



wwPDB EM Validation Summary Report ⓘ

Nov 17, 2022 – 01:41 AM EST

PDB ID : 7LAA
EMDB ID : EMD-23246
Title : Structure of SARS-CoV-2 S protein in complex with Receptor Binding Domain antibody DH1041
Authors : Manne, K.; Acharya, P.
Deposited on : 2021-01-06
Resolution : 3.42 Å (reported)
Based on initial model : 6VXX

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

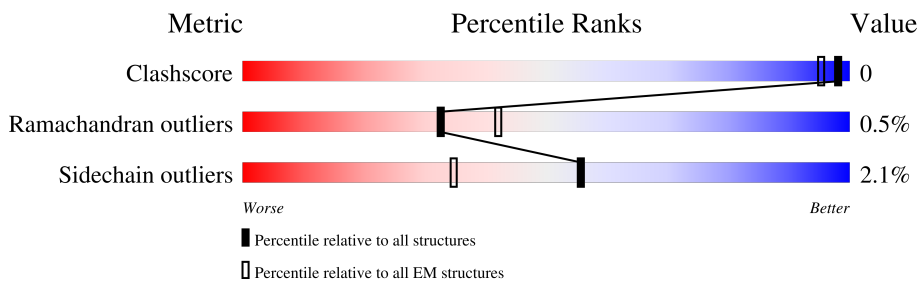
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.42 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.



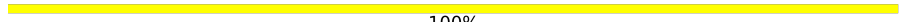
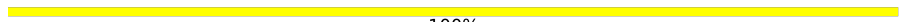

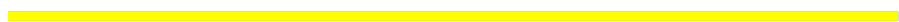






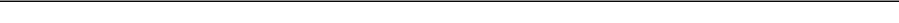

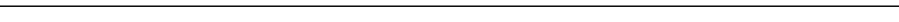
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1121	
1	B	1121	
1	C	1121	
2	H	226	
3	L	217	
4	D	2	
4	E	2	
4	F	2	
4	G	2	

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Mol	Chain	Length	Quality of chain
4	I	2	 100%
4	M	2	 100%
4	O	2	 100%
4	Q	2	 100%
4	R	2	 100%
4	T	2	 100%
4	V	2	 100%
5	J	3	 100%
5	K	3	 100%
5	N	3	 100%
5	P	3	 100%
5	S	3	 100%
5	U	3	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 46691 atoms, of which 22979 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
			Total	C	H	N	O	S		
1	A	991	14998	4878	7376	1269	1441	34	0	0
1	B	788	11871	3855	5846	1000	1144	26	0	0
1	C	789	11876	3858	5846	1001	1145	26	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	607	GLU	GLN	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	607	GLU	GLN	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	607	GLU	GLN	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 is a protein called DH1041 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	H	217	3227	1031	1592	283	314	7	0	0

- Molecule 3 is a protein called DH1041 light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	L	217	3182	1009	1562	273	333	5	0	0

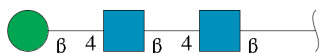
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	E	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	F	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	G	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	I	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	M	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	O	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	Q	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	R	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	T	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	V	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	K	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	N	3	Total	C	H	N	O	0	0
			76	22	37	2	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	S	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	U	3	Total	C	H	N	O	0	0
			76	22	37	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	A	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	A	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	A	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	A	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	B	1	Total	C	H	N	O	0
			168	48	84	6	30	
6	B	1	Total	C	H	N	O	0
			168	48	84	6	30	
6	B	1	Total	C	H	N	O	0
			168	48	84	6	30	

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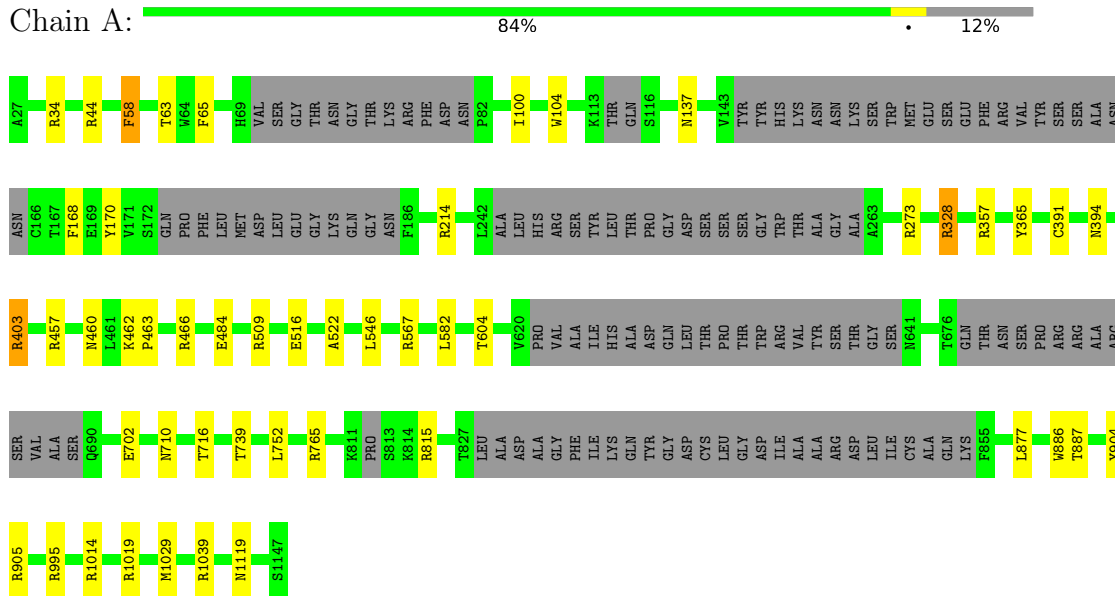
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Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total 168	C 48	H 84	N 6	O 30	0
6	B	1	Total 168	C 48	H 84	N 6	O 30	0
6	B	1	Total 168	C 48	H 84	N 6	O 30	0
6	C	1	Total 168	C 48	H 84	N 6	O 30	0
6	C	1	Total 168	C 48	H 84	N 6	O 30	0
6	C	1	Total 168	C 48	H 84	N 6	O 30	0
6	C	1	Total 168	C 48	H 84	N 6	O 30	0
6	C	1	Total 168	C 48	H 84	N 6	O 30	0
6	C	1	Total 168	C 48	H 84	N 6	O 30	0

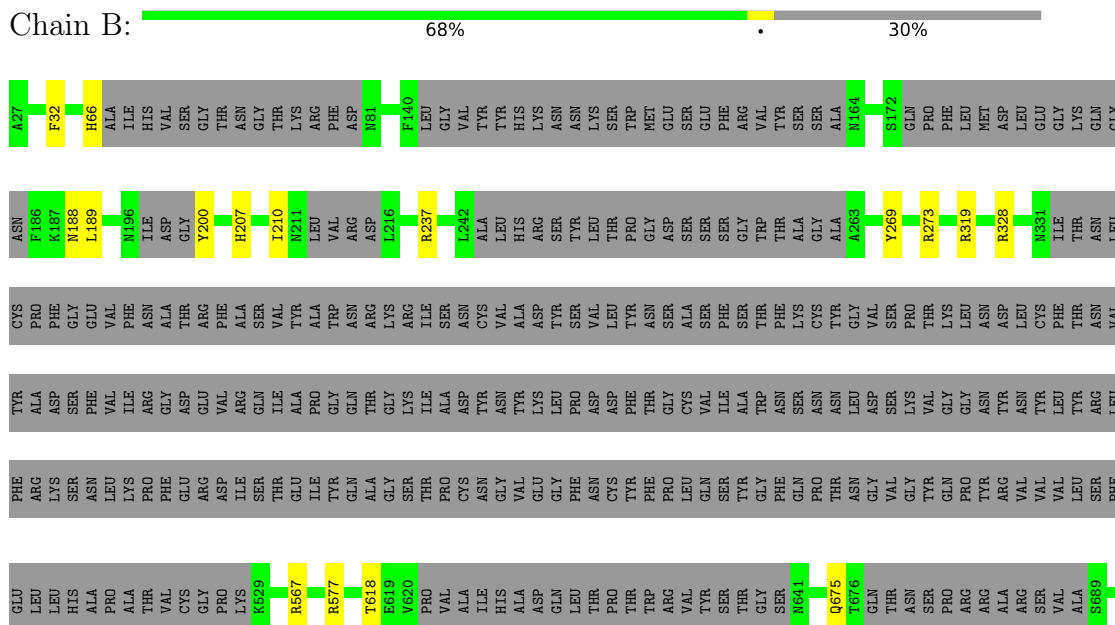
3 Residue-property plots

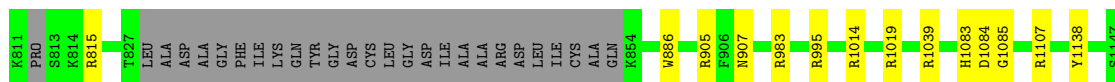
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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

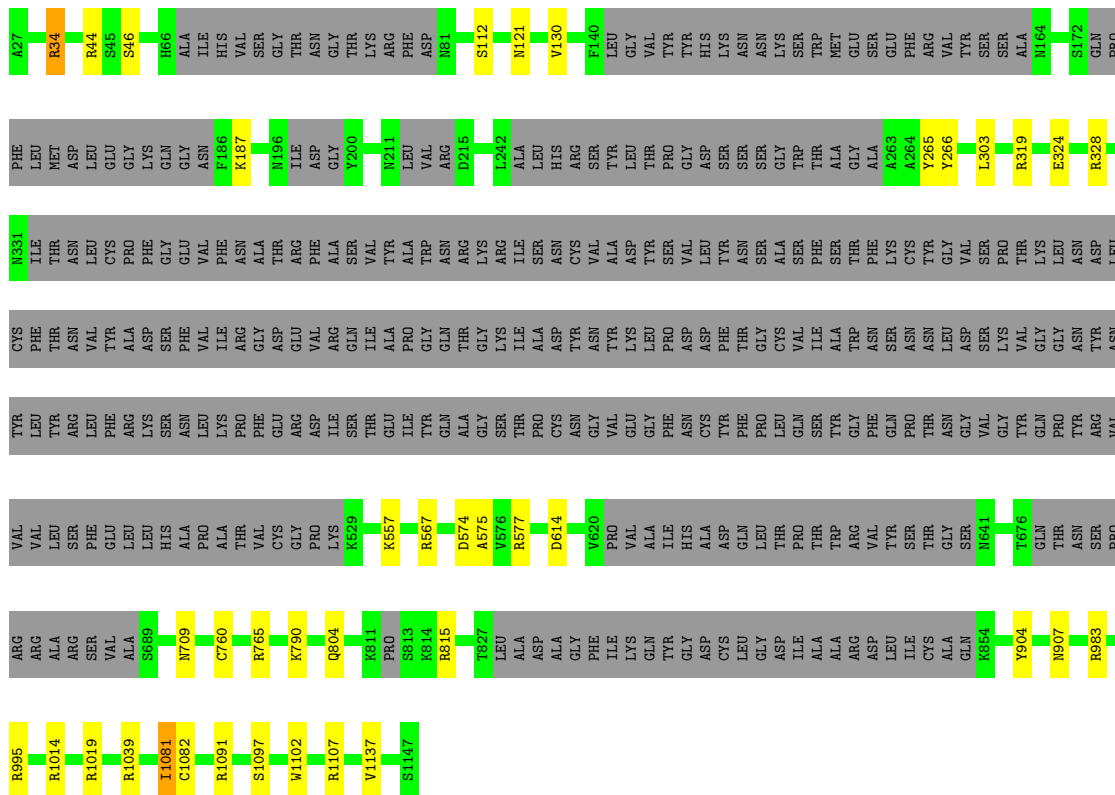


- Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein



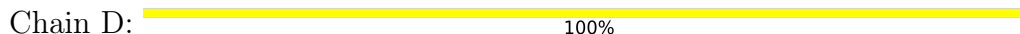
• Molecule 2: DH1041 heavy chain



• Molecule 3: DH1041 light chain




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



MAG1
MAG2


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

Chain E:  100%MAG1
MAG2


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

Chain F:  100%MAG1
MAG2


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

Chain G:  100%MAG1
MAG2

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

Chain I:  100%MAG1
MAG2


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

Chain M:  100%MAG1
MAG2

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


Chain O:  100%MAG1
MAG2

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

Chain Q:  100%

MAG1
MAG2

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

Chain R:  100%

MAG1
MAG2

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

Chain T:  100%

MAG1
MAG2

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

Chain V:  100%


MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2
BMA3

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

Chain K:  100%

MAG1
MAG2
BMA3

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

Chain N:  100%

MAG1
MAG2
BMA3

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

Chain P:  100%MAG1
MAG2
BMA3

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

Chain S:  100%MAG1
MAG2
BMA3

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

Chain U:  100%MAG1
MAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151384	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 ($e^-/\text{\AA}^2$)	65.94	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k 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: NAG, BMA

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	0.65	0/7792	1.01	22/10615 (0.2%)
1	B	0.63	0/6149	0.97	15/8373 (0.2%)
1	C	0.63	0/6154	0.99	16/8380 (0.2%)
2	H	0.71	0/1674	1.10	4/2276 (0.2%)
3	L	0.69	0/1660	1.09	3/2269 (0.1%)
All	All	0.65	0/23429	1.01	60/31913 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	1
2	H	0	2
All	All	0	9

There are no bond length outliers.

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1014	ARG	NE-CZ-NH1	8.28	124.44	120.30
2	H	97	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	A	904	TYR	CB-CG-CD1	-7.75	116.35	121.00
2	H	96	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	B	1014	ARG	NE-CZ-NH1	7.35	123.97	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	ARG	Sidechain
1	A	365	TYR	Sidechain
1	A	65	PHE	Sidechain
1	B	200	TYR	Sidechain
1	B	269	TYR	Sidechain

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	7622	7376	7364	3	0
1	B	6025	5846	5832	2	0
1	C	6030	5846	5832	5	0
2	H	1635	1592	1591	3	0
3	L	1620	1562	1562	4	0
4	D	28	27	25	0	0
4	E	28	27	25	0	0
4	F	28	27	25	0	0
4	G	28	27	25	0	0
4	I	28	27	25	0	0
4	M	28	27	25	0	0
4	O	28	27	25	0	0
4	Q	28	27	25	0	0
4	R	28	27	25	0	0
4	T	28	27	25	0	0
4	V	28	27	25	0	0
5	J	39	37	34	0	0
5	K	39	37	34	0	0
5	N	39	37	34	0	0
5	P	39	37	34	0	0
5	S	39	37	34	0	0
5	U	39	37	34	0	0
6	A	70	70	65	0	0
6	B	84	84	78	0	0
6	C	84	84	78	0	0
All	All	23712	22979	22881	15	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 0.

The worst 5 of 15 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)
3:L:21:ILE:HG22	3:L:22:SER:H	1.65	0.60
1:C:1081:ILE:HD11	1:C:1137:VAL:HG23	1.87	0.56
2:H:100(H):PHE:H	3:L:46:LEU:HD22	1.76	0.51
1:C:1081:ILE:HD11	1:C:1137:VAL:CG2	2.42	0.50
2:H:144:ASP:H	2:H:171:GLN:NE2	2.11	0.48

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	971/1121 (87%)	892 (92%)	74 (8%)	5 (0%)	29 65
1	B	764/1121 (68%)	713 (93%)	48 (6%)	3 (0%)	34 69
1	C	765/1121 (68%)	714 (93%)	47 (6%)	4 (0%)	29 65
2	H	213/226 (94%)	197 (92%)	15 (7%)	1 (0%)	29 65
3	L	215/217 (99%)	192 (89%)	21 (10%)	2 (1%)	17 53
All	All	2928/3806 (77%)	2708 (92%)	205 (7%)	15 (0%)	32 65

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	187	LYS
1	B	207	HIS
1	A	604	THR
1	A	137	ASN
1	A	582	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	834/972 (86%)	816 (98%)	18 (2%)	52	78
1	B	661/972 (68%)	655 (99%)	6 (1%)	78	90
1	C	661/972 (68%)	647 (98%)	14 (2%)	53	79
2	H	178/188 (95%)	171 (96%)	7 (4%)	32	64
3	L	183/183 (100%)	176 (96%)	7 (4%)	33	64
All	All	2517/3287 (77%)	2465 (98%)	52 (2%)	56	79

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	101	ASP
3	L	119	PHE
1	C	907	ASN
2	H	146	PHE
3	L	49	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

40 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	D	1	4,1	14,14,15	1.38	2 (14%)	17,19,21	0.85	0
4	NAG	D	2	4	14,14,15	1.29	3 (21%)	17,19,21	1.20	1 (5%)
4	NAG	E	1	4,1	14,14,15	1.30	2 (14%)	17,19,21	0.86	0
4	NAG	E	2	4	14,14,15	1.18	2 (14%)	17,19,21	0.83	0
4	NAG	F	1	4,1	14,14,15	1.18	2 (14%)	17,19,21	1.57	3 (17%)
4	NAG	F	2	4	14,14,15	1.04	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	G	1	4,1	14,14,15	1.05	0	17,19,21	1.01	1 (5%)
4	NAG	G	2	4	14,14,15	1.06	1 (7%)	17,19,21	1.15	1 (5%)
4	NAG	I	1	4,1	14,14,15	1.34	2 (14%)	17,19,21	0.82	0
4	NAG	I	2	4	14,14,15	1.35	3 (21%)	17,19,21	1.55	3 (17%)
5	NAG	J	1	1,5	14,14,15	1.14	1 (7%)	17,19,21	1.27	3 (17%)
5	NAG	J	2	5	14,14,15	1.18	2 (14%)	17,19,21	1.28	2 (11%)
5	BMA	J	3	5	11,11,12	1.13	1 (9%)	15,15,17	0.91	0
5	NAG	K	1	1,5	14,14,15	1.23	2 (14%)	17,19,21	1.17	2 (11%)
5	NAG	K	2	5	14,14,15	1.14	1 (7%)	17,19,21	0.92	1 (5%)
5	BMA	K	3	5	11,11,12	1.20	2 (18%)	15,15,17	0.74	0
4	NAG	M	1	4,1	14,14,15	1.28	2 (14%)	17,19,21	1.05	1 (5%)
4	NAG	M	2	4	14,14,15	1.29	3 (21%)	17,19,21	0.89	1 (5%)
5	NAG	N	1	1,5	14,14,15	1.05	2 (14%)	17,19,21	0.96	1 (5%)
5	NAG	N	2	5	14,14,15	1.11	0	17,19,21	0.87	1 (5%)
5	BMA	N	3	5	11,11,12	1.14	1 (9%)	15,15,17	1.45	2 (13%)
4	NAG	O	1	4,1	14,14,15	0.98	0	17,19,21	0.89	1 (5%)
4	NAG	O	2	4	14,14,15	1.17	2 (14%)	17,19,21	0.86	0
5	NAG	P	1	1,5	14,14,15	1.23	1 (7%)	17,19,21	1.70	4 (23%)
5	NAG	P	2	5	14,14,15	1.16	2 (14%)	17,19,21	0.88	1 (5%)
5	BMA	P	3	5	11,11,12	1.10	1 (9%)	15,15,17	0.90	1 (6%)
4	NAG	Q	1	4,1	14,14,15	1.34	3 (21%)	17,19,21	0.89	0
4	NAG	Q	2	4	14,14,15	1.18	2 (14%)	17,19,21	1.08	1 (5%)
4	NAG	R	1	4,1	14,14,15	1.35	3 (21%)	17,19,21	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	R	2	4	14,14,15	1.27	2 (14%)	17,19,21	0.85	1 (5%)
5	NAG	S	1	1,5	14,14,15	1.04	1 (7%)	17,19,21	0.69	0
5	NAG	S	2	5	14,14,15	1.19	1 (7%)	17,19,21	0.76	0
5	BMA	S	3	5	11,11,12	1.24	1 (9%)	15,15,17	0.73	0
4	NAG	T	1	4,1	14,14,15	1.26	2 (14%)	17,19,21	0.81	0
4	NAG	T	2	4	14,14,15	1.33	2 (14%)	17,19,21	0.77	0
5	NAG	U	1	1,5	14,14,15	1.09	0	17,19,21	1.18	2 (11%)
5	NAG	U	2	5	14,14,15	1.26	2 (14%)	17,19,21	0.89	1 (5%)
5	BMA	U	3	5	11,11,12	1.15	1 (9%)	15,15,17	1.45	2 (13%)
4	NAG	V	1	4,1	14,14,15	1.25	3 (21%)	17,19,21	0.70	0
4	NAG	V	2	4	14,14,15	1.29	2 (14%)	17,19,21	0.91	1 (5%)

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	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	BMA	J	3	5	-	1/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	1/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	BMA	N	3	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	O	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	1/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	BMA	P	3	5	-	0/2/19/22	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
5	NAG	S	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	0/6/23/26	0/1/1/1
5	BMA	S	3	5	-	0/2/19/22	0/1/1/1
4	NAG	T	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	1/6/23/26	0/1/1/1
5	NAG	U	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1
5	BMA	U	3	5	-	0/2/19/22	0/1/1/1
4	NAG	V	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	1/6/23/26	0/1/1/1

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	2	NAG	O5-C5	2.88	1.49	1.43
4	Q	1	NAG	O5-C5	2.78	1.49	1.43
4	D	2	NAG	O5-C5	2.75	1.49	1.43
4	I	2	NAG	O5-C5	2.71	1.48	1.43
4	T	2	NAG	O5-C5	2.71	1.48	1.43

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	3	BMA	C1-O5-C5	4.37	118.11	112.19
4	F	1	NAG	C2-N2-C7	3.90	128.46	122.90
4	G	2	NAG	C1-O5-C5	3.76	117.29	112.19
5	U	3	BMA	C1-O5-C5	3.56	117.02	112.19
4	D	2	NAG	C1-O5-C5	3.47	116.89	112.19

There are no chirality outliers.

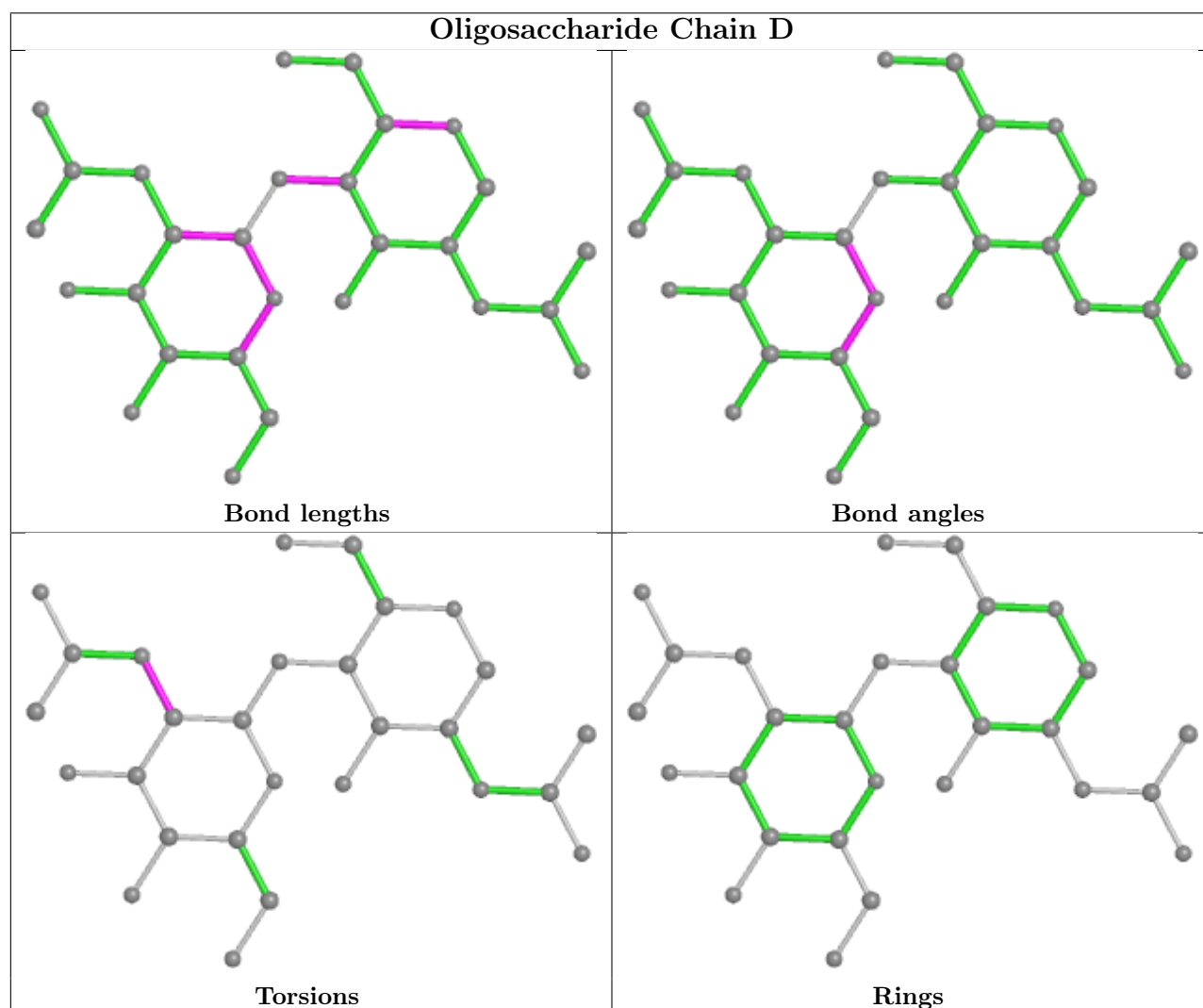
5 of 19 torsion outliers are listed below:

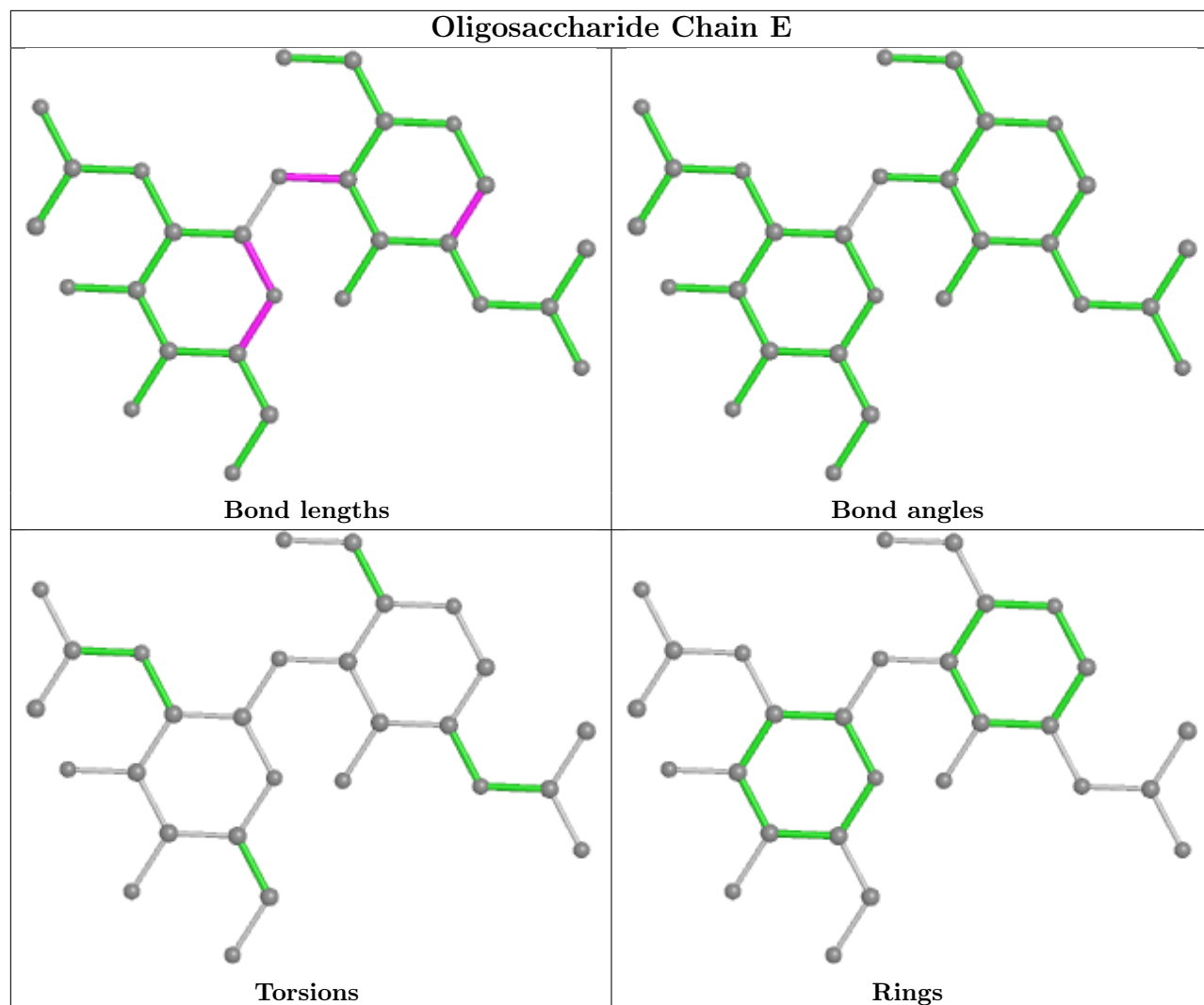
Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C1-C2-N2-C7
5	P	1	NAG	C1-C2-N2-C7
5	J	1	NAG	C4-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6

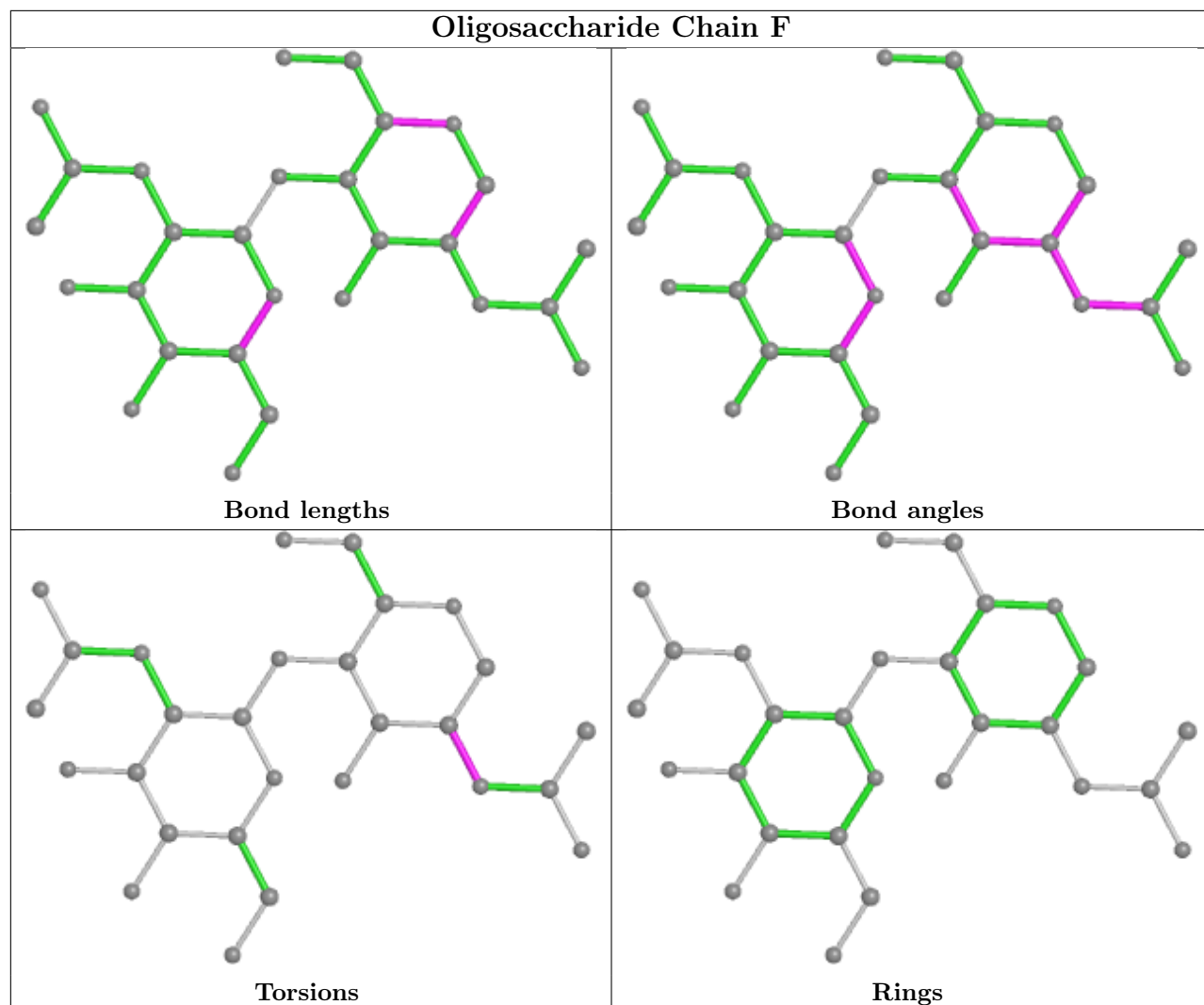
There are no ring outliers.

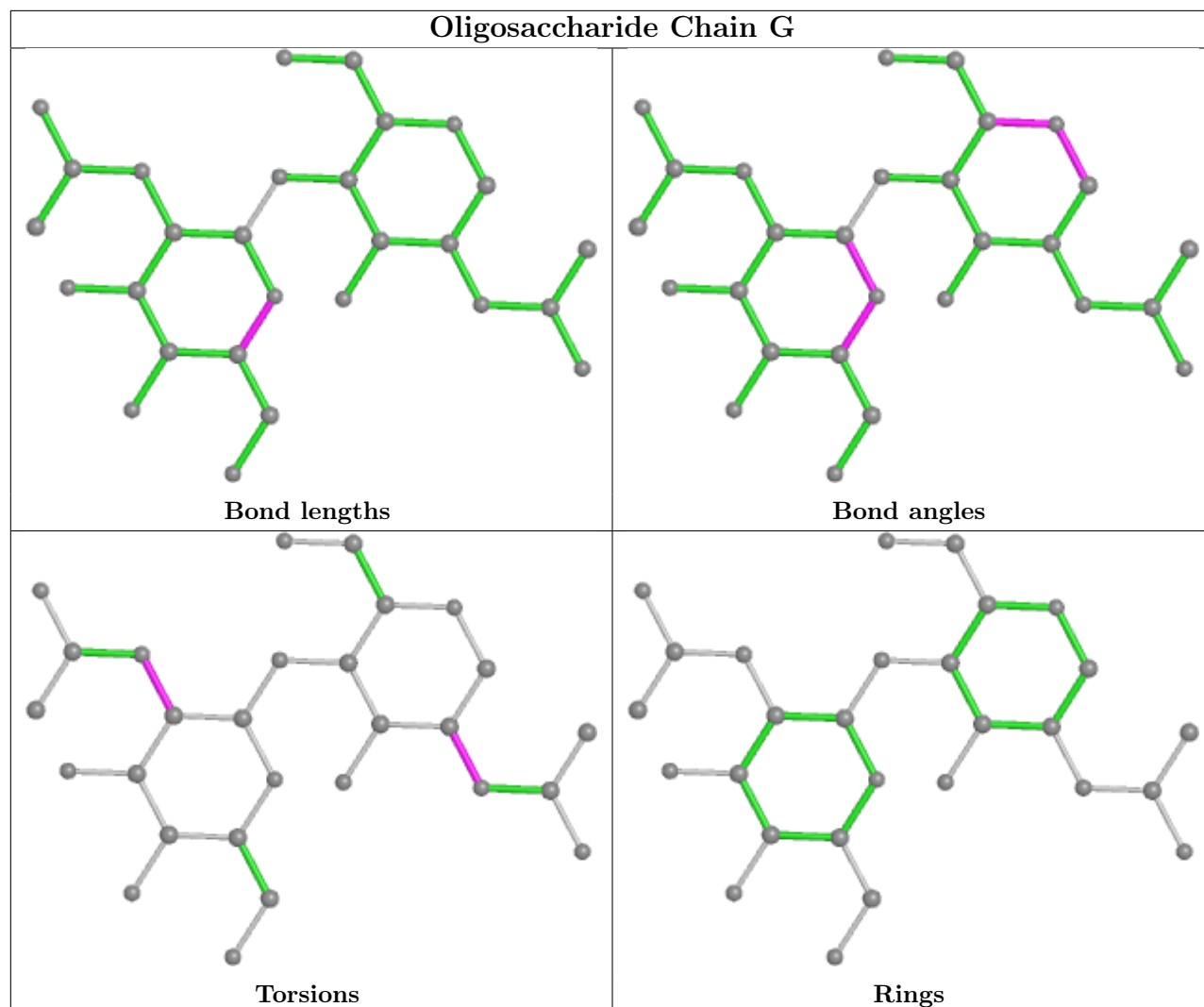
No monomer is involved in short contacts.

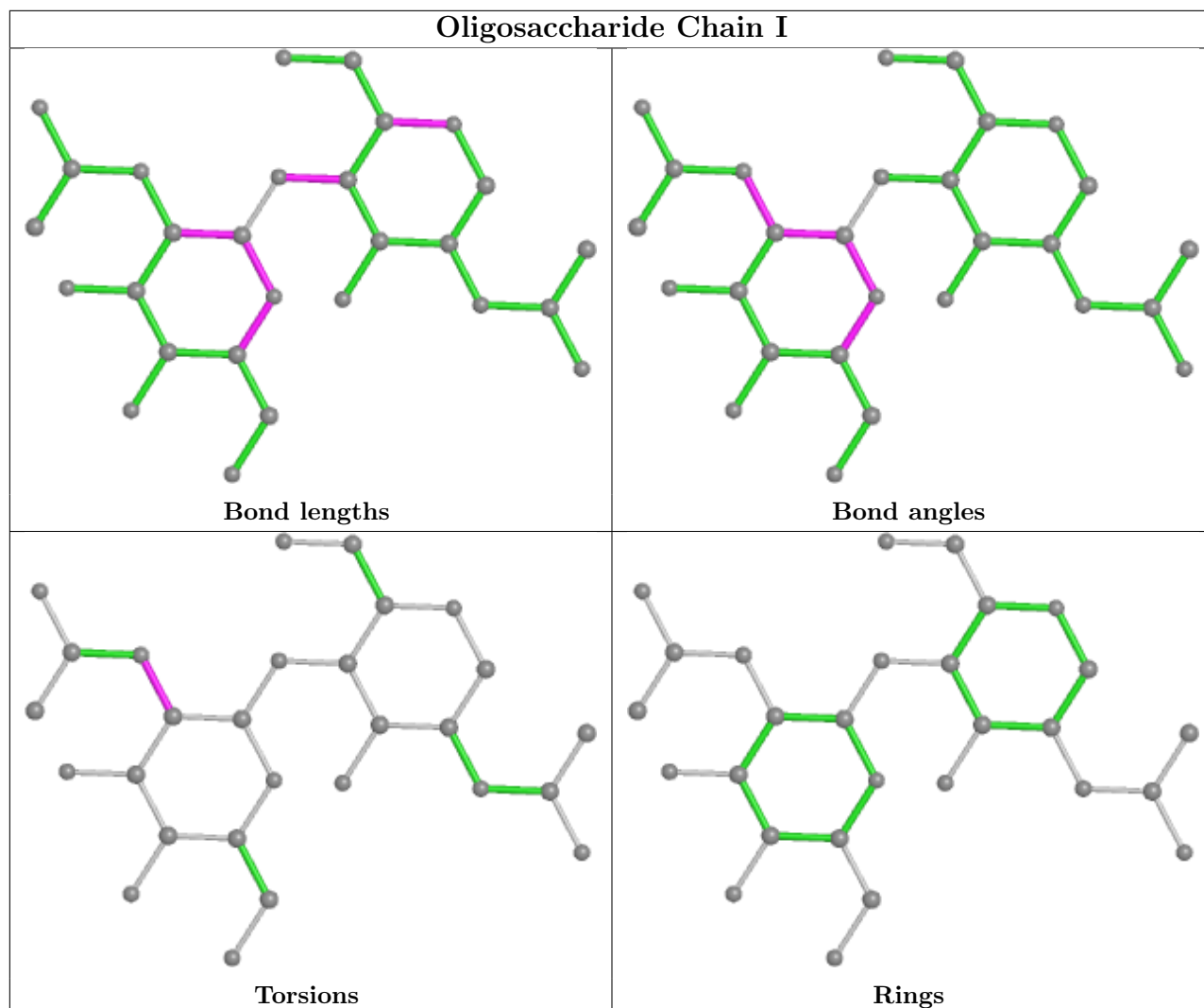
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

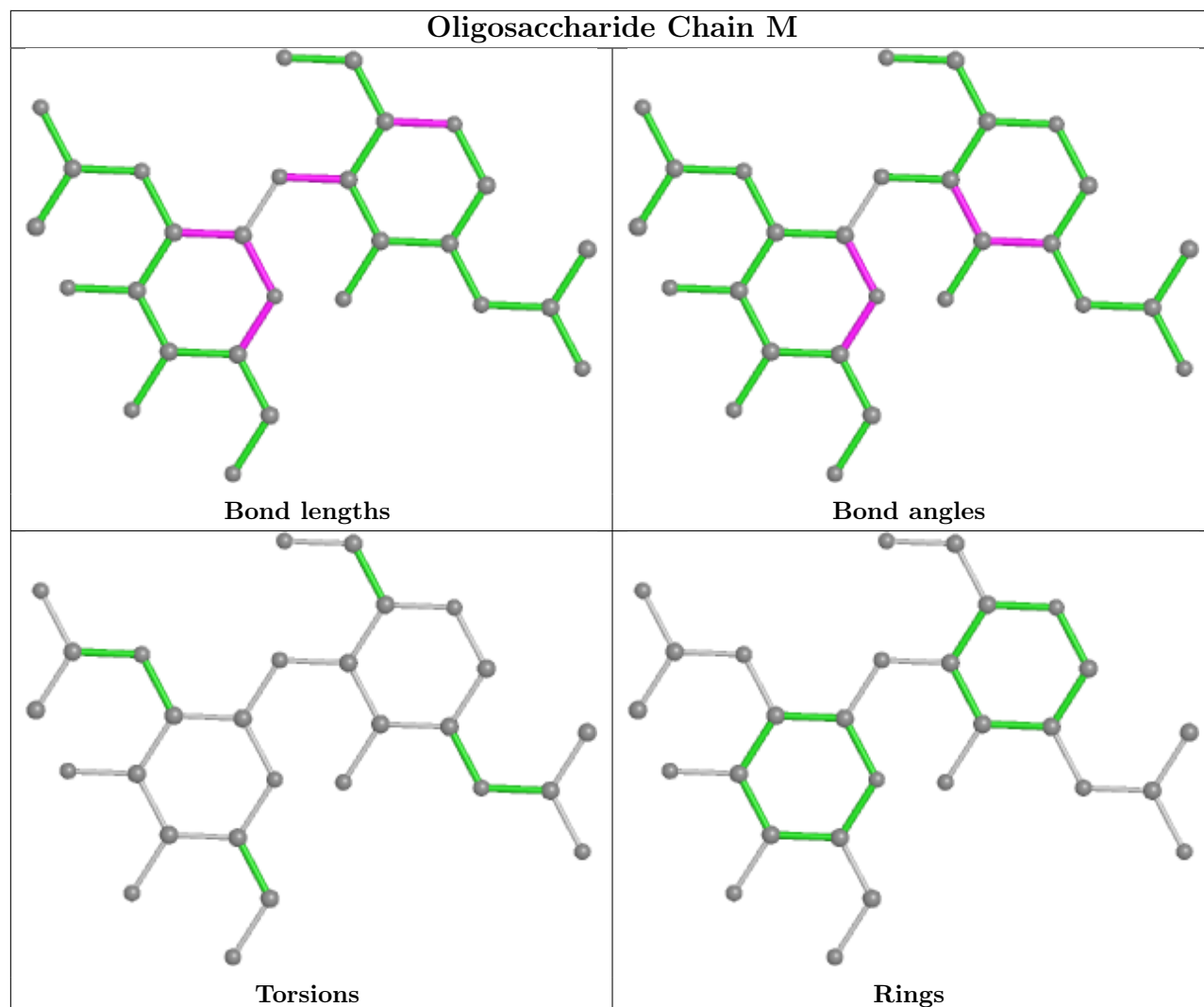


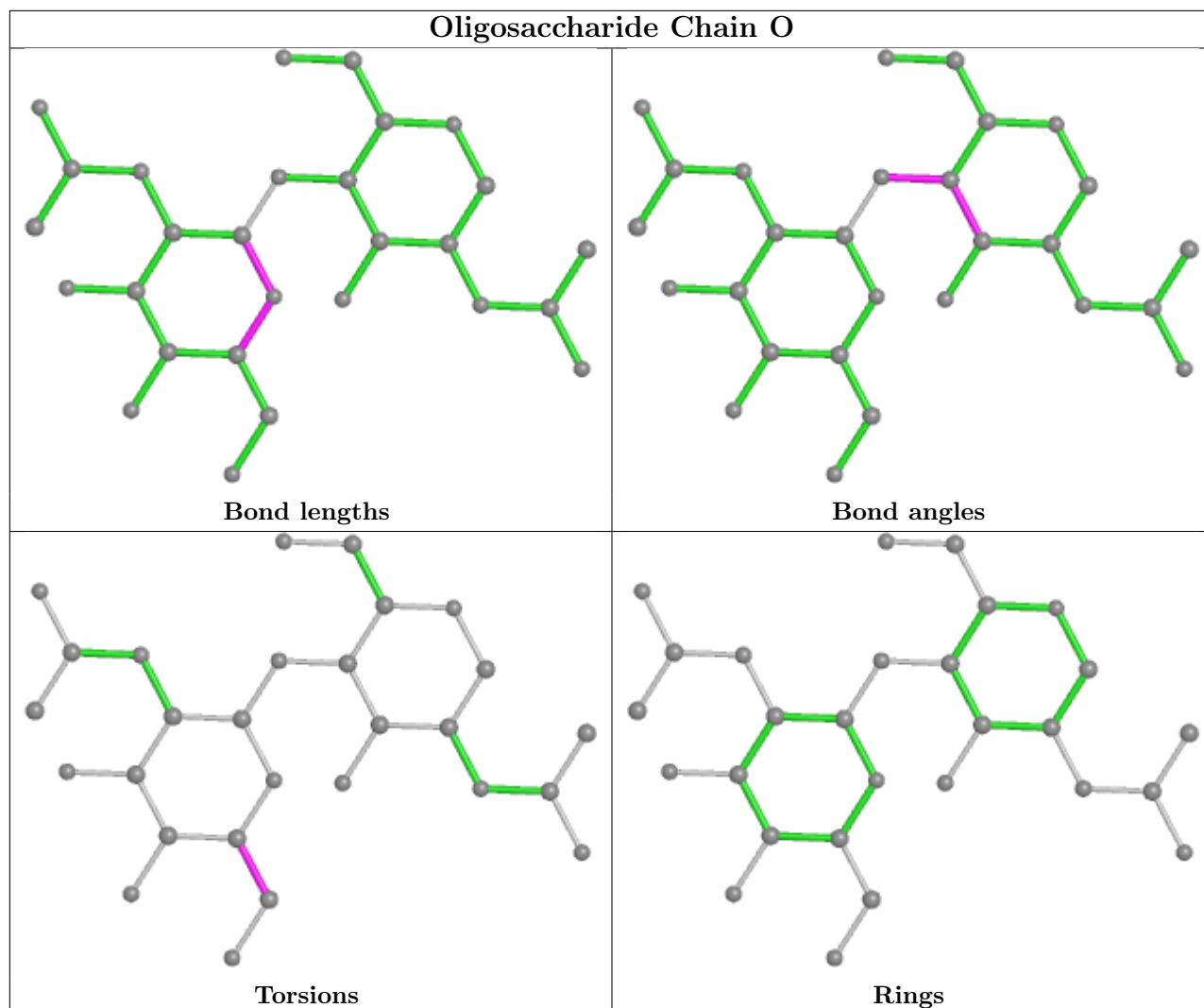


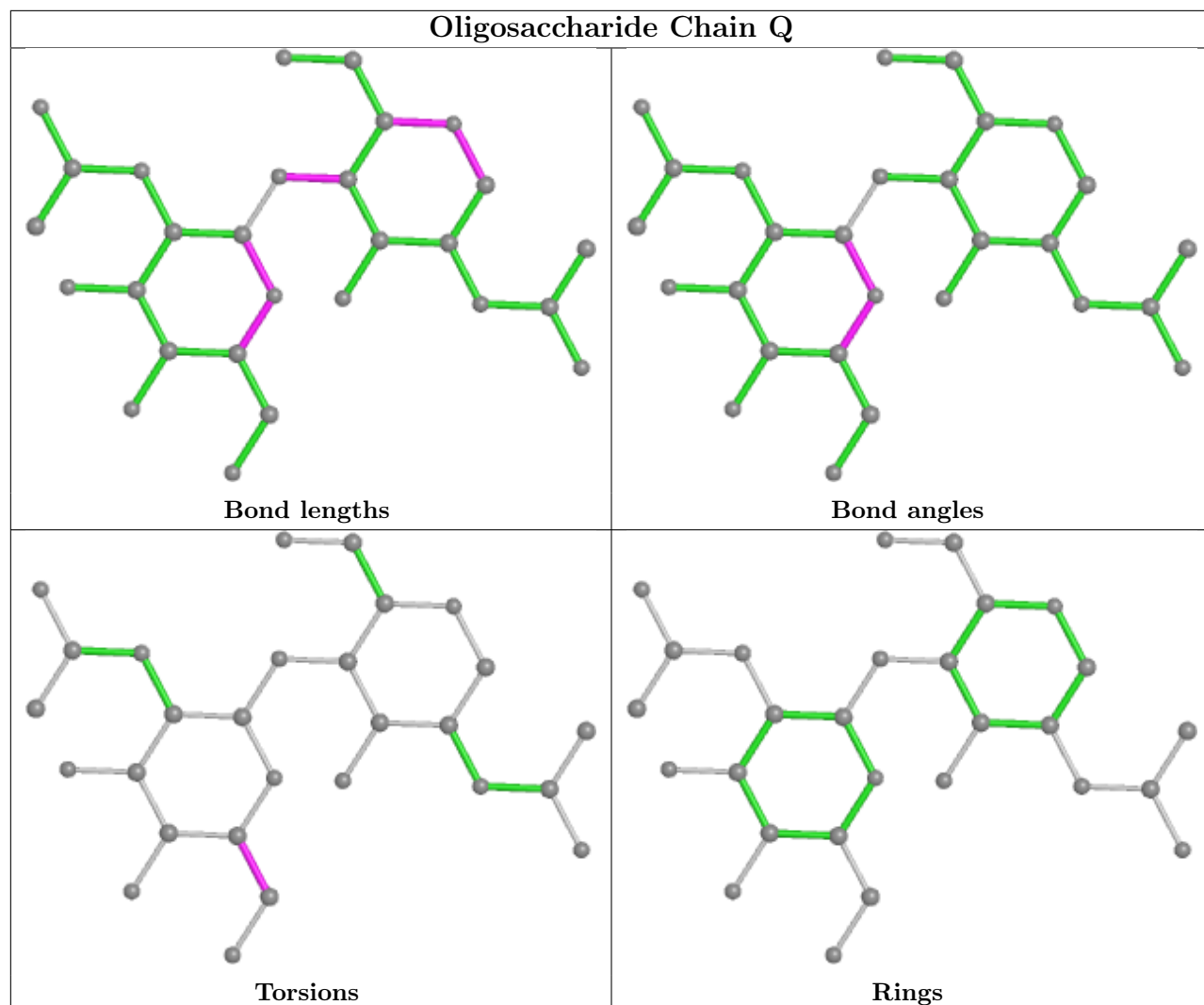


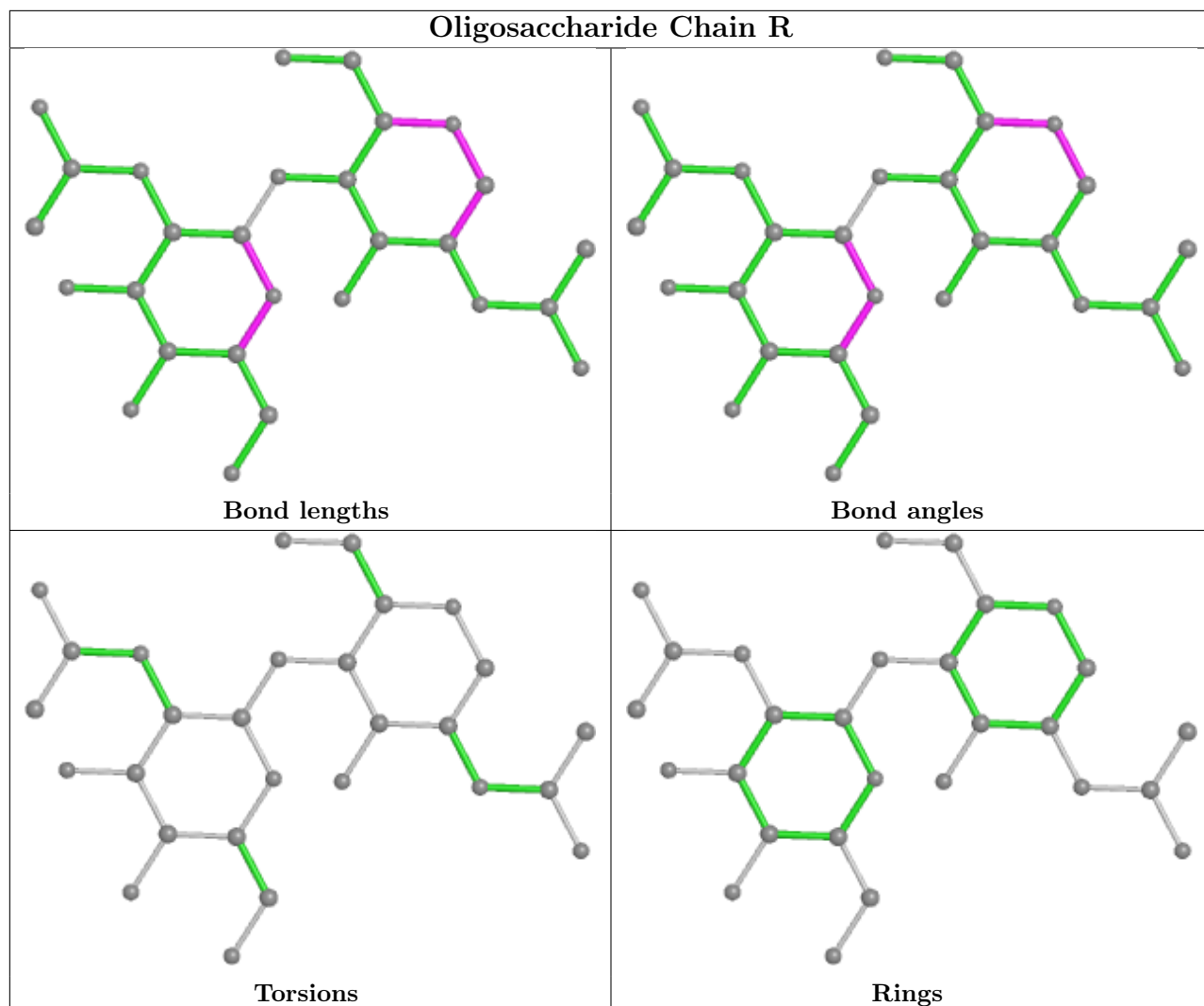


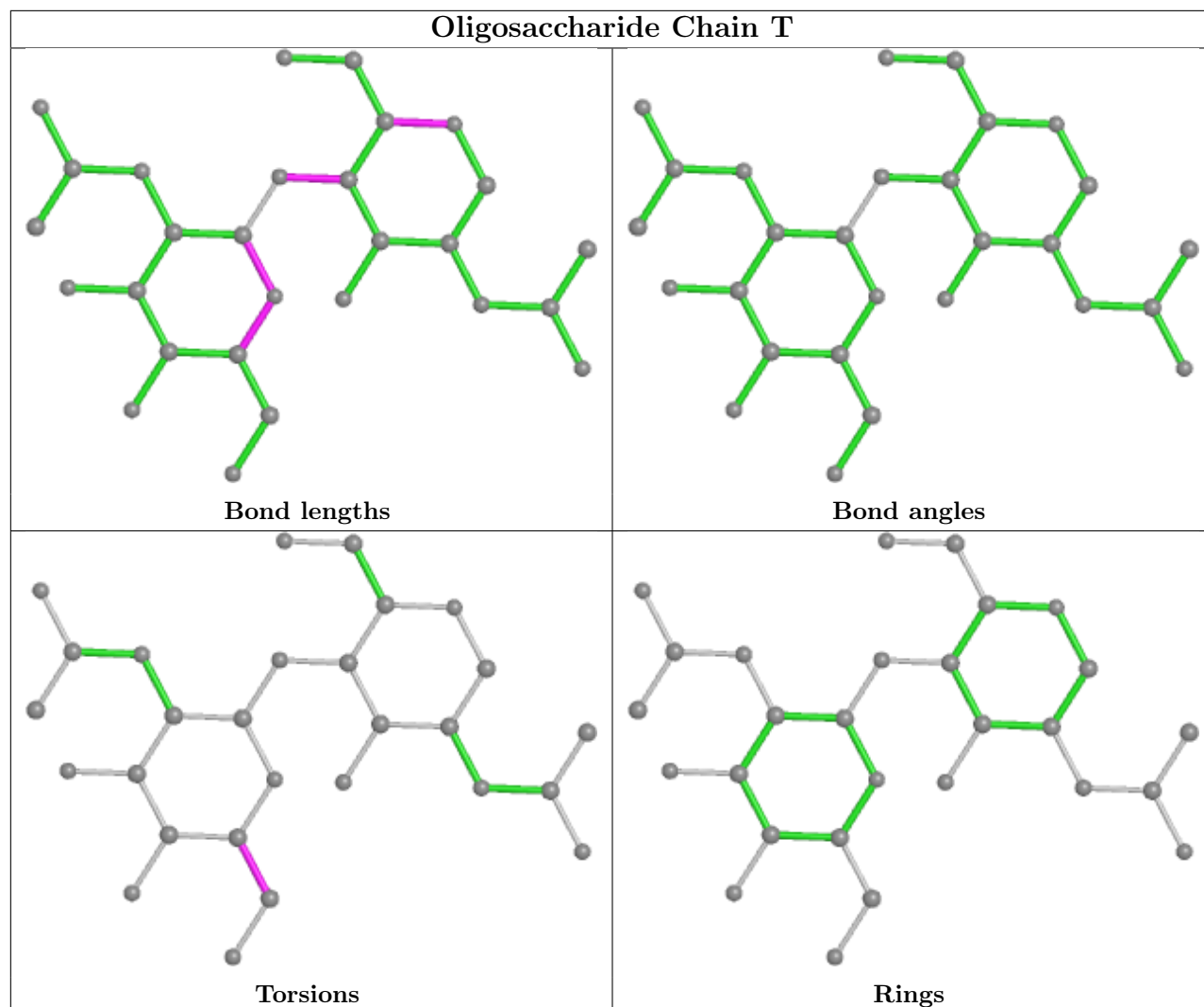


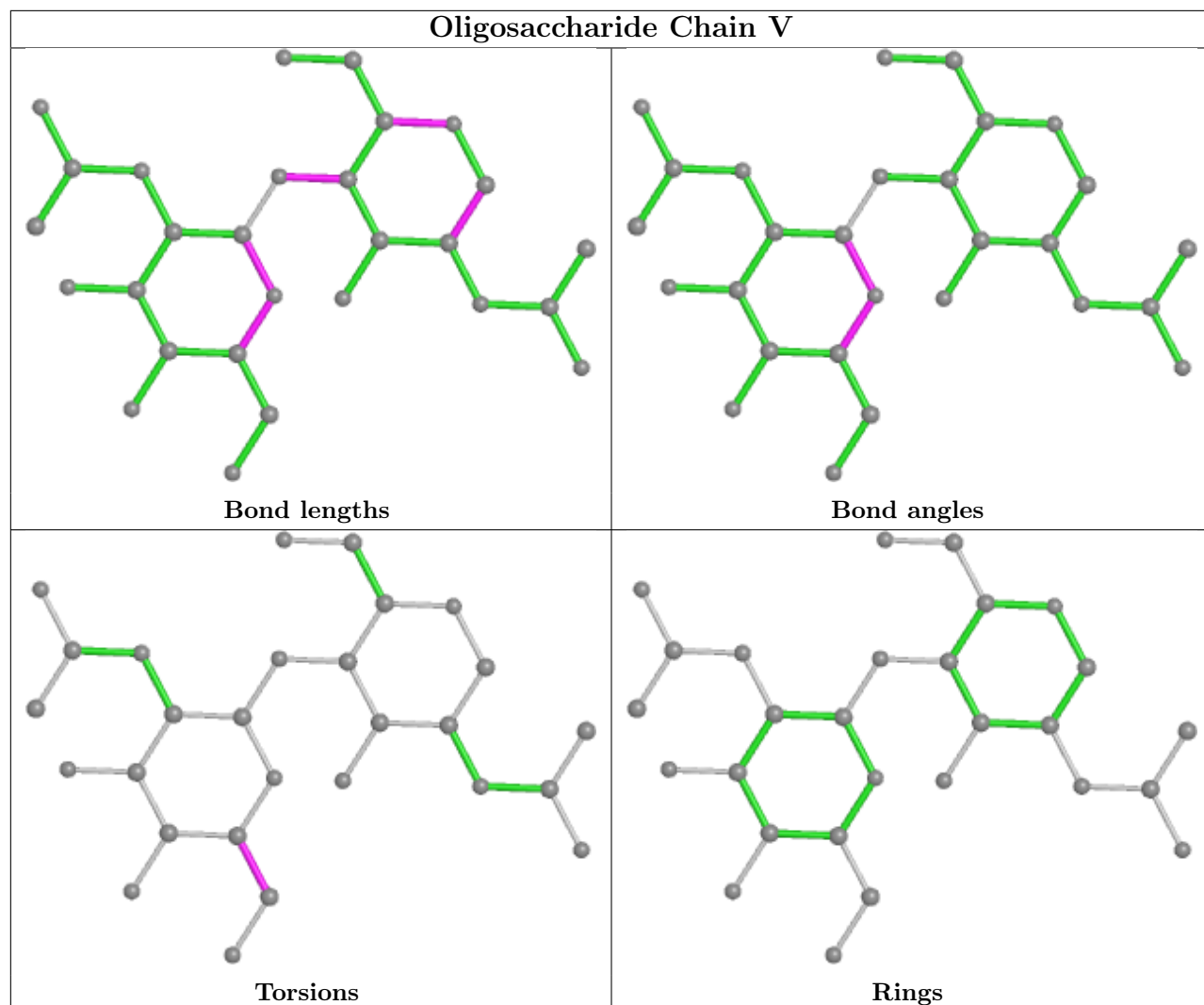


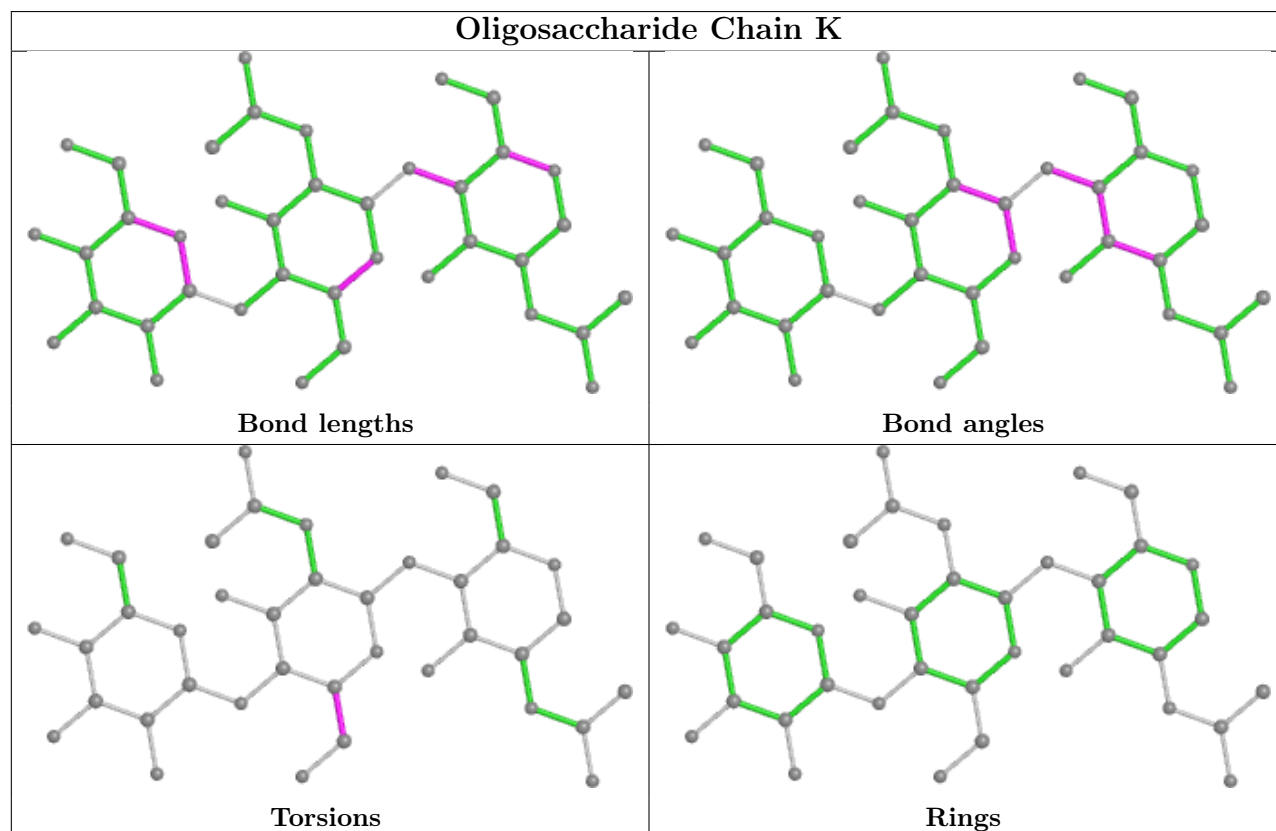
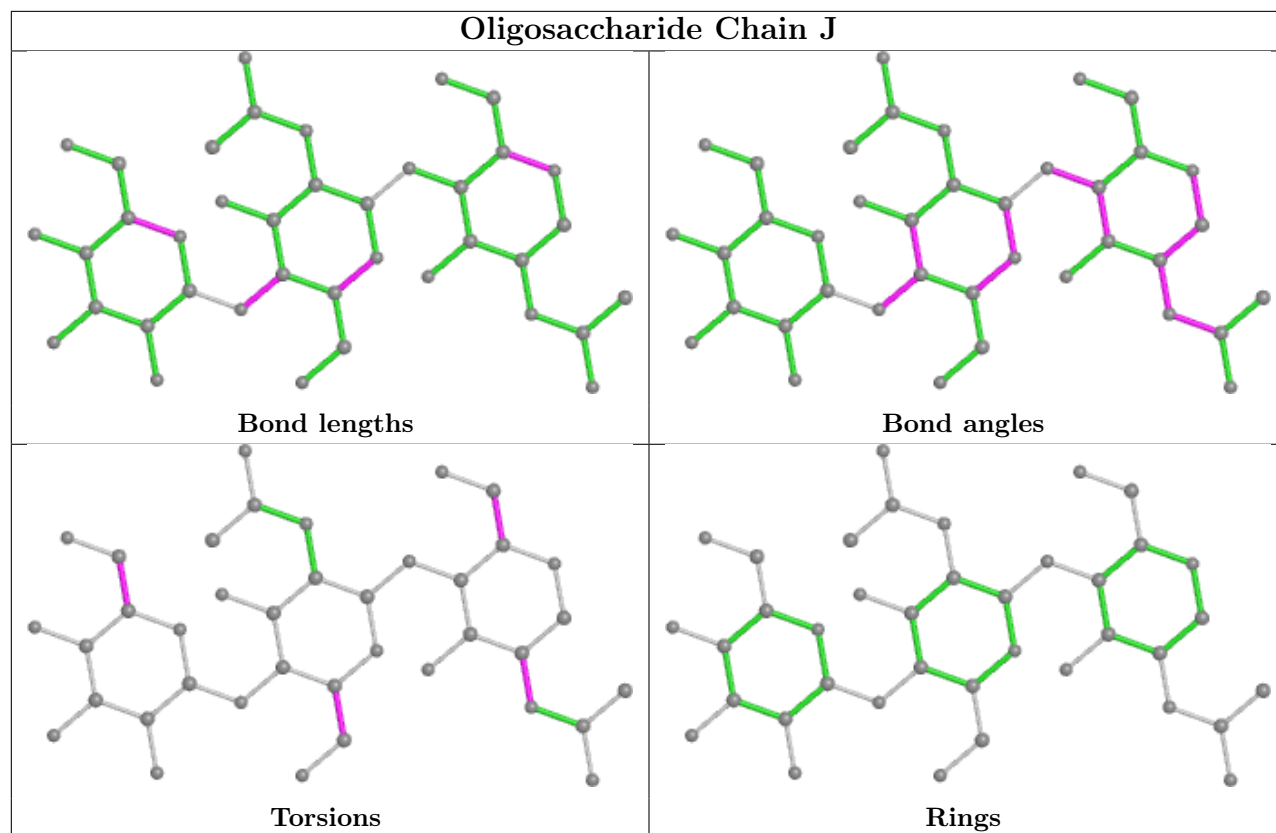


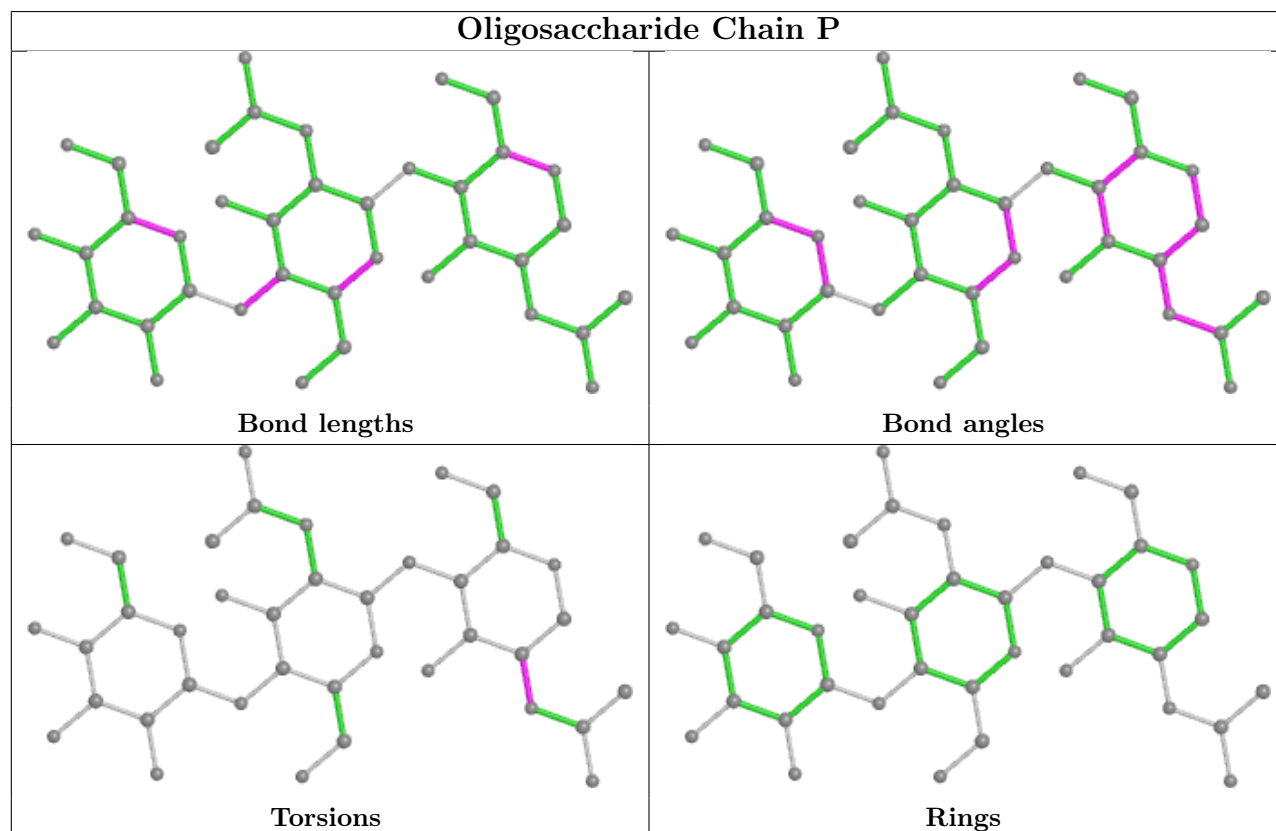
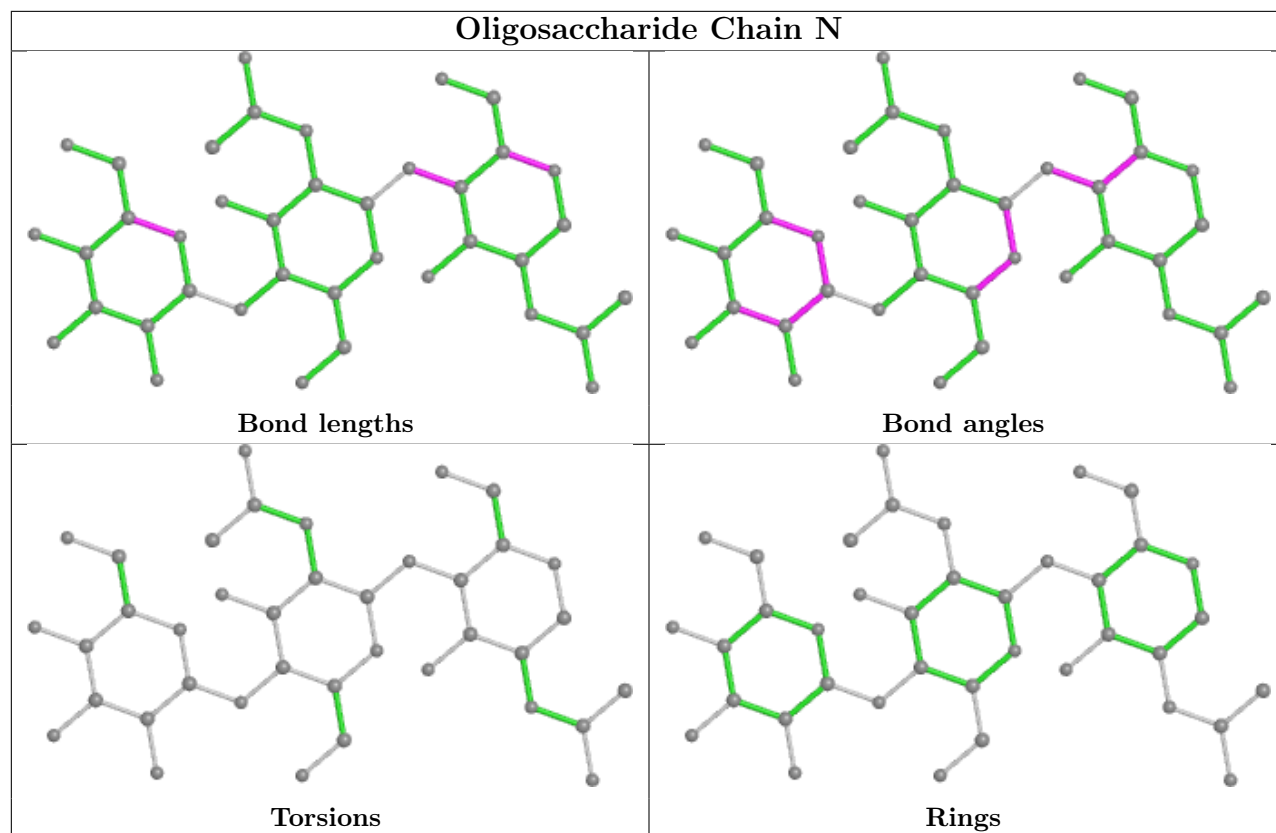


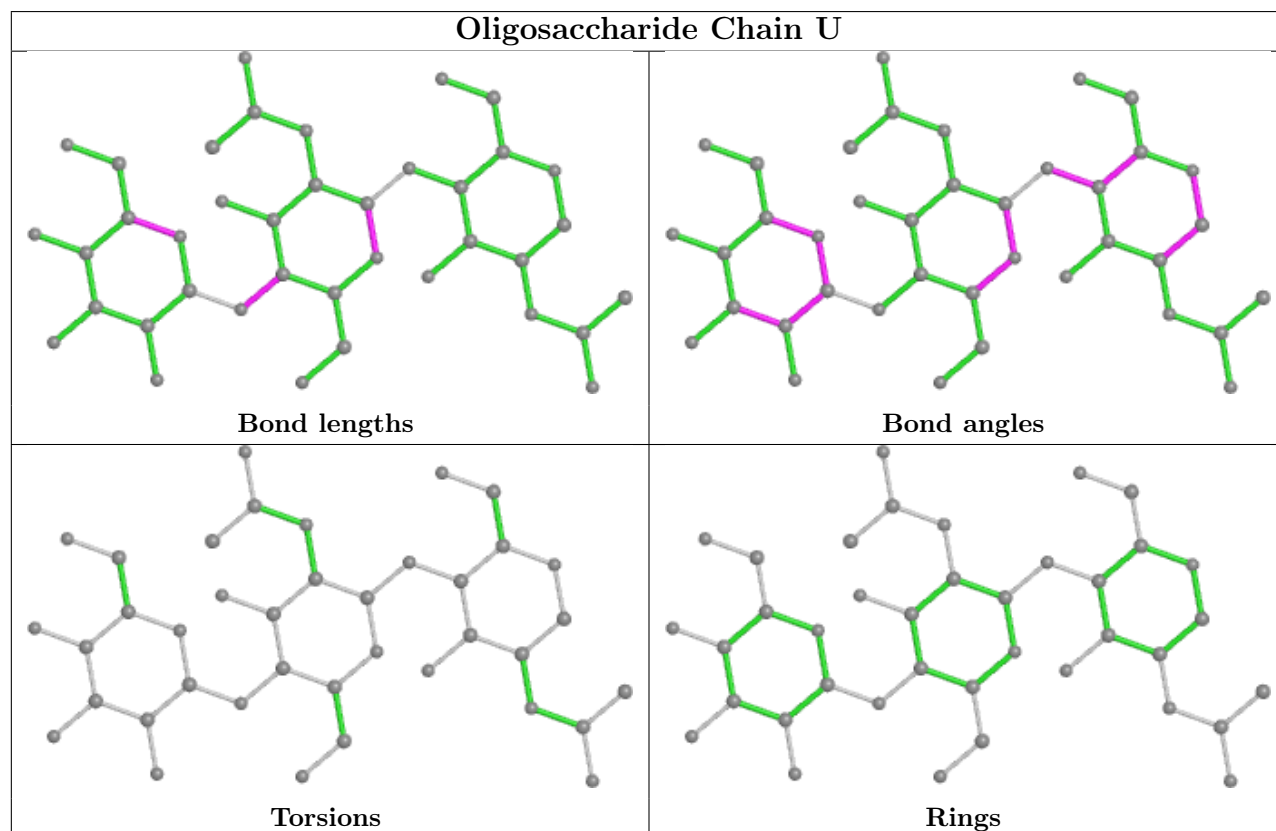
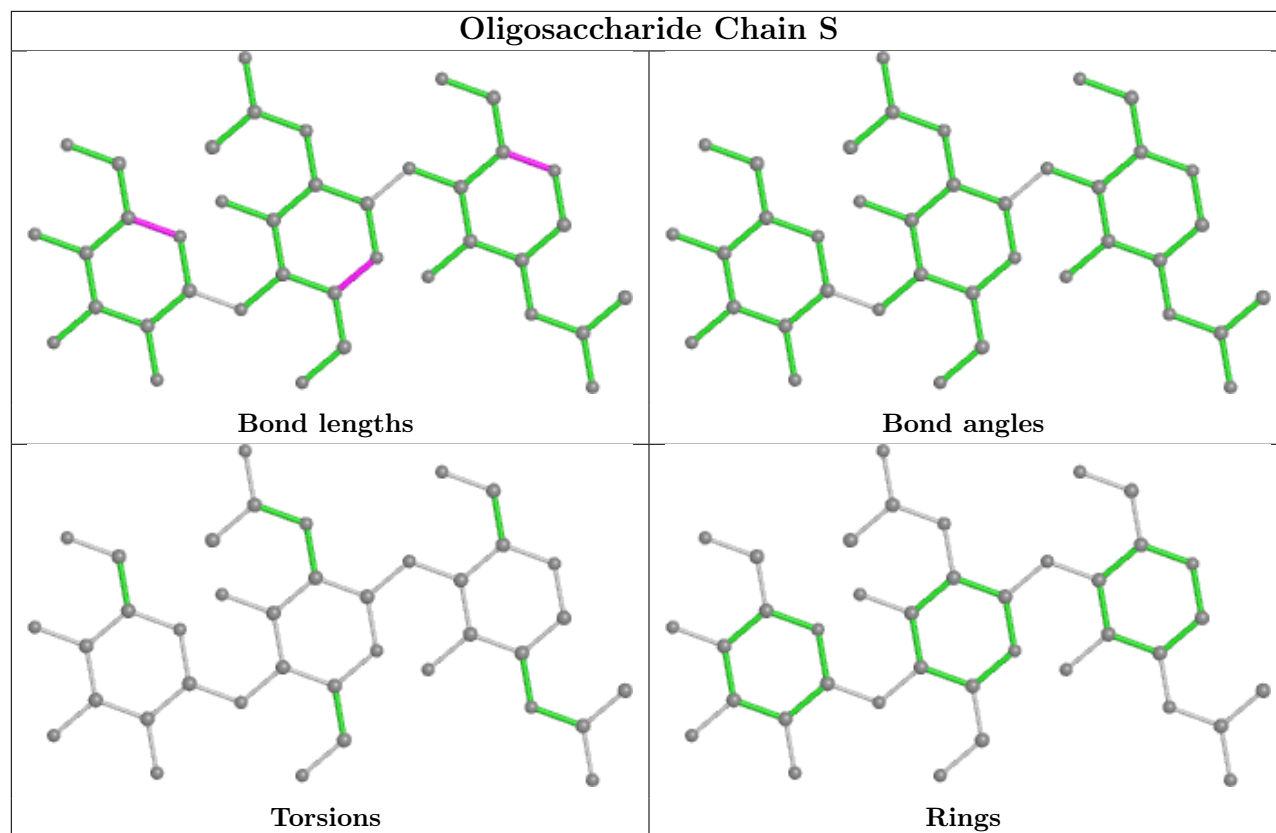












5.6 Ligand geometry [i](#)

17 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	B	1203	1	14,14,15	1.29	2 (14%)	17,19,21	0.89	0
6	NAG	A	1201	1	14,14,15	1.37	3 (21%)	17,19,21	0.89	0
6	NAG	C	1203	1	14,14,15	1.15	2 (14%)	17,19,21	1.07	1 (5%)
6	NAG	C	1202	1	14,14,15	0.99	0	17,19,21	0.88	0
6	NAG	C	1204	1	14,14,15	1.13	1 (7%)	17,19,21	0.72	0
6	NAG	A	1204	1	14,14,15	1.09	1 (7%)	17,19,21	0.87	0
6	NAG	B	1201	1	14,14,15	1.24	2 (14%)	17,19,21	0.83	0
6	NAG	B	1202	1	14,14,15	1.35	3 (21%)	17,19,21	0.91	1 (5%)
6	NAG	C	1205	1	14,14,15	1.18	1 (7%)	17,19,21	0.81	0
6	NAG	A	1202	1	14,14,15	1.19	1 (7%)	17,19,21	0.84	1 (5%)
6	NAG	C	1206	1	14,14,15	1.17	1 (7%)	17,19,21	0.62	0
6	NAG	A	1205	1	14,14,15	1.29	3 (21%)	17,19,21	1.04	1 (5%)
6	NAG	B	1205	1	14,14,15	1.03	1 (7%)	17,19,21	0.79	0
6	NAG	B	1206	1	14,14,15	1.26	3 (21%)	17,19,21	1.03	1 (5%)
6	NAG	A	1203	1	14,14,15	1.17	2 (14%)	17,19,21	0.77	0
6	NAG	C	1201	1	14,14,15	1.15	2 (14%)	17,19,21	0.86	0
6	NAG	B	1204	1	14,14,15	1.15	1 (7%)	17,19,21	0.56	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	B	1203	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1201	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1203	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1202	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1204	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1204	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1201	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1202	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1205	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1202	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1206	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1205	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1205	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1206	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1203	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1201	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1204	1	-	0/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1203	NAG	O5-C5	2.89	1.49	1.43
6	B	1202	NAG	O5-C5	2.81	1.49	1.43
6	A	1205	NAG	C1-C2	2.79	1.56	1.52
6	A	1201	NAG	O5-C5	2.77	1.49	1.43
6	A	1202	NAG	O5-C5	2.75	1.49	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1203	NAG	C1-O5-C5	3.78	117.31	112.19
6	B	1206	NAG	C1-O5-C5	3.52	116.96	112.19
6	A	1205	NAG	C1-O5-C5	3.46	116.88	112.19
6	A	1202	NAG	C1-O5-C5	2.35	115.37	112.19
6	B	1202	NAG	C1-O5-C5	2.27	115.27	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1204	NAG	O5-C5-C6-O6
6	B	1205	NAG	O5-C5-C6-O6
6	C	1205	NAG	O5-C5-C6-O6
6	B	1201	NAG	C1-C2-N2-C7
6	C	1202	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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-23246. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

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

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.