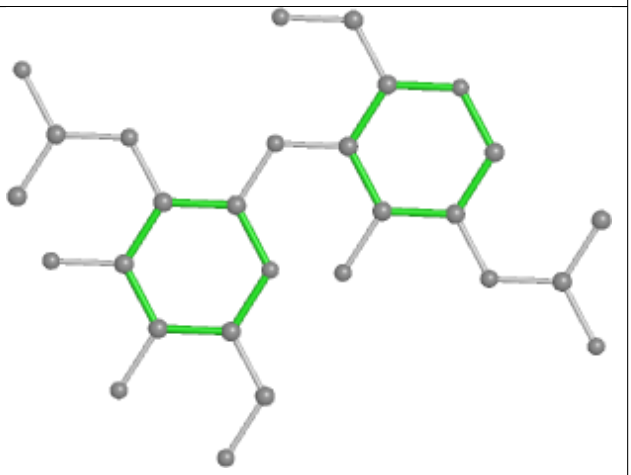

Rings

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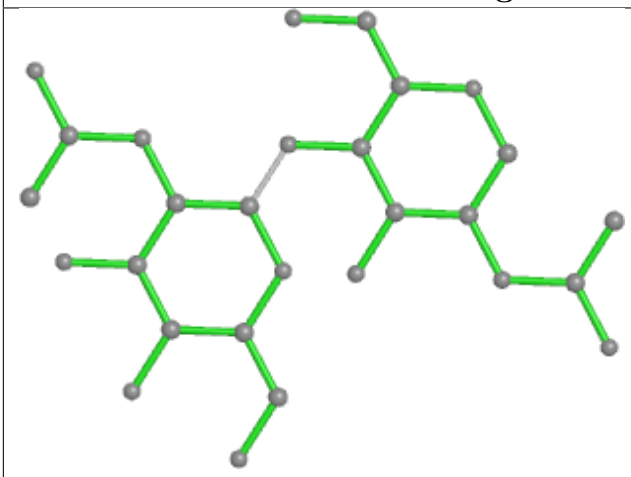
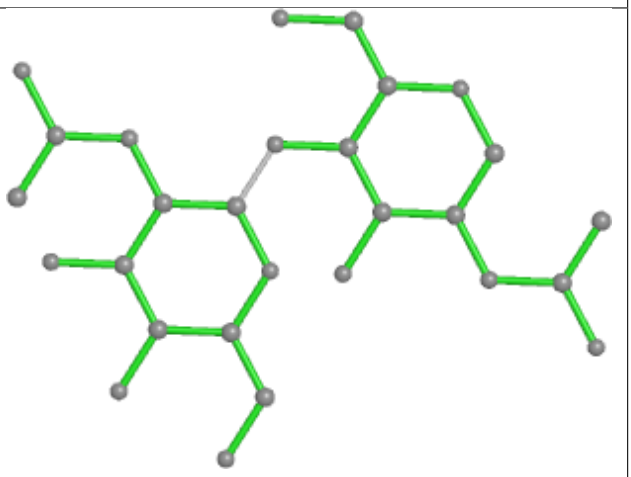
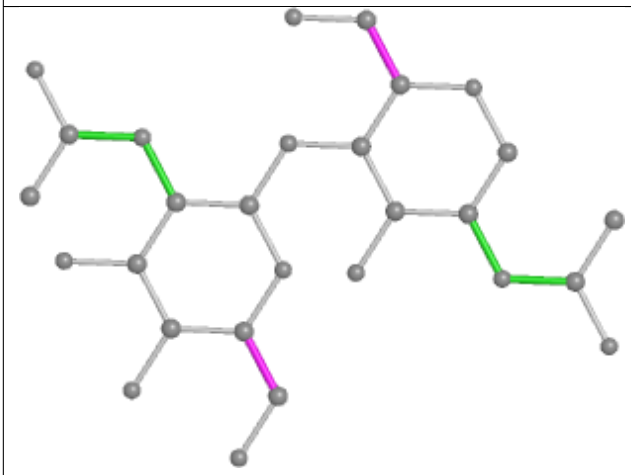
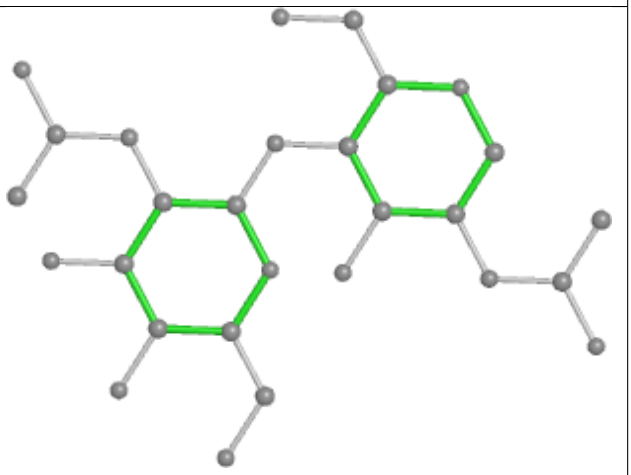
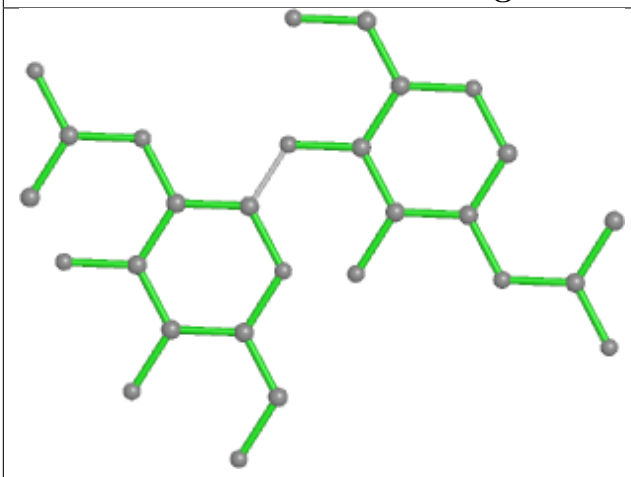
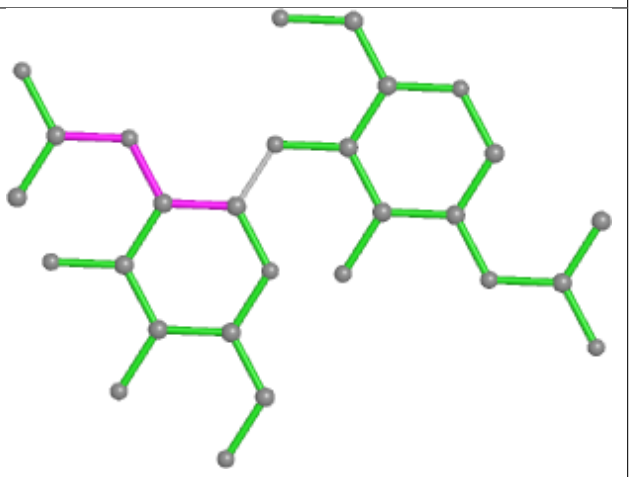
 Bond lengths	 Bond angles
 Torsions	 Rings

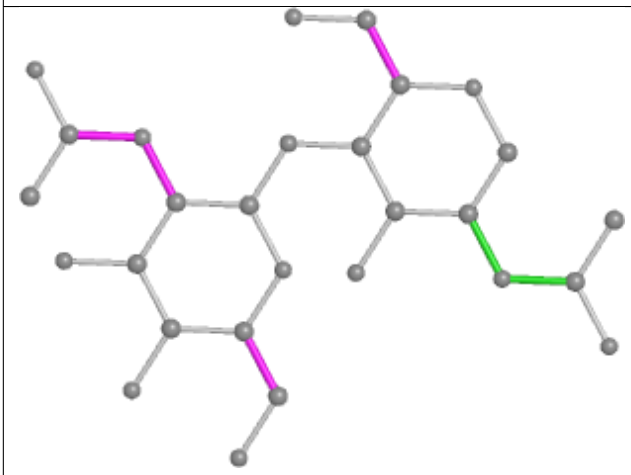
Oligosaccharide Chain R



Bond lengths



Bond angles



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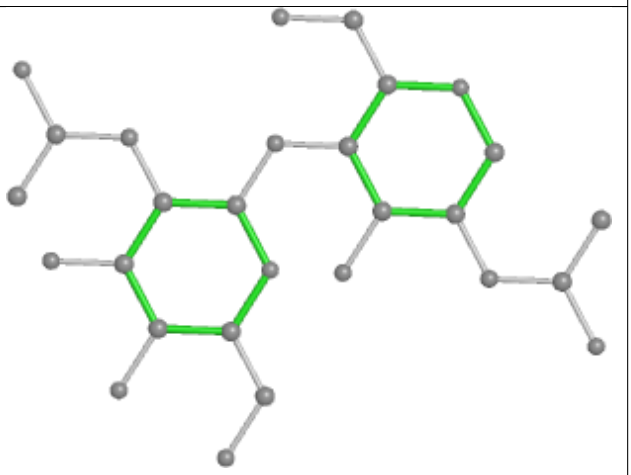
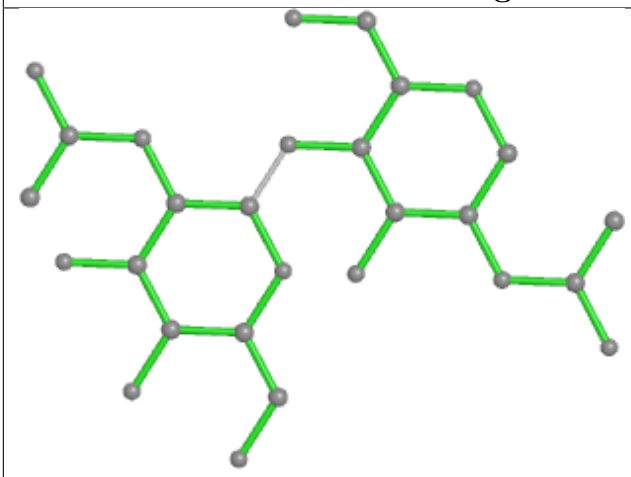


Rings

Oligosaccharide Chain U



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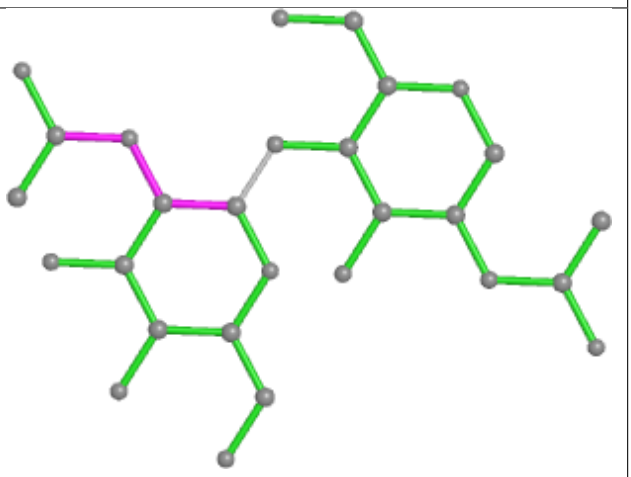

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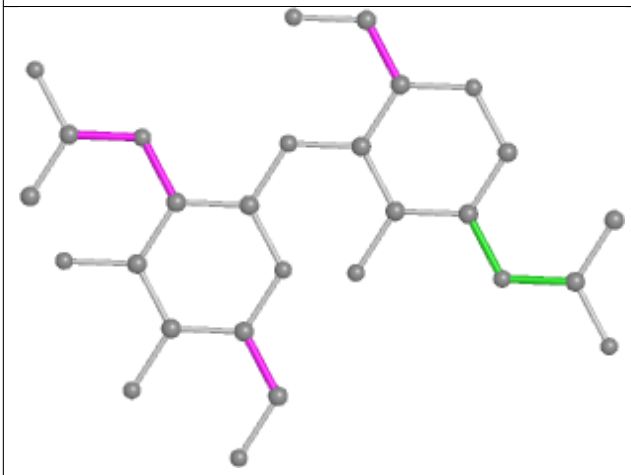

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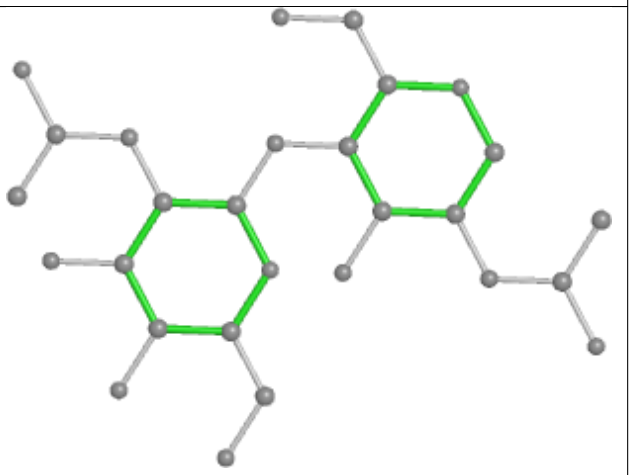
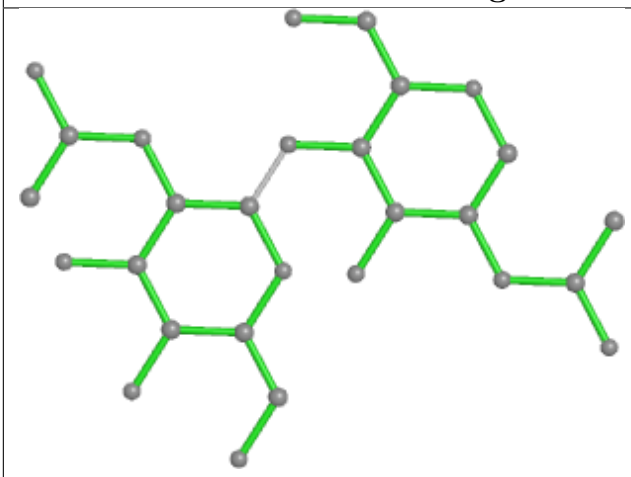
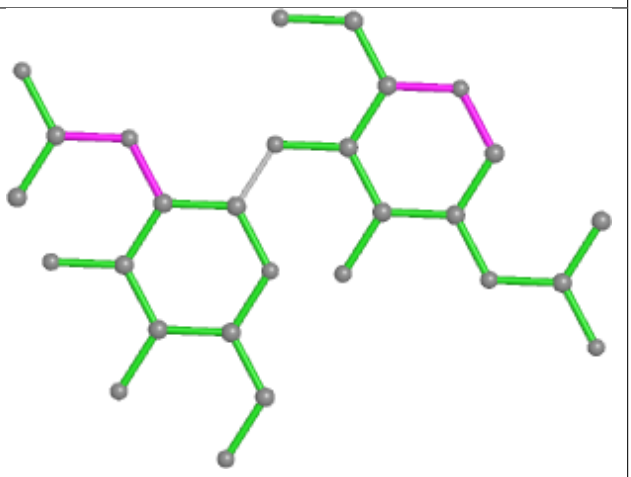


Rings

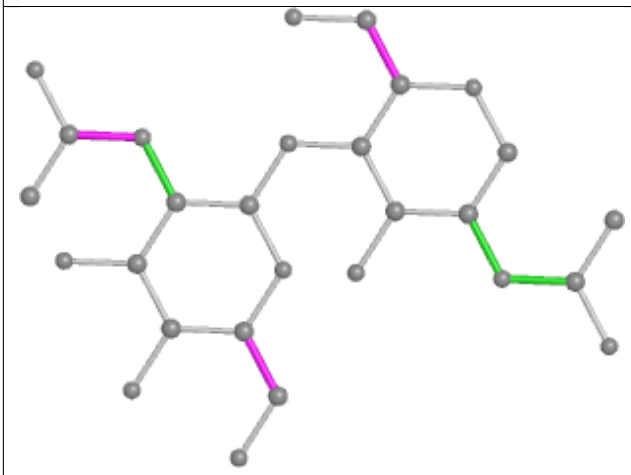
Oligosaccharide Chain W



Bond lengths



Bond angles



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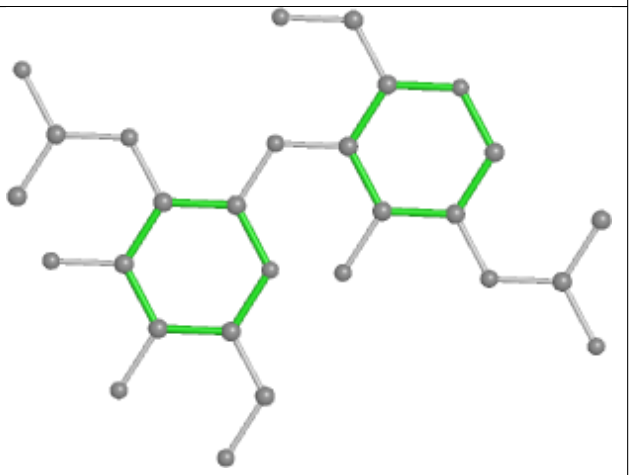
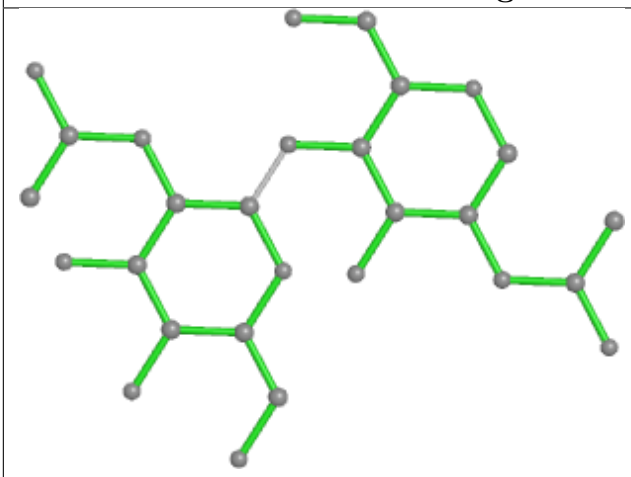


Rings

Oligosaccharide Chain Z



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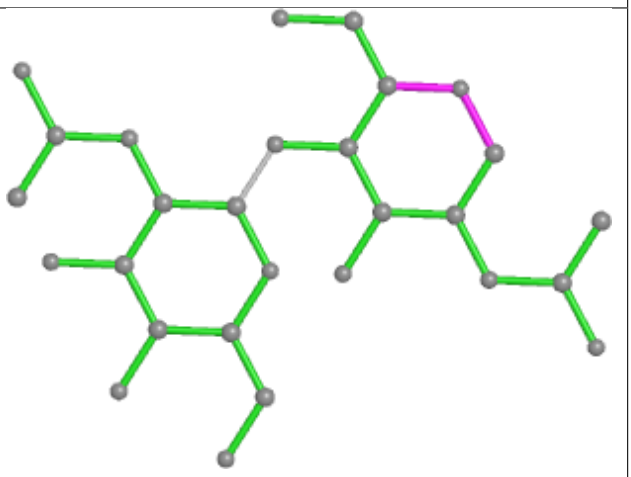
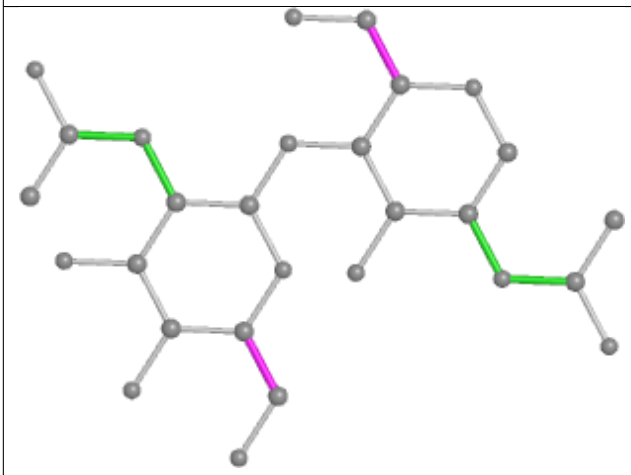


Bond angles



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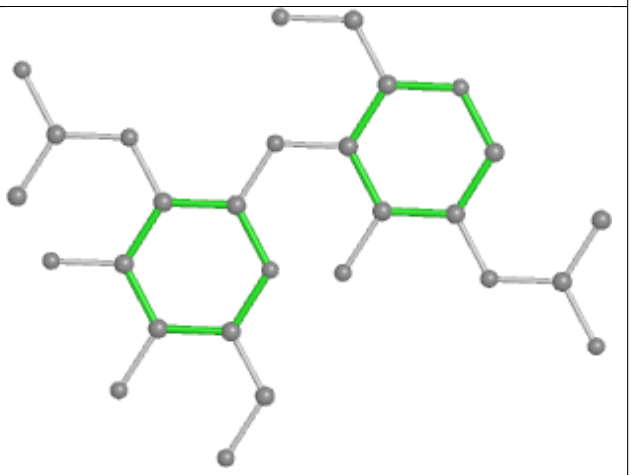
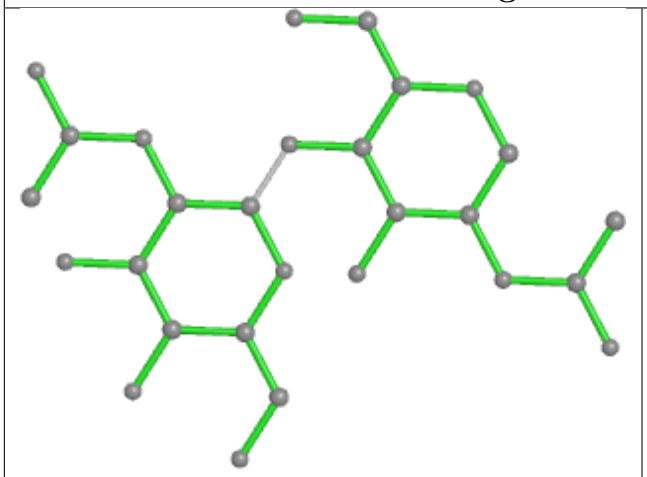


Rings

Oligosaccharide Chain b



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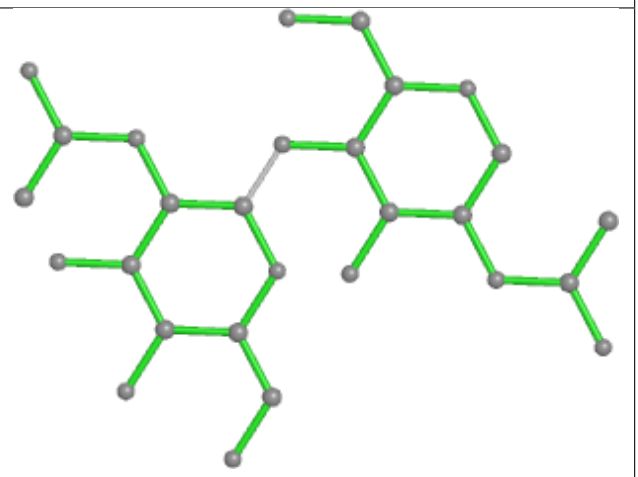

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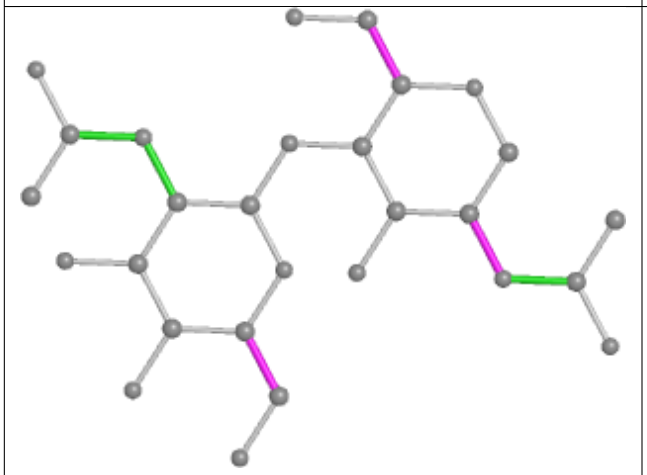

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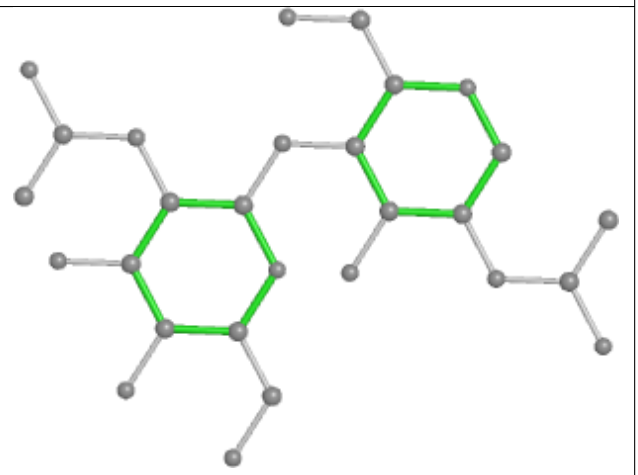
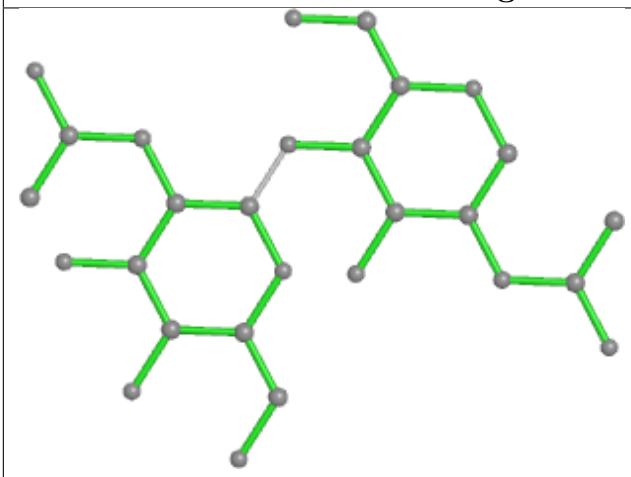
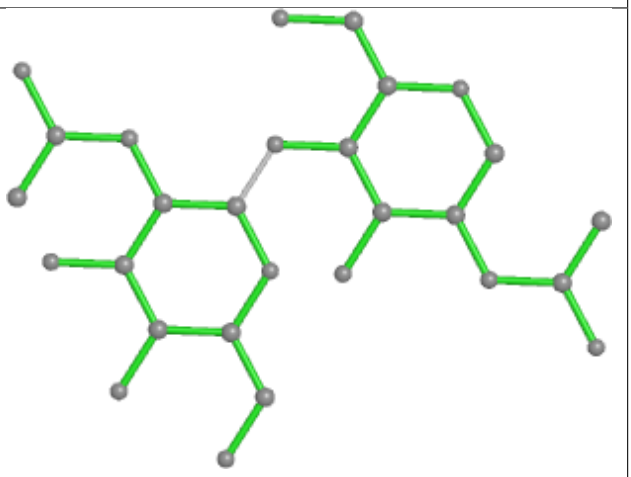
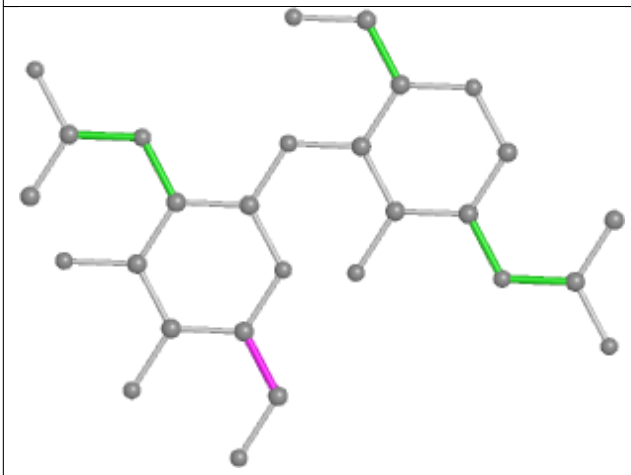
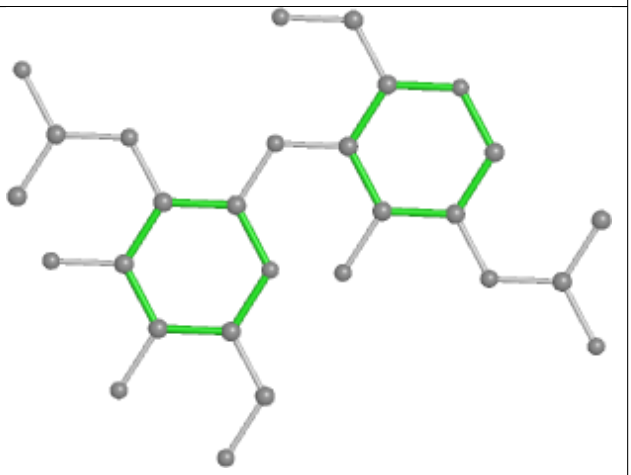
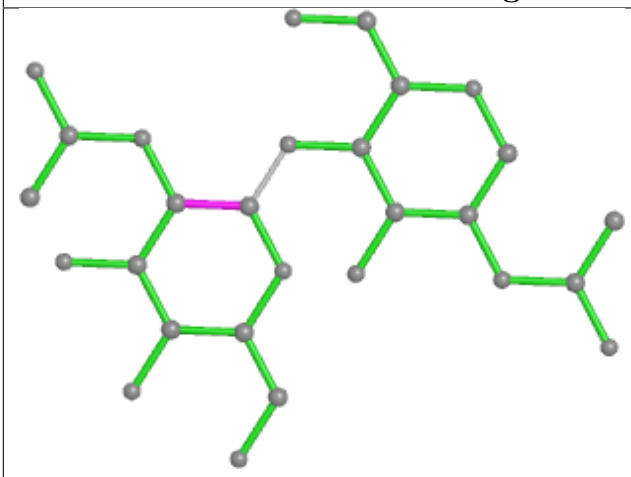


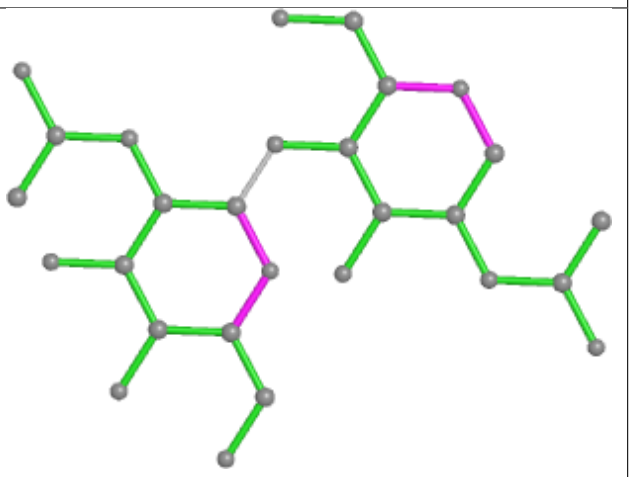
Rings

Oligosaccharide Chain h	
 Bond lengths	 Bond angles
 Torsions	 Rings

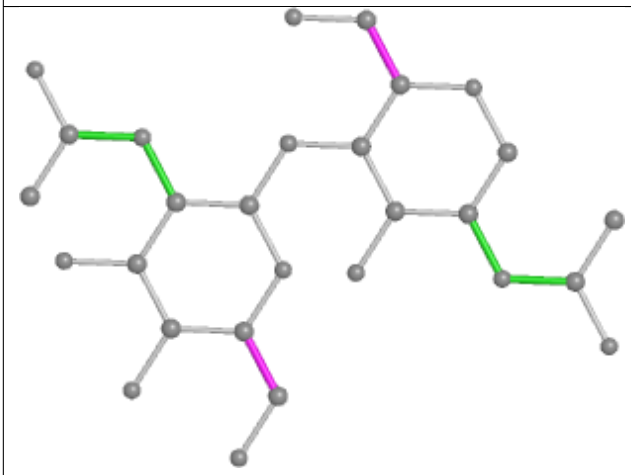
Oligosaccharide Chain l



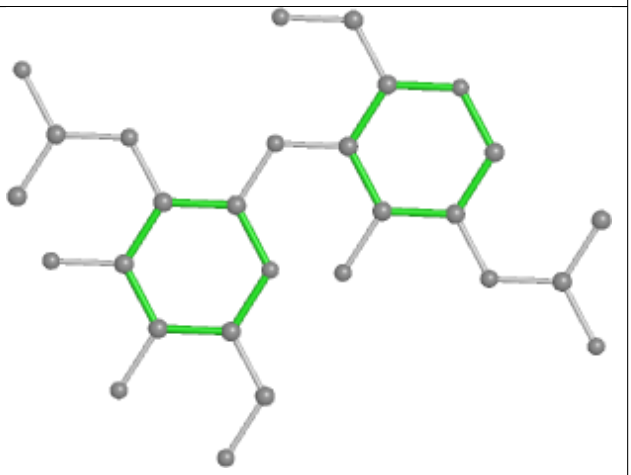
Bond lengths



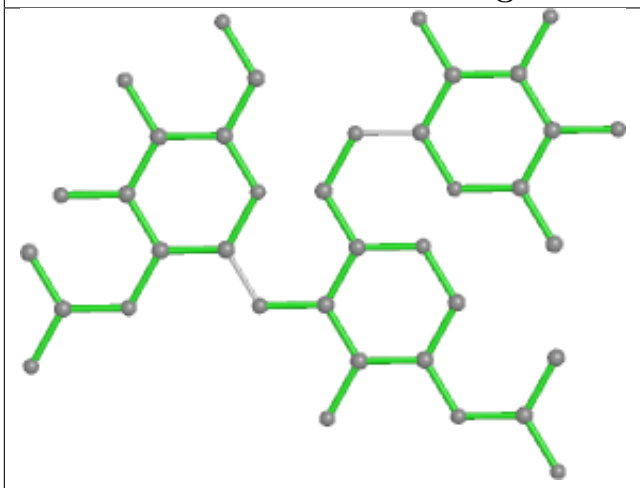
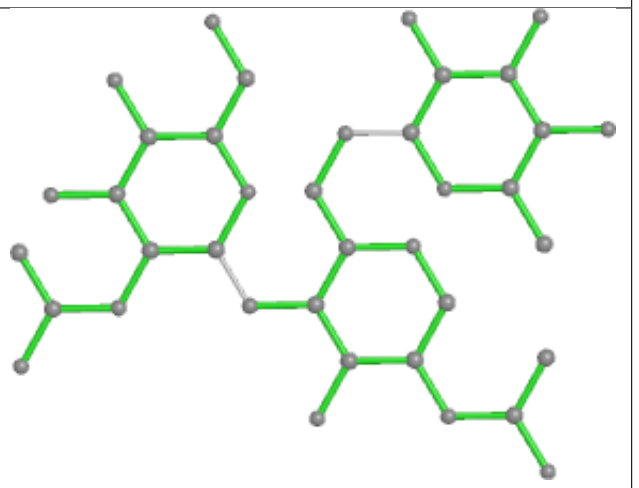
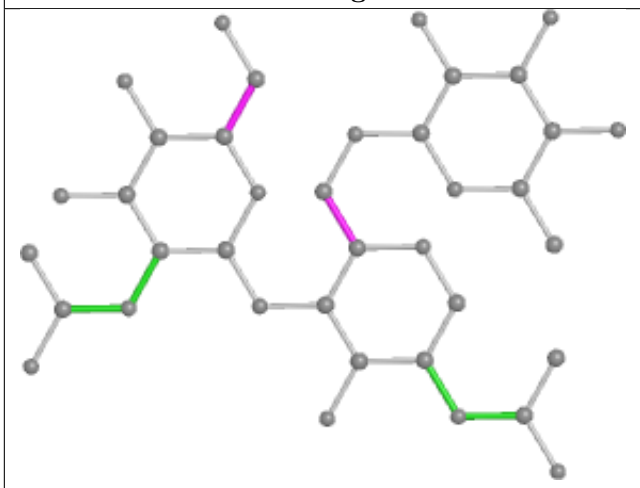
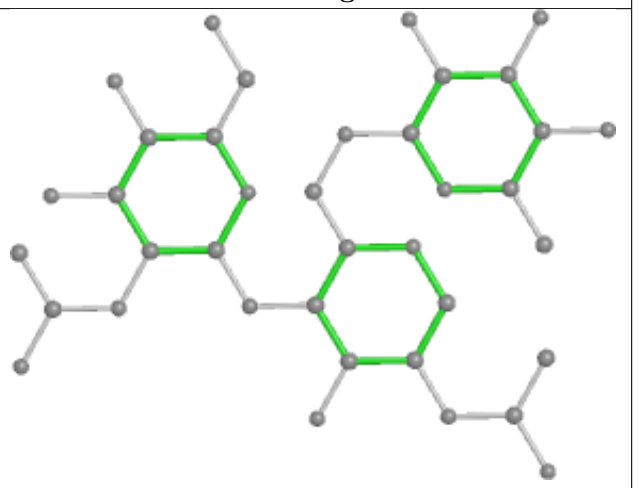
Bond angles



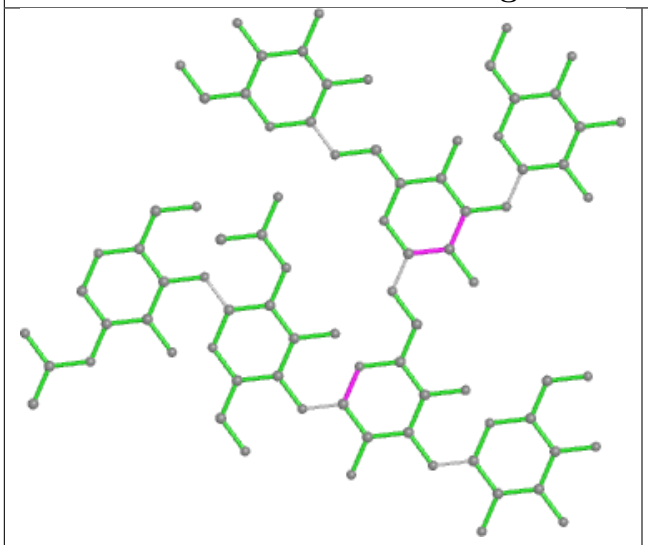
Torsions



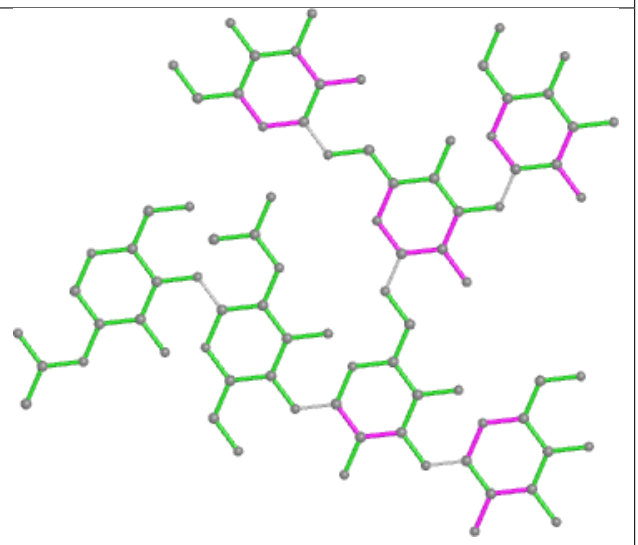
Rings

Oligosaccharide Chain T	
 Bond lengths	 Bond angles
 Torsions	 Rings

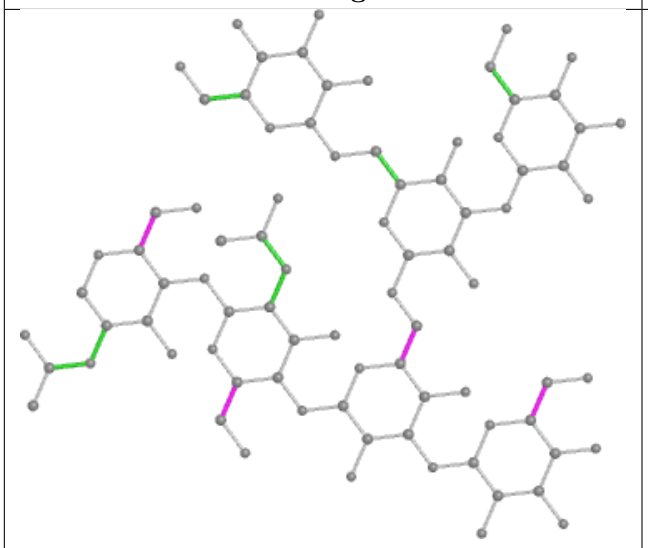
Oligosaccharide Chain a



Bond lengths



Bond angles



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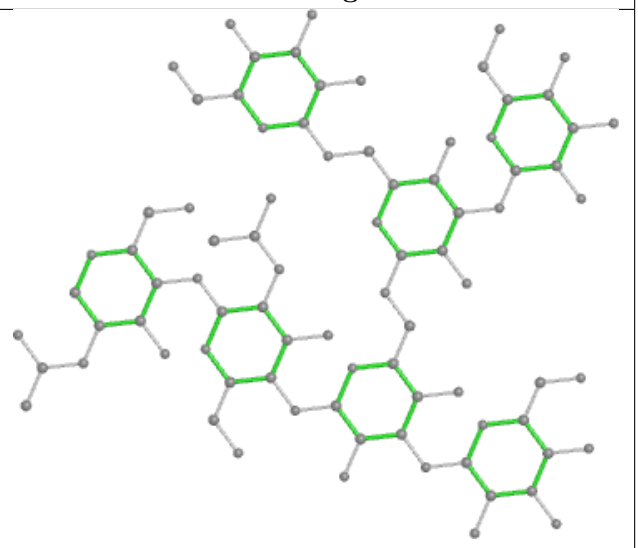
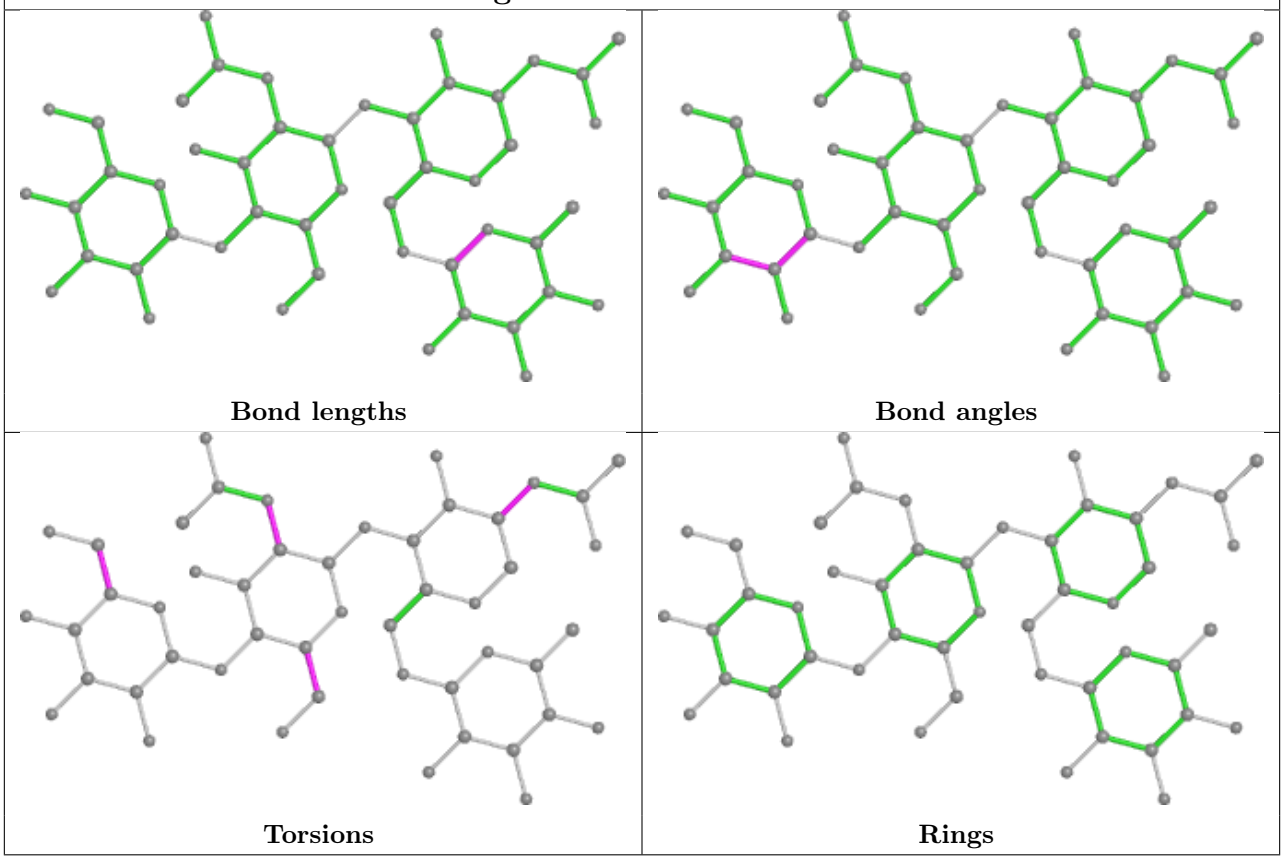


Rings

Oligosaccharide Chain m



5.6 Ligand geometry (i)

44 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	NAG	A	641	1	14,14,15	0.22	0	17,19,21	0.39	0
12	NAG	E	629	1	14,14,15	0.21	0	17,19,21	0.39	0
12	NAG	C	615	1	14,14,15	0.20	0	17,19,21	0.39	0
12	NAG	A	609	1	14,14,15	0.19	0	17,19,21	0.49	0
12	NAG	A	615	1	14,14,15	0.24	0	17,19,21	0.81	1 (5%)
12	NAG	A	640	1	14,14,15	0.21	0	17,19,21	0.82	1 (5%)
12	NAG	D	901	2	14,14,15	0.23	0	17,19,21	0.40	0
12	NAG	E	654	1	14,14,15	0.23	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	NAG	E	630	1	14,14,15	0.22	0	17,19,21	0.78	1 (5%)
12	NAG	B	903	2	14,14,15	0.20	0	17,19,21	0.72	1 (5%)
12	NAG	E	634	1	14,14,15	0.20	0	17,19,21	0.78	1 (5%)
12	NAG	C	618	1	14,14,15	0.20	0	17,19,21	0.42	0
12	NAG	C	602	1	14,14,15	0.24	0	17,19,21	0.43	0
12	NAG	A	621	1	14,14,15	0.25	0	17,19,21	0.41	0
12	NAG	F	902	2	14,14,15	0.60	0	17,19,21	0.55	0
12	NAG	E	625	1	14,14,15	0.20	0	17,19,21	0.39	0
12	NAG	C	620	1	14,14,15	0.29	0	17,19,21	1.10	2 (11%)
12	NAG	C	622	1	14,14,15	0.40	0	17,19,21	1.53	2 (11%)
12	NAG	C	614	1	14,14,15	0.34	0	17,19,21	0.44	0
12	NAG	A	639	1	14,14,15	0.17	0	17,19,21	0.52	0
12	NAG	A	601	1	14,14,15	0.91	1 (7%)	17,19,21	1.72	2 (11%)
12	NAG	C	627	1	14,14,15	0.19	0	17,19,21	0.45	0
12	NAG	C	621	1	14,14,15	0.20	0	17,19,21	0.73	1 (5%)
12	NAG	A	626	1	14,14,15	0.22	0	17,19,21	0.40	0
12	NAG	C	630	1	14,14,15	0.20	0	17,19,21	0.76	1 (5%)
12	NAG	A	629	1	14,14,15	0.22	0	17,19,21	0.76	1 (5%)
12	NAG	A	638	1	14,14,15	0.31	0	17,19,21	0.40	0
12	NAG	A	622	1	14,14,15	0.18	0	17,19,21	0.46	0
12	NAG	C	619	1	14,14,15	0.26	0	17,19,21	0.75	1 (5%)
12	NAG	E	653	1	14,14,15	0.22	0	17,19,21	0.77	1 (5%)
12	NAG	A	631	1	14,14,15	0.21	0	17,19,21	0.82	1 (5%)
12	NAG	A	628	1	14,14,15	0.28	0	17,19,21	1.10	2 (11%)
12	NAG	C	623	1	14,14,15	0.22	0	17,19,21	0.83	1 (5%)
12	NAG	C	601	1	14,14,15	0.32	0	17,19,21	1.57	2 (11%)
12	NAG	A	637	1	14,14,15	0.27	0	17,19,21	0.49	0
12	NAG	E	646	1	14,14,15	0.27	0	17,19,21	0.45	0
12	NAG	A	608	1	14,14,15	0.23	0	17,19,21	0.46	0
12	NAG	E	619	1	14,14,15	0.25	0	17,19,21	0.40	0
12	NAG	F	901	2	14,14,15	0.21	0	17,19,21	0.40	0
12	NAG	C	629	1	14,14,15	0.20	0	17,19,21	0.41	0
12	NAG	A	630	1	14,14,15	0.41	0	17,19,21	1.53	2 (11%)
12	NAG	E	601	1	14,14,15	0.75	1 (7%)	17,19,21	1.68	3 (17%)
12	NAG	A	627	1	14,14,15	0.23	0	17,19,21	0.74	1 (5%)
12	NAG	C	628	1	14,14,15	0.25	0	17,19,21	0.44	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
12	NAG	A	641	1	-	0/6/23/26	0/1/1/1
12	NAG	E	629	1	-	2/6/23/26	0/1/1/1
12	NAG	C	615	1	-	2/6/23/26	0/1/1/1
12	NAG	A	609	1	-	2/6/23/26	0/1/1/1
12	NAG	A	615	1	-	4/6/23/26	0/1/1/1
12	NAG	A	640	1	-	4/6/23/26	0/1/1/1
12	NAG	D	901	2	-	0/6/23/26	0/1/1/1
12	NAG	E	654	1	-	2/6/23/26	0/1/1/1
12	NAG	E	630	1	-	3/6/23/26	0/1/1/1
12	NAG	B	903	2	-	2/6/23/26	0/1/1/1
12	NAG	E	634	1	-	4/6/23/26	0/1/1/1
12	NAG	C	618	1	-	2/6/23/26	0/1/1/1
12	NAG	C	602	1	-	2/6/23/26	0/1/1/1
12	NAG	A	621	1	-	2/6/23/26	0/1/1/1
12	NAG	F	902	2	-	4/6/23/26	0/1/1/1
12	NAG	E	625	1	-	2/6/23/26	0/1/1/1
12	NAG	C	620	1	-	2/6/23/26	0/1/1/1
12	NAG	C	622	1	-	5/6/23/26	0/1/1/1
12	NAG	C	614	1	-	0/6/23/26	0/1/1/1
12	NAG	A	639	1	-	1/6/23/26	0/1/1/1
12	NAG	A	601	1	-	3/6/23/26	0/1/1/1
12	NAG	C	627	1	-	2/6/23/26	0/1/1/1
12	NAG	C	621	1	-	4/6/23/26	0/1/1/1
12	NAG	A	626	1	-	2/6/23/26	0/1/1/1
12	NAG	C	630	1	-	2/6/23/26	0/1/1/1
12	NAG	A	629	1	-	4/6/23/26	0/1/1/1
12	NAG	A	638	1	-	3/6/23/26	0/1/1/1
12	NAG	A	622	1	-	2/6/23/26	0/1/1/1
12	NAG	C	619	1	-	4/6/23/26	0/1/1/1
12	NAG	E	653	1	-	4/6/23/26	0/1/1/1
12	NAG	A	631	1	-	2/6/23/26	0/1/1/1
12	NAG	A	628	1	-	2/6/23/26	0/1/1/1
12	NAG	C	623	1	-	4/6/23/26	0/1/1/1
12	NAG	C	601	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	A	637	1	-	2/6/23/26	0/1/1/1
12	NAG	E	646	1	-	2/6/23/26	0/1/1/1
12	NAG	A	608	1	-	0/6/23/26	0/1/1/1
12	NAG	E	619	1	-	0/6/23/26	0/1/1/1
12	NAG	F	901	2	-	2/6/23/26	0/1/1/1
12	NAG	C	629	1	-	2/6/23/26	0/1/1/1
12	NAG	A	630	1	-	5/6/23/26	0/1/1/1
12	NAG	E	601	1	-	4/6/23/26	0/1/1/1
12	NAG	A	627	1	-	4/6/23/26	0/1/1/1
12	NAG	C	628	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	601	NAG	O5-C1	2.88	1.48	1.43
12	E	601	NAG	O5-C1	2.18	1.47	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	622	NAG	C2-N2-C7	5.10	130.17	122.90
12	C	601	NAG	C2-N2-C7	4.95	129.95	122.90
12	A	630	NAG	C2-N2-C7	4.91	129.90	122.90
12	A	601	NAG	C2-N2-C7	4.54	129.37	122.90
12	E	601	NAG	C1-O5-C5	4.53	118.33	112.19
12	A	601	NAG	C1-O5-C5	4.47	118.24	112.19
12	E	601	NAG	C2-N2-C7	4.24	128.94	122.90
12	A	630	NAG	C1-C2-N2	3.18	115.92	110.49
12	A	628	NAG	C1-O5-C5	3.13	116.43	112.19
12	C	601	NAG	C1-C2-N2	3.13	115.83	110.49
12	C	620	NAG	C1-O5-C5	3.11	116.41	112.19
12	A	631	NAG	C2-N2-C7	2.83	126.93	122.90
12	A	615	NAG	C2-N2-C7	2.80	126.89	122.90
12	A	640	NAG	C2-N2-C7	2.80	126.89	122.90
12	C	623	NAG	C2-N2-C7	2.66	126.68	122.90
12	A	629	NAG	C2-N2-C7	2.60	126.60	122.90
12	E	630	NAG	C2-N2-C7	2.59	126.59	122.90
12	C	619	NAG	C2-N2-C7	2.57	126.56	122.90
12	C	622	NAG	C1-C2-N2	2.55	114.84	110.49
12	A	627	NAG	C2-N2-C7	2.53	126.50	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	E	653	NAG	C2-N2-C7	2.50	126.46	122.90
12	E	634	NAG	C2-N2-C7	2.49	126.45	122.90
12	C	630	NAG	C2-N2-C7	2.48	126.43	122.90
12	B	903	NAG	C2-N2-C7	2.45	126.40	122.90
12	C	621	NAG	C2-N2-C7	2.43	126.36	122.90
12	C	620	NAG	C2-N2-C7	2.39	126.31	122.90
12	A	628	NAG	C2-N2-C7	2.28	126.15	122.90
12	E	601	NAG	C1-C2-N2	2.13	114.13	110.49

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	630	NAG	C4-C5-C6-O6
12	A	621	NAG	O5-C5-C6-O6
12	A	627	NAG	O5-C5-C6-O6
12	A	638	NAG	O5-C5-C6-O6
12	E	646	NAG	O5-C5-C6-O6
12	C	622	NAG	C4-C5-C6-O6
12	F	902	NAG	C1-C2-N2-C7
12	A	630	NAG	O5-C5-C6-O6
12	A	615	NAG	O5-C5-C6-O6
12	A	637	NAG	O5-C5-C6-O6
12	C	615	NAG	O5-C5-C6-O6
12	C	622	NAG	O5-C5-C6-O6
12	A	609	NAG	O5-C5-C6-O6
12	C	601	NAG	O5-C5-C6-O6
12	C	619	NAG	O5-C5-C6-O6
12	E	625	NAG	O5-C5-C6-O6
12	A	626	NAG	C4-C5-C6-O6
12	A	622	NAG	O5-C5-C6-O6
12	E	634	NAG	C4-C5-C6-O6
12	A	629	NAG	O5-C5-C6-O6
12	E	634	NAG	O5-C5-C6-O6
12	A	637	NAG	C4-C5-C6-O6
12	C	615	NAG	C4-C5-C6-O6
12	A	640	NAG	O5-C5-C6-O6
12	E	629	NAG	O5-C5-C6-O6
12	F	901	NAG	O5-C5-C6-O6
12	A	626	NAG	O5-C5-C6-O6
12	F	902	NAG	O5-C5-C6-O6
12	A	627	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	A	621	NAG	C4-C5-C6-O6
12	C	627	NAG	O5-C5-C6-O6
12	E	646	NAG	C4-C5-C6-O6
12	E	654	NAG	C4-C5-C6-O6
12	C	629	NAG	C4-C5-C6-O6
12	A	622	NAG	C4-C5-C6-O6
12	A	638	NAG	C4-C5-C6-O6
12	E	629	NAG	C4-C5-C6-O6
12	E	625	NAG	C4-C5-C6-O6
12	F	901	NAG	C4-C5-C6-O6
12	C	623	NAG	O5-C5-C6-O6
12	A	615	NAG	C4-C5-C6-O6
12	A	601	NAG	C8-C7-N2-C2
12	A	601	NAG	O7-C7-N2-C2
12	A	615	NAG	C8-C7-N2-C2
12	A	615	NAG	O7-C7-N2-C2
12	A	627	NAG	C8-C7-N2-C2
12	A	627	NAG	O7-C7-N2-C2
12	A	628	NAG	C8-C7-N2-C2
12	A	628	NAG	O7-C7-N2-C2
12	A	629	NAG	C8-C7-N2-C2
12	A	629	NAG	O7-C7-N2-C2
12	A	630	NAG	C8-C7-N2-C2
12	A	630	NAG	O7-C7-N2-C2
12	A	631	NAG	C8-C7-N2-C2
12	A	631	NAG	O7-C7-N2-C2
12	A	640	NAG	C8-C7-N2-C2
12	A	640	NAG	O7-C7-N2-C2
12	B	903	NAG	C8-C7-N2-C2
12	B	903	NAG	O7-C7-N2-C2
12	C	601	NAG	C8-C7-N2-C2
12	C	601	NAG	O7-C7-N2-C2
12	C	619	NAG	C8-C7-N2-C2
12	C	619	NAG	O7-C7-N2-C2
12	C	620	NAG	C8-C7-N2-C2
12	C	620	NAG	O7-C7-N2-C2
12	C	621	NAG	C8-C7-N2-C2
12	C	621	NAG	O7-C7-N2-C2
12	C	622	NAG	C8-C7-N2-C2
12	C	622	NAG	O7-C7-N2-C2
12	C	623	NAG	C8-C7-N2-C2
12	C	623	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
12	C	630	NAG	C8-C7-N2-C2
12	C	630	NAG	O7-C7-N2-C2
12	E	601	NAG	C8-C7-N2-C2
12	E	601	NAG	O7-C7-N2-C2
12	E	630	NAG	C8-C7-N2-C2
12	E	630	NAG	O7-C7-N2-C2
12	E	634	NAG	C8-C7-N2-C2
12	E	634	NAG	O7-C7-N2-C2
12	E	653	NAG	C8-C7-N2-C2
12	E	653	NAG	O7-C7-N2-C2
12	E	653	NAG	O5-C5-C6-O6
12	A	640	NAG	C4-C5-C6-O6
12	C	627	NAG	C4-C5-C6-O6
12	F	902	NAG	C4-C5-C6-O6
12	A	609	NAG	C4-C5-C6-O6
12	C	623	NAG	C4-C5-C6-O6
12	C	601	NAG	C4-C5-C6-O6
12	C	619	NAG	C4-C5-C6-O6
12	E	654	NAG	O5-C5-C6-O6
12	A	629	NAG	C4-C5-C6-O6
12	C	629	NAG	O5-C5-C6-O6
12	C	621	NAG	O5-C5-C6-O6
12	E	653	NAG	C4-C5-C6-O6
12	C	618	NAG	O5-C5-C6-O6
12	C	602	NAG	C4-C5-C6-O6
12	C	628	NAG	C4-C5-C6-O6
12	A	639	NAG	O5-C5-C6-O6
12	C	602	NAG	O5-C5-C6-O6
12	C	628	NAG	O5-C5-C6-O6
12	A	638	NAG	C1-C2-N2-C7
12	A	601	NAG	C3-C2-N2-C7
12	C	622	NAG	C3-C2-N2-C7
12	F	902	NAG	C3-C2-N2-C7
12	C	601	NAG	C1-C2-N2-C7
12	A	630	NAG	C1-C2-N2-C7
12	E	601	NAG	C1-C2-N2-C7
12	E	630	NAG	C4-C5-C6-O6
12	C	621	NAG	C4-C5-C6-O6
12	E	601	NAG	C3-C2-N2-C7
12	C	618	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

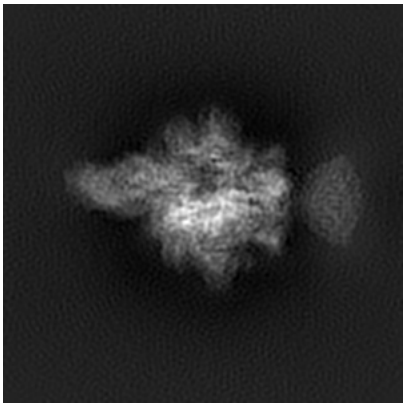
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20813. These allow visual inspection of the internal detail of the map and identification of artifacts.

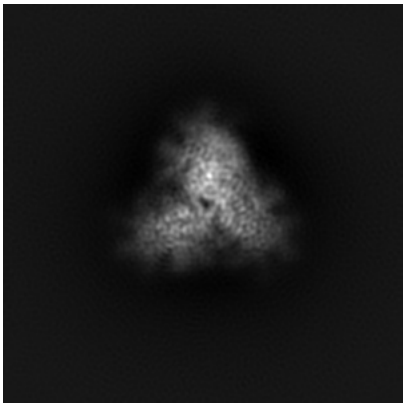
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

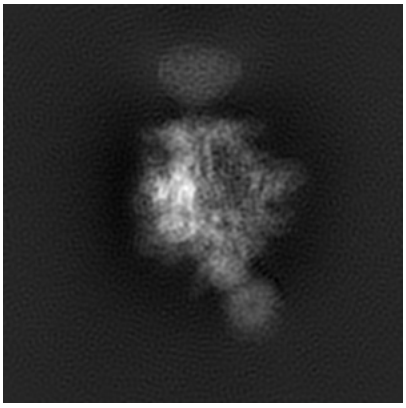
6.1.1 Primary map



X



Y

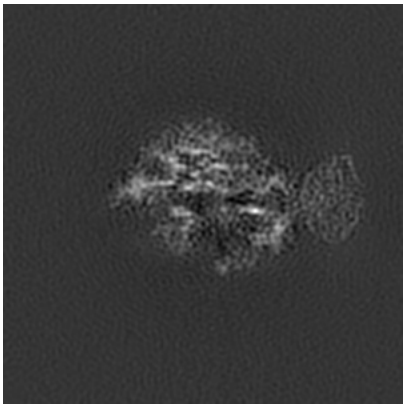


Z

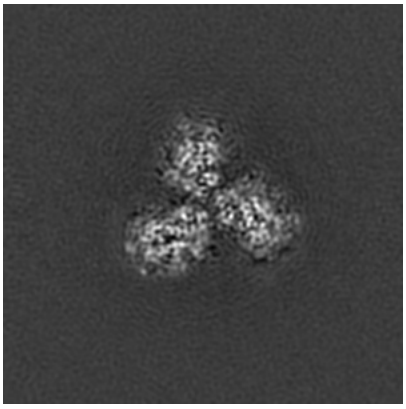
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

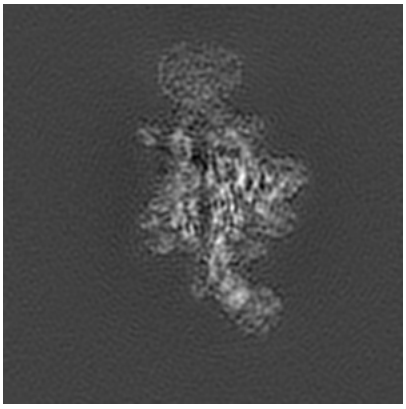
6.2.1 Primary map



X Index: 96



Y Index: 96

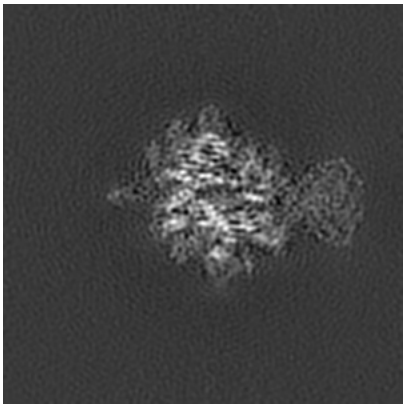


Z Index: 96

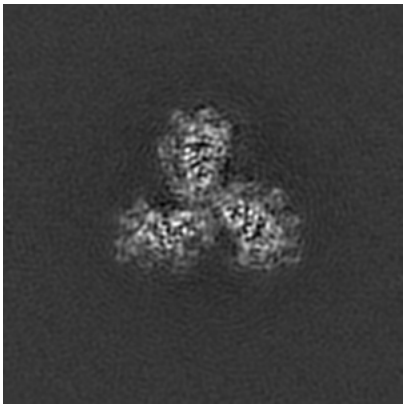
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

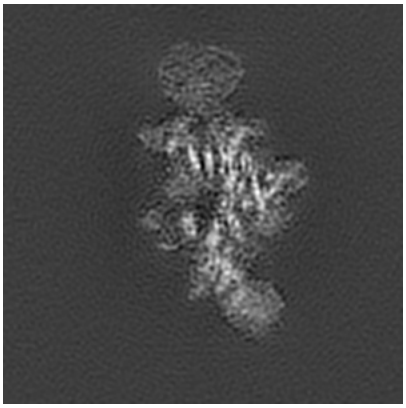
6.3.1 Primary map



X Index: 90



Y Index: 103

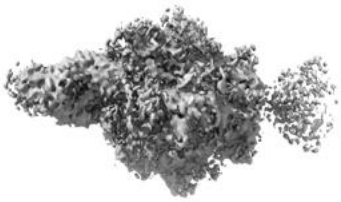


Z Index: 99

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

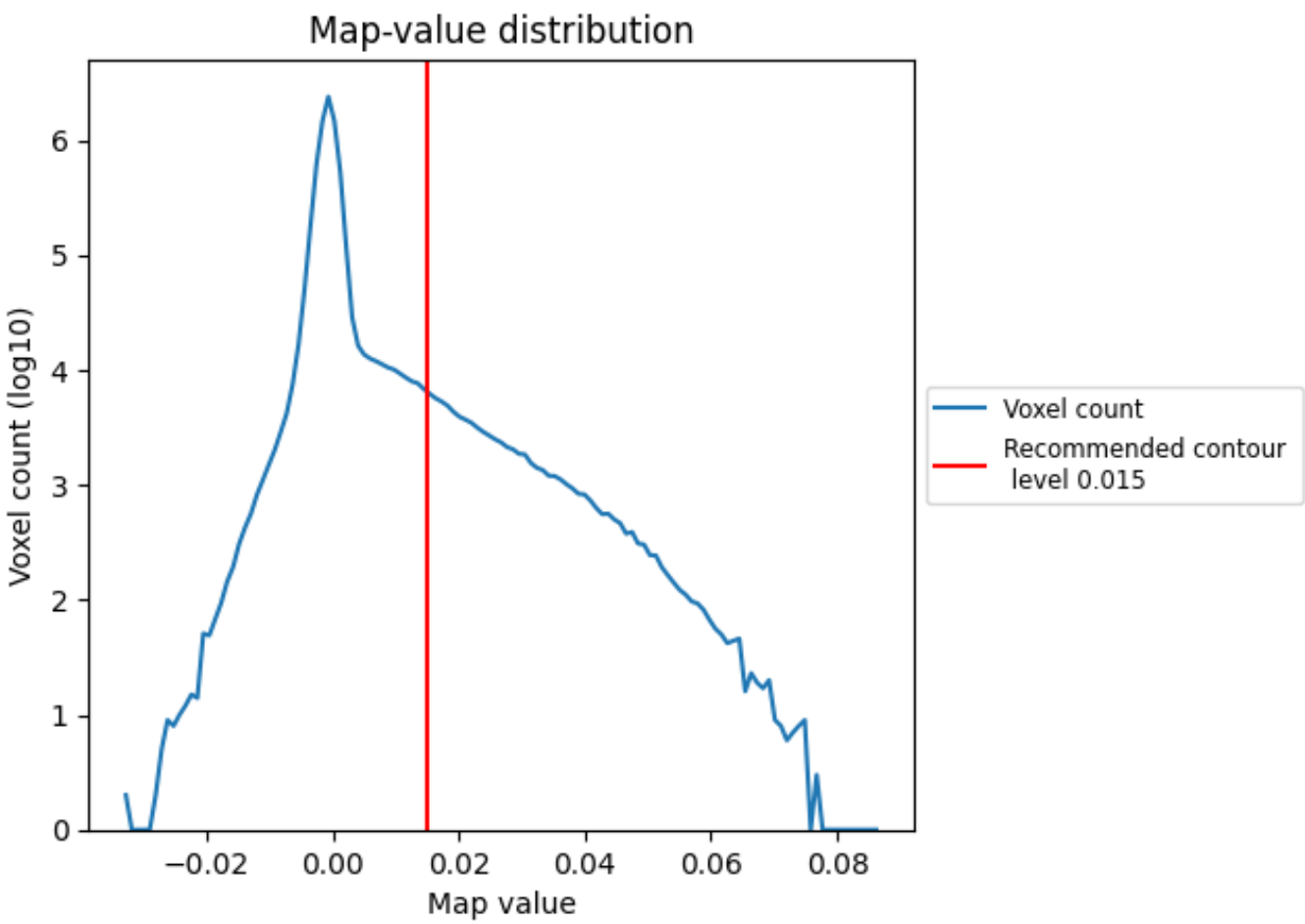
6.5 Mask visualisation (i)

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

7 Map analysis (i)

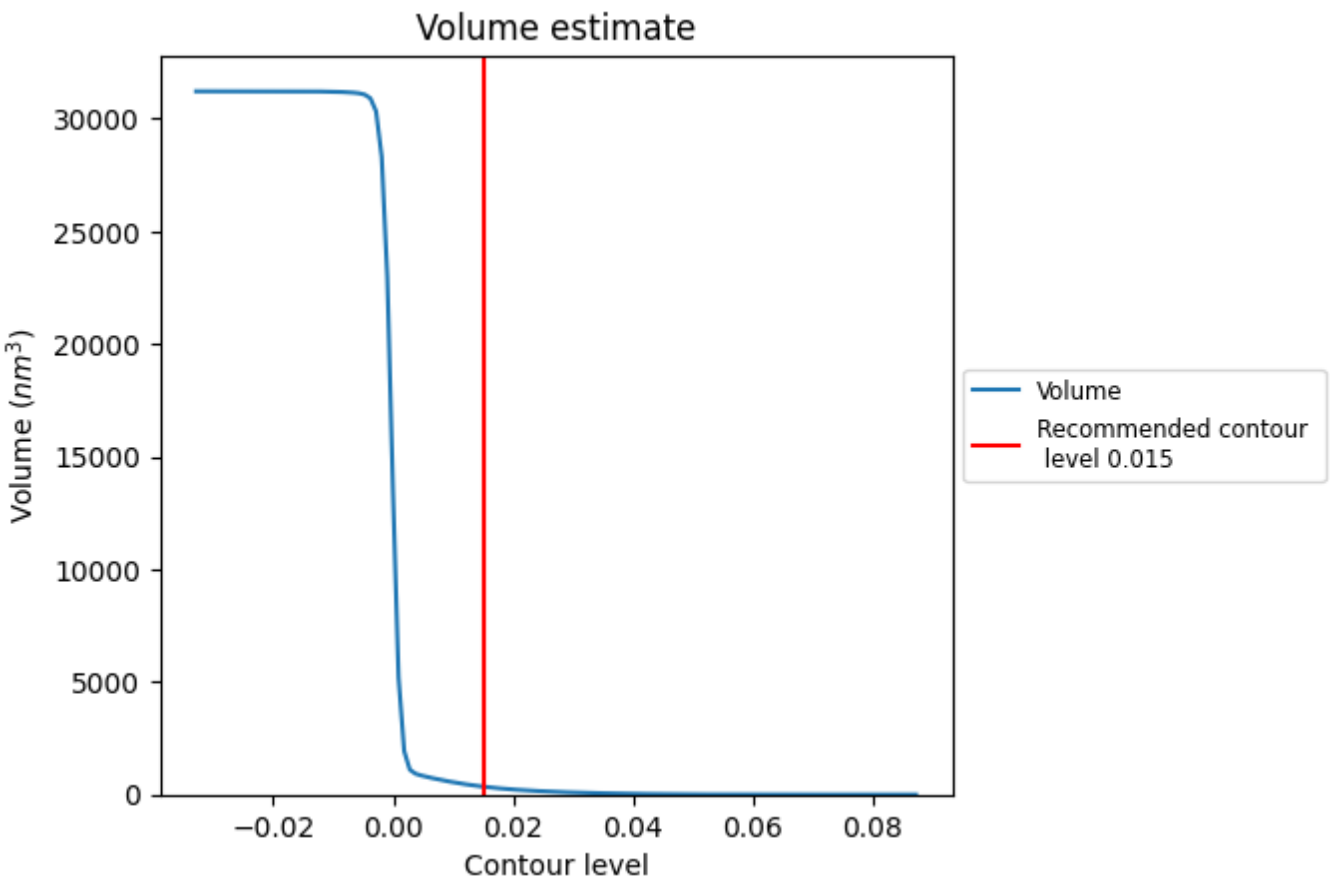
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

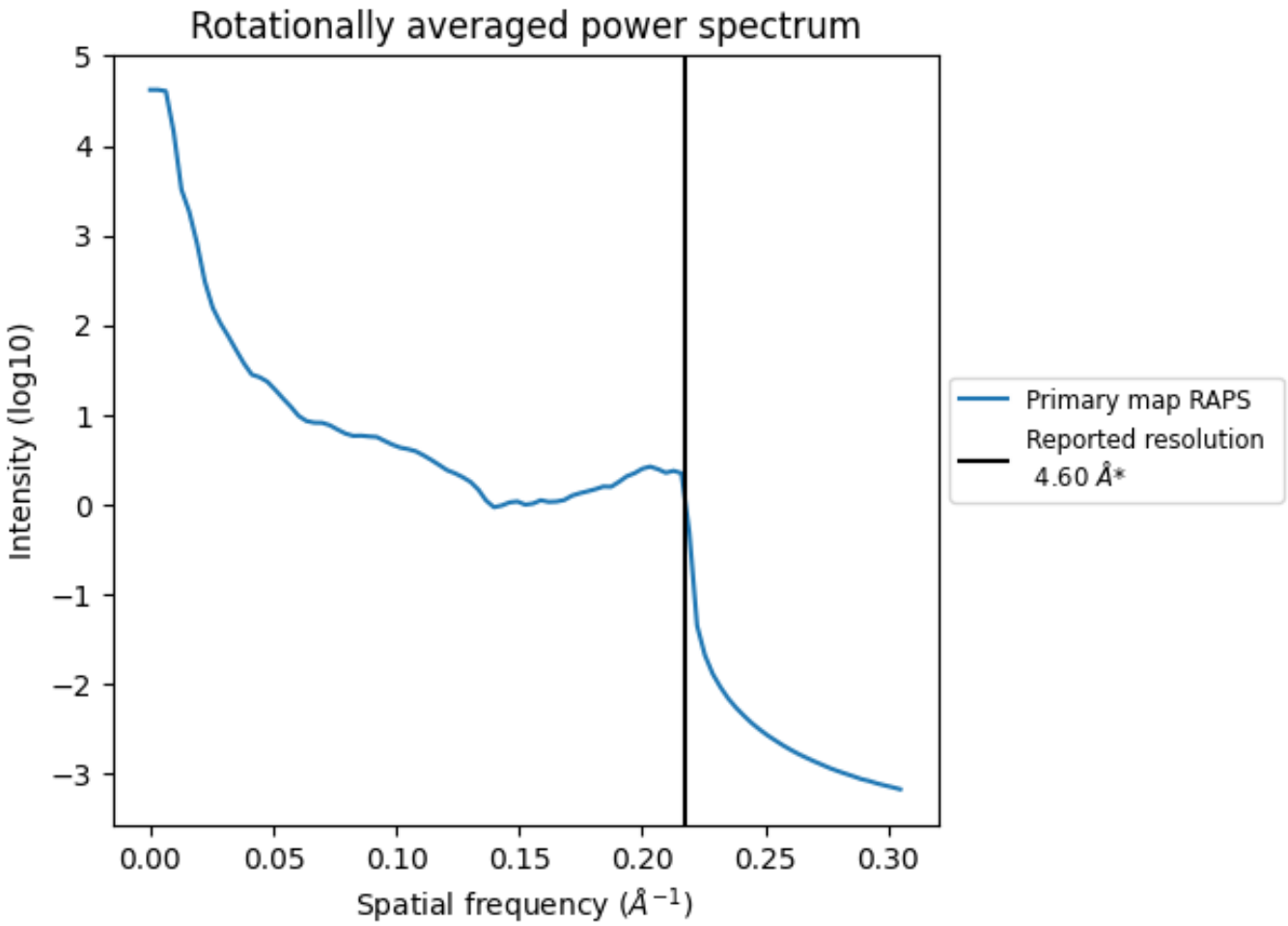
7.2 Volume estimate (i)



The volume at the recommended contour level is 351 nm^3; this corresponds to an approximate mass of 317 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)

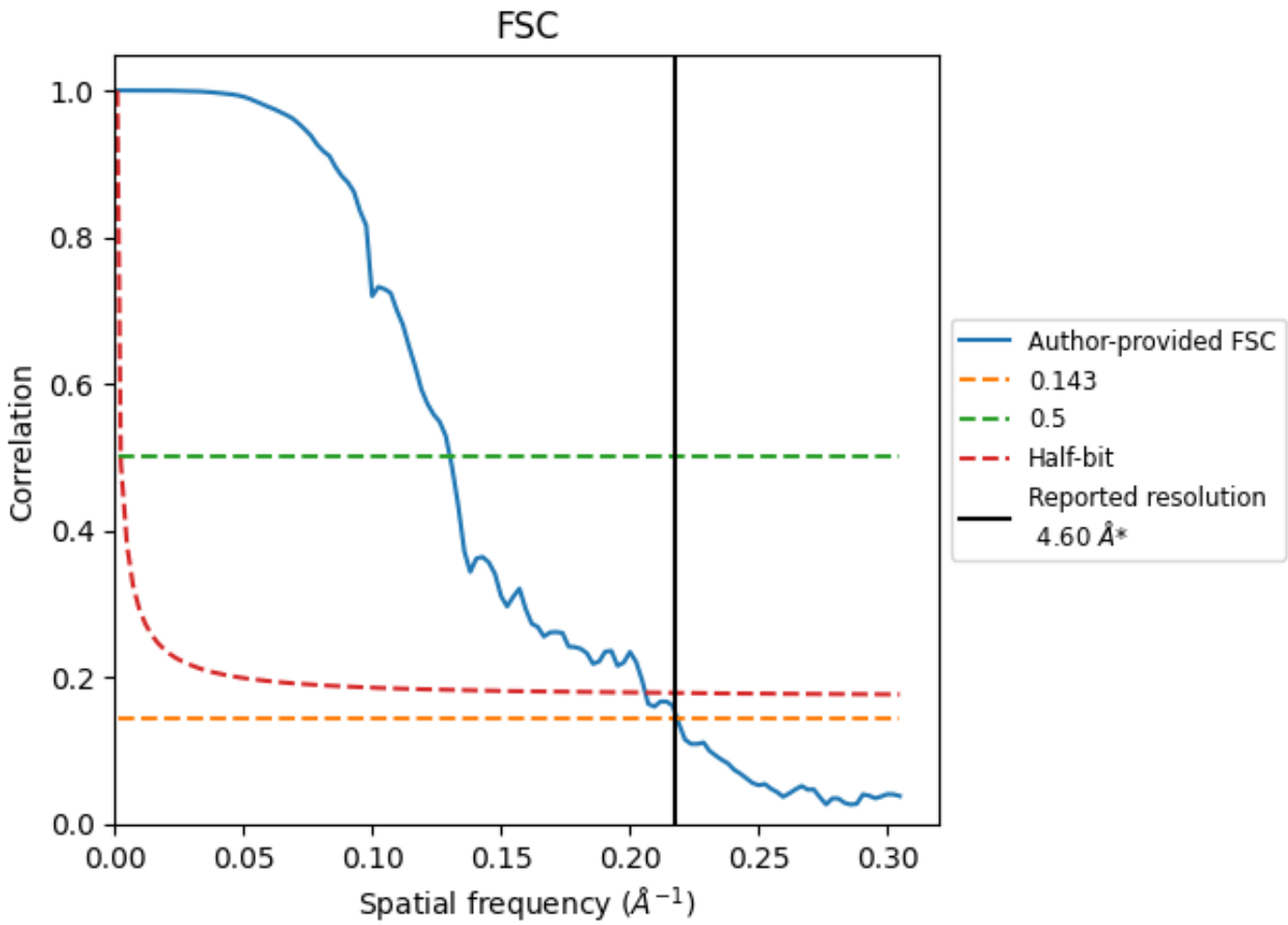


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8.2 Resolution estimates (i)

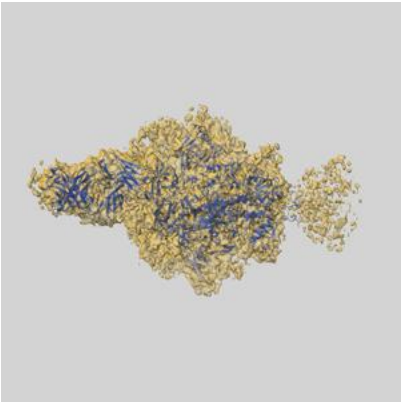
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.58	7.68	4.85
Unmasked-calculated*	-	-	-

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

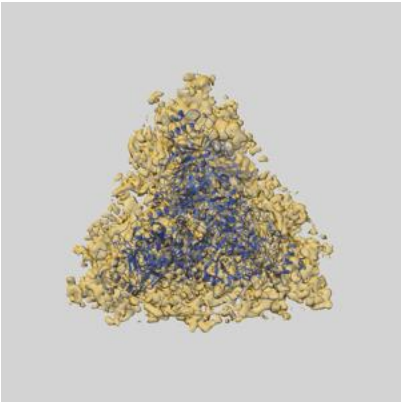
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20813 and PDB model 6ULC. Per-residue inclusion information can be found in section 3 on page 12.

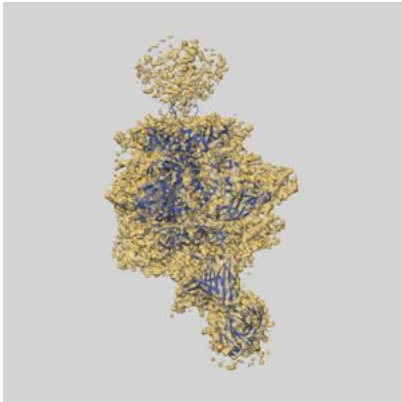
9.1 Map-model overlay (i)



X



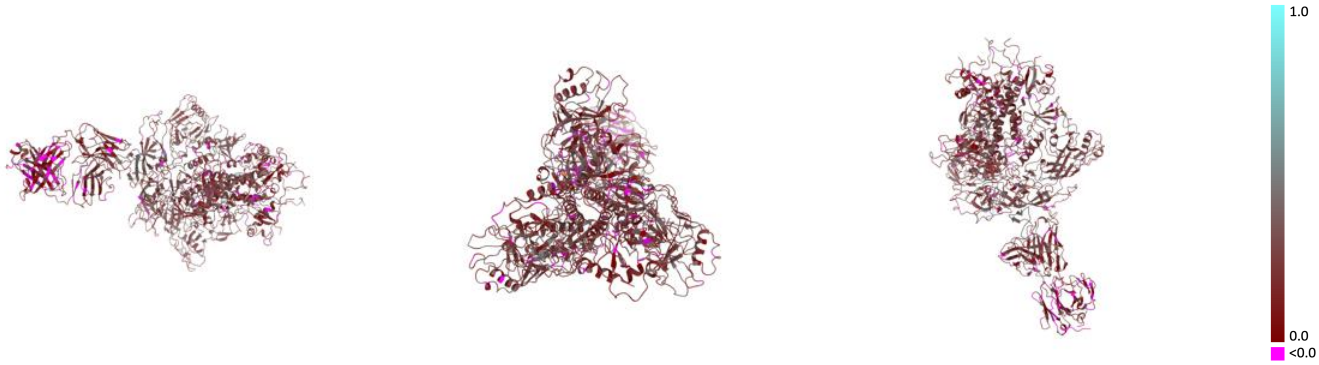
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

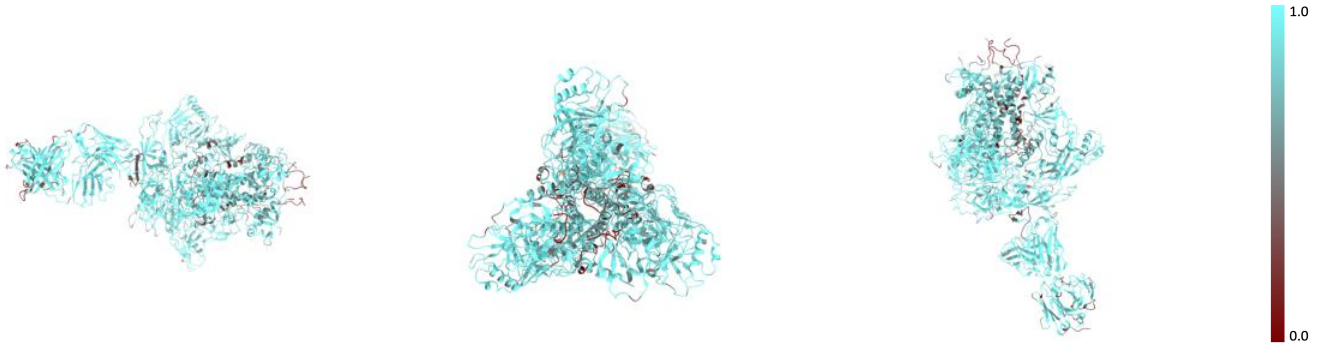
9.2 Q-score mapped to coordinate model (i)



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.

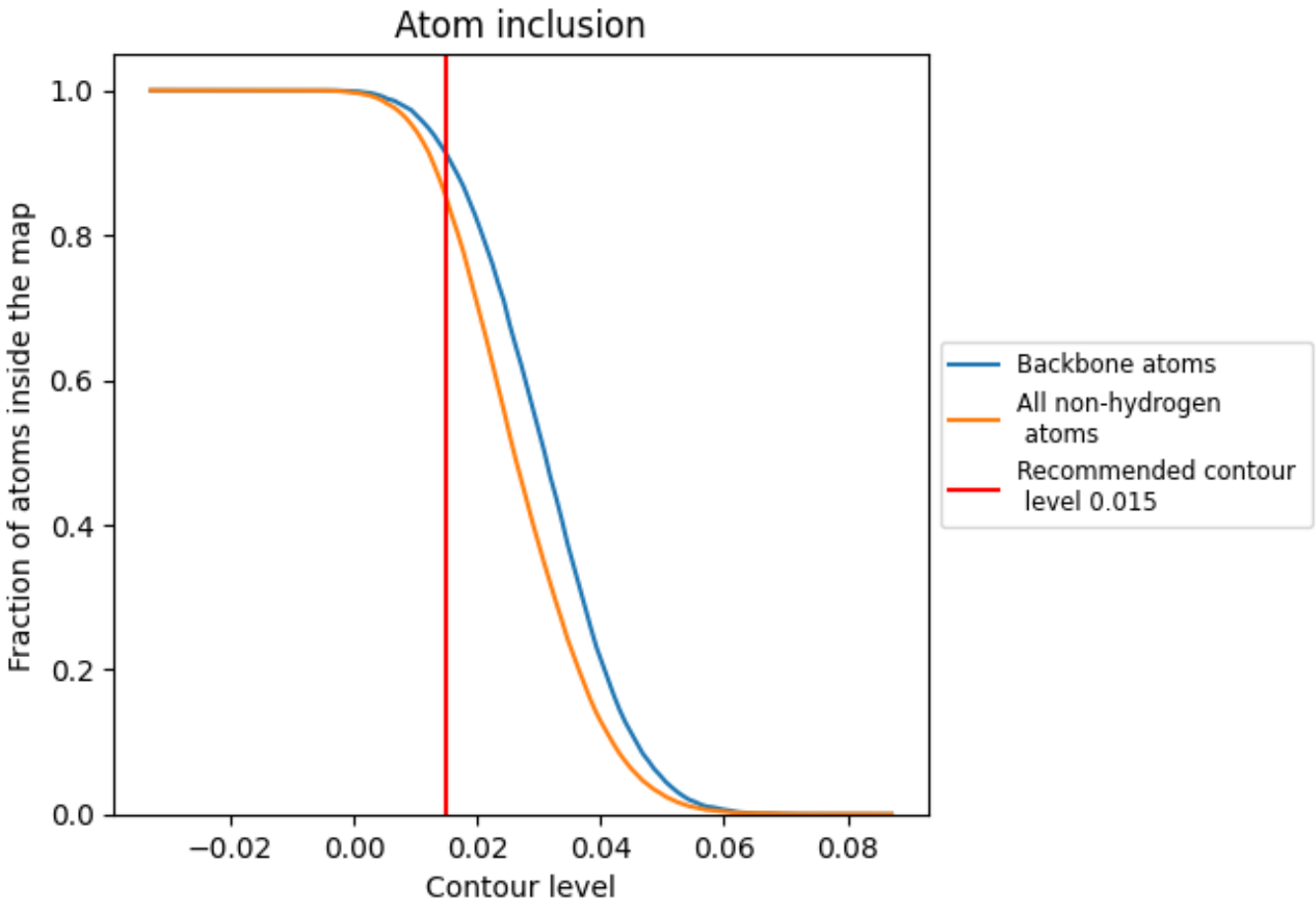
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8519	0.2400
A	0.8877	0.2610
B	0.6833	0.1900
C	0.8969	0.2600
D	0.6903	0.1960
E	0.8889	0.2720
F	0.6837	0.1970
G	0.8267	0.2830
H	0.8720	0.1930
I	0.9508	0.3050
J	0.8197	0.2790
K	0.9231	0.3360
L	0.9156	0.1840
M	0.9643	0.3280
N	0.9231	0.2880
O	0.5357	0.1540
P	0.6429	0.2920
Q	0.8974	0.3530
R	0.9643	0.3080
S	0.8205	0.2740
T	0.7632	0.2570
U	0.7857	0.2630
V	0.9744	0.2680
W	1.0000	0.4120
X	0.9231	0.3220
Y	0.7949	0.1900
Z	0.8929	0.2810
a	0.9518	0.3140
b	0.9643	0.3720
c	0.5641	0.1860
d	0.9744	0.4160
e	0.9744	0.2590
f	0.7949	0.1110
g	0.6923	0.2640
h	0.9286	0.3290

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Chain	Atom inclusion	Q-score
i	0.9487	0.3680
j	0.8205	0.2080
k	0.4103	0.2220
l	0.6429	0.1590
m	0.9388	0.1240
n	0.8205	0.3040