



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 03:41 AM UTC

PDB ID : 6DG8 / pdb_00006dg8
EMDB ID : EMD-7883
Title : Full-length 5-HT3A receptor in a serotonin-bound conformation- State 2
Authors : Basak, S.; Chakrapani, S.
Deposited on : 2018-05-17
Resolution : 3.89 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 : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

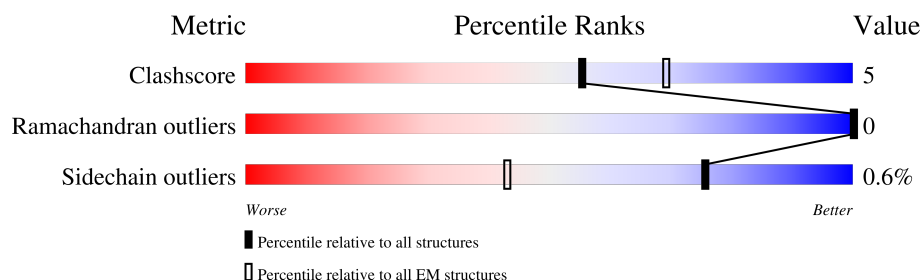
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.89 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	455	71% 15% 14%
1	B	455	72% 14% 14%
1	C	455	73% 13% 14%
1	D	455	73% 13% 14%
1	E	455	72% 14% 14%
2	F	2	100%
2	H	2	100%
2	J	2	100%
2	K	2	100%

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Mol	Chain	Length	Quality of chain
2	M	2	 100%
2	N	2	 100%
2	P	2	 50% 50%
2	Q	2	 100%
2	S	2	 50% 50%
2	T	2	 100%
3	G	3	 100%
3	I	3	 33% 67%
3	L	3	 67% 33%
3	O	3	 33% 67%
3	R	3	 67% 33%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16715 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 5-hydroxytryptamine receptor 3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	391	Total	C	N	O	S	0	0
			3235	2132	530	564	9		
1	B	391	Total	C	N	O	S	0	0
			3235	2132	530	564	9		
1	C	391	Total	C	N	O	S	0	0
			3235	2132	530	564	9		
1	D	391	Total	C	N	O	S	0	0
			3235	2132	530	564	9		
1	E	391	Total	C	N	O	S	0	0
			3235	2132	530	564	9		

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



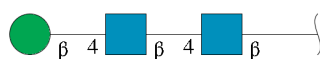
Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		

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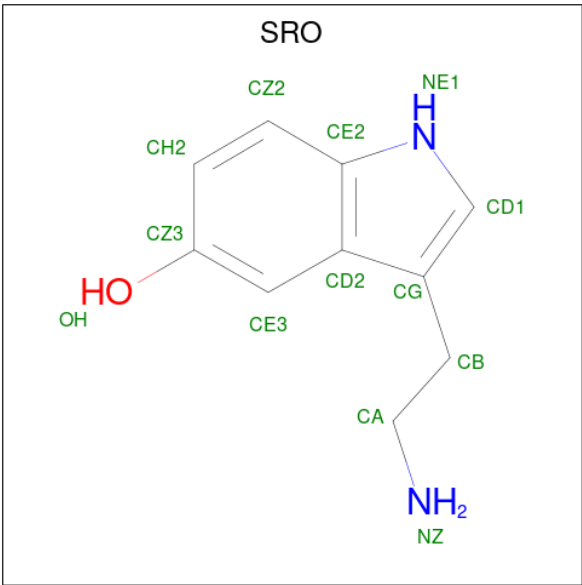
Mol	Chain	Residues	Atoms				AltConf	Trace
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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.

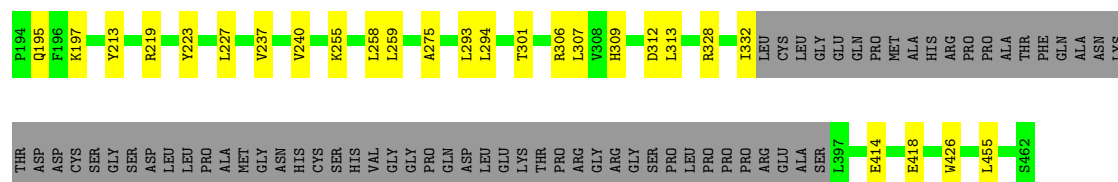


Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	L	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		
3	R	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is SEROTONIN (CCD ID: SRO) (formula: C₁₀H₁₂N₂O).

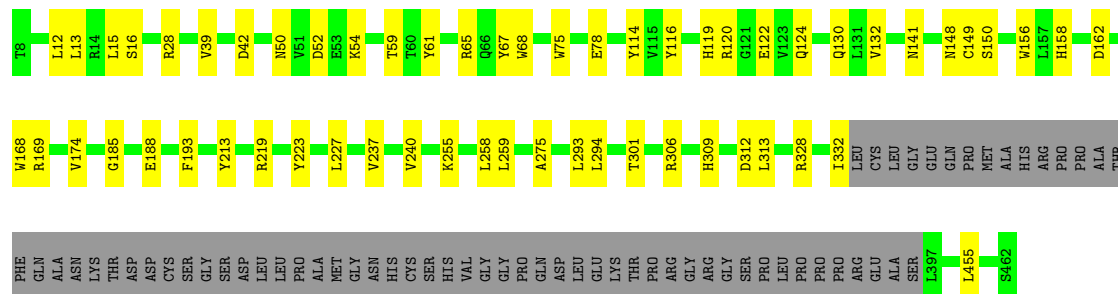


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			13	10	2	1	
4	B	1	Total	C	N	O	0
			13	10	2	1	
4	B	1	Total	C	N	O	0
			13	10	2	1	
4	D	1	Total	C	N	O	0
			13	10	2	1	
4	E	1	Total	C	N	O	0
			13	10	2	1	



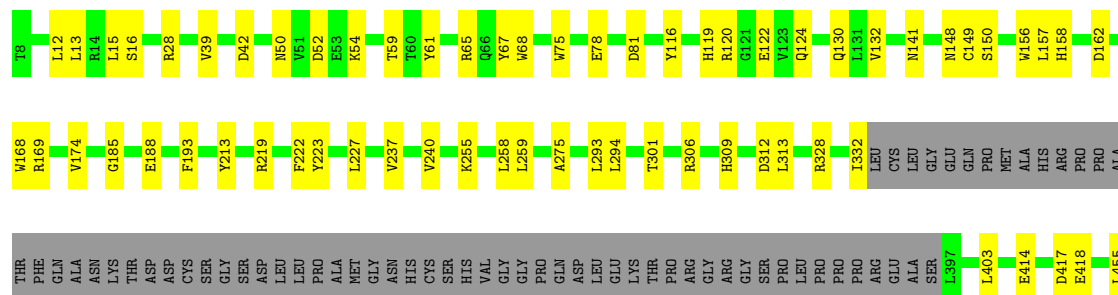
- Molecule 1: 5-hydroxytryptamine receptor 3A

Chain D: 73% 13% 14%



- Molecule 1: 5-hydroxytryptamine receptor 3A

Chain E: 72% 14% 14%



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

Chain F: 100%



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

Chain H: 100%



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

Chain J:  100%



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

Chain K:  100%



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

Chain M:  100%



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

Chain N:  100%



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

Chain P:  50% 50%



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

Chain Q:  100%

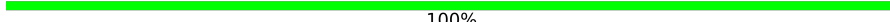


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  50% 50%

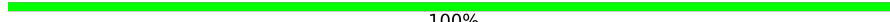


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%



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

Chain G:  100%



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

Chain I:  33% 67%



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

Chain L:  67% 33%



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

Chain O:  33% 67%



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

Chain R:  67% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18839	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (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: NAG, SRO, 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	0.23	0/3325	0.62	4/4542 (0.1%)
1	B	0.23	0/3325	0.62	4/4542 (0.1%)
1	C	0.23	0/3325	0.62	4/4542 (0.1%)
1	D	0.23	0/3325	0.62	4/4542 (0.1%)
1	E	0.23	0/3325	0.62	4/4542 (0.1%)
All	All	0.23	0/16625	0.62	20/22710 (0.1%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	78	GLU	CA-C-N	6.07	132.07	122.61
1	C	78	GLU	C-N-CA	6.07	132.07	122.61
1	A	78	GLU	CA-C-N	6.05	132.05	122.61
1	A	78	GLU	C-N-CA	6.05	132.05	122.61
1	D	78	GLU	CA-C-N	6.05	132.05	122.61

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	3235	0	3264	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3235	0	3263	35	0
1	C	3235	0	3264	31	0
1	D	3235	0	3263	32	0
1	E	3235	0	3264	38	0
2	F	28	0	25	0	0
2	H	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
3	G	39	0	34	0	0
3	I	39	0	34	0	0
3	L	39	0	34	0	0
3	O	39	0	34	0	0
3	R	39	0	34	0	0
4	A	13	0	12	0	0
4	B	26	0	24	0	0
4	D	13	0	12	1	0
4	E	13	0	12	1	0
All	All	16715	0	16798	167	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 5.

The worst 5 of 167 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:C:306:ARG:NH1	1:C:312:ASP:OD2	1.92	1.03
1:D:306:ARG:NH1	1:D:312:ASP:OD2	1.92	1.03
1:E:306:ARG:NH1	1:E:312:ASP:OD2	1.92	1.02
1:A:306:ARG:NH1	1:A:312:ASP:OD2	1.92	1.02
1:B:306:ARG:NH1	1:B:312:ASP:OD2	1.92	1.01

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	387/455 (85%)	370 (96%)	17 (4%)	0	100	100
1	B	387/455 (85%)	370 (96%)	17 (4%)	0	100	100
1	C	387/455 (85%)	370 (96%)	17 (4%)	0	100	100
1	D	387/455 (85%)	370 (96%)	17 (4%)	0	100	100
1	E	387/455 (85%)	370 (96%)	17 (4%)	0	100	100
All	All	1935/2275 (85%)	1850 (96%)	85 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	362/417 (87%)	360 (99%)	2 (1%)	78	80
1	B	362/417 (87%)	360 (99%)	2 (1%)	78	80
1	C	362/417 (87%)	360 (99%)	2 (1%)	78	80
1	D	362/417 (87%)	360 (99%)	2 (1%)	78	80
1	E	362/417 (87%)	360 (99%)	2 (1%)	78	80
All	All	1810/2085 (87%)	1800 (99%)	10 (1%)	76	80

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	293	LEU
1	E	132	VAL
1	E	293	LEU
1	B	293	LEU
1	C	132	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	74	GLN
1	D	309	HIS
1	D	164	ASN
1	D	411	HIS
1	B	309	HIS

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](#)

35 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	F	1	2	14,14,15	0.27	0	17,19,21	0.56	0
2	NAG	F	2	2	14,14,15	0.34	0	17,19,21	0.52	0
3	NAG	G	1	3	14,14,15	0.27	0	17,19,21	0.50	0
3	NAG	G	2	3	14,14,15	0.34	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	G	3	3	11,11,12	0.80	0	15,15,17	0.76	0
2	NAG	H	1	2	14,14,15	0.33	0	17,19,21	0.57	0
2	NAG	H	2	2	14,14,15	0.39	0	17,19,21	0.51	0
3	NAG	I	1	3,1	14,14,15	1.17	1 (7%)	17,19,21	2.27	2 (11%)
3	NAG	I	2	3	14,14,15	0.26	0	17,19,21	0.56	0
3	BMA	I	3	3	11,11,12	0.73	0	15,15,17	0.97	1 (6%)
2	NAG	J	1	2	14,14,15	0.21	0	17,19,21	0.53	0
2	NAG	J	2	2	14,14,15	0.36	0	17,19,21	0.55	0
2	NAG	K	1	2	14,14,15	0.42	0	17,19,21	0.53	0
2	NAG	K	2	2	14,14,15	0.38	0	17,19,21	0.56	0
3	NAG	L	1	3	14,14,15	0.21	0	17,19,21	0.51	0
3	NAG	L	2	3	14,14,15	0.36	0	17,19,21	0.72	1 (5%)
3	BMA	L	3	3	11,11,12	0.84	0	15,15,17	0.72	0
2	NAG	M	1	2	14,14,15	0.22	0	17,19,21	0.51	0
2	NAG	M	2	2	14,14,15	0.35	0	17,19,21	0.56	0
2	NAG	N	1	2	14,14,15	0.39	0	17,19,21	0.59	0
2	NAG	N	2	2	14,14,15	0.37	0	17,19,21	0.47	0
3	NAG	O	1	3	14,14,15	0.21	0	17,19,21	0.54	0
3	NAG	O	2	3	14,14,15	0.31	0	17,19,21	0.62	1 (5%)
3	BMA	O	3	3	11,11,12	1.46	2 (18%)	15,15,17	1.80	4 (26%)
2	NAG	P	1	2,1	14,14,15	0.97	1 (7%)	17,19,21	0.83	1 (5%)
2	NAG	P	2	2	14,14,15	0.61	0	17,19,21	0.47	0
2	NAG	Q	1	2	14,14,15	0.47	0	17,19,21	0.57	0
2	NAG	Q	2	2	14,14,15	0.40	0	17,19,21	0.40	0
3	NAG	R	1	3	14,14,15	0.40	0	17,19,21	0.75	0
3	NAG	R	2	3	14,14,15	0.27	0	17,19,21	0.57	0
3	BMA	R	3	3	11,11,12	0.76	0	15,15,17	0.91	1 (6%)
2	NAG	S	1	2	14,14,15	0.20	0	17,19,21	0.51	0
2	NAG	S	2	2	14,14,15	1.26	1 (7%)	17,19,21	1.47	1 (5%)
2	NAG	T	1	2	14,14,15	0.29	0	17,19,21	0.53	0
2	NAG	T	2	2	14,14,15	0.37	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
2	NAG	F	1	2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
2	NAG	J	1	2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	3/6/23/26	0/1/1/1
2	NAG	K	1	2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	3/6/23/26	0/1/1/1
3	NAG	L	1	3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
2	NAG	M	1	2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	3/6/23/26	0/1/1/1
2	NAG	N	1	2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	BMA	O	3	3	-	0/2/19/22	0/1/1/1
2	NAG	P	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	BMA	R	3	3	-	0/2/19/22	0/1/1/1
2	NAG	S	1	2	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	NAG	T	1	2	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	2	NAG	O5-C1	4.45	1.51	1.43
3	I	1	NAG	C1-C2	3.89	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	3	BMA	C2-C3	3.11	1.57	1.52
2	P	1	NAG	C1-C2	3.02	1.56	1.52
3	O	3	BMA	C1-C2	2.97	1.59	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	NAG	C2-N2-C7	7.76	133.29	122.90
2	S	2	NAG	C1-O5-C5	5.88	120.07	112.19
3	I	1	NAG	C1-C2-N2	4.17	117.00	110.43
3	O	3	BMA	C1-O5-C5	4.13	117.72	112.19
3	O	3	BMA	C1-C2-C3	3.33	114.49	109.64

There are no chirality outliers.

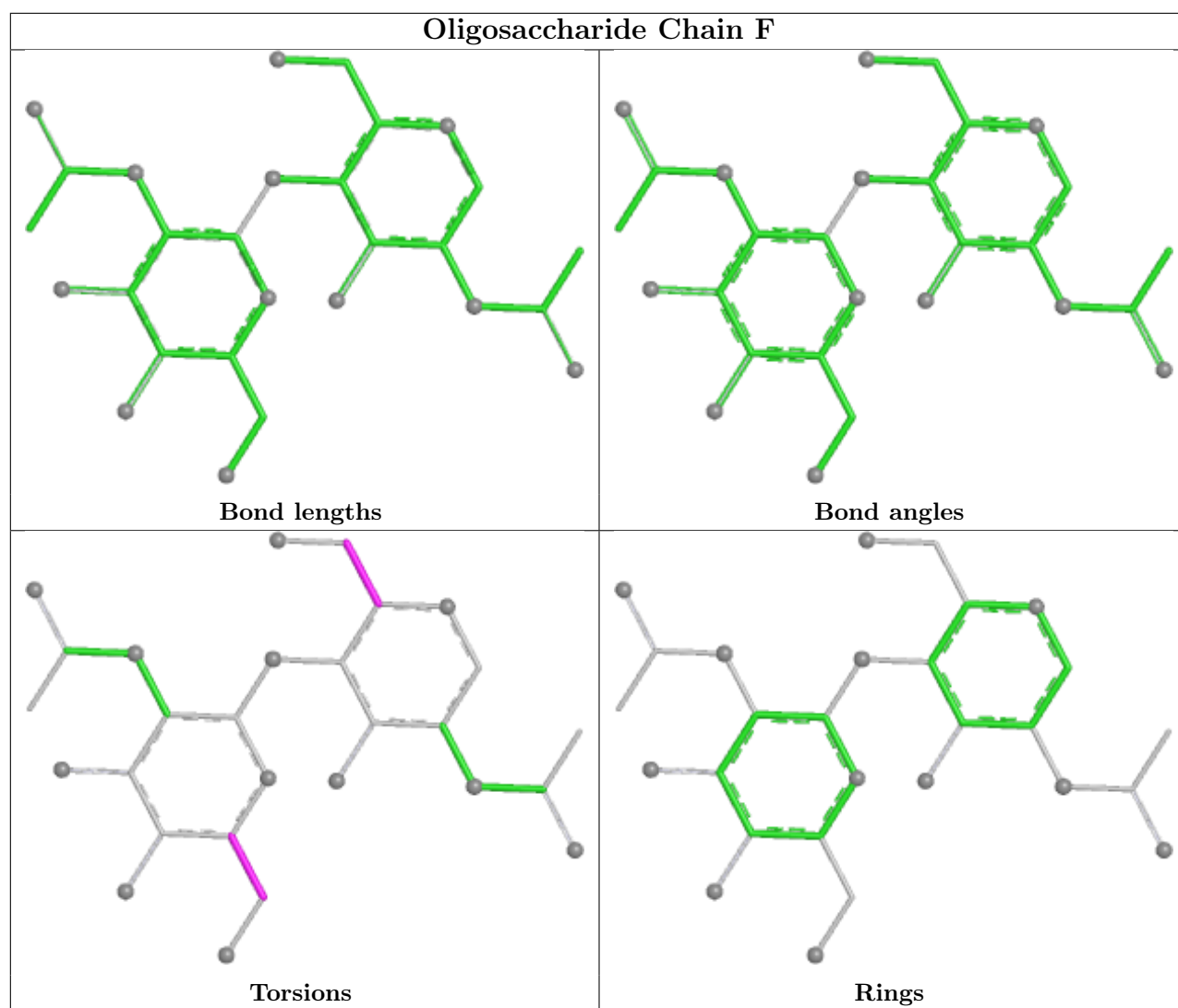
5 of 38 torsion outliers are listed below:

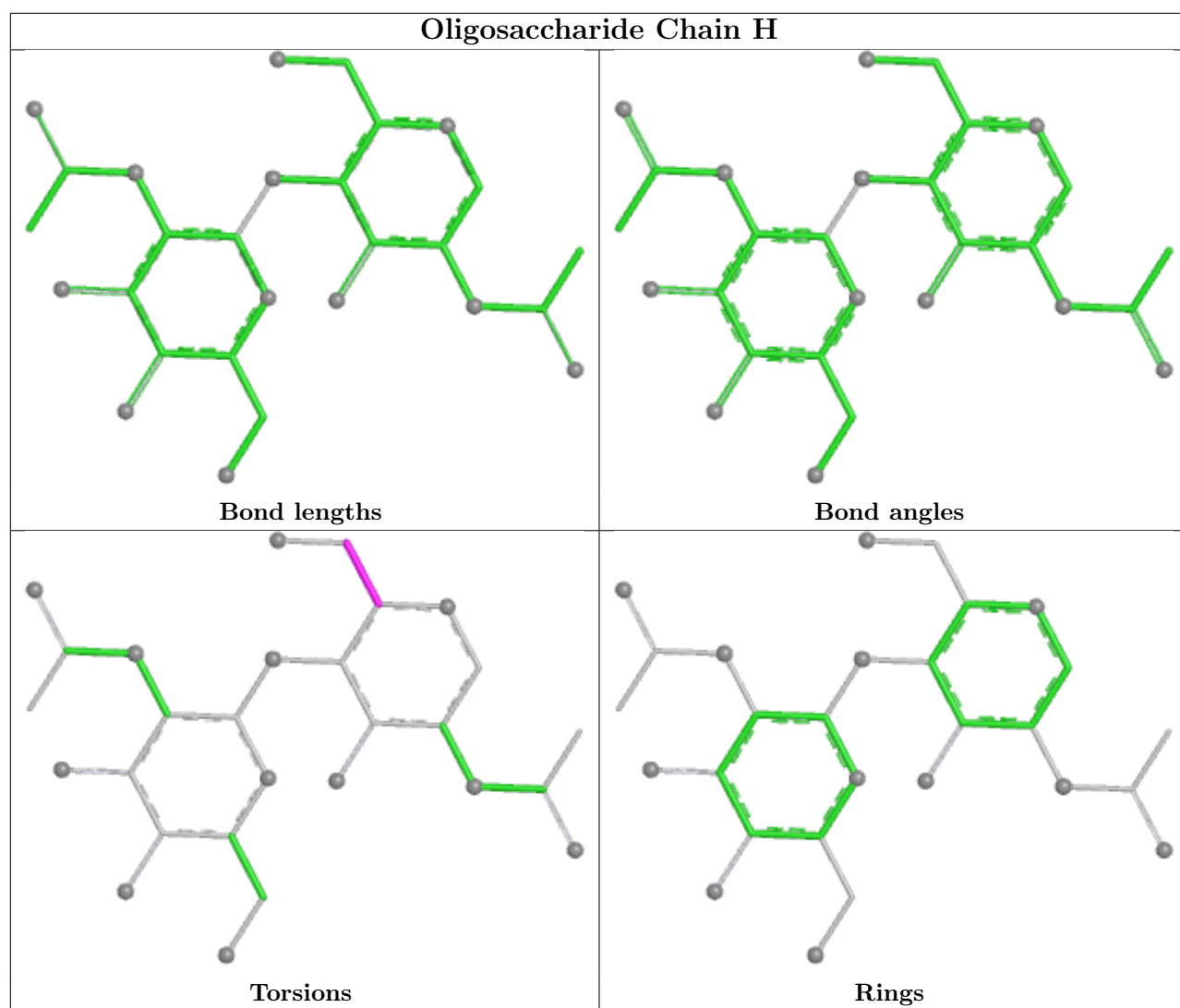
Mol	Chain	Res	Type	Atoms
2	P	2	NAG	C4-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6

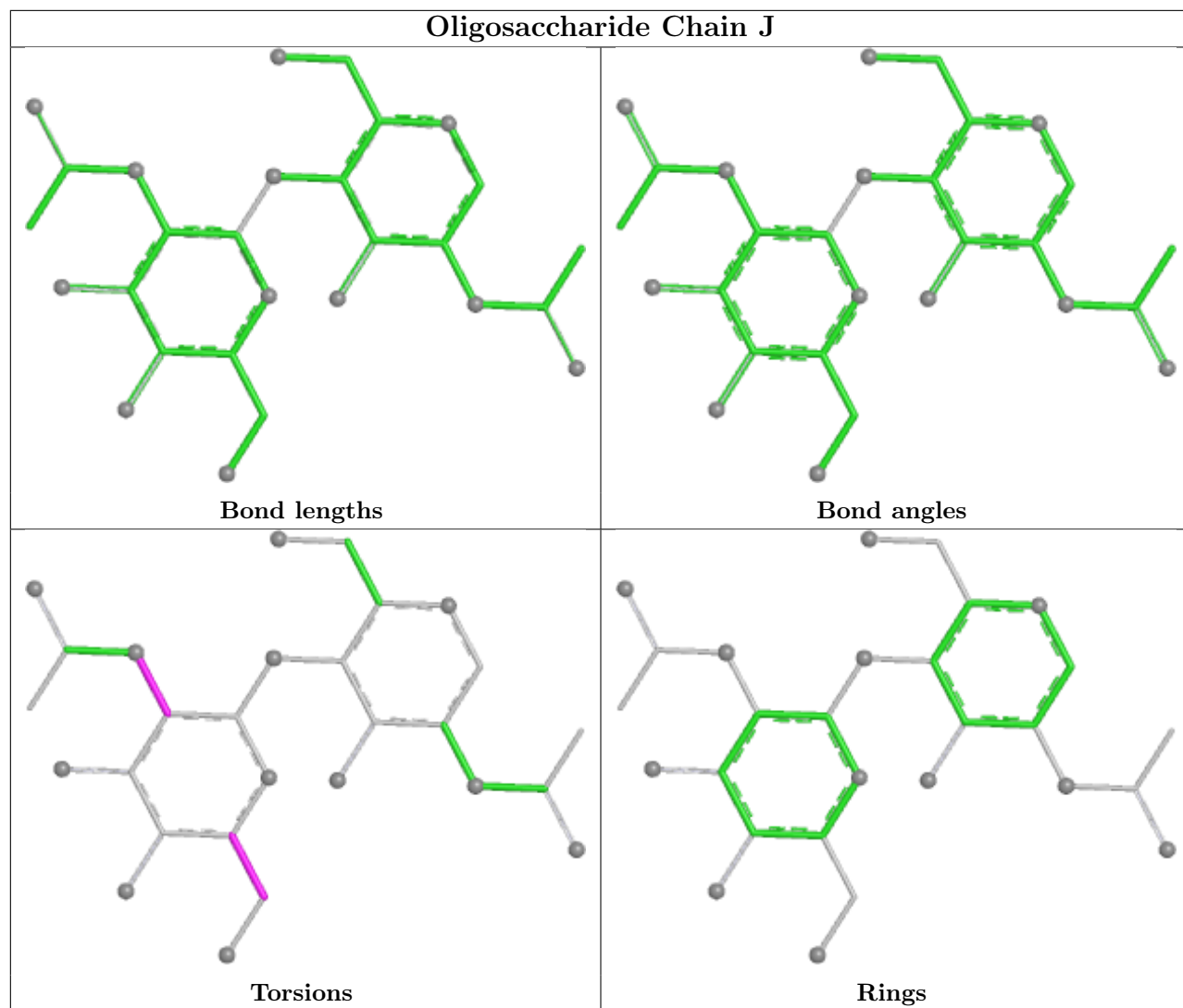
There are no ring outliers.

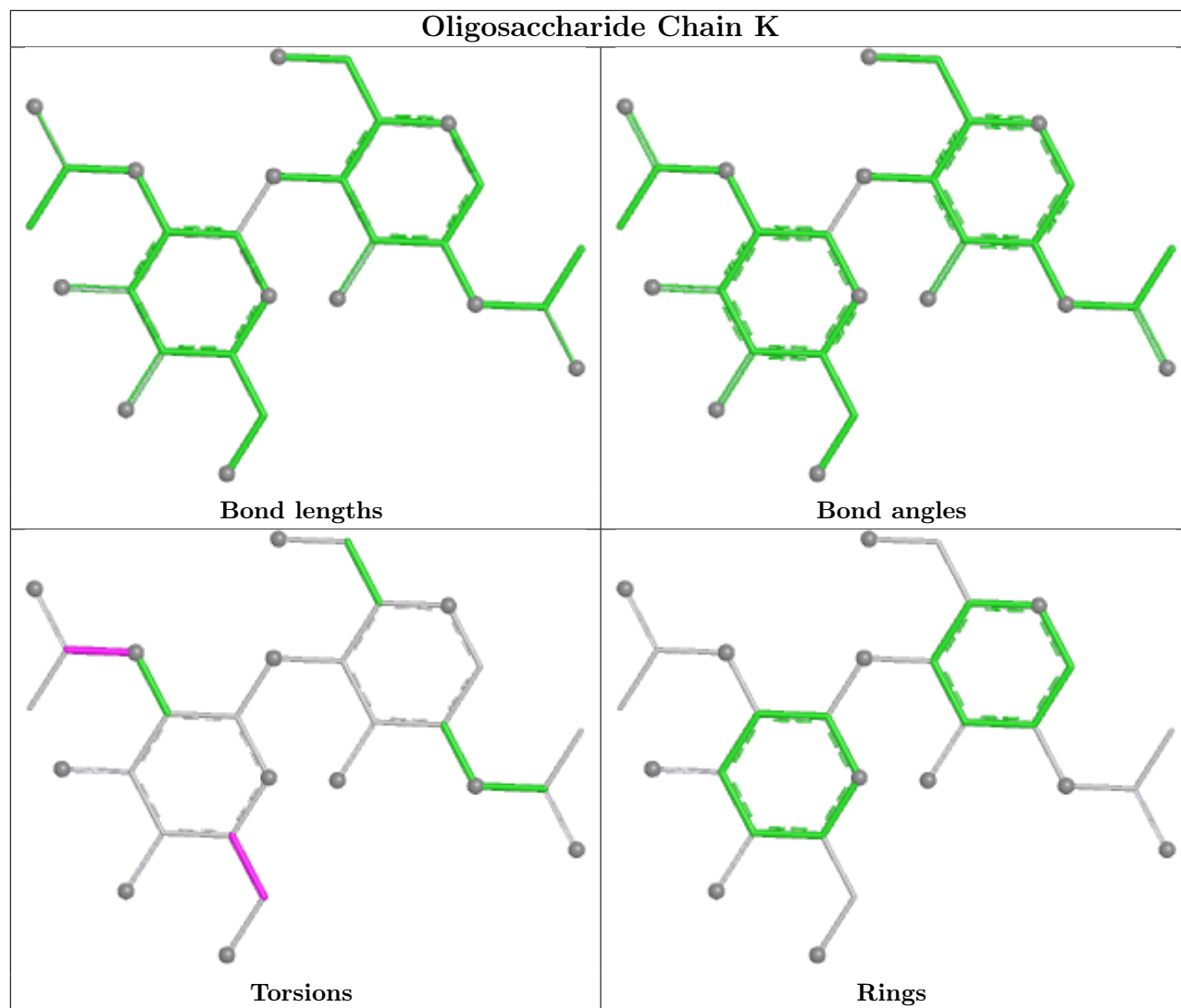
No monomer is involved in short contacts.

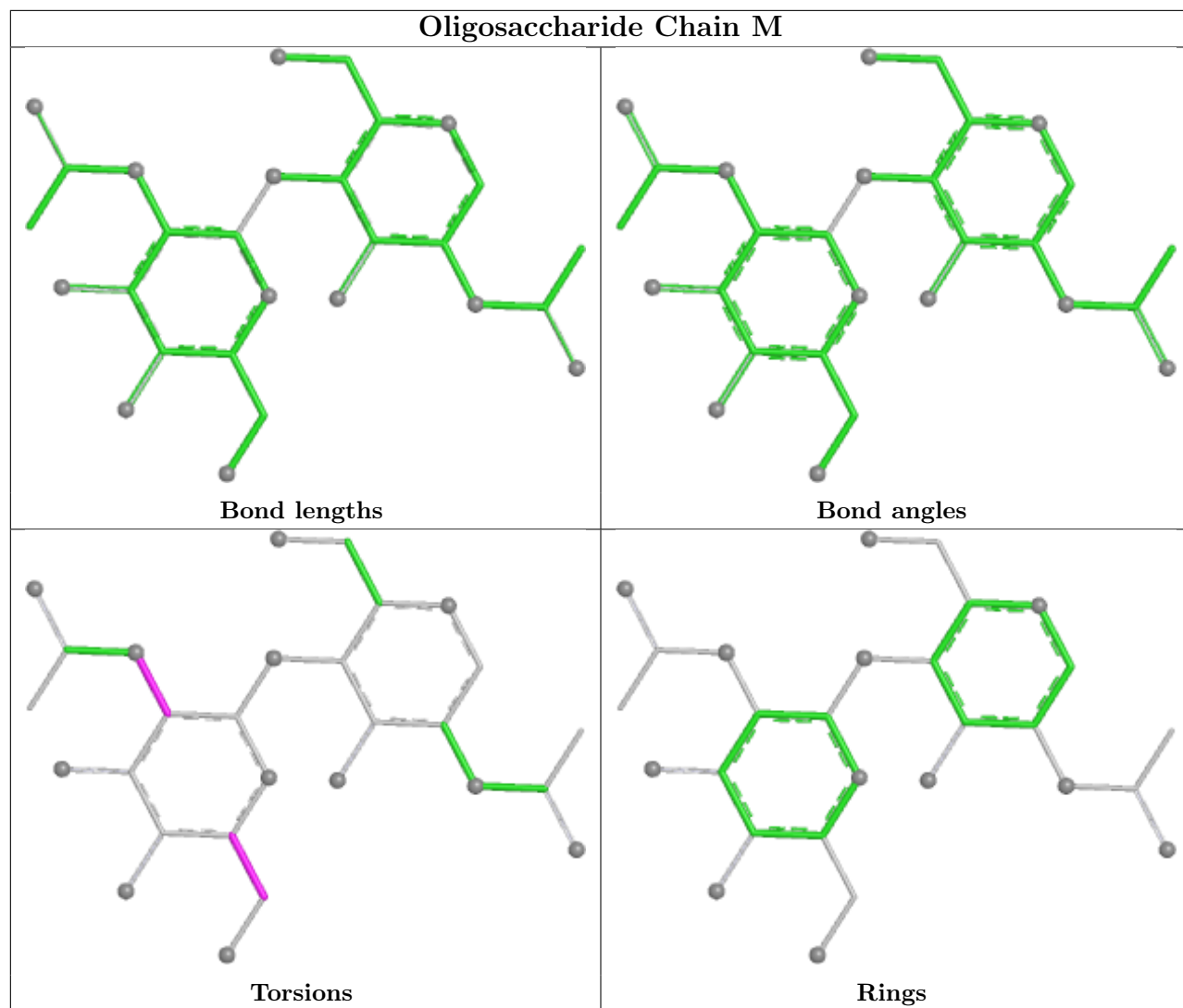
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

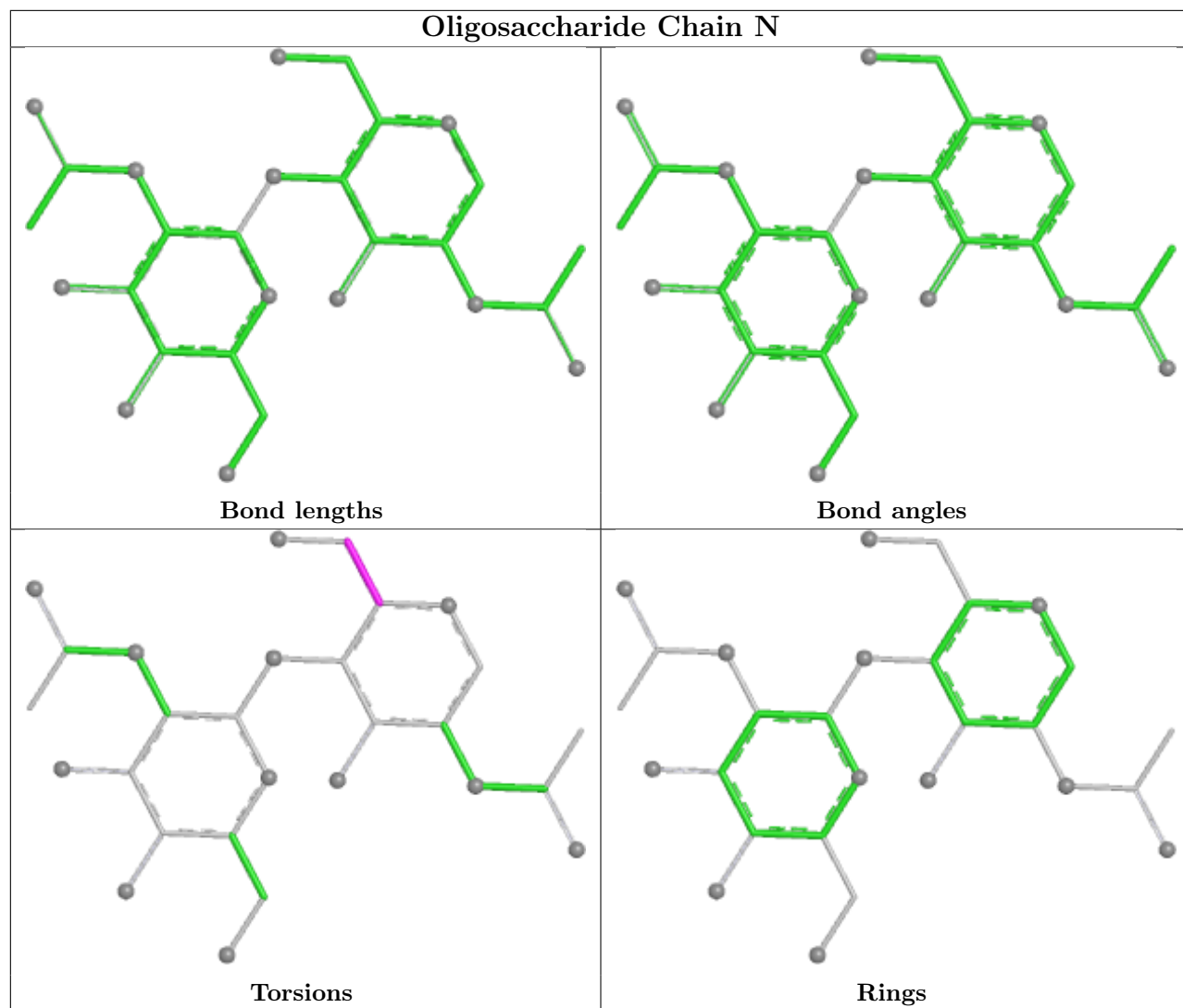


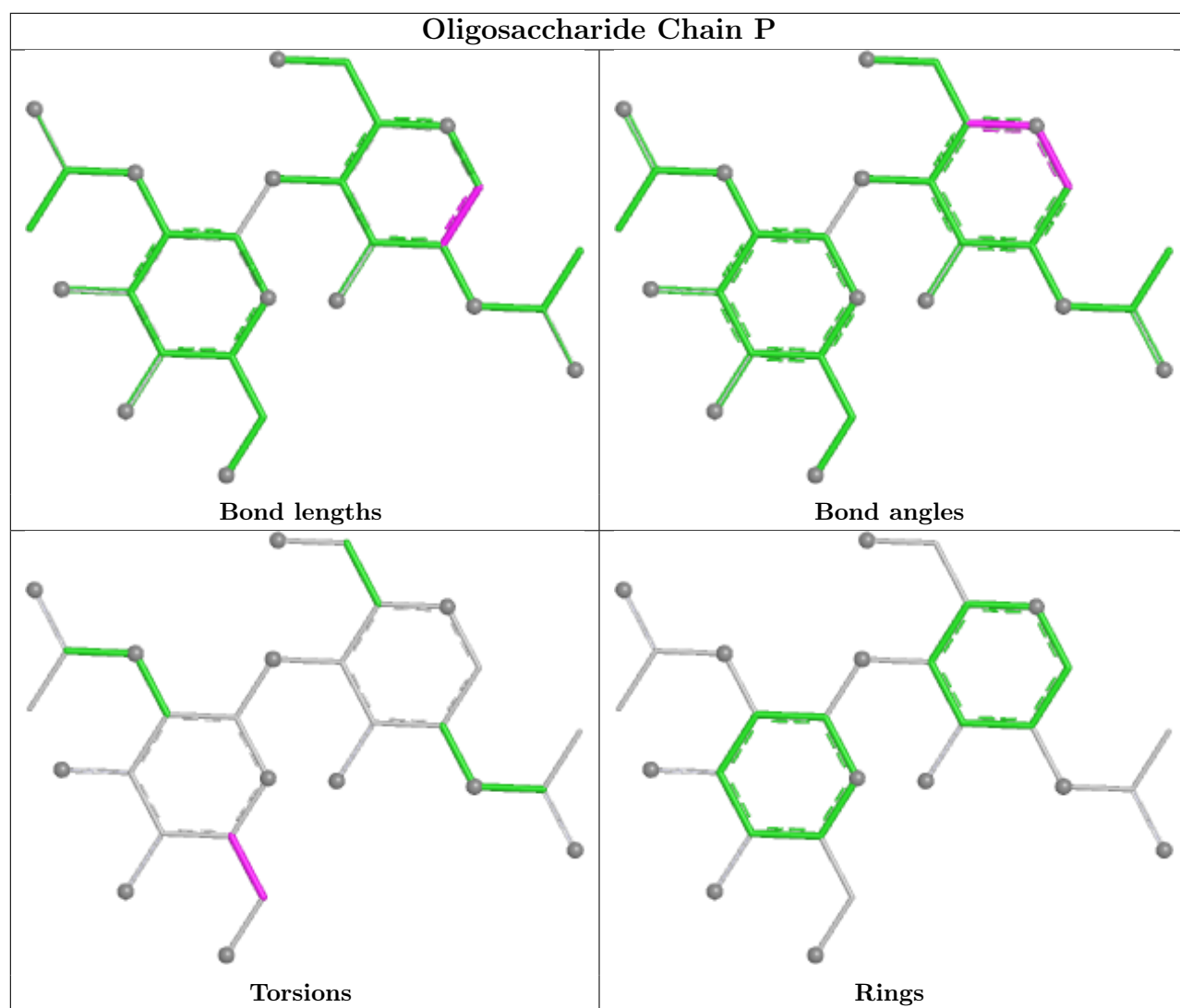


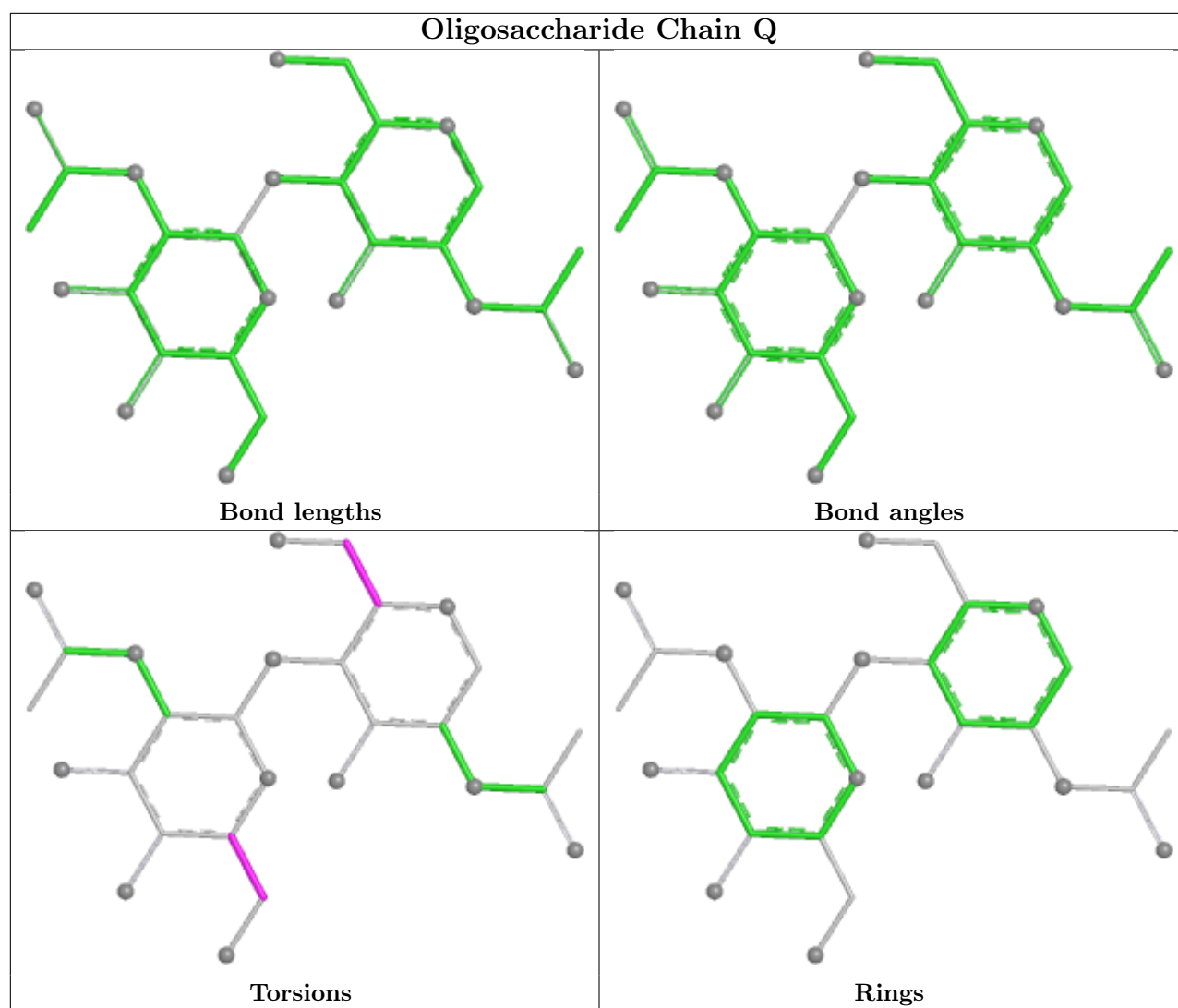


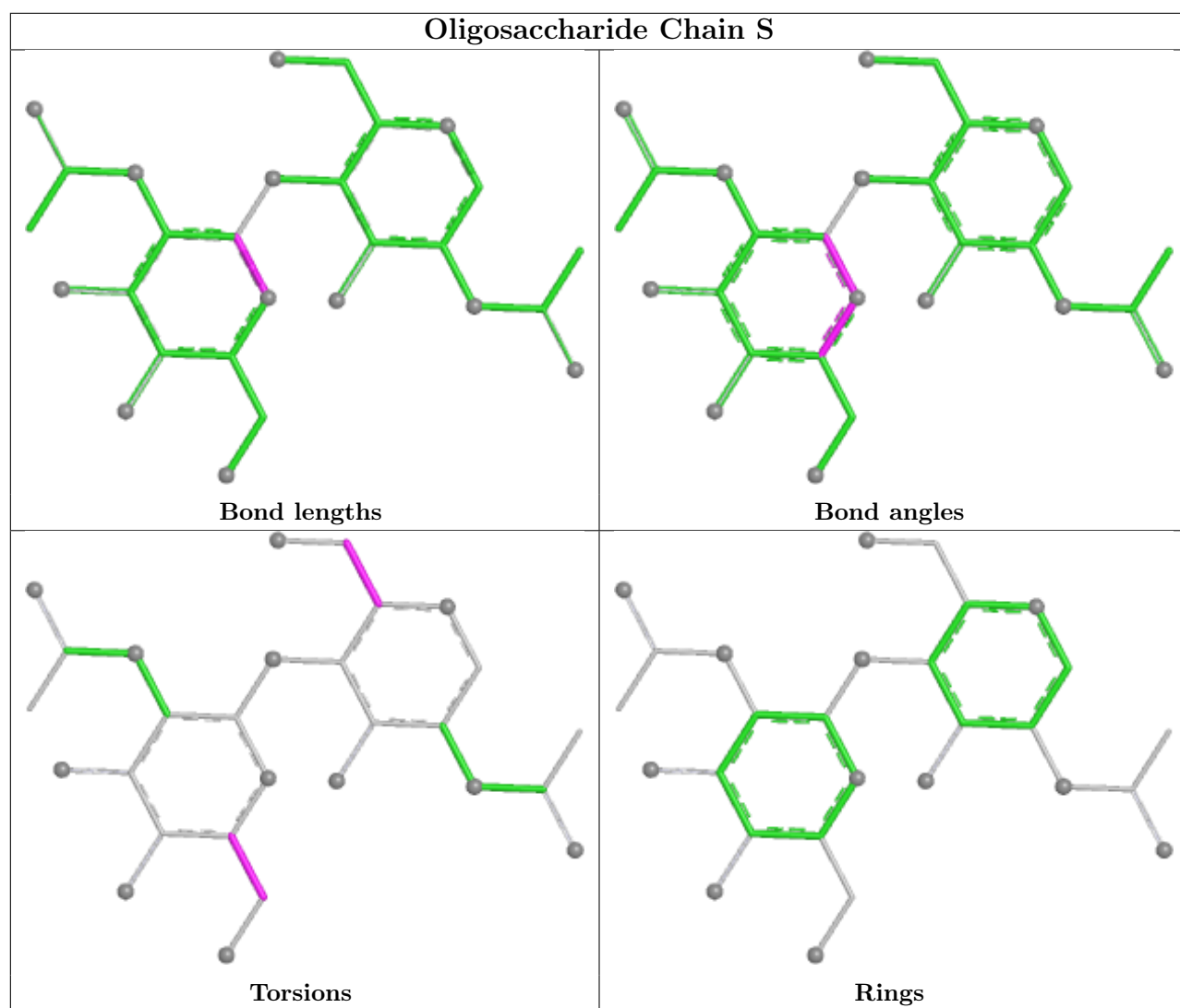


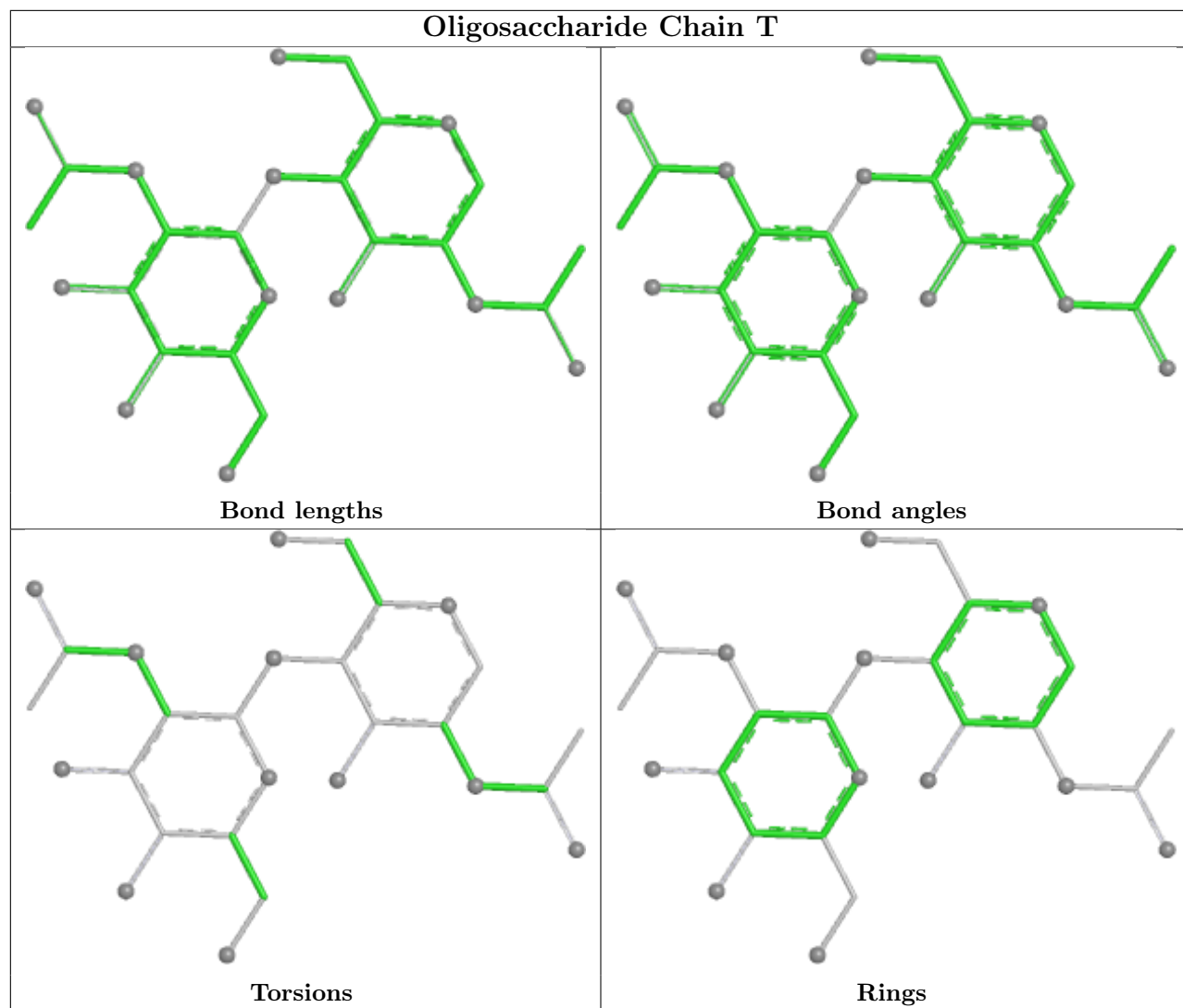


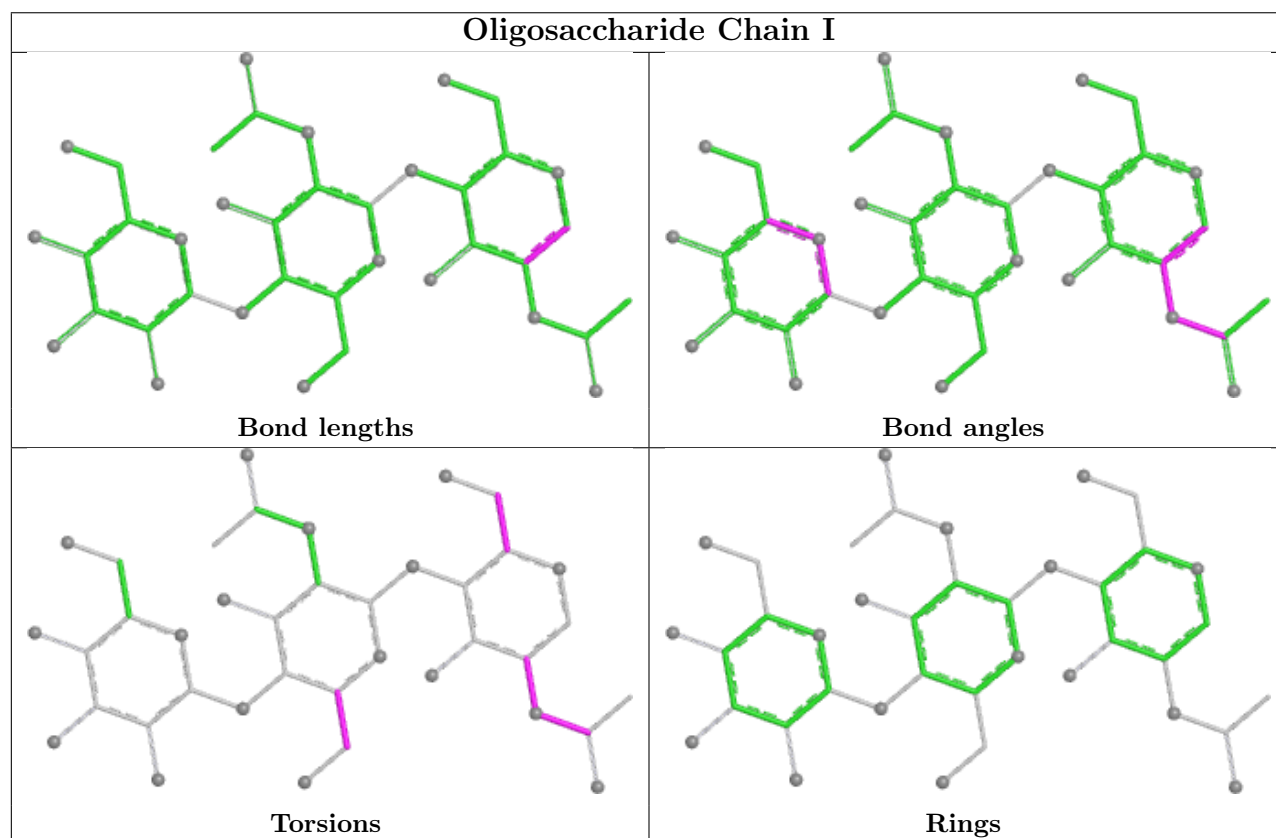
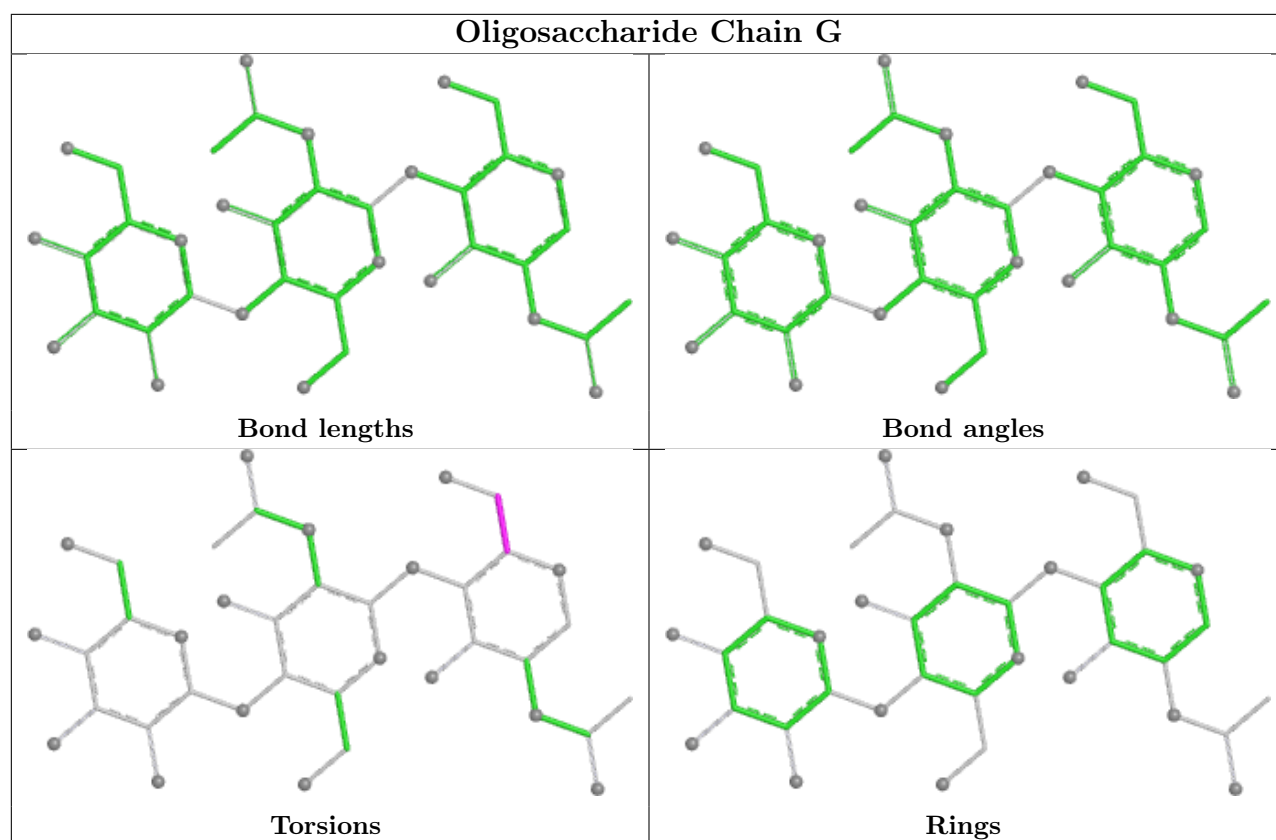


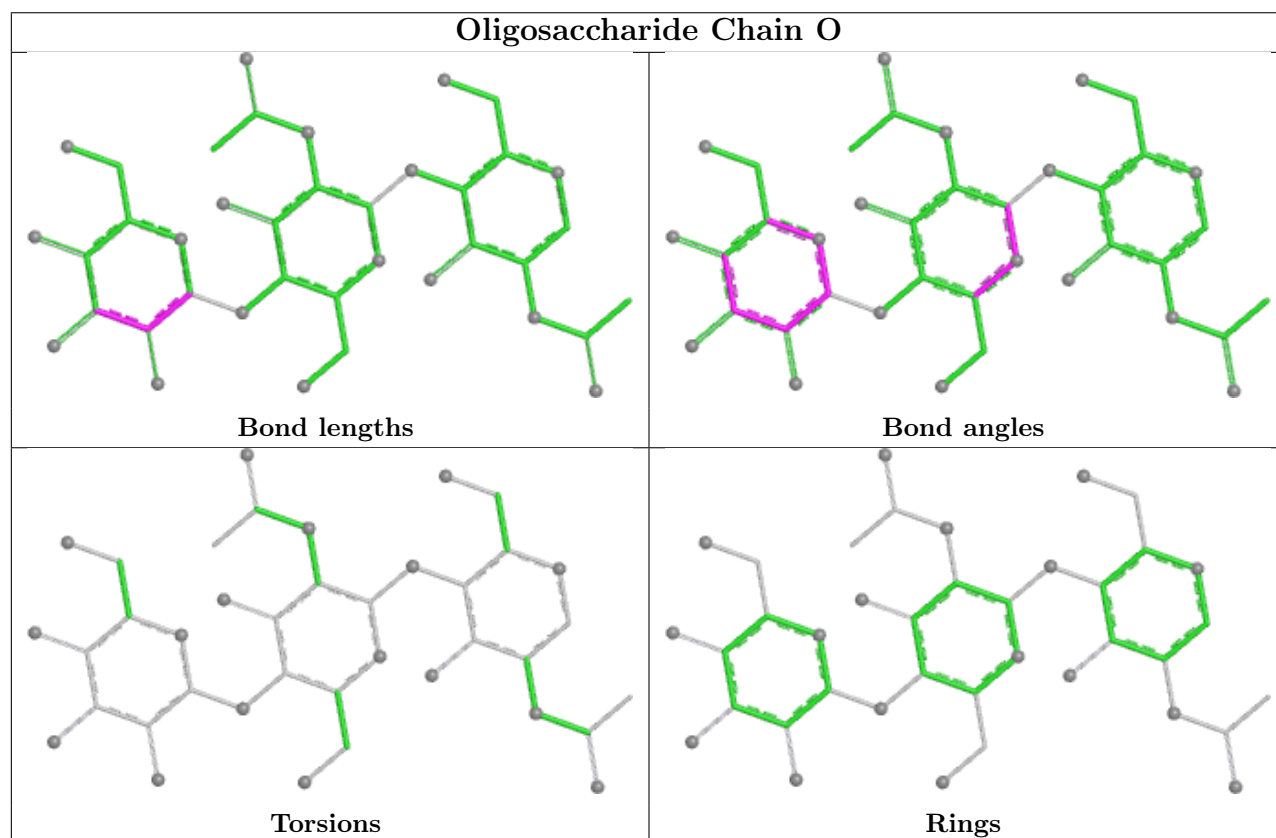
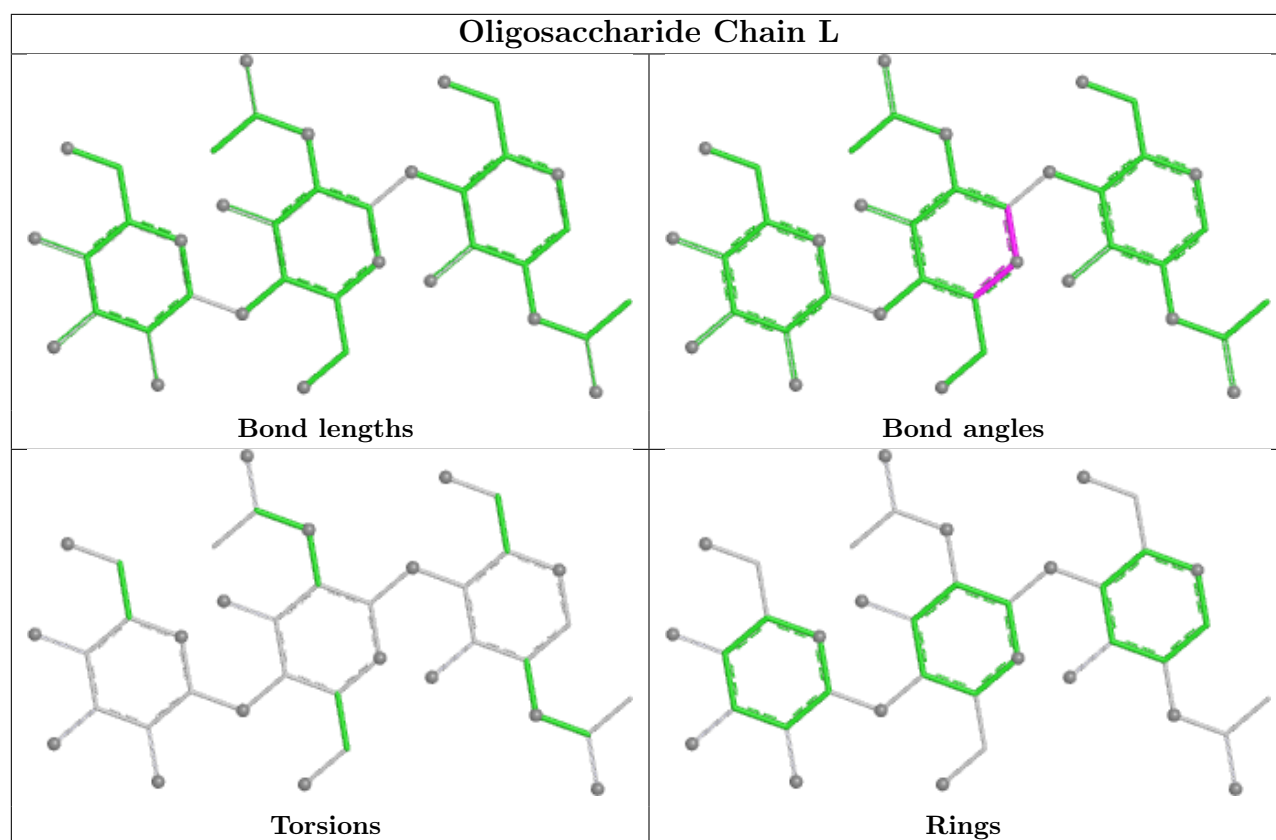


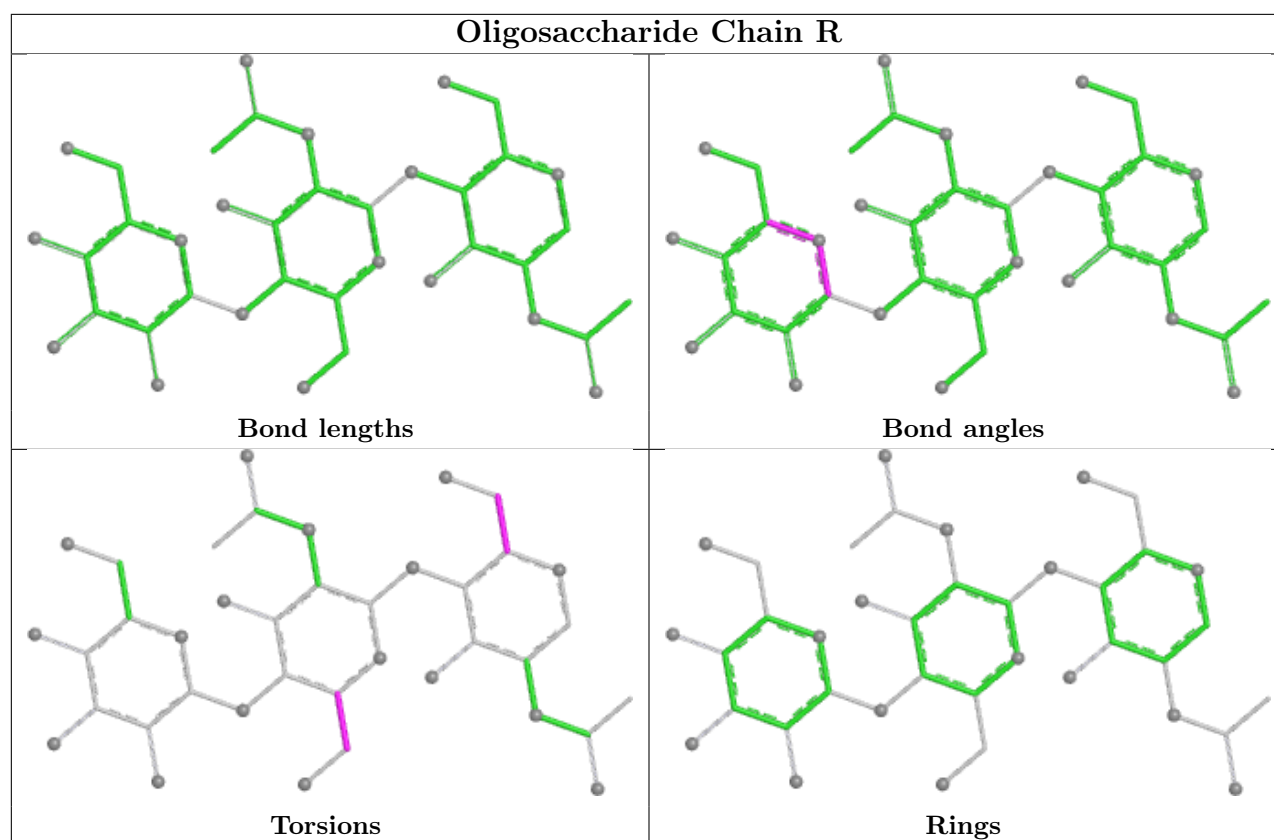












5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
4	SRO	D	501	-	14,14,14	1.55	2 (14%)	19,19,19	0.81	1 (5%)
4	SRO	B	501	-	14,14,14	1.55	2 (14%)	19,19,19	0.81	1 (5%)
4	SRO	E	501	-	14,14,14	1.56	2 (14%)	19,19,19	0.86	1 (5%)
4	SRO	A	501	-	14,14,14	1.54	2 (14%)	19,19,19	0.79	1 (5%)
4	SRO	B	502	-	14,14,14	1.56	2 (14%)	19,19,19	0.83	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	SRO	D	501	-	-	1/3/3/3	0/2/2/2
4	SRO	B	501	-	-	2/3/3/3	0/2/2/2
4	SRO	E	501	-	-	2/3/3/3	0/2/2/2
4	SRO	A	501	-	-	1/3/3/3	0/2/2/2
4	SRO	B	502	-	-	1/3/3/3	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	501	SRO	CD2-CE2	-3.24	1.37	1.41
4	B	502	SRO	CD2-CE2	-3.22	1.37	1.41
4	A	501	SRO	CD2-CE2	-3.18	1.37	1.41
4	B	501	SRO	CD2-CE2	-3.16	1.37	1.41
4	D	501	SRO	CD2-CE2	-3.16	1.37	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	SRO	CZ2-CE2-CD2	-2.28	119.98	122.19
4	A	501	SRO	CZ2-CE2-CD2	-2.22	120.04	122.19
4	E	501	SRO	CZ2-CE2-CD2	-2.20	120.06	122.19
4	D	501	SRO	CZ2-CE2-CD2	-2.19	120.07	122.19
4	B	501	SRO	CZ2-CE2-CD2	-2.05	120.20	122.19

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	SRO	NZ-CA-CB-CG
4	B	501	SRO	NZ-CA-CB-CG
4	B	502	SRO	NZ-CA-CB-CG
4	D	501	SRO	NZ-CA-CB-CG
4	E	501	SRO	NZ-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	501	SRO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	501	SRO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7883. 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

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 standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 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.