



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2025 – 07:40 pm GMT

PDB ID : 9GXG
EMDB ID : EMD-51660
Title : Structure of the SARS-CoV spike glycoprotein in complex with a biparatopic Bicycle molecule
Authors : Drulyte, I.; Pellegrino, S.; Harman, M.; Bezerra, G.A.
Deposited on : 2024-09-30
Resolution : 1.92 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis	: FAILED
Mogul	: 1.8.4, CSD as541be (2020)
MolProbity	: 4.02b-467
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	: FAILED
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.41

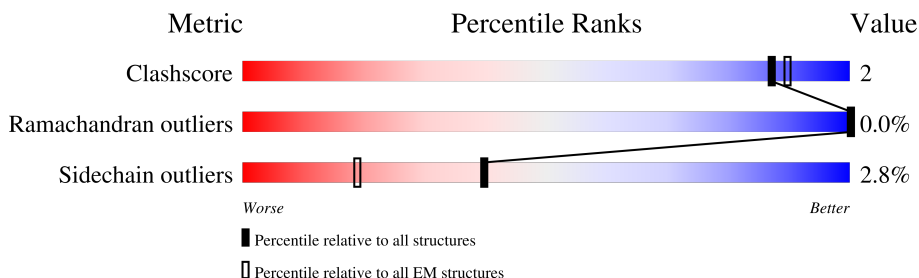
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.92 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1133	89% 8% .
1	B	1133	90% 7% .
1	C	1133	90% 7% .
2	D	15	87% 13%
2	E	15	93% 7%
2	F	15	100%
3	G	16	94% 6%
3	H	16	94% 6%
3	I	16	94% 6%

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Mol	Chain	Length	Quality of chain
4	AA	2	100%
4	AB	2	100%
4	AC	2	100%
4	AD	2	50%
4	AE	2	100%
4	AF	2	100%
4	AG	2	50%
4	AH	2	100%
4	BA	2	50%
4	BB	2	50%
4	BC	2	100%
4	BD	2	100%
4	BE	2	50%
4	BF	2	100%
4	BG	2	50%
4	BH	2	100%
4	BI	2	100%
4	CA	2	100%
4	CB	2	50%
4	CC	2	50%
4	CD	2	100%
4	CE	2	100%
4	CF	2	100%
4	CG	2	100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28265 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	1102	Total	C	N	O	S	1	0
			8620	5498	1440	1642	40		
1	B	1101	Total	C	N	O	S	2	0
			8620	5499	1442	1639	40		
1	C	1102	Total	C	N	O	S	1	0
			8620	5498	1440	1642	40		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Biparatopic bicycle molecule (14mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	15	Total	C	N	O	S	0	1
			100	64	15	17	4		
2	E	15	Total	C	N	O	S	0	1
			100	64	15	17	4		
2	F	15	Total	C	N	O	S	0	1
			100	64	15	17	4		

- Molecule 3 is a protein called Biparatopic bicycle molecule (15mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	16	Total	C	N	O	S	0	1
			101	63	18	17	3		
3	H	16	Total	C	N	O	S	0	1
			101	63	18	17	3		
3	I	16	Total	C	N	O	S	0	1
			101	63	18	17	3		

- Molecule 4 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
4	AA	2	Total	C	N	O	0	0
			28	16	2	10		
4	AB	2	Total	C	N	O	0	0
			28	16	2	10		
4	AC	2	Total	C	N	O	0	0
			28	16	2	10		
4	AD	2	Total	C	N	O	0	0
			28	16	2	10		
4	AE	2	Total	C	N	O	0	0
			28	16	2	10		
4	AF	2	Total	C	N	O	0	0
			28	16	2	10		
4	AG	2	Total	C	N	O	0	0
			28	16	2	10		
4	AH	2	Total	C	N	O	0	0
			28	16	2	10		
4	BA	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	BB	2	Total	C	N	O	0	0
			28	16	2	10		
4	BC	2	Total	C	N	O	0	0
			28	16	2	10		
4	BD	2	Total	C	N	O	0	0
			28	16	2	10		
4	BE	2	Total	C	N	O	0	0
			28	16	2	10		
4	BF	2	Total	C	N	O	0	0
			28	16	2	10		
4	BG	2	Total	C	N	O	0	0
			28	16	2	10		
4	BH	2	Total	C	N	O	0	0
			28	16	2	10		
4	BI	2	Total	C	N	O	0	0
			28	16	2	10		
4	CA	2	Total	C	N	O	0	0
			28	16	2	10		
4	CB	2	Total	C	N	O	0	0
			28	16	2	10		
4	CC	2	Total	C	N	O	0	0
			28	16	2	10		
4	CD	2	Total	C	N	O	0	0
			28	16	2	10		
4	CE	2	Total	C	N	O	0	0
			28	16	2	10		
4	CF	2	Total	C	N	O	0	0
			28	16	2	10		
4	CG	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



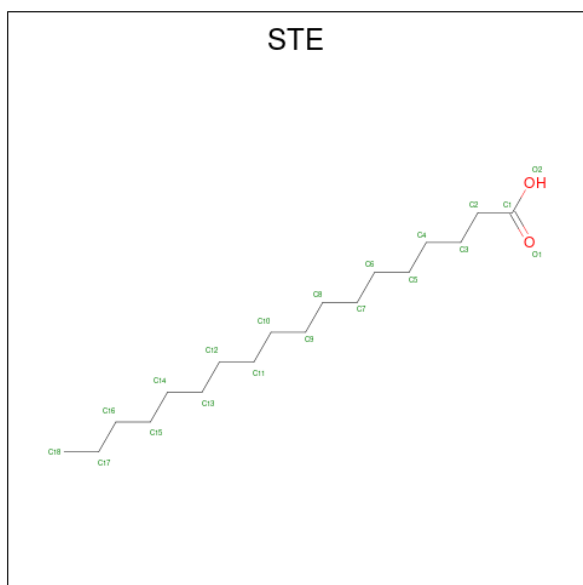
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5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

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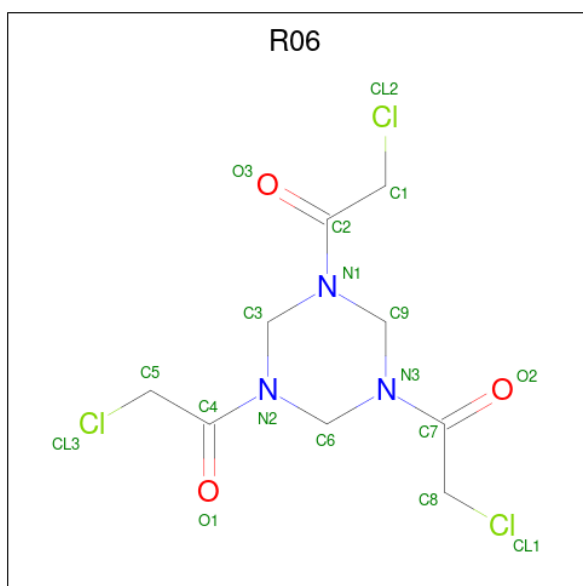
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5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

- Molecule 6 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



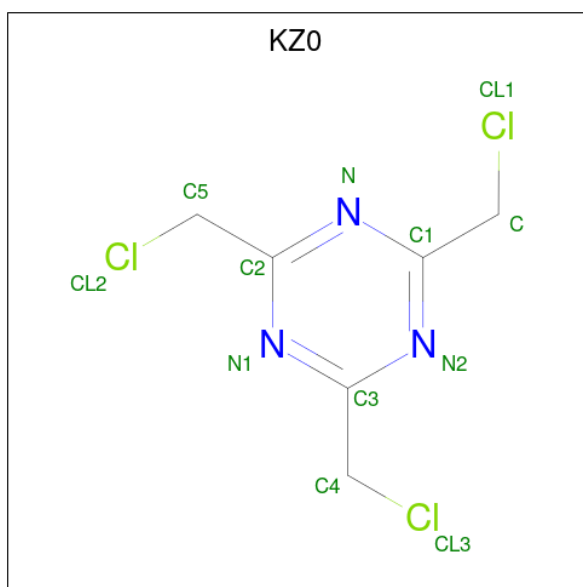
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			20	18	2	
6	B	1	Total	C	O	0
			20	18	2	
6	C	1	Total	C	O	0
			20	18	2	

- Molecule 7 is 1-[3,5-bis(2-chloranylethanoyl)-1,3,5-triazinan-1-yl]-2-chloranyl-ethanone (three-letter code: R06) (formula: $C_9H_{12}Cl_3N_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	D	1	Total	C	N	O	0
			15	9	3	3	
7	E	1	Total	C	N	O	0
			15	9	3	3	
7	F	1	Total	C	N	O	0
			15	9	3	3	

- Molecule 8 is 2,4,6-tris(chloromethyl)-1,3,5-triazine (three-letter code: KZ0) (formula: $C_6H_6Cl_3N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	G	1	Total	C	N	0
			9	6	3	
8	H	1	Total	C	N	0
			9	6	3	
8	I	1	Total	C	N	0
			9	6	3	

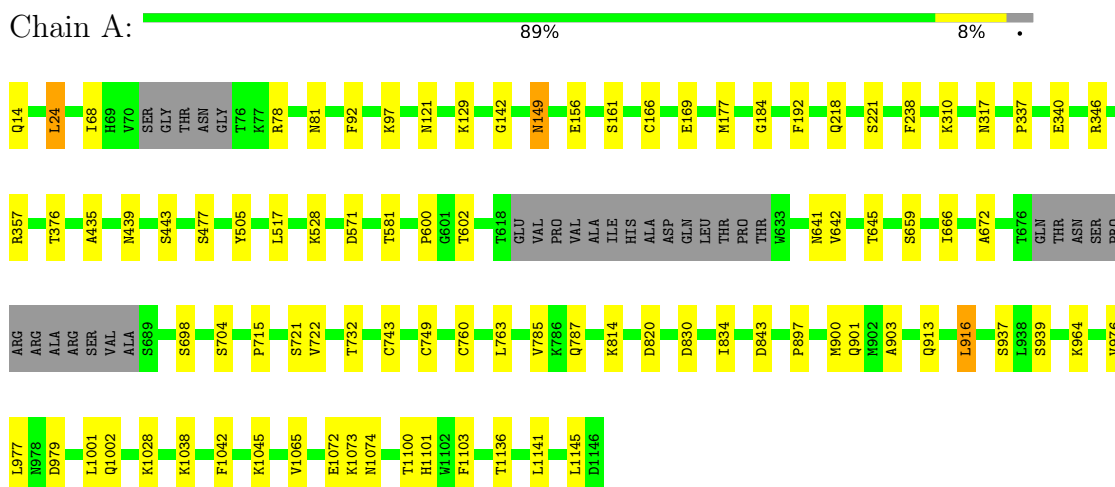
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	228	Total	O	0
			228	228	
9	B	217	Total	O	0
			217	217	
9	C	203	Total	O	0
			203	203	

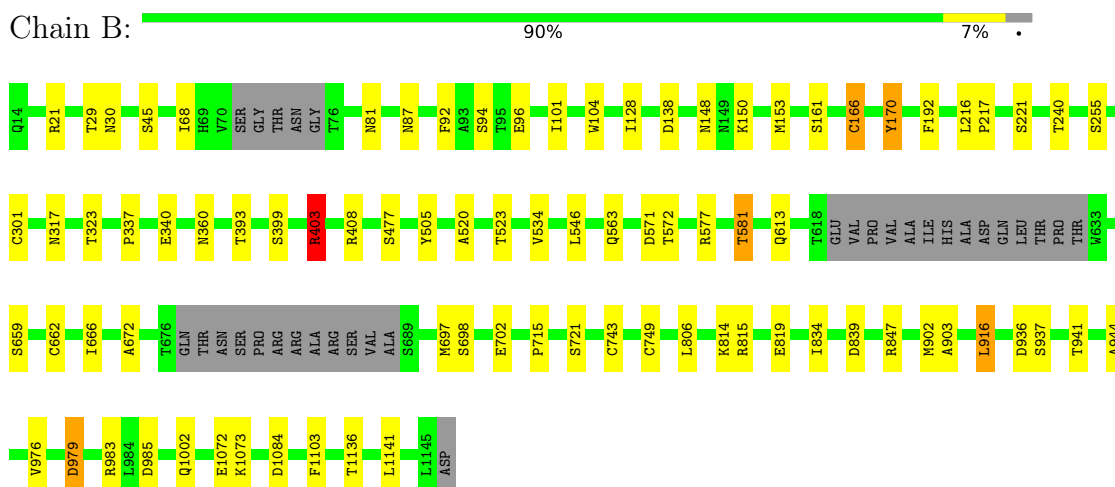
3 Residue-property plots

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. 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. 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.

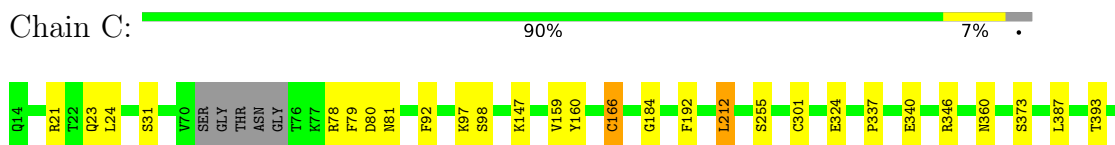
- Molecule 1: Spike glycoprotein

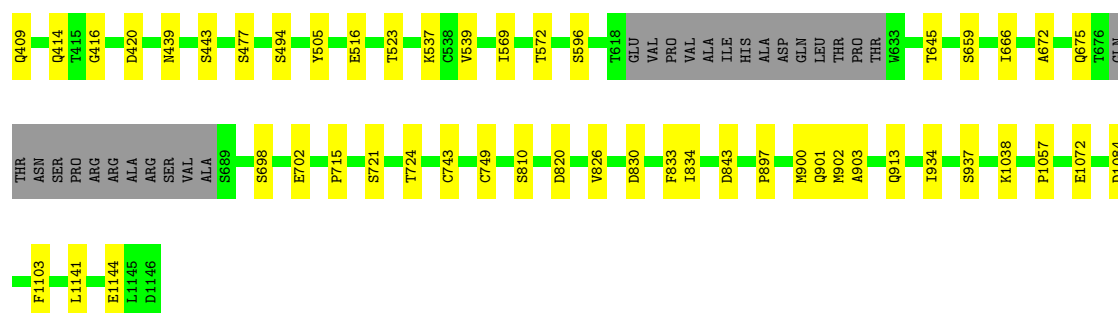


- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein





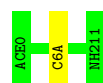
- Molecule 2: Biparatopic bicycle molecule (14mer)

Chain D: 87% 13%



- Molecule 2: Biparatopic bicycle molecule (14mer)

Chain E: 93% 7%



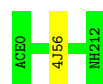
- Molecule 2: Biparatopic bicycle molecule (14mer)

Chain F: 100%

There are no outlier residues recorded for this chain.

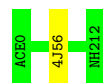
- Molecule 3: Biparatopic bicycle molecule (15mer)

Chain G: 94% 6%



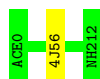
- Molecule 3: Biparatopic bicycle molecule (15mer)

Chain H: 94% 6%



- Molecule 3: Biparatopic bicycle molecule (15mer)

Chain I: 94% 6%



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

Chain AA:  100%



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

Chain AB:  100%



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

Chain AC:  100%



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

Chain AD:  50% 50%



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

Chain AE:  100%



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

Chain AF:  100%



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

Chain AG:  50% 50%



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

Chain AH:  100%



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

Chain BA:  50% 50%



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

Chain BB:  50% 50%



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

Chain BC:  100%



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

Chain BD:  100%



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

Chain BE:  50% 50%



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

Chain BF:  100%



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

Chain BG:  50% 50%



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

Chain BH:  100%



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

Chain BI:  100%



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

Chain CA:  100%



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

Chain CB:  50% 50%



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

Chain CC:  50% 50%



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

Chain CD:  100%



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

Chain CE:  100%



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

Chain CF:  100%



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

Chain CG:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117262	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	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: 0JY, R06, ACE, NH2, 4J5, STE, NAG, DAL, KZ0

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	0.31	0/8827	0.55	5/12018 (0.0%)
1	B	0.31	0/8830	0.55	4/12021 (0.0%)
1	C	0.32	0/8827	0.54	3/12018 (0.0%)
2	D	0.64	1/99 (1.0%)	0.57	0/136
2	E	0.61	0/99	0.56	0/136
2	F	0.61	0/99	0.53	0/136
3	G	0.71	0/73	0.57	0/97
3	H	0.71	0/73	0.55	0/97
3	I	0.72	0/73	0.55	0/97
All	All	0.33	1/27000 (0.0%)	0.55	12/36756 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	0	ACE	C-N	5.32	1.46	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	CYS	CA-CB-SG	9.90	131.82	114.00
1	C	166	CYS	CA-CB-SG	9.60	131.28	114.00
1	A	166	CYS	CA-CB-SG	9.06	130.31	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	916	LEU	CB-CG-CD1	-6.06	100.70	111.00
1	A	916	LEU	CB-CG-CD1	-5.75	101.22	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	403	ARG	Sidechain
1	B	96	GLU	Peptide

5.2 Too-close contacts

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	8620	0	8391	37	0
1	B	8620	0	8400	35	0
1	C	8620	0	8391	36	0
2	D	100	0	95	0	0
2	E	100	0	95	0	0
2	F	100	0	95	0	0
3	G	101	0	88	0	0
3	H	101	0	88	0	0
3	I	101	0	88	0	0
4	AA	28	0	25	0	0
4	AB	28	0	25	0	0
4	AC	28	0	25	0	0
4	AD	28	0	25	1	0
4	AE	28	0	25	0	0
4	AF	28	0	25	0	0
4	AG	28	0	25	1	0
4	AH	28	0	25	0	0
4	BA	28	0	25	0	0
4	BB	28	0	25	0	0
4	BC	28	0	25	0	0
4	BD	28	0	25	0	0
4	BE	28	0	25	1	0
4	BF	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BG	28	0	25	1	0
4	BH	28	0	25	0	0
4	BI	28	0	25	0	0
4	CA	28	0	25	0	0
4	CB	28	0	25	1	0
4	CC	28	0	25	1	0
4	CD	28	0	25	0	0
4	CE	28	0	25	0	0
4	CF	28	0	25	0	0
4	CG	28	0	25	0	0
5	A	112	0	104	0	0
5	B	98	0	91	1	0
5	C	140	0	130	0	0
6	A	20	0	35	0	0
6	B	20	0	35	1	0
6	C	20	0	35	0	0
7	D	15	0	0	0	0
7	E	15	0	0	0	0
7	F	15	0	0	0	0
8	G	9	0	0	0	0
8	H	9	0	0	0	0
8	I	9	0	0	0	0
9	A	228	0	0	3	0
9	B	217	0	0	1	0
9	C	203	0	0	1	0
All	All	28265	0	26761	104	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 2.

The worst 5 of 104 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:B:902:MET:HG3	1:B:916:LEU:HD11	1.78	0.65
1:B:148:ASN:HD21	5:B:1402:NAG:H82	1.66	0.60
1:B:403:ARG:NH1	1:C:373:SER:OG	2.35	0.60
1:A:149:ASN:N	1:A:149:ASN:OD1	2.35	0.59
1:B:337:PRO:HB2	1:B:340:GLU:HB2	1.84	0.59

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	1095/1133 (97%)	1059 (97%)	36 (3%)	0	100	100
1	B	1095/1133 (97%)	1062 (97%)	33 (3%)	0	100	100
1	C	1095/1133 (97%)	1056 (96%)	39 (4%)	0	100	100
2	D	13/15 (87%)	12 (92%)	0	1 (8%)	1	0
2	E	13/15 (87%)	13 (100%)	0	0	100	100
2	F	13/15 (87%)	13 (100%)	0	0	100	100
3	G	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
3	H	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
3	I	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
All	All	3357/3492 (96%)	3245 (97%)	111 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	0(A)	CYS

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	963/987 (98%)	934 (97%)	29 (3%)	36	19
1	B	963/987 (98%)	933 (97%)	30 (3%)	35	18
1	C	963/987 (98%)	941 (98%)	22 (2%)	45	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	11/11 (100%)	11 (100%)	0	100	100
2	E	11/11 (100%)	10 (91%)	1 (9%)	7	1
2	F	11/11 (100%)	11 (100%)	0	100	100
3	G	8/8 (100%)	8 (100%)	0	100	100
3	H	8/8 (100%)	8 (100%)	0	100	100
3	I	8/8 (100%)	8 (100%)	0	100	100
All	All	2946/3018 (98%)	2864 (97%)	82 (3%)	40	22

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1084	ASP
1	C	675	GLN
1	C	98	SER
1	C	477	SER
1	C	820	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	4J5	H	6	3	8,9,10	2.16	2 (25%)	4,10,12	0.35	0
3	DAL	G	7	3	3,4,5	0.95	0	2,4,6	0.72	0
3	DAL	H	7	3	3,4,5	0.97	0	2,4,6	0.75	0
3	4J5	G	6	3	8,9,10	2.30	2 (25%)	4,10,12	0.44	0
3	4J5	I	6	3	8,9,10	2.15	2 (25%)	4,10,12	0.34	0
3	DAL	I	7	3	3,4,5	0.97	0	2,4,6	0.71	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
3	4J5	H	6	3	-	0/7/8/10	-
3	DAL	G	7	3	-	0/0/2/4	-
3	DAL	H	7	3	-	0/0/2/4	-
3	4J5	G	6	3	-	2/7/8/10	-
3	4J5	I	6	3	-	0/7/8/10	-
3	DAL	I	7	3	-	0/0/2/4	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	6	4J5	CE-ND	4.41	1.42	1.33
3	H	6	4J5	CE-ND	4.40	1.42	1.33
3	I	6	4J5	CE-ND	4.39	1.42	1.33
3	G	6	4J5	CE-NH2	3.80	1.47	1.32
3	I	6	4J5	CE-NH1	3.06	1.47	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	6	4J5	C-CA-CB-CG
3	G	6	4J5	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

48 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	$\# Z > 2$
4	NAG	AA	1	1,4	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	AA	2	4	14,14,15	0.30	0	17,19,21	0.48	0
4	NAG	AB	1	1,4	14,14,15	0.26	0	17,19,21	0.51	0
4	NAG	AB	2	4	14,14,15	0.33	0	17,19,21	0.45	0
4	NAG	AC	1	1,4	14,14,15	0.28	0	17,19,21	0.56	0
4	NAG	AC	2	4	14,14,15	0.31	0	17,19,21	0.46	0
4	NAG	AD	1	1,4	14,14,15	0.30	0	17,19,21	0.58	0
4	NAG	AD	2	4	14,14,15	0.33	0	17,19,21	0.44	0
4	NAG	AE	1	4	14,14,15	0.17	0	17,19,21	0.47	0
4	NAG	AE	2	4	14,14,15	0.32	0	17,19,21	0.50	0
4	NAG	AF	1	1,4	14,14,15	0.31	0	17,19,21	0.56	0
4	NAG	AF	2	4	14,14,15	0.30	0	17,19,21	0.48	0
4	NAG	AG	1	1,4	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	AG	2	4	14,14,15	0.31	0	17,19,21	0.43	0
4	NAG	AH	1	1,4	14,14,15	0.22	0	17,19,21	0.49	0
4	NAG	AH	2	4	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	BA	1	1,4	14,14,15	0.22	0	17,19,21	0.51	0
4	NAG	BA	2	4	14,14,15	0.32	0	17,19,21	0.58	1 (5%)
4	NAG	BB	1	4	14,14,15	0.76	1 (7%)	17,19,21	1.18	3 (17%)
4	NAG	BB	2	4	14,14,15	0.43	0	17,19,21	0.41	0
4	NAG	BC	1	1,4	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	BC	2	4	14,14,15	0.31	0	17,19,21	0.48	0
4	NAG	BD	1	1,4	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	BD	2	4	14,14,15	0.37	0	17,19,21	0.47	0
4	NAG	BE	1	1,4	14,14,15	0.27	0	17,19,21	0.60	1 (5%)
4	NAG	BE	2	4	14,14,15	0.32	0	17,19,21	0.45	0
4	NAG	BF	1	1,4	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	BF	2	4	14,14,15	0.33	0	17,19,21	0.55	0
4	NAG	BG	1	1,4	14,14,15	0.29	0	17,19,21	0.52	0
4	NAG	BG	2	4	14,14,15	0.34	0	17,19,21	0.42	0
4	NAG	BH	1	1,4	14,14,15	0.31	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	BH	2	4	14,14,15	0.31	0	17,19,21	0.46	0
4	NAG	BI	1	1,4	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	BI	2	4	14,14,15	0.29	0	17,19,21	0.48	0
4	NAG	CA	1	1,4	14,14,15	0.21	0	17,19,21	0.49	0
4	NAG	CA	2	4	14,14,15	0.30	0	17,19,21	0.56	0
4	NAG	CB	1	1,4	14,14,15	0.30	0	17,19,21	0.60	0
4	NAG	CB	2	4	14,14,15	0.34	0	17,19,21	0.44	0
4	NAG	CC	1	1,4	14,14,15	0.28	0	17,19,21	0.53	0
4	NAG	CC	2	4	14,14,15	0.33	0	17,19,21	0.44	0
4	NAG	CD	1	1,4	14,14,15	0.30	0	17,19,21	0.56	0
4	NAG	CD	2	4	14,14,15	0.30	0	17,19,21	0.47	0
4	NAG	CE	1	1,4	14,14,15	0.30	0	17,19,21	0.58	0
4	NAG	CE	2	4	14,14,15	0.30	0	17,19,21	0.47	0
4	NAG	CF	1	1,4	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	CF	2	4	14,14,15	0.33	0	17,19,21	0.45	0
4	NAG	CG	1	1,4	14,14,15	0.29	0	17,19,21	0.51	0
4	NAG	CG	2	4	14,14,15	0.29	0	17,19,21	0.48	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
4	NAG	AA	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	AA	2	4	-	0/6/23/26	0/1/1/1
4	NAG	AB	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	AB	2	4	-	0/6/23/26	0/1/1/1
4	NAG	AC	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	AC	2	4	-	2/6/23/26	0/1/1/1
4	NAG	AD	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	AD	2	4	-	0/6/23/26	0/1/1/1
4	NAG	AE	1	4	-	2/6/23/26	0/1/1/1
4	NAG	AE	2	4	-	2/6/23/26	0/1/1/1
4	NAG	AF	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	AF	2	4	-	0/6/23/26	0/1/1/1
4	NAG	AG	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	AG	2	4	-	2/6/23/26	0/1/1/1
4	NAG	AH	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	AH	2	4	-	0/6/23/26	0/1/1/1
4	NAG	BA	1	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	BA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	BB	1	4	-	2/6/23/26	0/1/1/1
4	NAG	BB	2	4	-	2/6/23/26	0/1/1/1
4	NAG	BC	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	BC	2	4	-	1/6/23/26	0/1/1/1
4	NAG	BD	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	BD	2	4	-	0/6/23/26	0/1/1/1
4	NAG	BE	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	BE	2	4	-	0/6/23/26	0/1/1/1
4	NAG	BF	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	BF	2	4	-	0/6/23/26	0/1/1/1
4	NAG	BG	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	BG	2	4	-	0/6/23/26	0/1/1/1
4	NAG	BH	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	BH	2	4	-	2/6/23/26	0/1/1/1
4	NAG	BI	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	BI	2	4	-	0/6/23/26	0/1/1/1
4	NAG	CA	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	CA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	CB	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	CB	2	4	-	0/6/23/26	0/1/1/1
4	NAG	CC	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	CC	2	4	-	0/6/23/26	0/1/1/1
4	NAG	CD	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	CD	2	4	-	0/6/23/26	0/1/1/1
4	NAG	CE	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	CE	2	4	-	2/6/23/26	0/1/1/1
4	NAG	CF	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	CF	2	4	-	0/6/23/26	0/1/1/1
4	NAG	CG	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	CG	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BB	1	NAG	C1-C2	2.47	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BB	1	NAG	O4-C4-C5	2.50	115.50	109.30
4	BB	1	NAG	C3-C4-C5	-2.32	106.09	110.24
4	BB	1	NAG	C1-O5-C5	2.05	114.97	112.19
4	BA	2	NAG	C1-O5-C5	2.01	114.91	112.19
4	BE	1	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

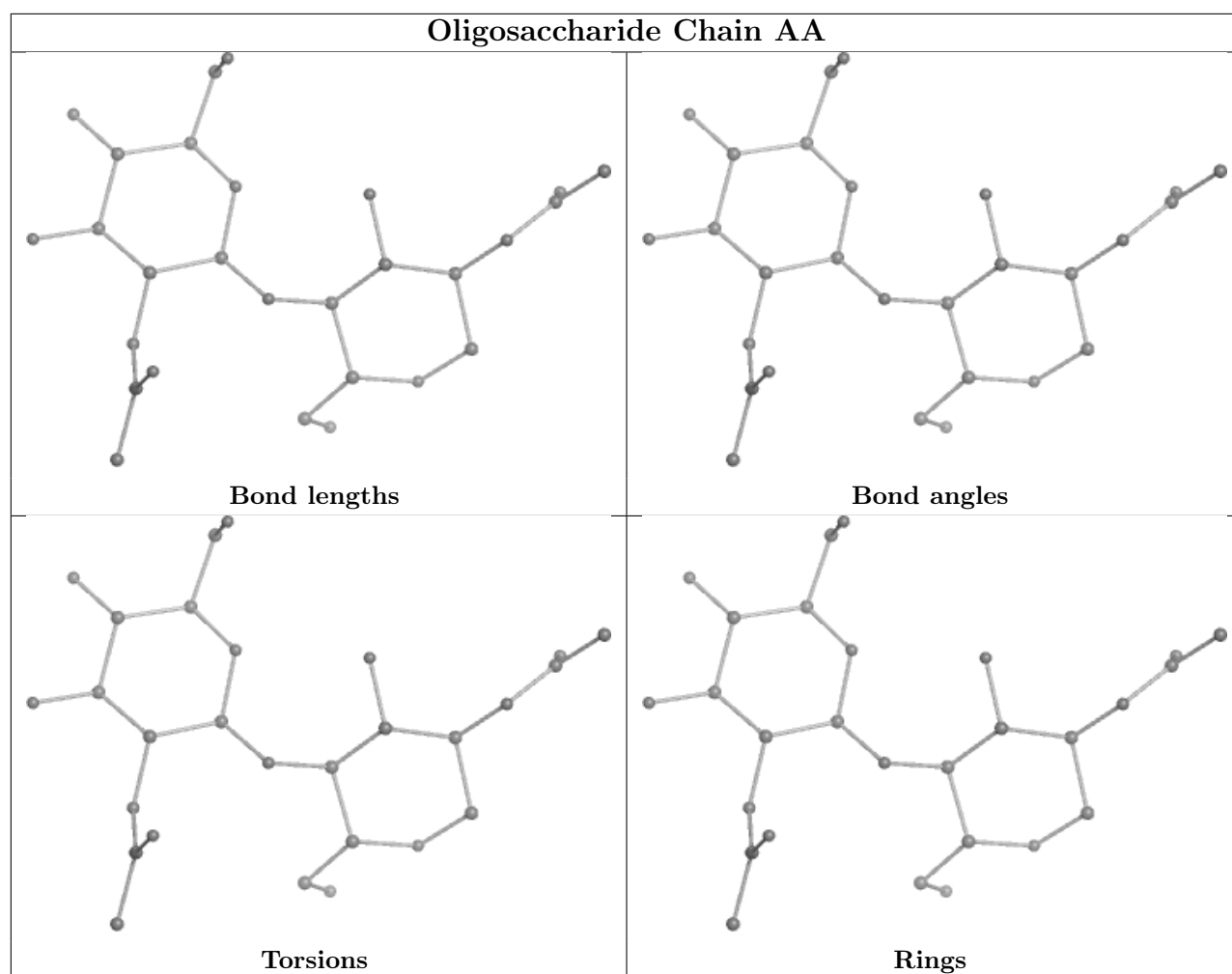
Mol	Chain	Res	Type	Atoms
4	AE	1	NAG	O5-C5-C6-O6
4	BB	2	NAG	O5-C5-C6-O6
4	AE	2	NAG	O5-C5-C6-O6
4	BI	1	NAG	O5-C5-C6-O6
4	CG	1	NAG	O5-C5-C6-O6

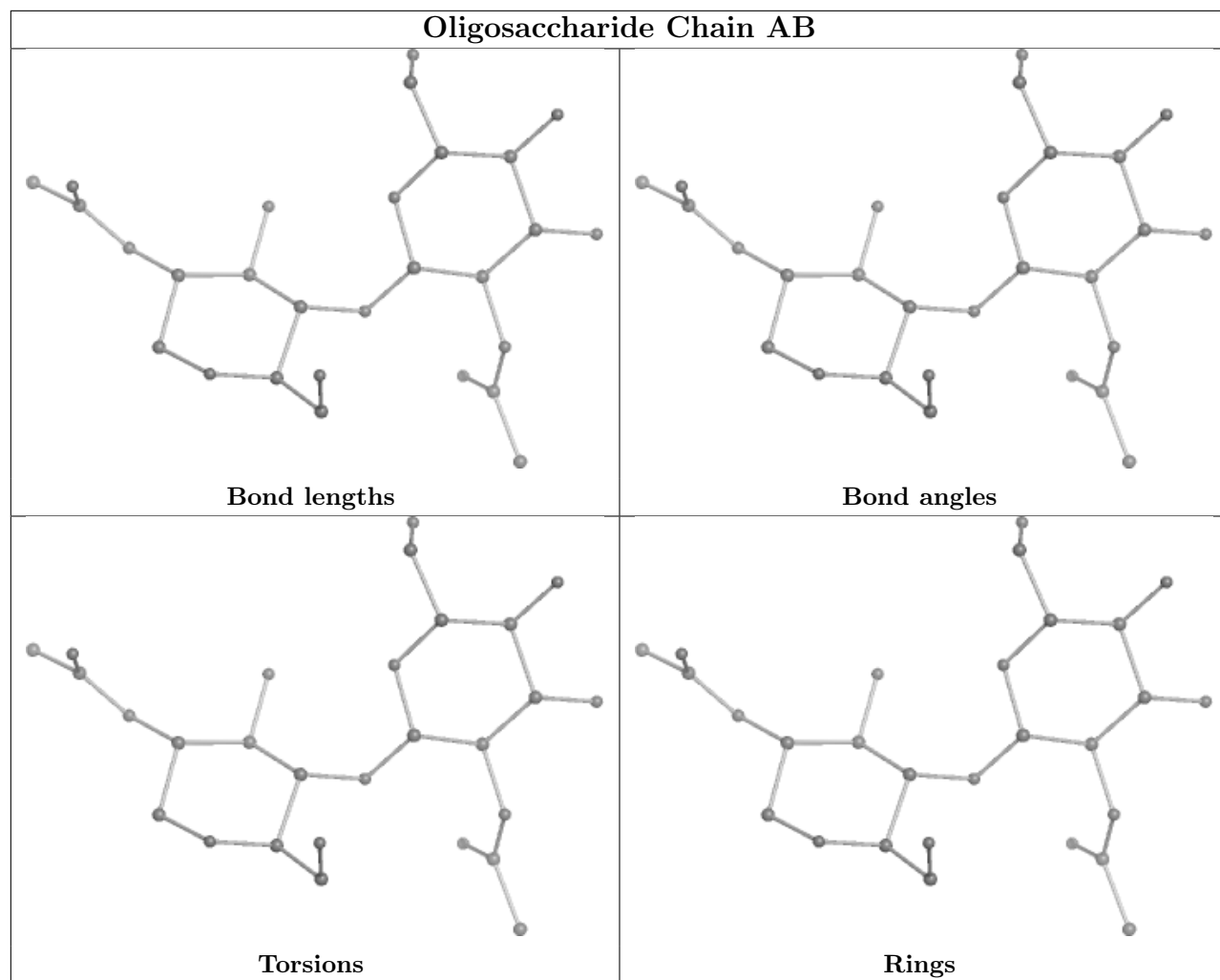
There are no ring outliers.

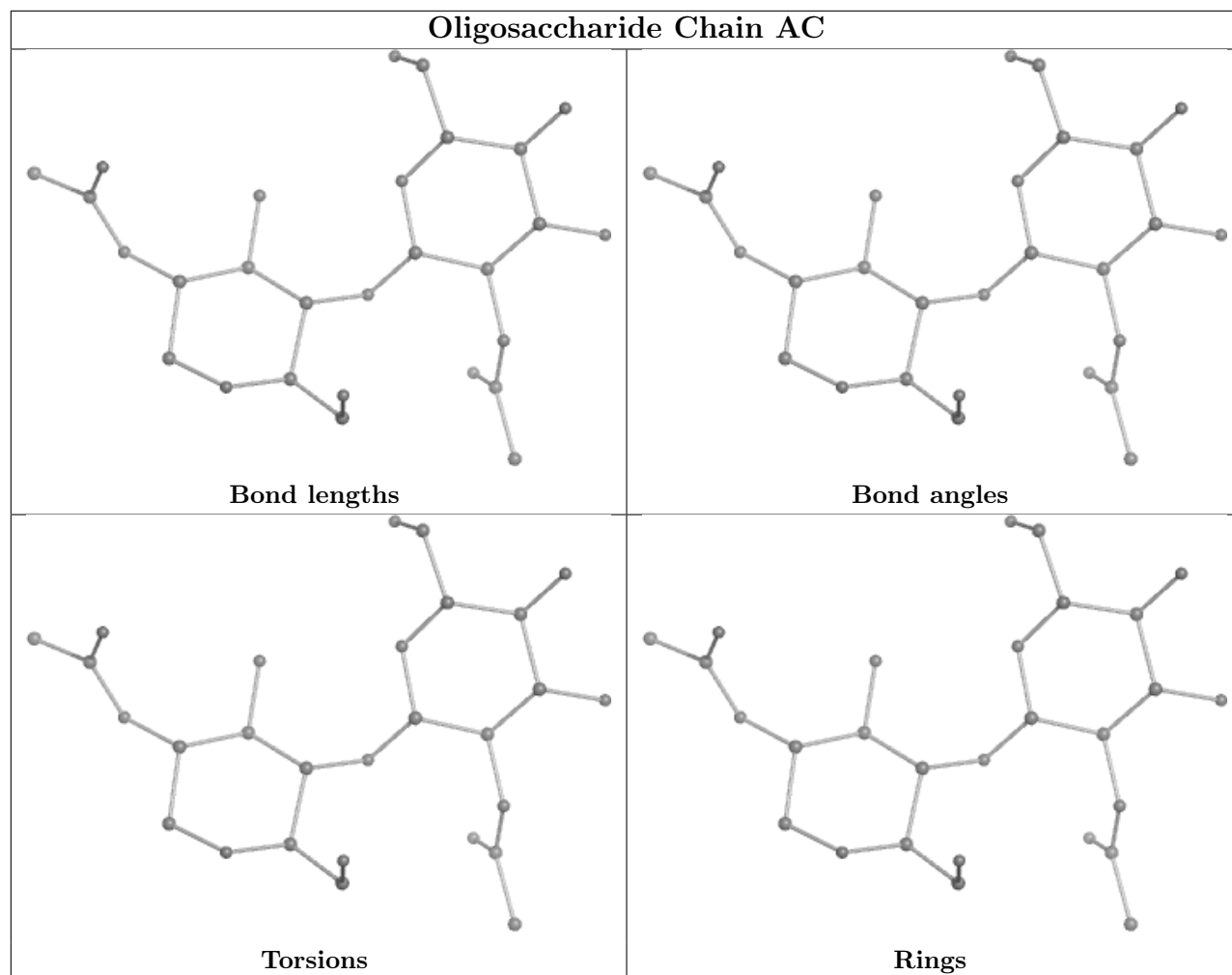
6 monomers are involved in 6 short contacts:

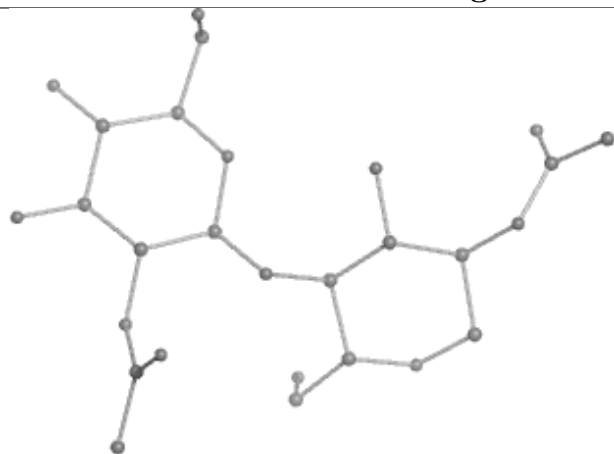
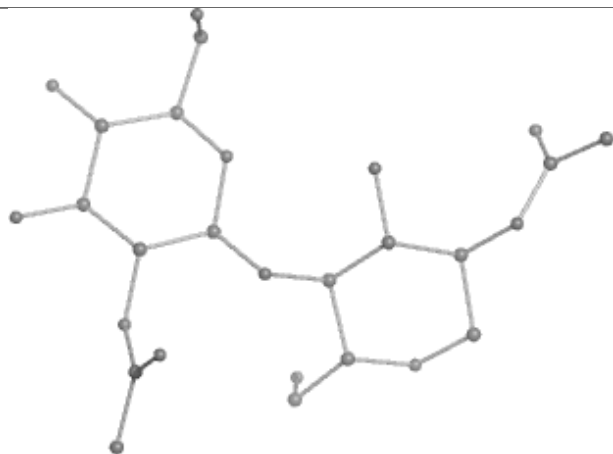
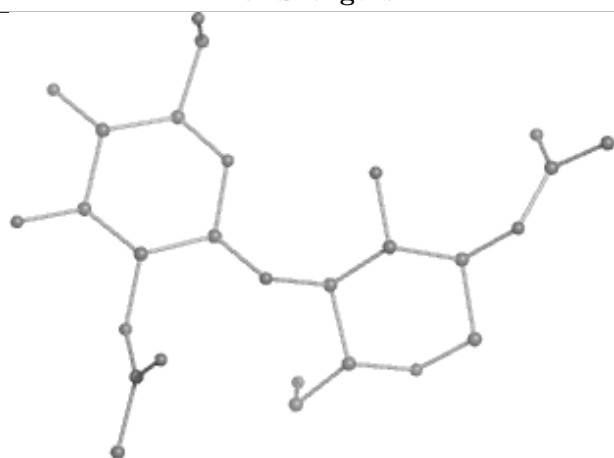
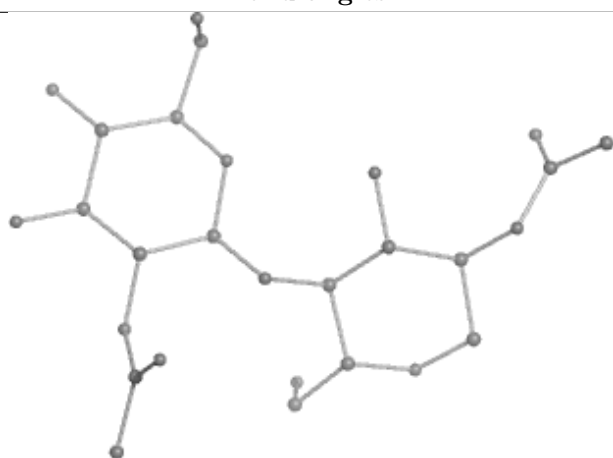
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CC	1	NAG	1	0
4	AD	1	NAG	1	0
4	AG	1	NAG	1	0
4	BG	1	NAG	1	0
4	CB	1	NAG	1	0
4	BE	1	NAG	1	0

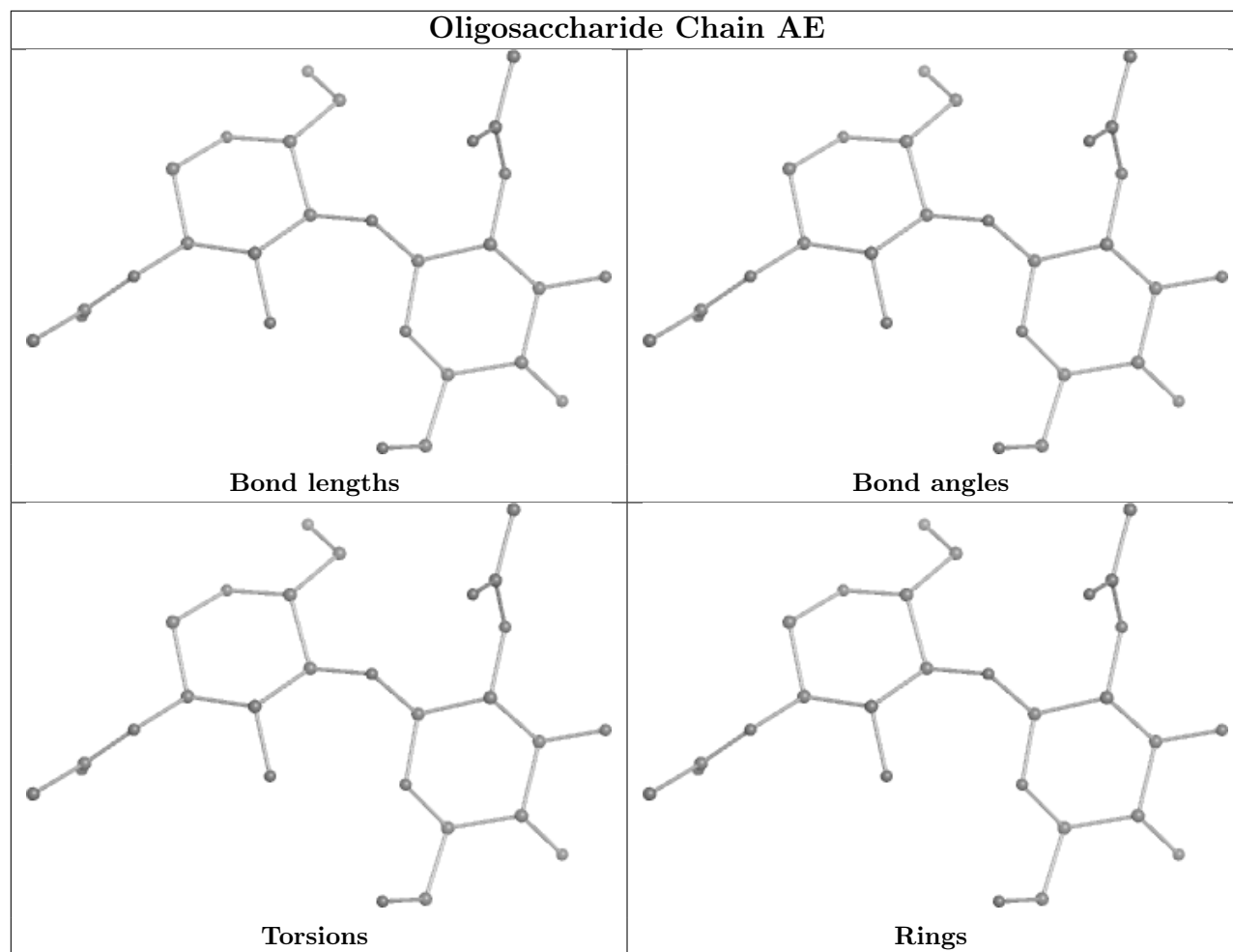
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

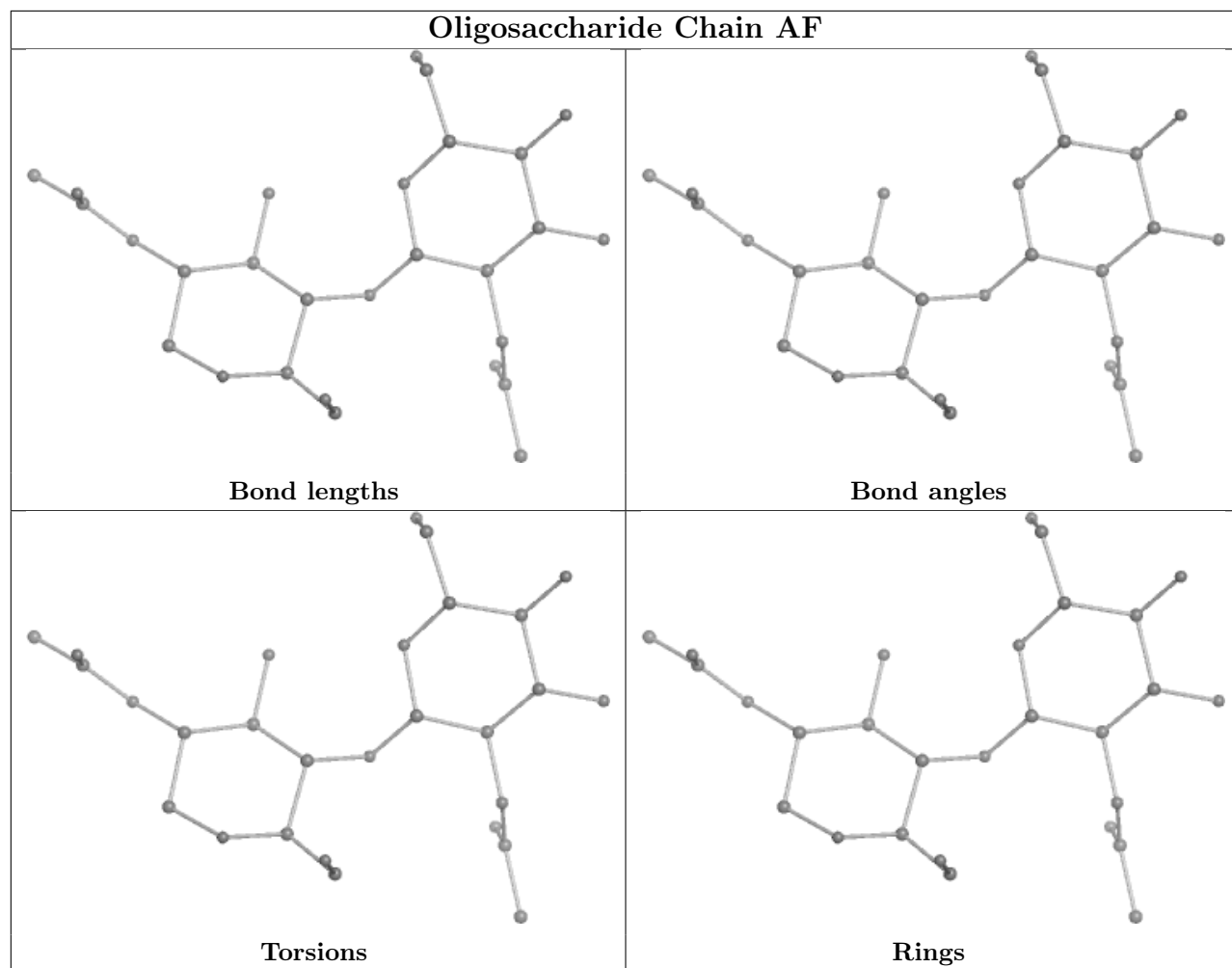




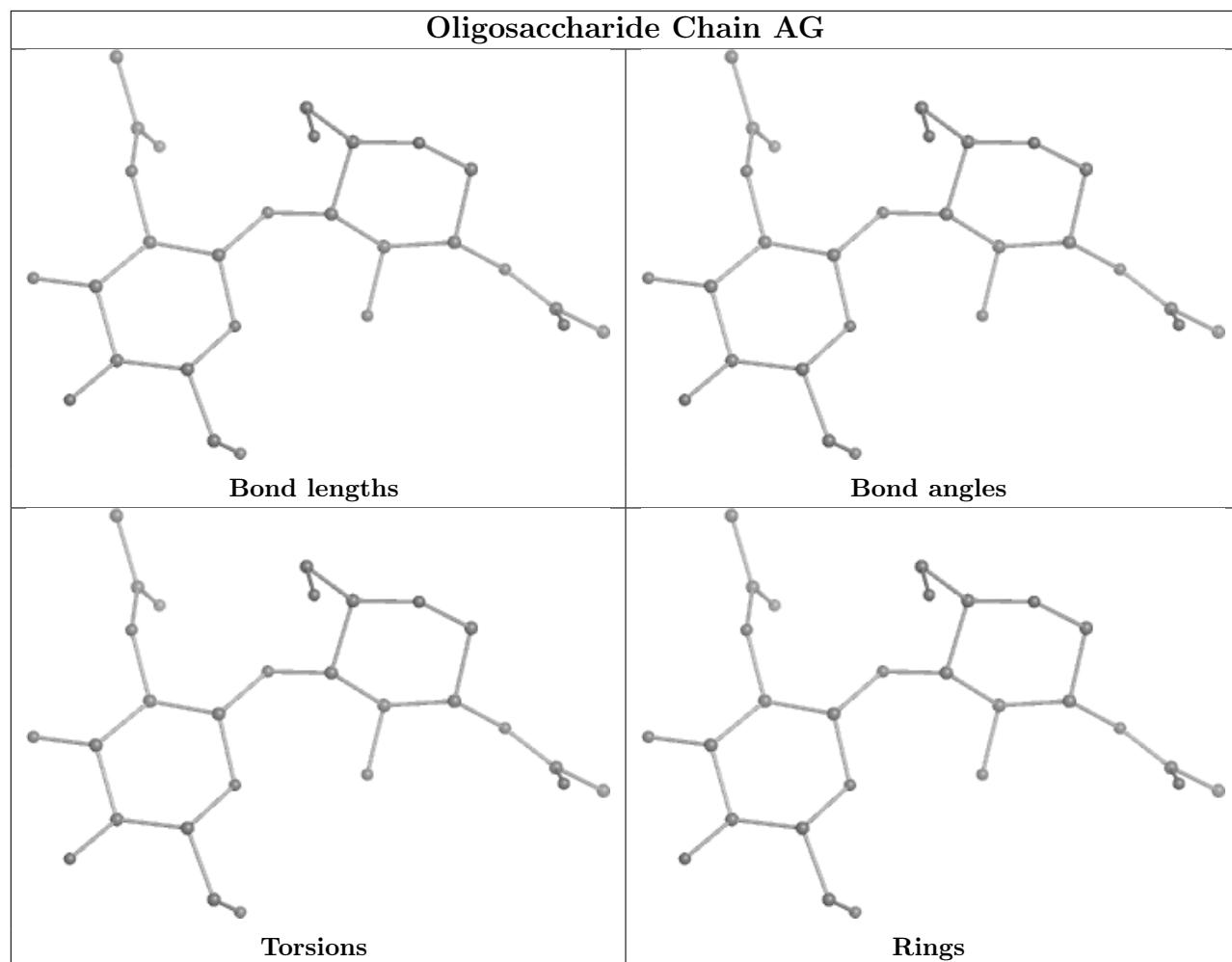


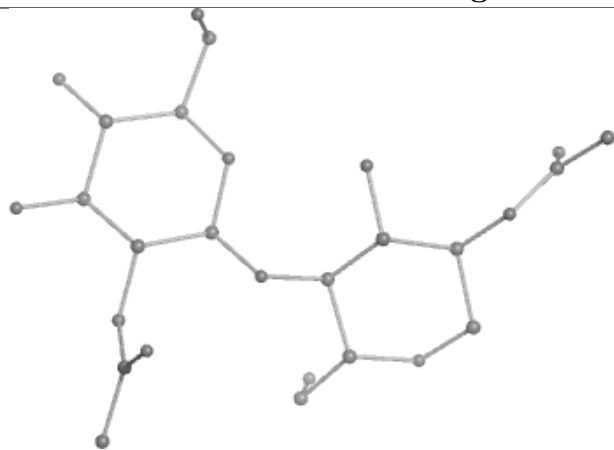
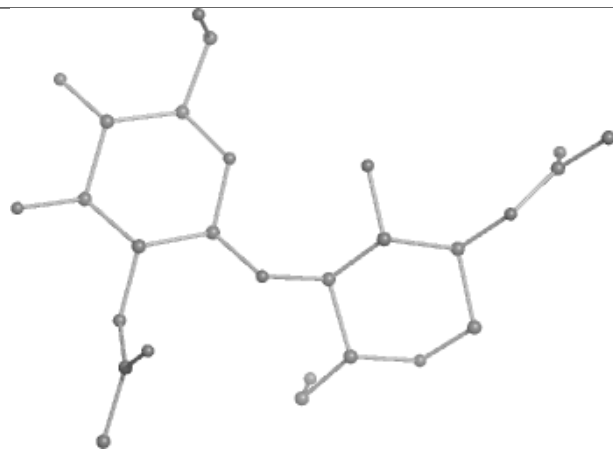
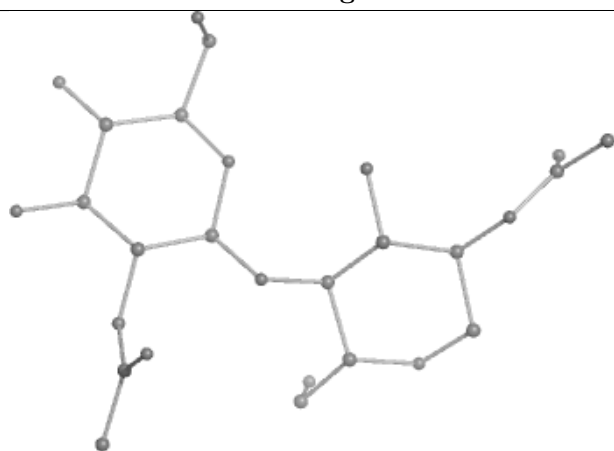
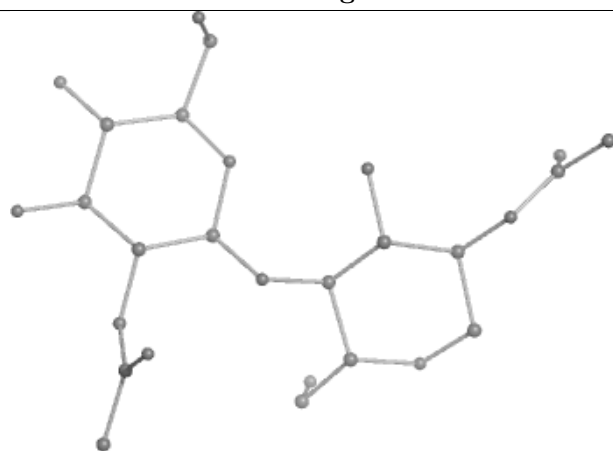
Oligosaccharide Chain AD**Bond lengths****Bond angles****Torsions****Rings**



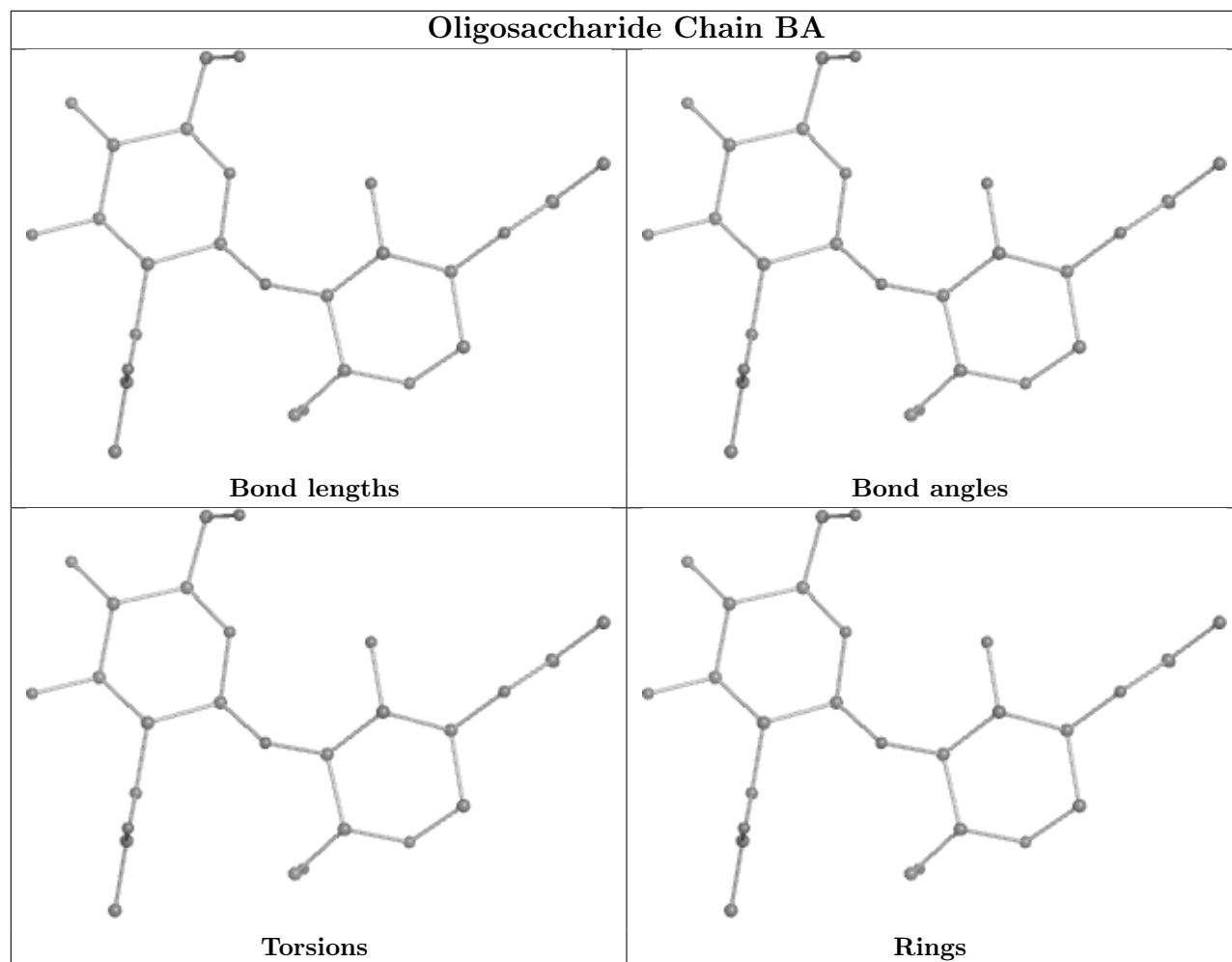


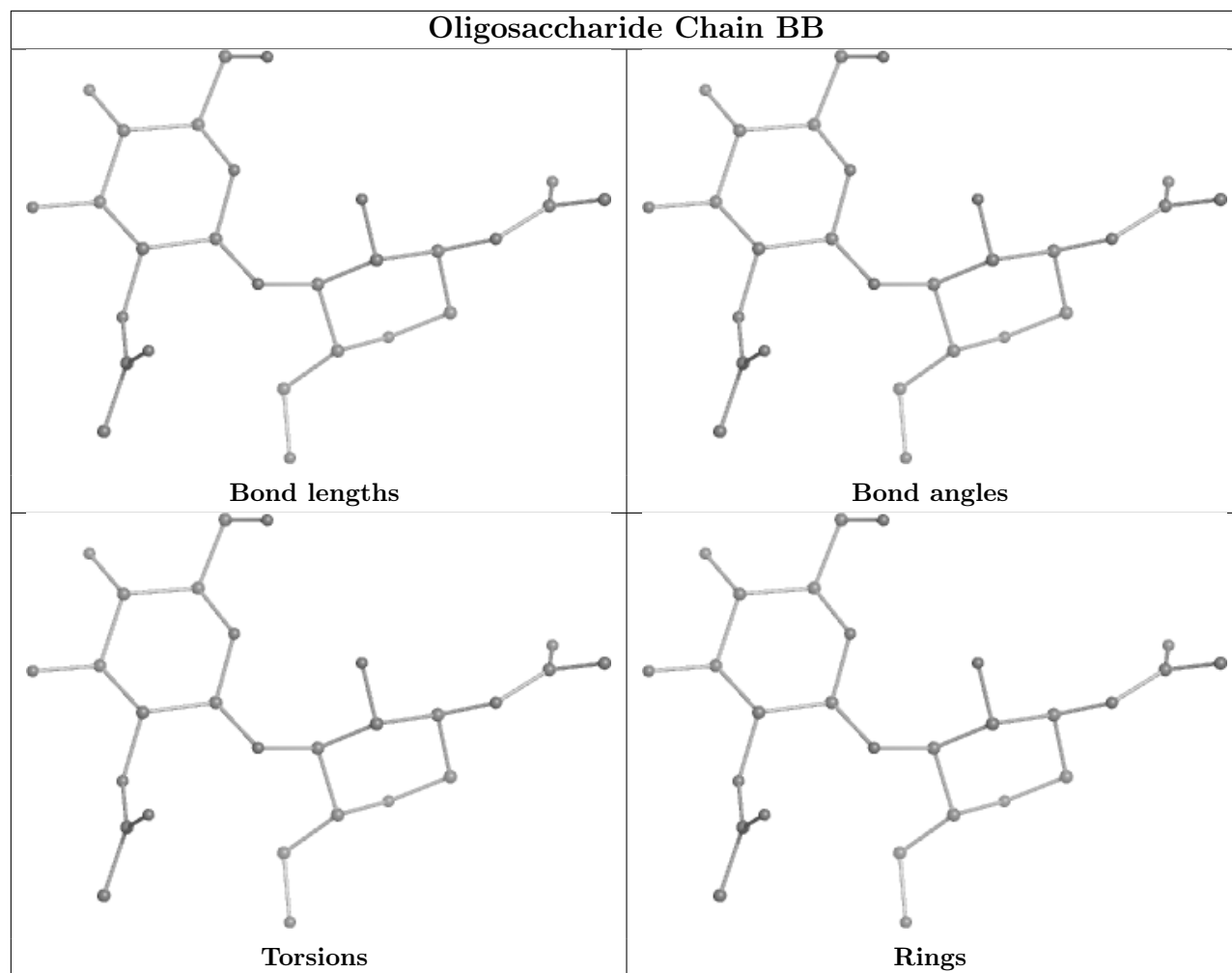
Oligosaccharide Chain AG



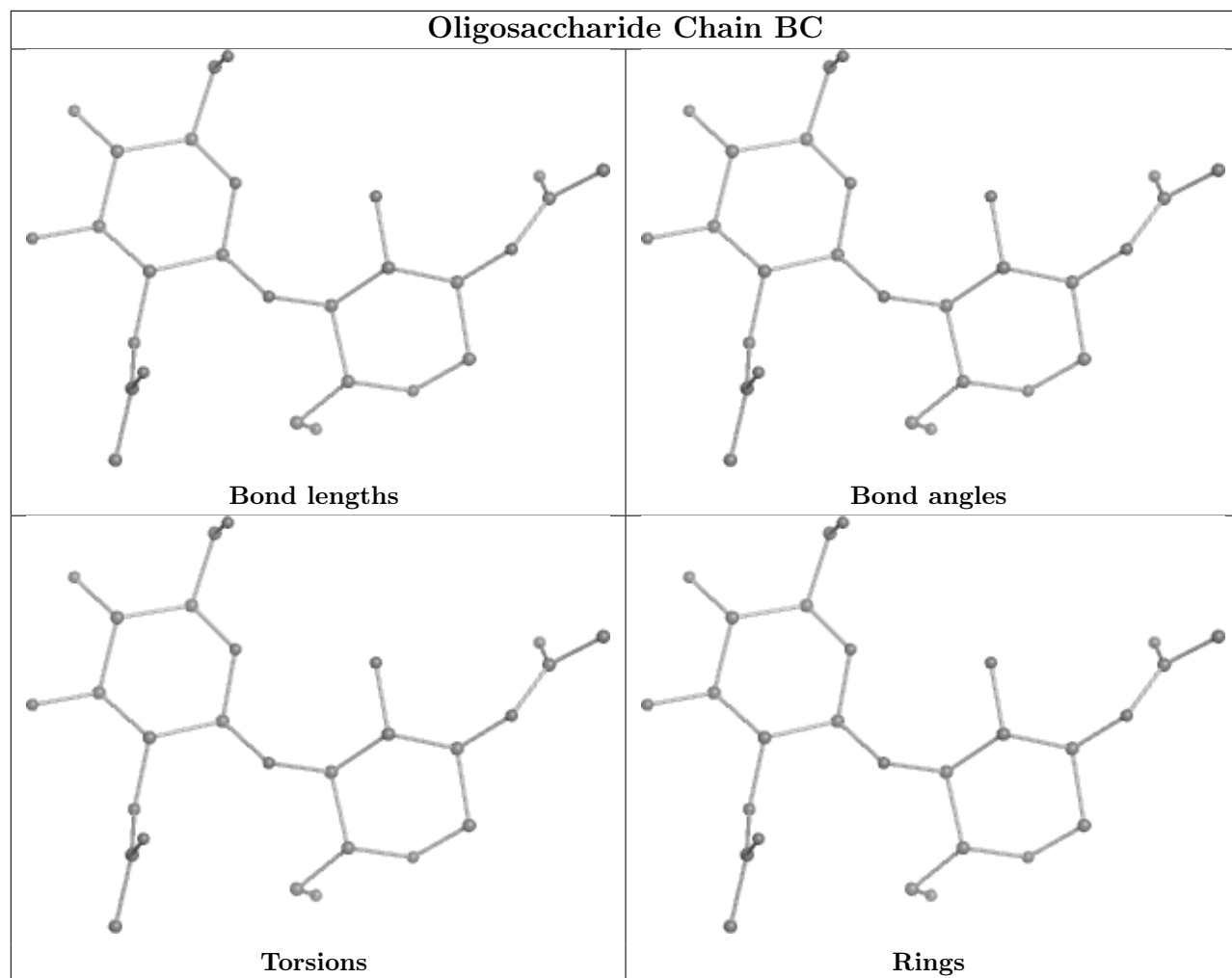
Oligosaccharide Chain AH**Bond lengths****Bond angles****Torsions****Rings**

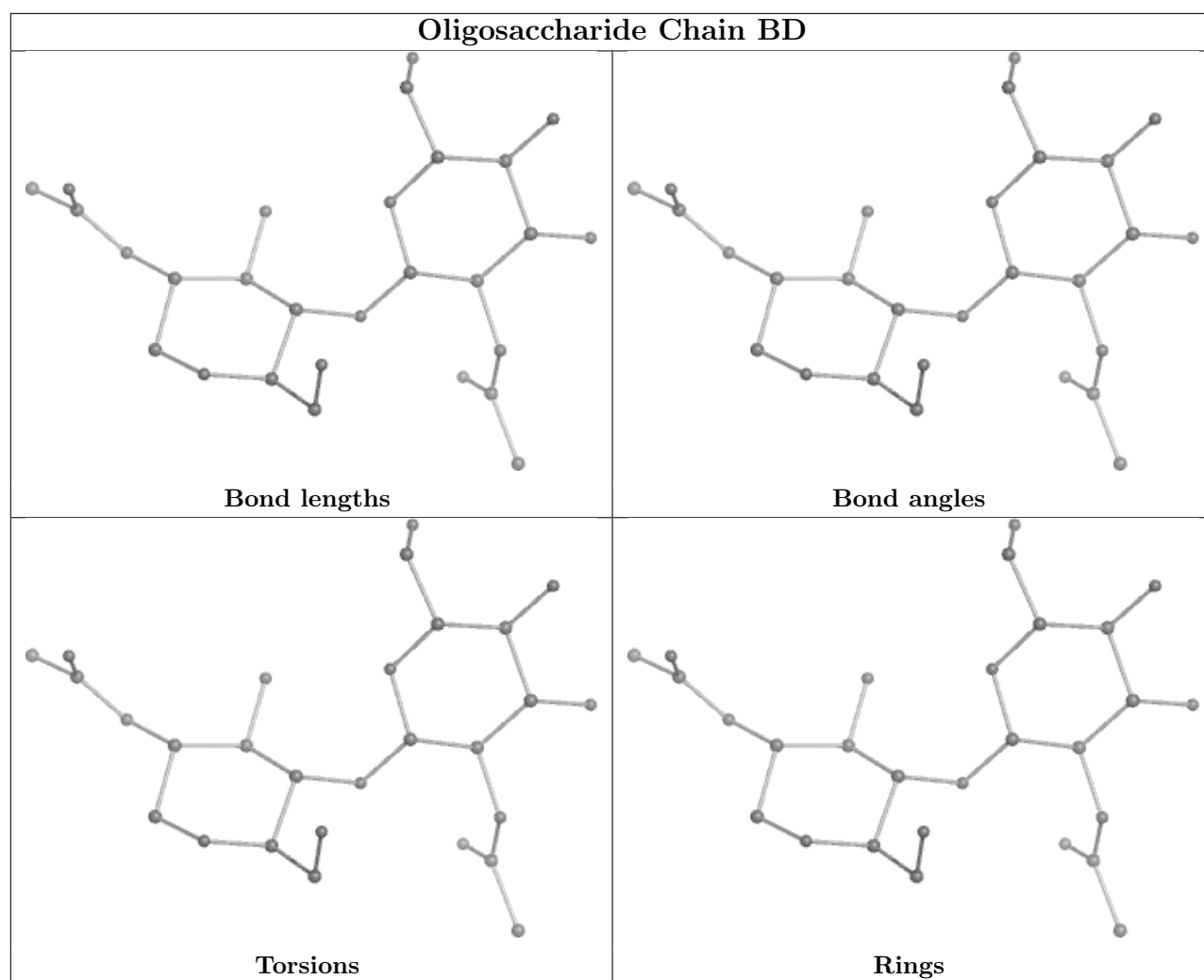
Oligosaccharide Chain BA

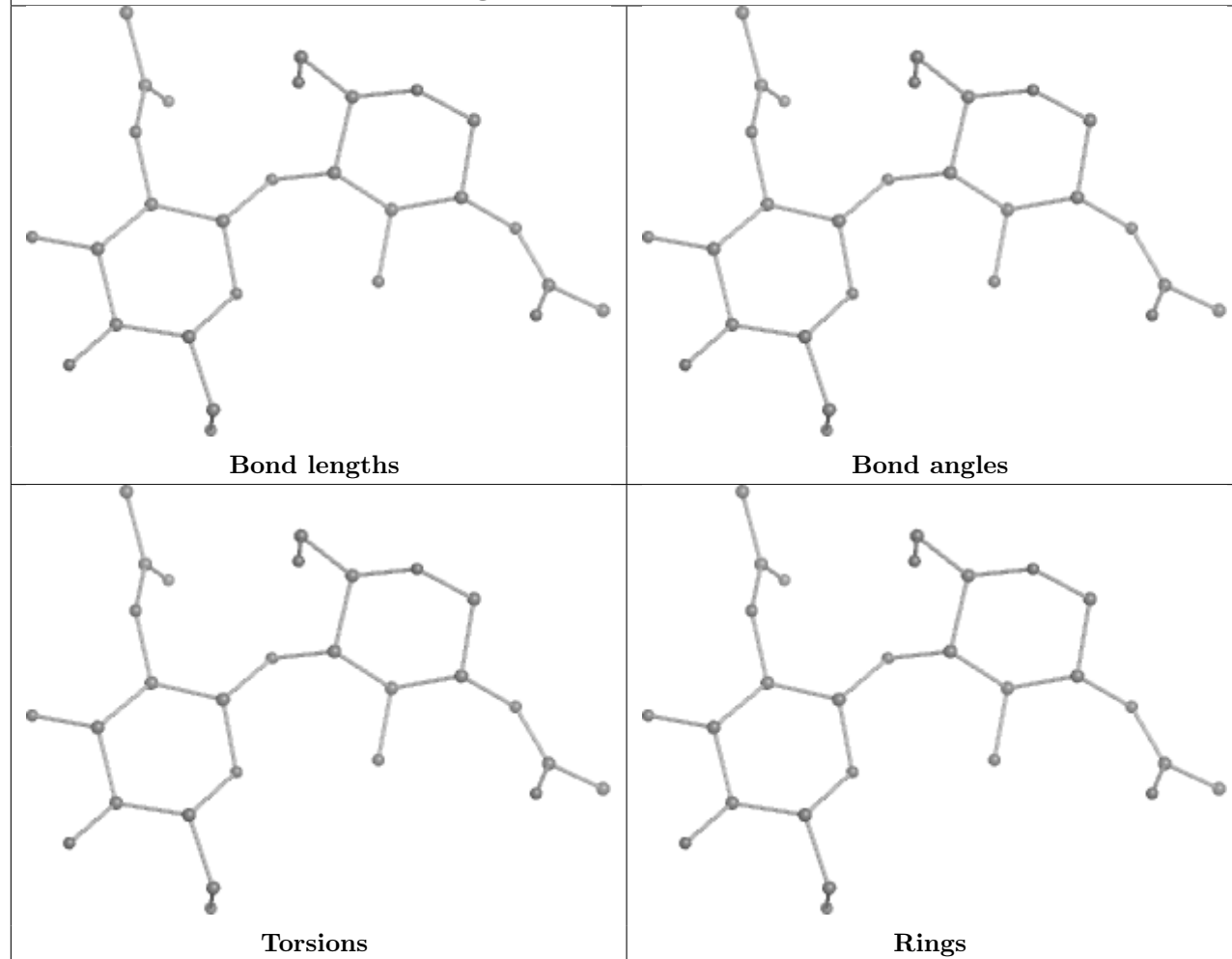


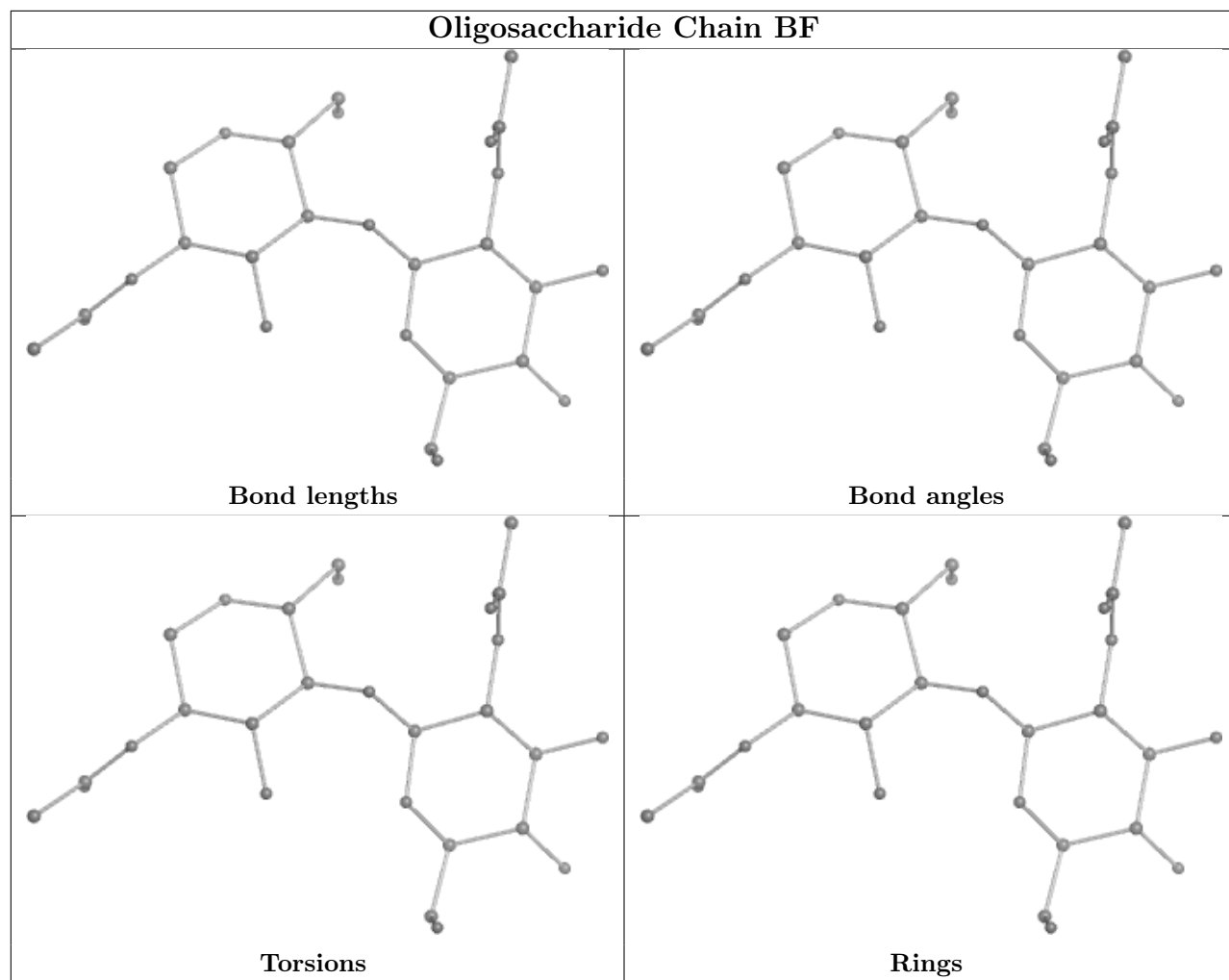


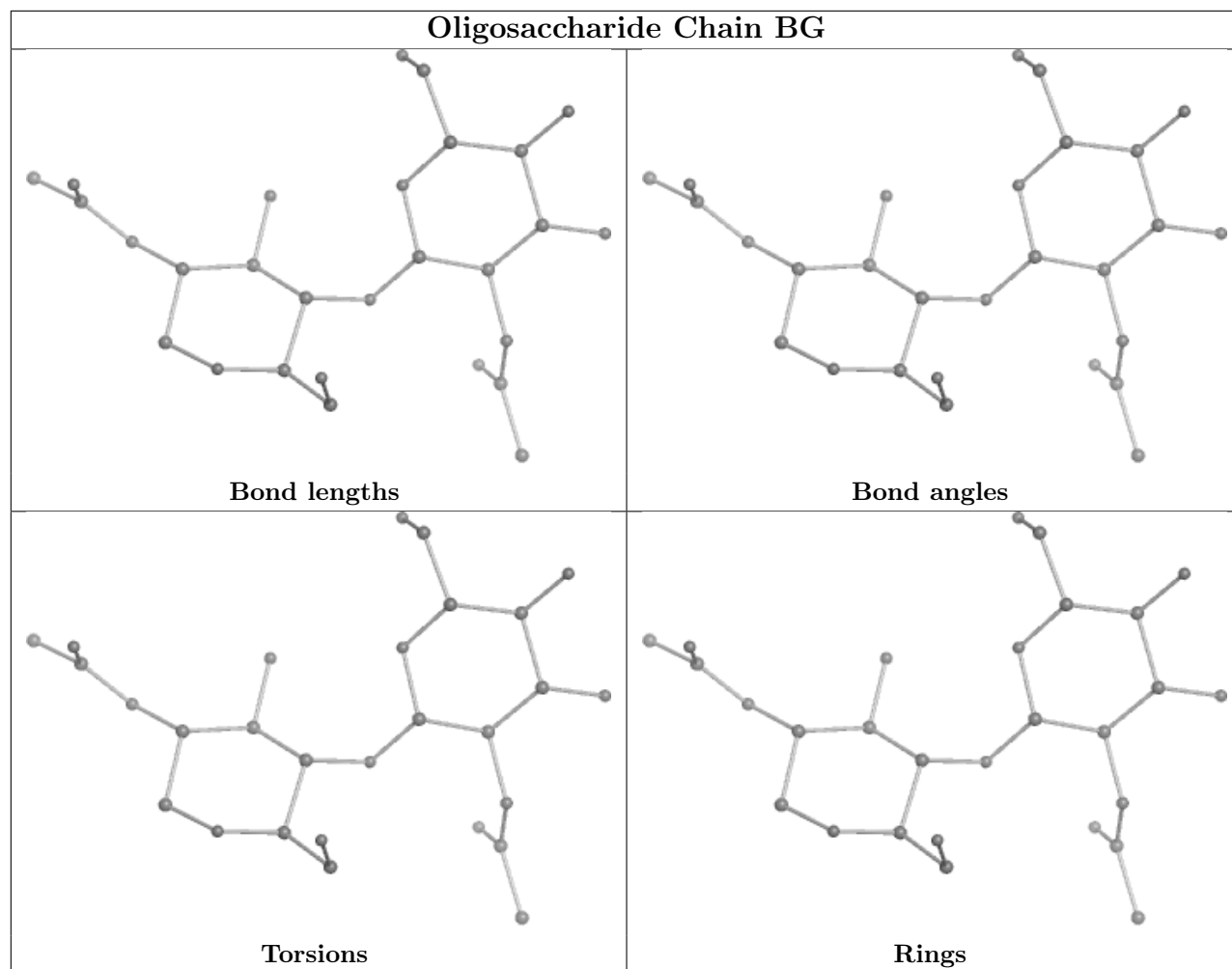
Oligosaccharide Chain BC

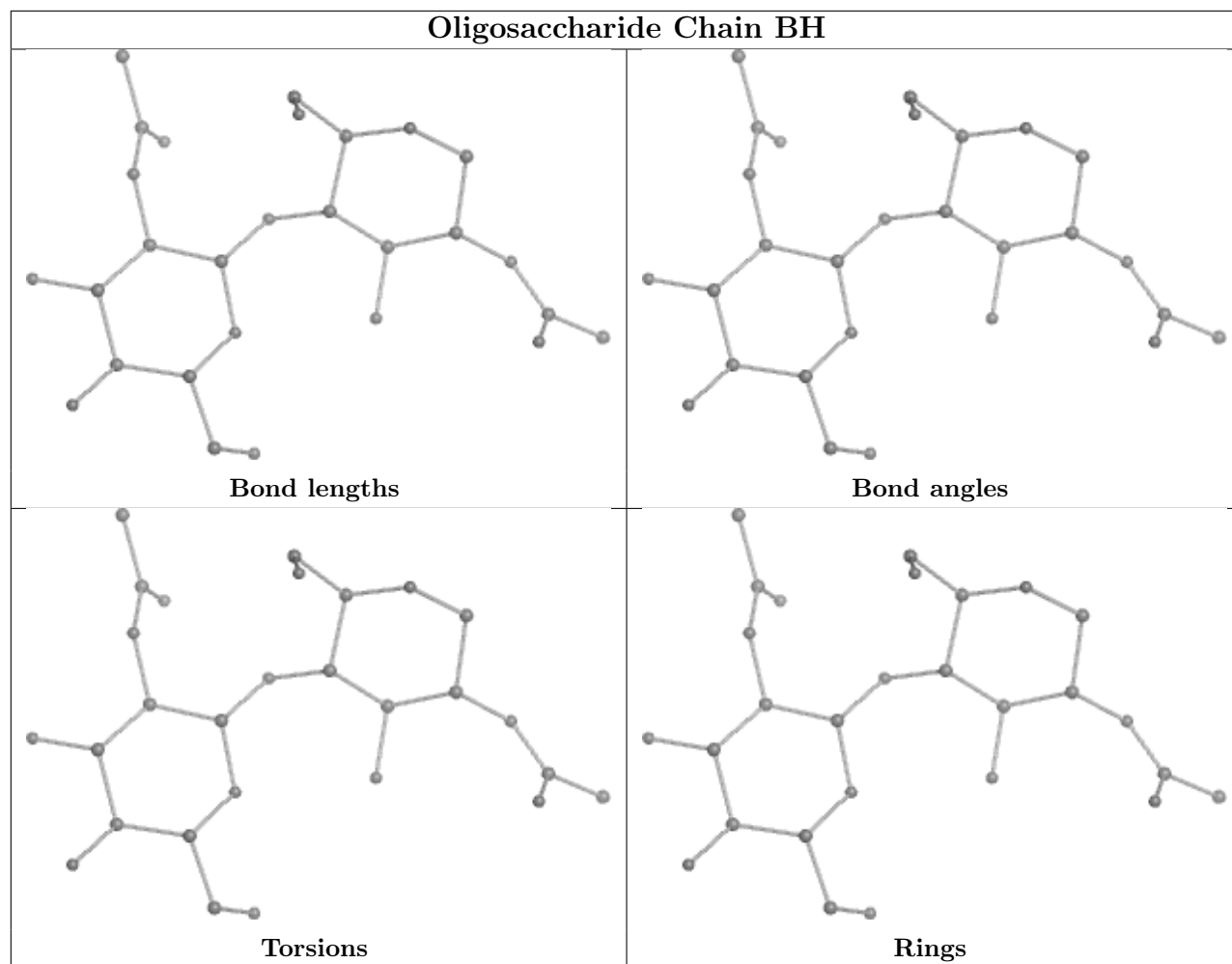


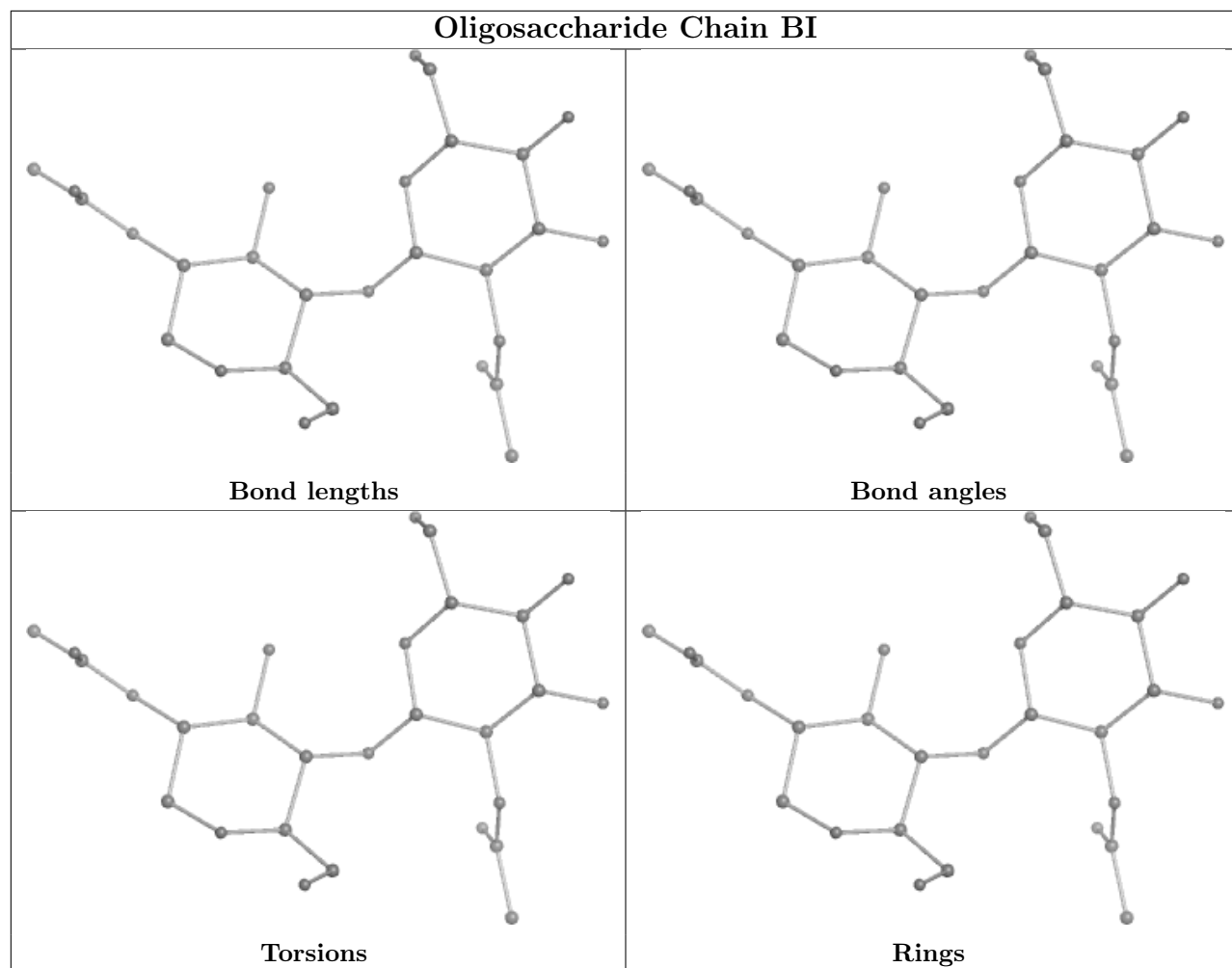


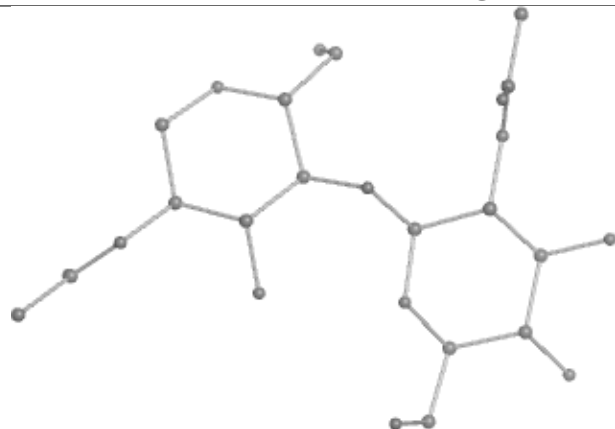
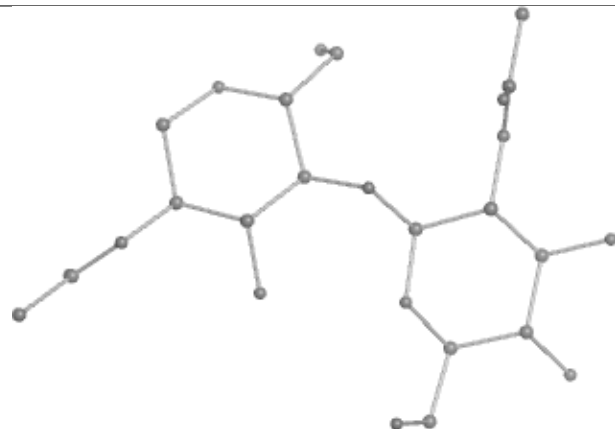
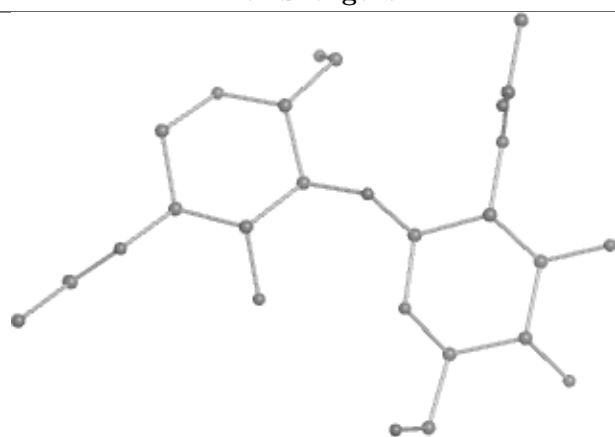
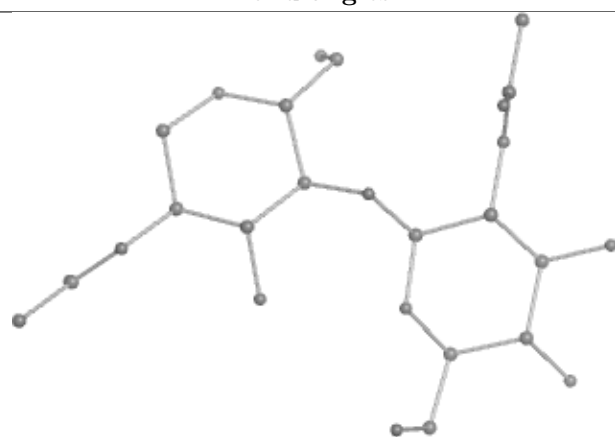
Oligosaccharide Chain BE

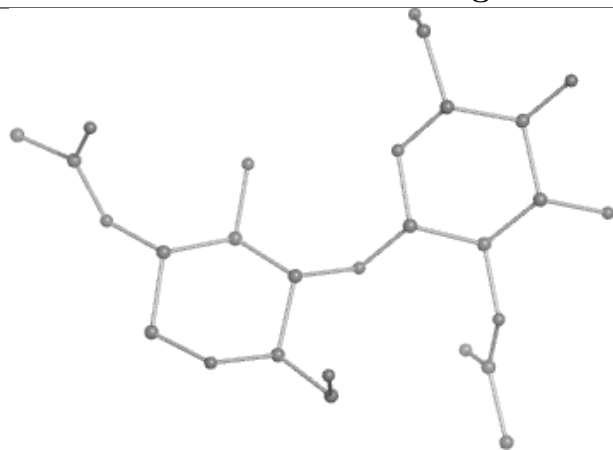
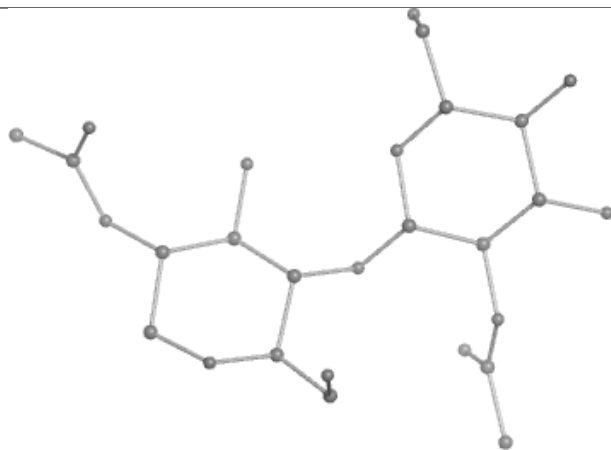
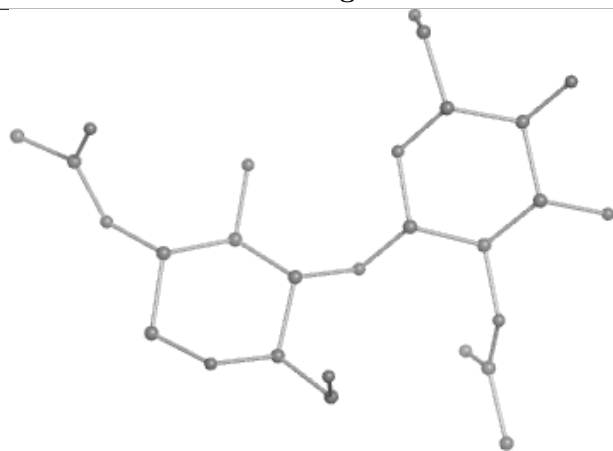
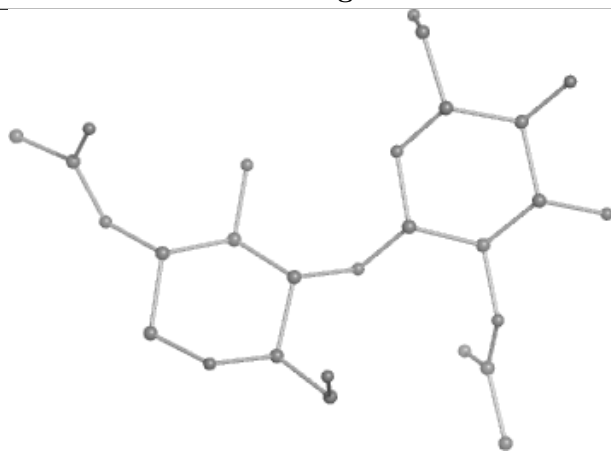


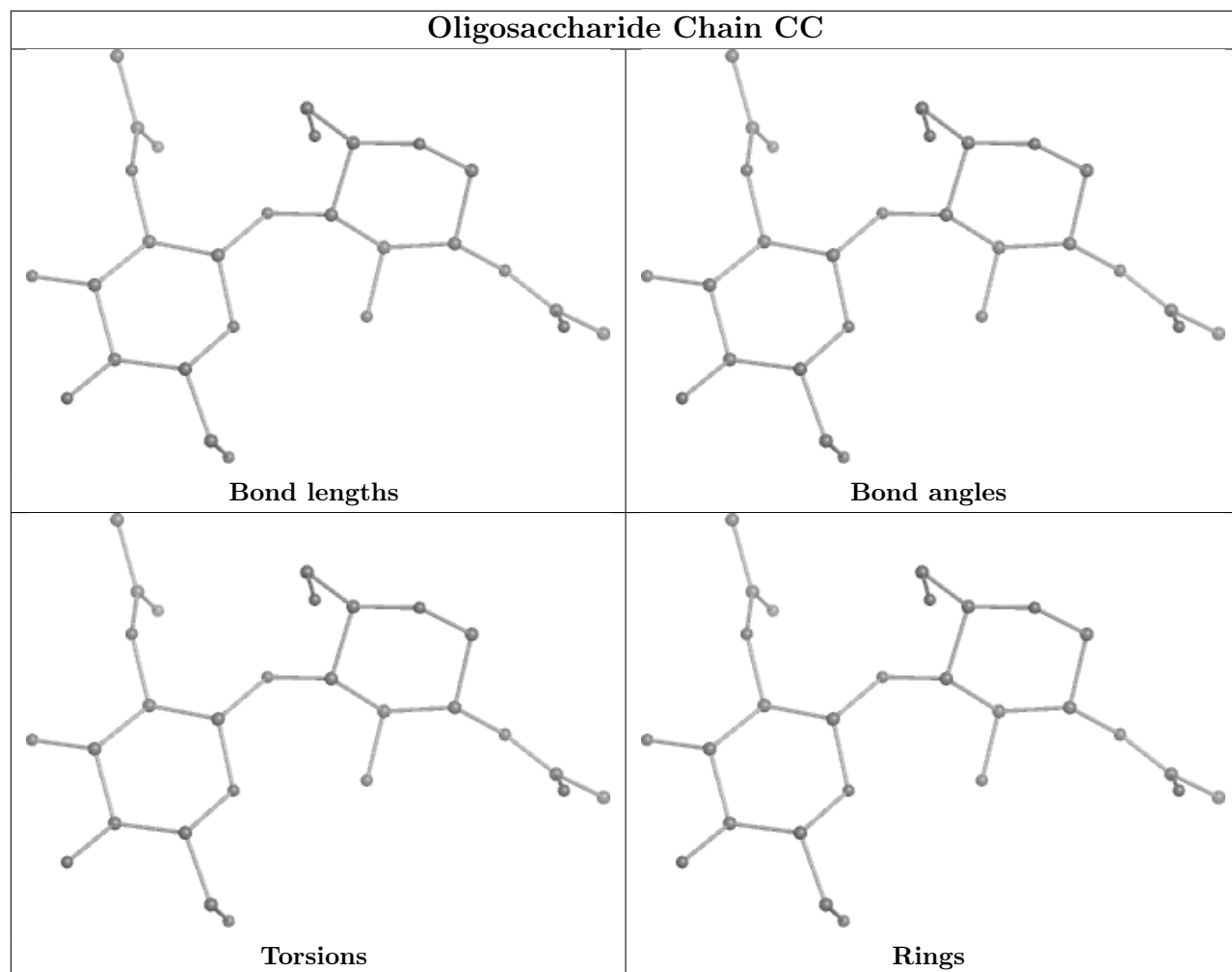


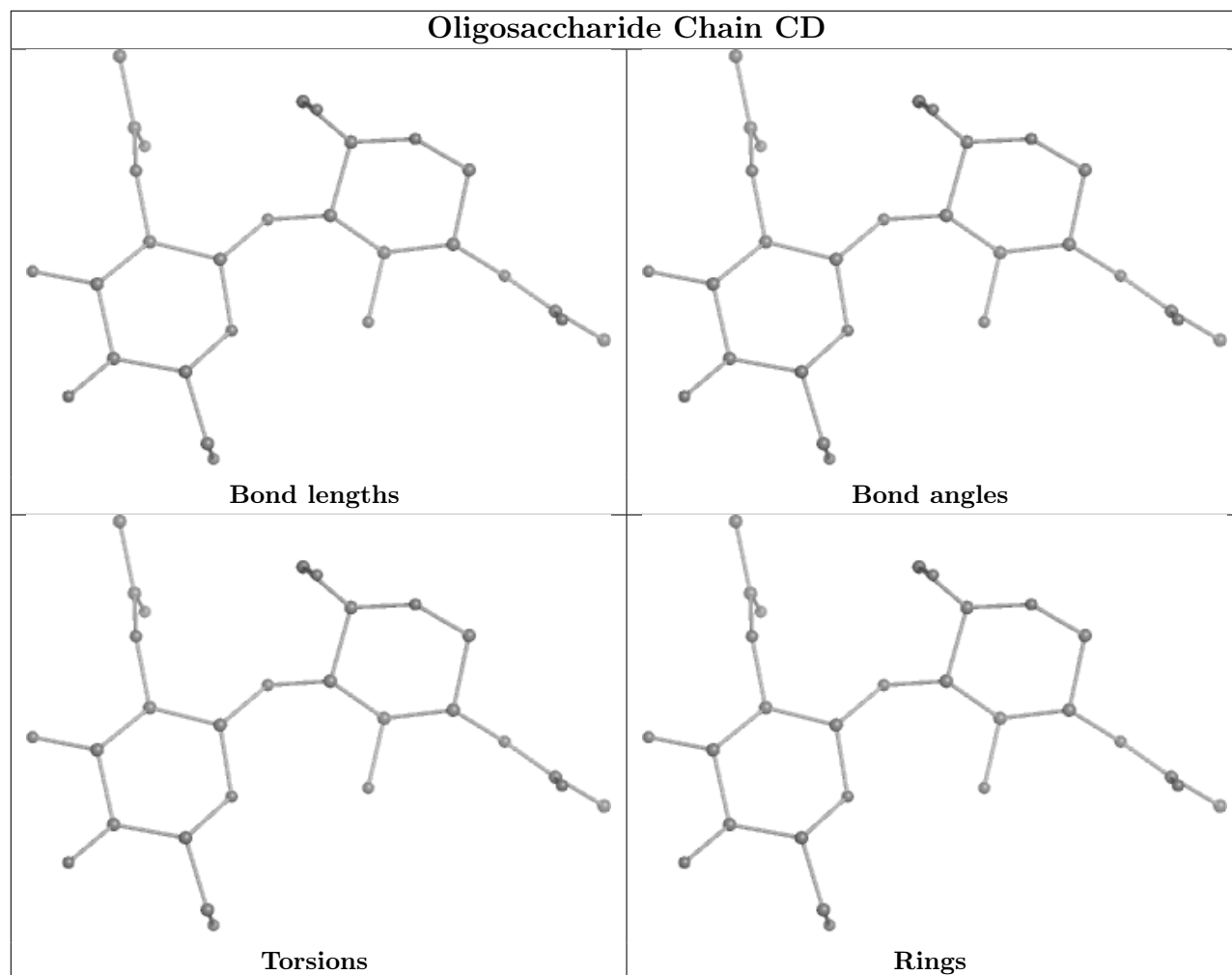


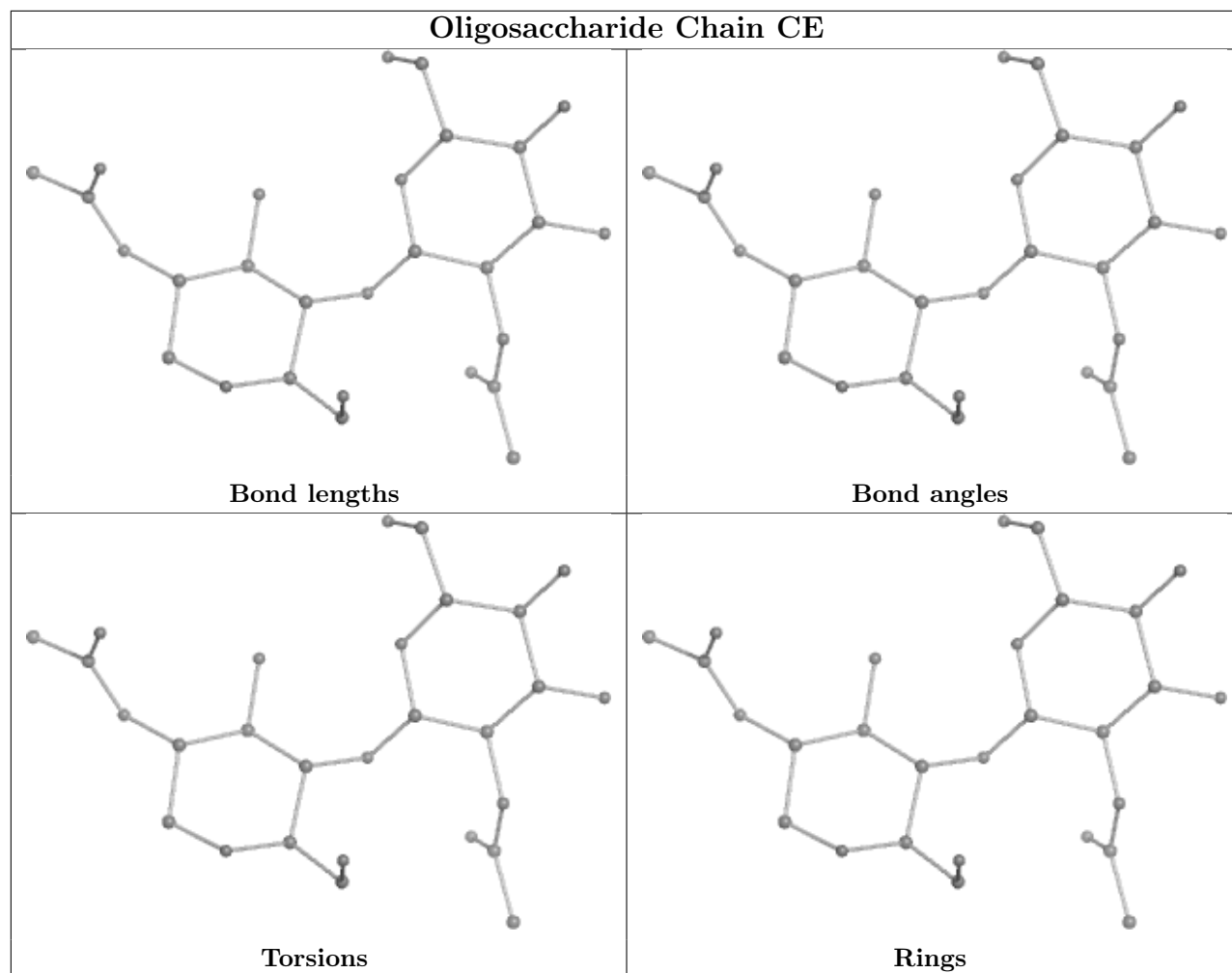


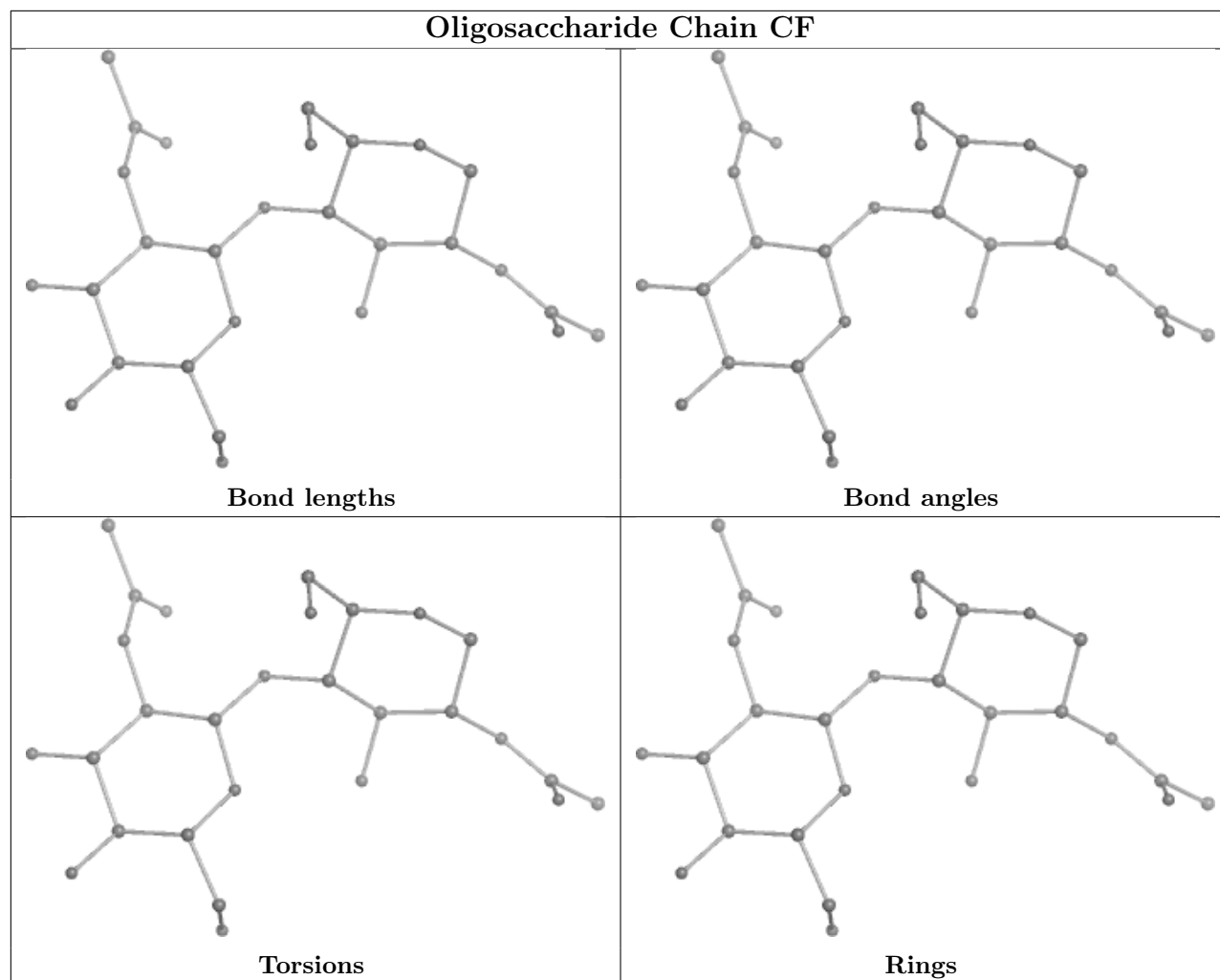
Oligosaccharide Chain CA**Bond lengths****Bond angles****Torsions****Rings**

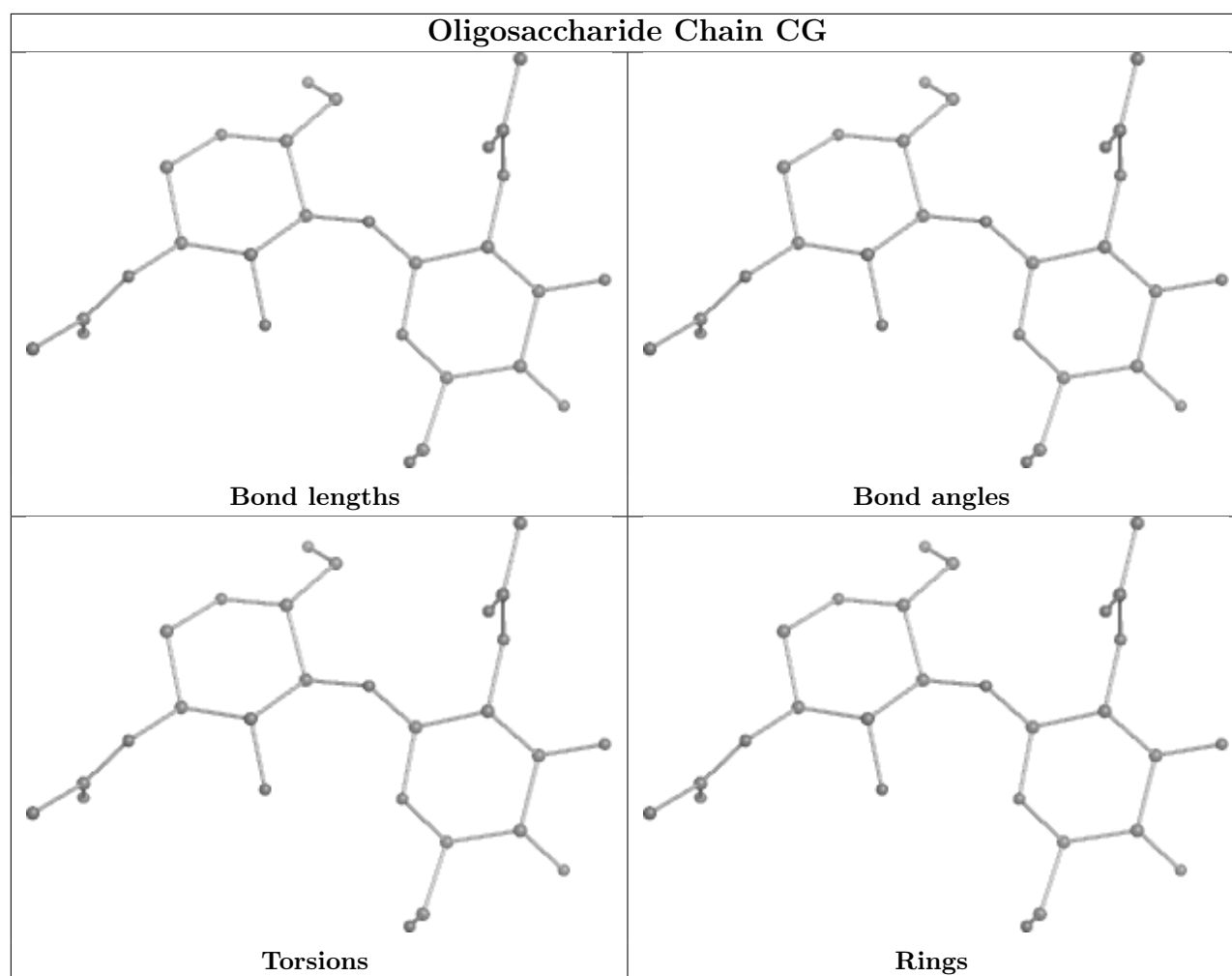
Oligosaccharide Chain CB**Bond lengths****Bond angles****Torsions****Rings**

Oligosaccharide Chain CC

Oligosaccharide Chain CD







5.6 Ligand geometry [i](#)

34 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	$\# Z > 2$
5	NAG	A	1204	1	14,14,15	0.37	0	17,19,21	0.45	0
5	NAG	B	1402	1	14,14,15	0.54	0	17,19,21	0.70	1 (5%)
5	NAG	C	1401	1	14,14,15	0.36	0	17,19,21	0.60	1 (5%)
5	NAG	B	1404	1	14,14,15	0.29	0	17,19,21	0.55	0
5	NAG	A	1202	1	14,14,15	0.35	0	17,19,21	0.58	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1404	-	14,14,15	0.41	0	17,19,21	0.46	0
5	NAG	C	1408	1	14,14,15	0.42	0	17,19,21	0.65	1 (5%)
5	NAG	B	1405	1	14,14,15	0.31	0	17,19,21	0.63	0
6	STE	B	1408	-	19,19,19	0.58	0	19,19,19	0.51	0
5	NAG	C	1407	1	14,14,15	0.32	0	17,19,21	0.53	0
8	KZ0	H	101	3	9,9,12	1.04	0	12,12,15	3.87	7 (58%)
5	NAG	A	1205	1	14,14,15	0.32	0	17,19,21	0.46	0
5	NAG	B	1406	1	14,14,15	0.29	0	17,19,21	0.60	0
5	NAG	B	1403	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	C	1406	1	14,14,15	0.30	0	17,19,21	0.53	0
5	NAG	C	1410	1	14,14,15	0.29	0	17,19,21	0.60	0
5	NAG	C	1405	-	14,14,15	0.24	0	17,19,21	0.54	0
6	STE	A	1209	-	19,19,19	0.59	0	19,19,19	0.57	0
5	NAG	A	1208	1	14,14,15	0.36	0	17,19,21	0.58	1 (5%)
5	NAG	A	1207	1	14,14,15	0.31	0	17,19,21	0.49	0
5	NAG	A	1203	1	14,14,15	0.36	0	17,19,21	0.59	0
5	NAG	A	1201	1	14,14,15	0.25	0	17,19,21	0.48	0
7	R06	F	101	2	15,15,18	1.88	3 (20%)	21,21,24	1.00	1 (4%)
5	NAG	C	1402	1	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	A	1206	1	14,14,15	0.32	0	17,19,21	0.57	0
7	R06	E	101	2	15,15,18	1.89	3 (20%)	21,21,24	0.88	0
7	R06	D	101	2	15,15,18	1.89	3 (20%)	21,21,24	0.99	1 (4%)
5	NAG	C	1409	1	14,14,15	0.33	0	17,19,21	0.46	0
5	NAG	B	1407	1	14,14,15	0.34	0	17,19,21	0.45	0
5	NAG	C	1403	1	14,14,15	0.64	1 (7%)	17,19,21	0.48	0
8	KZ0	G	101	3	9,9,12	1.04	0	12,12,15	3.86	7 (58%)
5	NAG	B	1401	1	14,14,15	0.37	0	17,19,21	0.65	1 (5%)
8	KZ0	I	101	3	9,9,12	1.04	0	12,12,15	3.84	7 (58%)
6	STE	C	1411	-	19,19,19	0.56	0	19,19,19	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1204	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1202	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1404	-	-	2/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
6	STE	B	1408	-	-	5/17/17/17	-
5	NAG	C	1407	1	-	2/6/23/26	0/1/1/1
8	KZ0	H	101	3	-	-	0/1/1/1
5	NAG	A	1205	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1410	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1405	-	-	0/6/23/26	0/1/1/1
6	STE	A	1209	-	-	5/17/17/17	-
5	NAG	A	1208	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1207	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1203	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1201	1	-	0/6/23/26	0/1/1/1
7	R06	F	101	2	-	0/12/24/30	0/0/1/1
5	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1206	1	-	0/6/23/26	0/1/1/1
7	R06	E	101	2	-	0/12/24/30	0/0/1/1
7	R06	D	101	2	-	0/12/24/30	0/0/1/1
5	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
8	KZ0	G	101	3	-	-	0/1/1/1
5	NAG	B	1401	1	-	4/6/23/26	0/1/1/1
8	KZ0	I	101	3	-	-	0/1/1/1
6	STE	C	1411	-	-	6/17/17/17	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	101	R06	C2-N1	3.45	1.45	1.35
7	E	101	R06	C2-N1	3.42	1.45	1.35
7	F	101	R06	C2-N1	3.41	1.45	1.35
7	F	101	R06	C7-N3	3.36	1.45	1.35
7	E	101	R06	C7-N3	3.36	1.45	1.35

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	101	KZ0	C2-N-C1	6.82	120.14	115.13
8	G	101	KZ0	C2-N-C1	6.78	120.11	115.13
8	I	101	KZ0	C2-N-C1	6.73	120.07	115.13
8	H	101	KZ0	C3-N1-C2	6.66	120.02	115.13
8	G	101	KZ0	C3-N1-C2	6.54	119.93	115.13

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

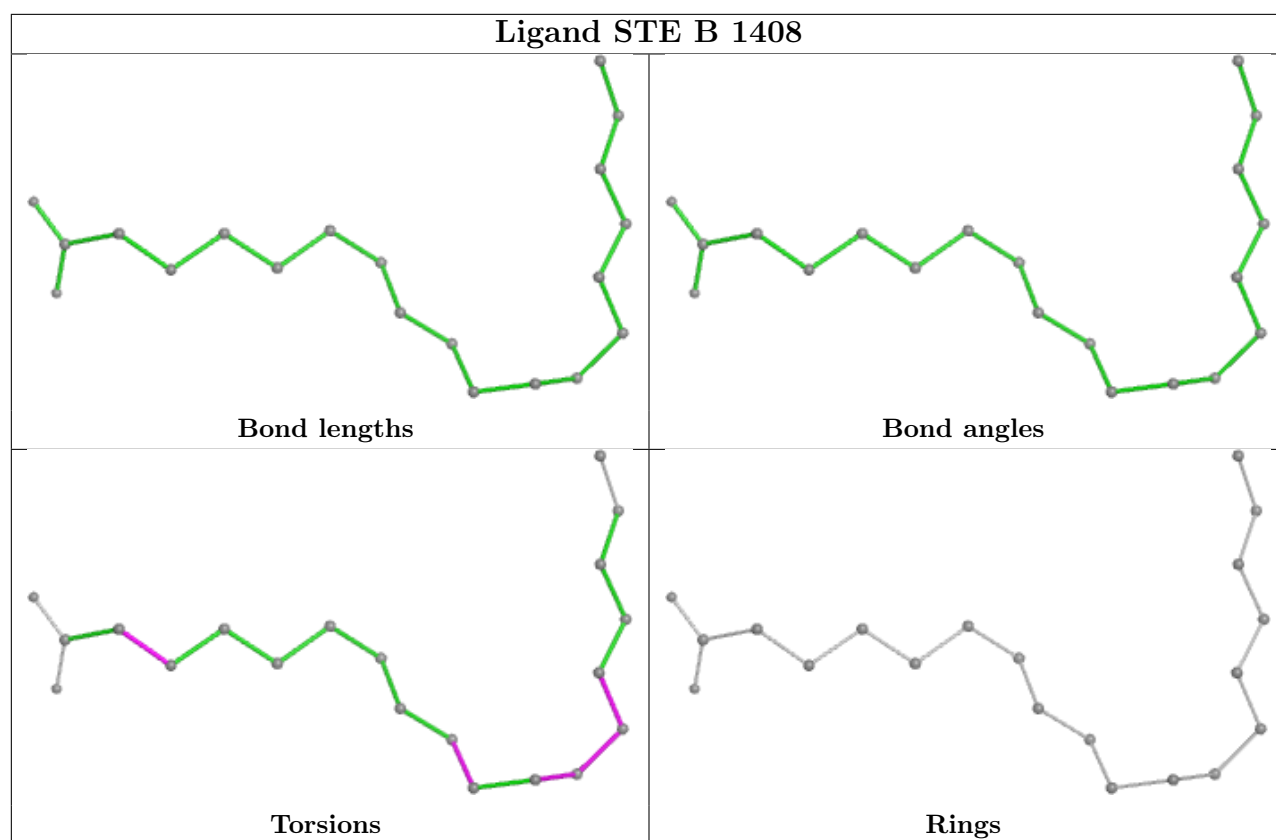
Mol	Chain	Res	Type	Atoms
5	A	1205	NAG	O5-C5-C6-O6
5	C	1403	NAG	O5-C5-C6-O6
5	B	1407	NAG	O5-C5-C6-O6
5	C	1409	NAG	O5-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6

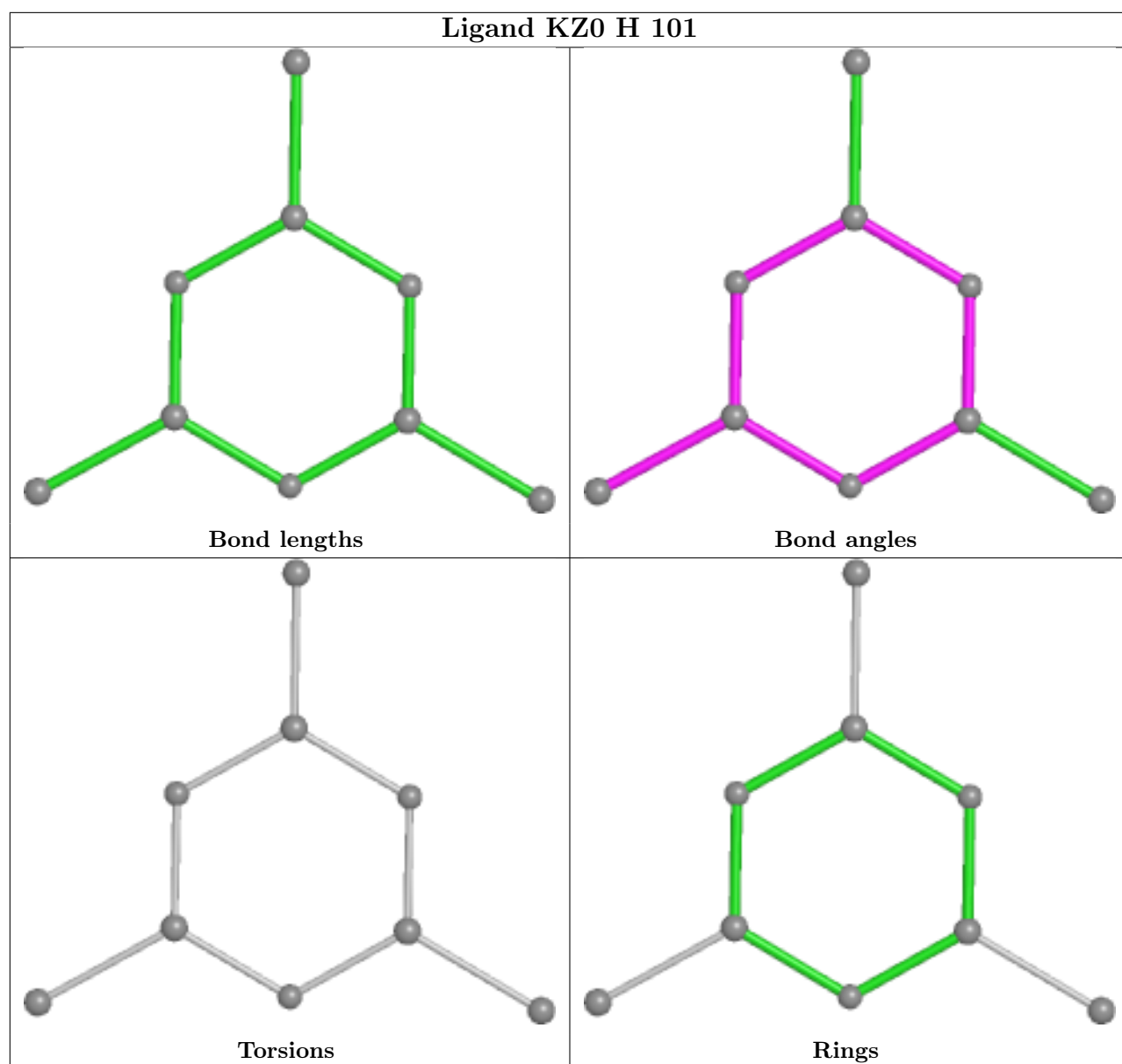
There are no ring outliers.

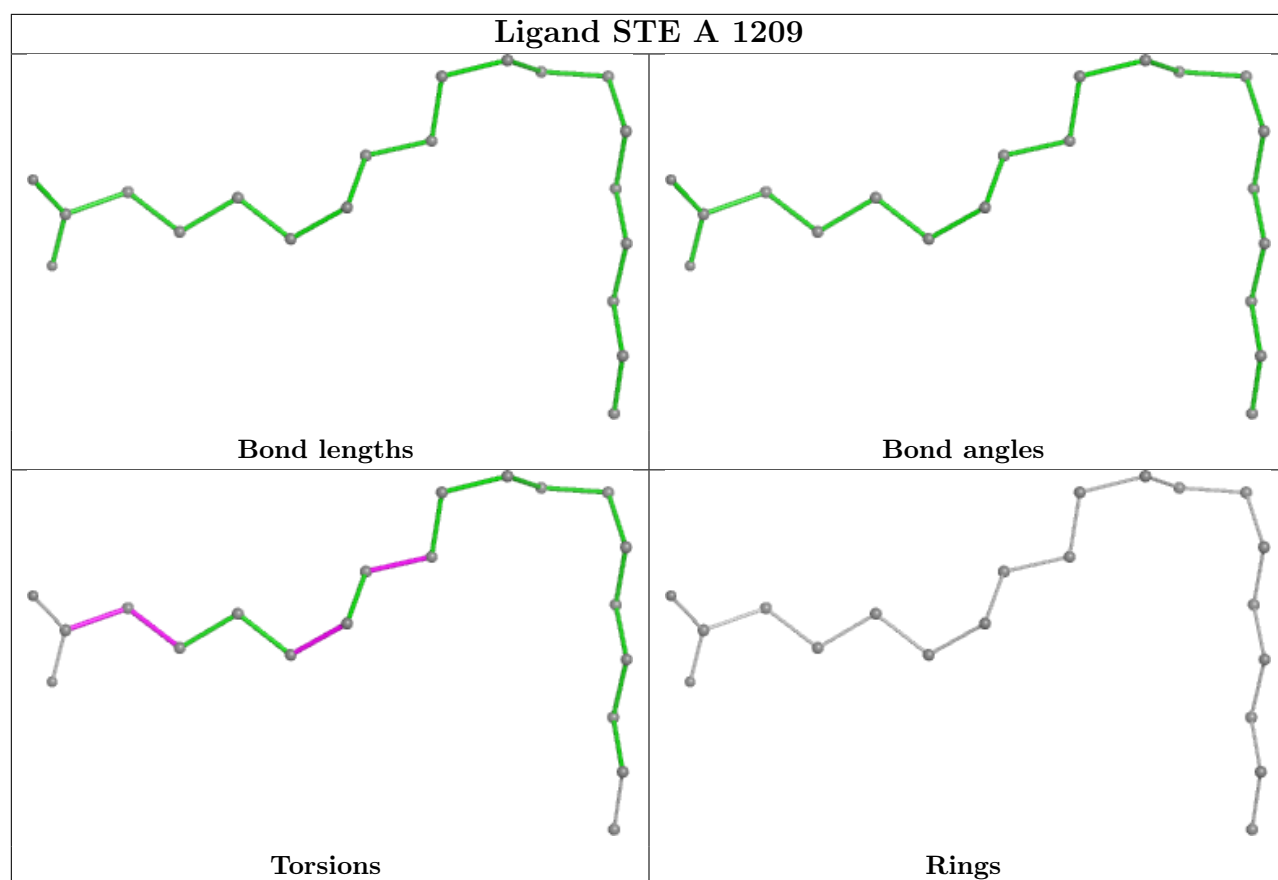
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1402	NAG	1	0
6	B	1408	STE	1	0

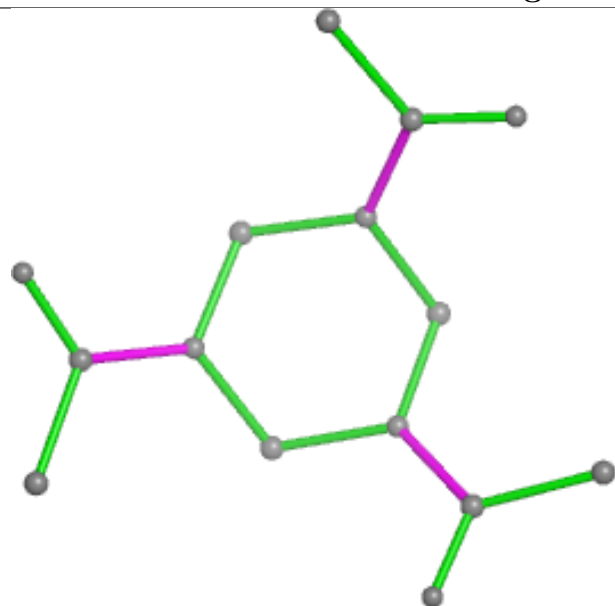
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



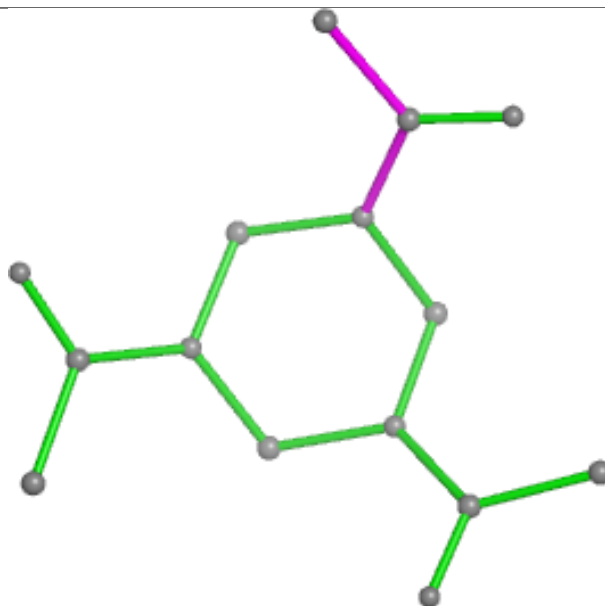




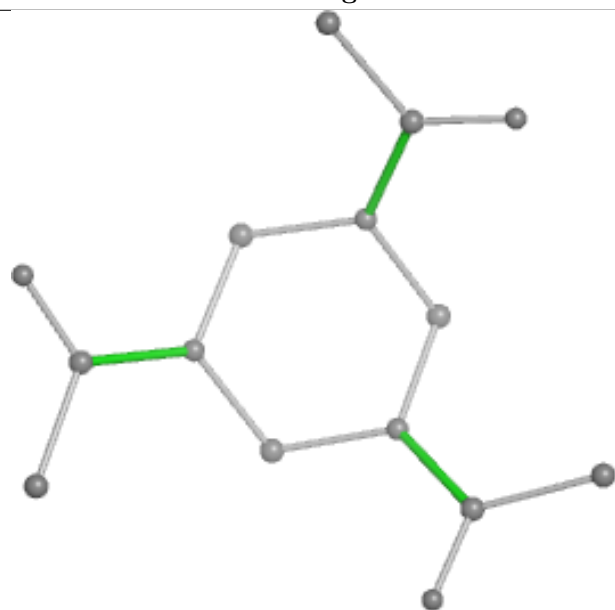
Ligand R06 F 101



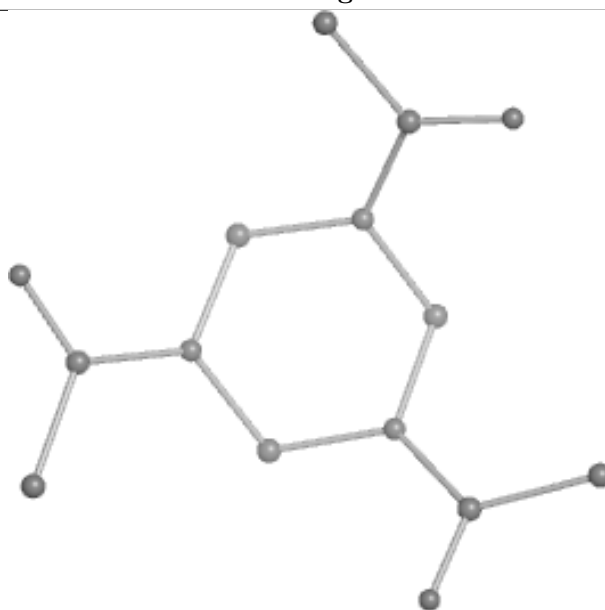
Bond lengths



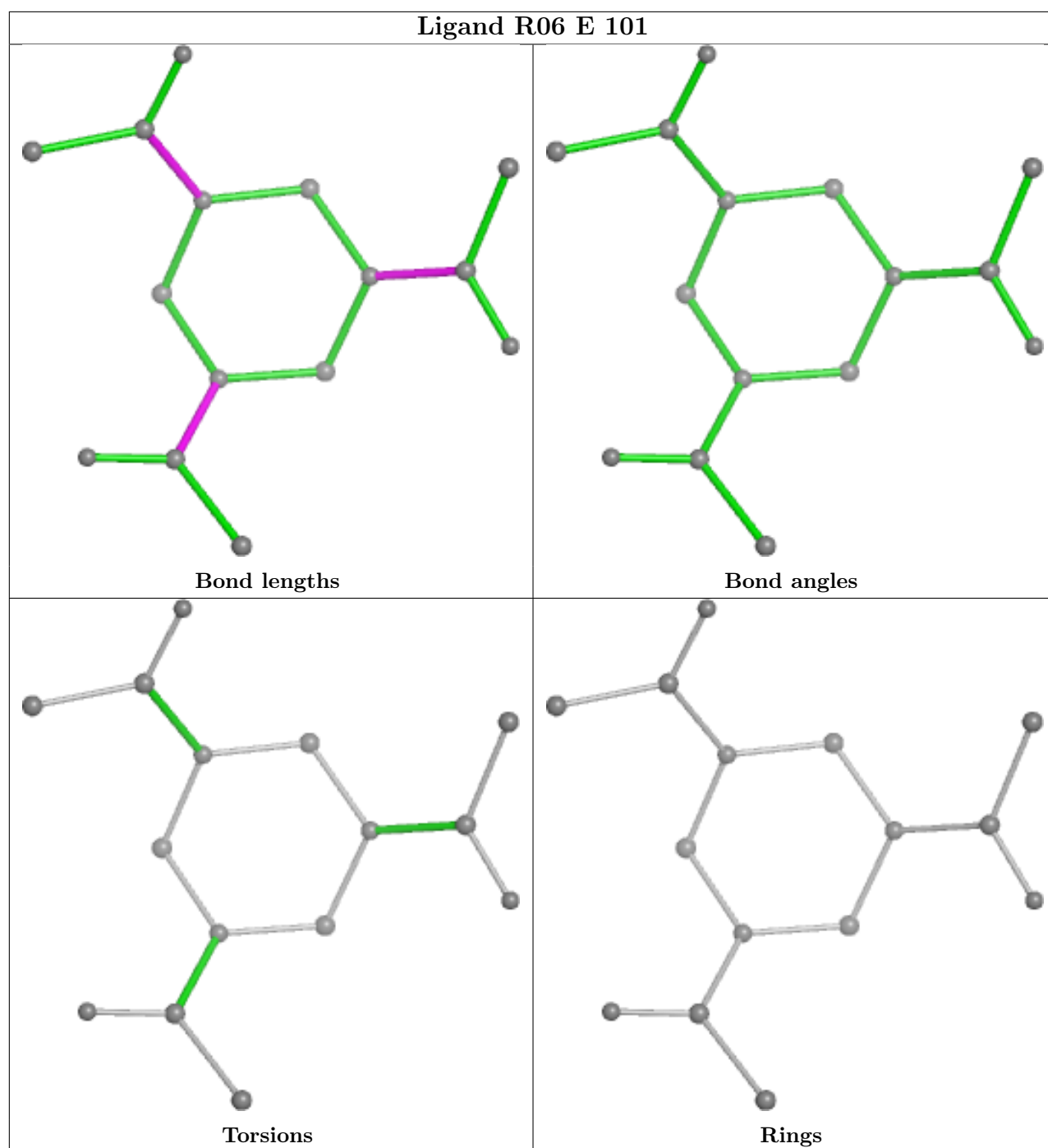
Bond angles



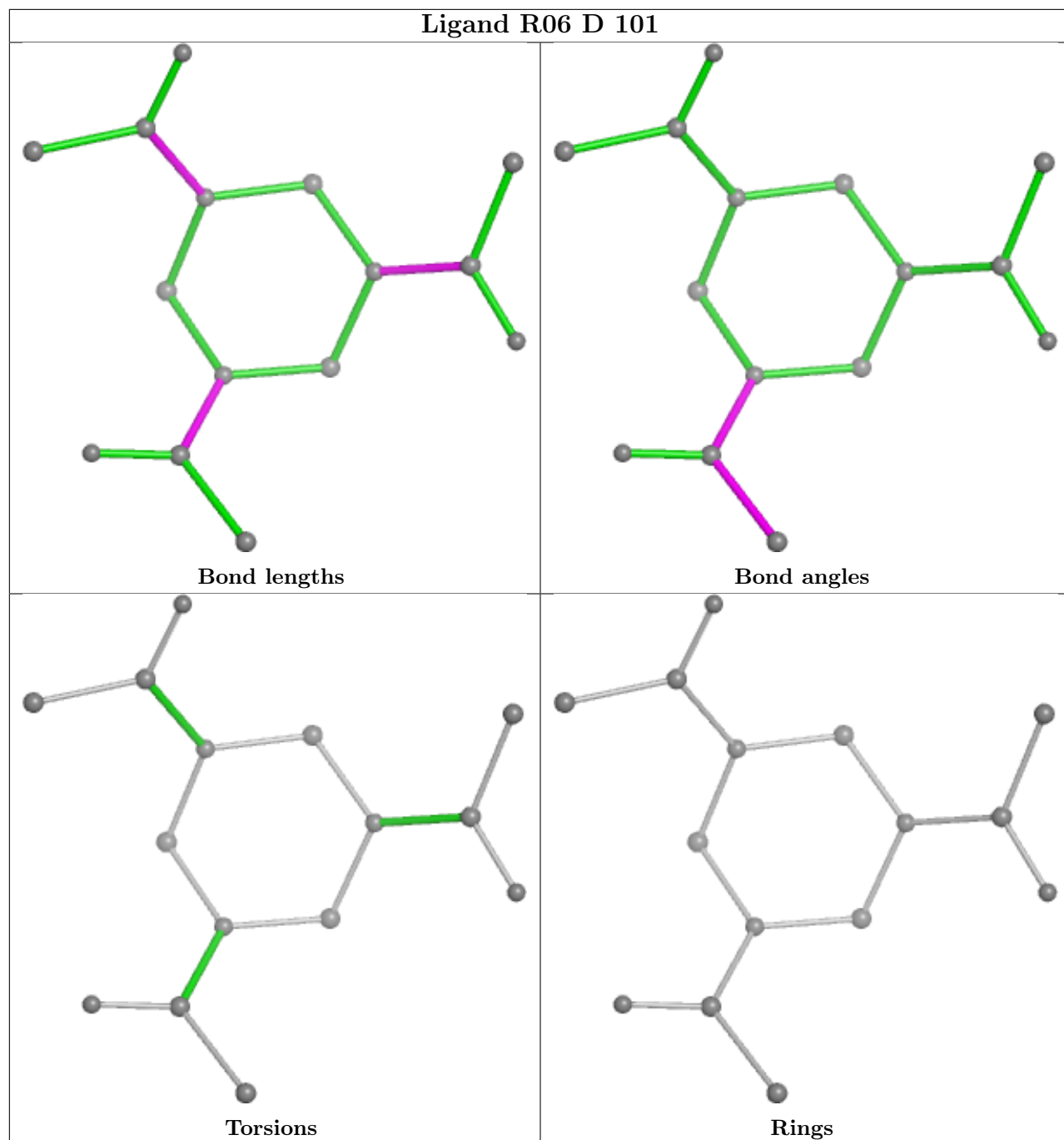
Torsions



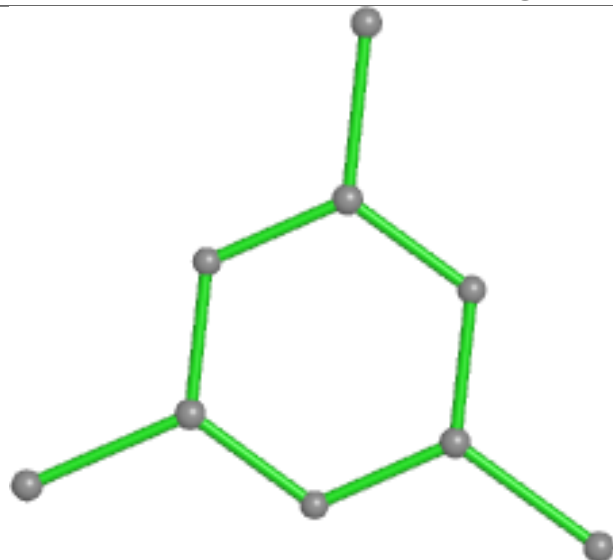
Rings



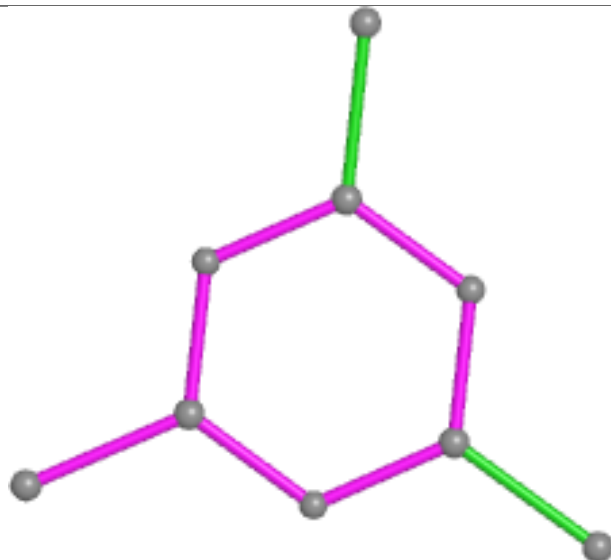
Ligand R06 D 101



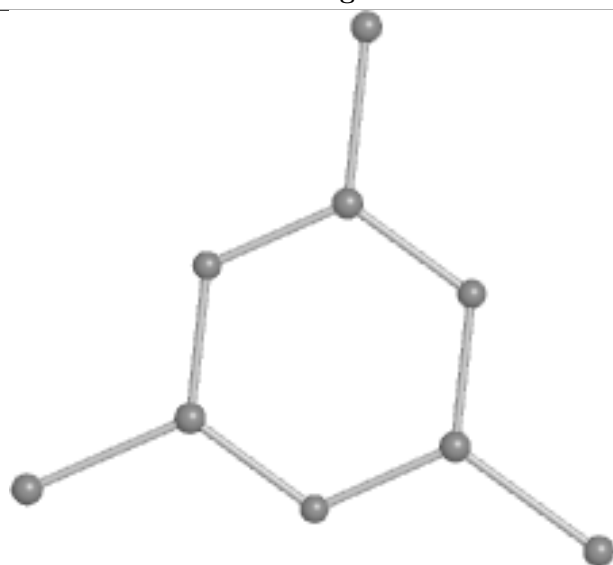
Ligand KZ0 G 101



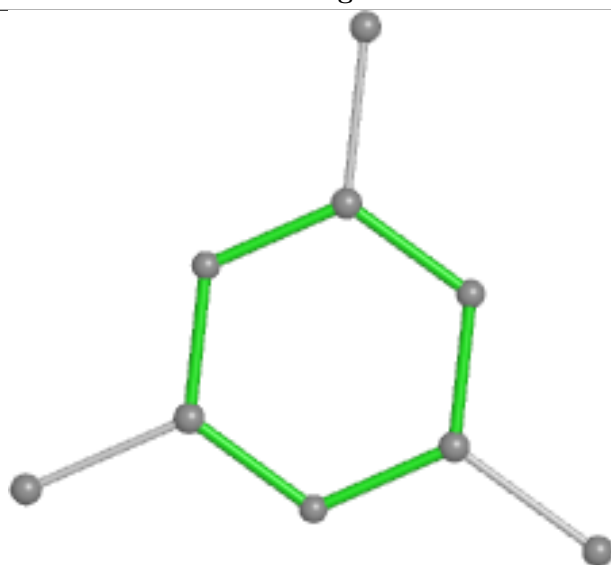
Bond lengths



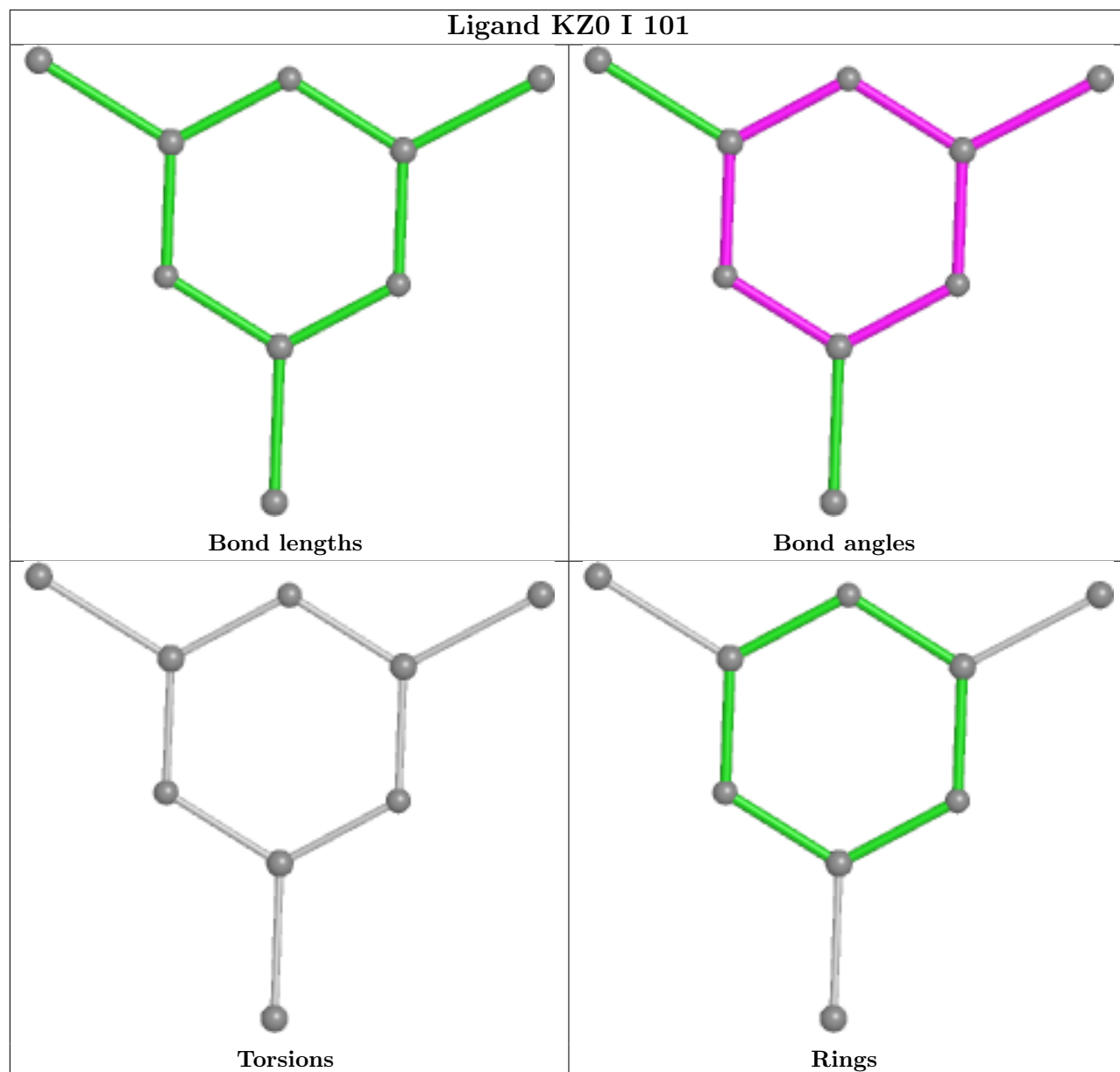
Bond angles

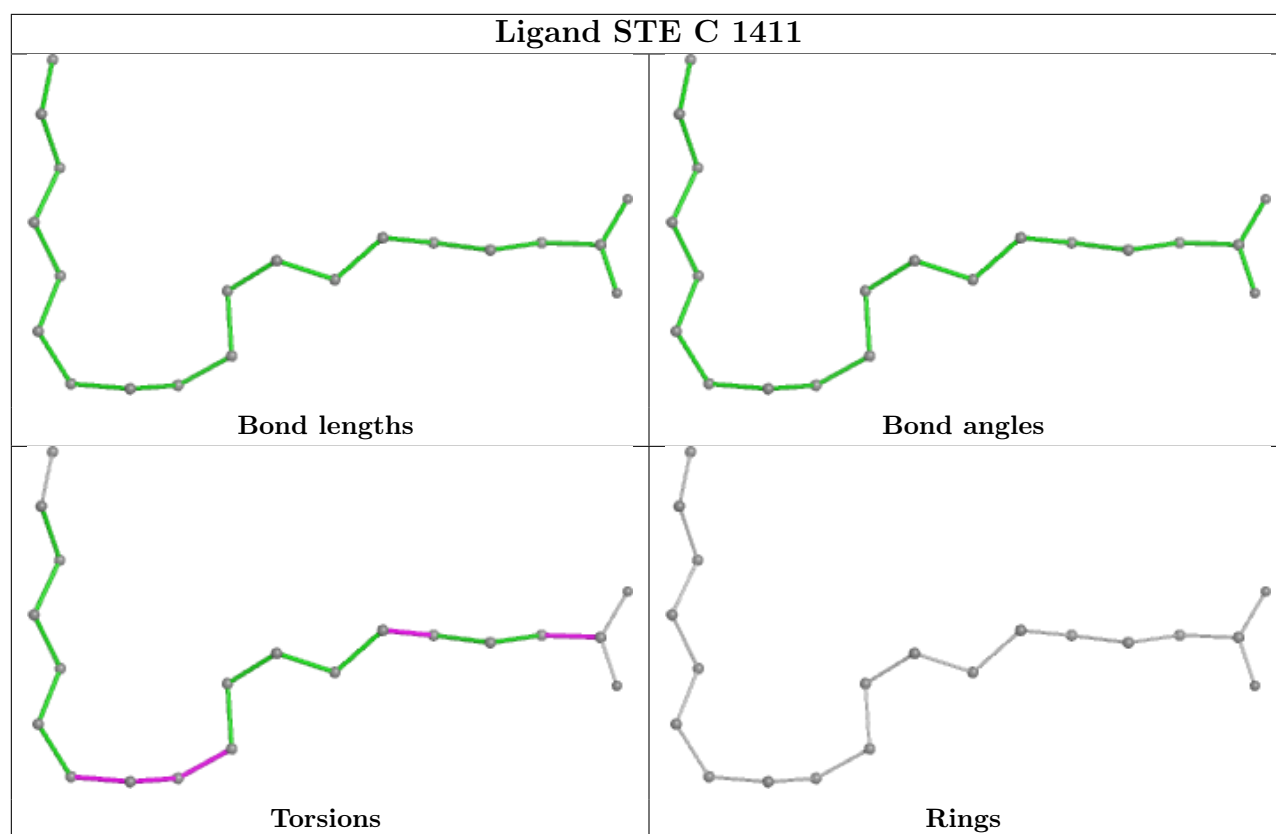


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.