Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 07:53 AM EST

PDB ID	:	6XR8
EMDB ID	:	EMD-22292
Title	:	Distinct conformational states of SARS-CoV-2 spike protein
Authors	:	Zhang, J.; Cai, Y.F.; Xiao, T.S.; Peng, H.Q.; Sterling, S.M.; Walsh Jr, R.M.; Rawson, S.; Volloch, S.R.; Chen, B.
Deposited on	:	2020-07-11
Resolution	:	2.90 Å(reported)
Based on initial model	:	6VXX

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

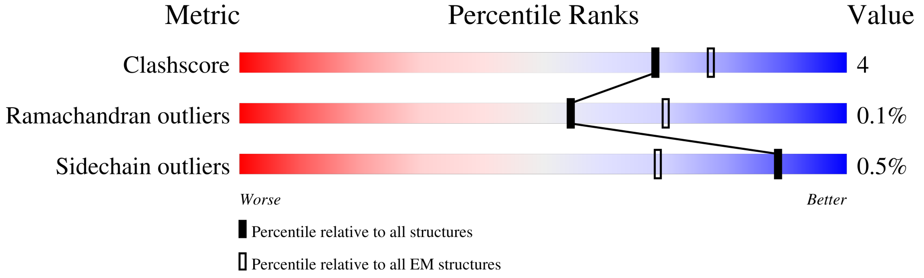
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	1310	• 78% 6% 15%
1	B	1310	• 78% 6% 15%
1	C	1310	• 79% 5% 15%
2	1A	3	33% 67% 33%
2	4A	3	33% 67% 33%
2	5	3	67% 67% 33%
2	DA	3	67% 33% 67%
2	GA	3	67% 67% 33%

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Mol	Chain	Length	Quality of chain
2	I	3	🟥 33% 🟩 33% 🟨 67%
2	JA	3	🟥 67% 🟩 67% 🟨 33%
2	MA	3	🟥 33% 🟩 67% 🟨 33%
2	PA	3	🟥 33% 🟩 67% 🟨 33%
2	Q	3	🟥 67% 🟨 100%
2	Y	3	🟥 33% 🟨 100%
2	b	3	🟥 67% 🟩 67% 🟨 33%
2	cA	3	🟩 67% 🟨 33%
2	e	3	🟥 67% 🟩 67% 🟨 33%
2	h	3	🟥 33% 🟩 67% 🟨 33%
2	k	3	🟥 33% 🟩 67% 🟨 33%
2	kA	3	🟥 67% 🟩 67% 🟨 33%
2	sA	3	🟥 33% 🟩 67% 🟨 33%
2	vA	3	🟥 67% 🟩 67% 🟨 33%
2	x	3	🟩 67% 🟨 33%
2	yA	3	🟥 67% 🟩 67% 🟨 33%
3	0	2	🟥 50% 🟩 100%
3	9	2	🟥 50% 🟧 100%
3	BA	2	🟥 50% 🟩 50% 🟨 50%
3	L	2	🟥 50% 🟩 100%
3	U	2	🟥 50% 🟨 50% 🟧 50%
3	W	2	🟥 50% 🟩 100%
3	fA	2	🟥 50% 🟩 100%
3	oA	2	🟥 50% 🟨 100%
3	qA	2	🟥 50% 🟩 100%

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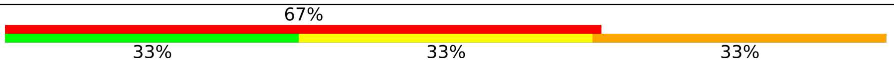
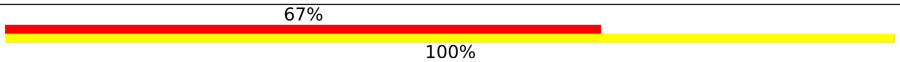
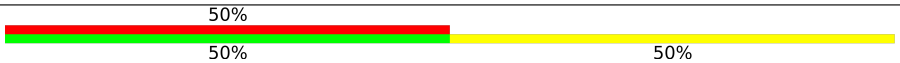
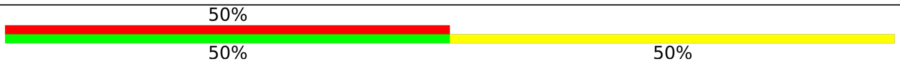
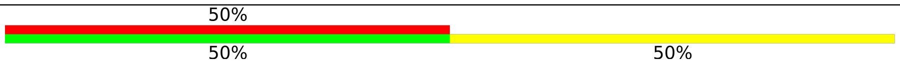
Mol	Chain	Length	Quality of chain
4	2	3	
4	N	3	
4	hA	3	
5	7A	4	
5	SA	4	
5	n	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	U	1	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 27627 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1107	Total 8666	C 5529	N 1446	O 1651	S 40	0	0
1	B	1107	Total 8666	C 5529	N 1446	O 1651	S 40	0	0
1	C	1107	Total 8666	C 5529	N 1446	O 1651	S 40	0	0

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	ALA	-	expression tag	UNP P0DTC2
A	1282	TRP	-	expression tag	UNP P0DTC2
A	1283	SER	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	PRO	-	expression tag	UNP P0DTC2
A	1286	GLN	-	expression tag	UNP P0DTC2
A	1287	PHE	-	expression tag	UNP P0DTC2
A	1288	GLU	-	expression tag	UNP P0DTC2
A	1289	LYS	-	expression tag	UNP P0DTC2
A	1290	GLY	-	expression tag	UNP P0DTC2
A	1291	GLY	-	expression tag	UNP P0DTC2
A	1292	GLY	-	expression tag	UNP P0DTC2
A	1293	SER	-	expression tag	UNP P0DTC2
A	1294	GLY	-	expression tag	UNP P0DTC2
A	1295	GLY	-	expression tag	UNP P0DTC2
A	1296	GLY	-	expression tag	UNP P0DTC2
A	1297	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1298	GLY	-	expression tag	UNP P0DTC2
A	1299	GLY	-	expression tag	UNP P0DTC2
A	1300	SER	-	expression tag	UNP P0DTC2
A	1301	SER	-	expression tag	UNP P0DTC2
A	1302	ALA	-	expression tag	UNP P0DTC2
A	1303	TRP	-	expression tag	UNP P0DTC2
A	1304	SER	-	expression tag	UNP P0DTC2
A	1305	HIS	-	expression tag	UNP P0DTC2
A	1306	PRO	-	expression tag	UNP P0DTC2
A	1307	GLN	-	expression tag	UNP P0DTC2
A	1308	PHE	-	expression tag	UNP P0DTC2
A	1309	GLU	-	expression tag	UNP P0DTC2
A	1310	LYS	-	expression tag	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	ALA	-	expression tag	UNP P0DTC2
B	1282	TRP	-	expression tag	UNP P0DTC2
B	1283	SER	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	PRO	-	expression tag	UNP P0DTC2
B	1286	GLN	-	expression tag	UNP P0DTC2
B	1287	PHE	-	expression tag	UNP P0DTC2
B	1288	GLU	-	expression tag	UNP P0DTC2
B	1289	LYS	-	expression tag	UNP P0DTC2
B	1290	GLY	-	expression tag	UNP P0DTC2
B	1291	GLY	-	expression tag	UNP P0DTC2
B	1292	GLY	-	expression tag	UNP P0DTC2
B	1293	SER	-	expression tag	UNP P0DTC2
B	1294	GLY	-	expression tag	UNP P0DTC2
B	1295	GLY	-	expression tag	UNP P0DTC2
B	1296	GLY	-	expression tag	UNP P0DTC2
B	1297	SER	-	expression tag	UNP P0DTC2
B	1298	GLY	-	expression tag	UNP P0DTC2
B	1299	GLY	-	expression tag	UNP P0DTC2
B	1300	SER	-	expression tag	UNP P0DTC2
B	1301	SER	-	expression tag	UNP P0DTC2
B	1302	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1303	TRP	-	expression tag	UNP P0DTC2
B	1304	SER	-	expression tag	UNP P0DTC2
B	1305	HIS	-	expression tag	UNP P0DTC2
B	1306	PRO	-	expression tag	UNP P0DTC2
B	1307	GLN	-	expression tag	UNP P0DTC2
B	1308	PHE	-	expression tag	UNP P0DTC2
B	1309	GLU	-	expression tag	UNP P0DTC2
B	1310	LYS	-	expression tag	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	ALA	-	expression tag	UNP P0DTC2
C	1282	TRP	-	expression tag	UNP P0DTC2
C	1283	SER	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	PRO	-	expression tag	UNP P0DTC2
C	1286	GLN	-	expression tag	UNP P0DTC2
C	1287	PHE	-	expression tag	UNP P0DTC2
C	1288	GLU	-	expression tag	UNP P0DTC2
C	1289	LYS	-	expression tag	UNP P0DTC2
C	1290	GLY	-	expression tag	UNP P0DTC2
C	1291	GLY	-	expression tag	UNP P0DTC2
C	1292	GLY	-	expression tag	UNP P0DTC2
C	1293	SER	-	expression tag	UNP P0DTC2
C	1294	GLY	-	expression tag	UNP P0DTC2
C	1295	GLY	-	expression tag	UNP P0DTC2
C	1296	GLY	-	expression tag	UNP P0DTC2
C	1297	SER	-	expression tag	UNP P0DTC2
C	1298	GLY	-	expression tag	UNP P0DTC2
C	1299	GLY	-	expression tag	UNP P0DTC2
C	1300	SER	-	expression tag	UNP P0DTC2
C	1301	SER	-	expression tag	UNP P0DTC2
C	1302	ALA	-	expression tag	UNP P0DTC2
C	1303	TRP	-	expression tag	UNP P0DTC2
C	1304	SER	-	expression tag	UNP P0DTC2
C	1305	HIS	-	expression tag	UNP P0DTC2
C	1306	PRO	-	expression tag	UNP P0DTC2
C	1307	GLN	-	expression tag	UNP P0DTC2

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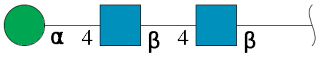
Chain	Residue	Modelled	Actual	Comment	Reference
C	1308	PHE	-	expression tag	UNP P0DTC2
C	1309	GLU	-	expression tag	UNP P0DTC2
C	1310	LYS	-	expression tag	UNP P0DTC2

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



Mol	Chain	Residues	Atoms	AltConf	Trace
2	I	3	Total C N O 39 22 2 15	0	0
2	Q	3	Total C N O 39 22 2 15	0	0
2	Y	3	Total C N O 39 22 2 15	0	0
2	b	3	Total C N O 39 22 2 15	0	0
2	e	3	Total C N O 39 22 2 15	0	0
2	h	3	Total C N O 39 22 2 15	0	0
2	k	3	Total C N O 39 22 2 15	0	0
2	x	3	Total C N O 39 22 2 15	0	0
2	5	3	Total C N O 39 22 2 15	0	0
2	DA	3	Total C N O 39 22 2 15	0	0
2	GA	3	Total C N O 39 22 2 15	0	0
2	JA	3	Total C N O 39 22 2 15	0	0
2	MA	3	Total C N O 39 22 2 15	0	0
2	PA	3	Total C N O 39 22 2 15	0	0
2	cA	3	Total C N O 39 22 2 15	0	0

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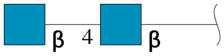
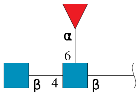
Mol	Chain	Residues	Atoms	AltConf	Trace
2	kA	3	Total C N O 39 22 2 15	0	0
2	sA	3	Total C N O 39 22 2 15	0	0
2	vA	3	Total C N O 39 22 2 15	0	0
2	yA	3	Total C N O 39 22 2 15	0	0
2	1A	3	Total C N O 39 22 2 15	0	0
2	4A	3	Total C N O 39 22 2 15	0	0

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



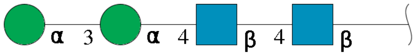
Mol	Chain	Residues	Atoms	AltConf	Trace
3	L	2	Total C N O 28 16 2 10	0	0
3	U	2	Total C N O 28 16 2 10	0	0
3	W	2	Total C N O 28 16 2 10	0	0
3	0	2	Total C N O 28 16 2 10	0	0
3	9	2	Total C N O 28 16 2 10	0	0
3	BA	2	Total C N O 28 16 2 10	0	0
3	fA	2	Total C N O 28 16 2 10	0	0
3	oA	2	Total C N O 28 16 2 10	0	0
3	qA	2	Total C N O 28 16 2 10	0	0

- Molecule 4 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.



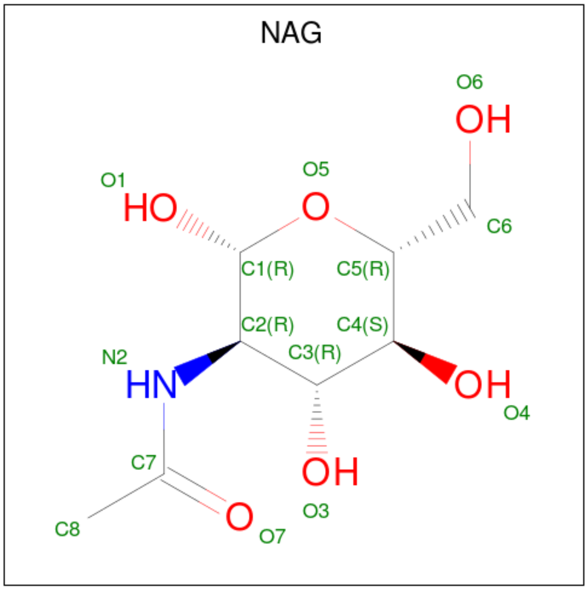
Mol	Chain	Residues	Atoms	AltConf	Trace
4	N	3	Total C N O 38 22 2 14	0	0
4	2	3	Total C N O 38 22 2 14	0	0
4	hA	3	Total C N O 38 22 2 14	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
5	n	4	Total C N O 50 28 2 20	0	0
5	SA	4	Total C N O 50 28 2 20	0	0
5	7A	4	Total C N O 50 28 2 20	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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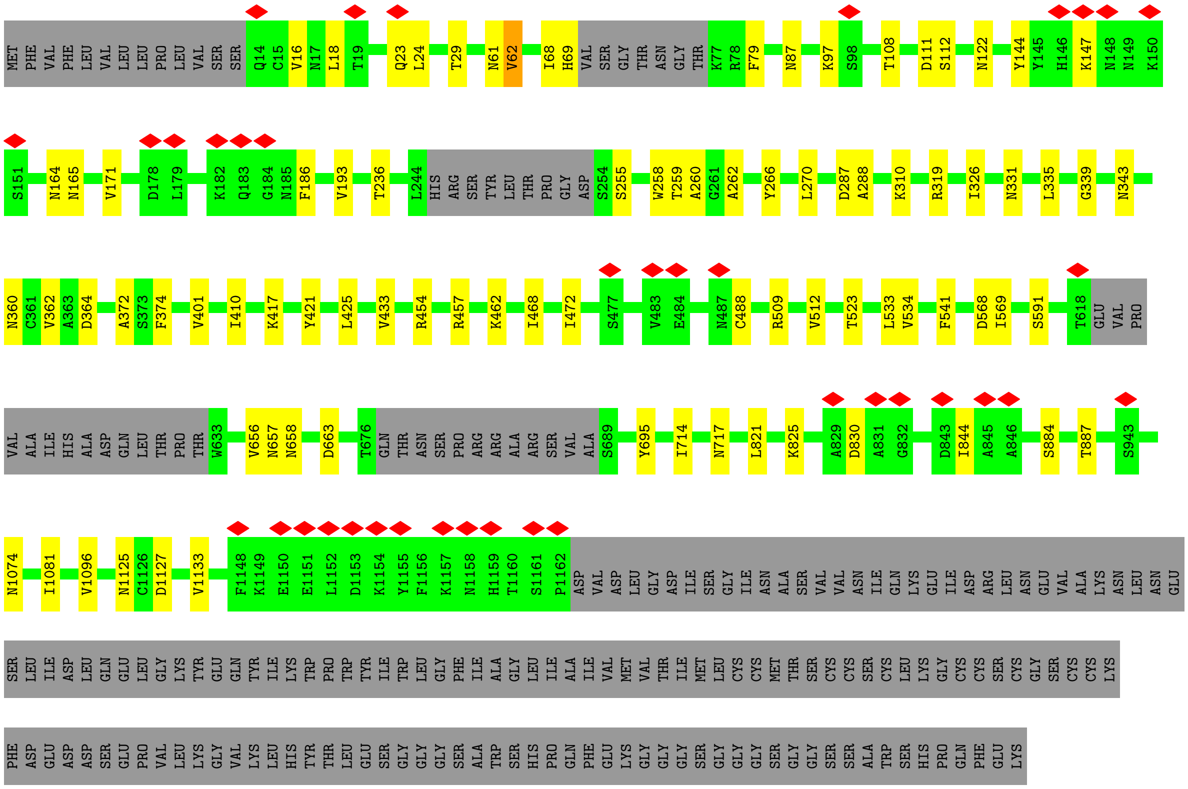
Mol	Chain	Residues	Atoms	AltConf
6	C	1	Total C N O 98 56 7 35	0
6	C	1	Total C N O 98 56 7 35	0
6	C	1	Total C N O 98 56 7 35	0
6	C	1	Total C N O 98 56 7 35	0
6	C	1	Total C N O 98 56 7 35	0
6	C	1	Total C N O 98 56 7 35	0
6	C	1	Total C N O 98 56 7 35	0

3 Residue-property plots ⓘ

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

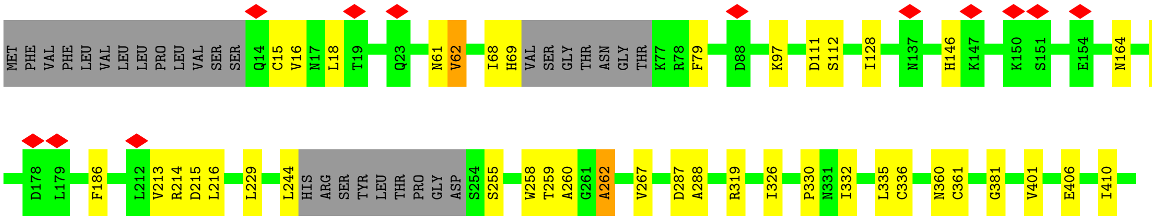
- Molecule 1: Spike glycoprotein

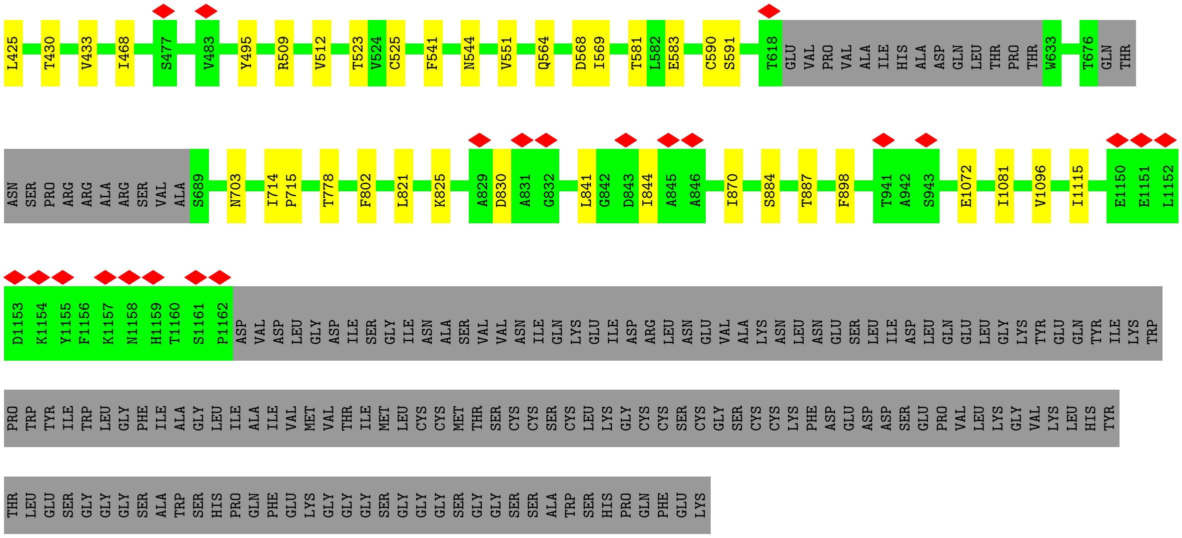
Chain A:



- Molecule 1: Spike glycoprotein

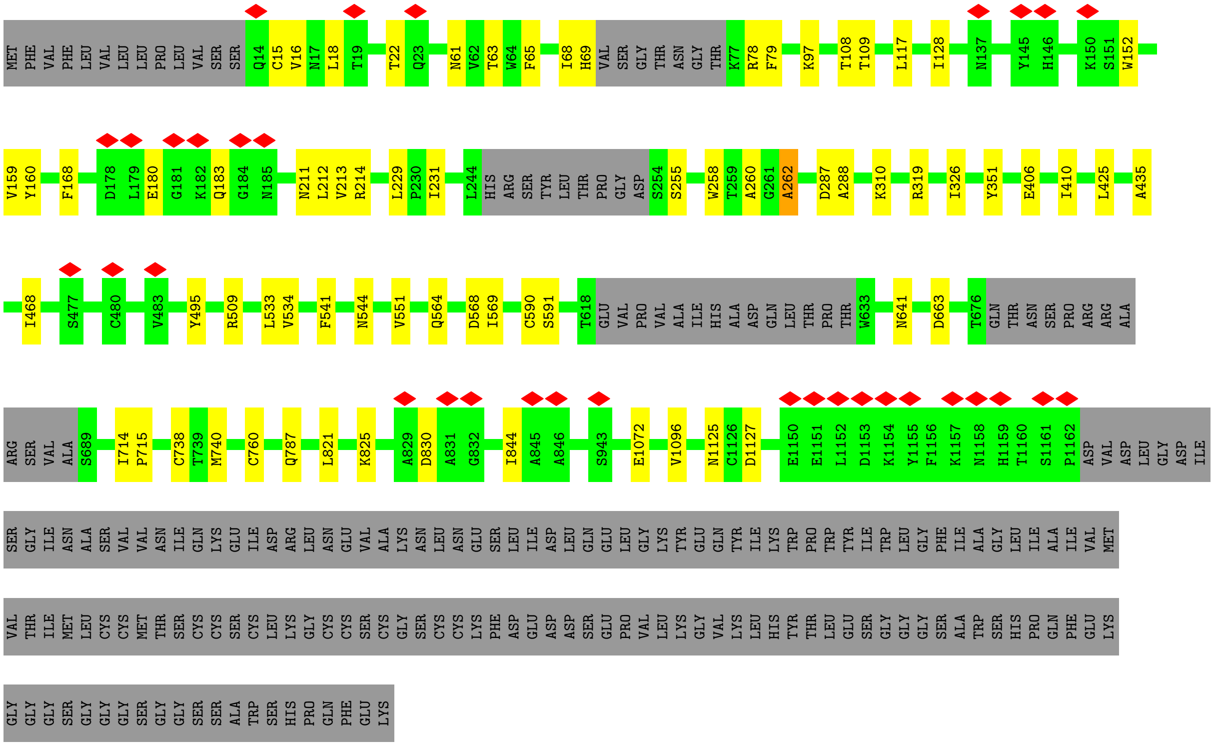
Chain B:





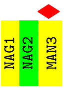
- Molecule 1: Spike glycoprotein

Chain C:



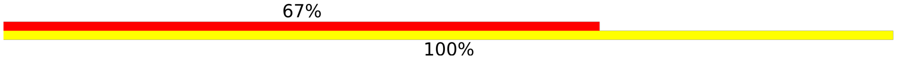
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



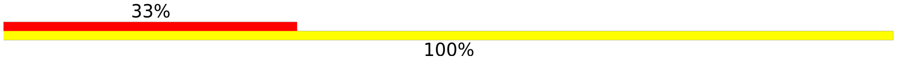
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



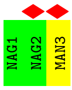
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



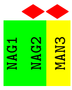
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



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

Chain e:

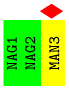


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

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

Chain k:

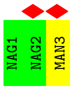


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:

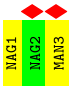
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5:



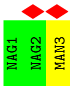
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:



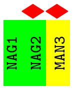
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA:



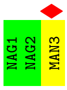
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JA:



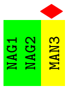
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain MA:



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

Chain PA:

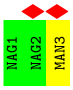


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain cA:

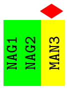
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain kA:



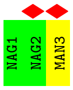
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain sA:



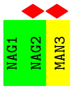
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain vA:



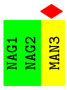
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain yA:



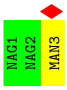
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1A:



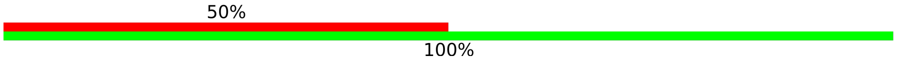
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4A:



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

Chain L:

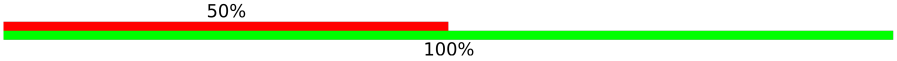


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

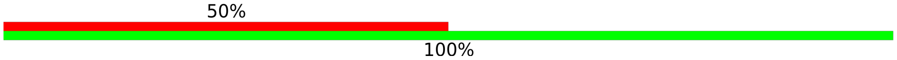
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



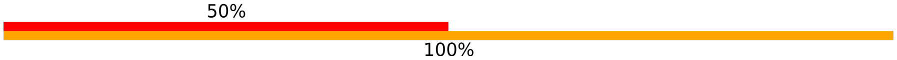
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:



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

Chain 9:

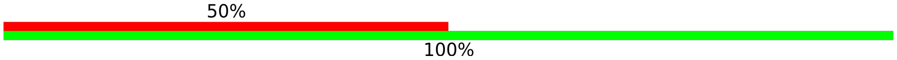


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA:

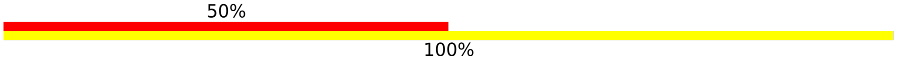
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain fA:



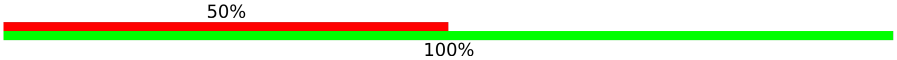
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain oA:



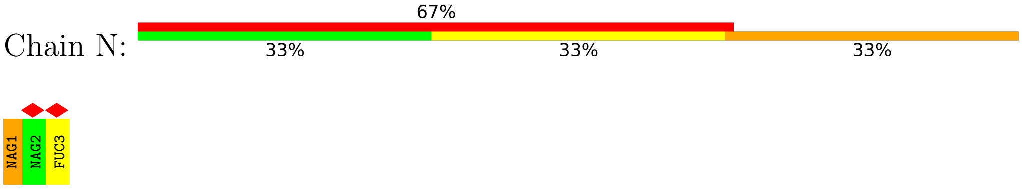
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain qA:



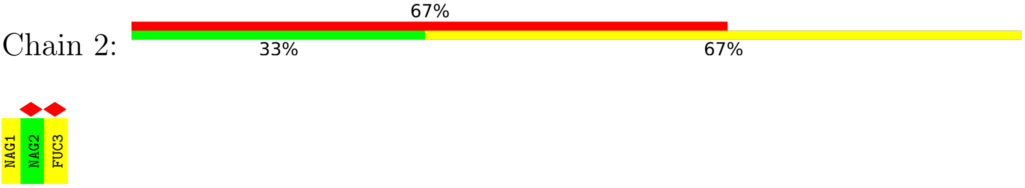
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



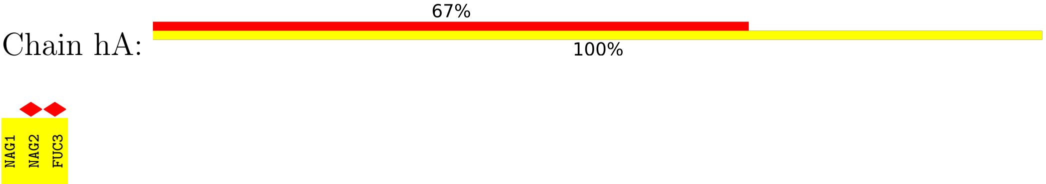
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:



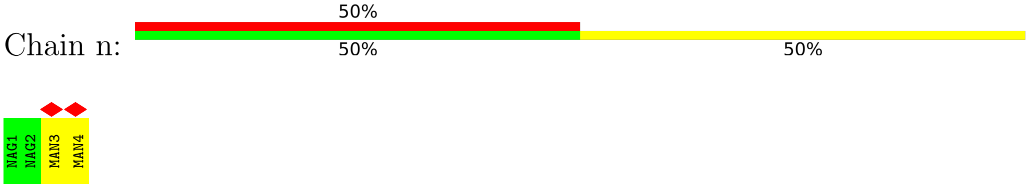
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain hA:



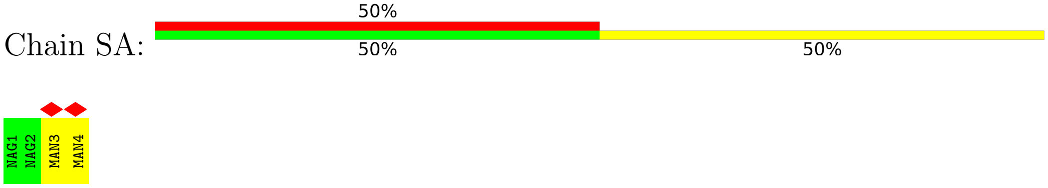
- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:



- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain SA:



- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7A:


NAG1
NAG2
MAN3
MAN4

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	71339	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	54.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/8866	0.45	0/12058
1	B	0.28	0/8866	0.44	0/12058
1	C	0.28	0/8866	0.44	0/12058
All	All	0.28	0/26598	0.44	0/36174

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8666	0	8436	86	0
1	B	8666	0	8429	63	0
1	C	8666	0	8429	52	0
2	1A	39	0	34	0	0
2	4A	39	0	34	0	0
2	5	39	0	34	0	0
2	DA	39	0	34	1	0
2	GA	39	0	34	0	0
2	I	39	0	34	5	0
2	JA	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	MA	39	0	34	0	0
2	PA	39	0	34	0	0
2	Q	39	0	34	4	0
2	Y	39	0	34	4	0
2	b	39	0	34	0	0
2	cA	39	0	34	0	0
2	e	39	0	34	0	0
2	h	39	0	34	0	0
2	k	39	0	34	0	0
2	kA	39	0	34	0	0
2	sA	39	0	34	0	0
2	vA	39	0	34	0	0
2	x	39	0	34	0	0
2	yA	39	0	34	0	0
3	0	28	0	25	0	0
3	9	28	0	25	2	0
3	BA	28	0	25	1	0
3	L	28	0	25	0	0
3	U	28	0	25	8	0
3	W	28	0	25	0	0
3	fA	28	0	25	0	0
3	oA	28	0	25	0	0
3	qA	28	0	25	0	0
4	2	38	0	34	0	0
4	N	38	0	34	3	0
4	hA	38	0	34	0	0
5	7A	50	0	43	0	0
5	SA	50	0	43	0	0
5	n	50	0	43	0	0
6	A	98	0	91	10	0
6	B	98	0	91	1	0
6	C	98	0	91	1	0
All	All	27627	0	26737	203	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:HD21	2:Q:1:NAG:C1	1.01	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASN:HD21	6:A:1402:NAG:C1	0.97	1.57
1:A:1074:ASN:HD21	4:N:1:NAG:C1	1.01	1.55
1:A:717:ASN:HD21	2:I:1:NAG:C1	1.17	1.53
1:A:343:ASN:ND2	6:A:1402:NAG:C1	1.80	1.43
1:A:657:ASN:ND2	6:A:1404:NAG:C1	1.79	1.43
1:A:657:ASN:HD21	6:A:1404:NAG:C1	1.33	1.40
1:A:122:ASN:ND2	2:Q:1:NAG:C1	1.79	1.38
1:A:717:ASN:ND2	2:I:1:NAG:C1	1.78	1.38
1:A:1074:ASN:ND2	4:N:1:NAG:C1	1.77	1.38
1:A:331:ASN:ND2	3:U:1:NAG:C1	1.89	1.34
1:A:69:HIS:C	1:A:260:ALA:H	1.50	1.12
1:A:97:LYS:HE2	1:A:262:ALA:HB3	1.30	1.10
1:A:61:ASN:ND2	6:A:1401:NAG:C1	2.15	1.10
1:A:331:ASN:HD21	3:U:1:NAG:C2	1.68	1.05
1:B:69:HIS:C	1:B:260:ALA:H	1.61	1.03
1:C:79:PHE:HB2	1:C:258:TRP:CH2	1.97	0.98
1:A:69:HIS:C	1:A:260:ALA:N	2.17	0.97
3:U:1:NAG:H62	3:U:2:NAG:HN2	1.32	0.92
1:A:97:LYS:CE	1:A:262:ALA:HB3	2.02	0.89
1:B:97:LYS:HE2	1:B:262:ALA:HB3	1.56	0.87
1:C:79:PHE:HB2	1:C:258:TRP:HH2	1.36	0.87
1:A:331:ASN:HD21	3:U:1:NAG:C1	1.76	0.87
1:A:717:ASN:CG	2:I:1:NAG:C1	2.46	0.84
1:B:69:HIS:C	1:B:260:ALA:N	2.32	0.82
1:C:97:LYS:NZ	1:C:183:GLN:O	2.11	0.82
1:C:79:PHE:CB	1:C:258:TRP:CH2	2.64	0.80
1:C:69:HIS:C	1:C:260:ALA:N	2.35	0.80
1:A:147:LYS:O	6:A:1406:NAG:H82	1.85	0.77
1:A:18:LEU:HD23	1:A:258:TRP:CD1	2.20	0.76
1:A:97:LYS:HE2	1:A:262:ALA:CB	2.14	0.76
1:C:68:ILE:O	1:C:260:ALA:HB3	1.85	0.76
1:A:61:ASN:HD21	6:A:1401:NAG:C1	1.99	0.73
1:C:69:HIS:C	1:C:260:ALA:H	1.92	0.73
1:A:1074:ASN:CG	4:N:1:NAG:C1	2.58	0.72
1:B:79:PHE:HB2	1:B:258:TRP:CH2	2.25	0.71
1:B:406:GLU:OE2	1:B:495:TYR:OH	2.09	0.71
1:C:544:ASN:ND2	1:C:564:GLN:OE1	2.23	0.70
1:B:97:LYS:CE	1:B:262:ALA:HB3	2.22	0.70
1:C:79:PHE:CB	1:C:258:TRP:HH2	2.00	0.70
1:A:360:ASN:H	1:A:523:THR:HG22	1.57	0.70
1:C:22:THR:O	1:C:78:ARG:NH1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:1:NAG:H62	3:U:2:NAG:N2	2.07	0.69
3:9:1:NAG:H62	3:9:2:NAG:HN2	1.58	0.69
1:A:186:PHE:HE1	1:A:262:ALA:O	1.74	0.69
1:C:326:ILE:HD12	1:C:534:VAL:HG22	1.75	0.69
1:A:79:PHE:HB2	1:A:258:TRP:CH2	2.27	0.68
1:C:406:GLU:OE2	1:C:495:TYR:OH	2.10	0.68
1:C:69:HIS:C	1:C:260:ALA:O	2.33	0.67
1:C:97:LYS:HE2	1:C:262:ALA:HB3	1.77	0.67
1:A:61:ASN:HD22	6:A:1401:NAG:C1	2.06	0.66
1:A:1081:ILE:HD13	1:A:1133:VAL:HG22	1.78	0.65
1:C:63:THR:HG21	1:C:65:PHE:CZ	2.32	0.64
1:A:18:LEU:HB3	1:A:258:TRP:HE1	1.63	0.64
1:A:335:LEU:HD11	1:A:364:ASP:HB3	1.80	0.64
1:C:128:ILE:HG21	1:C:229:LEU:HD13	1.80	0.63
1:A:236:THR:HG21	2:Y:2:NAG:H82	1.79	0.63
1:A:657:ASN:CG	6:A:1404:NAG:C1	2.66	0.62
1:C:128:ILE:HD13	1:C:229:LEU:HD11	1.81	0.62
1:B:128:ILE:HG21	1:B:229:LEU:CD1	2.29	0.62
1:A:16:VAL:HG11	1:A:255:SER:HB2	1.81	0.62
3:9:1:NAG:H62	3:9:2:NAG:N2	2.13	0.62
1:A:68:ILE:O	1:A:260:ALA:HB3	1.99	0.62
1:C:97:LYS:CE	1:C:262:ALA:HB3	2.30	0.61
1:B:381:GLY:HA3	1:B:430:THR:HG23	1.82	0.61
1:C:63:THR:CG2	1:C:65:PHE:CZ	2.84	0.60
1:A:1125:ASN:ND2	1:A:1127:ASP:OD2	2.35	0.59
1:A:122:ASN:CG	2:Q:1:NAG:C1	2.66	0.59
1:A:331:ASN:CG	3:U:1:NAG:C1	2.68	0.59
1:B:258:TRP:HZ3	1:B:260:ALA:HB2	1.68	0.59
1:B:581:THR:O	1:B:583:GLU:N	2.35	0.59
1:C:1125:ASN:ND2	1:C:1127:ASP:OD2	2.36	0.59
1:B:62:VAL:HG23	1:B:267:VAL:O	2.03	0.58
1:A:331:ASN:ND2	3:U:1:NAG:N2	2.48	0.58
1:C:128:ILE:HG21	1:C:229:LEU:CD1	2.34	0.58
1:A:258:TRP:HZ3	1:A:260:ALA:HB2	1.69	0.58
1:B:79:PHE:HB2	1:B:258:TRP:HH2	1.69	0.58
1:A:147:LYS:O	6:A:1406:NAG:C8	2.54	0.56
1:B:326:ILE:HG23	1:B:541:PHE:HA	1.87	0.56
1:C:258:TRP:HZ3	1:C:260:ALA:HB2	1.69	0.56
1:B:146:HIS:O	1:B:146:HIS:ND1	2.39	0.56
1:C:16:VAL:HG11	1:C:255:SER:HB2	1.88	0.56
1:B:360:ASN:H	1:B:523:THR:HG22	1.71	0.56

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:B:62:VAL:HG23	1:B:267:VAL:C	2.25	0.55
1:B:244:LEU:HD11	1:B:258:TRP:CG	2.42	0.55
1:A:79:PHE:HB2	1:A:258:TRP:HH2	1.69	0.54
1:B:128:ILE:HD13	1:B:229:LEU:HD11	1.89	0.54
1:B:168:PHE:CZ	1:B:229:LEU:HD22	2.42	0.54
1:A:29:THR:HG23	1:A:62:VAL:HG23	1.88	0.53
1:A:331:ASN:HD22	3:U:1:NAG:C1	2.09	0.53
1:C:211:ASN:O	1:C:212:LEU:HD12	2.09	0.53
1:B:544:ASN:OD1	1:B:564:GLN:NE2	2.42	0.52
1:B:468:ILE:O	1:B:468:ILE:HG22	2.09	0.52
1:A:108:THR:OG1	2:Y:1:NAG:H62	2.10	0.52
1:B:79:PHE:CB	1:B:258:TRP:CH2	2.92	0.52
1:C:568:ASP:OD1	1:C:569:ILE:N	2.39	0.51
1:A:335:LEU:HD12	1:A:362:VAL:O	2.11	0.51
1:C:211:ASN:C	1:C:212:LEU:HD12	2.31	0.51
1:A:69:HIS:O	1:A:259:THR:HA	2.11	0.51
1:B:258:TRP:CZ3	1:B:260:ALA:HB2	2.46	0.51
1:B:215:ASP:OD1	1:B:216:LEU:N	2.42	0.51
1:B:568:ASP:OD1	1:B:569:ILE:N	2.40	0.51
1:B:128:ILE:HG21	1:B:229:LEU:HD13	1.93	0.50
1:A:23:GLN:C	1:A:24:LEU:HD22	2.31	0.50
1:A:193:VAL:HG13	1:A:270:LEU:HD11	1.94	0.50
1:C:168:PHE:CZ	1:C:229:LEU:HD22	2.47	0.49
1:A:79:PHE:CB	1:A:258:TRP:CH2	2.95	0.49
1:A:326:ILE:HD11	1:A:533:LEU:HA	1.95	0.49
1:B:186:PHE:HE1	1:B:262:ALA:O	1.95	0.49
1:C:410:ILE:O	1:C:425:LEU:HD12	2.12	0.49
1:A:462:LYS:HE2	2:DA:1:NAG:H82	1.93	0.48
1:A:468:ILE:HG22	1:A:468:ILE:O	2.13	0.48
1:A:568:ASP:OD1	1:A:569:ILE:N	2.43	0.48
2:Y:1:NAG:H61	2:Y:2:NAG:N2	2.28	0.48
1:B:332:ILE:HG21	1:B:360:ASN:C	2.33	0.48
1:B:68:ILE:O	1:B:260:ALA:HB3	2.13	0.48
1:B:18:LEU:HB3	1:B:258:TRP:HE1	1.78	0.48
1:C:326:ILE:HD11	1:C:533:LEU:HA	1.96	0.48
1:A:69:HIS:O	1:A:260:ALA:N	2.38	0.48
1:A:326:ILE:HG23	1:A:541:PHE:HA	1.96	0.48
1:C:551:VAL:HG23	1:C:590:CYS:SG	2.54	0.47
1:A:258:TRP:CZ3	1:A:260:ALA:HB2	2.49	0.47
1:A:164:ASN:OD1	1:A:165:ASN:N	2.47	0.47
1:B:287:ASP:OD1	1:B:288:ALA:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:VAL:HG13	1:C:214:ARG:HG2	1.97	0.47
1:B:591:SER:HB3	1:C:740:MET:HE1	1.97	0.47
1:A:717:ASN:OD1	2:I:1:NAG:C1	2.62	0.47
1:C:326:ILE:HG23	1:C:541:PHE:HA	1.97	0.46
1:B:714:ILE:HD12	1:B:1096:VAL:HG11	1.97	0.46
1:B:1081:ILE:CD1	1:B:1115:ILE:HD13	2.46	0.46
1:B:703:ASN:ND2	1:C:787:GLN:OE1	2.46	0.46
1:C:61:ASN:HD21	6:C:1401:NAG:C7	2.29	0.46
1:A:319:ARG:HB2	1:A:591:SER:OG	2.15	0.46
1:B:551:VAL:HG23	1:B:590:CYS:SG	2.56	0.46
1:C:213:VAL:HG13	1:C:214:ARG:N	2.32	0.45
1:A:326:ILE:HD12	1:A:534:VAL:HG22	1.99	0.45
1:C:468:ILE:HG22	1:C:468:ILE:O	2.17	0.45
1:C:715:PRO:HA	1:C:1072:GLU:HA	2.00	0.45
1:B:213:VAL:HG13	1:B:214:ARG:N	2.32	0.44
1:C:18:LEU:HD23	1:C:258:TRP:CD1	2.52	0.44
1:A:287:ASP:OD1	1:A:288:ALA:N	2.47	0.44
1:A:433:VAL:HG22	1:A:512:VAL:HG13	1.99	0.44
1:B:410:ILE:O	1:B:425:LEU:HD12	2.17	0.44
1:C:714:ILE:HD12	1:C:1096:VAL:HG11	1.98	0.44
1:A:884:SER:OG	1:A:887:THR:OG1	2.31	0.44
1:B:16:VAL:HG11	1:B:255:SER:HB2	2.00	0.44
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.99	0.44
1:B:111:ASP:O	1:B:112:SER:OG	2.26	0.44
1:A:111:ASP:O	1:A:112:SER:OG	2.24	0.43
1:A:410:ILE:O	1:A:410:ILE:HG22	2.18	0.43
1:A:79:PHE:CB	1:A:258:TRP:HH2	2.31	0.43
1:A:472:ILE:HG21	1:A:488:CYS:HB3	2.01	0.43
1:B:841:LEU:HD12	1:B:841:LEU:C	2.38	0.43
1:A:410:ILE:O	1:A:425:LEU:HD12	2.17	0.43
1:A:717:ASN:ND2	2:I:1:NAG:O5	2.23	0.43
1:C:821:LEU:O	1:C:825:LYS:HG2	2.18	0.43
1:A:714:ILE:HD12	1:A:1096:VAL:HG11	2.01	0.43
1:B:335:LEU:HD12	1:B:335:LEU:N	2.33	0.43
1:A:1081:ILE:CD1	1:A:1133:VAL:HG22	2.47	0.43
1:C:159:VAL:HG13	1:C:160:TYR:CD2	2.54	0.43
1:B:319:ARG:CB	1:B:591:SER:OG	2.67	0.42
1:B:591:SER:HB3	1:C:740:MET:CE	2.49	0.42
1:B:61:ASN:HD21	6:B:1401:NAG:C7	2.33	0.42
1:B:244:LEU:HD11	1:B:258:TRP:CD2	2.55	0.42
1:B:336:CYS:HA	1:B:361:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:ASP:N	1:B:830:ASP:OD1	2.53	0.42
1:A:417:LYS:O	1:A:421:TYR:HB2	2.20	0.42
1:B:61:ASN:N	1:B:61:ASN:OD1	2.53	0.42
1:B:715:PRO:HA	1:B:1072:GLU:HA	2.02	0.42
1:A:454:ARG:HD3	1:A:457:ARG:HG2	2.02	0.41
1:A:830:ASP:OD1	1:A:830:ASP:N	2.53	0.41
1:A:87:ASN:OD1	1:A:87:ASN:N	2.52	0.41
1:B:401:VAL:HG22	1:B:509:ARG:HG2	2.02	0.41
1:B:802:PHE:HZ	1:B:898:PHE:CZ	2.38	0.41
1:C:117:LEU:HD22	1:C:231:ILE:HD13	2.02	0.41
1:C:319:ARG:HB3	1:C:591:SER:OG	2.20	0.41
1:B:523:THR:HG22	1:B:523:THR:O	2.20	0.41
1:C:435:ALA:HA	1:C:509:ARG:O	2.20	0.41
1:B:97:LYS:HE2	1:B:262:ALA:CB	2.39	0.41
1:A:372:ALA:HB1	1:A:374:PHE:CZ	2.56	0.41
1:B:821:LEU:O	1:B:825:LYS:HG2	2.20	0.41
1:C:108:THR:HG23	1:C:109:THR:N	2.34	0.41
1:C:319:ARG:CB	1:C:591:SER:OG	2.68	0.41
1:A:108:THR:OG1	2:Y:1:NAG:C6	2.69	0.41
1:A:821:LEU:O	1:A:825:LYS:HG2	2.21	0.41
1:B:79:PHE:CB	1:B:258:TRP:HH2	2.31	0.41
1:B:164:ASN:HD21	3:BA:1:NAG:C6	2.33	0.41
1:A:319:ARG:CB	1:A:591:SER:OG	2.69	0.41
1:A:339:GLY:O	1:A:343:ASN:HB2	2.20	0.41
1:A:656:VAL:HG23	1:A:695:TYR:HB3	2.03	0.41
1:B:258:TRP:HB2	1:B:259:THR:H	1.73	0.41
1:B:433:VAL:HG22	1:B:512:VAL:HG13	2.02	0.41
1:B:778:THR:CG2	1:B:870:ILE:HD11	2.51	0.41
1:A:171:VAL:HG21	2:Q:2:NAG:H82	2.03	0.41
1:A:310:LYS:NZ	1:A:663:ASP:OD2	2.44	0.41
1:A:326:ILE:CG2	1:A:541:PHE:HA	2.51	0.40
1:C:152:TRP:CD1	1:C:180:GLU:HB3	2.55	0.40
1:C:310:LYS:NZ	1:C:663:ASP:OD2	2.44	0.40
1:B:330:PRO:HD2	1:B:525:CYS:SG	2.61	0.40
1:C:287:ASP:OD1	1:C:288:ALA:N	2.52	0.40
1:C:830:ASP:OD1	1:C:830:ASP:N	2.50	0.40
1:B:360:ASN:N	1:B:523:THR:HG22	2.36	0.40
1:B:884:SER:HG	1:B:887:THR:HG1	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1097/1310 (84%)	1068 (97%)	29 (3%)	0	100	100
1	B	1097/1310 (84%)	1074 (98%)	22 (2%)	1 (0%)	51	82
1	C	1097/1310 (84%)	1065 (97%)	31 (3%)	1 (0%)	51	82
All	All	3291/3930 (84%)	3207 (97%)	82 (2%)	2 (0%)	54	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	262	ALA
1	C	262	ALA

5.3.2 Protein sidechains ⓘ

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	965/1136 (85%)	960 (100%)	5 (0%)	88	96
1	B	965/1136 (85%)	962 (100%)	3 (0%)	92	98
1	C	965/1136 (85%)	959 (99%)	6 (1%)	86	96
All	All	2895/3408 (85%)	2881 (100%)	14 (0%)	89	96

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

Mol	Chain	Res	Type
1	A	62	VAL

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Mol	Chain	Res	Type
1	A	144	TYR
1	A	266	TYR
1	A	658	ASN
1	A	844	ILE
1	B	15	CYS
1	B	62	VAL
1	B	844	ILE
1	C	15	CYS
1	C	351	TYR
1	C	641	ASN
1	C	738	CYS
1	C	760	CYS
1	C	844	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	122	ASN
1	A	331	ASN
1	A	343	ASN
1	A	657	ASN
1	B	164	ASN
1	B	544	ASN
1	B	564	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

102 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	$\#\|Z\|>2$
3	NAG	0	1	1,3	14,14,15	0.26	0	17,19,21	0.34	0
3	NAG	0	2	3	14,14,15	0.28	0	17,19,21	0.46	0
2	NAG	1A	1	1,2	14,14,15	0.28	0	17,19,21	0.41	0
2	NAG	1A	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	MAN	1A	3	2	11,11,12	0.79	0	15,15,17	1.13	2 (13%)
4	NAG	2	1	1,4	14,14,15	0.25	0	17,19,21	0.89	1 (5%)
4	NAG	2	2	4	14,14,15	0.17	0	17,19,21	0.55	0
4	FUC	2	3	4	10,10,11	1.48	2 (20%)	14,14,16	1.59	3 (21%)
2	NAG	4A	1	1,2	14,14,15	0.23	0	17,19,21	0.51	0
2	NAG	4A	2	2	14,14,15	0.23	0	17,19,21	0.38	0
2	MAN	4A	3	2	11,11,12	0.76	0	15,15,17	1.12	2 (13%)
2	NAG	5	1	1,2	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	5	2	2	14,14,15	0.22	0	17,19,21	0.51	0
2	MAN	5	3	2	11,11,12	0.75	0	15,15,17	1.16	2 (13%)
5	NAG	7A	1	1,5	14,14,15	0.23	0	17,19,21	0.48	0
5	NAG	7A	2	5	14,14,15	0.23	0	17,19,21	0.42	0
5	MAN	7A	3	5	11,11,12	0.76	0	15,15,17	1.04	2 (13%)
5	MAN	7A	4	5	11,11,12	0.62	0	15,15,17	1.17	2 (13%)
3	NAG	9	1	1,3	14,14,15	1.22	1 (7%)	17,19,21	1.13	2 (11%)
3	NAG	9	2	3	14,14,15	0.30	0	17,19,21	0.63	1 (5%)
3	NAG	BA	1	3	14,14,15	0.26	0	17,19,21	0.50	0
3	NAG	BA	2	3	14,14,15	0.25	0	17,19,21	0.47	0
2	NAG	DA	1	1,2	14,14,15	0.26	0	17,19,21	0.54	0
2	NAG	DA	2	2	14,14,15	0.22	0	17,19,21	0.48	0
2	MAN	DA	3	2	11,11,12	0.76	0	15,15,17	1.04	2 (13%)
2	NAG	GA	1	2	14,14,15	0.31	0	17,19,21	0.44	0
2	NAG	GA	2	2	14,14,15	0.20	0	17,19,21	0.40	0
2	MAN	GA	3	2	11,11,12	0.72	0	15,15,17	1.03	2 (13%)
2	NAG	I	1	2	14,14,15	0.32	0	17,19,21	0.50	0
2	NAG	I	2	2	14,14,15	0.26	0	17,19,21	0.38	0
2	MAN	I	3	2	11,11,12	0.76	0	15,15,17	1.20	2 (13%)
2	NAG	JA	1	1,2	14,14,15	0.24	0	17,19,21	0.43	0
2	NAG	JA	2	2	14,14,15	0.27	0	17,19,21	0.40	0
2	MAN	JA	3	2	11,11,12	0.86	0	15,15,17	1.38	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	L	1	1,3	14,14,15	0.26	0	17,19,21	0.37	0
3	NAG	L	2	3	14,14,15	0.29	0	17,19,21	0.43	0
2	NAG	MA	1	1,2	14,14,15	0.34	0	17,19,21	0.39	0
2	NAG	MA	2	2	14,14,15	0.23	0	17,19,21	0.39	0
2	MAN	MA	3	2	11,11,12	0.77	0	15,15,17	1.07	2 (13%)
4	NAG	N	1	4	14,14,15	0.15	0	17,19,21	0.81	1 (5%)
4	NAG	N	2	4	14,14,15	0.19	0	17,19,21	0.57	0
4	FUC	N	3	4	10,10,11	1.67	2 (20%)	14,14,16	1.54	4 (28%)
2	NAG	PA	1	1,2	14,14,15	0.21	0	17,19,21	0.53	0
2	NAG	PA	2	2	14,14,15	0.22	0	17,19,21	0.41	0
2	MAN	PA	3	2	11,11,12	0.84	1 (9%)	15,15,17	1.18	2 (13%)
2	NAG	Q	1	2	14,14,15	0.22	0	17,19,21	0.37	0
2	NAG	Q	2	2	14,14,15	0.22	0	17,19,21	0.45	0
2	MAN	Q	3	2	11,11,12	0.75	0	15,15,17	1.18	2 (13%)
5	NAG	SA	1	5	14,14,15	0.23	0	17,19,21	0.50	0
5	NAG	SA	2	5	14,14,15	0.22	0	17,19,21	0.46	0
5	MAN	SA	3	5	11,11,12	0.78	0	15,15,17	1.02	2 (13%)
5	MAN	SA	4	5	11,11,12	0.66	0	15,15,17	1.25	2 (13%)
3	NAG	U	1	3	14,14,15	1.26	1 (7%)	17,19,21	1.16	2 (11%)
3	NAG	U	2	3	14,14,15	0.35	0	17,19,21	0.61	0
3	NAG	W	1	1,3	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	W	2	3	14,14,15	0.34	0	17,19,21	0.47	0
2	NAG	Y	1	1,2	14,14,15	0.29	0	17,19,21	0.59	0
2	NAG	Y	2	2	14,14,15	0.19	0	17,19,21	0.48	0
2	MAN	Y	3	2	11,11,12	0.77	0	15,15,17	0.88	1 (6%)
2	NAG	b	1	2	14,14,15	0.34	0	17,19,21	0.43	0
2	NAG	b	2	2	14,14,15	0.21	0	17,19,21	0.42	0
2	MAN	b	3	2	11,11,12	0.75	0	15,15,17	1.10	2 (13%)
2	NAG	cA	1	1,2	14,14,15	0.33	0	17,19,21	0.49	0
2	NAG	cA	2	2	14,14,15	0.27	0	17,19,21	0.43	0
2	MAN	cA	3	2	11,11,12	0.79	0	15,15,17	1.22	2 (13%)
2	NAG	e	1	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	e	2	2	14,14,15	0.28	0	17,19,21	0.40	0
2	MAN	e	3	2	11,11,12	0.77	0	15,15,17	1.17	2 (13%)
3	NAG	fA	1	1,3	14,14,15	0.25	0	17,19,21	0.39	0
3	NAG	fA	2	3	14,14,15	0.30	0	17,19,21	0.47	0
2	NAG	h	1	2	14,14,15	0.26	0	17,19,21	0.41	0
2	NAG	h	2	2	14,14,15	0.22	0	17,19,21	0.40	0
2	MAN	h	3	2	11,11,12	0.77	0	15,15,17	1.23	2 (13%)
4	NAG	hA	1	1,4	14,14,15	0.16	0	17,19,21	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	hA	2	4	14,14,15	0.20	0	17,19,21	0.66	1 (5%)
4	FUC	hA	3	4	10,10,11	1.66	2 (20%)	14,14,16	1.60	4 (28%)
2	NAG	k	1	1,2	14,14,15	0.22	0	17,19,21	0.56	0
2	NAG	k	2	2	14,14,15	0.21	0	17,19,21	0.46	0
2	MAN	k	3	2	11,11,12	0.77	0	15,15,17	1.20	2 (13%)
2	NAG	kA	1	1,2	14,14,15	0.24	0	17,19,21	0.39	0
2	NAG	kA	2	2	14,14,15	0.22	0	17,19,21	0.50	0
2	MAN	kA	3	2	11,11,12	0.72	0	15,15,17	1.15	2 (13%)
5	NAG	n	1	1,5	14,14,15	0.21	0	17,19,21	0.48	0
5	NAG	n	2	5	14,14,15	0.26	0	17,19,21	0.45	0
5	MAN	n	3	5	11,11,12	0.74	0	15,15,17	0.98	2 (13%)
5	MAN	n	4	5	11,11,12	0.72	0	15,15,17	1.30	2 (13%)
3	NAG	oA	1	1,3	14,14,15	1.18	1 (7%)	17,19,21	1.11	1 (5%)
3	NAG	oA	2	3	14,14,15	0.35	0	17,19,21	0.64	1 (5%)
3	NAG	qA	1	1,3	14,14,15	0.30	0	17,19,21	0.54	0
3	NAG	qA	2	3	14,14,15	0.20	0	17,19,21	0.53	0
2	NAG	sA	1	1,2	14,14,15	0.26	0	17,19,21	0.55	0
2	NAG	sA	2	2	14,14,15	0.23	0	17,19,21	0.45	0
2	MAN	sA	3	2	11,11,12	0.79	0	15,15,17	0.99	2 (13%)
2	NAG	vA	1	1,2	14,14,15	0.35	0	17,19,21	0.42	0
2	NAG	vA	2	2	14,14,15	0.27	0	17,19,21	0.45	0
2	MAN	vA	3	2	11,11,12	0.73	0	15,15,17	1.05	2 (13%)
2	NAG	x	1	1,2	14,14,15	0.32	0	17,19,21	0.49	0
2	NAG	x	2	2	14,14,15	0.30	0	17,19,21	0.45	0
2	MAN	x	3	2	11,11,12	0.75	0	15,15,17	1.09	2 (13%)
2	NAG	yA	1	1,2	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	yA	2	2	14,14,15	0.26	0	17,19,21	0.47	0
2	MAN	yA	3	2	11,11,12	0.73	0	15,15,17	1.17	2 (13%)

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
3	NAG	0	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	0	2	3	-	0/6/23/26	0/1/1/1
2	NAG	1A	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	1A	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	1A	3	2	-	2/2/19/22	1/1/1/1
4	NAG	2	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	2	2	4	-	0/6/23/26	0/1/1/1
4	FUC	2	3	4	-	-	0/1/1/1
2	NAG	4A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	4A	2	2	-	0/6/23/26	0/1/1/1
2	MAN	4A	3	2	-	2/2/19/22	1/1/1/1
2	NAG	5	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	5	2	2	-	2/6/23/26	0/1/1/1
2	MAN	5	3	2	-	1/2/19/22	1/1/1/1
5	NAG	7A	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	7A	2	5	-	0/6/23/26	0/1/1/1
5	MAN	7A	3	5	-	0/2/19/22	1/1/1/1
5	MAN	7A	4	5	-	0/2/19/22	0/1/1/1
3	NAG	9	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	9	2	3	-	0/6/23/26	0/1/1/1
3	NAG	BA	1	3	-	0/6/23/26	0/1/1/1
3	NAG	BA	2	3	-	0/6/23/26	0/1/1/1
2	NAG	DA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	DA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	DA	3	2	-	0/2/19/22	1/1/1/1
2	NAG	GA	1	2	-	0/6/23/26	0/1/1/1
2	NAG	GA	2	2	-	1/6/23/26	0/1/1/1
2	MAN	GA	3	2	-	0/2/19/22	1/1/1/1
2	NAG	I	1	2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	MAN	I	3	2	-	1/2/19/22	1/1/1/1
2	NAG	JA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	JA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	JA	3	2	-	2/2/19/22	1/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
2	NAG	MA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	MA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	MA	3	2	-	2/2/19/22	1/1/1/1
4	NAG	N	1	4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	FUC	N	3	4	-	-	0/1/1/1
2	NAG	PA	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	PA	2	2	-	1/6/23/26	0/1/1/1
2	MAN	PA	3	2	-	2/2/19/22	1/1/1/1
2	NAG	Q	1	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	MAN	Q	3	2	-	2/2/19/22	1/1/1/1
5	NAG	SA	1	5	-	2/6/23/26	0/1/1/1
5	NAG	SA	2	5	-	2/6/23/26	0/1/1/1
5	MAN	SA	3	5	-	1/2/19/22	1/1/1/1
5	MAN	SA	4	5	-	0/2/19/22	0/1/1/1
3	NAG	U	1	3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
2	NAG	Y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	2/6/23/26	0/1/1/1
2	MAN	Y	3	2	-	0/2/19/22	1/1/1/1
2	NAG	b	1	2	-	2/6/23/26	0/1/1/1
2	NAG	b	2	2	-	1/6/23/26	0/1/1/1
2	MAN	b	3	2	-	0/2/19/22	1/1/1/1
2	NAG	cA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	cA	2	2	-	1/6/23/26	0/1/1/1
2	MAN	cA	3	2	-	1/2/19/22	1/1/1/1
2	NAG	e	1	2	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	2/6/23/26	0/1/1/1
2	MAN	e	3	2	-	0/2/19/22	1/1/1/1
3	NAG	fA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	fA	2	3	-	0/6/23/26	0/1/1/1
2	NAG	h	1	2	-	2/6/23/26	0/1/1/1
2	NAG	h	2	2	-	1/6/23/26	0/1/1/1
2	MAN	h	3	2	-	1/2/19/22	1/1/1/1
4	NAG	hA	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	hA	2	4	-	2/6/23/26	0/1/1/1
4	FUC	hA	3	4	-	-	0/1/1/1
2	NAG	k	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	k	2	2	-	0/6/23/26	0/1/1/1
2	MAN	k	3	2	-	2/2/19/22	1/1/1/1
2	NAG	kA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	kA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	kA	3	2	-	2/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	n	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	n	2	5	-	2/6/23/26	0/1/1/1
5	MAN	n	3	5	-	0/2/19/22	1/1/1/1
5	MAN	n	4	5	-	0/2/19/22	0/1/1/1
3	NAG	oA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	oA	2	3	-	0/6/23/26	0/1/1/1
3	NAG	qA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	qA	2	3	-	1/6/23/26	0/1/1/1
2	NAG	sA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	sA	2	2	-	0/6/23/26	0/1/1/1
2	MAN	sA	3	2	-	1/2/19/22	1/1/1/1
2	NAG	vA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	vA	2	2	-	1/6/23/26	0/1/1/1
2	MAN	vA	3	2	-	0/2/19/22	1/1/1/1
2	NAG	x	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	x	2	2	-	0/6/23/26	0/1/1/1
2	MAN	x	3	2	-	2/2/19/22	1/1/1/1
2	NAG	yA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	yA	2	2	-	2/6/23/26	0/1/1/1
2	MAN	yA	3	2	-	1/2/19/22	1/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	1	NAG	O5-C1	-4.63	1.36	1.43
3	9	1	NAG	O5-C1	-4.48	1.36	1.43
3	oA	1	NAG	O5-C1	-4.34	1.36	1.43
4	hA	3	FUC	C2-C3	3.87	1.58	1.52
4	N	3	FUC	C2-C3	3.74	1.58	1.52
4	2	3	FUC	C2-C3	3.56	1.57	1.52
4	hA	3	FUC	C1-C2	3.20	1.59	1.52
4	N	3	FUC	C1-C2	2.96	1.59	1.52
4	2	3	FUC	C1-C2	2.07	1.56	1.52
2	PA	3	MAN	O5-C5	2.07	1.47	1.43

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	JA	3	MAN	C1-O5-C5	3.93	117.52	112.19
5	n	4	MAN	C1-O5-C5	3.74	117.26	112.19
5	SA	4	MAN	C1-O5-C5	3.60	117.07	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	cA	3	MAN	C1-O5-C5	3.52	116.95	112.19
2	h	3	MAN	C1-O5-C5	3.38	116.77	112.19
2	I	3	MAN	C1-O5-C5	3.37	116.75	112.19
2	yA	3	MAN	C1-O5-C5	3.32	116.69	112.19
2	e	3	MAN	C1-O5-C5	3.27	116.62	112.19
4	2	3	FUC	C1-C2-C3	3.26	113.68	109.67
2	k	3	MAN	C1-O5-C5	3.26	116.61	112.19
5	7A	4	MAN	C1-O5-C5	3.21	116.54	112.19
2	Q	3	MAN	C1-O5-C5	3.20	116.53	112.19
2	PA	3	MAN	C1-O5-C5	3.13	116.44	112.19
2	5	3	MAN	C1-O5-C5	3.09	116.39	112.19
2	kA	3	MAN	C1-O5-C5	3.08	116.36	112.19
4	2	1	NAG	C1-O5-C5	3.07	116.36	112.19
4	2	3	FUC	C1-O5-C5	3.01	119.61	112.78
3	oA	1	NAG	C1-O5-C5	3.00	116.26	112.19
4	N	3	FUC	O2-C2-C1	2.98	115.24	109.15
2	1A	3	MAN	C1-O5-C5	2.95	116.19	112.19
2	b	3	MAN	C1-O5-C5	2.94	116.17	112.19
2	4A	3	MAN	C1-O5-C5	2.89	116.11	112.19
3	U	1	NAG	C1-O5-C5	2.88	116.09	112.19
2	x	3	MAN	C1-O5-C5	2.86	116.06	112.19
4	hA	3	FUC	C1-O5-C5	2.82	119.17	112.78
2	MA	3	MAN	C1-O5-C5	2.75	115.92	112.19
4	hA	1	NAG	C1-O5-C5	2.75	115.92	112.19
4	hA	3	FUC	O2-C2-C1	2.74	114.77	109.15
2	vA	3	MAN	C1-O5-C5	2.74	115.91	112.19
3	9	1	NAG	C1-O5-C5	2.74	115.90	112.19
4	N	1	NAG	C1-O5-C5	2.73	115.89	112.19
2	GA	3	MAN	C1-O5-C5	2.71	115.86	112.19
4	hA	3	FUC	C1-C2-C3	2.68	112.96	109.67
4	N	3	FUC	O5-C5-C4	2.68	114.33	109.52
2	DA	3	MAN	C1-O5-C5	2.63	115.76	112.19
5	7A	3	MAN	C1-O5-C5	2.62	115.74	112.19
5	SA	3	MAN	C1-O5-C5	2.56	115.66	112.19
4	N	3	FUC	C1-O5-C5	2.56	118.57	112.78
2	kA	3	MAN	O2-C2-C3	-2.47	105.20	110.14
2	sA	3	MAN	C1-O5-C5	2.46	115.53	112.19
5	n	3	MAN	C1-O5-C5	2.46	115.52	112.19
5	SA	3	MAN	O2-C2-C3	-2.46	105.22	110.14
2	PA	3	MAN	O2-C2-C3	-2.45	105.24	110.14
5	7A	3	MAN	O2-C2-C3	-2.44	105.25	110.14
2	Q	3	MAN	O2-C2-C3	-2.44	105.25	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	k	3	MAN	O2-C2-C3	-2.44	105.26	110.14
2	4A	3	MAN	O2-C2-C3	-2.44	105.26	110.14
2	5	3	MAN	O2-C2-C3	-2.43	105.27	110.14
2	I	3	MAN	O2-C2-C3	-2.43	105.28	110.14
4	hA	3	FUC	O5-C5-C4	2.42	113.86	109.52
2	1A	3	MAN	O2-C2-C3	-2.42	105.30	110.14
2	JA	3	MAN	O2-C2-C3	-2.40	105.32	110.14
5	n	3	MAN	O2-C2-C3	-2.40	105.32	110.14
2	x	3	MAN	O2-C2-C3	-2.40	105.34	110.14
2	h	3	MAN	O2-C2-C3	-2.38	105.36	110.14
2	DA	3	MAN	O2-C2-C3	-2.36	105.42	110.14
5	n	4	MAN	O2-C2-C3	-2.32	105.48	110.14
2	MA	3	MAN	O2-C2-C3	-2.32	105.48	110.14
2	b	3	MAN	O2-C2-C3	-2.30	105.53	110.14
2	yA	3	MAN	O2-C2-C3	-2.30	105.53	110.14
2	e	3	MAN	O2-C2-C3	-2.29	105.55	110.14
2	cA	3	MAN	O2-C2-C3	-2.28	105.57	110.14
5	SA	4	MAN	O2-C2-C3	-2.26	105.61	110.14
2	vA	3	MAN	O2-C2-C3	-2.26	105.62	110.14
5	7A	4	MAN	O2-C2-C3	-2.25	105.63	110.14
2	sA	3	MAN	O2-C2-C3	-2.25	105.63	110.14
2	GA	3	MAN	O2-C2-C3	-2.24	105.65	110.14
4	2	3	FUC	O2-C2-C1	2.24	113.73	109.15
4	hA	2	NAG	C1-O5-C5	2.21	115.19	112.19
2	Y	3	MAN	O2-C2-C3	-2.16	105.80	110.14
4	N	3	FUC	C1-C2-C3	2.12	112.28	109.67
3	oA	2	NAG	C1-O5-C5	2.06	114.99	112.19
3	U	1	NAG	C3-C4-C5	2.05	113.89	110.24
3	9	1	NAG	C3-C4-C5	2.03	113.87	110.24
3	9	2	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	2	1	NAG	O5-C5-C6-O6
4	hA	2	NAG	O5-C5-C6-O6
2	h	1	NAG	O5-C5-C6-O6
2	kA	3	MAN	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	hA	1	NAG	O5-C5-C6-O6
2	x	3	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	N	1	NAG	C4-C5-C6-O6
4	2	1	NAG	C4-C5-C6-O6
2	JA	3	MAN	O5-C5-C6-O6
2	h	1	NAG	C4-C5-C6-O6
4	hA	1	NAG	C4-C5-C6-O6
2	Q	3	MAN	O5-C5-C6-O6
2	x	3	MAN	C4-C5-C6-O6
2	JA	3	MAN	C4-C5-C6-O6
3	fA	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
4	hA	2	NAG	C4-C5-C6-O6
2	k	3	MAN	O5-C5-C6-O6
2	JA	2	NAG	O5-C5-C6-O6
5	SA	1	NAG	O5-C5-C6-O6
2	1A	3	MAN	O5-C5-C6-O6
2	4A	3	MAN	O5-C5-C6-O6
5	n	1	NAG	O5-C5-C6-O6
2	MA	3	MAN	O5-C5-C6-O6
2	PA	3	MAN	O5-C5-C6-O6
2	yA	2	NAG	O5-C5-C6-O6
2	5	3	MAN	O5-C5-C6-O6
2	JA	2	NAG	C4-C5-C6-O6
5	SA	1	NAG	C4-C5-C6-O6
5	n	1	NAG	C4-C5-C6-O6
2	yA	2	NAG	C4-C5-C6-O6
3	0	1	NAG	O5-C5-C6-O6
3	fA	1	NAG	C4-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
2	h	3	MAN	O5-C5-C6-O6
2	MA	1	NAG	O5-C5-C6-O6
2	1A	2	NAG	C4-C5-C6-O6
2	cA	2	NAG	O5-C5-C6-O6
3	U	1	NAG	C1-C2-N2-C7
3	9	1	NAG	C1-C2-N2-C7
3	9	1	NAG	O5-C5-C6-O6
2	I	3	MAN	O5-C5-C6-O6
3	oA	1	NAG	C1-C2-N2-C7
2	kA	3	MAN	C4-C5-C6-O6
2	Y	2	NAG	C4-C5-C6-O6
2	b	1	NAG	C4-C5-C6-O6
2	1A	2	NAG	O5-C5-C6-O6
5	n	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	Q	3	MAN	C4-C5-C6-O6
2	b	1	NAG	O5-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6
2	e	2	NAG	C4-C5-C6-O6
5	n	2	NAG	O5-C5-C6-O6
5	7A	1	NAG	C4-C5-C6-O6
2	e	2	NAG	O5-C5-C6-O6
5	7A	1	NAG	O5-C5-C6-O6
2	1A	3	MAN	C4-C5-C6-O6
2	k	3	MAN	C4-C5-C6-O6
2	1A	1	NAG	C4-C5-C6-O6
2	4A	3	MAN	C4-C5-C6-O6
5	SA	2	NAG	C4-C5-C6-O6
3	0	1	NAG	C4-C5-C6-O6
2	sA	3	MAN	O5-C5-C6-O6
2	MA	2	NAG	C4-C5-C6-O6
2	PA	3	MAN	C4-C5-C6-O6
2	PA	2	NAG	O5-C5-C6-O6
2	1A	1	NAG	O5-C5-C6-O6
2	vA	2	NAG	C4-C5-C6-O6
2	5	2	NAG	C4-C5-C6-O6
3	oA	1	NAG	O5-C5-C6-O6
2	GA	2	NAG	C4-C5-C6-O6
2	cA	3	MAN	C4-C5-C6-O6
2	MA	3	MAN	C4-C5-C6-O6
2	MA	2	NAG	O5-C5-C6-O6
2	DA	1	NAG	C4-C5-C6-O6
3	qA	2	NAG	C4-C5-C6-O6
5	SA	2	NAG	O5-C5-C6-O6
5	SA	3	MAN	C4-C5-C6-O6
3	U	1	NAG	C3-C2-N2-C7
3	9	1	NAG	C3-C2-N2-C7
3	oA	1	NAG	C3-C2-N2-C7
2	MA	1	NAG	C4-C5-C6-O6
2	h	2	NAG	C4-C5-C6-O6
2	5	2	NAG	O5-C5-C6-O6
2	yA	3	MAN	C4-C5-C6-O6
2	DA	1	NAG	O5-C5-C6-O6
2	b	2	NAG	C4-C5-C6-O6

All (24) ring outliers are listed below:

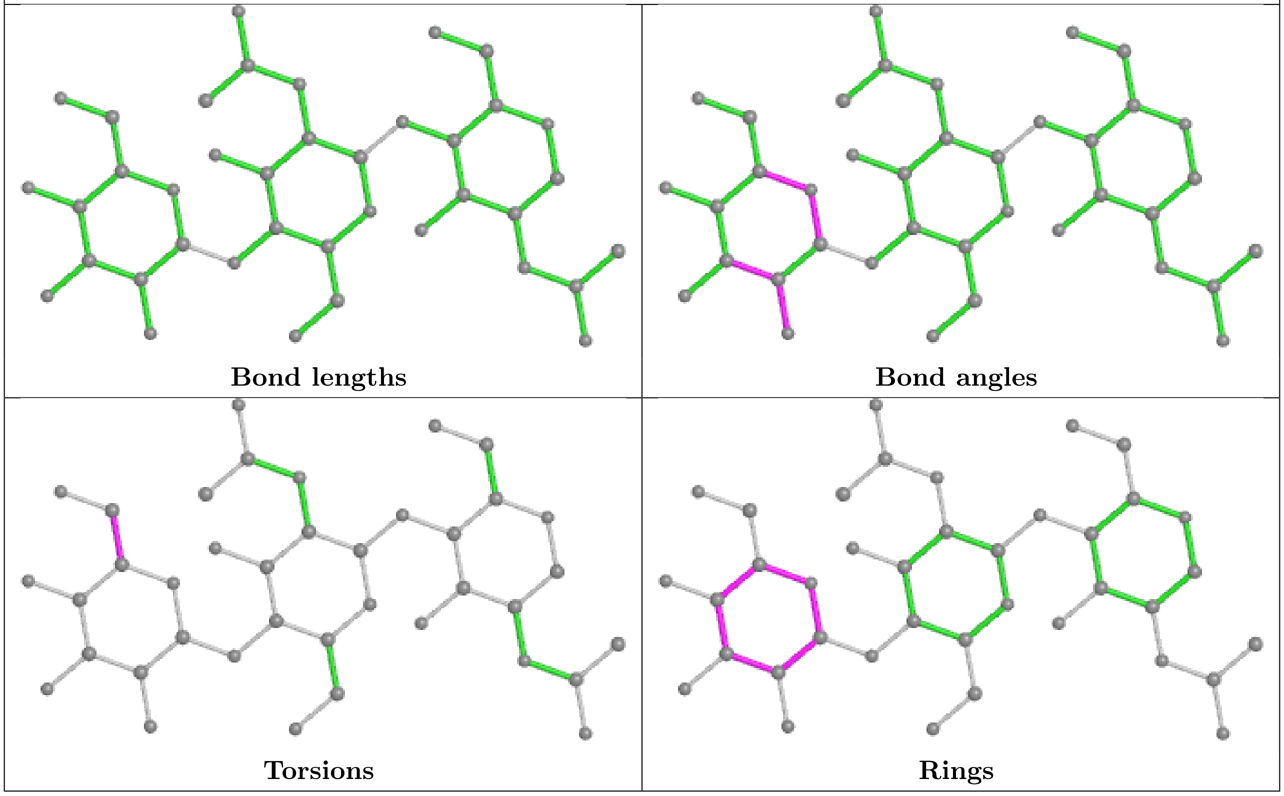
Mol	Chain	Res	Type	Atoms
5	n	3	MAN	C1-C2-C3-C4-C5-O5
5	7A	3	MAN	C1-C2-C3-C4-C5-O5
5	SA	3	MAN	C1-C2-C3-C4-C5-O5
2	Y	3	MAN	C1-C2-C3-C4-C5-O5
2	sA	3	MAN	C1-C2-C3-C4-C5-O5
2	JA	3	MAN	C1-C2-C3-C4-C5-O5
2	DA	3	MAN	C1-C2-C3-C4-C5-O5
2	GA	3	MAN	C1-C2-C3-C4-C5-O5
2	yA	3	MAN	C1-C2-C3-C4-C5-O5
2	MA	3	MAN	C1-C2-C3-C4-C5-O5
2	vA	3	MAN	C1-C2-C3-C4-C5-O5
2	e	3	MAN	C1-C2-C3-C4-C5-O5
2	Q	3	MAN	C1-C2-C3-C4-C5-O5
2	b	3	MAN	C1-C2-C3-C4-C5-O5
2	1A	3	MAN	C1-C2-C3-C4-C5-O5
2	5	3	MAN	C1-C2-C3-C4-C5-O5
2	4A	3	MAN	C1-C2-C3-C4-C5-O5
2	h	3	MAN	C1-C2-C3-C4-C5-O5
2	x	3	MAN	C1-C2-C3-C4-C5-O5
2	PA	3	MAN	C1-C2-C3-C4-C5-O5
2	kA	3	MAN	C1-C2-C3-C4-C5-O5
2	cA	3	MAN	C1-C2-C3-C4-C5-O5
2	I	3	MAN	C1-C2-C3-C4-C5-O5
2	k	3	MAN	C1-C2-C3-C4-C5-O5

12 monomers are involved in 28 short contacts:

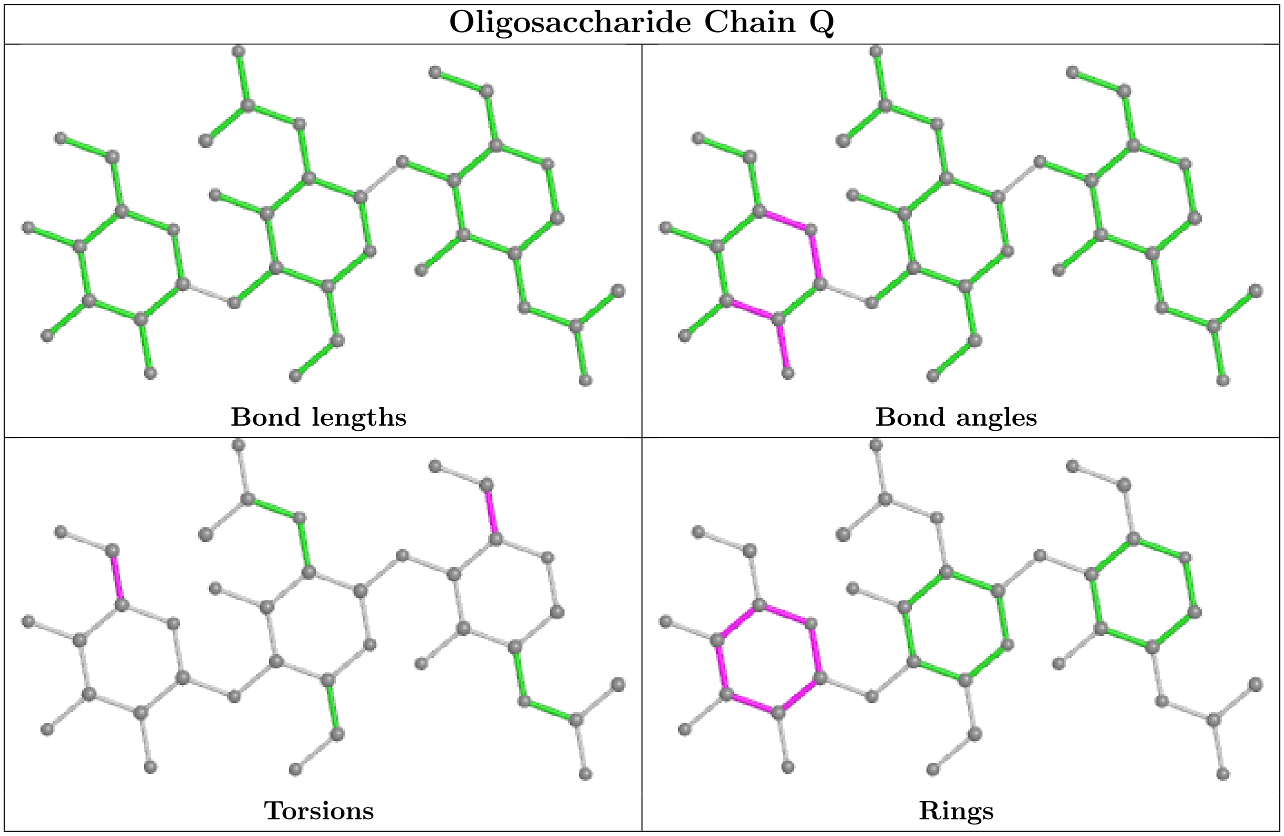
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	1	NAG	3	0
2	Y	1	NAG	3	0
3	9	1	NAG	2	0
3	9	2	NAG	2	0
2	Y	2	NAG	2	0
2	DA	1	NAG	1	0
4	N	1	NAG	3	0
3	BA	1	NAG	1	0
2	Q	2	NAG	1	0
3	U	2	NAG	2	0
3	U	1	NAG	8	0
2	I	1	NAG	5	0

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

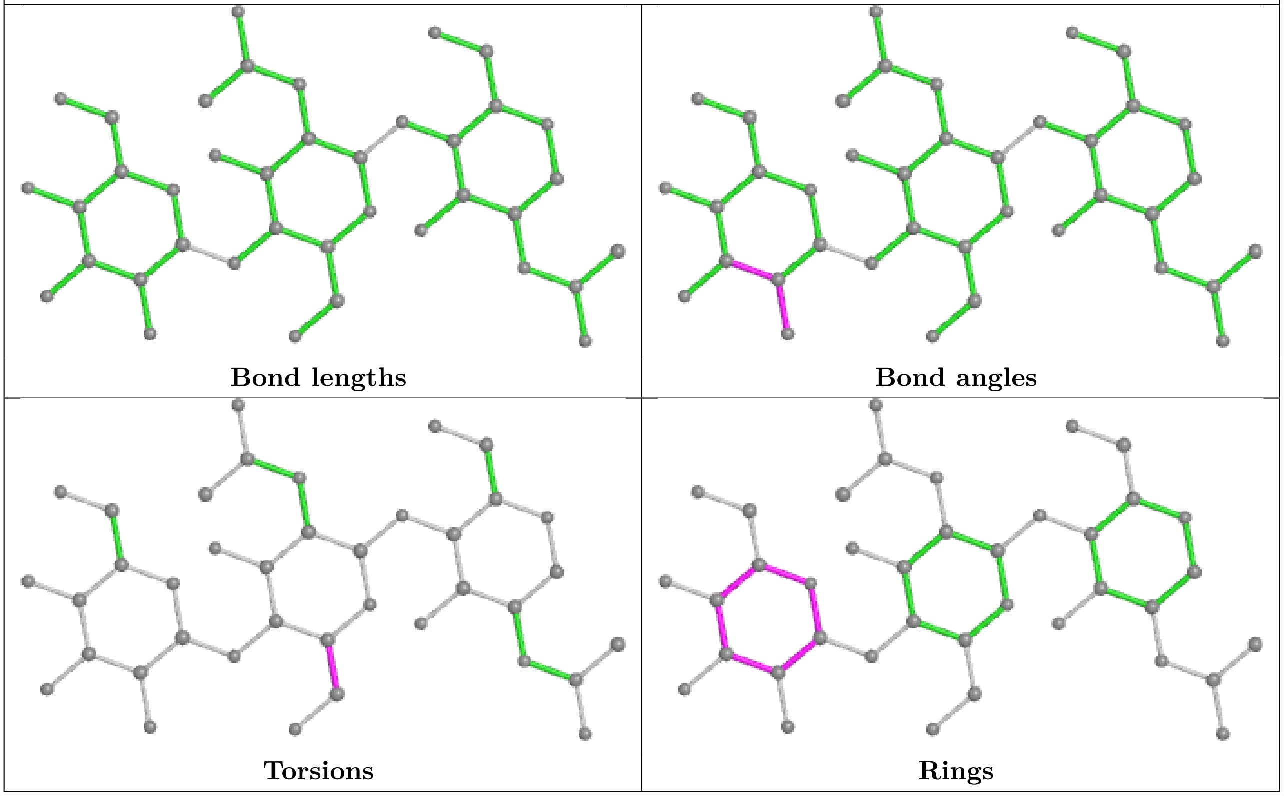
Oligosaccharide Chain I



Oligosaccharide Chain Q



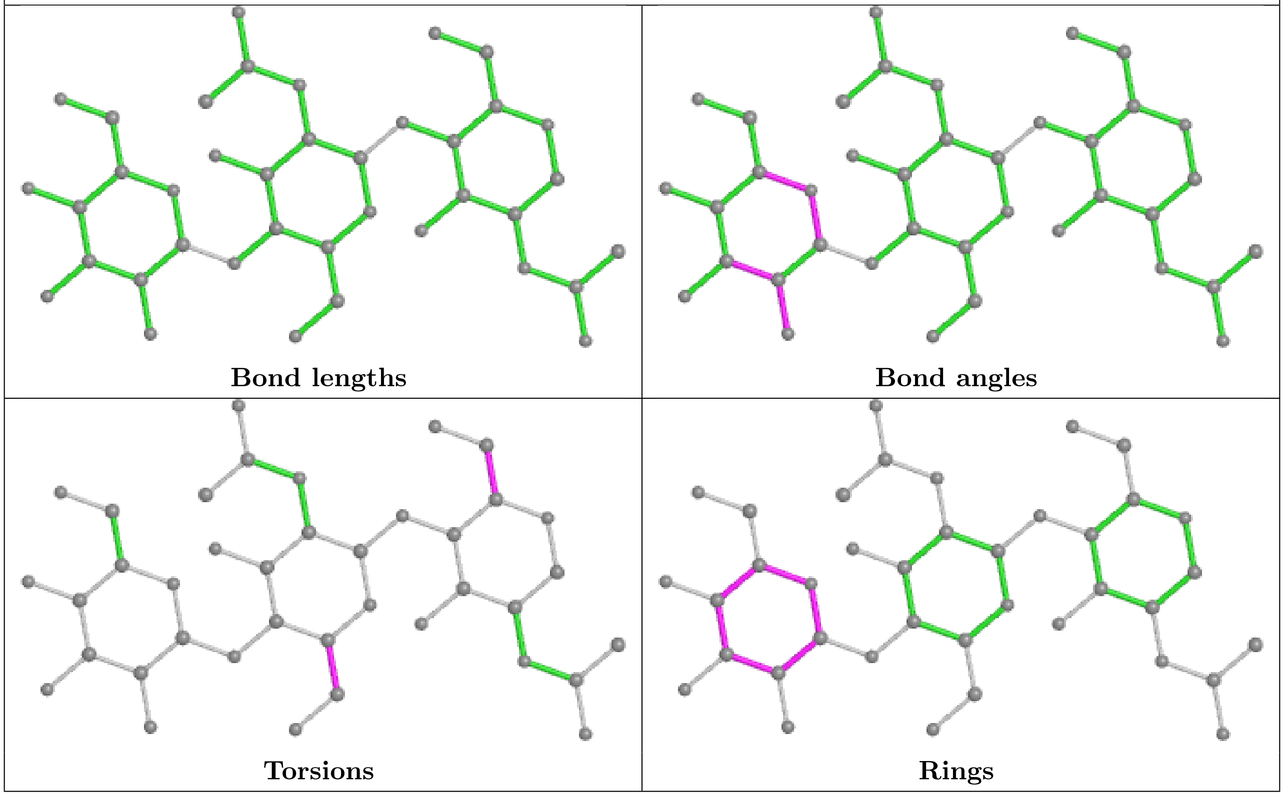
Oligosaccharide Chain Y



Bond lengths Bond angles

Torsions Rings

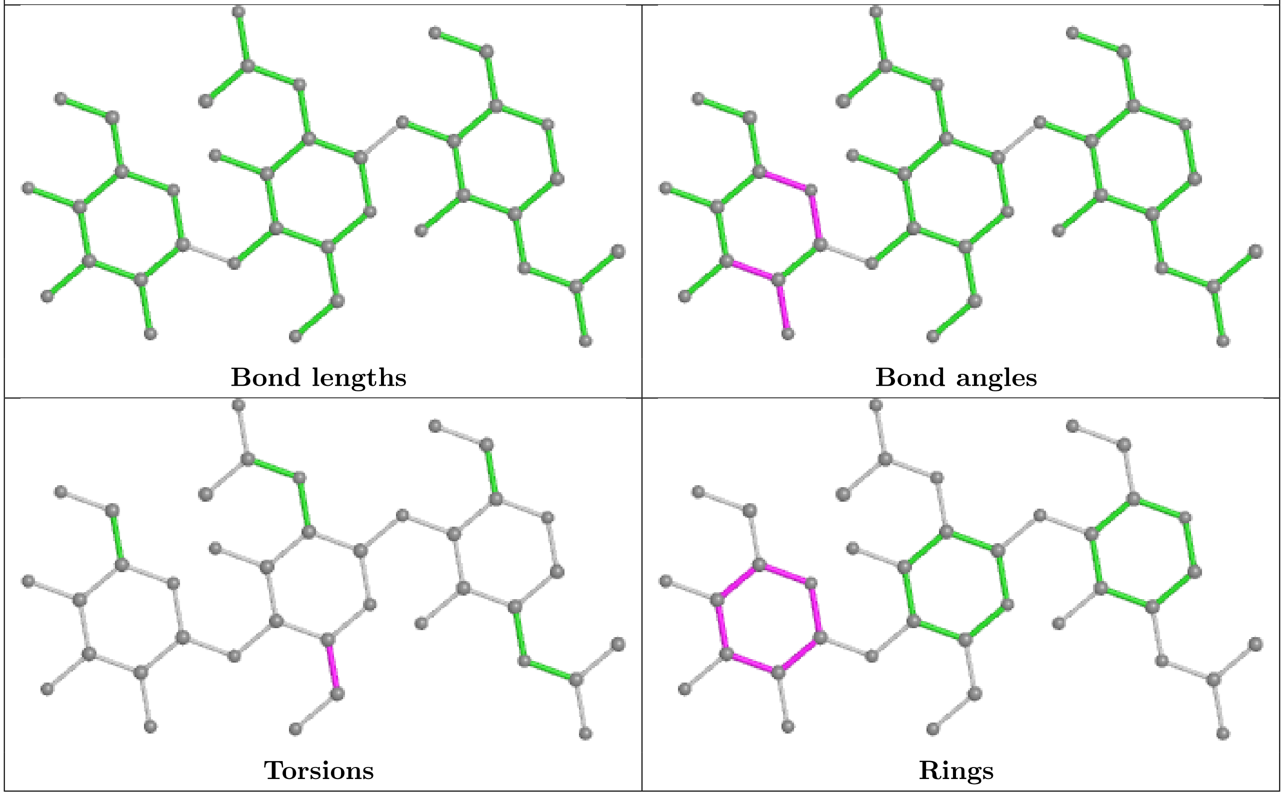
Oligosaccharide Chain b



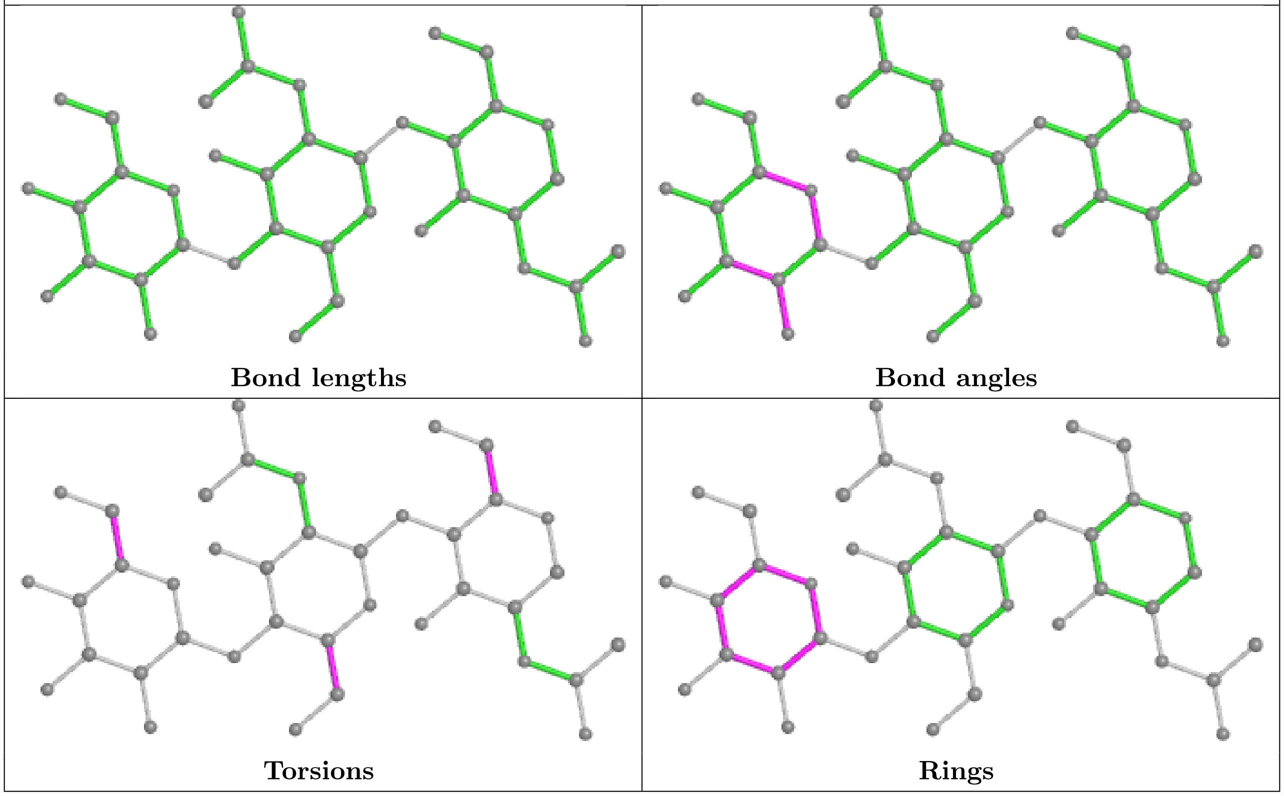
Bond lengths Bond angles

Torsions Rings

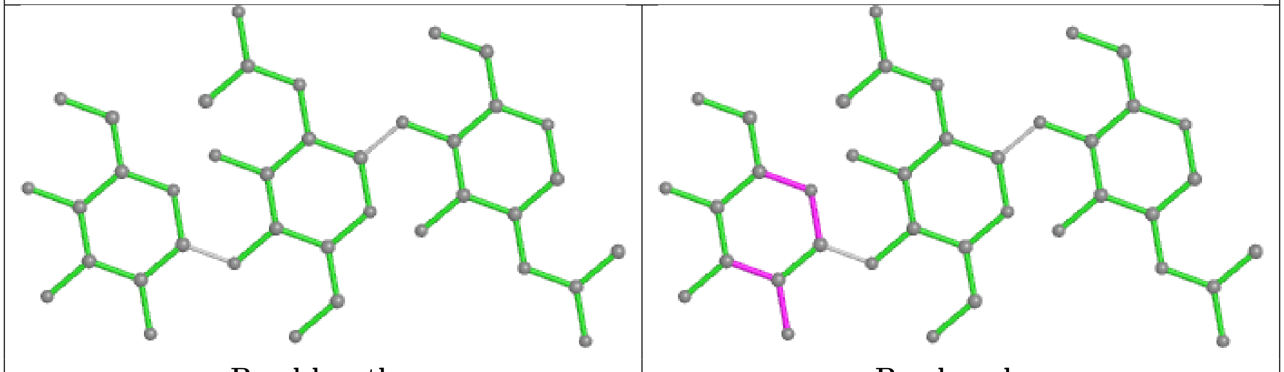
Oligosaccharide Chain e



Oligosaccharide Chain h

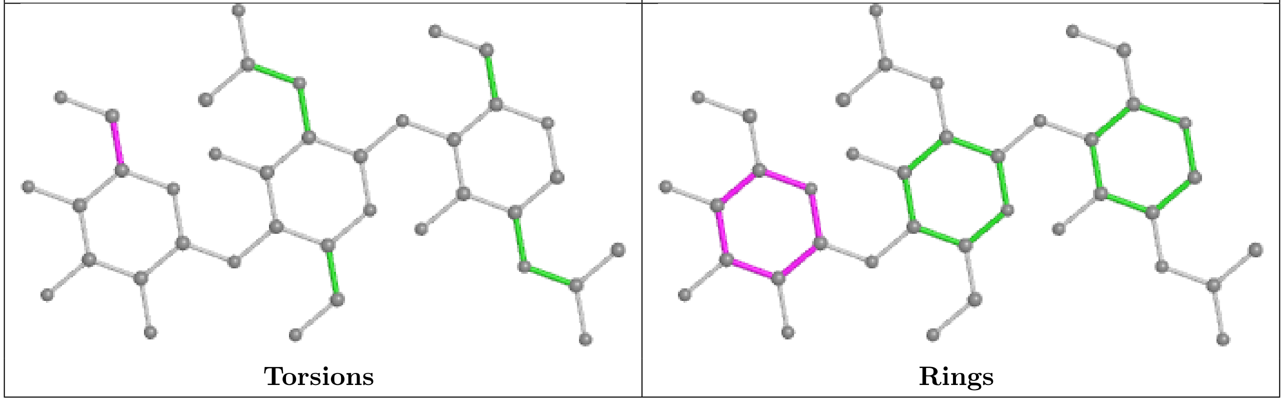


Oligosaccharide Chain k



Bond lengths

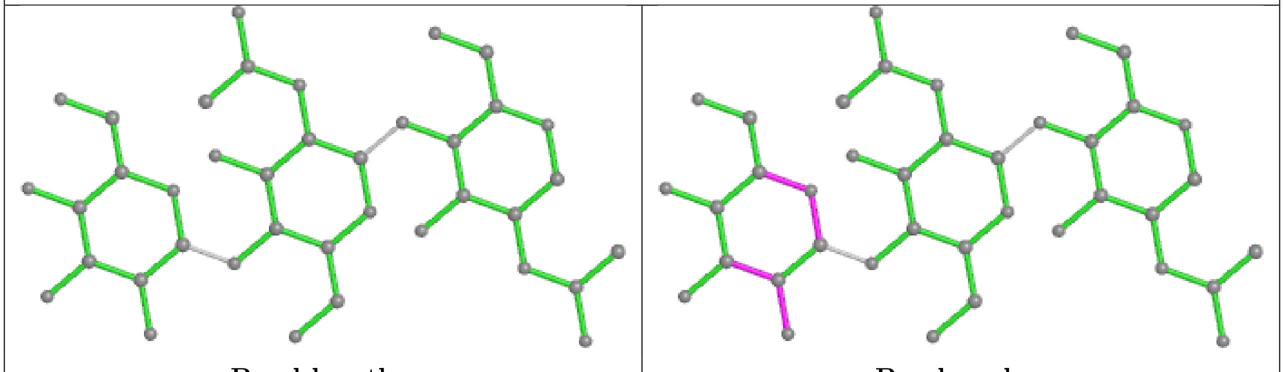
Bond angles



Torsions

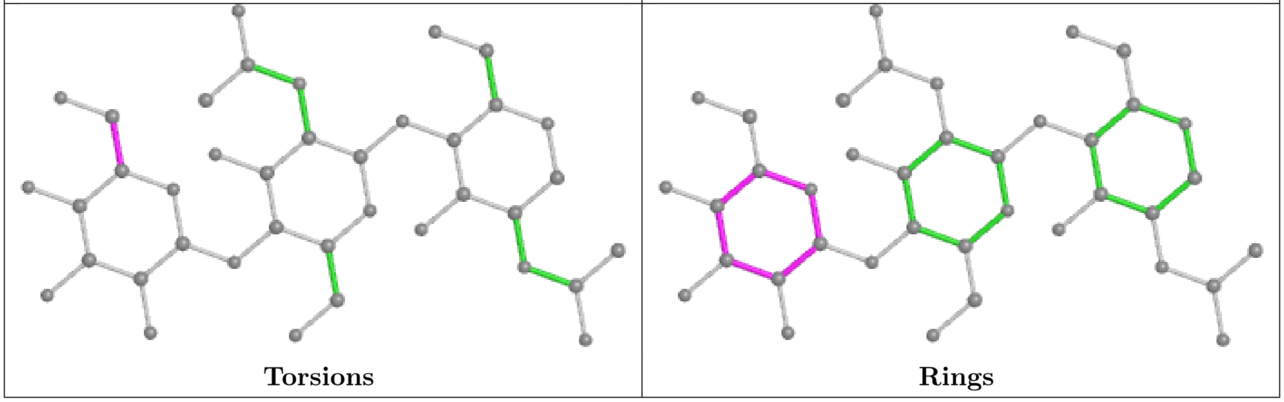
Rings

Oligosaccharide Chain x



Bond lengths

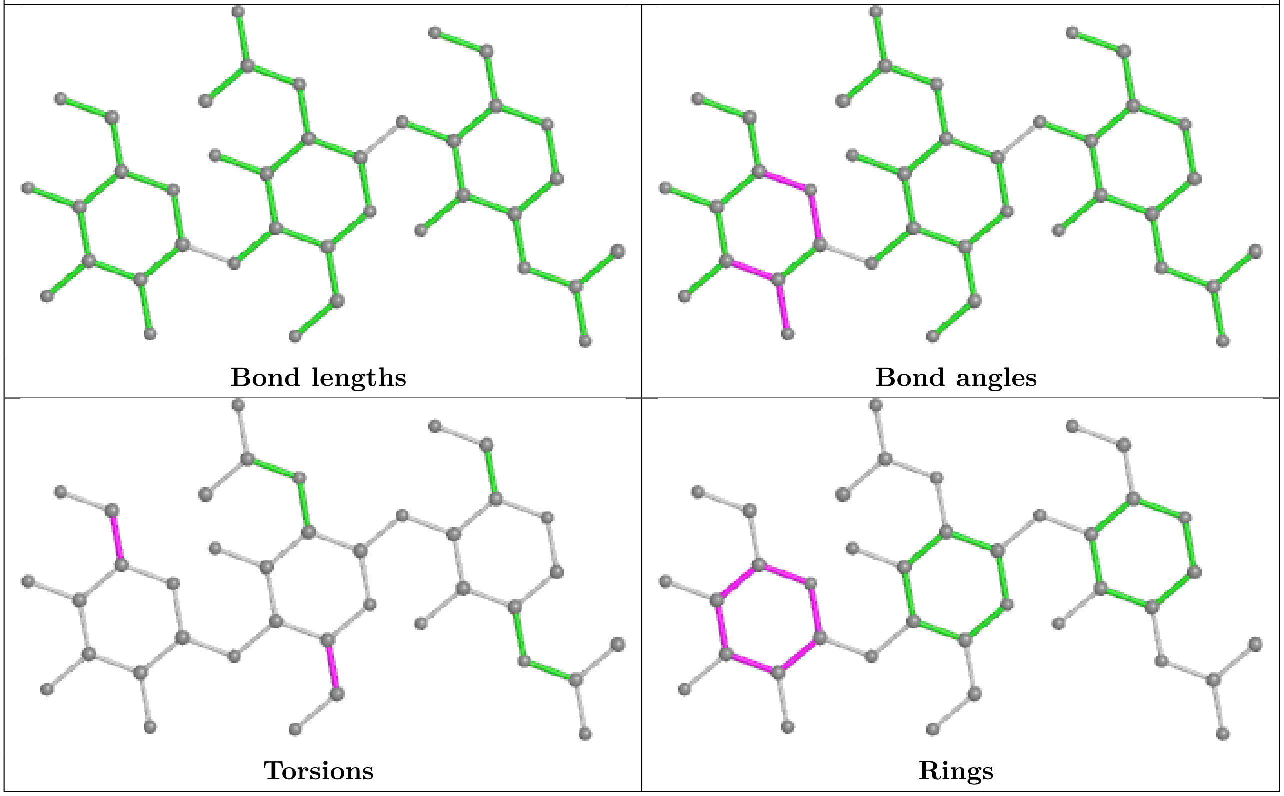
Bond angles



Torsions

Rings

Oligosaccharide Chain 5



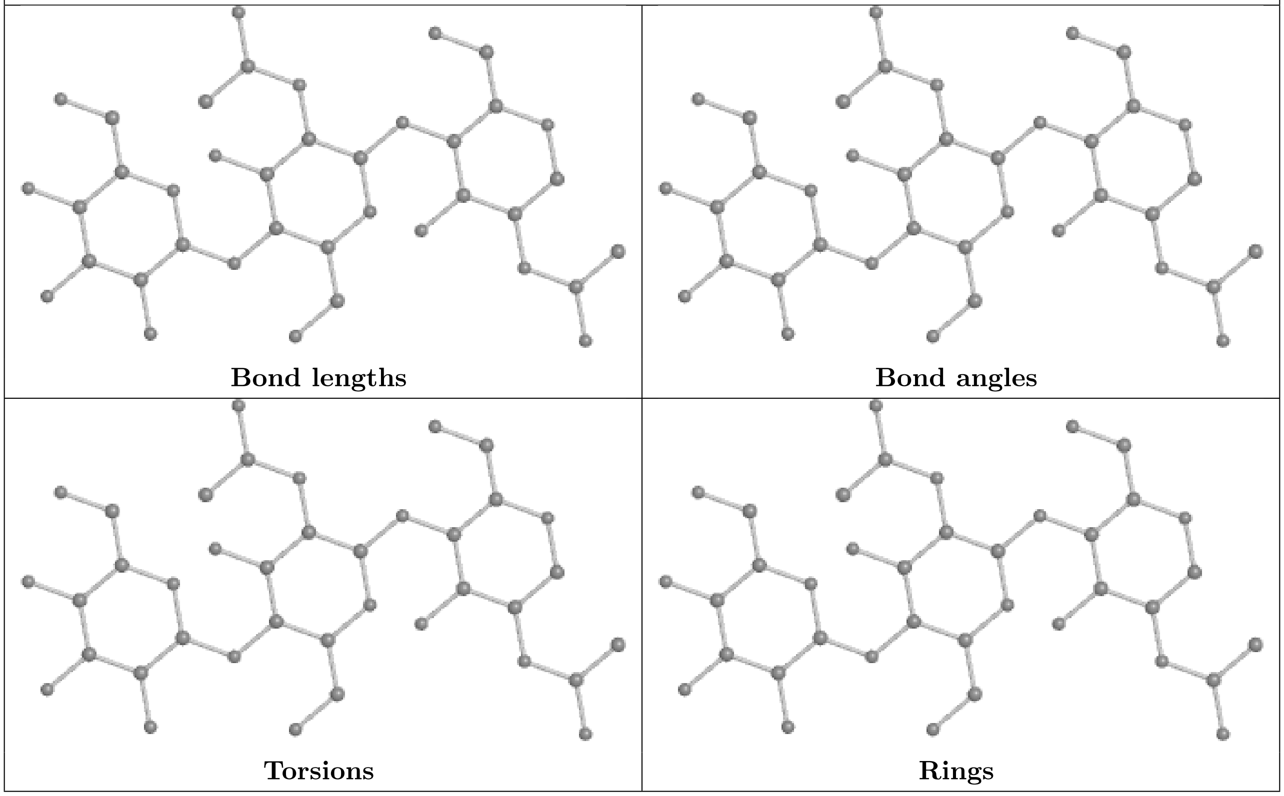
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain DA



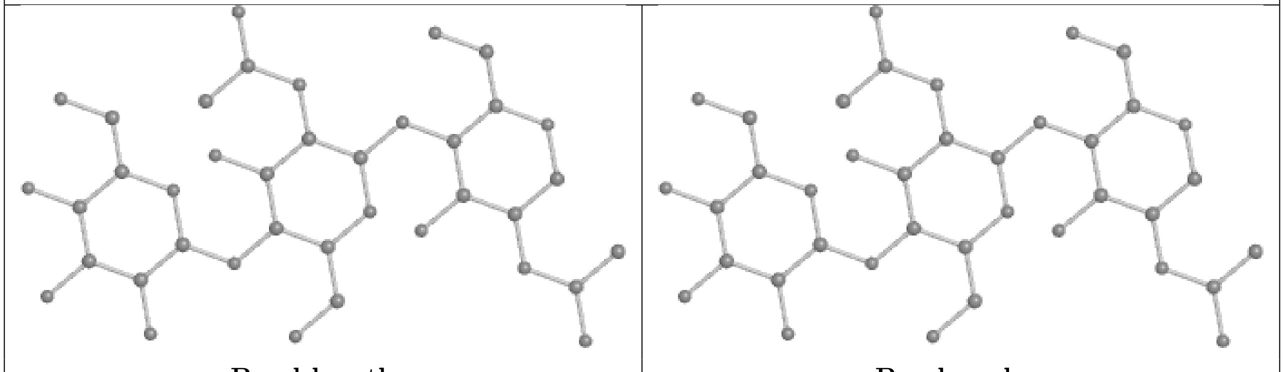
Bond lengths

Bond angles

Torsions

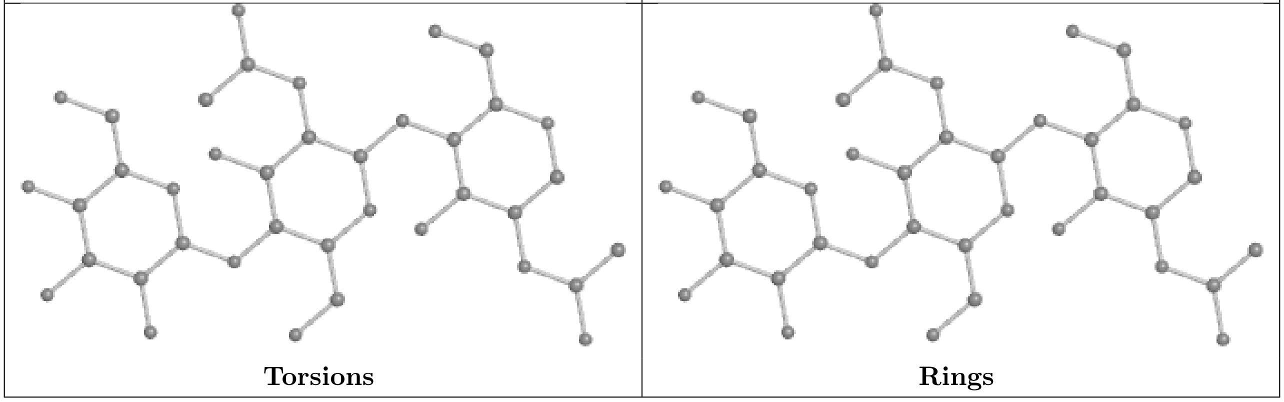
Rings

Oligosaccharide Chain GA



Bond lengths

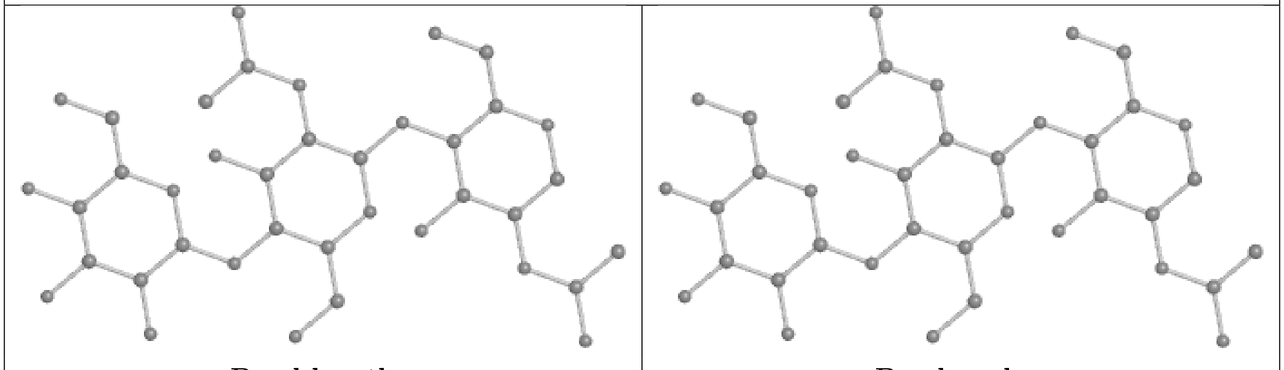
Bond angles



Torsions

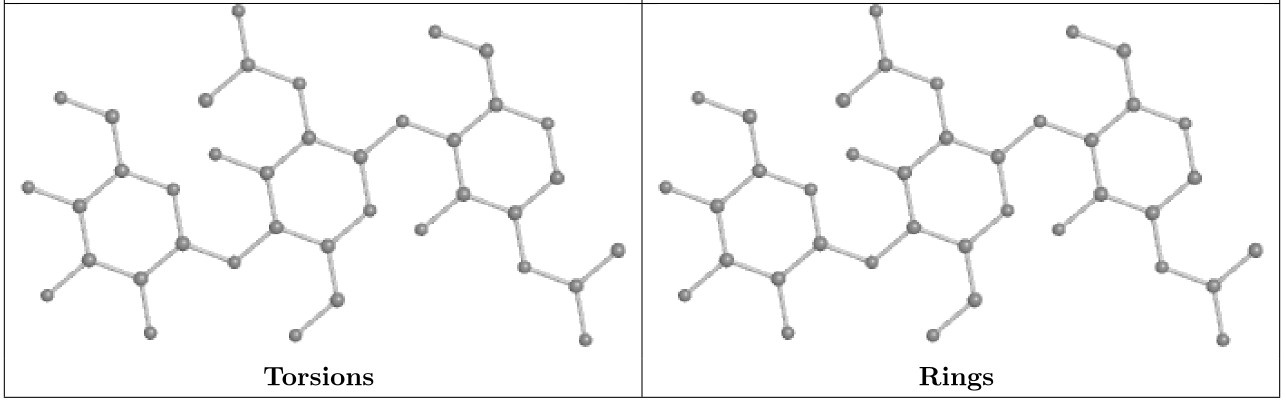
Rings

Oligosaccharide Chain JA



Bond lengths

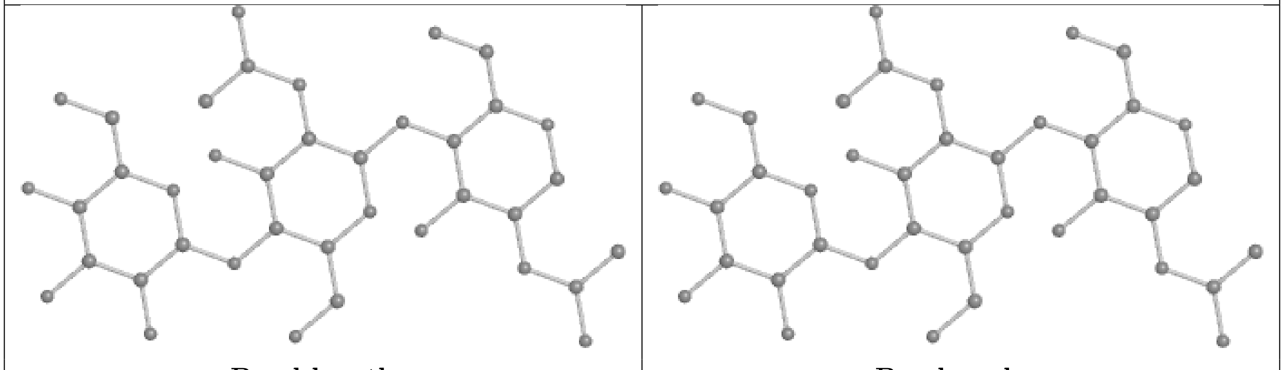
Bond angles



Torsions

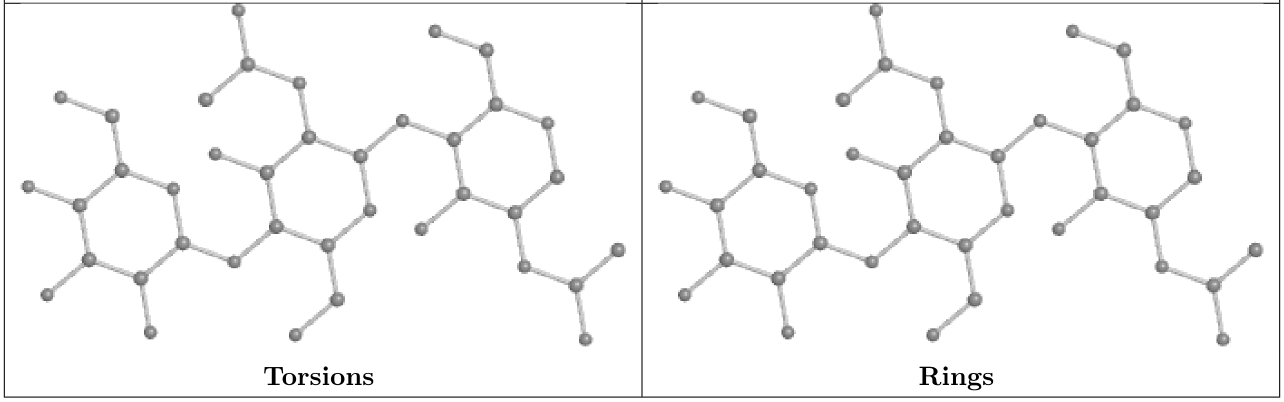
Rings

Oligosaccharide Chain MA



Bond lengths

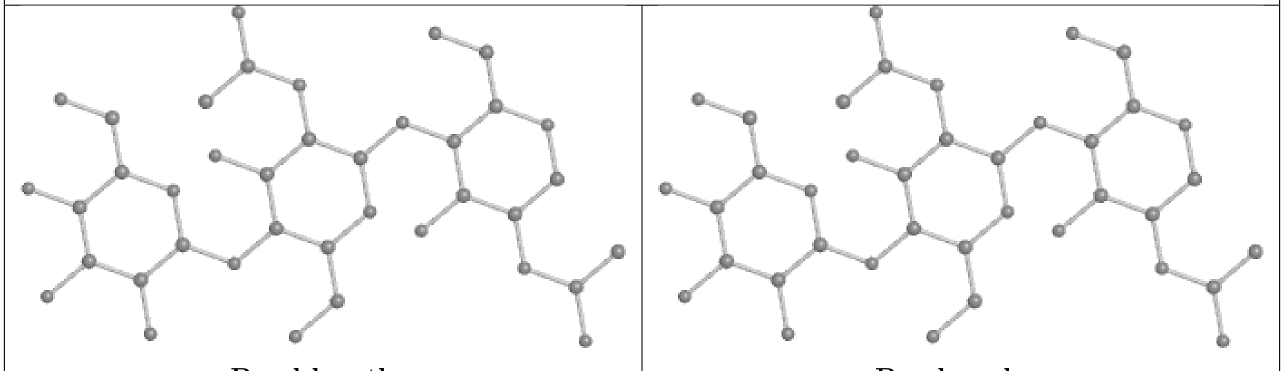
Bond angles



Torsions

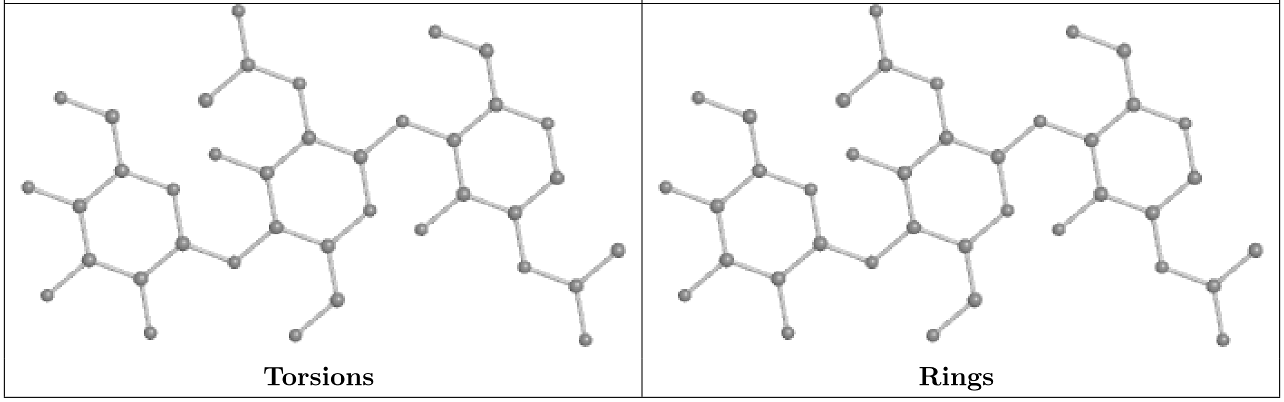
Rings

Oligosaccharide Chain PA



Bond lengths

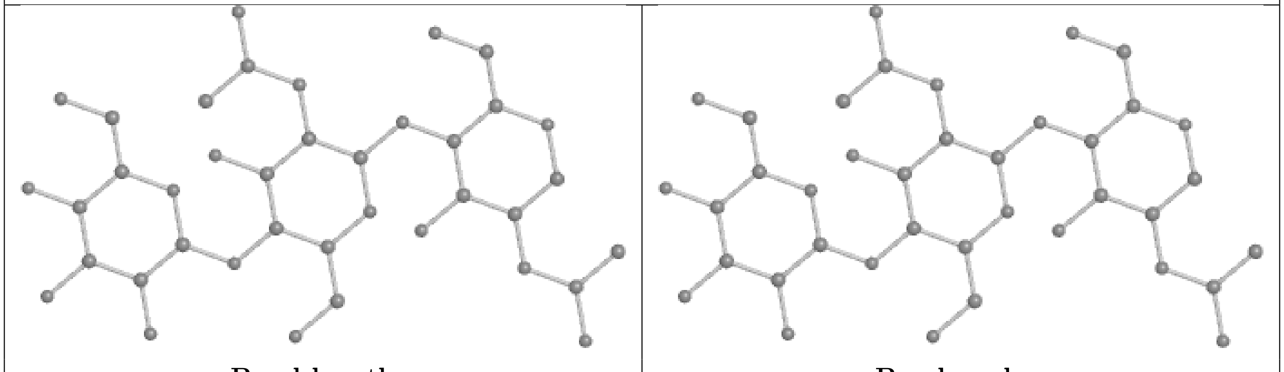
Bond angles



Torsions

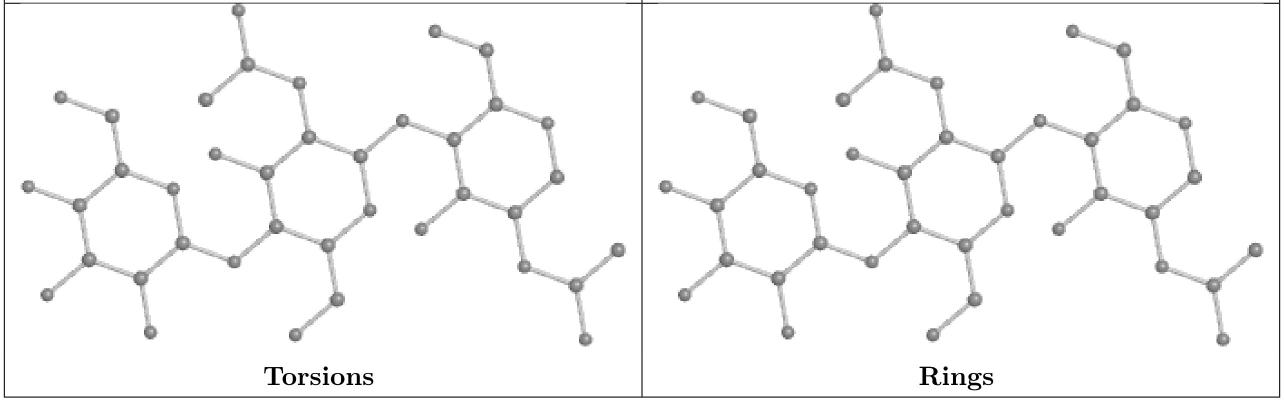
Rings

Oligosaccharide Chain cA



Bond lengths

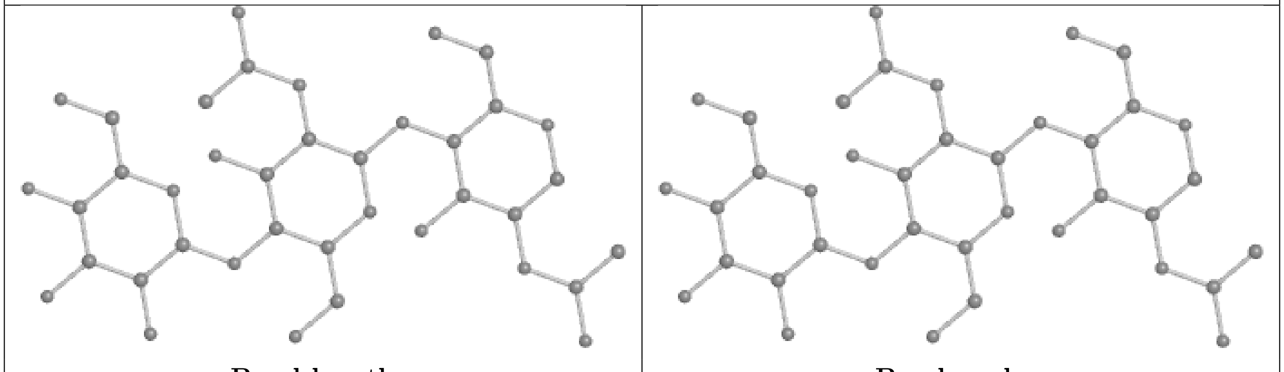
Bond angles



Torsions

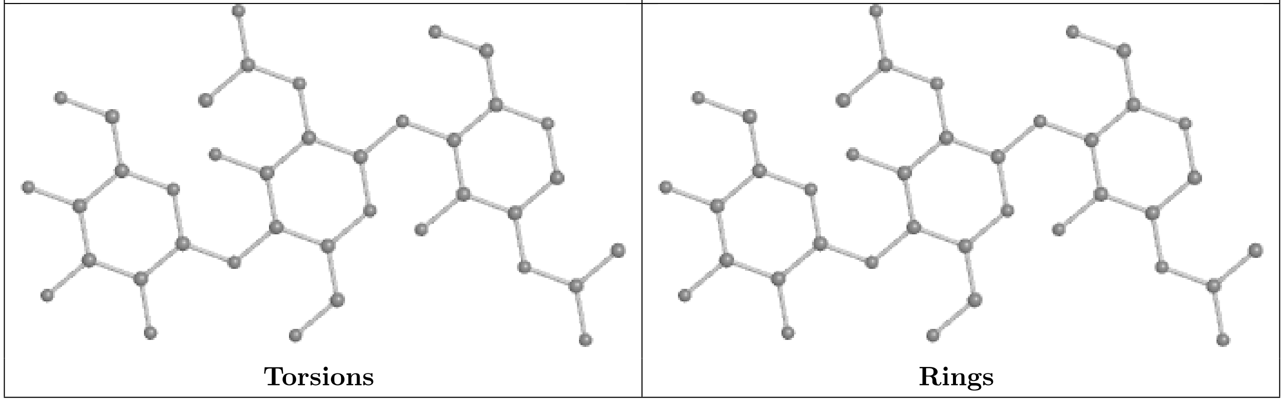
Rings

Oligosaccharide Chain kA



Bond lengths

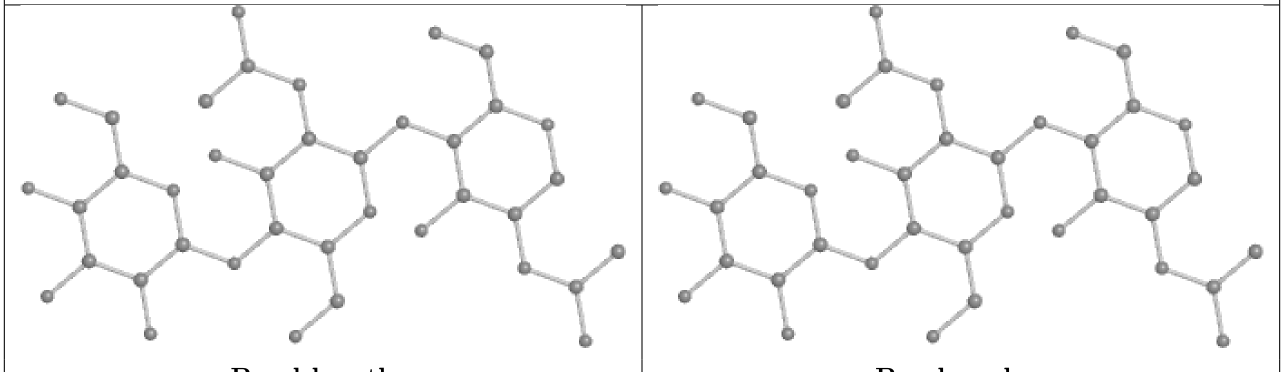
Bond angles



Torsions

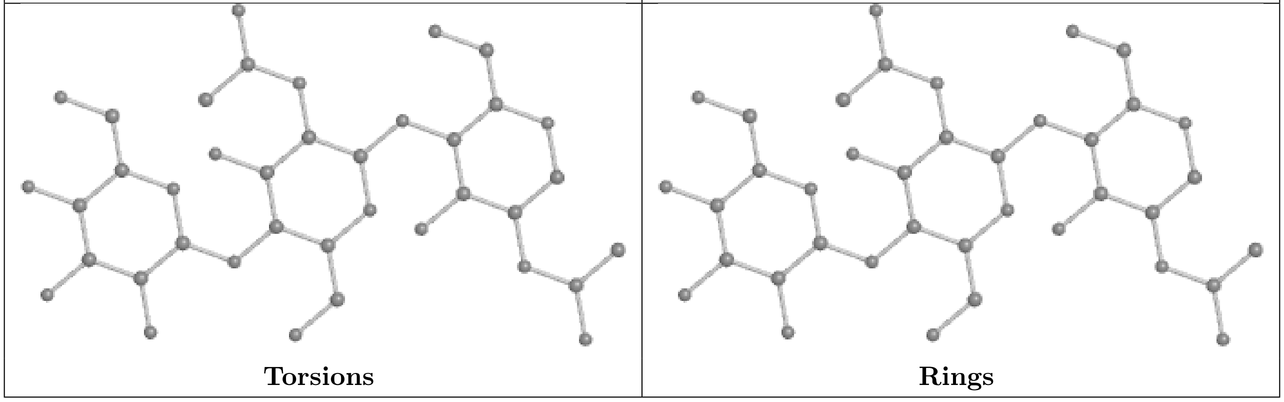
Rings

Oligosaccharide Chain sA



Bond lengths

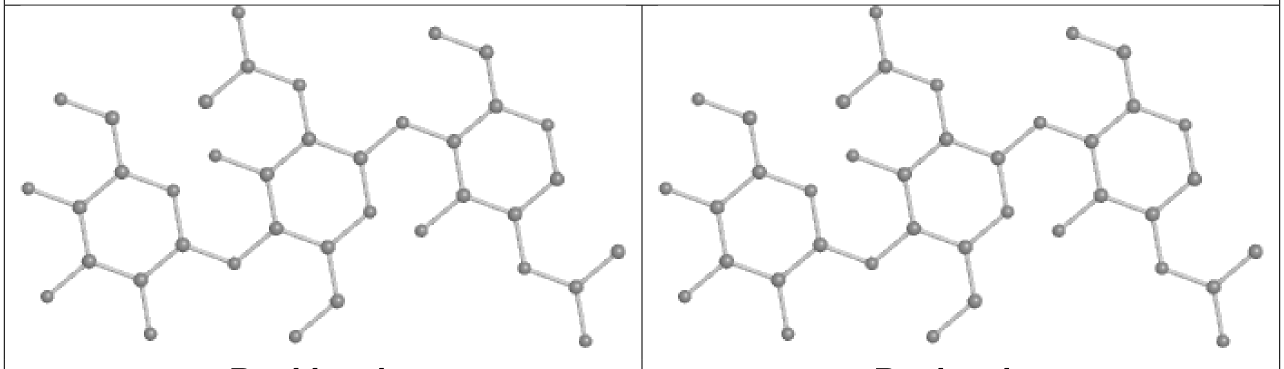
Bond angles



Torsions

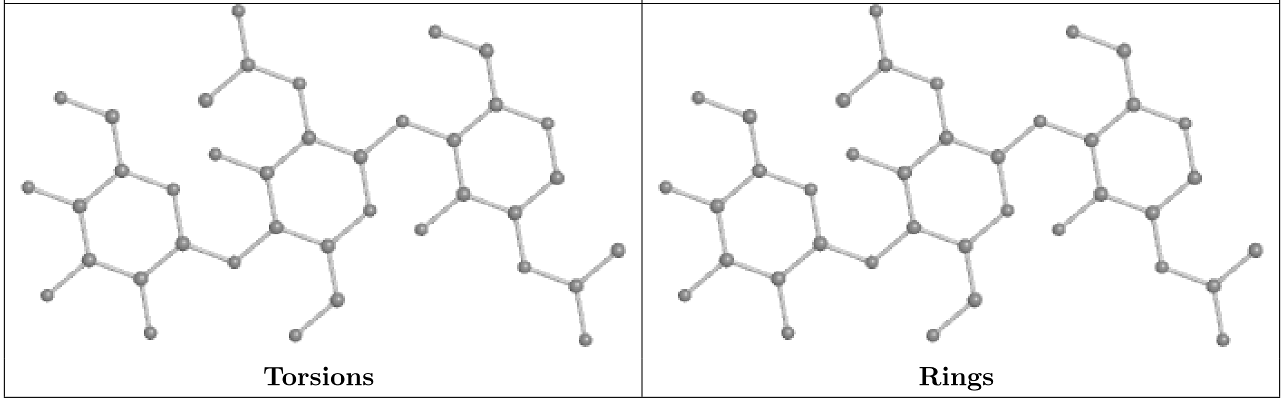
Rings

Oligosaccharide Chain vA



Bond lengths

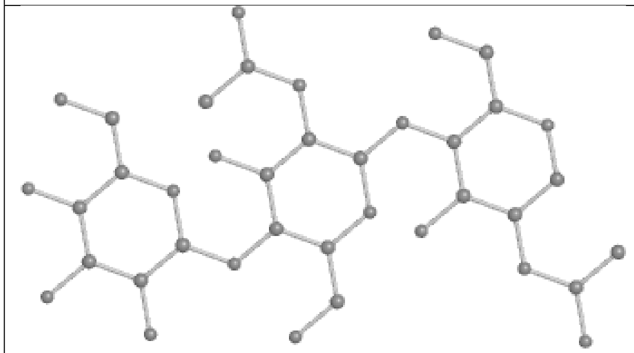
Bond angles



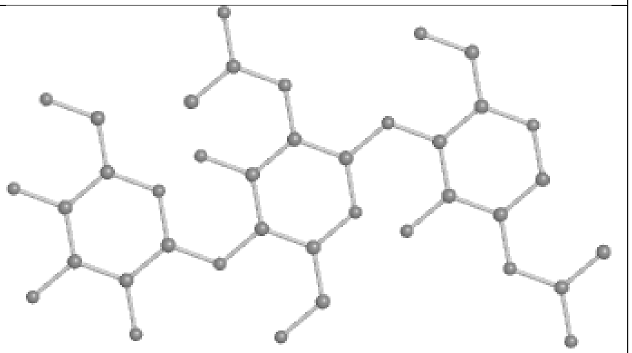
Torsions

Rings

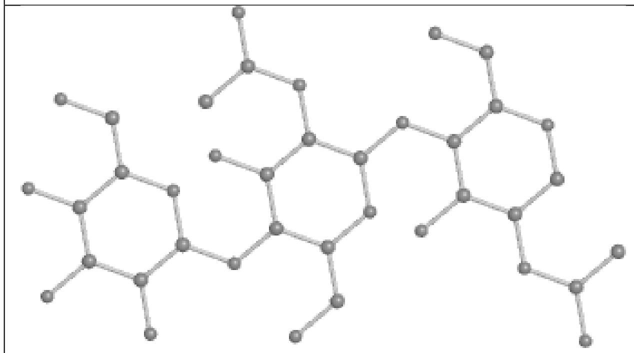
Oligosaccharide Chain yA



Bond lengths



Bond angles



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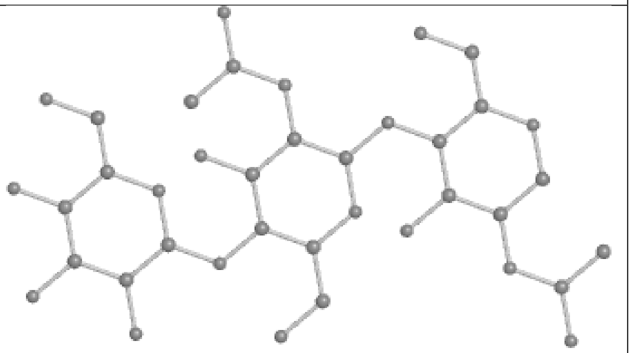
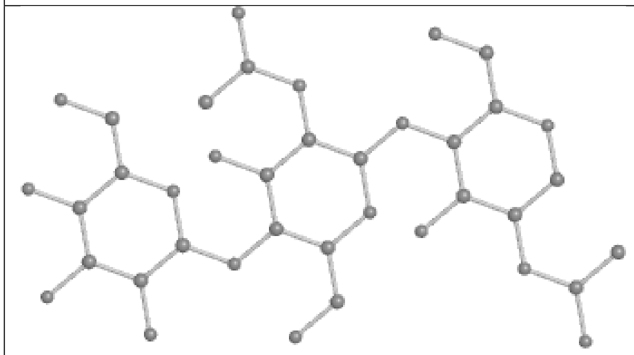
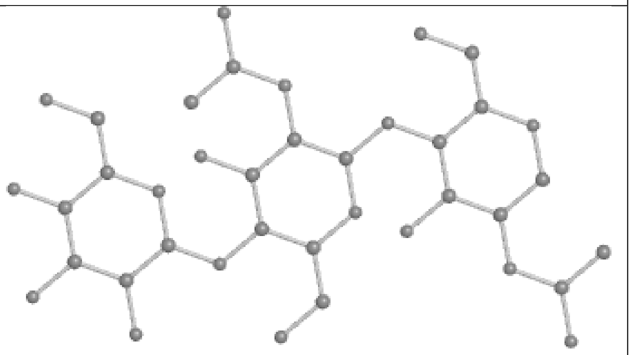


Rings

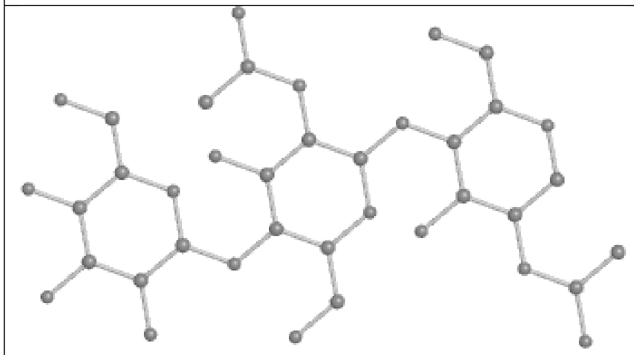
Oligosaccharide Chain 1A



Bond lengths



Bond angles



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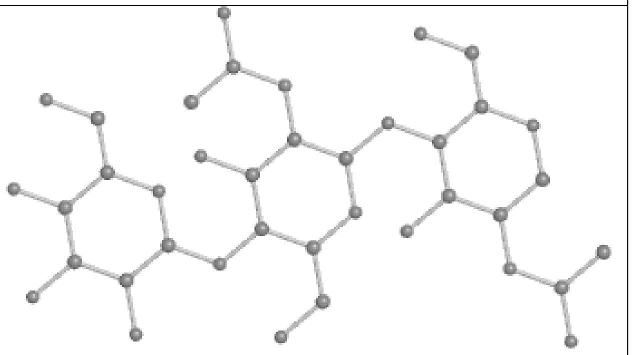
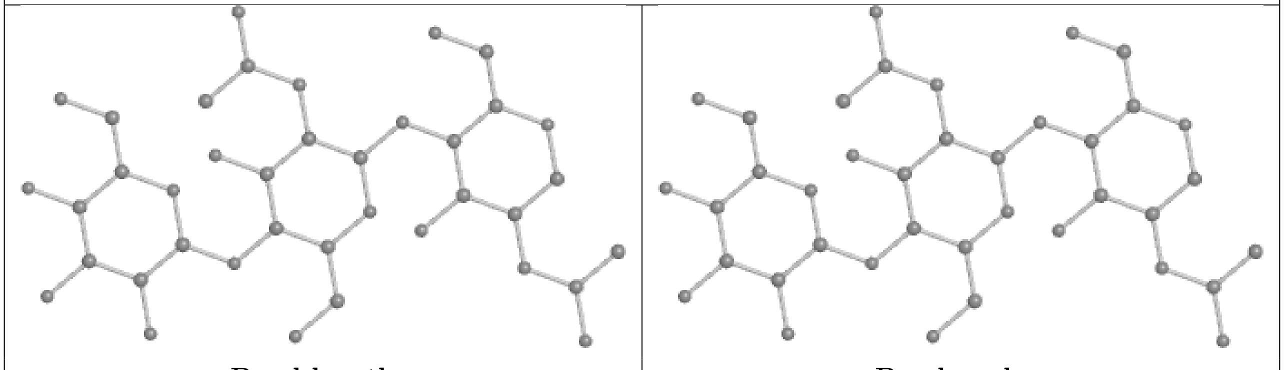
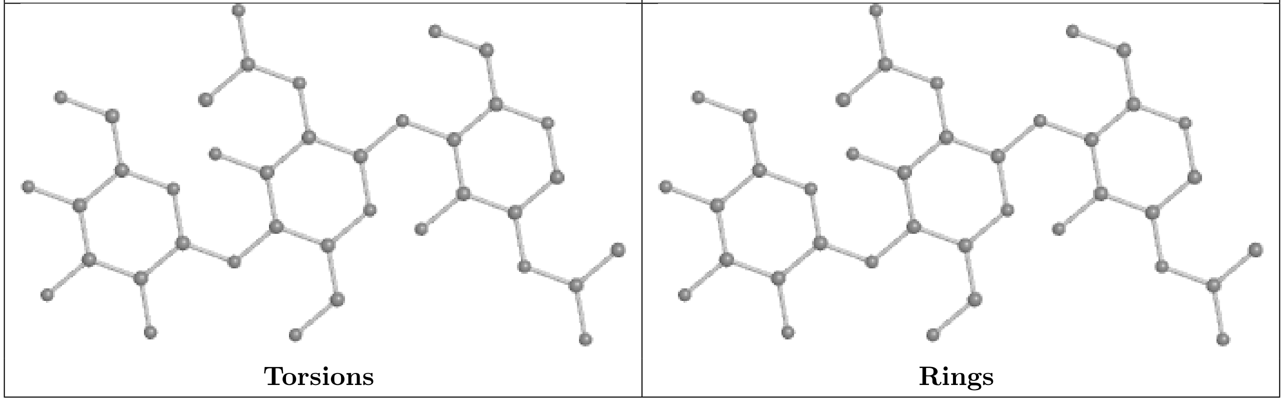


Rings

Oligosaccharide Chain 4A

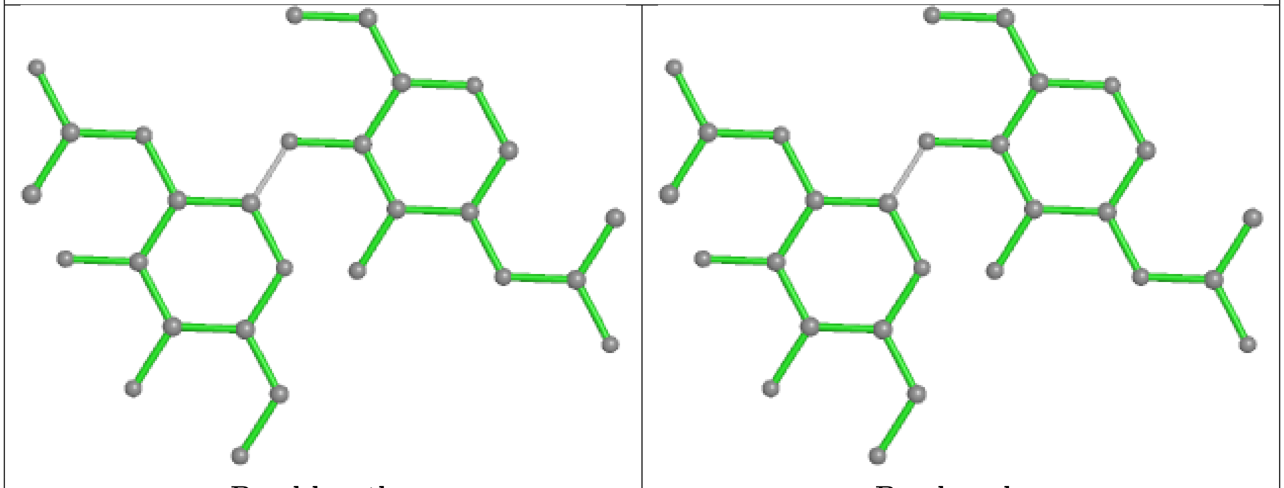


Bond lengths **Bond angles**



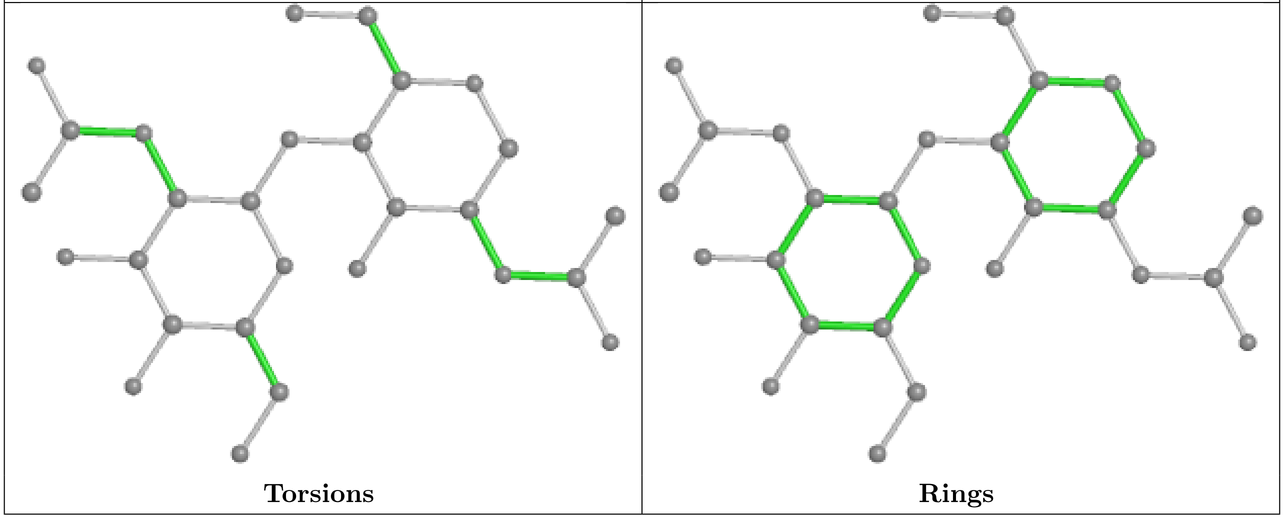
Torsions **Rings**

Oligosaccharide Chain L



Bond lengths

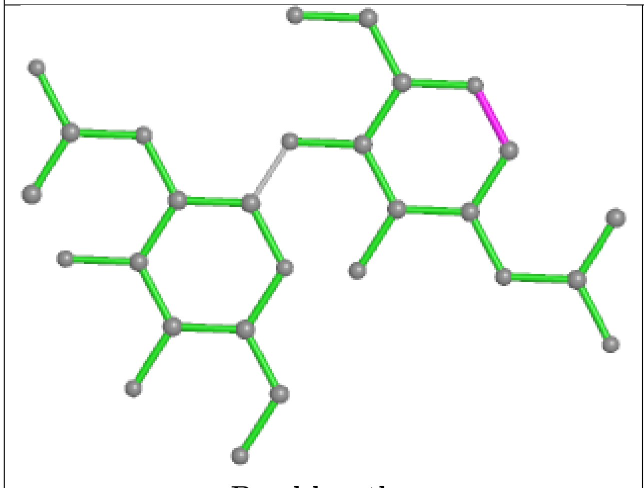
Bond angles



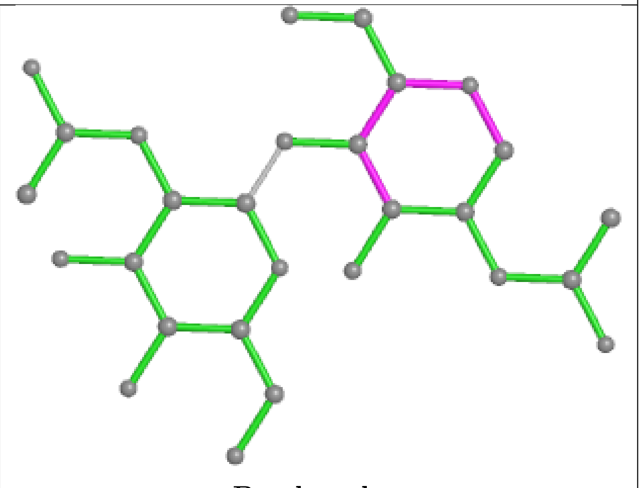
Torsions

Rings

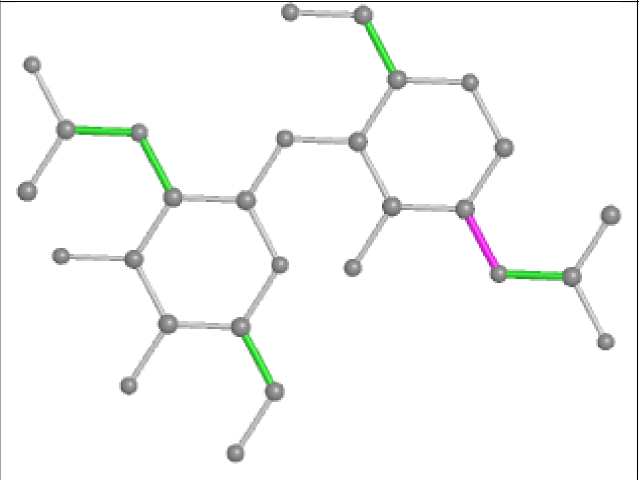
Oligosaccharide Chain U



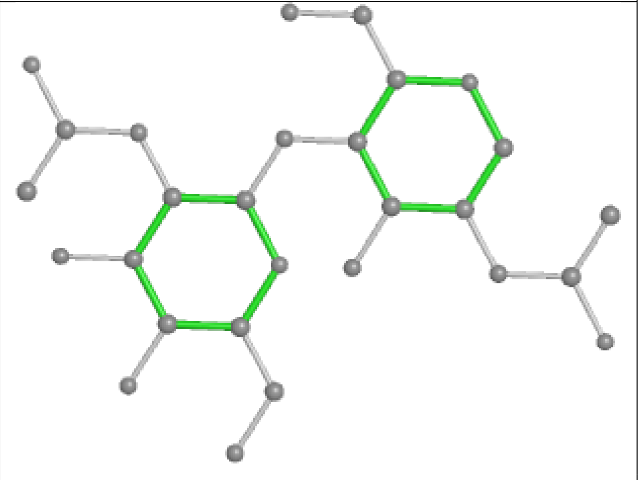
Bond lengths



Bond angles

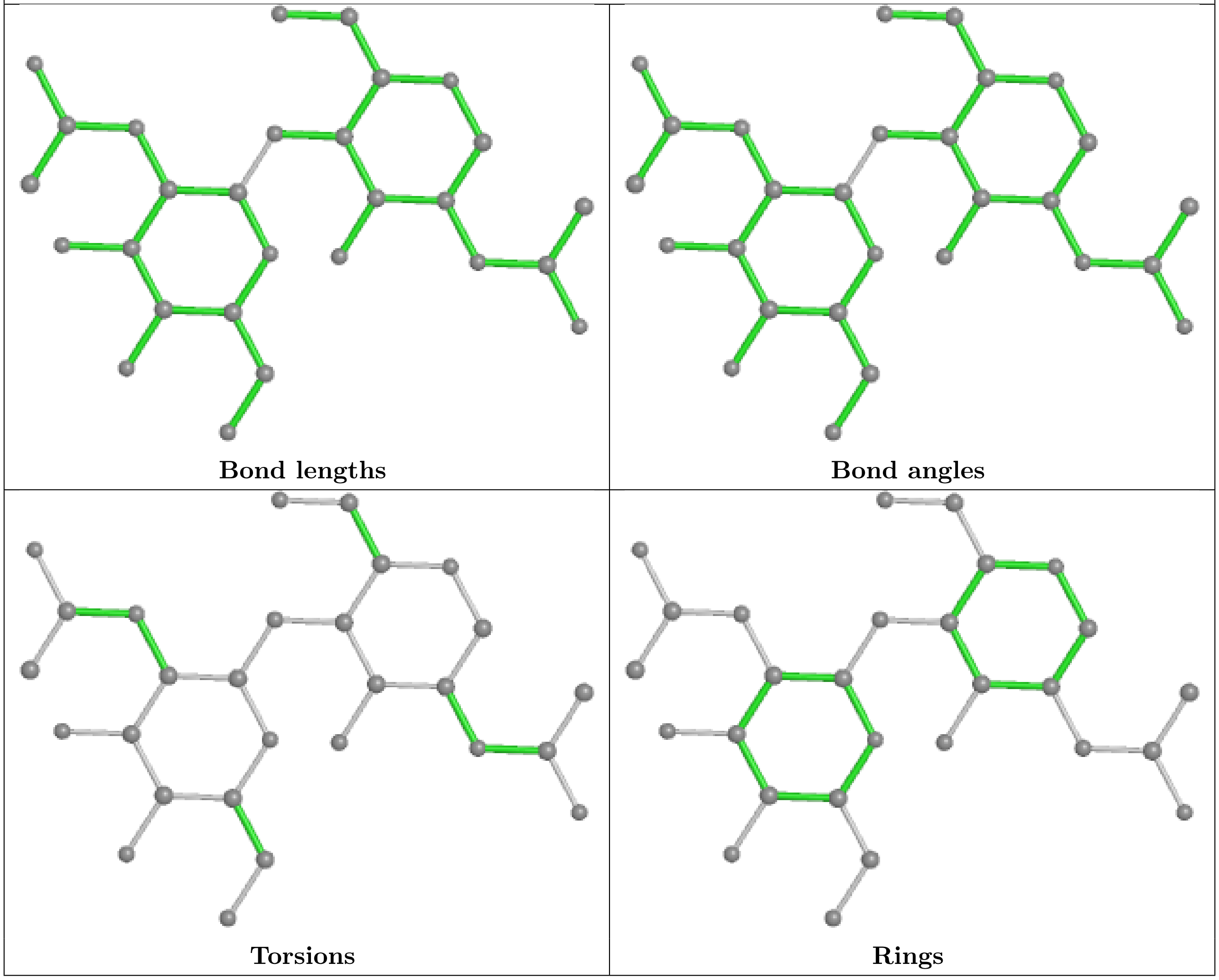


Torsions



Rings

Oligosaccharide Chain W



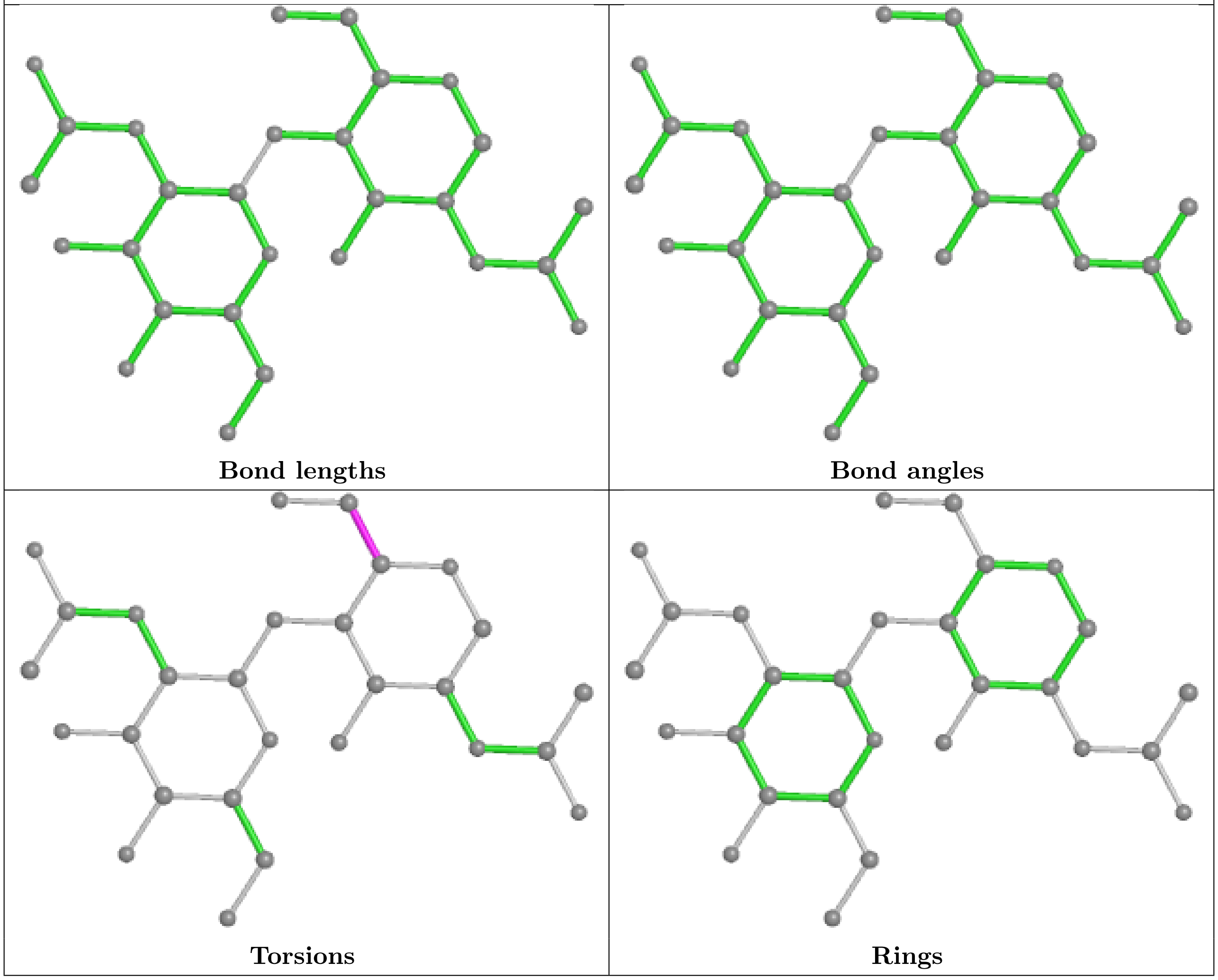
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain 0



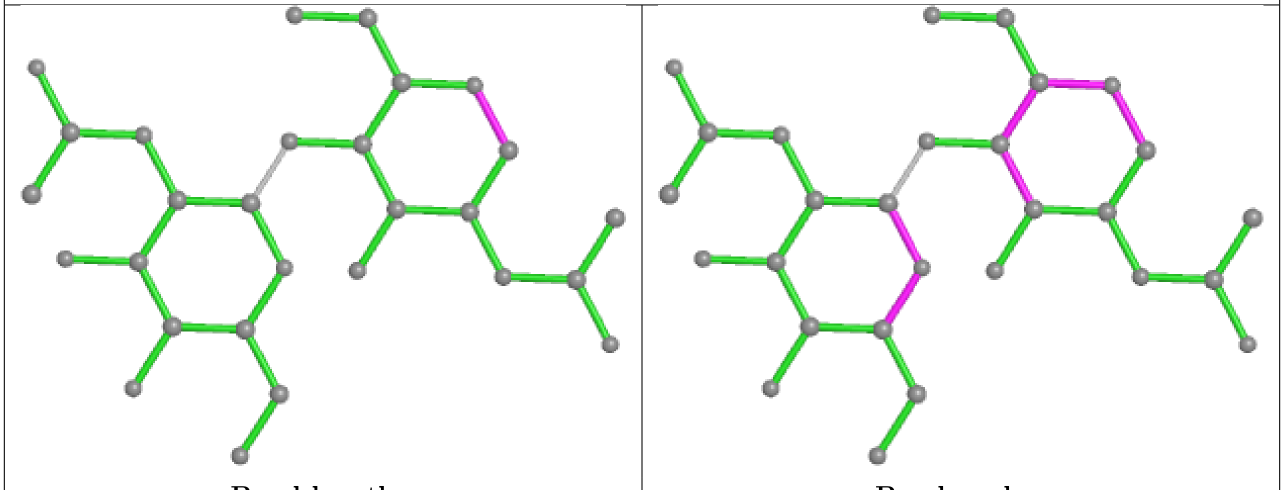
Bond lengths

Bond angles

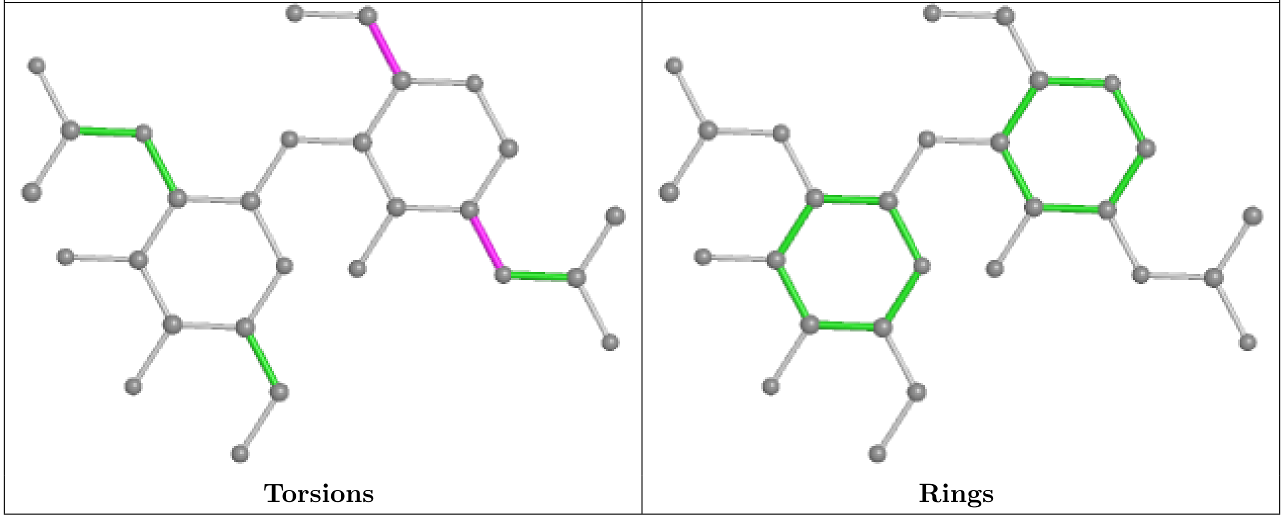
Torsions

Rings

Oligosaccharide Chain 9

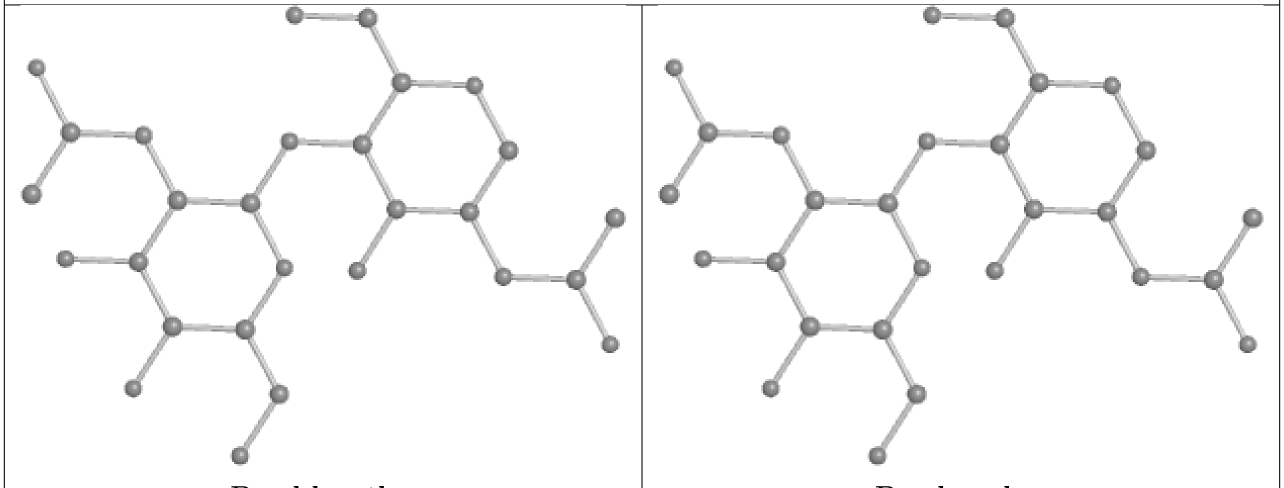


Bond lengths **Bond angles**

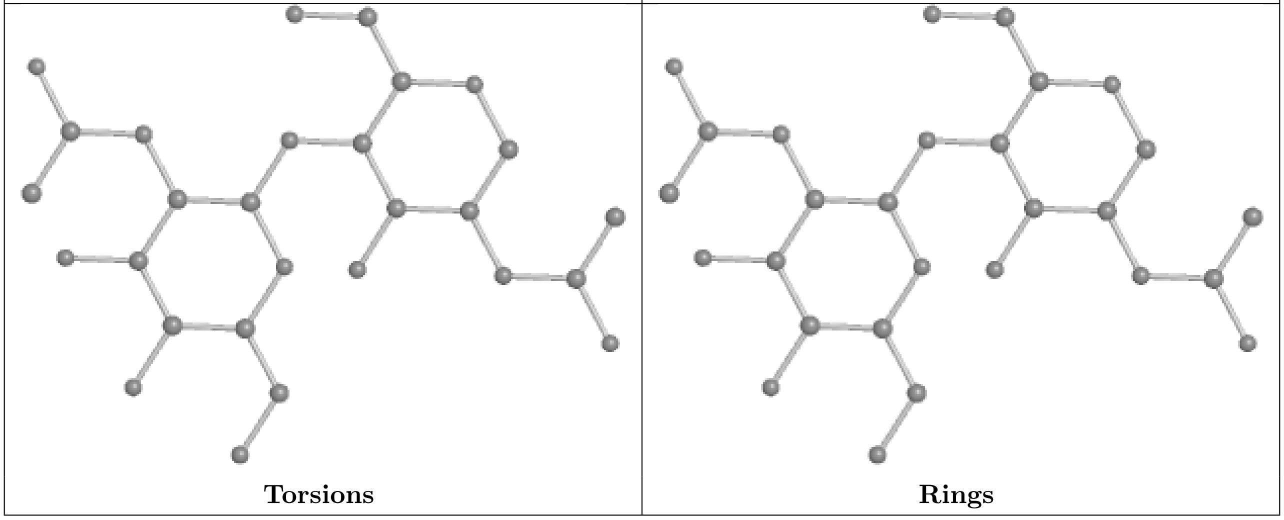


Torsions **Rings**

Oligosaccharide Chain BA

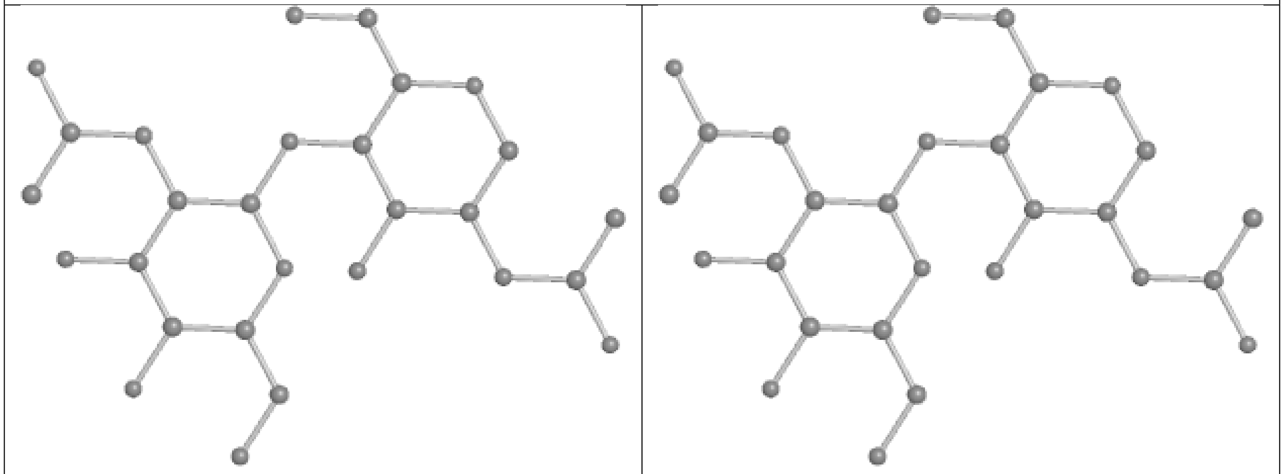


Bond lengths **Bond angles**



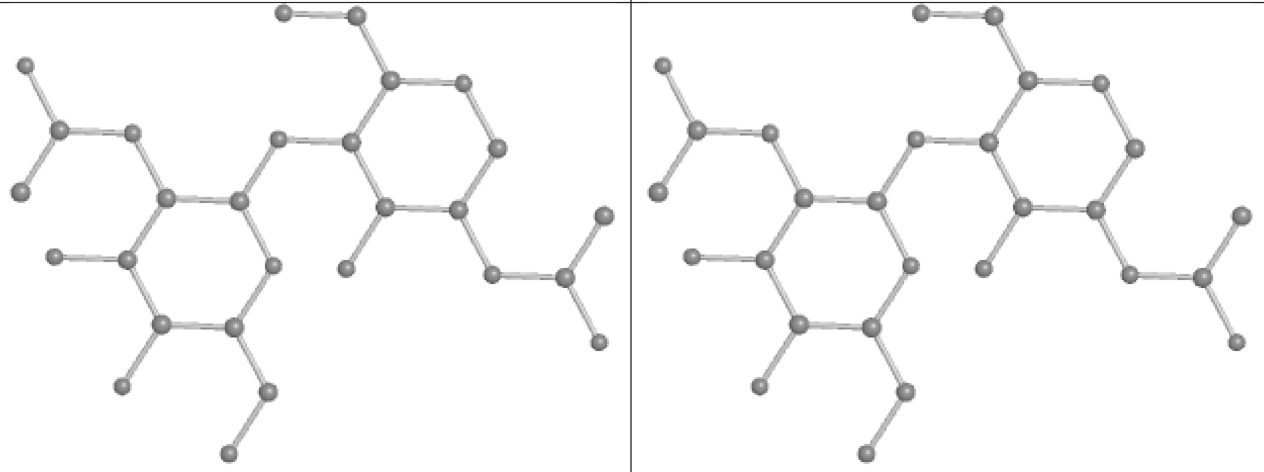
Torsions **Rings**

Oligosaccharide Chain fA



Bond lengths

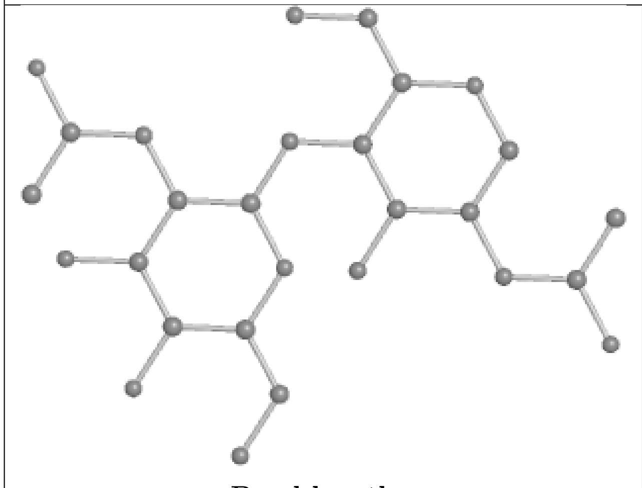
Bond angles



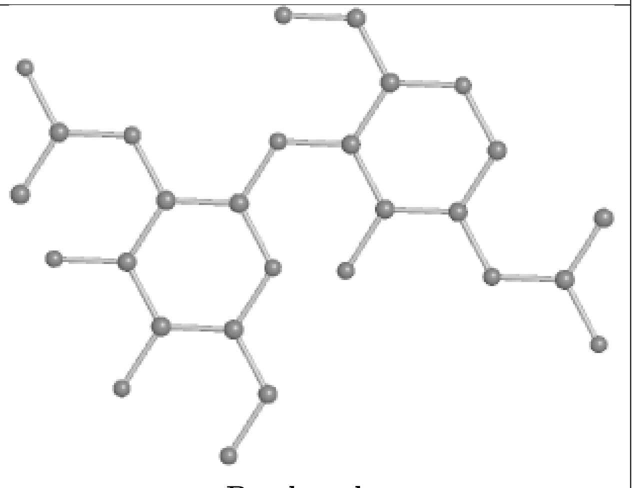
Torsions

Rings

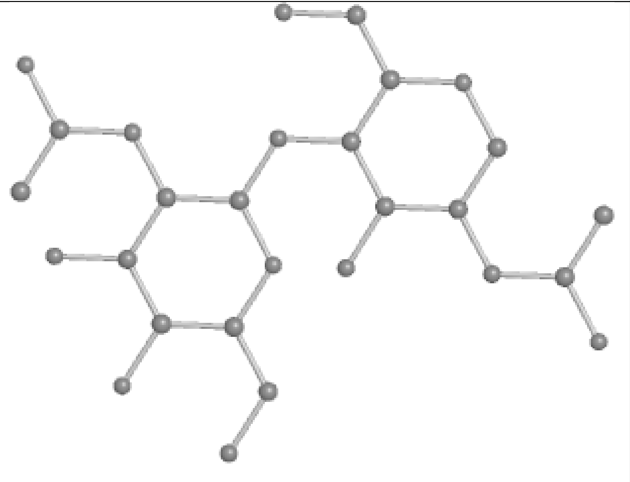
Oligosaccharide Chain oA



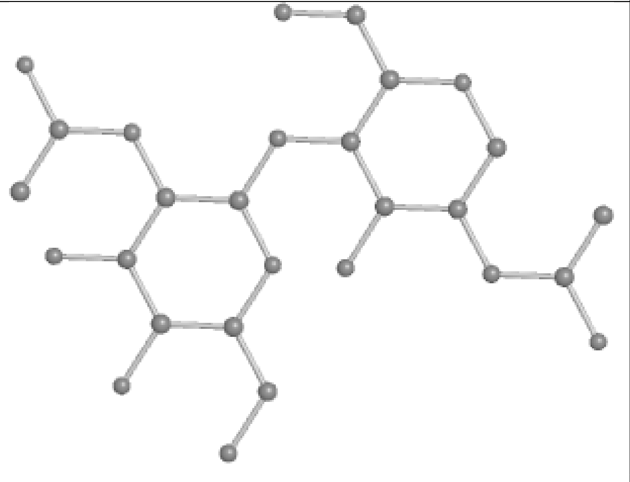
Bond lengths



Bond angles

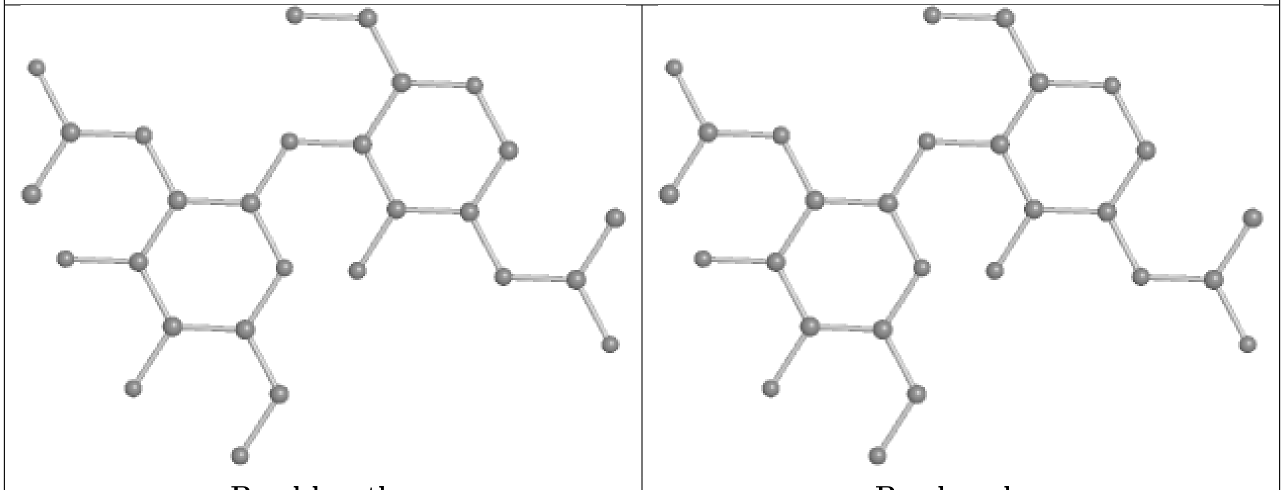


Torsions

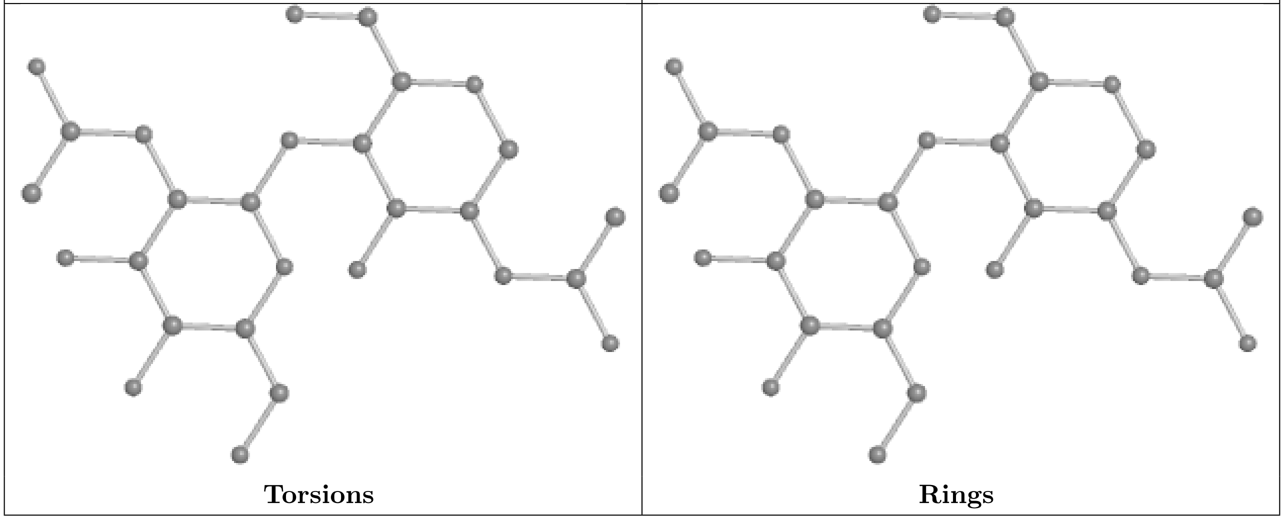


Rings

Oligosaccharide Chain qA

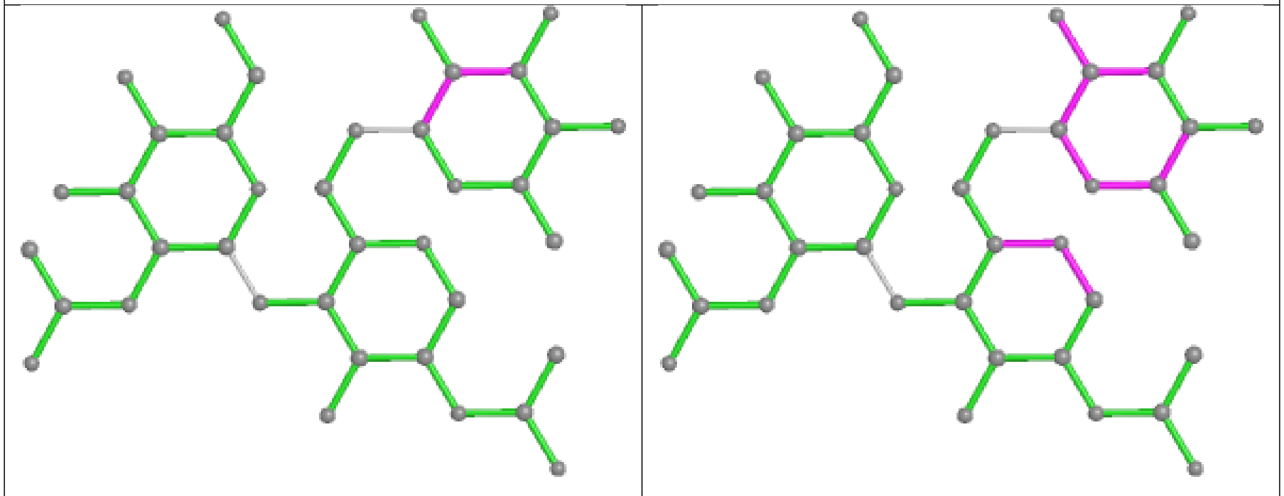


Bond lengths Bond angles

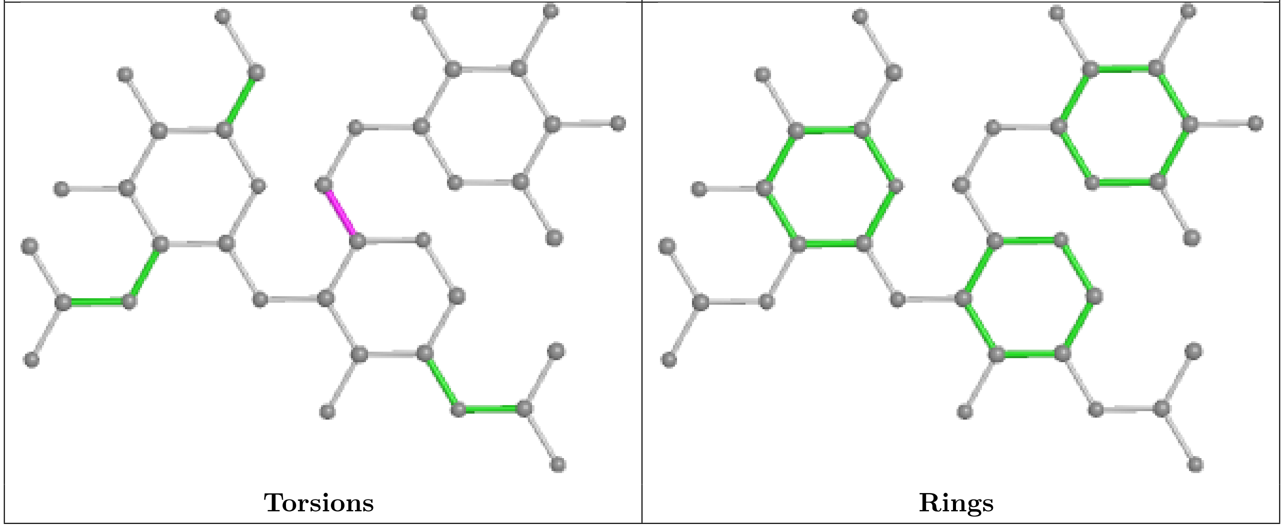


Torsions Rings

Oligosaccharide Chain N

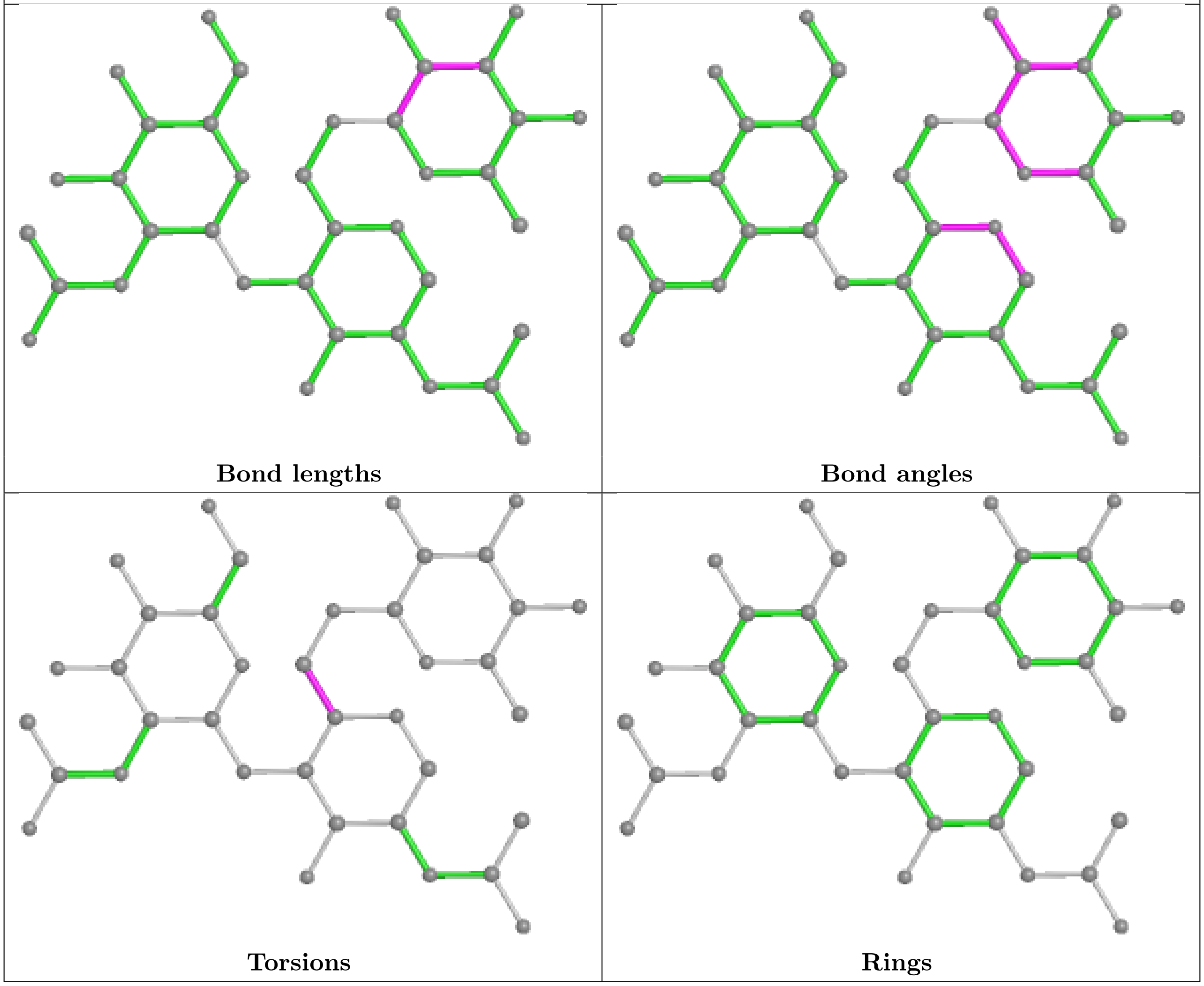


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain 2



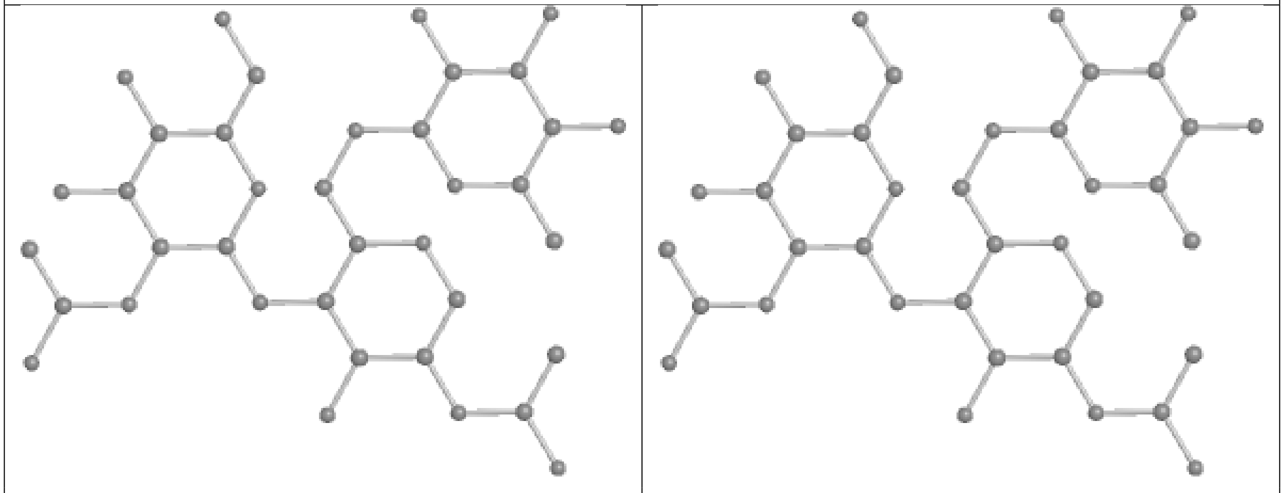
Bond lengths

Bond angles

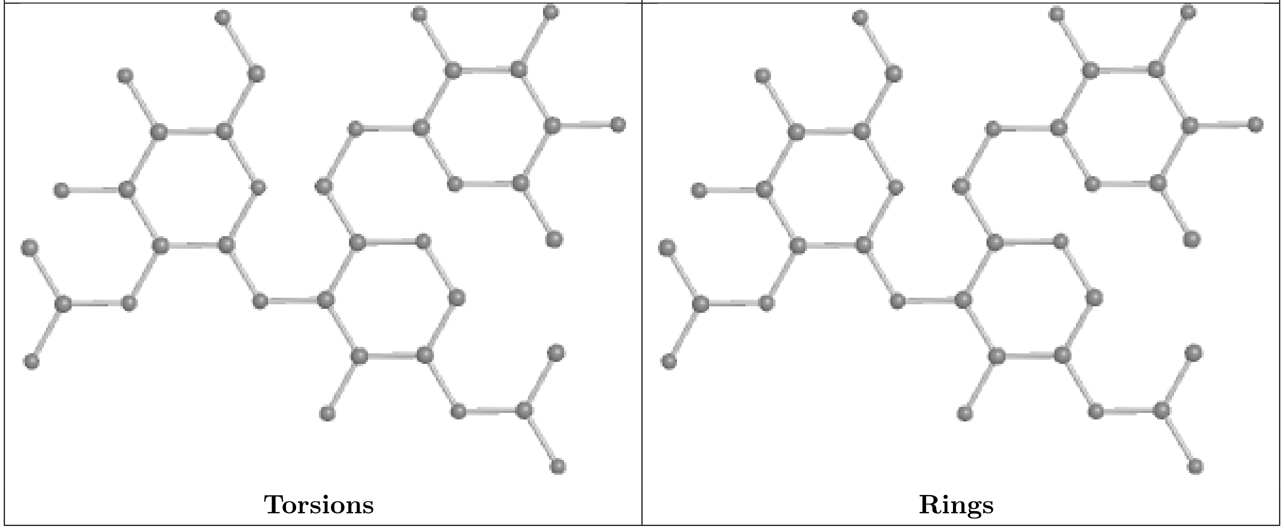
Torsions

Rings

Oligosaccharide Chain hA

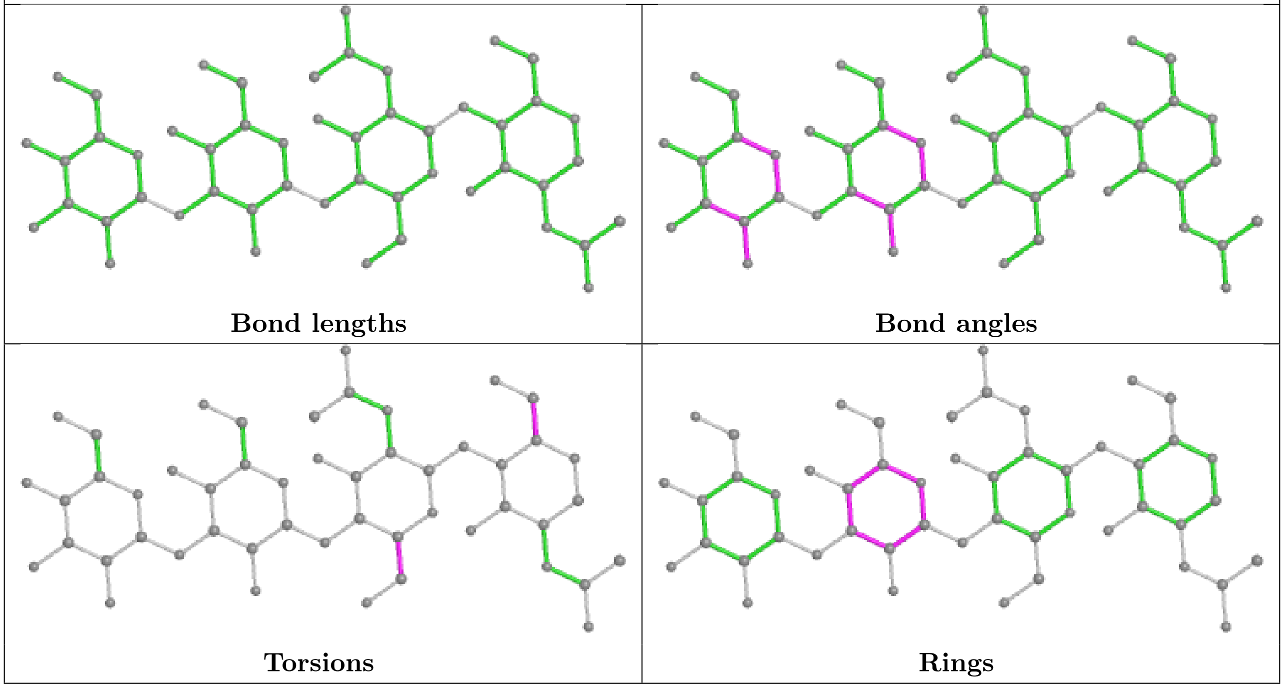


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain n



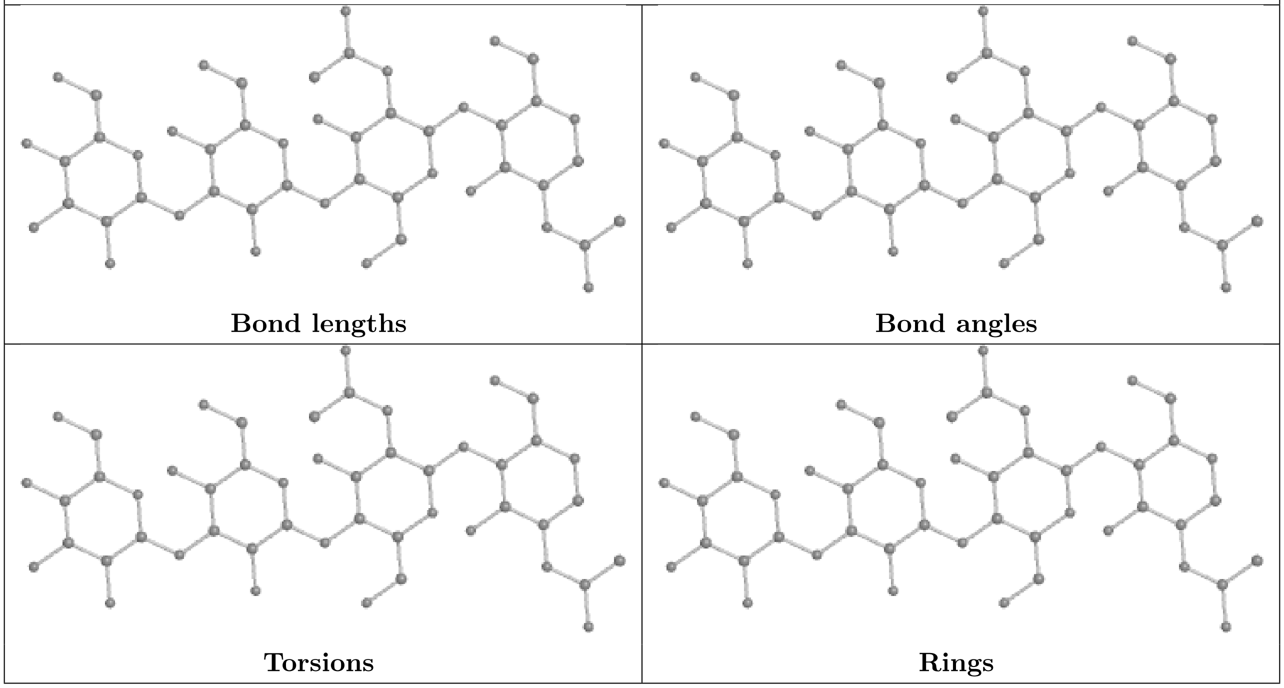
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain SA



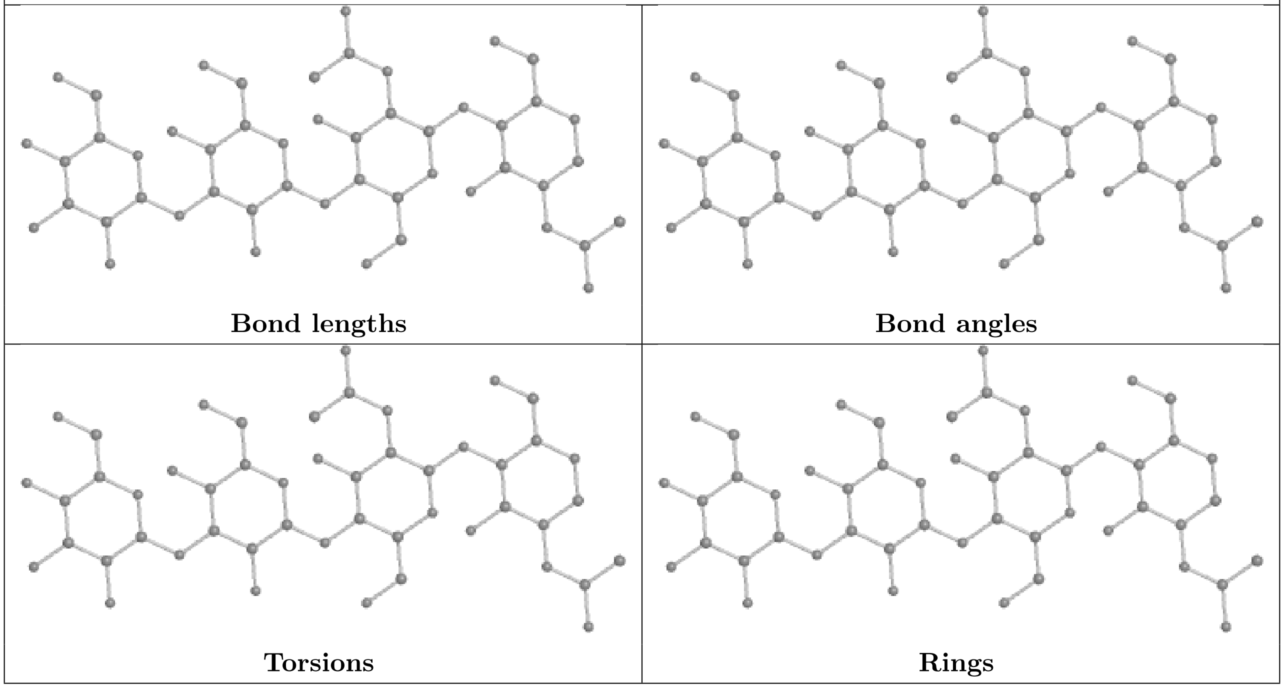
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain 7A


Bond lengths
Bond angles
Torsions
Rings

5.6 Ligand geometry

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	C	1401	1	14,14,15	0.58	0	17,19,21	0.44	0
6	NAG	B	1401	1	14,14,15	0.48	0	17,19,21	0.44	0
6	NAG	B	1406	1	14,14,15	0.54	0	17,19,21	0.65	1 (5%)
6	NAG	C	1406	1	14,14,15	0.45	0	17,19,21	0.65	1 (5%)
6	NAG	B	1402	1	14,14,15	0.29	0	17,19,21	0.44	0
6	NAG	B	1407	1	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	A	1405	1	14,14,15	0.26	0	17,19,21	0.44	0
6	NAG	A	1403	1	14,14,15	0.26	0	17,19,21	0.42	0
6	NAG	A	1407	1	14,14,15	0.26	0	17,19,21	0.42	0
6	NAG	C	1405	1	14,14,15	0.37	0	17,19,21	0.54	0
6	NAG	A	1401	-	14,14,15	0.18	0	17,19,21	0.46	0
6	NAG	C	1403	1	14,14,15	0.22	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	C	1407	1	14,14,15	0.27	0	17,19,21	0.43	0
6	NAG	A	1406	1	14,14,15	0.52	0	17,19,21	0.62	1 (5%)
6	NAG	B	1404	1	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	C	1404	1	14,14,15	0.25	0	17,19,21	0.37	0
6	NAG	B	1403	1	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	C	1402	1	14,14,15	0.32	0	17,19,21	0.45	0
6	NAG	B	1405	1	14,14,15	0.23	0	17,19,21	0.46	0
6	NAG	A	1402	-	14,14,15	0.28	0	17,19,21	0.42	0
6	NAG	A	1404	-	14,14,15	0.25	0	17,19,21	0.36	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
6	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1401	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1406	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1401	-	-	0/6/23/26	0/1/1/1
6	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1404	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1402	-	-	0/6/23/26	0/1/1/1
6	NAG	A	1404	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1406	NAG	C1-O5-C5	2.28	115.28	112.19
6	B	1406	NAG	C1-O5-C5	2.26	115.26	112.19
6	A	1406	NAG	C1-O5-C5	2.13	115.08	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1401	NAG	O5-C5-C6-O6
6	C	1401	NAG	C4-C5-C6-O6
6	A	1405	NAG	O5-C5-C6-O6
6	A	1406	NAG	O5-C5-C6-O6
6	B	1405	NAG	O5-C5-C6-O6
6	B	1406	NAG	O5-C5-C6-O6
6	C	1406	NAG	O5-C5-C6-O6
6	A	1405	NAG	C4-C5-C6-O6
6	B	1401	NAG	C4-C5-C6-O6
6	A	1406	NAG	C4-C5-C6-O6
6	B	1404	NAG	C4-C5-C6-O6
6	B	1407	NAG	C4-C5-C6-O6
6	B	1405	NAG	C4-C5-C6-O6
6	B	1406	NAG	C4-C5-C6-O6

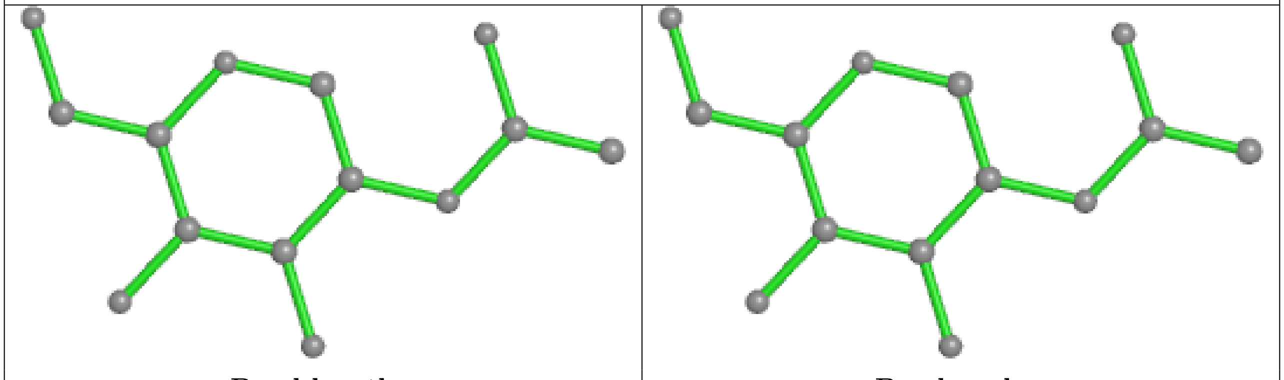
There are no ring outliers.

6 monomers are involved in 12 short contacts:

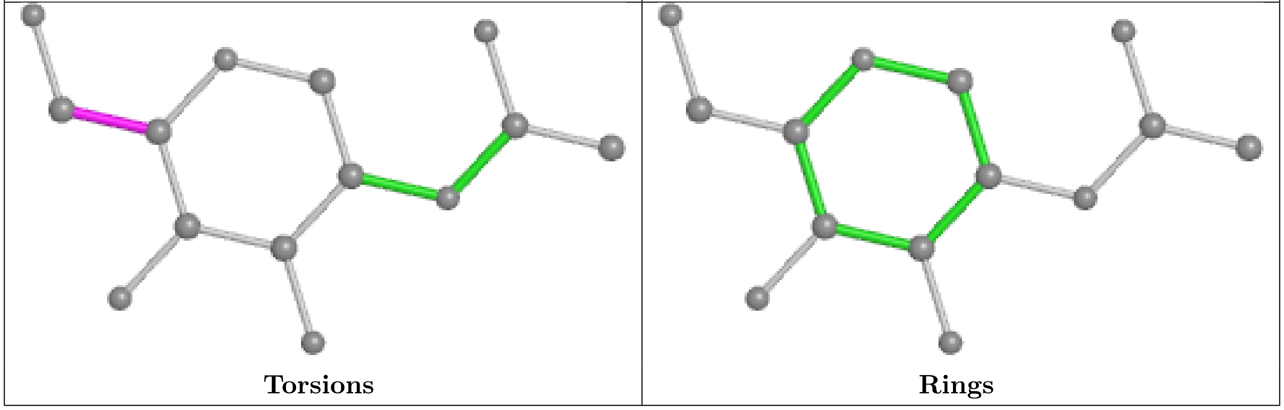
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1401	NAG	1	0
6	B	1401	NAG	1	0
6	A	1401	NAG	3	0
6	A	1406	NAG	2	0
6	A	1402	NAG	2	0
6	A	1404	NAG	3	0

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

Ligand NAG C 1401

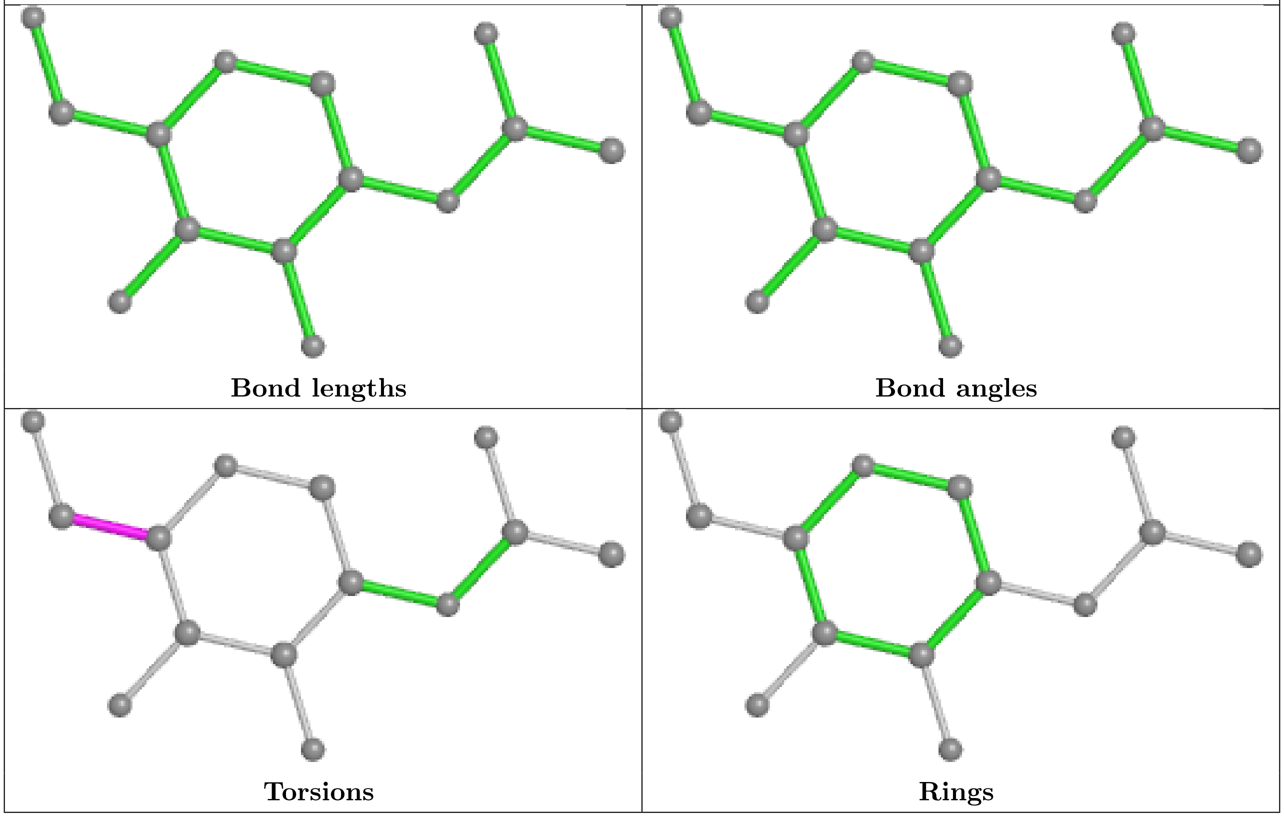


Bond lengths **Bond angles**



Torsions **Rings**

Ligand NAG B 1401



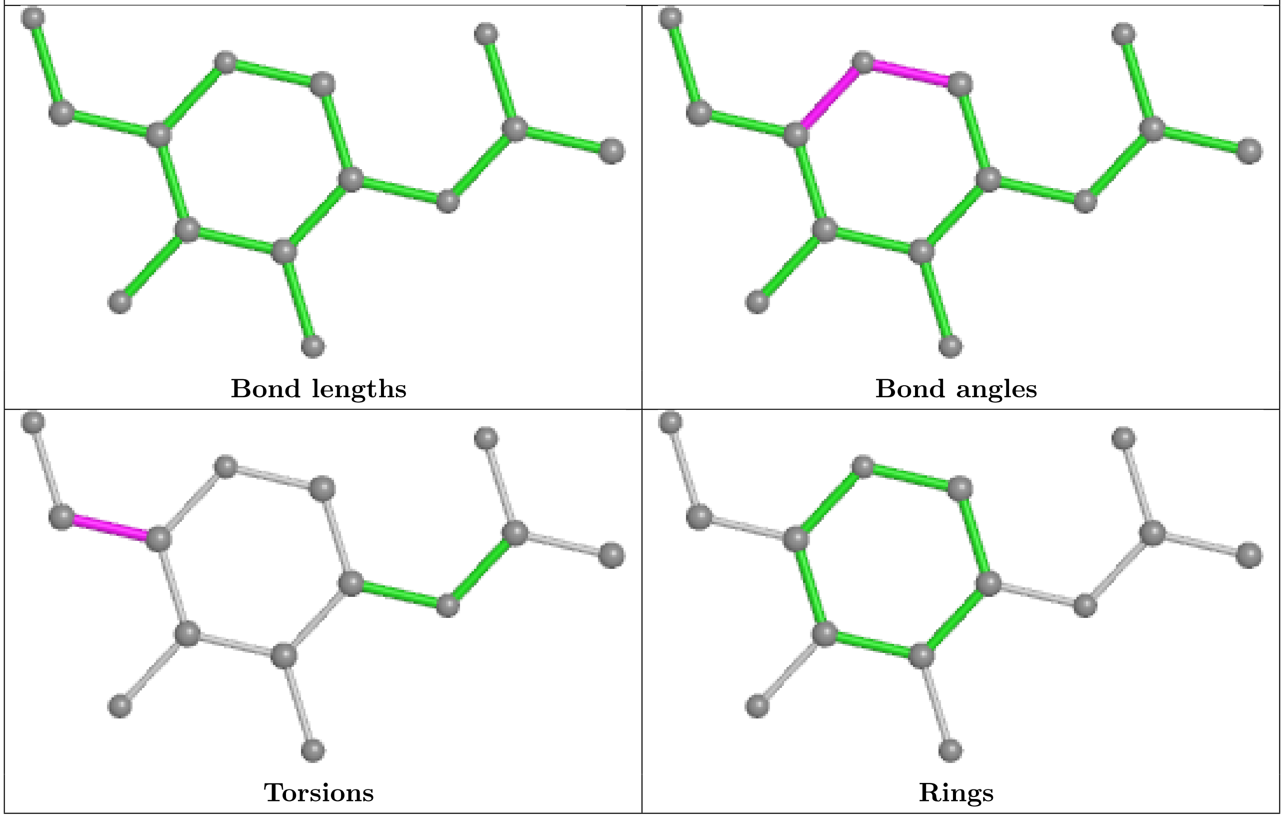
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 1406



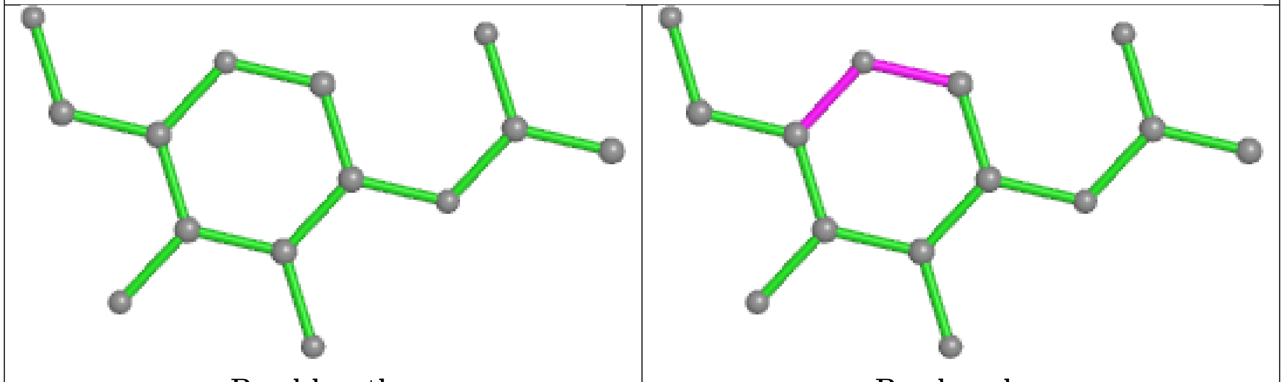
Bond lengths

Bond angles

Torsions

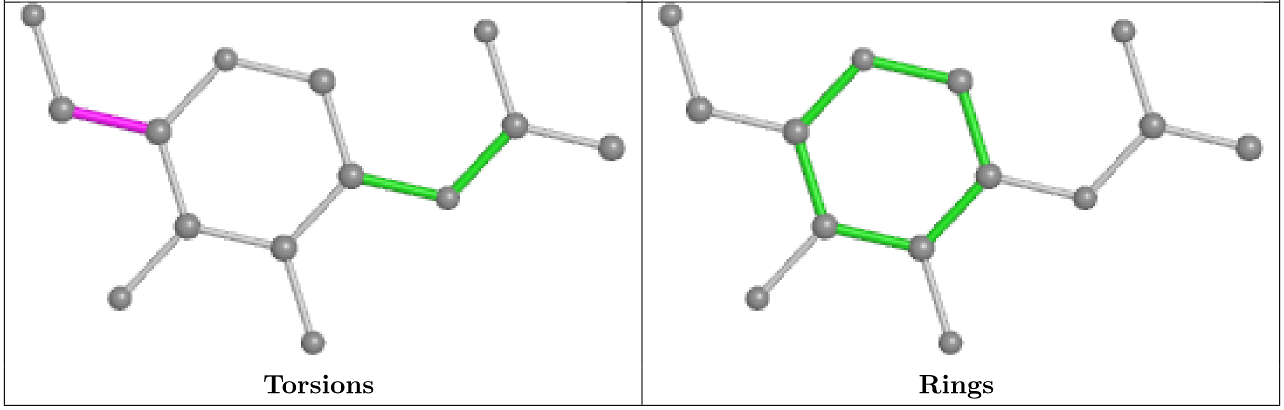
Rings

Ligand NAG C 1406



Bond lengths

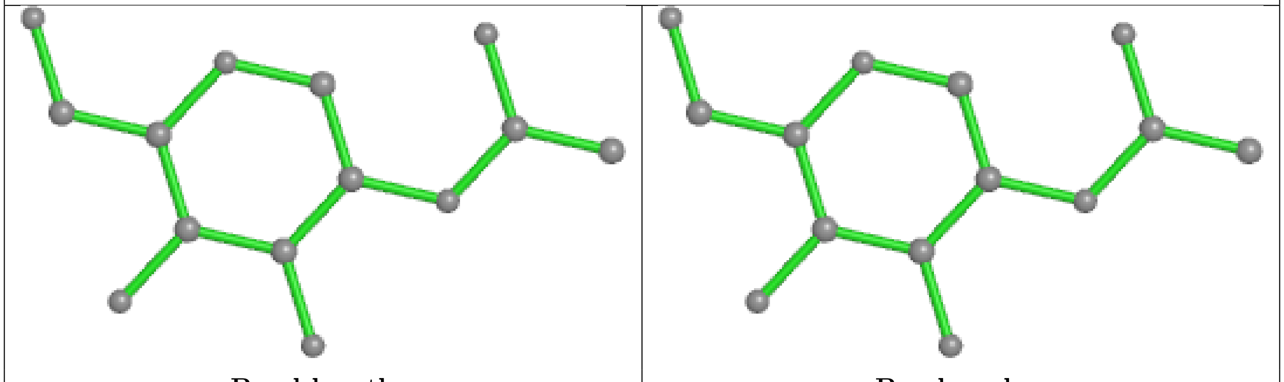
Bond angles



Torsions

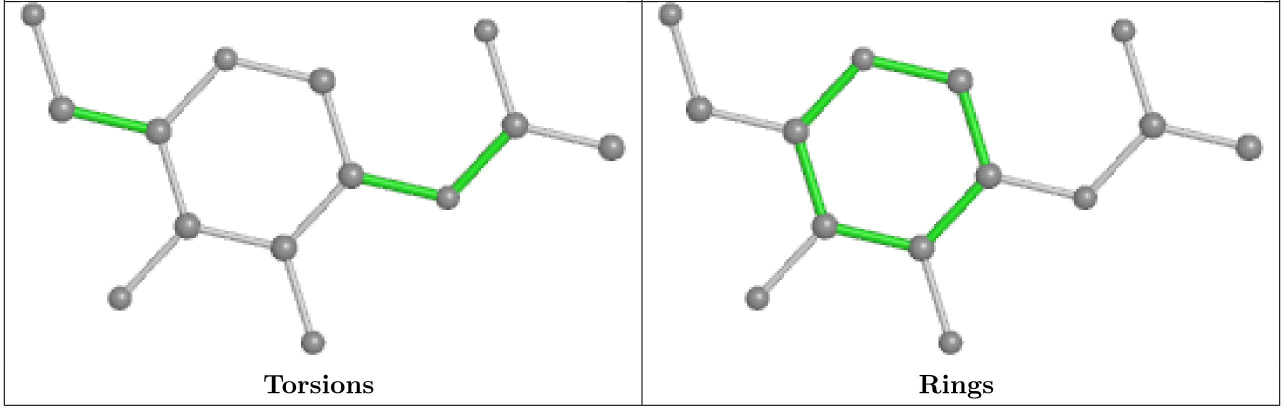
Rings

Ligand NAG B 1402



Bond lengths

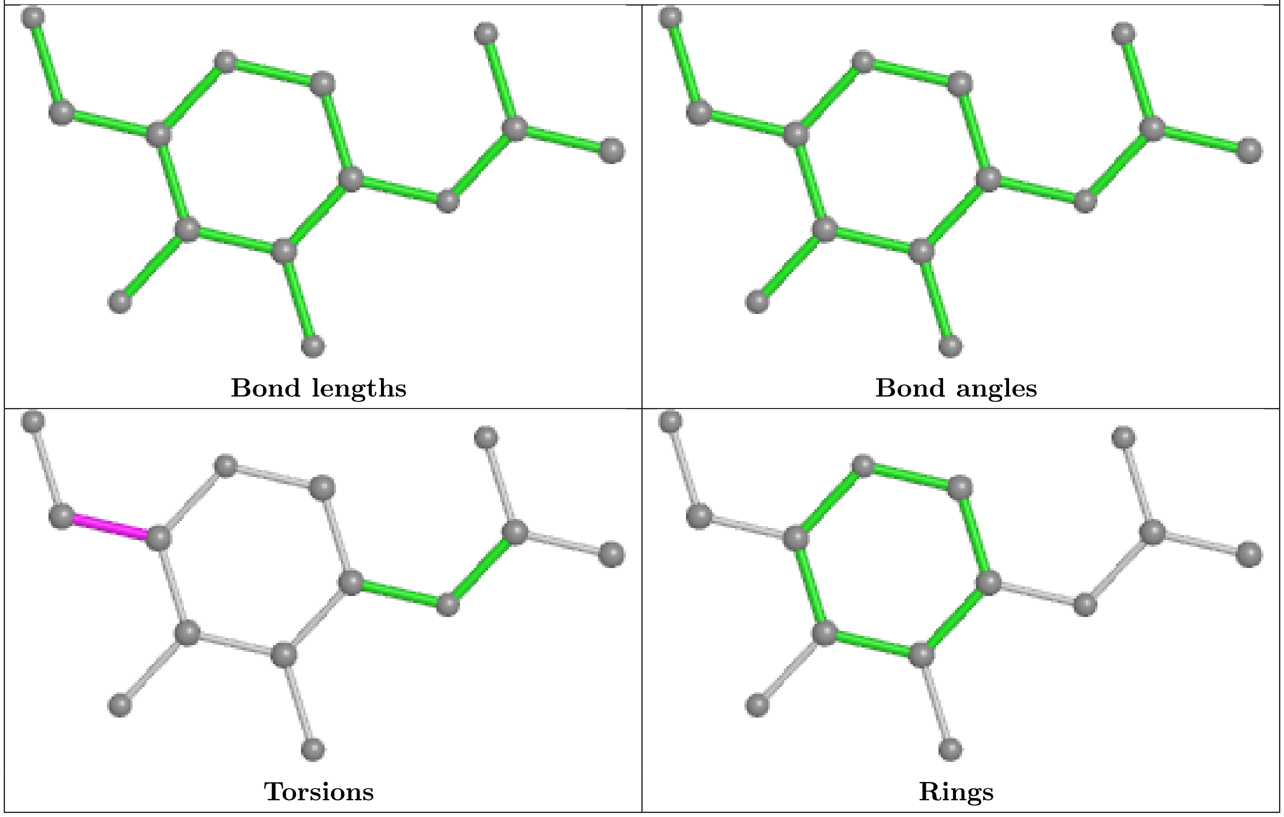
Bond angles



Torsions

Rings

Ligand NAG B 1407



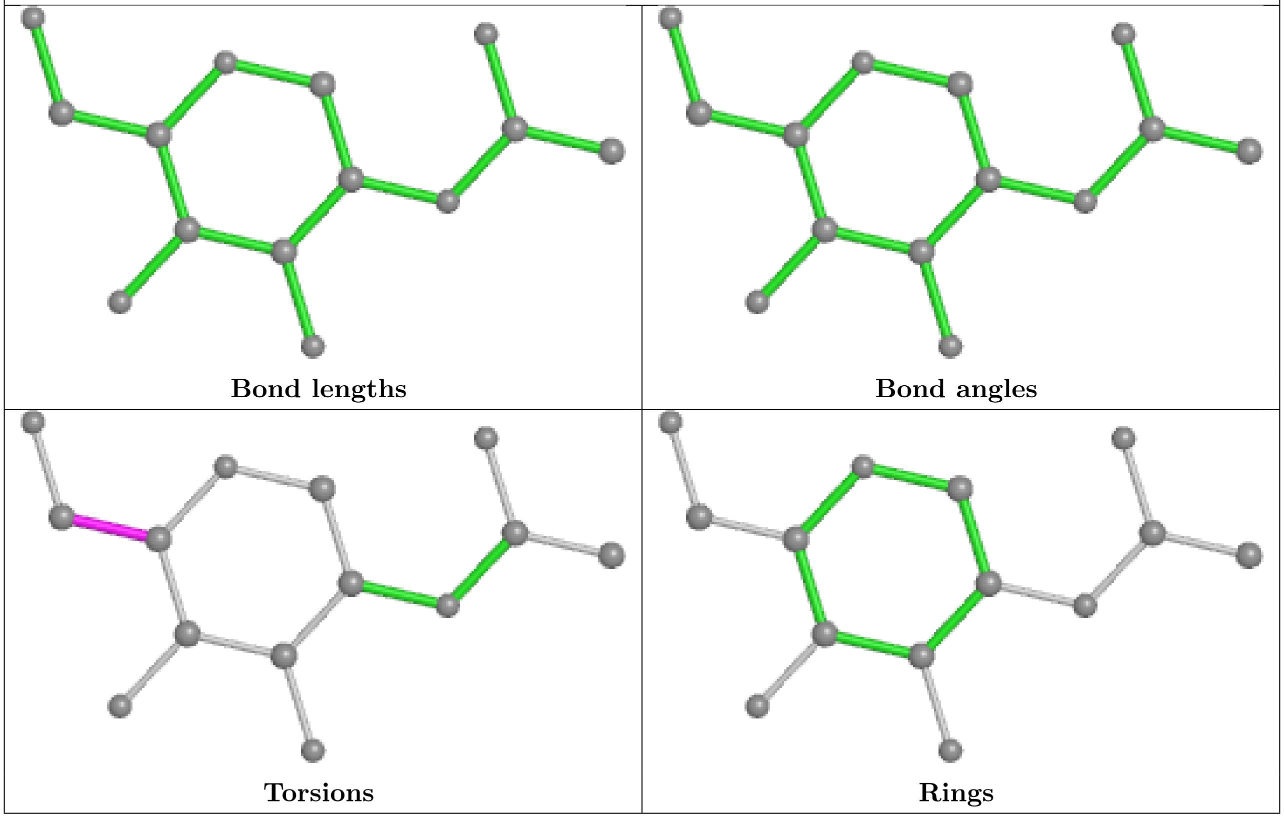
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 1405



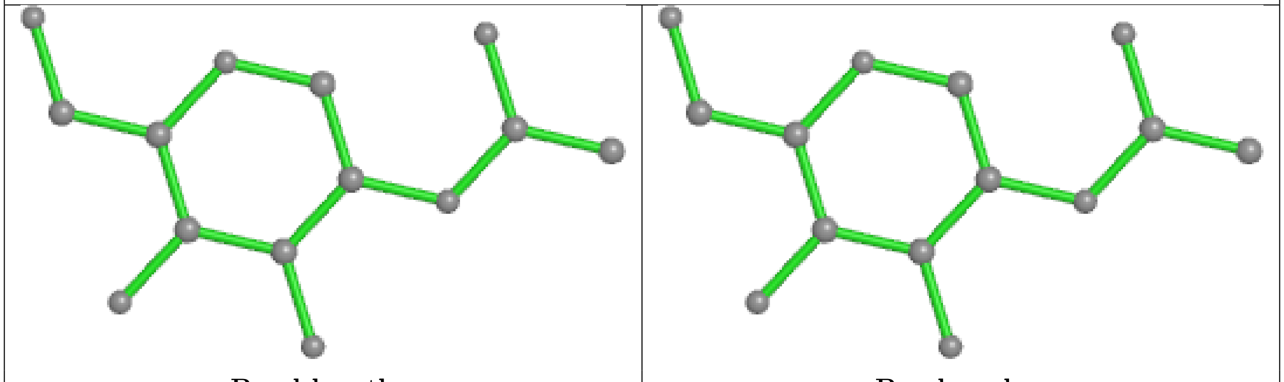
Bond lengths

Bond angles

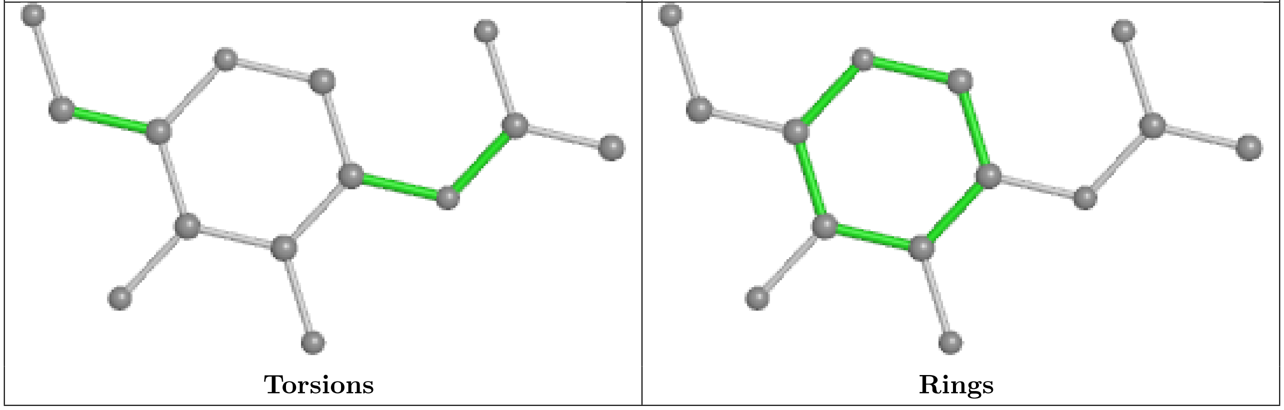
Torsions

Rings

Ligand NAG A 1403

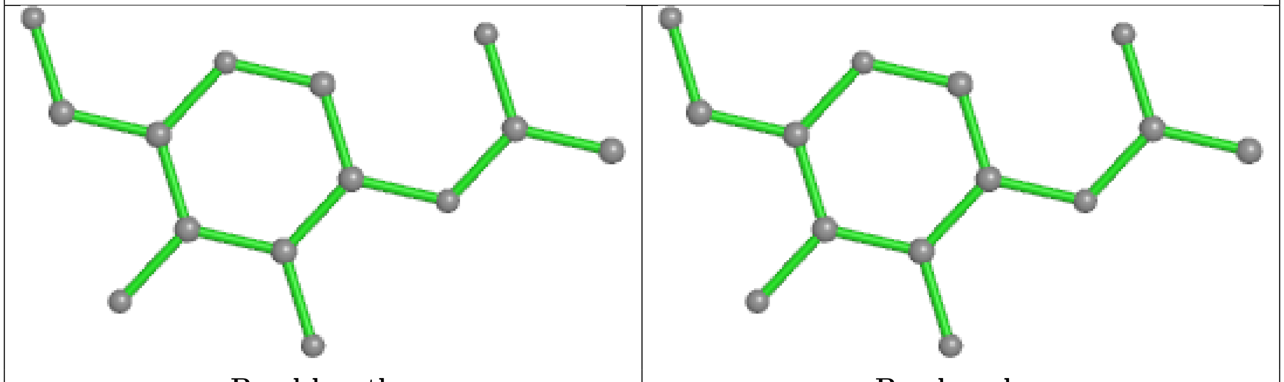


Bond lengths Bond angles

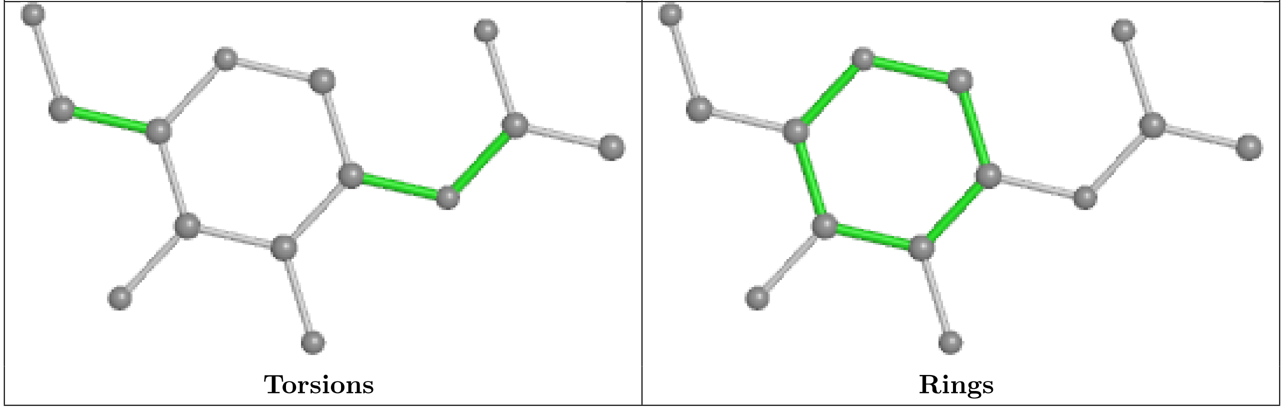


Torsions Rings

Ligand NAG A 1407

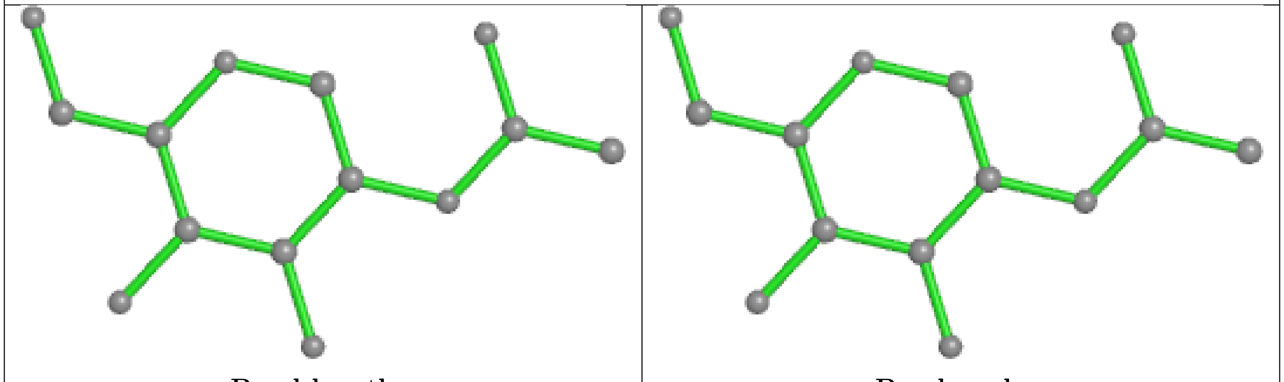


Bond lengths Bond angles



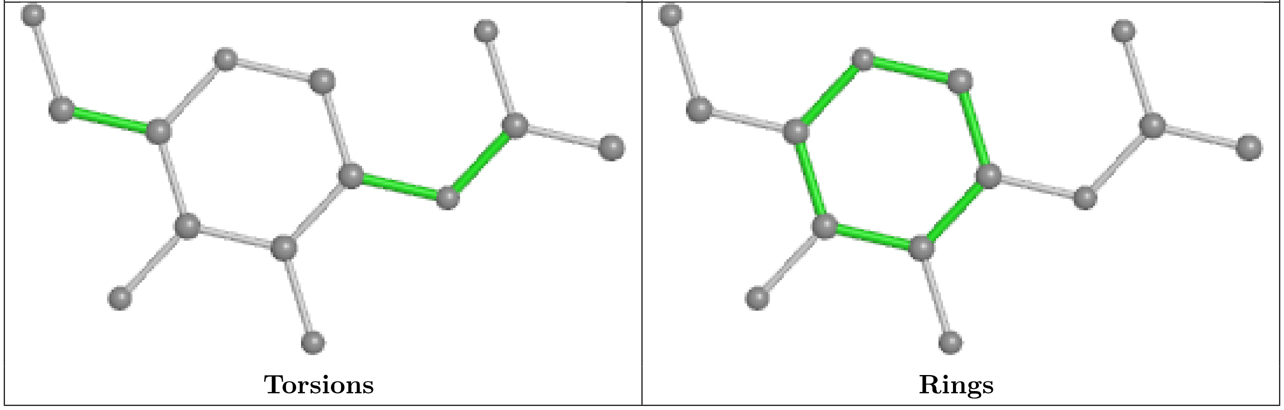
Torsions Rings

Ligand NAG C 1405



Bond lengths

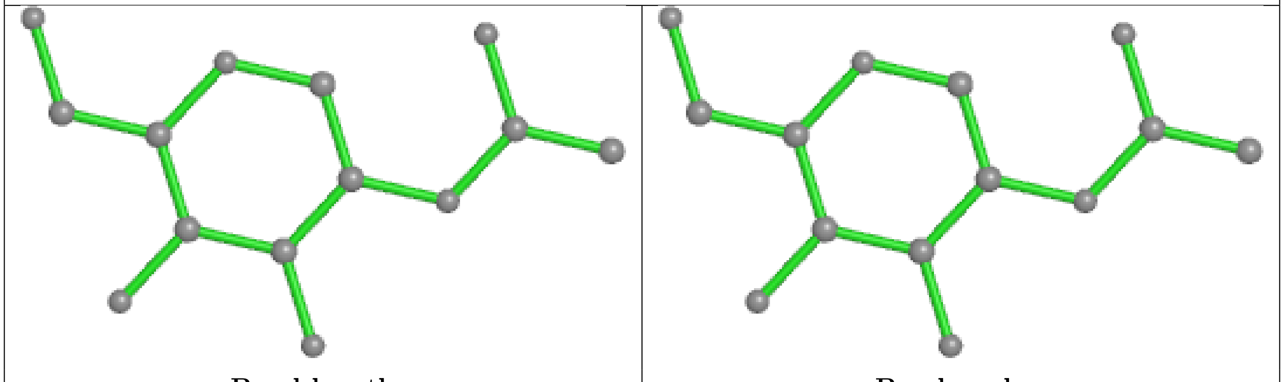
Bond angles



Torsions

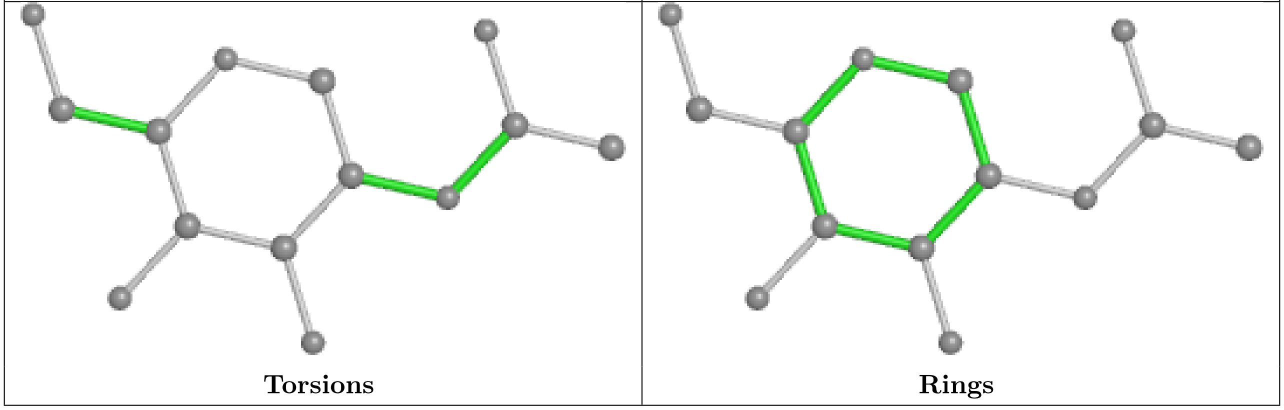
Rings

Ligand NAG A 1401



Bond lengths

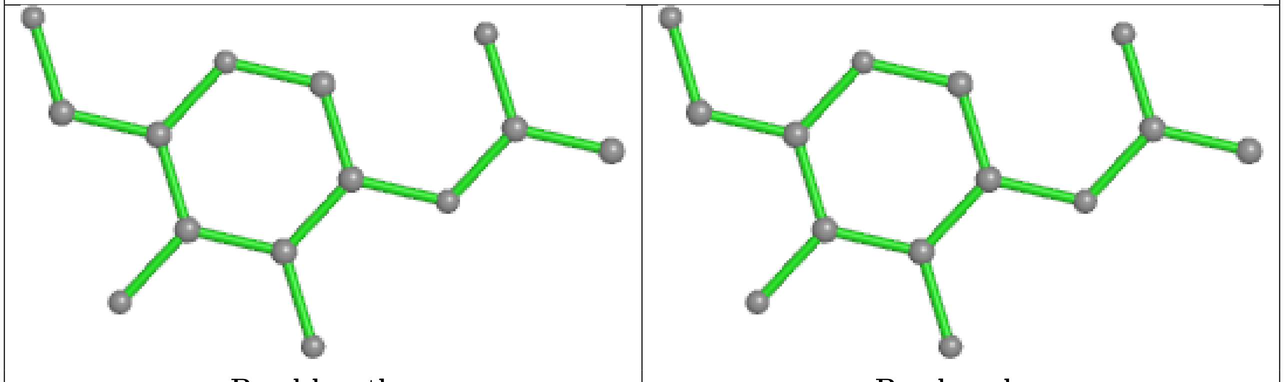
Bond angles



Torsions

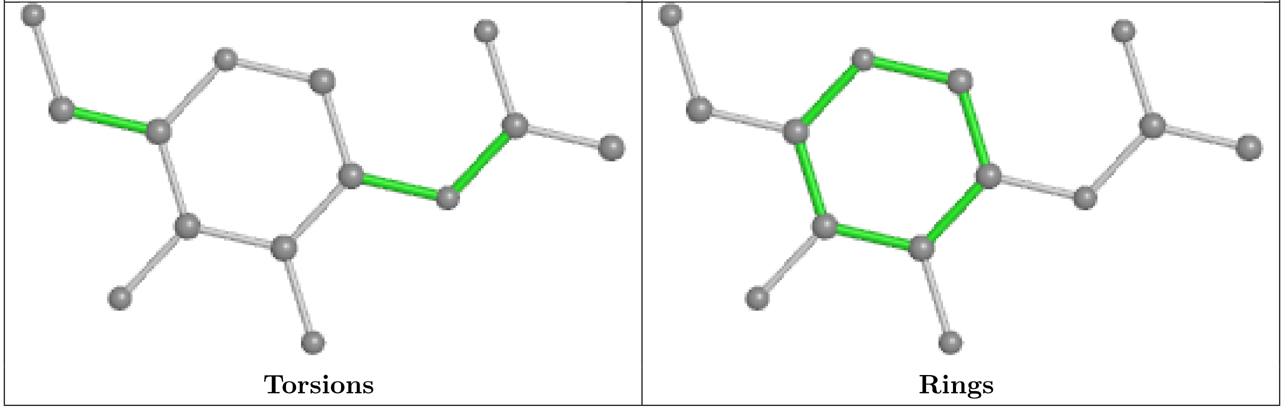
Rings

Ligand NAG C 1403



Bond lengths

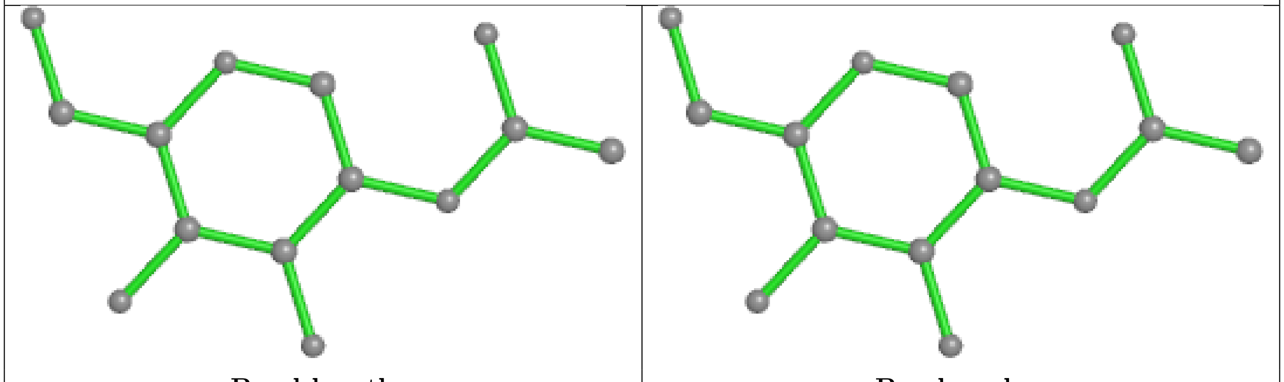
Bond angles



Torsions

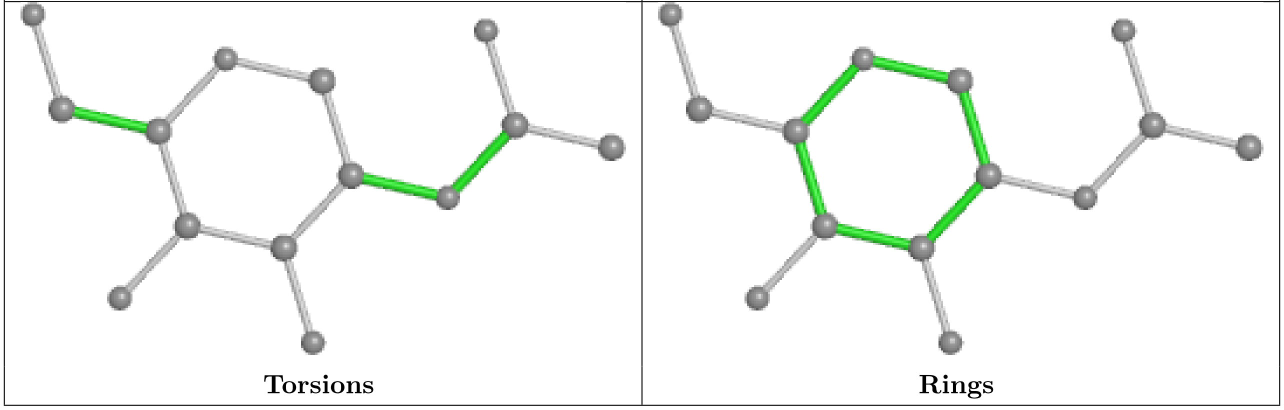
Rings

Ligand NAG C 1407



Bond lengths

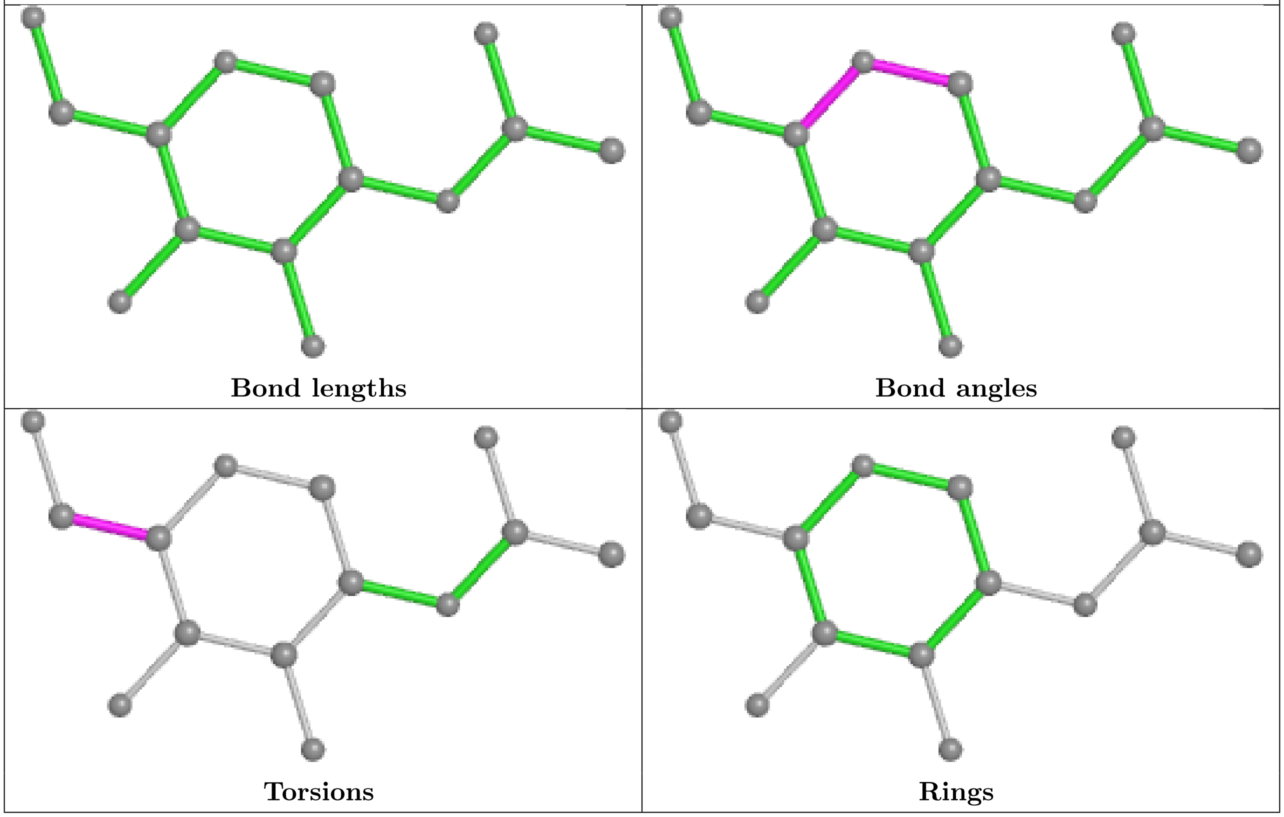
Bond angles



Torsions

Rings

Ligand NAG A 1406



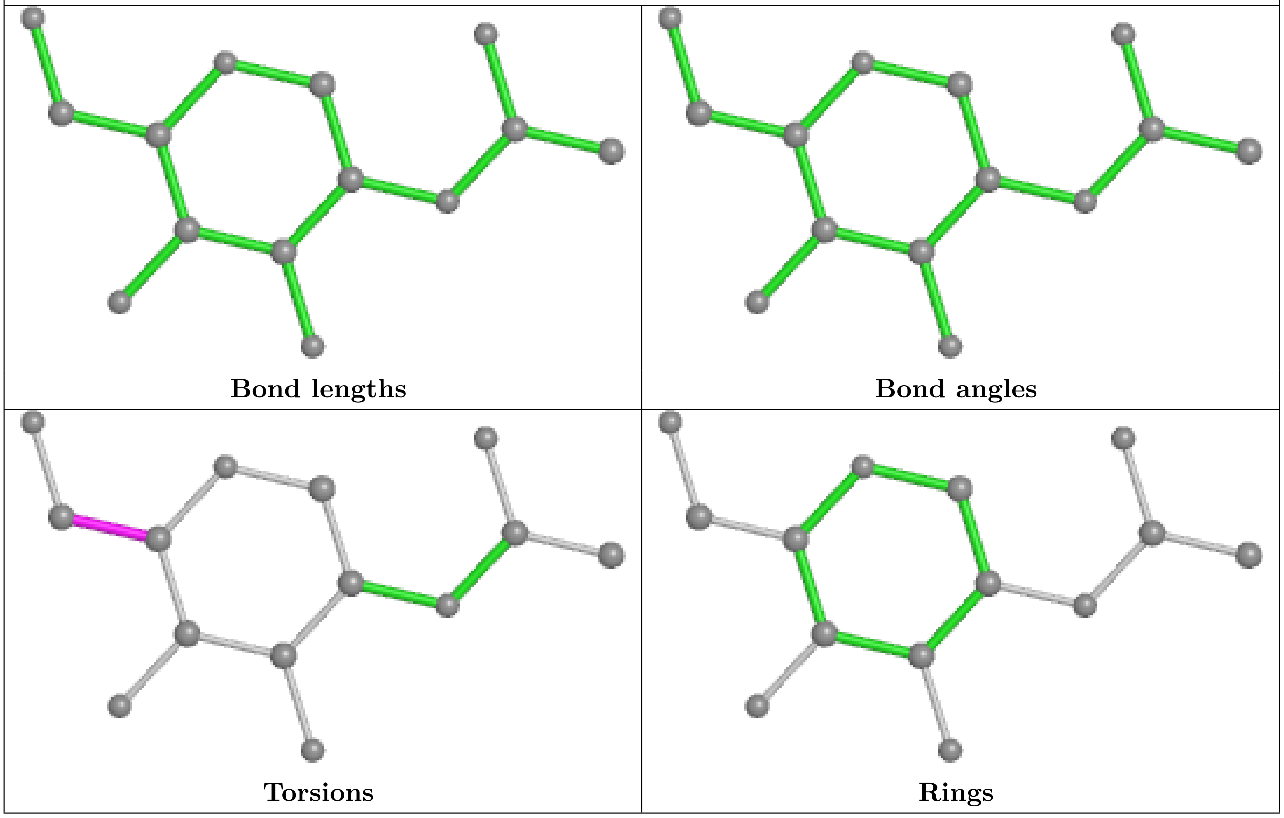
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 1404



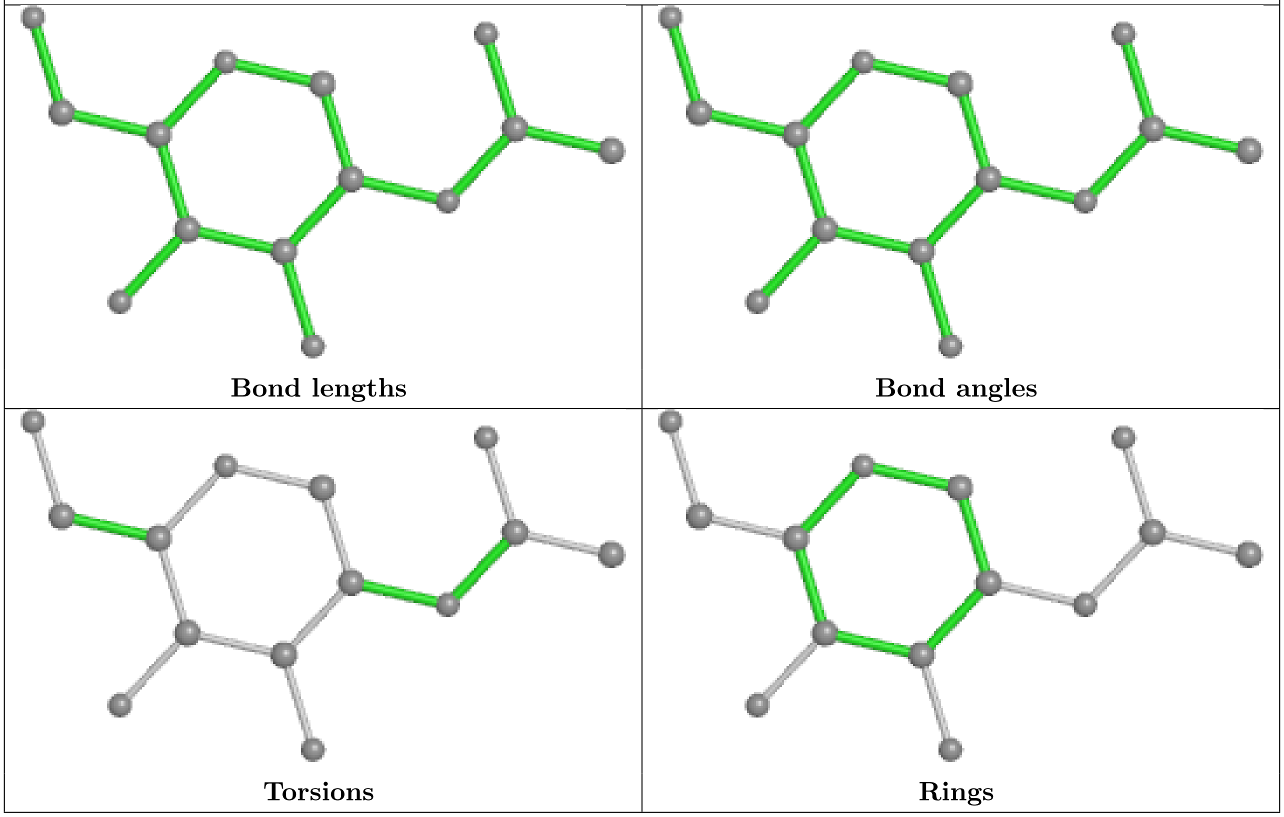
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 1404



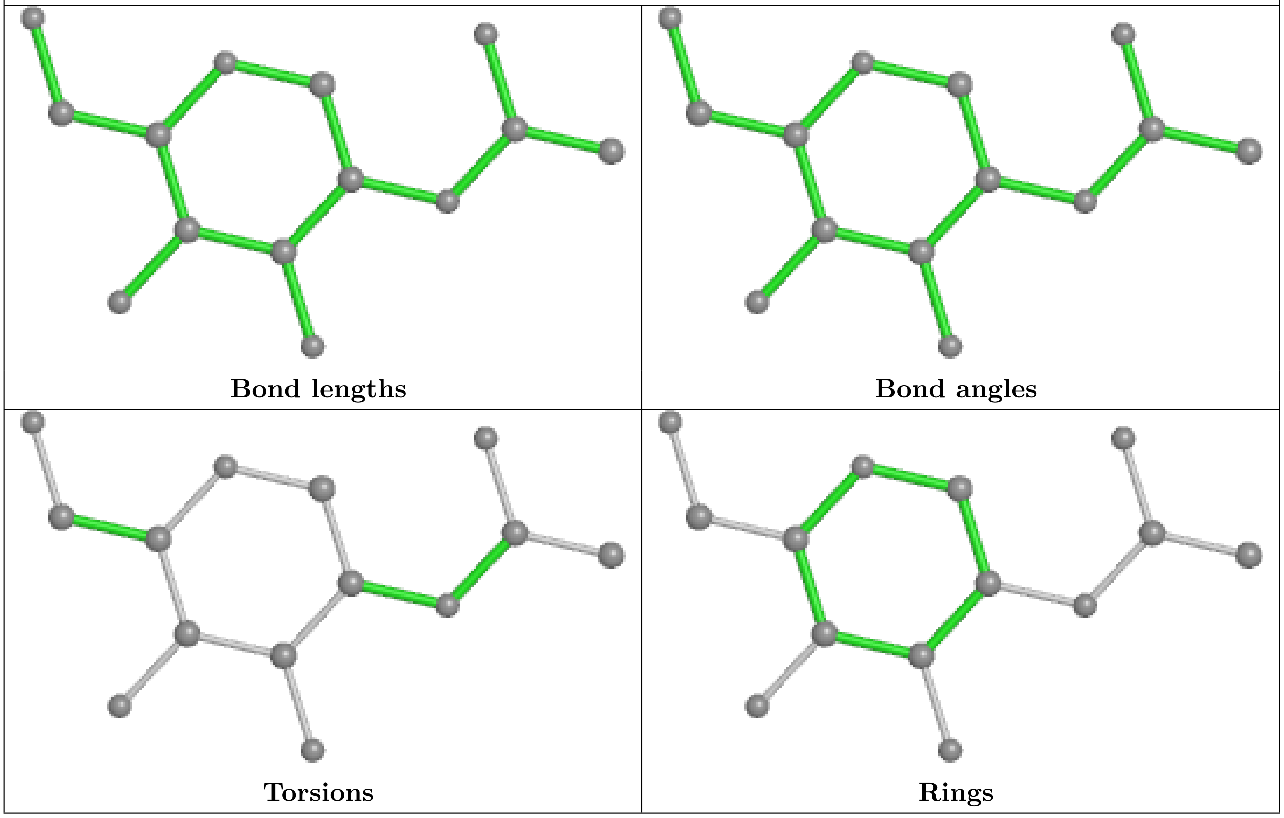
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 1403



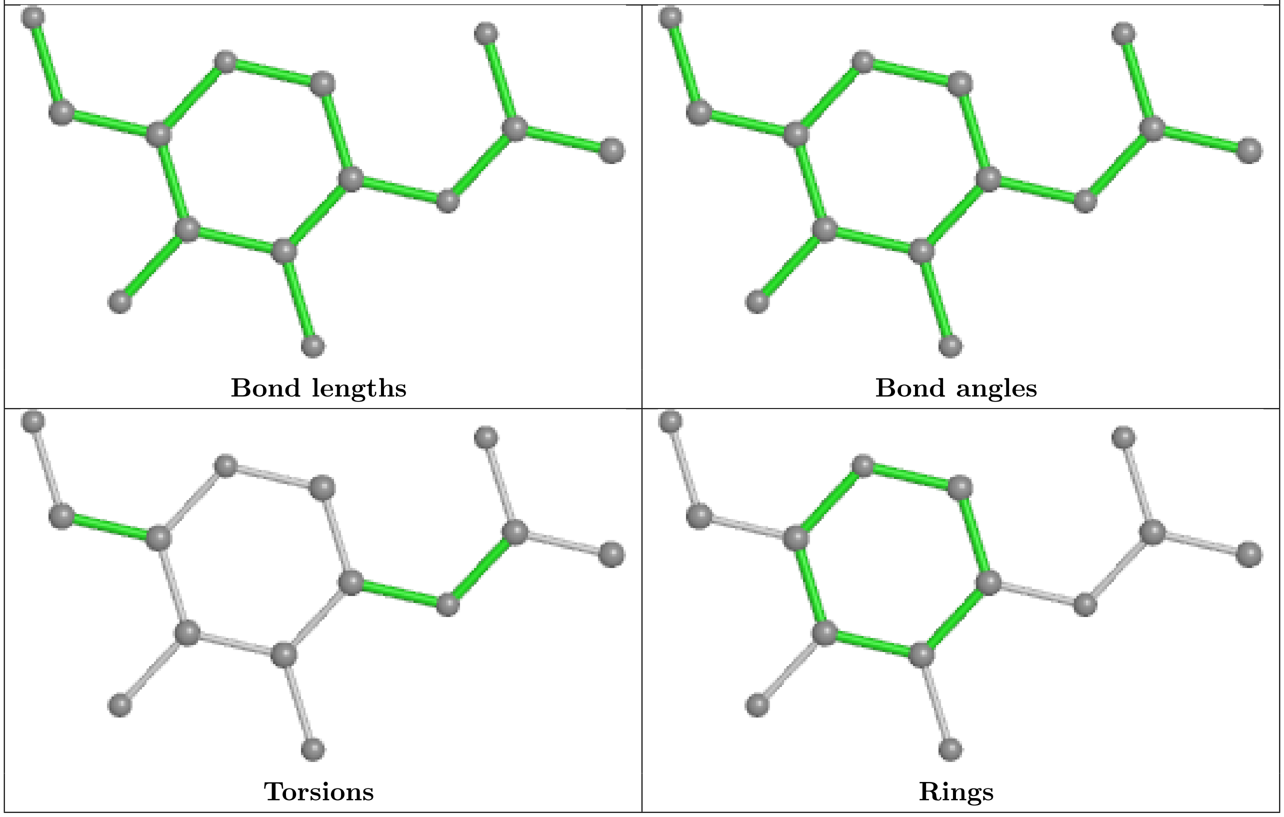
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 1402



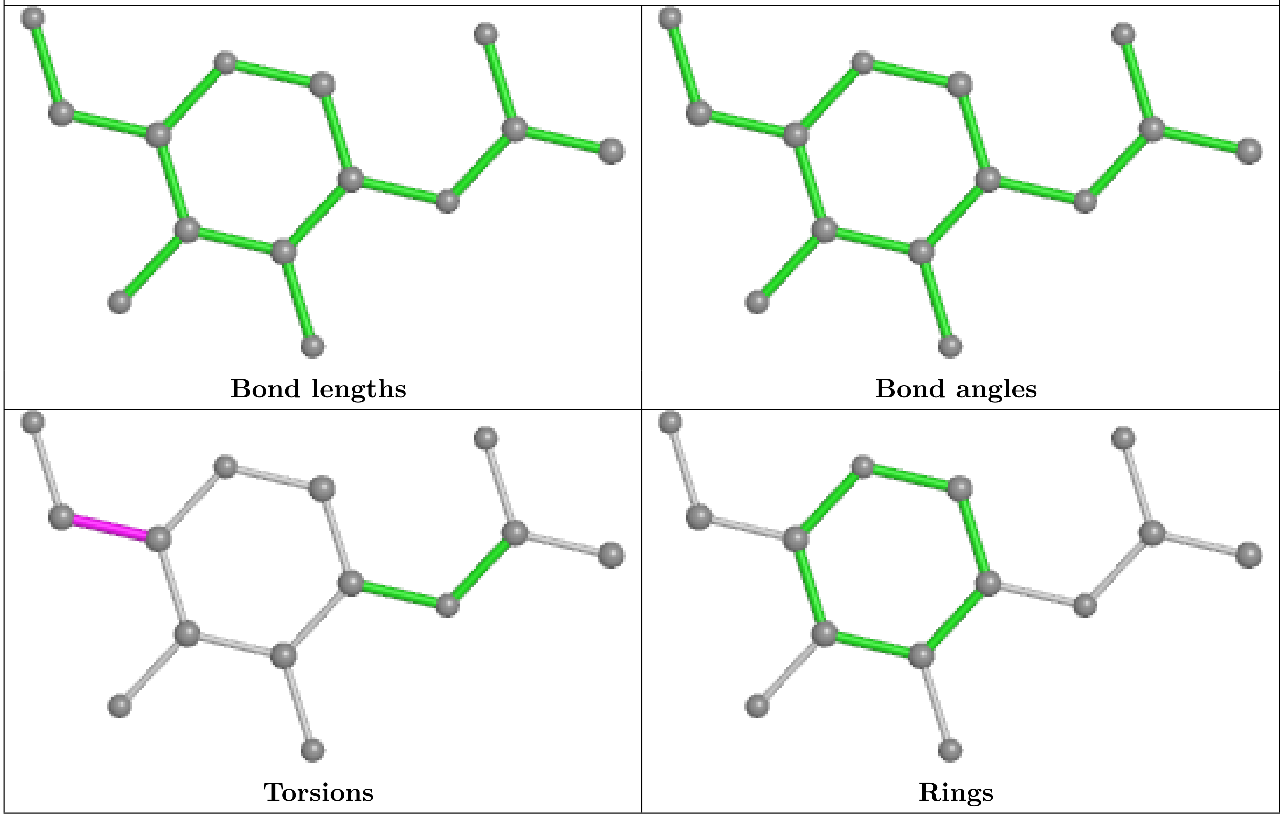
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 1405



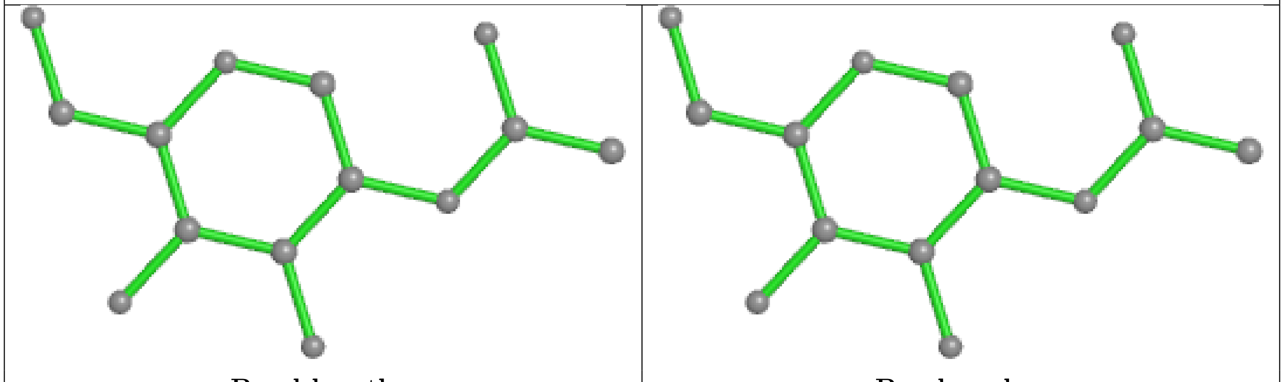
Bond lengths

Bond angles

Torsions

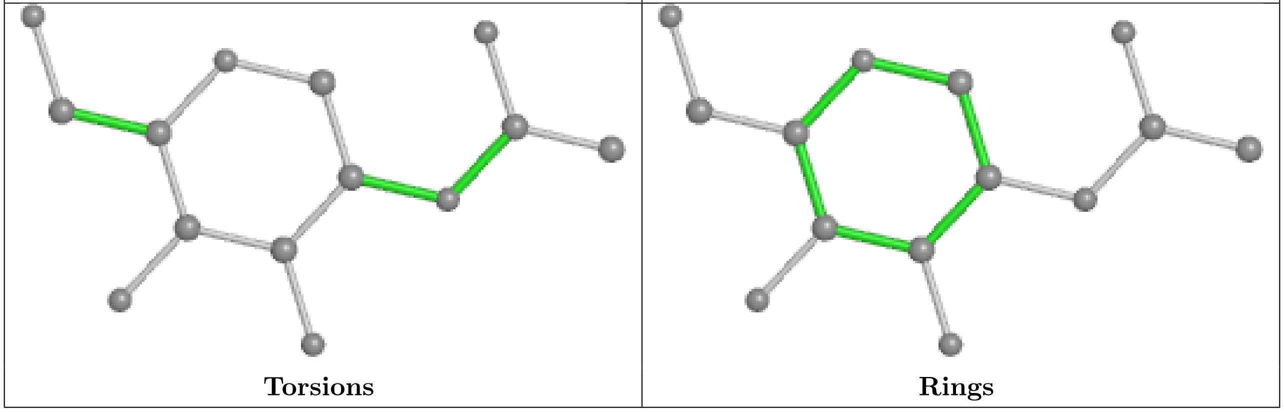
Rings

Ligand NAG A 1402



Bond lengths

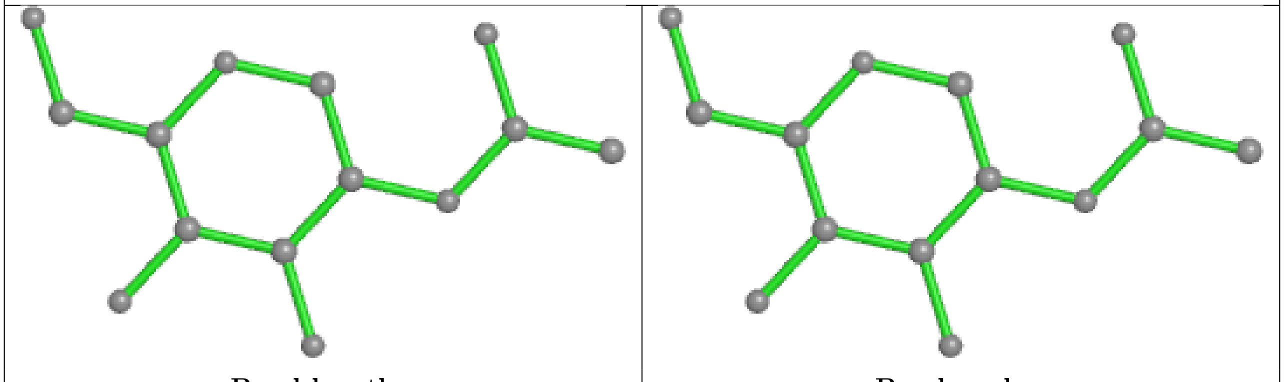
Bond angles



Torsions

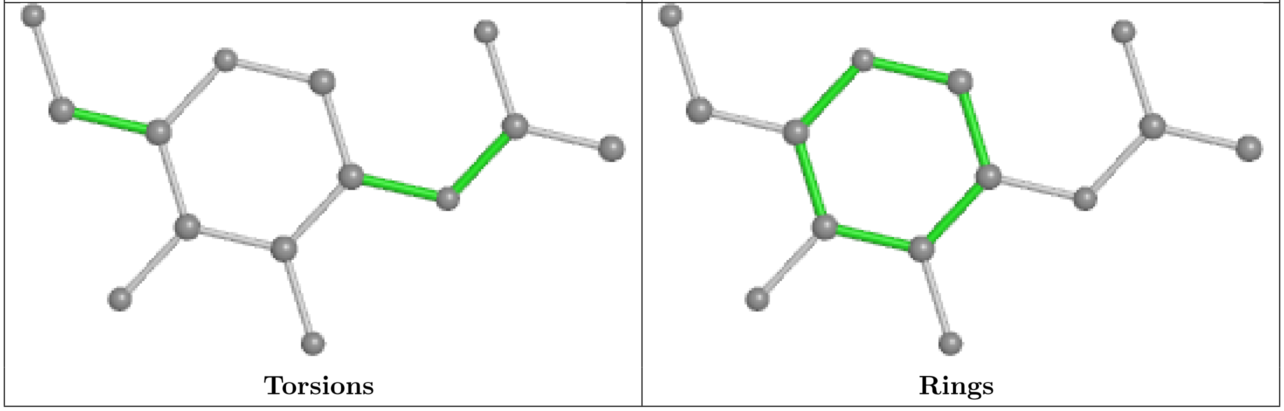
Rings

Ligand NAG A 1404



Bond lengths

Bond angles



Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

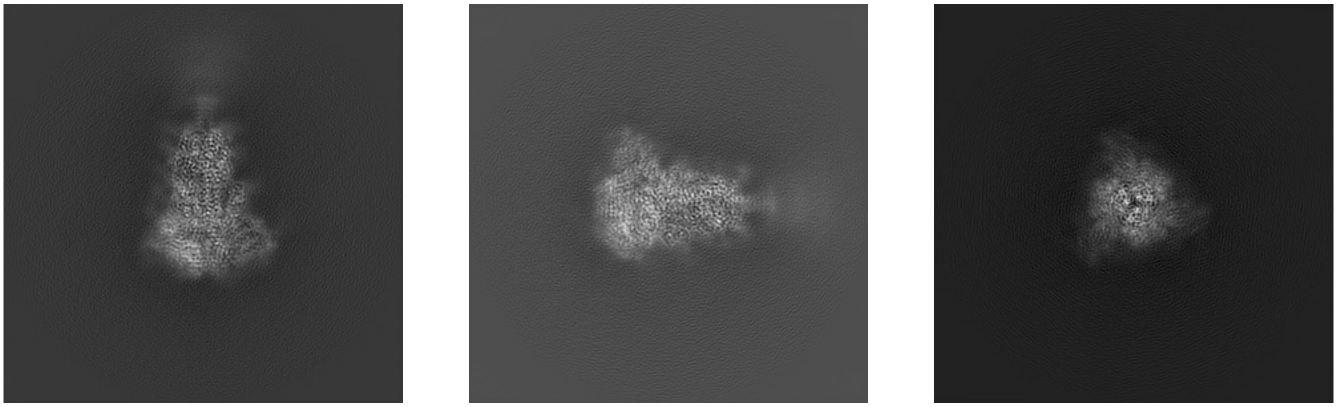
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-22292. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

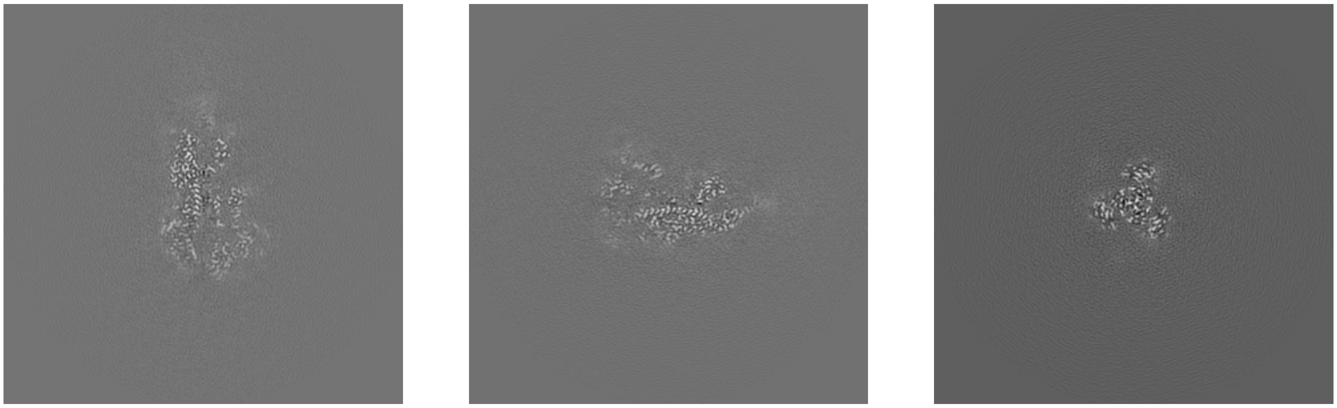


X Y Z

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

6.2 Central slices ⓘ

6.2.1 Primary map

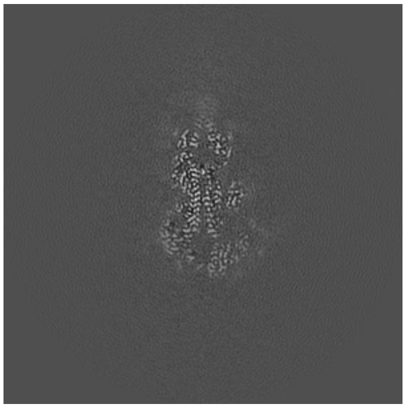


X Index: 240 Y Index: 240 Z Index: 240

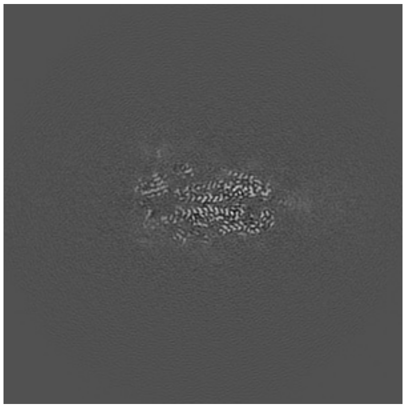
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

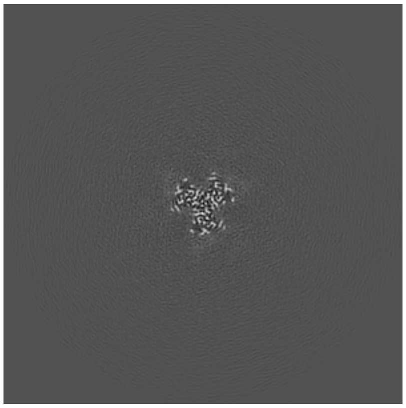
6.3.1 Primary map



X Index: 243



Y Index: 244



Z Index: 279

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

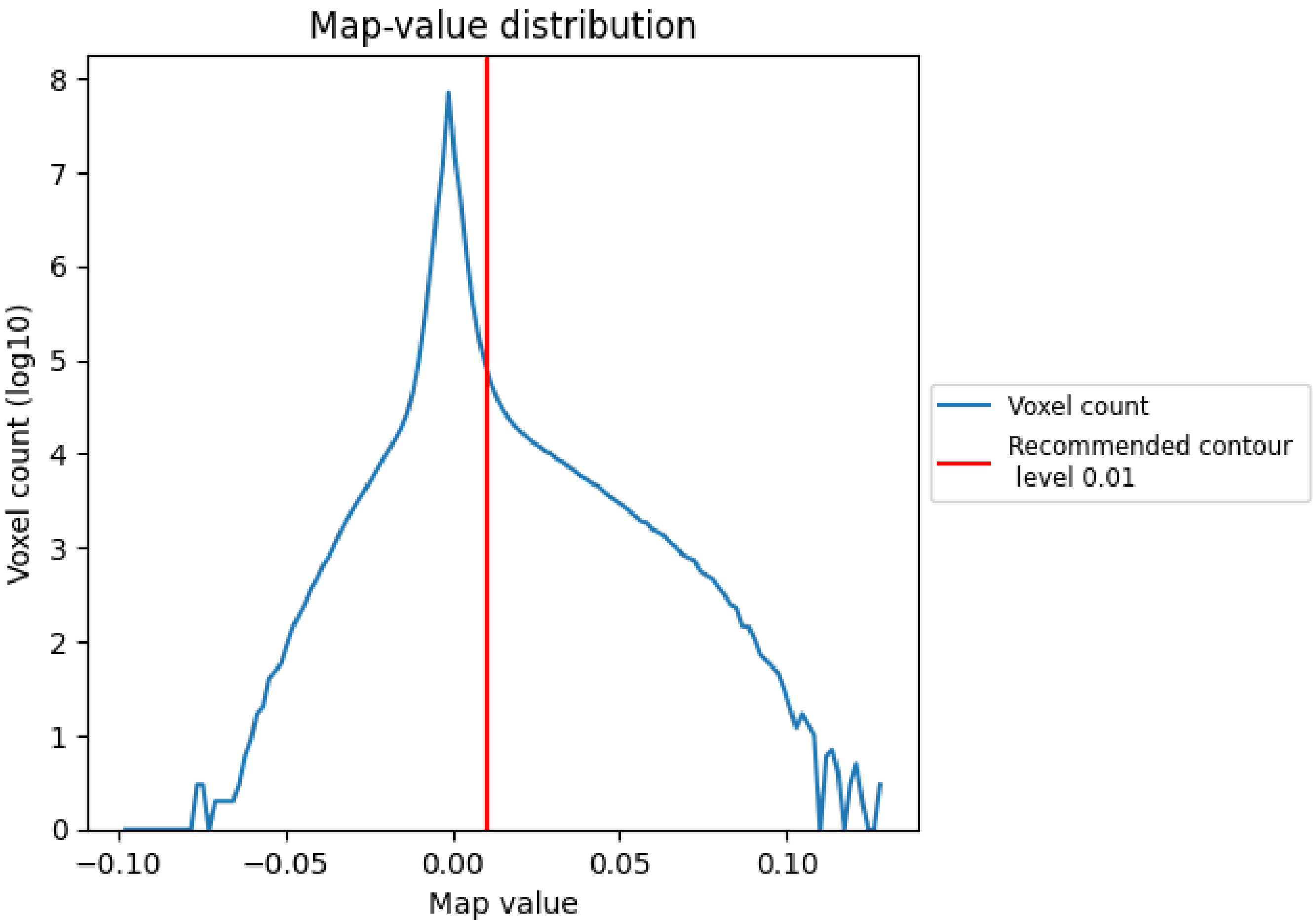
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

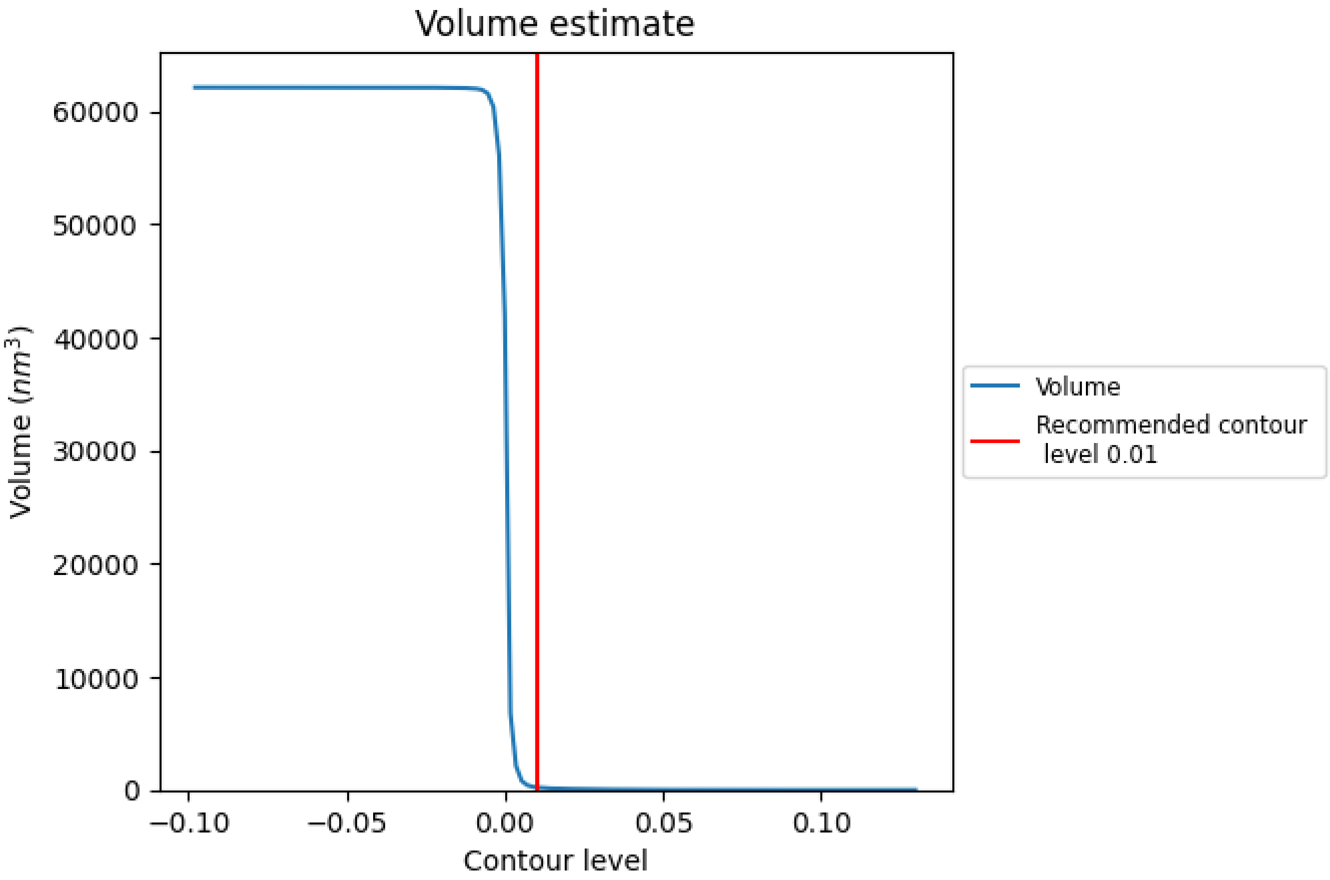
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

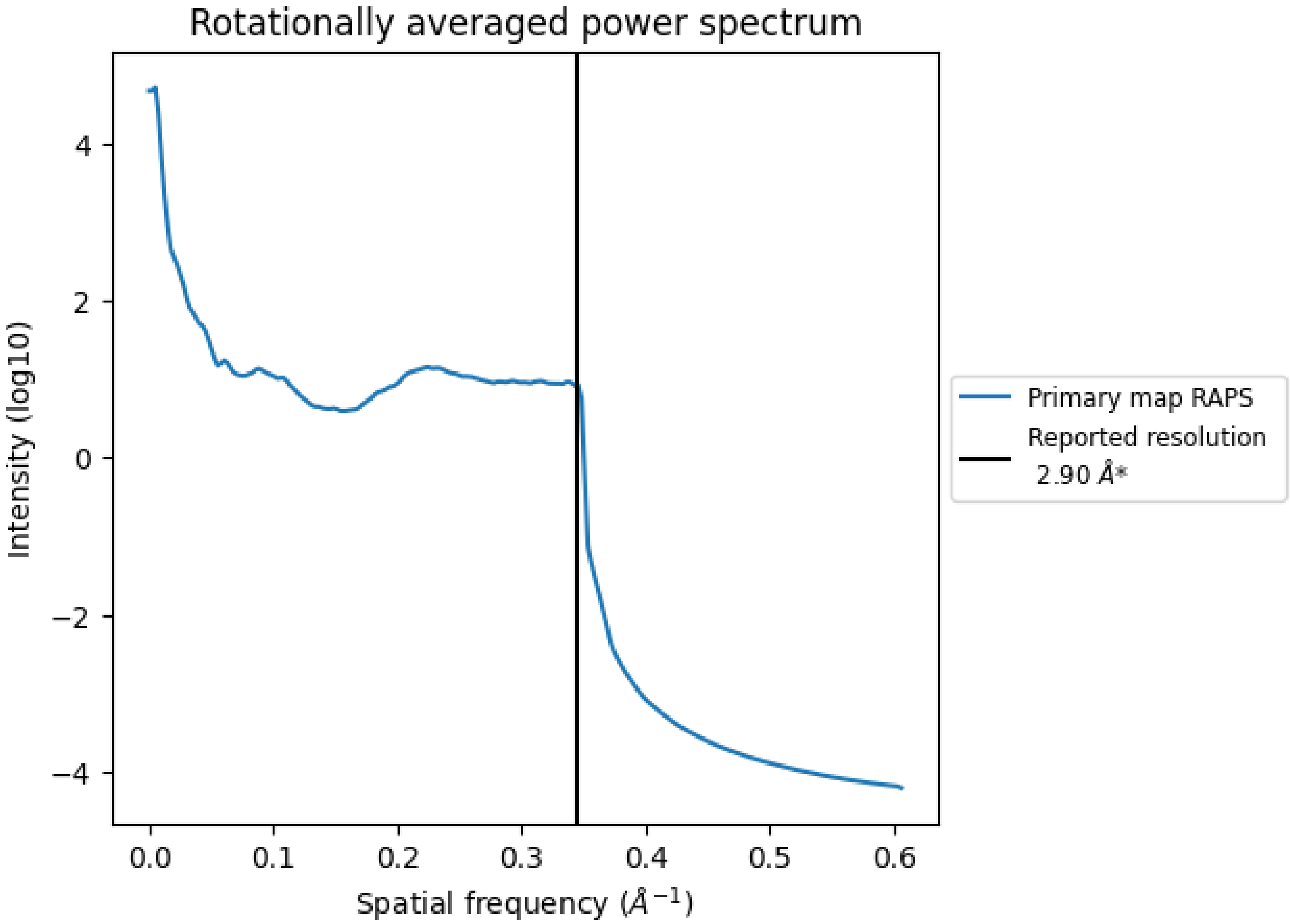
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 232 nm^3; this corresponds to an approximate mass of 210 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation (i)

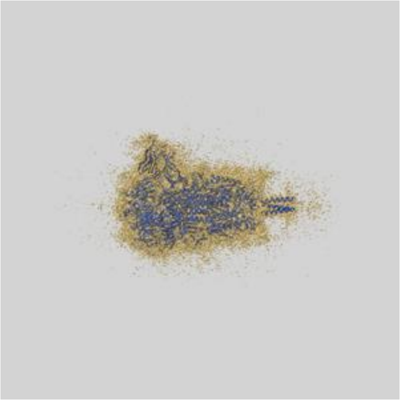
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

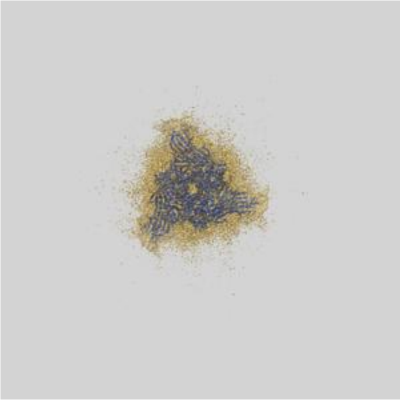
This section contains information regarding the fit between EMDB map EMD-22292 and PDB model 6XR8. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay

X



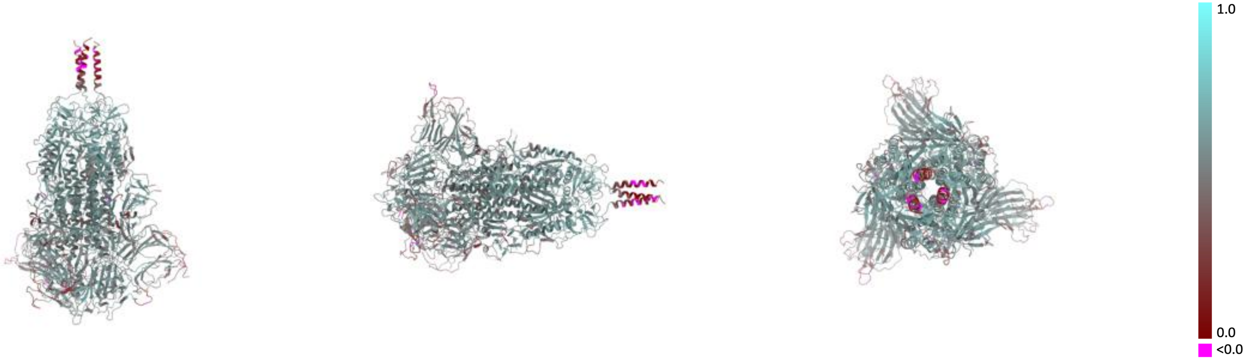
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

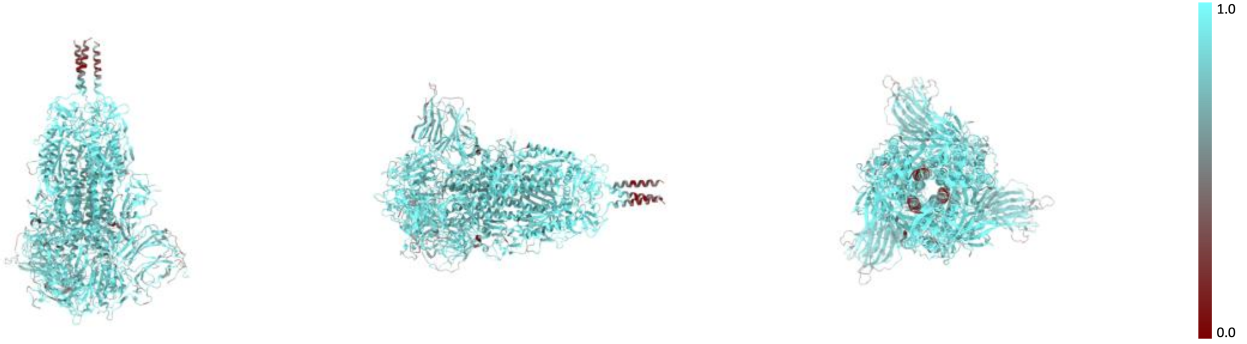
9.2 Q-score mapped to coordinate model ⓘ



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.

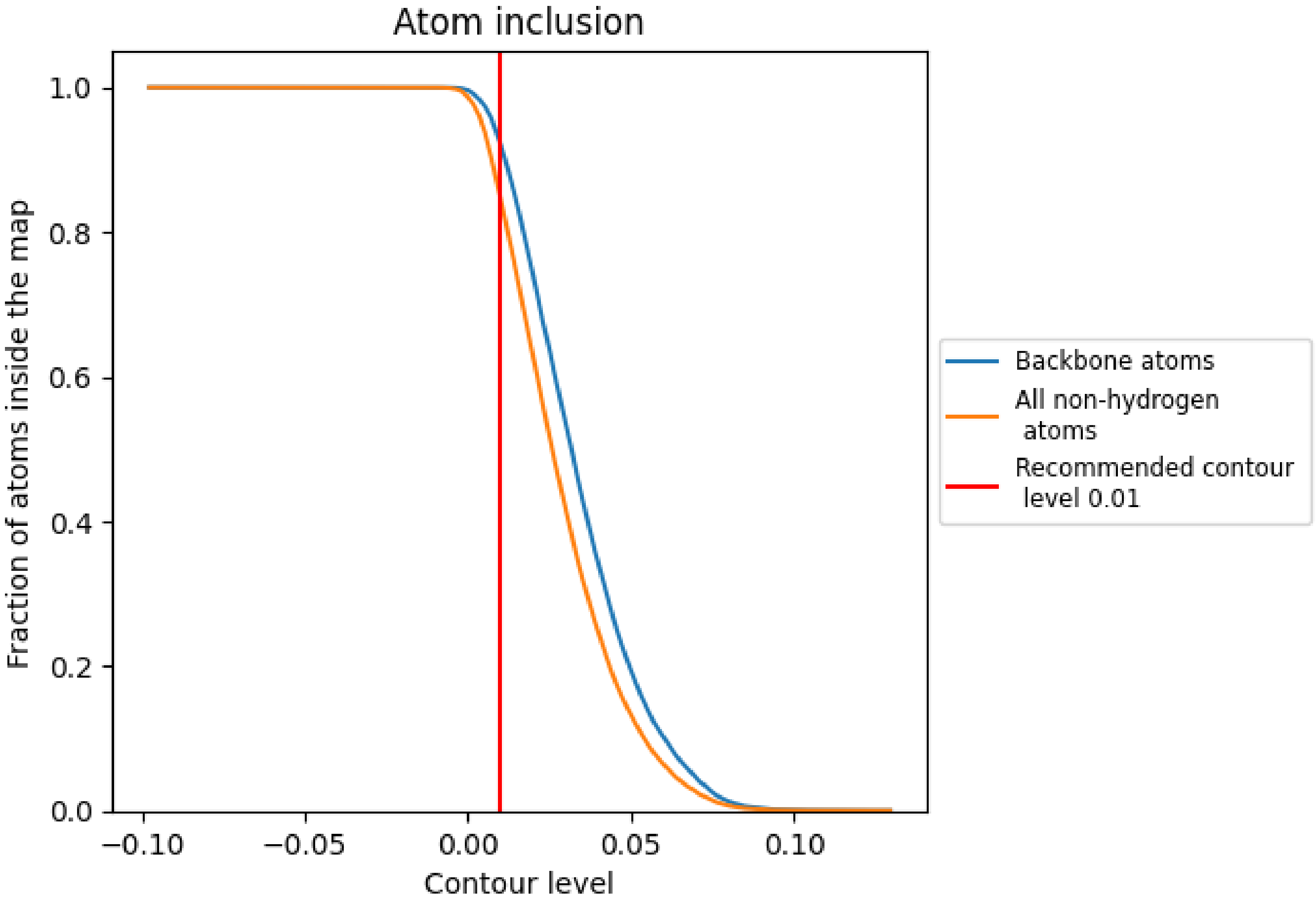
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.01).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8468	0.5090
0	0.5000	0.2710
1A	0.4615	0.2460
2	0.4737	0.2660
4A	0.6410	0.2910
5	0.4872	0.4000
7A	0.4600	0.1740
9	0.3214	0.1470
A	0.8645	0.5210
B	0.8645	0.5210
BA	0.4286	0.3190
C	0.8663	0.5200
DA	0.4615	0.3200
GA	0.4103	0.2100
I	0.6667	0.3550
JA	0.3590	0.2560
L	0.5000	0.2360
MA	0.5128	0.2770
N	0.5000	0.2860
PA	0.6667	0.3470
Q	0.4872	0.3830
SA	0.4600	0.1870
U	0.3929	0.1580
W	0.5357	0.3020
Y	0.4872	0.3090
b	0.4359	0.2200
cA	0.7436	0.4280
e	0.4359	0.2550
fA	0.4643	0.2610
h	0.4872	0.2490
hA	0.4737	0.2650
k	0.6923	0.3390
kA	0.4359	0.3670
n	0.4400	0.1730
oA	0.3571	0.1660

Continued on next page...

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Chain	Atom inclusion	Q-score
qA	0.4286	0.3460
sA	0.4615	0.3530
vA	0.4103	0.2070
x	0.7179	0.3890
yA	0.4359	0.2480