



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 08:26 PM UTC

PDB ID : 7N6W / pdb_00007n6w
EMDB ID : EMD-23861
Title : Structure of uncleaved HIV-1 JR-FL Env glycoprotein trimer in state U2
bound to small Molecule HIV-1 Entry Inhibitor BMS-378806
Authors : Zhang, S.; Wang, K.; Mao, Y.
Deposited on : 2021-06-09
Resolution : 4.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

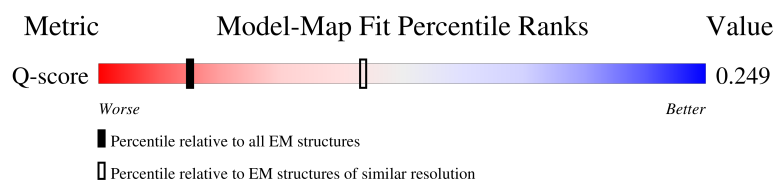
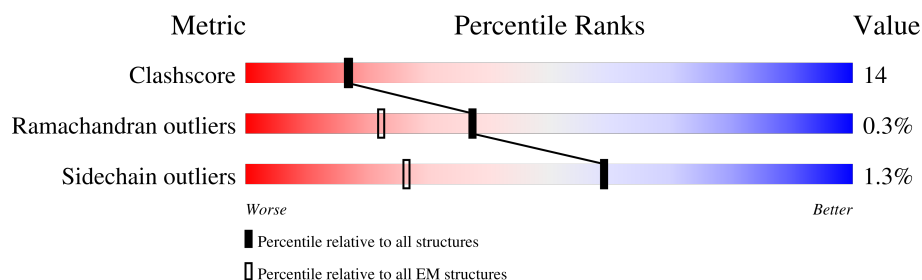
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1989 (4.20 - 5.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	848	12% 45% 24% 30%
1	B	848	13% 48% 22% 30%
1	C	848	10% 46% 23% 31%
2	D	3	67% 33% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	3	
2	K	3	
2	M	3	
2	N	3	
2	Q	3	
2	W	3	
2	X	3	
2	Y	3	
2	Z	3	
2	e	3	
2	k	3	
2	m	3	
2	n	3	
3	E	2	
3	H	2	
3	I	2	
3	J	2	
3	L	2	
3	O	2	
3	R	2	
3	S	2	
3	T	2	
3	V	2	
3	a	2	
3	b	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	2	50% 50%
3	d	2	100% 50%
3	f	2	50% 50%
3	i	2	50% 50%
3	j	2	50% 50%
3	l	2	50% 50%
3	p	2	100% 50%
3	q	2	100% 100%
4	G	7	43% 43% 57%
4	U	7	71% 29% 57% 14%
5	P	4	75% 75% 25%
5	o	4	50% 50% 25% 25%
6	g	4	50% 75% 25%
7	h	5	80% 40% 60%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	A	901	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15705 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	591	Total	C	N	O	S	0	0
			4686	2953	816	885	32		
1	B	595	Total	C	N	O	S	0	0
			4711	2967	820	892	32		
1	C	585	Total	C	N	O	S	0	0
			4637	2919	809	877	32		

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP Q75760
A	?	-	ILE	deletion	UNP Q75760
A	?	-	ARG	deletion	UNP Q75760
A	5	GLU	LYS	conflict	UNP Q75760
A	6	LYS	SER	conflict	UNP Q75760
A	9	HIS	TYR	conflict	UNP Q75760
A	12	ARG	LYS	conflict	UNP Q75760
A	13	TRP	GLY	conflict	UNP Q75760
A	15	TRP	-	insertion	UNP Q75760
A	16	ARG	-	insertion	UNP Q75760
A	17	TRP	-	insertion	UNP Q75760
A	18	GLY	-	insertion	UNP Q75760
A	20	MET	LEU	conflict	UNP Q75760
A	24	MET	ILE	conflict	UNP Q75760
A	31	THR	VAL	conflict	UNP Q75760
A	508	SER	ARG	conflict	UNP Q75760
A	511	SER	ARG	conflict	UNP Q75760
A	752	SER	PHE	conflict	UNP Q75760
A	758	ASP	VAL	conflict	UNP Q75760
A	777	ILE	THR	conflict	UNP Q75760
A	792	ALA	VAL	conflict	UNP Q75760
A	829	VAL	ILE	conflict	UNP Q75760
A	832	VAL	ALA	conflict	UNP Q75760
A	833	VAL	LEU	conflict	UNP Q75760

Continued on next page...

Continued from previous page...

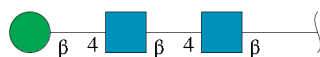
Chain	Residue	Modelled	Actual	Comment	Reference
A	835	GLY	ARG	conflict	UNP Q75760
A	836	ALA	THR	conflict	UNP Q75760
A	837	CYS	TYR	conflict	UNP Q75760
A	841	ARG	LEU	conflict	UNP Q75760
A	845	ARG	THR	conflict	UNP Q75760
A	854	ILE	ALA	conflict	UNP Q75760
B	?	-	GLY	deletion	UNP Q75760
B	?	-	ILE	deletion	UNP Q75760
B	?	-	ARG	deletion	UNP Q75760
B	5	GLU	LYS	conflict	UNP Q75760
B	6	LYS	SER	conflict	UNP Q75760
B	9	HIS	TYR	conflict	UNP Q75760
B	12	ARG	LYS	conflict	UNP Q75760
B	13	TRP	GLY	conflict	UNP Q75760
B	15	TRP	-	insertion	UNP Q75760
B	16	ARG	-	insertion	UNP Q75760
B	17	TRP	-	insertion	UNP Q75760
B	18	GLY	-	insertion	UNP Q75760
B	20	MET	LEU	conflict	UNP Q75760
B	24	MET	ILE	conflict	UNP Q75760
B	31	THR	VAL	conflict	UNP Q75760
B	508	SER	ARG	conflict	UNP Q75760
B	511	SER	ARG	conflict	UNP Q75760
B	752	SER	PHE	conflict	UNP Q75760
B	758	ASP	VAL	conflict	UNP Q75760
B	777	ILE	THR	conflict	UNP Q75760
B	792	ALA	VAL	conflict	UNP Q75760
B	829	VAL	ILE	conflict	UNP Q75760
B	832	VAL	ALA	conflict	UNP Q75760
B	833	VAL	LEU	conflict	UNP Q75760
B	835	GLY	ARG	conflict	UNP Q75760
B	836	ALA	THR	conflict	UNP Q75760
B	837	CYS	TYR	conflict	UNP Q75760
B	841	ARG	LEU	conflict	UNP Q75760
B	845	ARG	THR	conflict	UNP Q75760
B	854	ILE	ALA	conflict	UNP Q75760
C	?	-	GLY	deletion	UNP Q75760
C	?	-	ILE	deletion	UNP Q75760
C	?	-	ARG	deletion	UNP Q75760
C	5	GLU	LYS	conflict	UNP Q75760
C	6	LYS	SER	conflict	UNP Q75760
C	9	HIS	TYR	conflict	UNP Q75760

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	12	ARG	LYS	conflict	UNP Q75760
C	13	TRP	GLY	conflict	UNP Q75760
C	15	TRP	-	insertion	UNP Q75760
C	16	ARG	-	insertion	UNP Q75760
C	17	TRP	-	insertion	UNP Q75760
C	18	GLY	-	insertion	UNP Q75760
C	20	MET	LEU	conflict	UNP Q75760
C	24	MET	ILE	conflict	UNP Q75760
C	31	THR	VAL	conflict	UNP Q75760
C	508	SER	ARG	conflict	UNP Q75760
C	511	SER	ARG	conflict	UNP Q75760
C	752	SER	PHE	conflict	UNP Q75760
C	758	ASP	VAL	conflict	UNP Q75760
C	777	ILE	THR	conflict	UNP Q75760
C	792	ALA	VAL	conflict	UNP Q75760
C	829	VAL	ILE	conflict	UNP Q75760
C	832	VAL	ALA	conflict	UNP Q75760
C	833	VAL	LEU	conflict	UNP Q75760
C	835	GLY	ARG	conflict	UNP Q75760
C	836	ALA	THR	conflict	UNP Q75760
C	837	CYS	TYR	conflict	UNP Q75760
C	841	ARG	LEU	conflict	UNP Q75760
C	845	ARG	THR	conflict	UNP Q75760
C	854	ILE	ALA	conflict	UNP Q75760

- Molecule 2 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
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	K	3	Total	C	N	O	0	0
			39	22	2	15		
2	M	3	Total	C	N	O	0	0
			39	22	2	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	3	Total	C	N	O	0	0
			39	22	2	15		
2	Q	3	Total	C	N	O	0	0
			39	22	2	15		
2	W	3	Total	C	N	O	0	0
			39	22	2	15		
2	X	3	Total	C	N	O	0	0
			39	22	2	15		
2	Y	3	Total	C	N	O	0	0
			39	22	2	15		
2	Z	3	Total	C	N	O	0	0
			39	22	2	15		
2	e	3	Total	C	N	O	0	0
			39	22	2	15		
2	k	3	Total	C	N	O	0	0
			39	22	2	15		
2	m	3	Total	C	N	O	0	0
			39	22	2	15		
2	n	3	Total	C	N	O	0	0
			39	22	2	15		

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



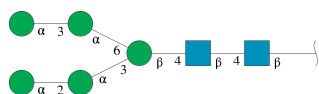
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		
3	b	2	Total	C	N	O	0	0
			28	16	2	10		
3	c	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	2	Total	C	N	O	0	0
			28	16	2	10		
3	f	2	Total	C	N	O	0	0
			28	16	2	10		
3	i	2	Total	C	N	O	0	0
			28	16	2	10		
3	j	2	Total	C	N	O	0	0
			28	16	2	10		
3	l	2	Total	C	N	O	0	0
			28	16	2	10		
3	p	2	Total	C	N	O	0	0
			28	16	2	10		
3	q	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	7	Total	C	N	O	0	0
			83	46	2	35		
4	U	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-

e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



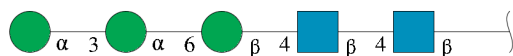
Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	4	Total	C	N	O	0	0
			50	28	2	20		
5	o	4	Total	C	N	O	0	0
			50	28	2	20		

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



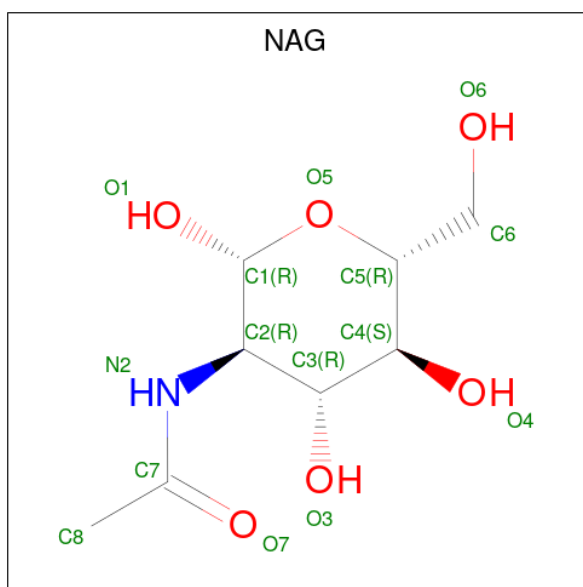
Mol	Chain	Residues	Atoms				AltConf	Trace
6	g	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



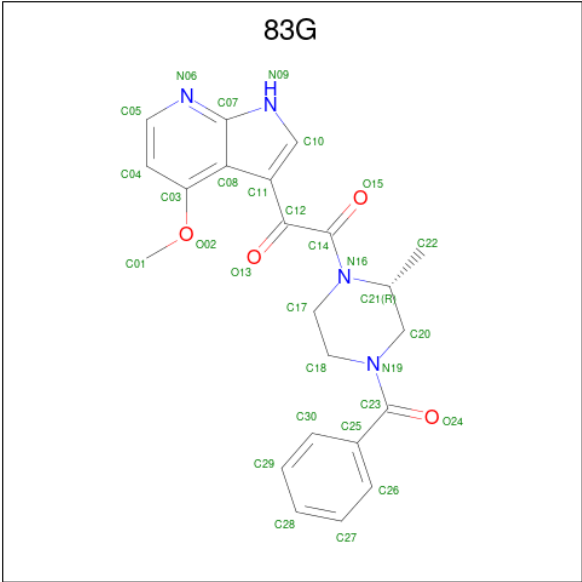
Mol	Chain	Residues	Atoms				AltConf	Trace
7	h	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is 1-[(2R)-4-(benzenecarbonyl)-2-methylpiperazin-1-yl]-2-(4-methoxy-1H-pyrrolo [2,3-b]pyridin-3-yl)ethane-1,2-dione (CCD ID: 83G) (formula: C₂₂H₂₂N₄O₄).

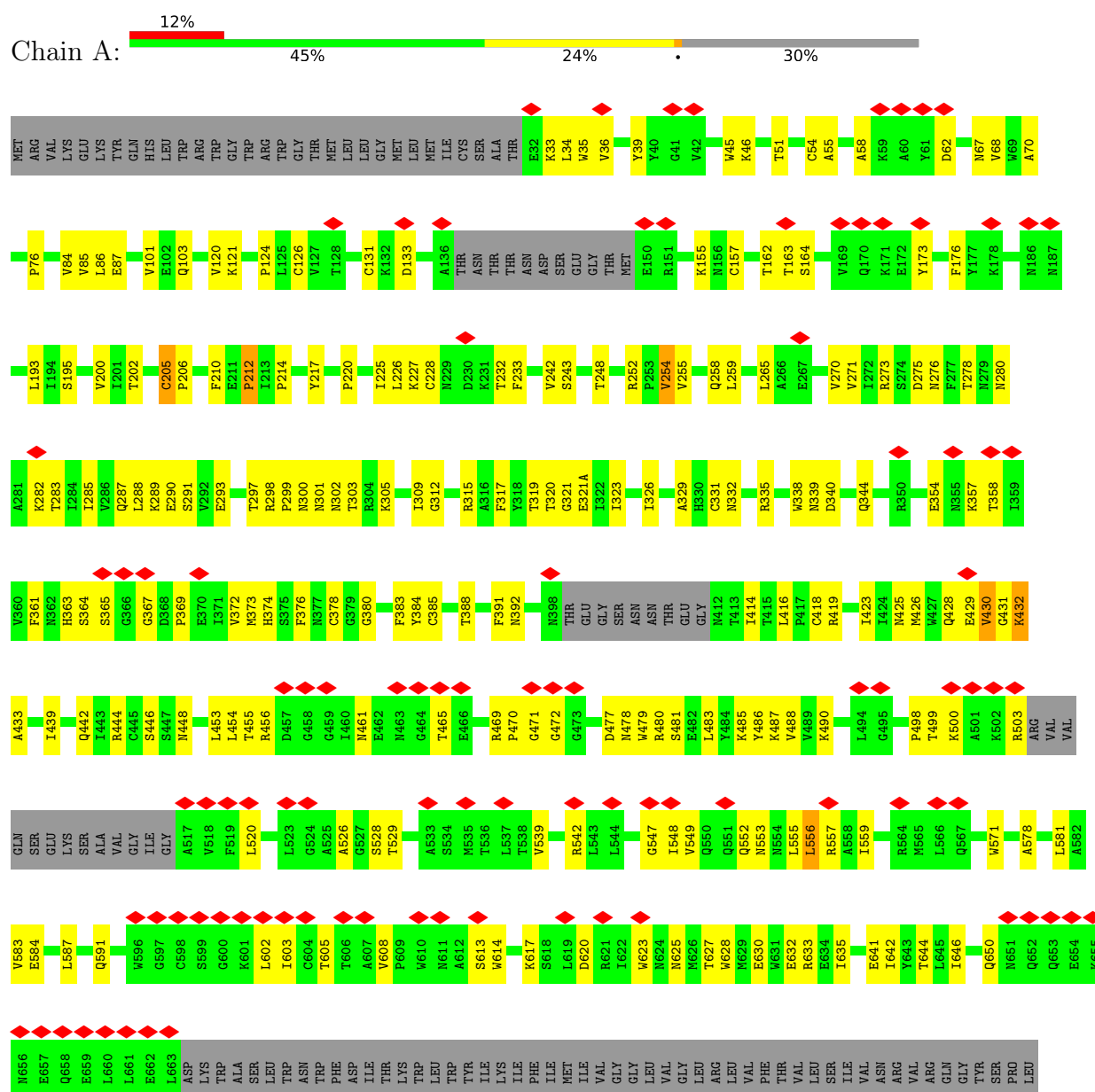


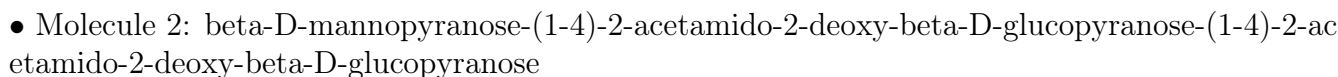
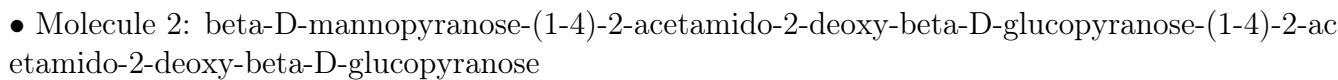
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			30	22	4	4	
9	B	1	Total	C	N	O	0
			30	22	4	4	
9	C	1	Total	C	N	O	0
			30	22	4	4	

3 Residue-property plots

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

• Molecule 1: Envelope glycoprotein gp160







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



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



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



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



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



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



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



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



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



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



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





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



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



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



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



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



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





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



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



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



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



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



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



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



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



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



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



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



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



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



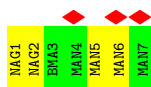
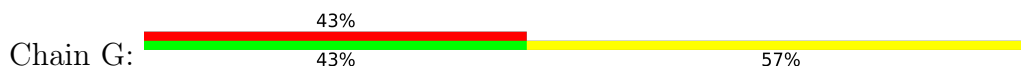
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

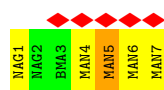


- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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





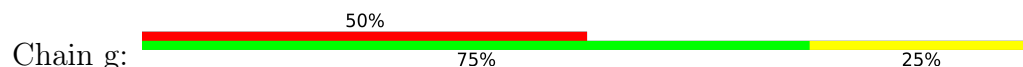
- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



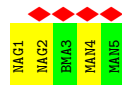
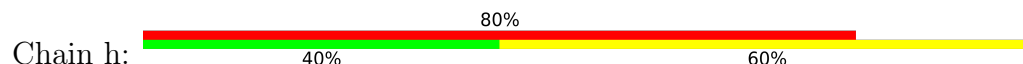
- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55571	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	230.16, 230.16, 230.16	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	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: 83G, BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	1/4779 (0.0%)	0.76	5/6487 (0.1%)
1	B	0.40	0/4804	0.81	7/6522 (0.1%)
1	C	0.38	0/4729	0.79	4/6419 (0.1%)
All	All	0.39	1/14312 (0.0%)	0.79	16/19428 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	608	VAL	C-N	5.68	1.40	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	VAL	N-CA-C	8.88	121.61	109.80
1	B	388	THR	CA-CB-OG1	-8.50	96.85	109.60
1	B	229	ASN	CB-CA-C	8.18	123.69	111.17
1	C	553	ASN	CA-C-N	6.25	133.48	121.54
1	C	553	ASN	C-N-CA	6.25	133.48	121.54
1	B	314	GLY	N-CA-C	-6.02	105.32	115.80
1	B	173	TYR	N-CA-CB	-5.70	101.43	111.40
1	B	230	ASP	CA-C-N	-5.64	114.83	123.07
1	B	230	ASP	C-N-CA	-5.64	114.83	123.07
1	A	212	PRO	CA-C-N	-5.32	117.48	123.02
1	A	212	PRO	C-N-CA	-5.32	117.48	123.02
1	C	93	PHE	CA-C-N	5.32	129.96	122.46
1	C	93	PHE	C-N-CA	5.32	129.96	122.46
1	B	440	ARG	N-CA-C	-5.21	107.44	112.97
1	A	195	SER	CA-C-N	5.10	131.28	121.54
1	A	195	SER	C-N-CA	5.10	131.28	121.54

There are no chirality outliers.

There are no planarity outliers.

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	4686	0	4604	142	0
1	B	4711	0	4622	133	0
1	C	4637	0	4551	146	0
2	D	39	0	34	0	0
2	F	39	0	34	1	0
2	K	39	0	34	0	0
2	M	39	0	34	1	0
2	N	39	0	34	2	0
2	Q	39	0	34	2	0
2	W	39	0	34	1	0
2	X	39	0	34	1	0
2	Y	39	0	34	3	0
2	Z	39	0	34	1	0
2	e	39	0	34	2	0
2	k	39	0	34	0	0
2	m	39	0	34	0	0
2	n	39	0	34	0	0
3	E	28	0	25	0	0
3	H	28	0	25	4	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	L	28	0	25	0	0
3	O	28	0	25	4	0
3	R	28	0	25	3	0
3	S	28	0	25	6	0
3	T	28	0	25	0	0
3	V	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	2	0
3	c	28	0	25	1	0
3	d	28	0	25	4	0
3	f	28	0	25	0	0
3	i	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	j	28	0	25	4	0
3	l	28	0	25	1	0
3	p	28	0	25	0	0
3	q	28	0	25	0	0
4	G	83	0	70	5	0
4	U	83	0	70	3	0
5	P	50	0	43	0	0
5	o	50	0	43	1	0
6	g	50	0	42	0	0
7	h	61	0	52	2	0
8	A	42	0	39	9	0
8	B	28	0	26	0	0
8	C	28	0	26	4	0
9	A	30	0	0	0	0
9	B	30	0	0	0	0
9	C	30	0	0	1	0
All	All	15705	0	15164	430	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 14.

All (430) 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)
4:G:1:NAG:H61	4:G:2:NAG:H82	1.47	0.97
1:A:278:THR:OG1	3:H:1:NAG:C1	2.15	0.95
7:h:1:NAG:H61	7:h:2:NAG:H82	1.47	0.94
1:B:175:LEU:HD11	3:R:1:NAG:H82	1.49	0.94
1:A:388:THR:HG21	2:N:1:NAG:H5	1.55	0.89
1:C:257:THR:HG1	1:C:374:HIS:HD1	1.23	0.87
1:A:87:GLU:HB3	8:A:901:NAG:C8	2.06	0.85
1:A:87:GLU:HB3	8:A:901:NAG:C7	2.09	0.82
1:A:378:CYS:SG	4:G:1:NAG:H3	2.20	0.81
1:C:397:ASN:HA	8:C:901:NAG:H81	1.62	0.79
1:A:87:GLU:HB3	8:A:901:NAG:H81	1.66	0.77
1:B:376:PHE:HB2	1:B:383:PHE:HB2	1.69	0.74
1:B:87:GLU:OE2	2:Q:1:NAG:C7	2.36	0.74
1:B:334:SER:HA	1:B:413:THR:HA	1.70	0.74
1:A:549:VAL:HG22	1:A:557:ARG:H	1.56	0.71
1:A:87:GLU:HB3	8:A:901:NAG:O7	1.90	0.70
1:A:392:ASN:HD22	3:O:1:NAG:C7	2.03	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:MET:HE3	1:A:432:LYS:H	1.54	0.70
1:B:378:CYS:HB3	4:U:1:NAG:H83	1.72	0.69
1:B:362:ASN:OD1	2:Y:1:NAG:N2	2.25	0.69
1:C:125:LEU:HB3	1:C:196:CYS:HB2	1.74	0.68
1:C:618:SER:H	1:C:621:ARG:HH21	1.41	0.68
1:B:362:ASN:CG	2:Y:1:NAG:N2	2.52	0.67
1:A:87:GLU:OE1	8:A:901:NAG:H81	1.94	0.67
1:C:323:ILE:HG21	3:j:1:NAG:O5	1.93	0.67
1:A:288:LEU:HG	1:A:290:GLU:H	1.61	0.66
1:A:312:GLY:HA3	1:A:315:ARG:HH21	1.61	0.66
1:B:36:VAL:HA	1:B:498:PRO:HA	1.78	0.65
1:C:80:ASN:HB3	1:C:82:GLN:HG2	1.79	0.65
1:B:67:ASN:HB2	1:B:208:ILE:HA	1.77	0.65
1:C:491:ILE:O	1:C:585:ARG:NH2	2.30	0.65
1:A:552:GLN:HG2	1:A:555:LEU:H	1.63	0.64
1:C:86:LEU:HA	1:C:523:LEU:HD21	1.79	0.64
1:B:530:MET:HG2	1:B:627:THR:HA	1.80	0.64
1:B:182:VAL:HG23	1:B:194:ILE:HA	1.80	0.64
2:F:1:NAG:H83	2:F:2:NAG:H2	1.80	0.63
1:B:266:ALA:HB3	1:B:289:LYS:HA	1.81	0.63
3:H:1:NAG:H5	3:H:2:NAG:HN2	1.64	0.63
1:A:34:LEU:HD12	1:A:503:ARG:HH11	1.63	0.63
1:C:34:LEU:HB2	1:C:610:TRP:HB2	1.81	0.62
1:B:559:ILE:HA	1:B:562:GLN:HB3	1.82	0.61
1:A:265:LEU:O	1:A:287:GLN:NE2	2.33	0.61
1:A:289:LYS:HG3	1:A:290:GLU:HG3	1.82	0.61
1:A:297:THR:OG1	1:A:444:ARG:NH1	2.33	0.61
1:A:87:GLU:CB	8:A:901:NAG:C8	2.79	0.61
1:A:121:LYS:HA	1:A:202:THR:HA	1.83	0.61
1:A:227:LYS:HE2	1:A:486:TYR:HE1	1.65	0.61
1:C:270:VAL:HG22	1:C:289:LYS:H	1.64	0.60
1:A:45:TRP:O	1:A:633:ARG:NH2	2.35	0.60
1:A:298:ARG:NH1	1:A:300:ASN:O	2.34	0.60
1:C:268:GLU:HA	1:C:289:LYS:HG3	1.83	0.60
1:C:163:THR:OG1	1:C:166:ARG:NH2	2.35	0.60
1:B:575:GLN:O	1:B:579:ARG:NE	2.32	0.59
1:A:291:SER:HB2	1:A:448:ASN:HB3	1.84	0.59
1:A:84:VAL:HG21	1:A:520:LEU:HB2	1.84	0.59
1:B:530:MET:SD	1:B:530:MET:N	2.76	0.59
1:A:87:GLU:CB	8:A:901:NAG:H81	2.33	0.59
1:C:292:VAL:HB	1:C:449:ILE:HB	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ASN:HA	1:C:322:ILE:HA	1.85	0.58
1:C:620:ASP:HA	1:C:623:TRP:HD1	1.68	0.58
5:o:1:NAG:H83	5:o:1:NAG:H3	1.85	0.58
1:A:276:ASN:OD1	3:H:1:NAG:N2	2.37	0.58
1:B:192:ARG:NH1	1:B:196:CYS:SG	2.76	0.58
1:C:131:CYS:HA	1:C:157:CYS:HA	1.84	0.58
1:A:556:LEU:HD12	1:A:559:ILE:HG13	1.86	0.58
1:B:634:GLU:HA	3:d:1:NAG:H81	1.84	0.58
1:B:567:GLN:HE21	1:C:577:GLN:HE22	1.52	0.58
1:C:159:PHE:HB2	1:C:174:ALA:HB2	1.85	0.58
3:S:1:NAG:O3	3:S:2:NAG:O5	2.20	0.58
1:A:214:PRO:HG3	1:A:252:ARG:HG3	1.85	0.57
1:B:335:ARG:NH1	1:B:411:GLY:O	2.37	0.57
1:B:74:CYS:SG	1:B:75:VAL:N	2.77	0.57
1:B:298:ARG:HD3	1:B:442:GLN:HG2	1.86	0.57
1:C:36:VAL:HA	1:C:498:PRO:HA	1.86	0.57
1:A:301:ASN:HB3	1:A:323:ILE:HB	1.86	0.57
1:C:257:THR:OG1	1:C:374:HIS:ND1	2.30	0.57
1:C:475:MET:SD	1:C:475:MET:N	2.78	0.57
1:A:220:PRO:HG3	1:A:578:ALA:HB1	1.86	0.57
1:A:298:ARG:HH11	1:A:442:GLN:HA	1.70	0.57
1:B:56:SER:HB2	1:B:59:LYS:HB3	1.85	0.57
1:A:620:ASP:H	1:A:623:TRP:HB2	1.70	0.57
1:C:547:GLY:HA2	1:C:555:LEU:HB2	1.87	0.57
1:B:439:ILE:HG22	4:U:5:MAN:O6	2.04	0.56
1:B:328:GLN:NE2	1:B:418:CYS:O	2.37	0.56
1:B:179:LEU:O	1:B:421:LYS:NZ	2.38	0.56
1:C:31:THR:N	1:C:500:LYS:O	2.37	0.56
1:C:49:THR:HG22	1:C:99:ASN:HD22	1.70	0.56
1:B:344:GLN:HA	1:B:347:ILE:HD12	1.88	0.56
1:C:298:ARG:HD3	1:C:443:ILE:H	1.70	0.56
1:B:158:SER:HA	1:B:172:GLU:HB3	1.88	0.56
1:B:562:GLN:HG2	1:B:563:GLN:HB2	1.87	0.56
1:A:101:VAL:HG13	1:A:479:TRP:HB2	1.88	0.56
1:C:308:HIS:HA	1:C:316:ALA:HA	1.88	0.56
1:C:353:PHE:HB3	1:C:357:LYS:HB2	1.88	0.56
1:C:308:HIS:NE2	1:C:312:GLY:O	2.39	0.55
1:C:529:THR:HA	1:C:628:TRP:HE1	1.70	0.55
1:A:87:GLU:CG	8:A:901:NAG:H81	2.36	0.55
1:A:217:TYR:O	1:A:248:THR:N	2.39	0.55
1:C:47:GLU:OE2	1:C:99:ASN:ND2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ILE:HD11	1:C:331:CYS:HB3	1.87	0.55
1:A:299:PRO:HG3	1:A:329:ALA:H	1.72	0.55
1:A:499:THR:O	1:A:503:ARG:NE	2.35	0.55
1:C:547:GLY:H	1:C:552:GLN:HE22	1.54	0.55
1:B:363:HIS:CE1	1:B:388:THR:HA	2.42	0.55
1:C:166:ARG:NH2	1:C:309:ILE:O	2.37	0.55
1:C:323:ILE:HG21	3:j:1:NAG:O6	2.06	0.55
1:A:173:TYR:O	1:A:305:LYS:NZ	2.37	0.55
1:B:170:GLN:NE2	3:S:1:NAG:O7	2.40	0.55
1:C:546:SER:OG	1:C:552:GLN:NE2	2.40	0.55
1:C:257:THR:H	1:C:376:PHE:HE1	1.55	0.54
1:C:279:ASN:O	1:C:456:ARG:NH2	2.40	0.54
1:C:397:ASN:HA	8:C:901:NAG:C8	2.34	0.54
3:R:1:NAG:H61	3:R:2:NAG:HN2	1.72	0.54
1:B:360:VAL:HA	1:B:394:THR:HB	1.89	0.54
1:B:360:VAL:HB	1:B:467:ILE:HA	1.89	0.54
1:C:156:ASN:ND2	2:e:1:NAG:O7	2.40	0.54
1:A:58:ALA:O	1:A:62:ASP:N	2.38	0.54
1:C:40:TYR:HB3	1:C:602:LEU:HD13	1.89	0.54
1:C:65:VAL:HG12	1:C:73:ALA:HB3	1.90	0.54
1:A:283:THR:HB	1:A:453:LEU:HD11	1.89	0.54
1:B:371:ILE:HG23	1:B:472:GLY:HA3	1.90	0.54
1:B:647:GLU:O	1:B:651:ASN:N	2.40	0.54
1:B:126:CYS:HA	1:B:193:LEU:HD22	1.90	0.54
1:B:651:ASN:ND2	1:B:654:GLU:OE1	2.40	0.54
1:A:528:SER:HA	1:A:627:THR:H	1.73	0.53
1:B:151:ARG:NH2	1:B:327:ARG:O	2.40	0.53
1:B:86:LEU:HD22	1:B:523:LEU:HB2	1.90	0.53
1:A:335:ARG:O	1:A:339:ASN:N	2.37	0.53
1:B:68:VAL:O	1:B:72:HIS:N	2.40	0.53
1:C:599:SER:OG	1:C:601:LYS:NZ	2.42	0.53
1:A:228:CYS:O	1:A:485:LYS:NZ	2.37	0.53
1:B:59:LYS:NZ	1:B:72:HIS:O	2.39	0.53
1:C:592:LEU:HA	1:C:595:ILE:HB	1.91	0.53
1:C:593:LEU:HD11	1:C:600:GLY:H	1.73	0.53
1:B:102:GLU:O	1:B:105:GLN:NE2	2.41	0.53
1:A:193:LEU:HD11	1:A:423:ILE:HG21	1.91	0.53
1:B:376:PHE:O	1:B:383:PHE:N	2.38	0.53
1:A:376:PHE:HB3	1:A:383:PHE:HB2	1.91	0.53
1:B:296:CYS:HA	1:B:331:CYS:HA	1.91	0.53
1:C:97:LYS:HA	1:C:480:ARG:HH22	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ILE:HG23	4:G:5:MAN:O6	2.08	0.52
1:C:642:ILE:HA	1:C:645:LEU:HB2	1.90	0.52
1:C:397:ASN:HD22	8:C:901:NAG:H82	1.74	0.52
1:C:297:THR:OG1	1:C:298:ARG:N	2.42	0.52
1:A:46:LYS:O	1:A:490:LYS:N	2.42	0.52
1:A:163:THR:HB	1:A:309:ILE:HG23	1.91	0.52
1:A:363:HIS:ND1	1:A:364:SER:O	2.36	0.52
1:B:126:CYS:SG	1:B:192:ARG:NH1	2.75	0.52
1:B:385:CYS:HA	1:B:418:CYS:HA	1.89	0.52
1:A:642:ILE:O	1:A:646:ILE:N	2.39	0.52
1:B:523:LEU:O	1:B:527:GLY:N	2.41	0.52
1:C:258:GLN:HB2	1:C:374:HIS:HE1	1.74	0.52
1:A:340:ASP:OD2	1:A:344:GLN:NE2	2.42	0.52
1:A:628:TRP:CD1	1:A:630:GLU:H	2.28	0.52
1:B:276:ASN:OD1	1:B:279:ASN:ND2	2.43	0.52
1:B:342:LEU:HA	1:B:345:ILE:HD12	1.92	0.52
1:A:461:ASN:ND2	1:A:465:THR:O	2.38	0.52
1:A:646:ILE:O	1:A:650:GLN:N	2.37	0.52
1:B:69:TRP:NE1	1:B:560:GLU:OE2	2.34	0.52
1:A:298:ARG:NH2	1:A:302:ASN:OD1	2.38	0.52
1:B:301:ASN:HB3	1:B:323:ILE:HB	1.92	0.52
1:C:598:CYS:O	1:C:601:LYS:NZ	2.43	0.52
1:A:584:GLU:HA	1:A:587:LEU:HB2	1.91	0.51
1:A:367:GLY:H	1:A:372:VAL:HG11	1.76	0.51
1:C:333:ILE:O	1:C:414:ILE:N	2.43	0.51
1:A:587:LEU:O	1:A:591:GLN:N	2.41	0.51
1:B:192:ARG:HD2	1:B:193:LEU:HB2	1.92	0.51
1:C:113:ASP:OD1	9:C:903:83G:N09	2.43	0.51
1:C:163:THR:OG1	1:C:309:ILE:O	2.29	0.51
1:C:52:LEU:HB3	1:C:219:ALA:HA	1.93	0.51
1:B:33:LYS:HB3	1:B:35:TRP:CD1	2.45	0.51
1:B:330:HIS:HB3	1:B:415:THR:HB	1.92	0.51
1:C:342:LEU:HA	1:C:345:ILE:HD12	1.93	0.51
1:C:619:LEU:HA	1:C:622:ILE:HD12	1.92	0.51
1:B:55:ALA:HB3	1:B:216:HIS:HB2	1.93	0.51
1:C:218:CYS:HA	1:C:247:CYS:HA	1.92	0.51
1:C:41:GLY:N	1:C:493:PRO:O	2.35	0.51
2:M:1:NAG:H61	2:M:2:NAG:C7	2.40	0.51
1:C:159:PHE:HB3	1:C:172:GLU:HB2	1.93	0.50
1:B:542:ARG:HH21	1:B:546:SER:HB2	1.75	0.50
1:A:54:CYS:SG	1:A:55:ALA:N	2.84	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LEU:HD23	1:A:472:GLY:HA2	1.92	0.50
1:A:499:THR:HB	1:A:503:ARG:HH21	1.77	0.50
1:B:592:LEU:O	1:B:596:TRP:N	2.38	0.50
1:C:335:ARG:O	1:C:339:ASN:N	2.39	0.50
1:B:286:VAL:HB	1:B:452:LEU:HB3	1.93	0.50
1:A:76:PRO:O	1:A:553:ASN:ND2	2.35	0.50
1:C:614:TRP:HB3	1:C:635:ILE:HG12	1.94	0.50
1:A:613:SER:HG	1:A:614:TRP:CD1	2.30	0.50
1:B:231:LYS:HE2	1:B:268:GLU:HG2	1.93	0.50
1:C:226:LEU:HB2	1:C:487:LYS:HB3	1.94	0.50
1:C:529:THR:OG1	1:C:623:TRP:O	2.30	0.50
1:A:126:CYS:HB3	1:C:165:ILE:HG21	1.94	0.49
1:B:164:SER:OG	1:B:165:ILE:N	2.45	0.49
1:B:228:CYS:HA	1:B:242:VAL:HA	1.94	0.49
1:C:627:THR:OG1	1:C:630:GLU:OE1	2.29	0.49
1:B:362:ASN:OD1	2:Y:1:NAG:C7	2.60	0.49
1:C:179:LEU:HD11	1:C:419:ARG:HE	1.76	0.49
1:C:286:VAL:N	1:C:452:LEU:O	2.40	0.49
1:A:87:GLU:CD	8:A:901:NAG:H81	2.37	0.49
1:A:454:LEU:HD12	1:A:470:PRO:HA	1.95	0.49
1:B:151:ARG:HH21	1:B:328:GLN:HA	1.76	0.49
1:B:475:MET:SD	1:B:475:MET:N	2.85	0.49
1:C:101:VAL:HG13	1:C:479:TRP:HB2	1.94	0.49
1:C:576:LEU:HD13	1:C:579:ARG:HG3	1.93	0.49
1:C:132:LYS:O	1:C:156:ASN:N	2.46	0.49
1:A:275:ASP:HB3	1:A:282:LYS:HD2	1.94	0.49
1:B:304:ARG:NH2	1:B:438:PRO:O	2.46	0.49
1:B:653:GLN:NE2	1:B:657:GLU:OE1	2.46	0.49
1:A:526:ALA:HB3	1:A:529:THR:HG22	1.94	0.49
1:B:258:GLN:HB2	1:B:374:HIS:CE1	2.48	0.49
1:B:576:LEU:HA	1:B:579:ARG:HH21	1.78	0.49
1:A:428:GLN:HG3	1:A:429:GLU:HG3	1.94	0.48
1:A:617:LYS:HD2	1:A:635:ILE:HG12	1.95	0.48
1:B:66:HIS:O	1:B:70:ALA:N	2.46	0.48
1:B:648:GLU:O	1:B:652:GLN:N	2.45	0.48
1:C:574:LYS:HA	1:C:577:GLN:HB2	1.95	0.48
1:A:303:THR:OG1	1:A:321(A):GLU:N	2.45	0.48
1:C:66:HIS:HB3	1:C:72:HIS:CE1	2.48	0.48
1:C:195:SER:HG	1:C:198:THR:HG1	1.55	0.48
1:C:397:ASN:CA	8:C:901:NAG:H81	2.39	0.48
1:B:108:ILE:O	1:B:112:TRP:N	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ASN:HA	1:B:279:ASN:HB2	1.95	0.48
1:B:294:ILE:HG13	1:B:333:ILE:HD13	1.95	0.48
1:A:85:VAL:HA	1:A:243:SER:HA	1.95	0.48
1:B:388:THR:HG21	2:Z:1:NAG:H3	1.95	0.48
2:X:1:NAG:O7	2:X:1:NAG:O3	2.27	0.48
1:A:259:LEU:HD11	1:A:374:HIS:HB3	1.95	0.48
1:B:248:THR:OG1	1:B:249:HIS:N	2.47	0.48
1:B:581:LEU:O	1:B:585:ARG:NH1	2.45	0.48
1:B:110:SER:O	1:B:114:GLN:NE2	2.46	0.48
1:C:64:GLU:HB3	1:C:67:ASN:HB2	1.95	0.48
1:A:305:LYS:HB2	1:A:321:GLY:HA2	1.95	0.47
1:C:31:THR:OG1	1:C:35:TRP:NE1	2.32	0.47
2:N:1:NAG:H61	2:N:2:NAG:H82	1.96	0.47
1:B:592:LEU:HA	1:B:595:ILE:HB	1.96	0.47
1:C:198:THR:OG1	1:C:199:SER:N	2.48	0.47
1:B:627:THR:HG22	1:B:629:MET:H	1.78	0.47
1:A:373:MET:HG2	1:A:384:TYR:HB3	1.97	0.47
1:B:552:GLN:HB3	1:B:556:LEU:HB2	1.94	0.47
1:C:31:THR:HG1	1:C:35:TRP:HE1	1.59	0.47
1:A:155:LYS:O	1:A:176:PHE:N	2.46	0.47
1:A:300:ASN:OD1	1:A:300:ASN:N	2.46	0.47
1:B:542:ARG:HA	1:B:546:SER:HB3	1.95	0.47
1:A:309:ILE:HG13	1:A:317:PHE:H	1.80	0.47
1:B:39:TYR:N	1:B:495:GLY:O	2.44	0.47
1:C:55:ALA:HB3	1:C:216:HIS:HB2	1.96	0.47
1:C:323:ILE:HD12	3:j:1:NAG:O6	2.14	0.47
1:A:51:THR:HA	1:A:103:GLN:HE22	1.80	0.47
1:A:528:SER:OG	1:A:625:ASN:O	2.22	0.47
1:A:384:TYR:O	1:A:419:ARG:N	2.46	0.47
1:B:202:THR:OG1	1:B:433:ALA:O	2.33	0.47
1:C:192:ARG:NH1	1:C:193:LEU:O	2.47	0.47
1:B:151:ARG:HE	1:B:328:GLN:HA	1.79	0.46
1:B:170:GLN:HE22	3:S:1:NAG:C7	2.27	0.46
1:C:91:GLU:HB2	1:C:93:PHE:CZ	2.51	0.46
1:C:252:ARG:HH22	7:h:1:NAG:C1	2.28	0.46
1:C:357:LYS:HD3	1:C:357:LYS:HA	1.58	0.46
1:C:163:THR:OG1	1:C:164:SER:N	2.49	0.46
1:B:200:VAL:HA	1:B:433:ALA:H	1.80	0.46
1:B:460:ILE:HD11	1:B:463:ASN:HA	1.98	0.46
1:C:323:ILE:CG2	3:j:1:NAG:O6	2.64	0.46
1:B:529:THR:HB	1:B:532:ALA:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:LEU:HA	1:C:486:TYR:HD2	1.80	0.46
1:C:610:TRP:HH2	1:C:645:LEU:HB3	1.80	0.46
1:A:549:VAL:HA	1:A:556:LEU:HA	1.98	0.46
1:C:304:ARG:HB2	1:C:440:ARG:HH21	1.80	0.46
1:A:483:LEU:HA	1:A:486:TYR:HD2	1.80	0.46
1:A:526:ALA:HA	1:A:628:TRP:HZ3	1.80	0.46
1:A:233:PHE:O	1:A:273:ARG:NH2	2.49	0.46
1:B:170:GLN:HE22	3:S:1:NAG:H81	1.80	0.46
3:b:1:NAG:C3	3:b:1:NAG:O7	2.64	0.45
3:b:1:NAG:O7	3:b:1:NAG:H3	2.16	0.45
1:A:319:THR:OG1	1:A:320:THR:N	2.49	0.45
1:A:478:ASN:O	1:A:481:SER:OG	2.28	0.45
3:d:1:NAG:H62	3:d:2:NAG:N2	2.31	0.45
1:A:602:LEU:O	1:A:605:THR:OG1	2.34	0.45
1:C:56:SER:O	1:C:78:ASP:N	2.49	0.45
1:A:641:GLU:O	1:A:644:THR:OG1	2.27	0.45
1:C:535:MET:O	1:C:538:THR:OG1	2.27	0.45
1:A:454:LEU:HA	1:A:471:GLY:H	1.81	0.45
1:C:538:THR:O	1:C:542:ARG:N	2.47	0.45
1:C:641:GLU:O	1:C:644:THR:OG1	2.30	0.45
3:O:1:NAG:H61	3:O:2:NAG:C7	2.46	0.45
1:B:227:LYS:O	1:B:243:SER:N	2.49	0.45
1:B:256:SER:HB2	1:B:261:LEU:HD12	1.99	0.45
1:C:157:CYS:N	1:C:174:ALA:O	2.45	0.45
1:C:614:TRP:HE3	1:C:635:ILE:HD11	1.82	0.45
1:B:555:LEU:HD23	1:C:581:LEU:HD13	1.98	0.45
1:A:193:LEU:HD11	1:A:423:ILE:HD13	1.98	0.45
1:B:637:ASN:OD1	3:d:1:NAG:N2	2.50	0.45
1:C:84:VAL:HG23	1:C:86:LEU:HD11	1.98	0.45
1:C:583:VAL:O	1:C:587:LEU:N	2.40	0.44
1:B:611:ASN:ND2	3:c:1:NAG:C7	2.81	0.44
1:C:230:ASP:N	1:C:241:ASN:HB3	2.32	0.44
1:A:581:LEU:HA	1:A:584:GLU:HG3	1.98	0.44
1:B:335:ARG:O	1:B:339:ASN:N	2.47	0.44
1:C:552:GLN:HG3	1:C:553:ASN:H	1.82	0.44
1:A:270:VAL:HG23	1:A:289:LYS:HE3	2.00	0.44
1:C:52:LEU:HB2	1:C:217:TYR:CE2	2.53	0.44
1:A:162:THR:OG1	1:A:164:SER:O	2.32	0.44
1:A:258:GLN:NE2	1:A:453:LEU:O	2.50	0.44
1:A:254:VAL:HB	1:A:478:ASN:HB3	1.99	0.44
1:A:300:ASN:HB3	1:A:326:ILE:HG23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ASN:OD1	1:B:191:TYR:OH	2.30	0.44
1:A:86:LEU:N	1:A:242:VAL:O	2.40	0.44
1:A:232:THR:HA	1:A:271:VAL:HG11	2.00	0.44
1:A:293:GLU:OE1	1:A:446:SER:OG	2.34	0.44
1:A:392:ASN:ND2	3:O:1:NAG:C7	2.74	0.44
1:A:455:THR:HG23	1:A:471:GLY:HA3	2.00	0.44
1:B:59:LYS:HD3	1:B:213:ILE:HG21	2.00	0.44
1:B:182:VAL:HG12	1:B:184:ILE:HG23	2.00	0.44
1:C:627:THR:N	1:C:630:GLU:OE2	2.41	0.44
1:A:85:VAL:HG22	1:A:243:SER:HB2	1.99	0.44
1:C:38:VAL:HA	1:C:496:VAL:HG22	1.99	0.43
1:A:131:CYS:SG	1:A:155:LYS:HB3	2.58	0.43
1:B:596:TRP:HZ3	1:B:646:ILE:HG23	1.83	0.43
1:C:96:TRP:O	1:C:98:ASN:ND2	2.51	0.43
1:C:232:THR:HA	1:C:273:ARG:HD2	2.00	0.43
1:C:262:ASN:N	1:C:448:ASN:O	2.43	0.43
1:A:280:ASN:OD1	1:A:456:ARG:NE	2.51	0.43
1:B:304:ARG:HH11	4:U:5:MAN:HO4	1.64	0.43
1:B:590:GLN:HA	1:B:593:LEU:HB2	2.00	0.43
1:C:165:ILE:HG22	1:C:166:ARG:HH11	1.81	0.43
1:C:273:ARG:N	1:C:287:GLN:OE1	2.50	0.43
1:C:270:VAL:HG13	1:C:288:LEU:HA	1.99	0.43
1:C:303:THR:HA	1:C:440:ARG:HG2	2.01	0.43
1:C:642:ILE:O	1:C:646:ILE:N	2.45	0.43
1:A:331:CYS:HB2	1:A:416:LEU:HD22	2.01	0.43
1:B:182:VAL:HG23	1:B:194:ILE:HD13	2.00	0.43
1:B:323:ILE:HD11	2:W:1:NAG:H82	2.00	0.43
1:C:195:SER:O	1:C:198:THR:OG1	2.35	0.43
1:C:156:ASN:CG	2:e:1:NAG:O7	2.61	0.43
1:C:334:SER:HA	1:C:413:THR:H	1.82	0.43
1:B:34:LEU:HB3	1:B:610:TRP:HB3	2.00	0.43
1:B:652:GLN:HA	1:B:655:LYS:HG2	2.00	0.43
1:C:161:ILE:O	1:C:170:GLN:N	2.45	0.43
1:A:212:PRO:HB2	1:A:252:ARG:HG2	2.01	0.43
1:A:365:SER:H	1:A:469:ARG:NH1	2.16	0.43
1:B:200:VAL:HB	1:B:433:ALA:HB3	1.99	0.43
1:B:295:ASN:OD1	1:B:332:ASN:HB3	2.19	0.43
1:C:129:LEU:HD22	1:C:159:PHE:HA	2.00	0.43
1:C:491:ILE:H	1:C:585:ARG:HH22	1.65	0.43
3:S:1:NAG:C3	3:S:2:NAG:O5	2.66	0.43
1:C:96:TRP:CG	1:C:275:ASP:HB3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:LYS:NZ	1:C:229:ASN:OD1	2.52	0.43
1:C:362:ASN:ND2	3:l:1:NAG:C7	2.82	0.43
1:C:490:LYS:HE3	1:C:490:LYS:HB3	1.90	0.43
1:A:226:LEU:N	1:A:487:LYS:O	2.47	0.42
1:A:364:SER:HA	1:A:469:ARG:HD3	2.01	0.42
1:A:378:CYS:SG	4:G:1:NAG:C3	3.01	0.42
1:A:548:ILE:HG22	1:A:549:VAL:H	1.84	0.42
1:A:632:GLU:HA	1:A:635:ILE:HD12	2.01	0.42
1:B:112:TRP:O	1:B:115:SER:OG	2.36	0.42
1:C:55:ALA:N	1:C:216:HIS:O	2.51	0.42
1:A:547:GLY:N	1:B:591:GLN:OE1	2.44	0.42
1:B:633:ARG:O	3:d:1:NAG:O7	2.37	0.42
1:A:200:VAL:O	1:A:433:ALA:N	2.52	0.42
1:A:67:ASN:O	1:A:70:ALA:N	2.39	0.42
1:A:124:PRO:HA	1:C:165:ILE:HD11	2.02	0.42
1:A:297:THR:OG1	1:A:298:ARG:N	2.52	0.42
1:B:34:LEU:O	1:B:610:TRP:N	2.47	0.42
1:B:325:ASP:HB3	1:B:327:ARG:HH12	1.85	0.42
1:A:210:PHE:HD2	1:A:380:GLY:HA2	1.84	0.42
1:B:100:MET:SD	1:B:100:MET:N	2.92	0.42
1:B:300:ASN:HB2	1:B:326:ILE:HG23	2.00	0.42
1:A:439:ILE:CG2	4:G:5:MAN:O6	2.67	0.42
1:A:391:PHE:HE2	1:A:470:PRO:HG3	1.84	0.42
1:B:232:THR:HB	1:B:271:VAL:HG21	2.01	0.42
1:C:591:GLN:O	1:C:595:ILE:N	2.49	0.42
1:A:54:CYS:HB3	1:A:571:TRP:CH2	2.54	0.42
1:A:131:CYS:HA	1:A:157:CYS:HA	2.02	0.42
1:A:385:CYS:HA	1:A:418:CYS:HA	2.02	0.42
1:A:392:ASN:ND2	3:O:1:NAG:O7	2.50	0.42
1:B:297:THR:OG1	1:B:330:HIS:N	2.41	0.42
1:C:584:GLU:HA	1:C:587:LEU:HB2	2.02	0.42
1:A:335:ARG:HA	1:A:338:TRP:HB3	2.02	0.42
1:B:359:ILE:HB	1:B:395:TRP:HB3	2.02	0.42
1:B:557:ARG:HD2	1:C:50:THR:HA	2.01	0.42
1:B:608:VAL:HG12	1:B:646:ILE:HD13	2.01	0.42
1:C:279:ASN:HB2	1:C:282:LYS:HG2	2.02	0.42
1:C:544:LEU:HD13	1:C:545:LEU:HG	2.02	0.42
1:C:157:CYS:HB2	1:C:174:ALA:HB3	2.02	0.42
1:A:364:SER:N	1:A:470:PRO:HD2	2.35	0.41
1:B:171:LYS:HB2	3:R:2:NAG:O7	2.20	0.41
1:C:54:CYS:SG	1:C:55:ALA:N	2.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:LYS:O	1:C:578:ALA:N	2.52	0.41
1:B:34:LEU:HB3	1:B:610:TRP:H	1.84	0.41
1:C:182:VAL:O	1:C:192:ARG:N	2.53	0.41
1:A:35:TRP:HA	1:A:498:PRO:HB3	2.01	0.41
1:A:369:PRO:HA	1:A:372:VAL:HG22	2.01	0.41
1:B:41:GLY:N	1:B:493:PRO:O	2.53	0.41
1:B:126:CYS:HB2	1:B:196:CYS:HB2	1.92	0.41
1:B:170:GLN:NE2	3:S:1:NAG:C7	2.83	0.41
1:A:273:ARG:HB2	1:A:285:ILE:HB	2.02	0.41
1:C:226:LEU:N	1:C:487:LYS:O	2.36	0.41
1:B:386:ASN:N	1:B:417:PRO:O	2.45	0.41
1:A:278:THR:CG2	3:H:1:NAG:HN2	2.33	0.41
1:A:332:ASN:HA	1:A:414:ILE:HG22	2.03	0.41
1:B:158:SER:HG	1:B:173:TYR:H	1.63	0.41
1:B:457:ASP:OD2	1:B:469:ARG:N	2.49	0.41
1:C:528:SER:O	1:C:628:TRP:NE1	2.54	0.41
1:A:205:CYS:HA	1:A:206:PRO:HD3	1.84	0.41
1:C:549:VAL:HG12	1:C:551:GLN:H	1.86	0.41
1:B:574:LYS:O	1:B:578:ALA:N	2.54	0.41
1:A:361:PHE:HD1	1:A:361:PHE:HA	1.74	0.41
1:B:53:PHE:HB2	1:B:220:PRO:HD3	2.02	0.41
1:C:67:ASN:HA	1:C:208:ILE:HA	2.03	0.41
1:C:193:LEU:HD13	1:C:193:LEU:HA	1.89	0.41
1:B:127:VAL:HG11	1:B:161:ILE:HD13	2.03	0.41
1:B:370:GLU:H	1:B:370:GLU:HG3	1.69	0.41
1:C:637:ASN:N	1:C:637:ASN:OD1	2.54	0.41
1:A:33:LYS:HB2	1:A:500:LYS:HD2	2.02	0.40
1:A:39:TYR:HE1	1:A:603:ILE:HG23	1.86	0.40
1:A:539:VAL:HA	1:A:542:ARG:HG2	2.03	0.40
1:A:583:VAL:O	1:A:587:LEU:N	2.38	0.40
1:C:360:VAL:HG13	1:C:394:THR:HA	2.03	0.40
1:C:364:SER:HB2	1:C:470:PRO:HG2	2.02	0.40
1:C:102:GLU:HA	1:C:105:GLN:HE21	1.86	0.40
1:C:130:ASN:OD1	1:C:130:ASN:N	2.54	0.40
1:A:300:ASN:HB3	1:A:326:ILE:HG12	2.03	0.40
1:C:259:LEU:HB2	1:C:376:PHE:CZ	2.57	0.40
1:A:225:ILE:HG12	1:A:488:VAL:HG22	2.03	0.40
1:A:477:ASP:HA	1:A:480:ARG:HB2	2.03	0.40
1:B:102:GLU:OE1	1:B:476:ARG:NH1	2.50	0.40
1:C:266:ALA:HB2	1:C:287:GLN:HB3	2.02	0.40
1:C:346:VAL:HA	1:C:349:LEU:HB3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ASN:ND2	2:Q:1:NAG:O7	2.55	0.40
1:B:483:LEU:HD13	1:B:483:LEU:HA	1.91	0.40
1:C:124:PRO:HB3	1:C:161:ILE:HD13	2.02	0.40

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	583/848 (69%)	513 (88%)	66 (11%)	4 (1%)	18	55
1	B	587/848 (69%)	517 (88%)	68 (12%)	2 (0%)	36	72
1	C	577/848 (68%)	491 (85%)	86 (15%)	0	100	100
All	All	1747/2544 (69%)	1521 (87%)	220 (13%)	6 (0%)	37	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	431	GLY
1	A	358	THR
1	B	299	PRO
1	A	68	VAL
1	B	548	ILE
1	A	430	VAL

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	523/744 (70%)	512 (98%)	11 (2%)	47	65
1	B	526/744 (71%)	519 (99%)	7 (1%)	61	72
1	C	518/744 (70%)	515 (99%)	3 (1%)	78	81
All	All	1567/2232 (70%)	1546 (99%)	21 (1%)	59	72

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	133	ASP
1	A	205	CYS
1	A	254	VAL
1	A	255	VAL
1	A	354	GLU
1	A	357	LYS
1	A	425	ASN
1	A	430	VAL
1	A	432	LYS
1	A	556	LEU
1	B	86	LEU
1	B	89	VAL
1	B	230	ASP
1	B	300	ASN
1	B	355	ASN
1	B	357	LYS
1	B	638	TYR
1	C	169	VAL
1	C	357	LYS
1	C	494	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	103	GLN
1	A	203	GLN
1	A	258	GLN
1	A	308	HIS
1	A	396	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	398	ASN
1	A	425	ASN
1	A	461	ASN
1	A	616	ASN
1	A	650	GLN
1	A	658	GLN
1	B	66	HIS
1	B	170	GLN
1	B	246	GLN
1	B	276	ASN
1	B	279	ASN
1	B	300	ASN
1	B	339	ASN
1	B	355	ASN
1	B	363	HIS
1	B	389	GLN
1	B	397	ASN
1	B	412	ASN
1	B	553	ASN
1	B	567	GLN
1	B	656	ASN
1	B	658	GLN
1	C	72	HIS
1	C	98	ASN
1	C	186	ASN
1	C	203	GLN
1	C	397	ASN
1	C	551	GLN
1	C	552	GLN
1	C	590	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

113 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	D	1	1,2	14,14,15	0.68	1 (7%)	17,19,21	0.52	0
2	NAG	D	2	2	14,14,15	0.17	0	17,19,21	0.74	1 (5%)
2	BMA	D	3	2	11,11,12	0.78	0	15,15,17	0.75	0
3	NAG	E	1	1,3	14,14,15	0.52	0	17,19,21	0.47	0
3	NAG	E	2	3	14,14,15	0.15	0	17,19,21	0.57	0
2	NAG	F	1	1,2	14,14,15	0.14	0	17,19,21	0.61	0
2	NAG	F	2	2	14,14,15	0.27	0	17,19,21	0.55	0
2	BMA	F	3	2	11,11,12	0.54	0	15,15,17	0.97	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.60	0	17,19,21	0.67	0
4	NAG	G	2	4	14,14,15	0.57	0	17,19,21	0.87	0
4	BMA	G	3	4	11,11,12	0.65	0	15,15,17	0.71	0
4	MAN	G	4	4	11,11,12	0.57	0	15,15,17	0.59	0
4	MAN	G	5	4	11,11,12	0.51	0	15,15,17	0.63	0
4	MAN	G	6	4	11,11,12	0.63	0	15,15,17	0.93	2 (13%)
4	MAN	G	7	4	11,11,12	0.64	0	15,15,17	0.54	0
3	NAG	H	1	1,3	14,14,15	0.63	1 (7%)	17,19,21	0.63	0
3	NAG	H	2	3	14,14,15	0.35	0	17,19,21	0.57	0
3	NAG	I	1	1,3	14,14,15	0.31	0	17,19,21	0.47	0
3	NAG	I	2	3	14,14,15	0.25	0	17,19,21	0.41	0
3	NAG	J	1	1,3	14,14,15	0.34	0	17,19,21	0.49	0
3	NAG	J	2	3	14,14,15	0.19	0	17,19,21	0.50	0
2	NAG	K	1	1,2	14,14,15	0.40	0	17,19,21	0.51	0
2	NAG	K	2	2	14,14,15	0.29	0	17,19,21	0.47	0
2	BMA	K	3	2	11,11,12	0.54	0	15,15,17	0.78	1 (6%)
3	NAG	L	1	1,3	14,14,15	0.39	0	17,19,21	0.52	0
3	NAG	L	2	3	14,14,15	0.32	0	17,19,21	0.43	0
2	NAG	M	1	1,2	14,14,15	0.56	0	17,19,21	0.45	0
2	NAG	M	2	2	14,14,15	0.28	0	17,19,21	0.57	0
2	BMA	M	3	2	11,11,12	0.54	0	15,15,17	0.70	0
2	NAG	N	1	1,2	14,14,15	0.68	1 (7%)	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	N	2	2	14,14,15	0.16	0	17,19,21	0.50	0
2	BMA	N	3	2	11,11,12	0.58	0	15,15,17	0.69	0
3	NAG	O	1	1,3	14,14,15	0.51	0	17,19,21	0.37	0
3	NAG	O	2	3	14,14,15	0.51	0	17,19,21	0.69	1 (5%)
5	NAG	P	1	1,5	14,14,15	0.49	0	17,19,21	0.54	0
5	NAG	P	2	5	14,14,15	0.20	0	17,19,21	0.62	0
5	BMA	P	3	5	11,11,12	0.52	0	15,15,17	0.83	0
5	MAN	P	4	5	11,11,12	0.89	1 (9%)	15,15,17	0.79	1 (6%)
2	NAG	Q	1	1,2	14,14,15	0.65	1 (7%)	17,19,21	0.69	0
2	NAG	Q	2	2	14,14,15	0.33	0	17,19,21	0.63	1 (5%)
2	BMA	Q	3	2	11,11,12	0.60	0	15,15,17	0.72	0
3	NAG	R	1	1,3	14,14,15	0.49	0	17,19,21	0.44	0
3	NAG	R	2	3	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	S	1	1,3	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
3	NAG	S	2	3	14,14,15	0.52	0	17,19,21	1.32	3 (17%)
3	NAG	T	1	1,3	14,14,15	0.51	0	17,19,21	2.28	3 (17%)
3	NAG	T	2	3	14,14,15	0.47	0	17,19,21	1.37	3 (17%)
4	NAG	U	1	1,4	14,14,15	0.53	0	17,19,21	0.44	0
4	NAG	U	2	4	14,14,15	0.46	0	17,19,21	0.82	0
4	BMA	U	3	4	11,11,12	0.71	0	15,15,17	0.79	0
4	MAN	U	4	4	11,11,12	0.65	0	15,15,17	1.29	2 (13%)
4	MAN	U	5	4	11,11,12	0.62	0	15,15,17	0.94	2 (13%)
4	MAN	U	6	4	11,11,12	0.59	0	15,15,17	0.88	1 (6%)
4	MAN	U	7	4	11,11,12	0.62	0	15,15,17	1.06	2 (13%)
3	NAG	V	1	1,3	14,14,15	0.38	0	17,19,21	0.43	0
3	NAG	V	2	3	14,14,15	0.18	0	17,19,21	0.51	0
2	NAG	W	1	1,2	14,14,15	0.32	0	17,19,21	0.60	0
2	NAG	W	2	2	14,14,15	0.16	0	17,19,21	0.62	0
2	BMA	W	3	2	11,11,12	0.49	0	15,15,17	0.85	0
2	NAG	X	1	1,2	14,14,15	0.60	0	17,19,21	0.68	1 (5%)
2	NAG	X	2	2	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
2	BMA	X	3	2	11,11,12	0.73	0	15,15,17	0.80	0
2	NAG	Y	1	1,2	14,14,15	0.74	1 (7%)	17,19,21	0.54	0
2	NAG	Y	2	2	14,14,15	0.18	0	17,19,21	0.48	0
2	BMA	Y	3	2	11,11,12	0.52	0	15,15,17	0.90	0
2	NAG	Z	1	1,2	14,14,15	0.46	0	17,19,21	0.49	0
2	NAG	Z	2	2	14,14,15	0.32	0	17,19,21	0.47	0
2	BMA	Z	3	2	11,11,12	0.66	0	15,15,17	0.85	0
3	NAG	a	1	1,3	14,14,15	0.50	0	17,19,21	2.27	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	a	2	3	14,14,15	0.53	0	17,19,21	1.32	3 (17%)
3	NAG	b	1	1,3	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
3	NAG	b	2	3	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
3	NAG	c	1	1,3	14,14,15	0.62	1 (7%)	17,19,21	0.54	0
3	NAG	c	2	3	14,14,15	0.17	0	17,19,21	0.42	0
3	NAG	d	1	1,3	14,14,15	1.16	1 (7%)	17,19,21	0.97	2 (11%)
3	NAG	d	2	3	14,14,15	0.23	0	17,19,21	0.60	0
2	NAG	e	1	1,2	14,14,15	0.93	1 (7%)	17,19,21	0.83	0
2	NAG	e	2	2	14,14,15	0.15	0	17,19,21	0.64	0
2	BMA	e	3	2	11,11,12	0.56	0	15,15,17	0.77	0
3	NAG	f	1	1,3	14,14,15	0.83	1 (7%)	17,19,21	0.65	0
3	NAG	f	2	3	14,14,15	0.29	0	17,19,21	0.49	0
6	NAG	g	1	1,6	14,14,15	0.21	0	17,19,21	0.63	0
6	NAG	g	2	6	14,14,15	0.18	0	17,19,21	0.53	0
6	BMA	g	3	6	11,11,12	0.52	0	15,15,17	0.89	0
6	MAN	g	4	6	11,11,12	0.62	0	15,15,17	1.02	2 (13%)
7	NAG	h	1	1,7	14,14,15	0.59	0	17,19,21	0.66	0
7	NAG	h	2	7	14,14,15	0.57	0	17,19,21	0.86	0
7	BMA	h	3	7	11,11,12	0.64	0	15,15,17	0.71	0
7	MAN	h	4	7	11,11,12	0.63	0	15,15,17	0.93	1 (6%)
7	MAN	h	5	7	11,11,12	0.61	0	15,15,17	0.54	0
3	NAG	i	1	1,3	14,14,15	0.78	1 (7%)	17,19,21	0.56	0
3	NAG	i	2	3	14,14,15	0.19	0	17,19,21	0.54	0
3	NAG	j	1	1,3	14,14,15	0.51	0	17,19,21	2.26	3 (17%)
3	NAG	j	2	3	14,14,15	0.49	0	17,19,21	1.32	3 (17%)
2	NAG	k	1	1,2	14,14,15	0.46	0	17,19,21	0.43	0
2	NAG	k	2	2	14,14,15	0.18	0	17,19,21	0.57	0
2	BMA	k	3	2	11,11,12	0.67	0	15,15,17	0.94	0
3	NAG	l	1	1,3	14,14,15	0.64	0	17,19,21	0.70	0
3	NAG	l	2	3	14,14,15	0.17	0	17,19,21	0.42	0
2	NAG	m	1	1,2	14,14,15	0.62	1 (7%)	17,19,21	0.44	0
2	NAG	m	2	2	14,14,15	0.20	0	17,19,21	0.54	0
2	BMA	m	3	2	11,11,12	0.65	0	15,15,17	0.92	1 (6%)
2	NAG	n	1	1,2	14,14,15	0.75	1 (7%)	17,19,21	0.76	0
2	NAG	n	2	2	14,14,15	0.27	0	17,19,21	0.52	0
2	BMA	n	3	2	11,11,12	0.76	0	15,15,17	0.88	0
5	NAG	o	1	1,5	14,14,15	0.73	1 (7%)	17,19,21	1.31	1 (5%)
5	NAG	o	2	5	14,14,15	0.24	0	17,19,21	0.42	0
5	BMA	o	3	5	11,11,12	0.54	0	15,15,17	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	o	4	5	11,11,12	1.28	3 (27%)	15,15,17	1.94	2 (13%)
3	NAG	p	1	1,3	14,14,15	1.51	4 (28%)	17,19,21	1.09	1 (5%)
3	NAG	p	2	3	14,14,15	1.34	2 (14%)	17,19,21	1.31	1 (5%)
3	NAG	q	1	1,3	14,14,15	0.44	0	17,19,21	0.61	0
3	NAG	q	2	3	14,14,15	0.31	0	17,19,21	0.58	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	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	MAN	G	5	4	-	2/2/19/22	0/1/1/1
4	MAN	G	6	4	-	2/2/19/22	0/1/1/1
4	MAN	G	7	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	n	2	2	-	2/6/23/26	0/1/1/1
2	BMA	n	3	2	-	2/2/19/22	0/1/1/1
5	NAG	o	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	o	2	5	-	2/6/23/26	0/1/1/1
5	BMA	o	3	5	-	2/2/19/22	0/1/1/1
5	MAN	o	4	5	-	2/2/19/22	0/1/1/1
3	NAG	p	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	p	2	3	-	0/6/23/26	0/1/1/1
3	NAG	q	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	q	2	3	-	2/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	d	1	NAG	O5-C1	-3.97	1.37	1.43
2	e	1	NAG	O5-C1	-3.40	1.38	1.43
3	f	1	NAG	O5-C1	-2.97	1.38	1.43
3	p	1	NAG	O5-C1	2.96	1.48	1.43
3	p	2	NAG	O5-C1	2.76	1.48	1.43
3	i	1	NAG	O5-C1	-2.70	1.39	1.43
5	o	4	MAN	O5-C5	2.68	1.48	1.43
3	p	1	NAG	O5-C5	2.63	1.48	1.43
5	o	1	NAG	O5-C1	-2.62	1.39	1.43
2	Y	1	NAG	O5-C1	-2.57	1.39	1.43
2	D	1	NAG	O5-C1	-2.50	1.39	1.43
5	P	4	MAN	O5-C1	-2.50	1.39	1.43
2	n	1	NAG	O5-C1	-2.47	1.39	1.43
2	Q	1	NAG	O5-C1	-2.31	1.39	1.43
2	N	1	NAG	O5-C1	-2.30	1.39	1.43
3	p	2	NAG	O5-C5	2.26	1.47	1.43
2	m	1	NAG	O5-C1	-2.23	1.39	1.43
5	o	4	MAN	O5-C1	2.22	1.47	1.43
3	c	1	NAG	O5-C1	-2.20	1.40	1.43
3	H	1	NAG	O5-C1	-2.17	1.40	1.43
3	p	1	NAG	O4-C4	2.05	1.48	1.43
3	p	1	NAG	C8-C7	2.02	1.54	1.50
5	o	4	MAN	C1-C2	2.00	1.57	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	1	NAG	O5-C1-C2	-7.53	99.64	111.29
3	T	1	NAG	O5-C1-C2	-7.52	99.66	111.29
3	S	1	NAG	O5-C1-C2	-7.51	99.67	111.29
3	j	1	NAG	O5-C1-C2	-7.49	99.70	111.29
3	a	1	NAG	O5-C1-C2	-7.49	99.71	111.29
5	o	4	MAN	C1-O5-C5	6.64	121.08	112.19
5	o	1	NAG	C2-N2-C7	4.53	128.97	122.90
3	p	2	NAG	C1-O5-C5	4.08	117.66	112.19
3	p	1	NAG	C1-O5-C5	3.37	116.70	112.19
4	U	4	MAN	C1-O5-C5	3.21	116.49	112.19
4	U	4	MAN	O2-C2-C3	-3.11	103.70	110.15
3	j	2	NAG	O5-C5-C6	-3.08	101.67	107.66
3	b	2	NAG	O5-C5-C6	-3.08	101.67	107.66
3	T	2	NAG	O5-C5-C6	-3.05	101.72	107.66
3	S	2	NAG	O5-C5-C6	-3.05	101.72	107.66
3	a	2	NAG	O5-C5-C6	-3.05	101.73	107.66
3	T	1	NAG	O7-C7-C8	-2.94	116.82	122.05
3	a	1	NAG	O7-C7-C8	-2.92	116.85	122.05
3	S	1	NAG	O7-C7-C8	-2.91	116.86	122.05
3	j	1	NAG	O7-C7-C8	-2.87	116.94	122.05
3	b	1	NAG	O7-C7-C8	-2.82	117.03	122.05
3	a	1	NAG	C4-C3-C2	-2.70	107.07	111.02
3	j	1	NAG	C4-C3-C2	-2.66	107.12	111.02
5	o	4	MAN	O2-C2-C3	-2.64	104.69	110.15
3	b	1	NAG	C4-C3-C2	-2.64	107.15	111.02
3	T	1	NAG	C4-C3-C2	-2.63	107.16	111.02
3	S	1	NAG	C4-C3-C2	-2.61	107.19	111.02
4	U	7	MAN	C1-O5-C5	2.54	115.59	112.19
3	T	2	NAG	O5-C1-C2	-2.43	107.54	111.29
6	g	4	MAN	O2-C2-C3	-2.40	105.18	110.15
4	U	7	MAN	O2-C2-C3	-2.37	105.25	110.15
3	T	2	NAG	C4-C3-C2	-2.36	107.56	111.02
3	b	2	NAG	O5-C1-C2	-2.33	107.69	111.29
3	j	2	NAG	O5-C1-C2	-2.30	107.73	111.29
3	S	2	NAG	O5-C1-C2	-2.30	107.74	111.29
3	a	2	NAG	O5-C1-C2	-2.30	107.74	111.29
4	U	6	MAN	O2-C2-C3	-2.26	105.47	110.15
6	g	4	MAN	C1-O5-C5	2.24	115.19	112.19
2	X	2	NAG	C1-O5-C5	2.23	115.18	112.19
3	a	2	NAG	C4-C3-C2	-2.22	107.77	111.02
3	O	2	NAG	C1-O5-C5	2.21	115.15	112.19
4	U	5	MAN	C1-O5-C5	2.21	115.15	112.19
3	S	2	NAG	C4-C3-C2	-2.19	107.81	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	2	NAG	C4-C3-C2	-2.16	107.85	111.02
2	K	3	BMA	O2-C2-C3	-2.16	105.68	110.15
4	U	5	MAN	O2-C2-C3	-2.14	105.72	110.15
3	j	2	NAG	C4-C3-C2	-2.11	107.92	111.02
3	d	1	NAG	C1-O5-C5	-2.10	109.37	112.19
5	P	4	MAN	O2-C2-C3	-2.09	105.82	110.15
3	d	1	NAG	C3-C4-C5	2.09	114.02	110.23
7	h	4	MAN	C1-O5-C5	-2.09	109.39	112.19
2	m	3	BMA	C1-O5-C5	2.05	114.93	112.19
2	F	3	BMA	C1-O5-C5	2.05	114.93	112.19
2	D	2	NAG	C1-O5-C5	2.05	114.93	112.19
4	G	6	MAN	C1-O5-C5	-2.04	109.45	112.19
4	G	6	MAN	O5-C5-C6	2.03	111.61	107.66
2	X	1	NAG	C1-O5-C5	2.03	114.90	112.19
2	Q	2	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (133) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	1	NAG	C1-C2-N2-C7
2	e	1	NAG	C1-C2-N2-C7
3	b	1	NAG	C3-C2-N2-C7
3	d	1	NAG	C1-C2-N2-C7
3	c	1	NAG	C4-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
3	q	1	NAG	C4-C5-C6-O6
2	e	1	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	f	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6
2	k	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	U	5	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	o	4	MAN	O5-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
3	c	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
3	q	1	NAG	O5-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
2	N	3	BMA	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
2	F	3	BMA	C4-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
2	m	1	NAG	O5-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
5	o	4	MAN	C4-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
2	n	1	NAG	O5-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
2	N	3	BMA	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
2	e	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
2	k	1	NAG	C4-C5-C6-O6
3	l	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
4	U	5	MAN	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	e	3	BMA	C4-C5-C6-O6
2	e	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	f	1	NAG	C4-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
5	o	1	NAG	C8-C7-N2-C2
5	o	1	NAG	O7-C7-N2-C2
2	X	1	NAG	O5-C5-C6-O6
2	m	1	NAG	C4-C5-C6-O6
2	n	3	BMA	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
2	n	2	NAG	O5-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	q	2	NAG	O5-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
3	l	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
7	h	2	NAG	C8-C7-N2-C2
2	n	1	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
5	o	3	BMA	O5-C5-C6-O6
5	o	3	BMA	C4-C5-C6-O6
4	G	6	MAN	C4-C5-C6-O6
7	h	4	MAN	C4-C5-C6-O6
2	e	3	BMA	O5-C5-C6-O6
4	G	6	MAN	O5-C5-C6-O6
7	h	4	MAN	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	e	2	NAG	C4-C5-C6-O6
2	n	3	BMA	O5-C5-C6-O6
4	G	2	NAG	O7-C7-N2-C2
7	h	2	NAG	O7-C7-N2-C2
2	e	1	NAG	C3-C2-N2-C7
5	o	2	NAG	C4-C5-C6-O6
6	g	1	NAG	O5-C5-C6-O6
2	n	2	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
5	P	1	NAG	C1-C2-N2-C7
3	q	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	o	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
2	m	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C3-C2-N2-C7
2	X	1	NAG	C3-C2-N2-C7
3	d	1	NAG	C3-C2-N2-C7
3	q	1	NAG	C3-C2-N2-C7
4	G	5	MAN	C4-C5-C6-O6
3	O	1	NAG	C1-C2-N2-C7
3	q	1	NAG	C1-C2-N2-C7
5	o	1	NAG	C1-C2-N2-C7
2	D	2	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	C3-C2-N2-C7
2	X	2	NAG	C3-C2-N2-C7
3	f	2	NAG	C3-C2-N2-C7
5	P	1	NAG	C3-C2-N2-C7
5	o	1	NAG	C3-C2-N2-C7
2	m	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
3	T	1	NAG	O7-C7-N2-C2
3	b	1	NAG	O7-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	a	1	NAG	O7-C7-N2-C2
3	j	1	NAG	O7-C7-N2-C2

There are no ring outliers.

34 monomers are involved in 54 short contacts:

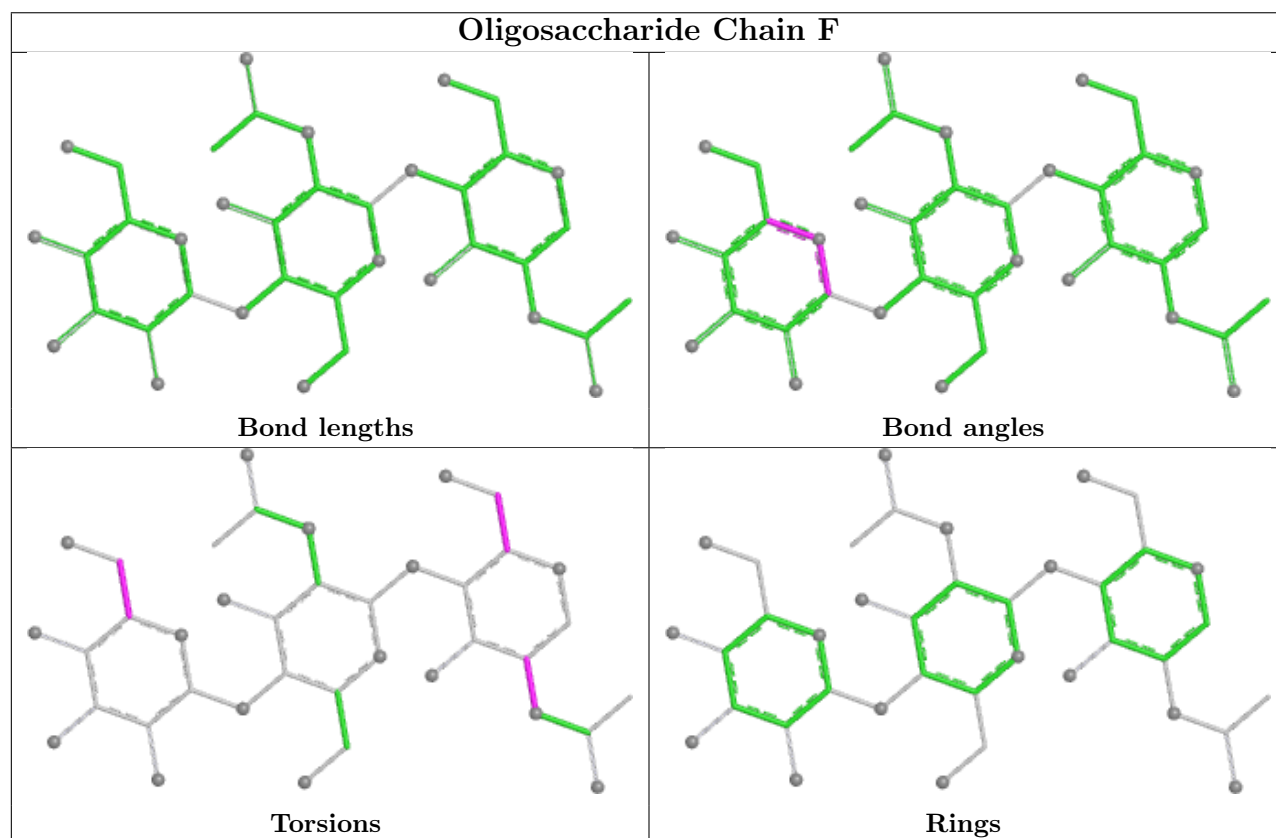
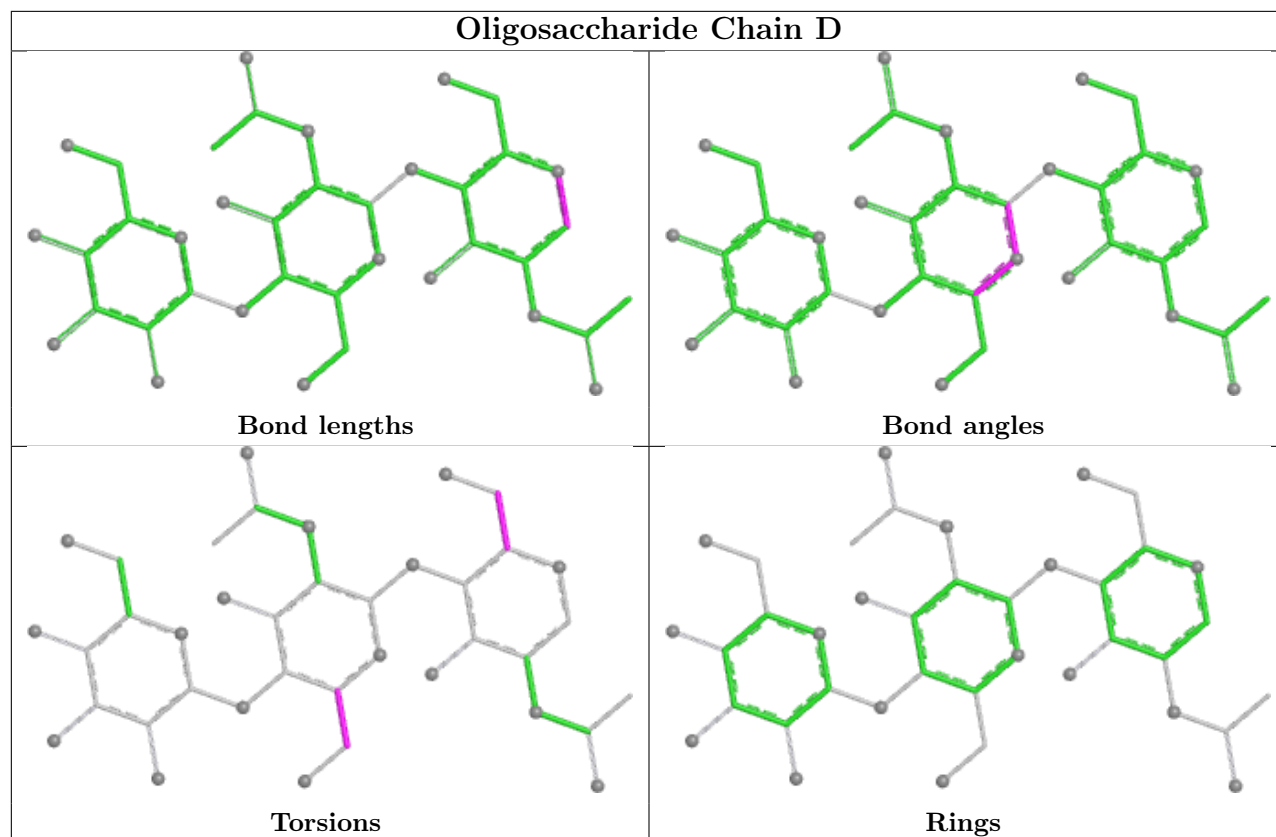
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	1	NAG	1	0
2	Q	1	NAG	2	0
3	H	1	NAG	4	0
7	h	1	NAG	2	0
5	o	1	NAG	1	0
4	G	5	MAN	2	0
4	G	1	NAG	3	0
2	N	1	NAG	2	0
2	W	1	NAG	1	0
3	H	2	NAG	1	0

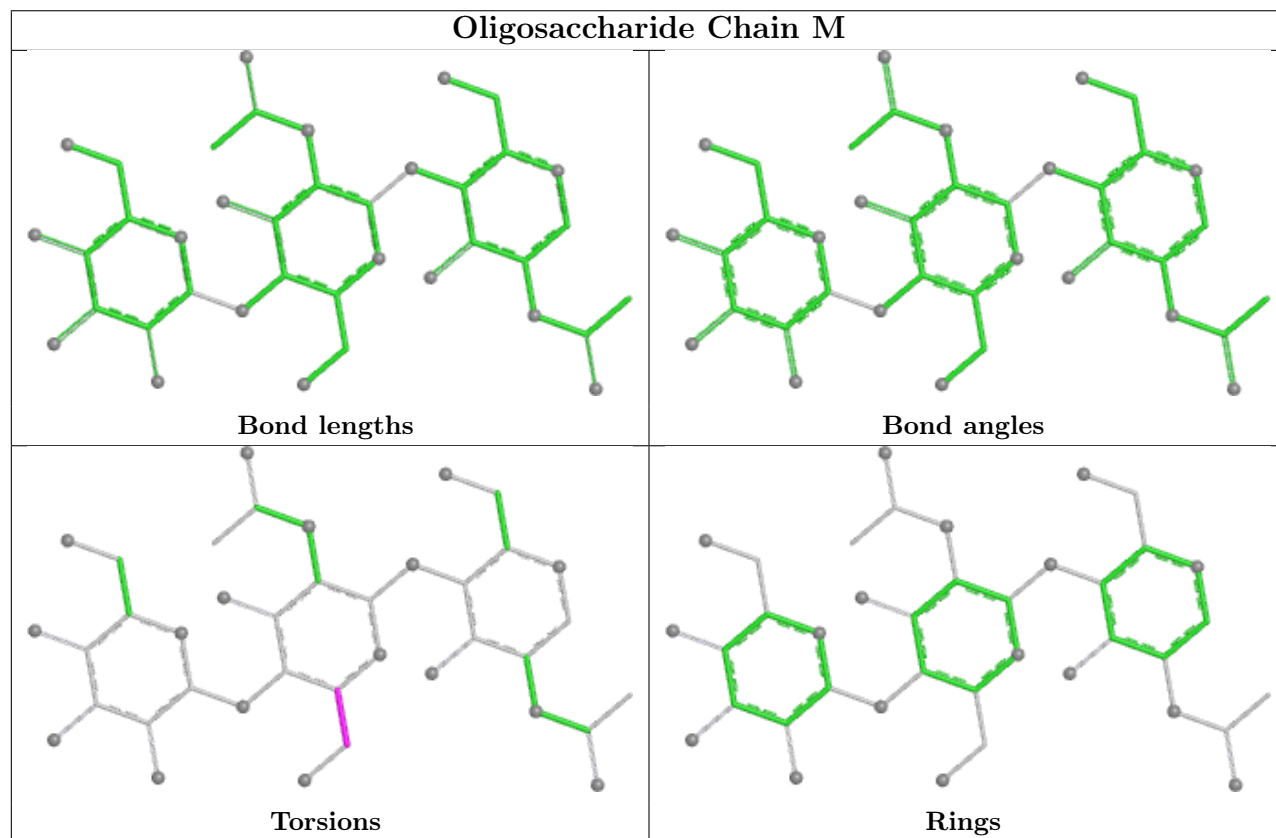
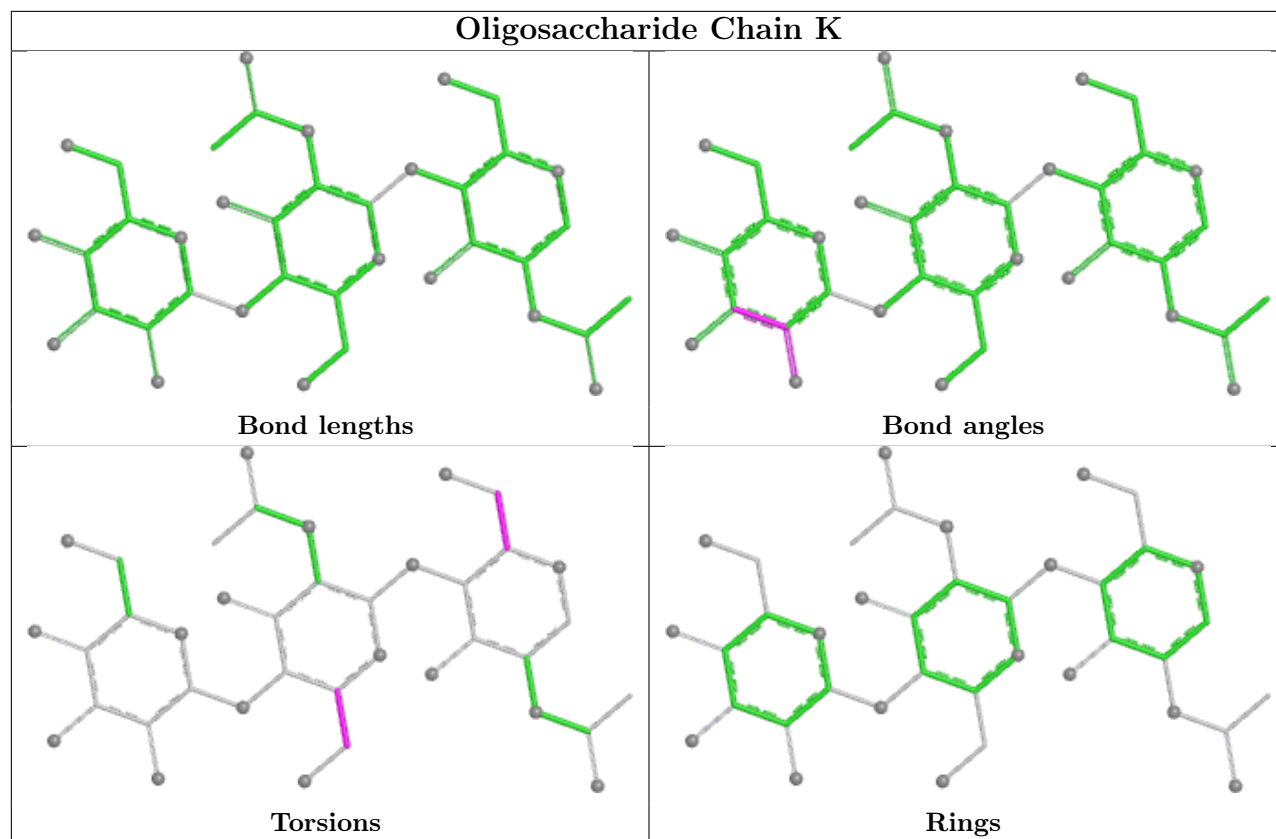
Continued on next page...

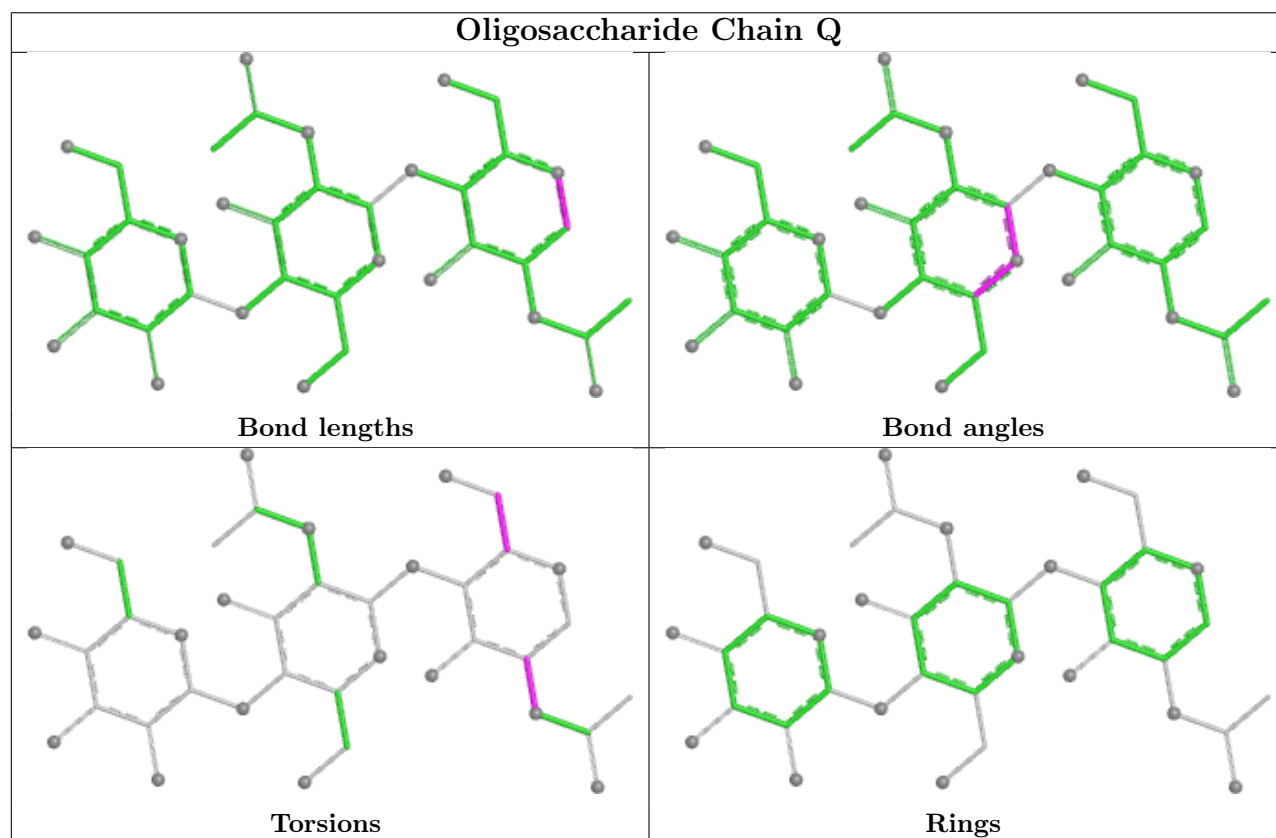
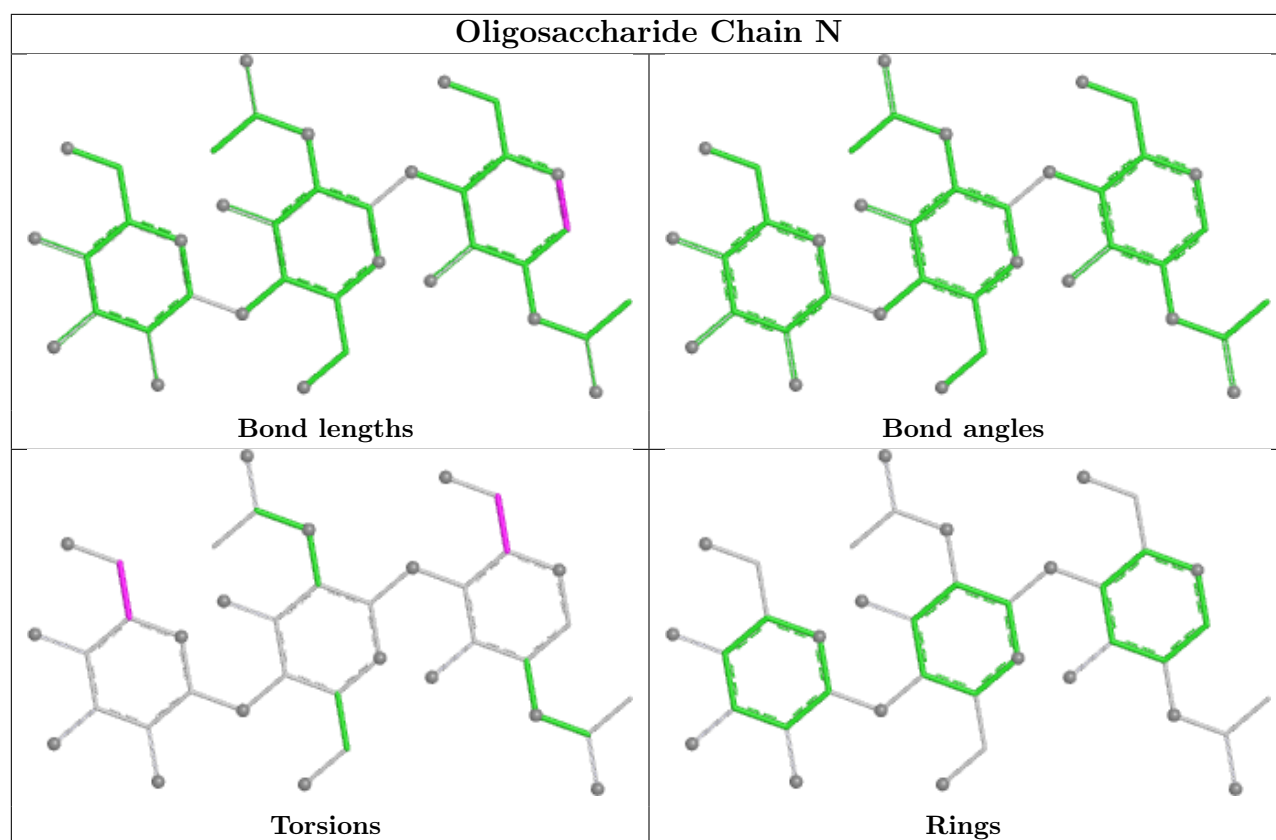
Continued from previous page...

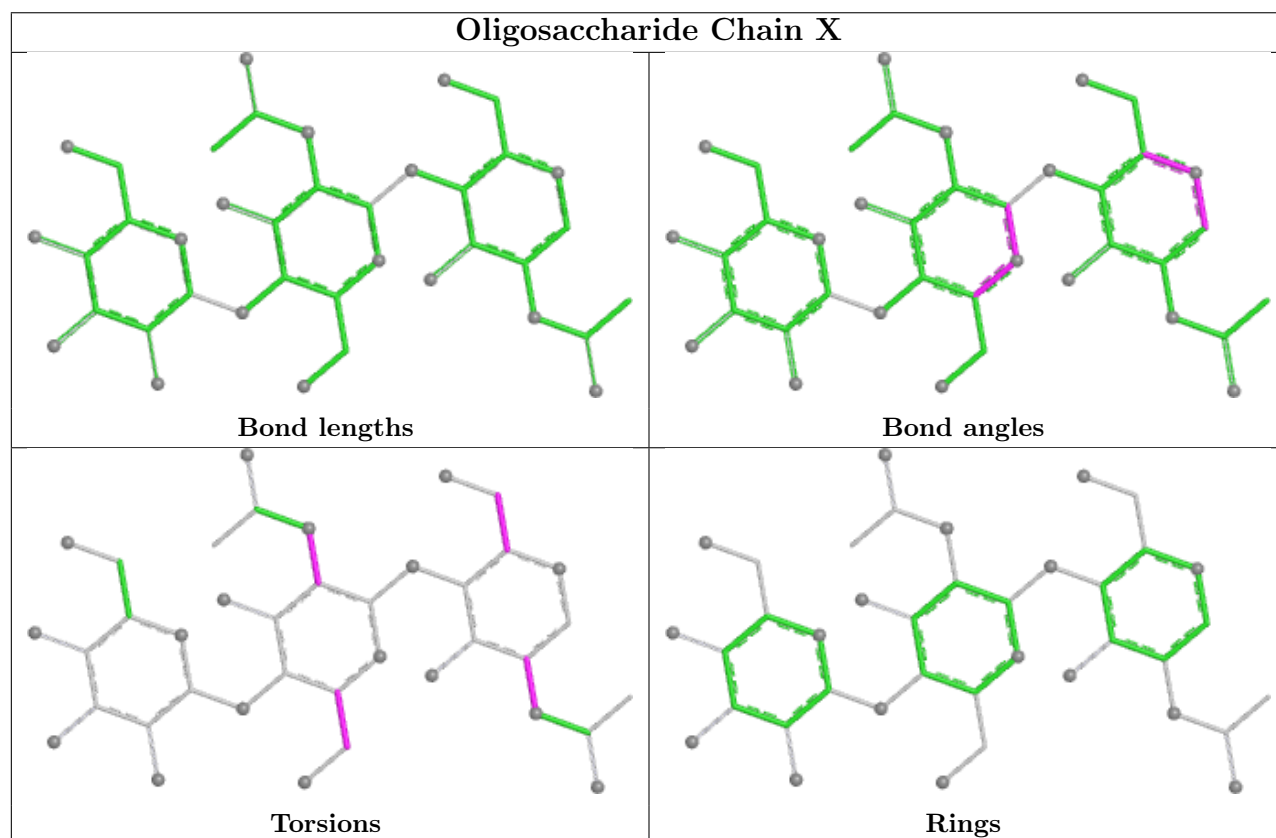
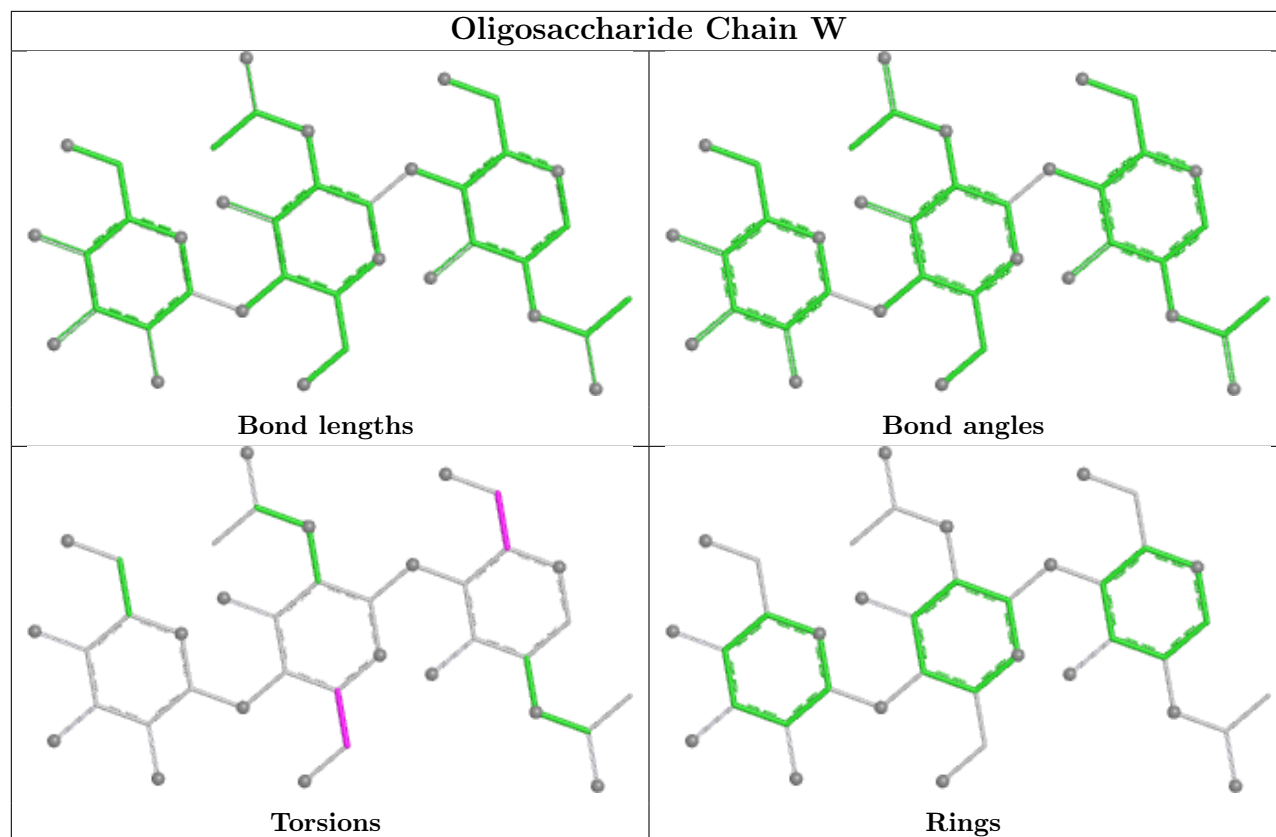
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	1	NAG	1	0
7	h	2	NAG	1	0
3	j	1	NAG	4	0
2	F	2	NAG	1	0
2	X	1	NAG	1	0
2	N	2	NAG	1	0
3	d	2	NAG	1	0
4	U	5	MAN	2	0
2	F	1	NAG	1	0
4	U	1	NAG	1	0
3	c	1	NAG	1	0
3	O	1	NAG	4	0
4	G	2	NAG	1	0
2	e	1	NAG	2	0
3	d	1	NAG	4	0
3	l	1	NAG	1	0
3	O	2	NAG	1	0
3	S	1	NAG	6	0
3	b	1	NAG	2	0
2	Y	1	NAG	3	0
3	R	1	NAG	2	0
3	R	2	NAG	2	0
2	M	2	NAG	1	0
3	S	2	NAG	2	0

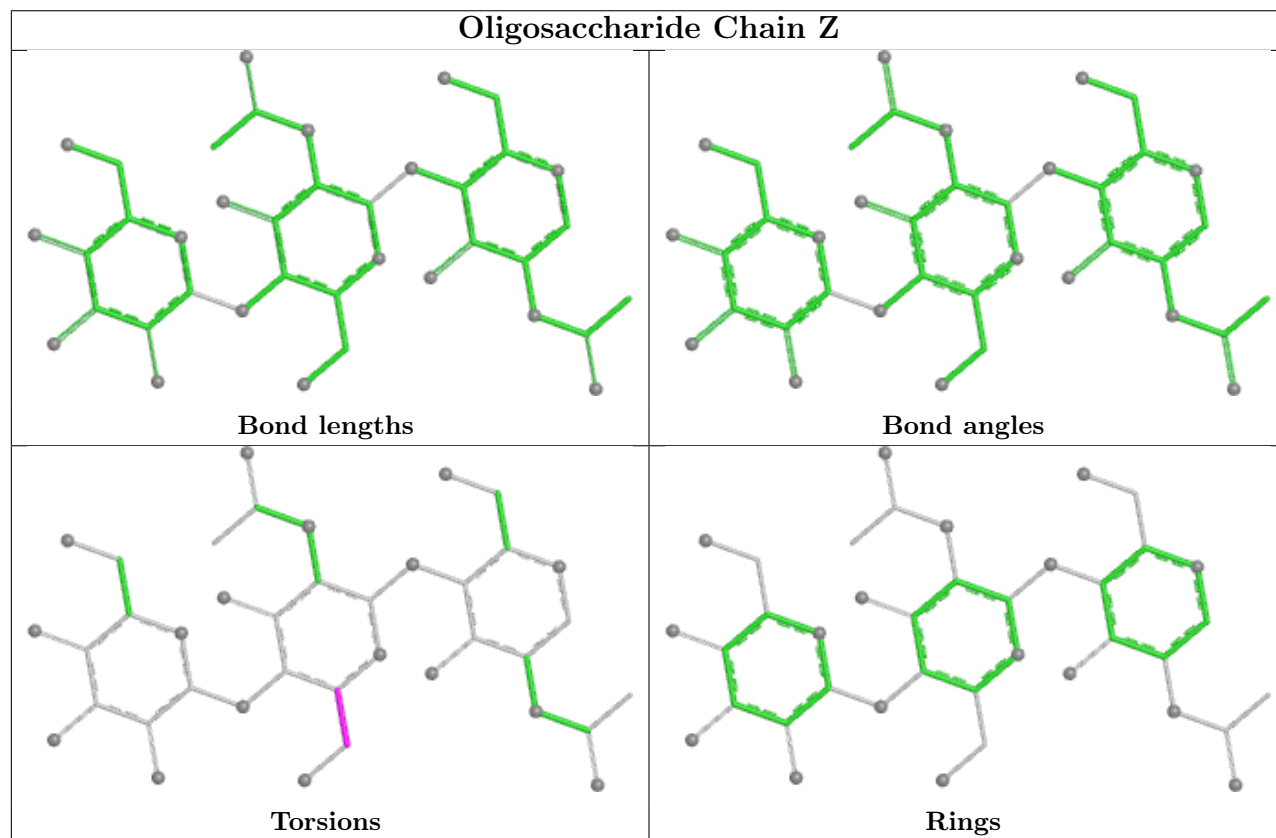
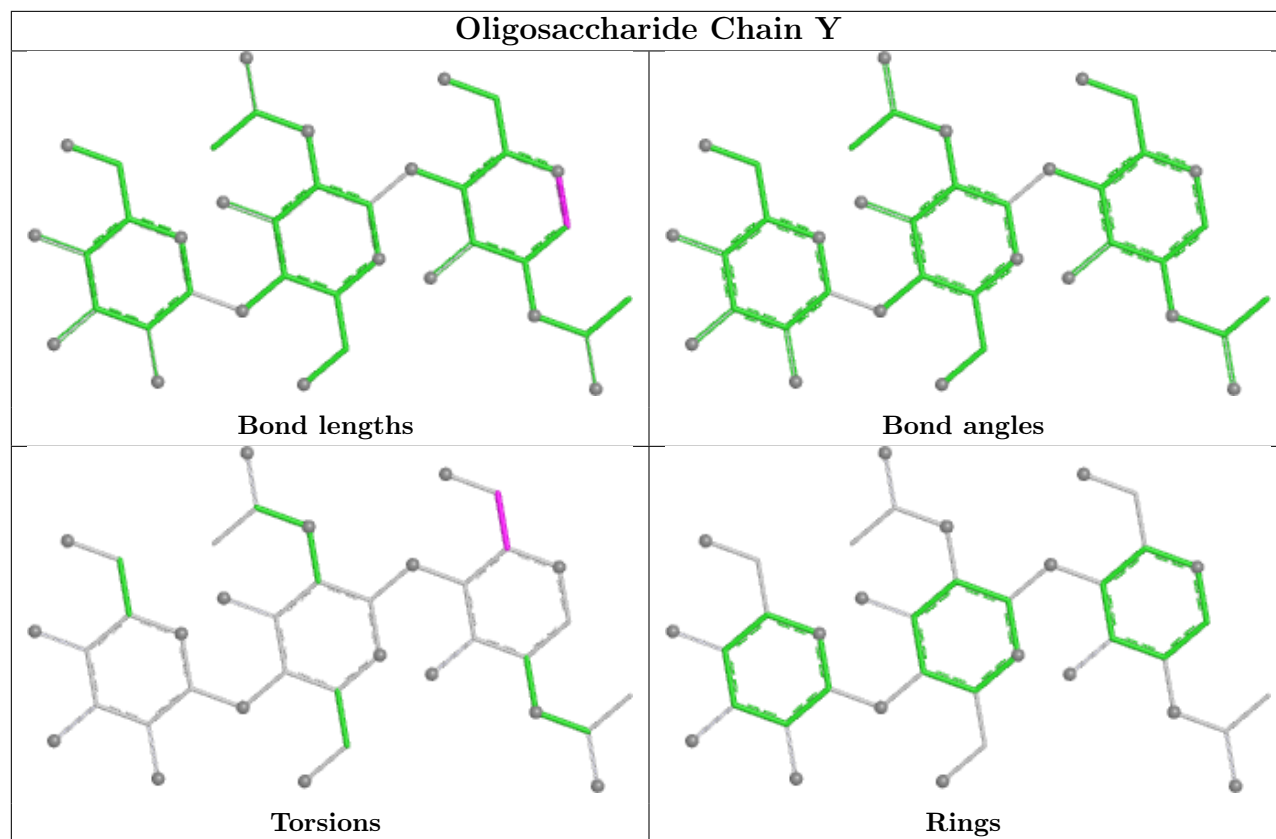
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

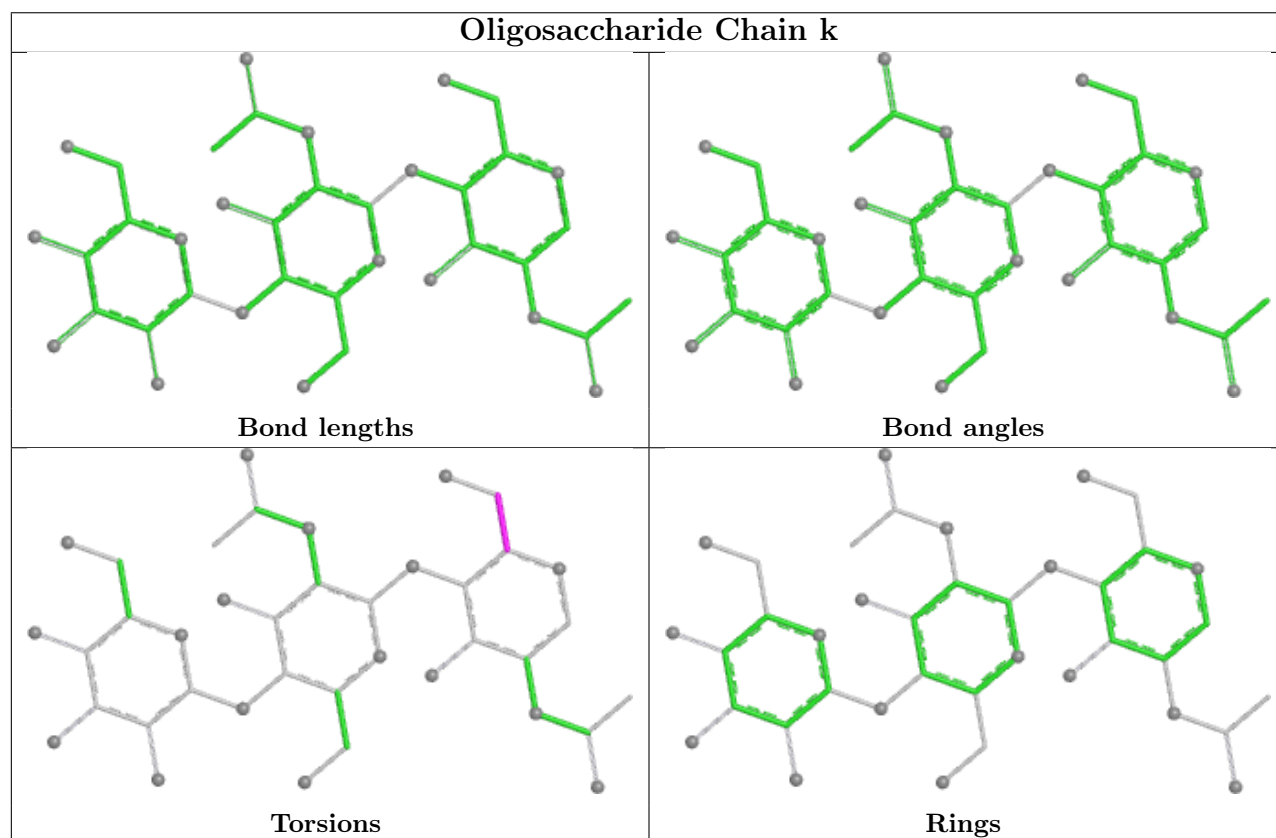
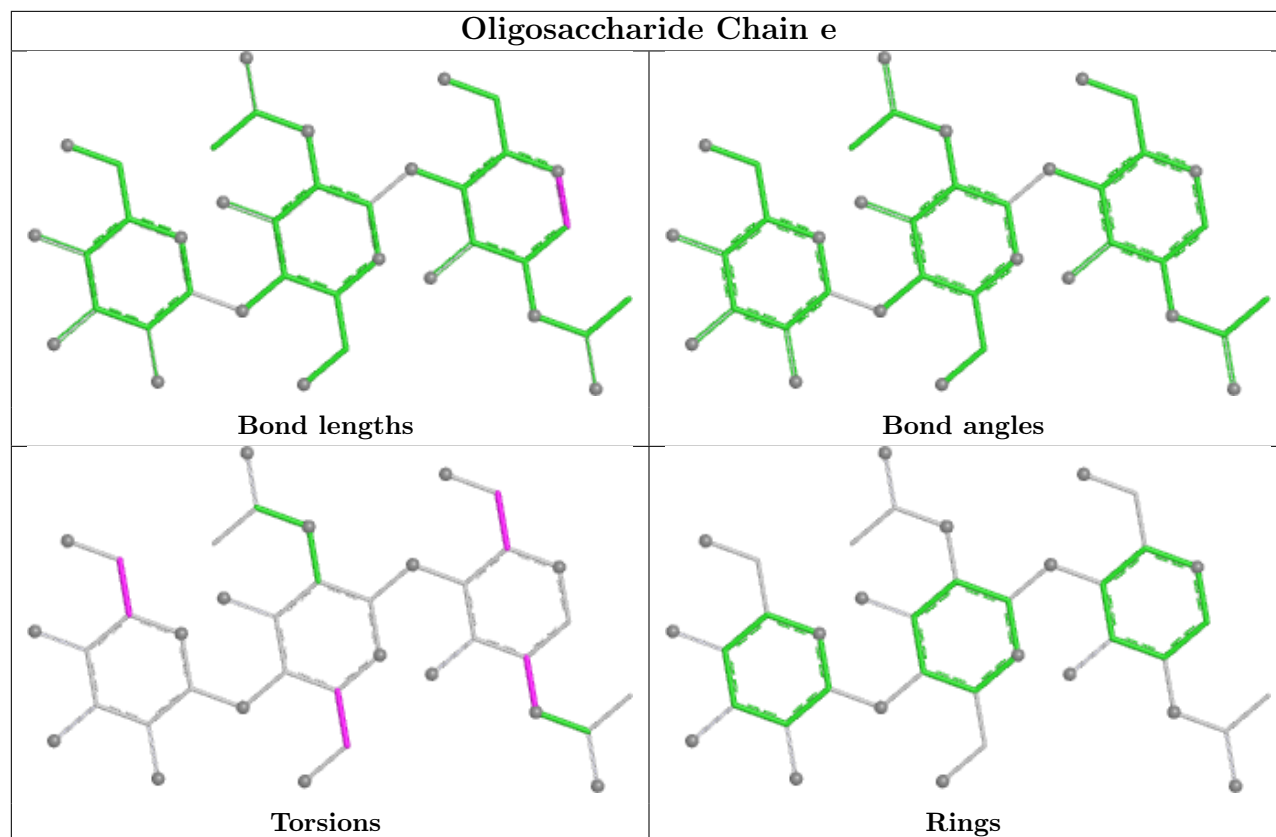


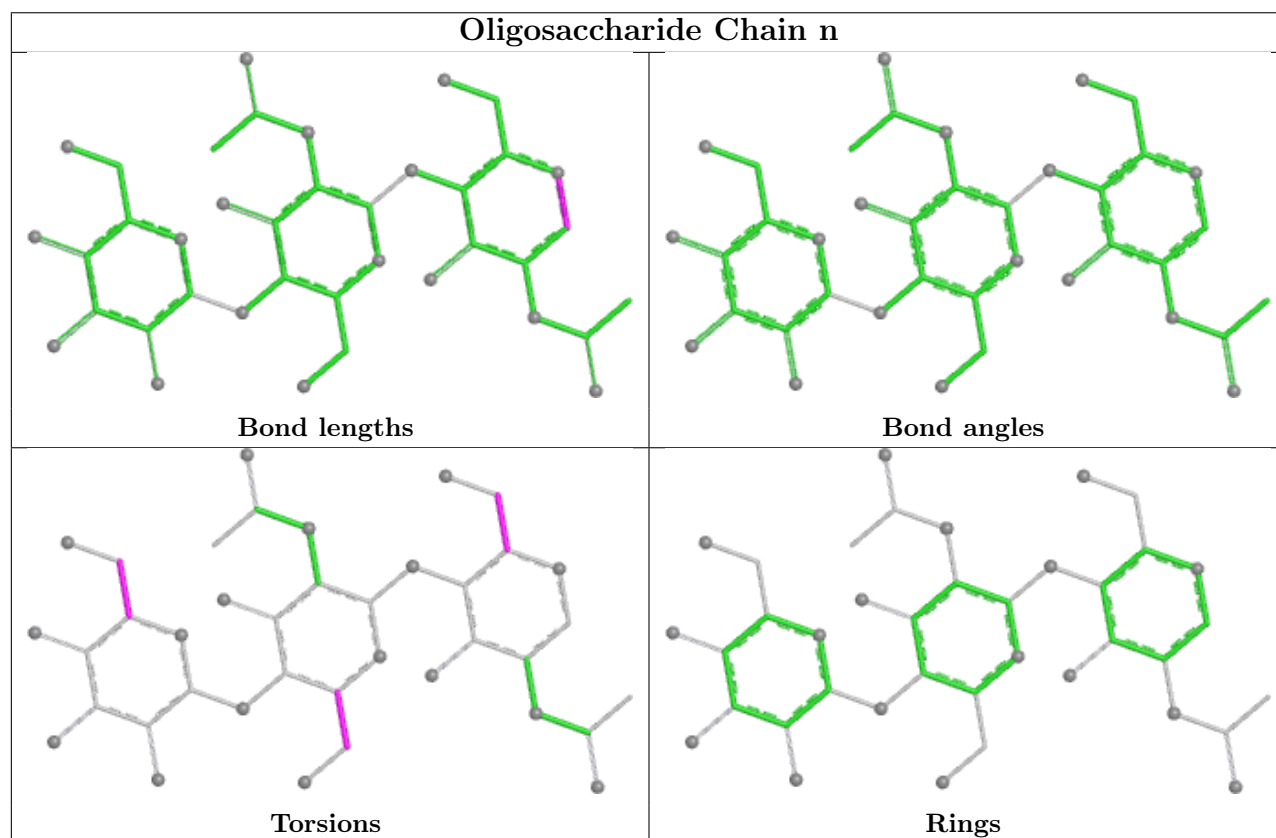
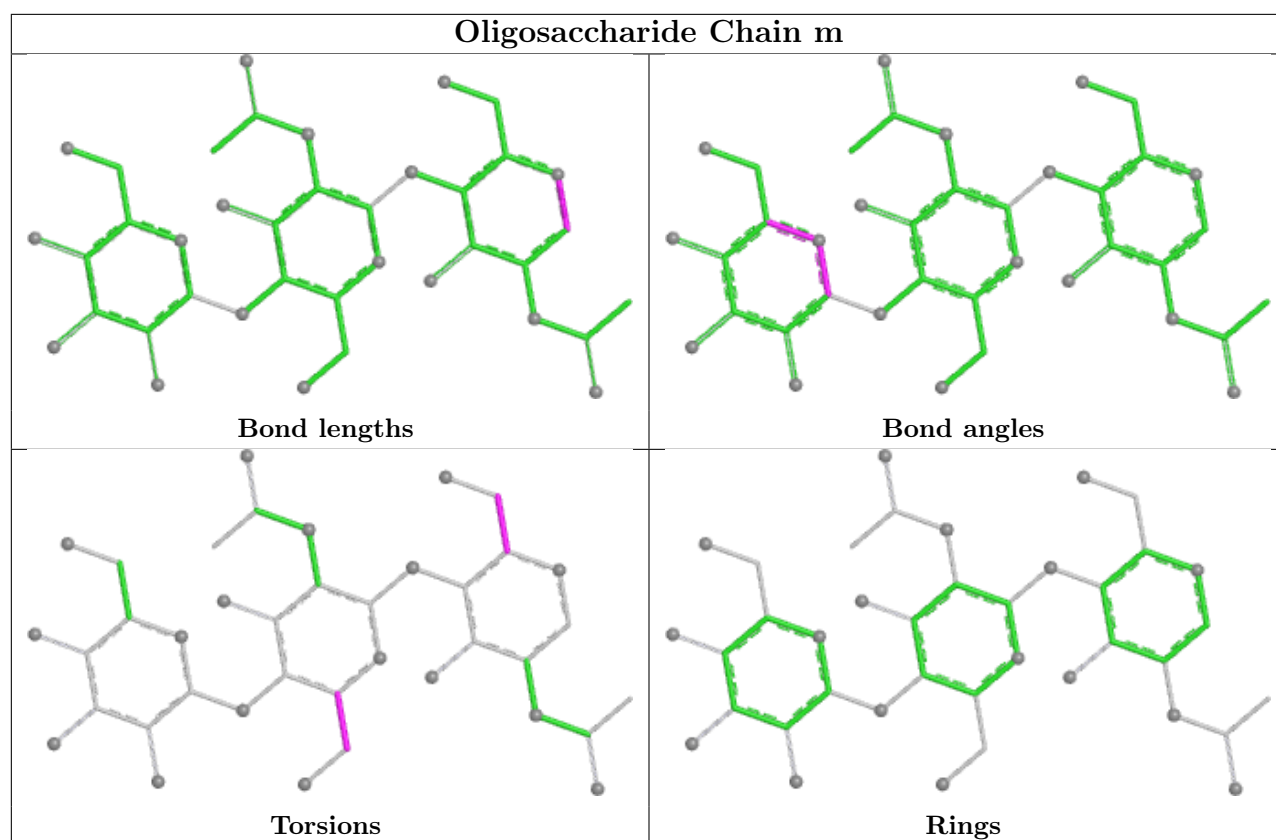


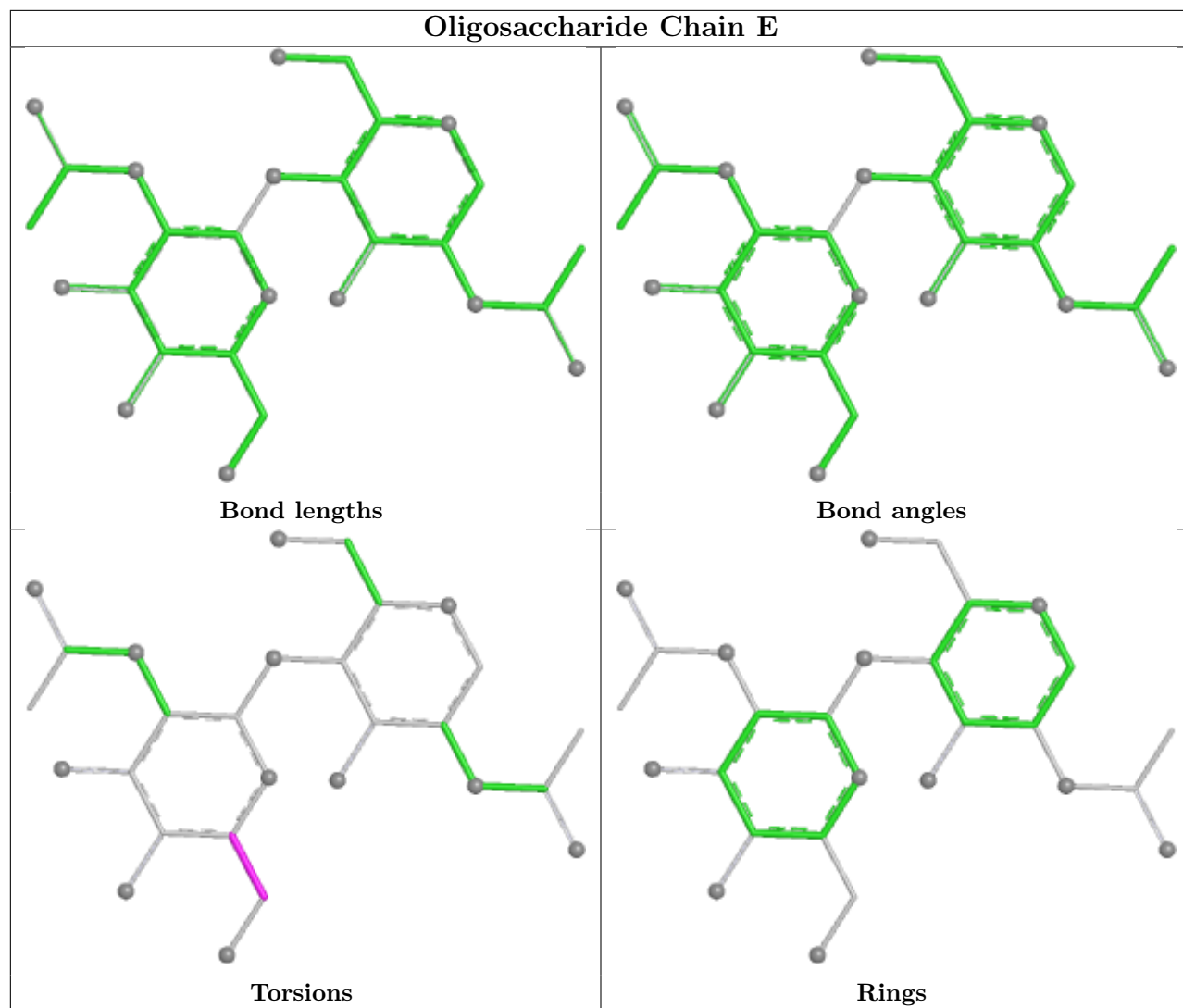


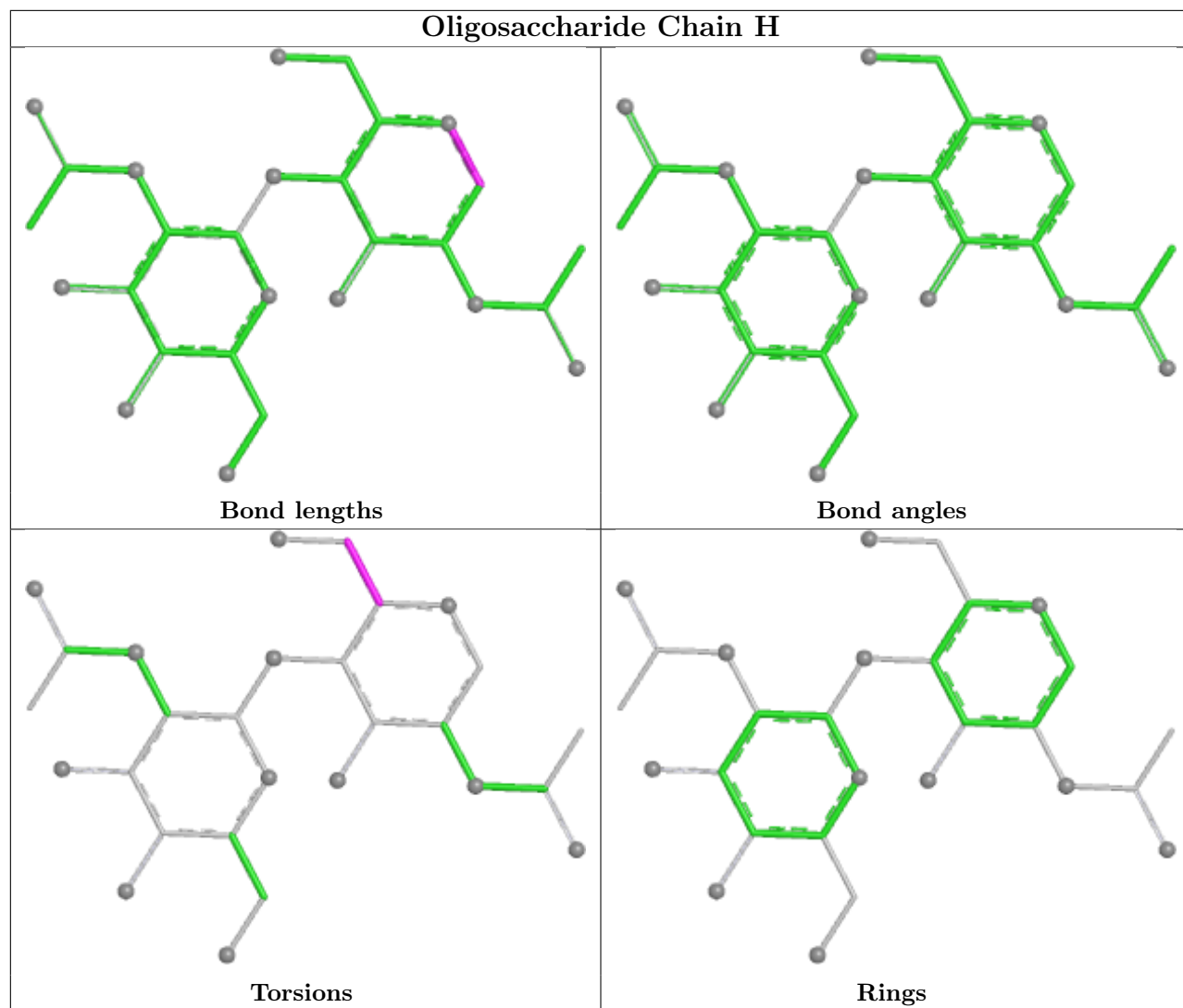


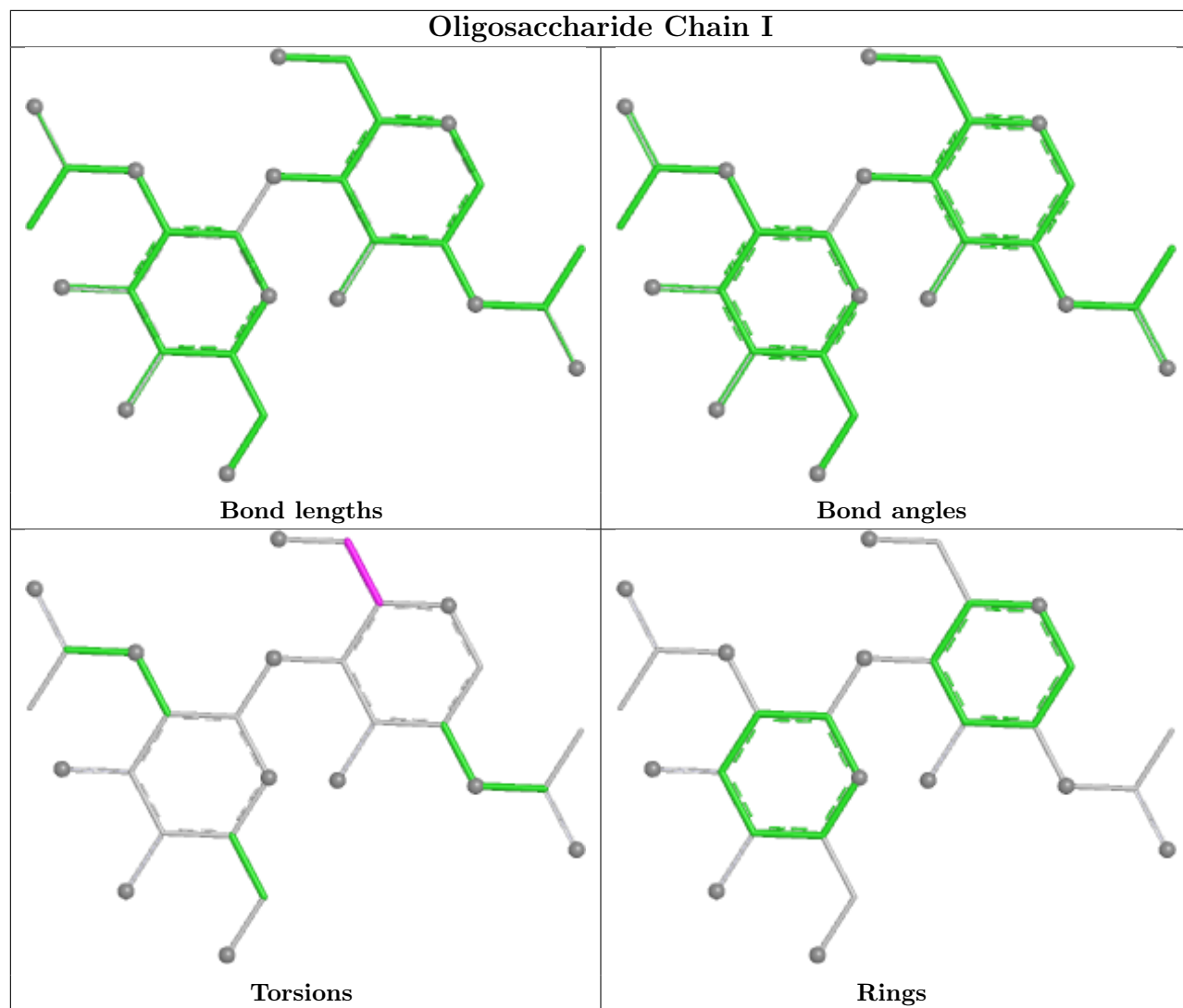


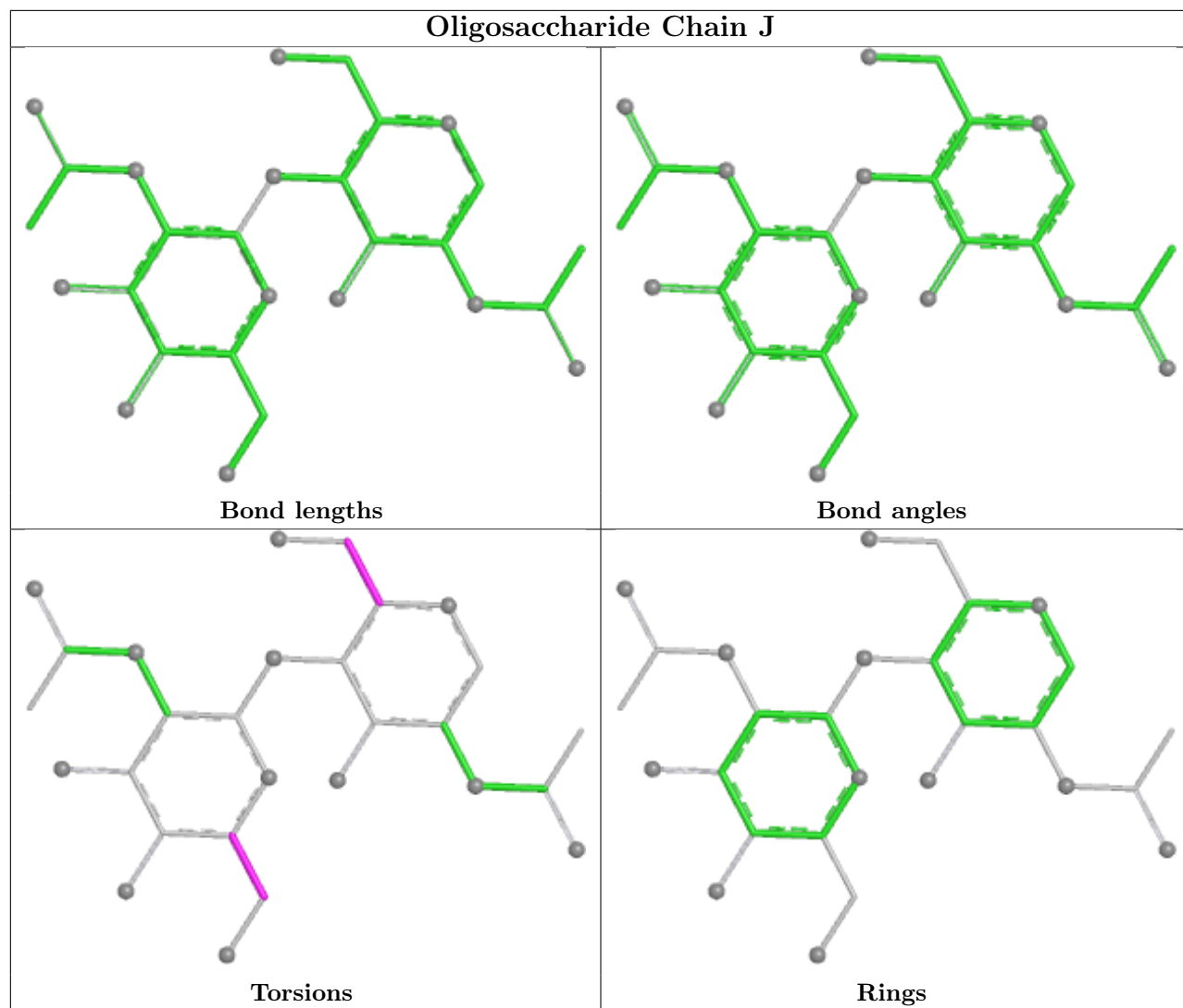


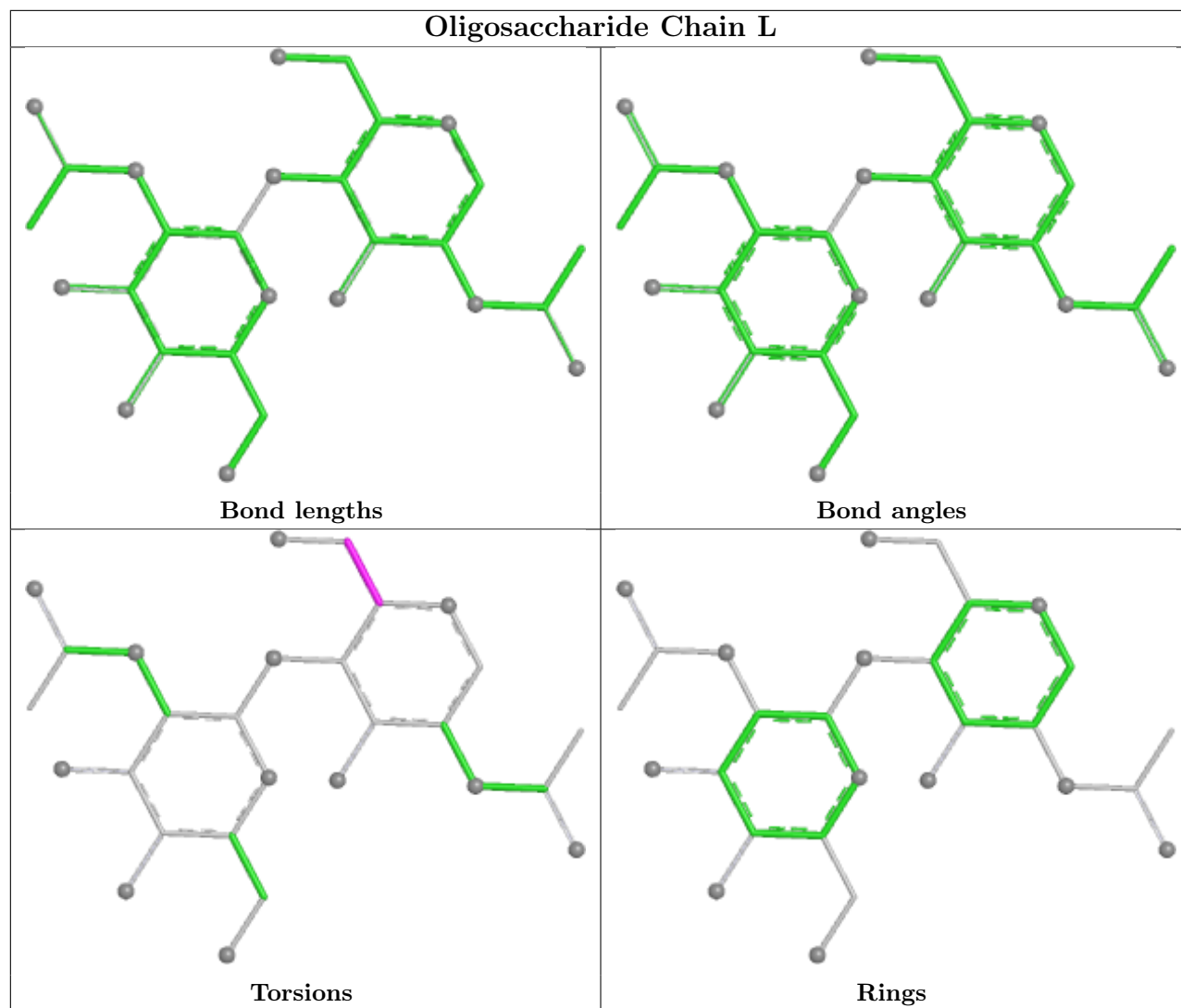


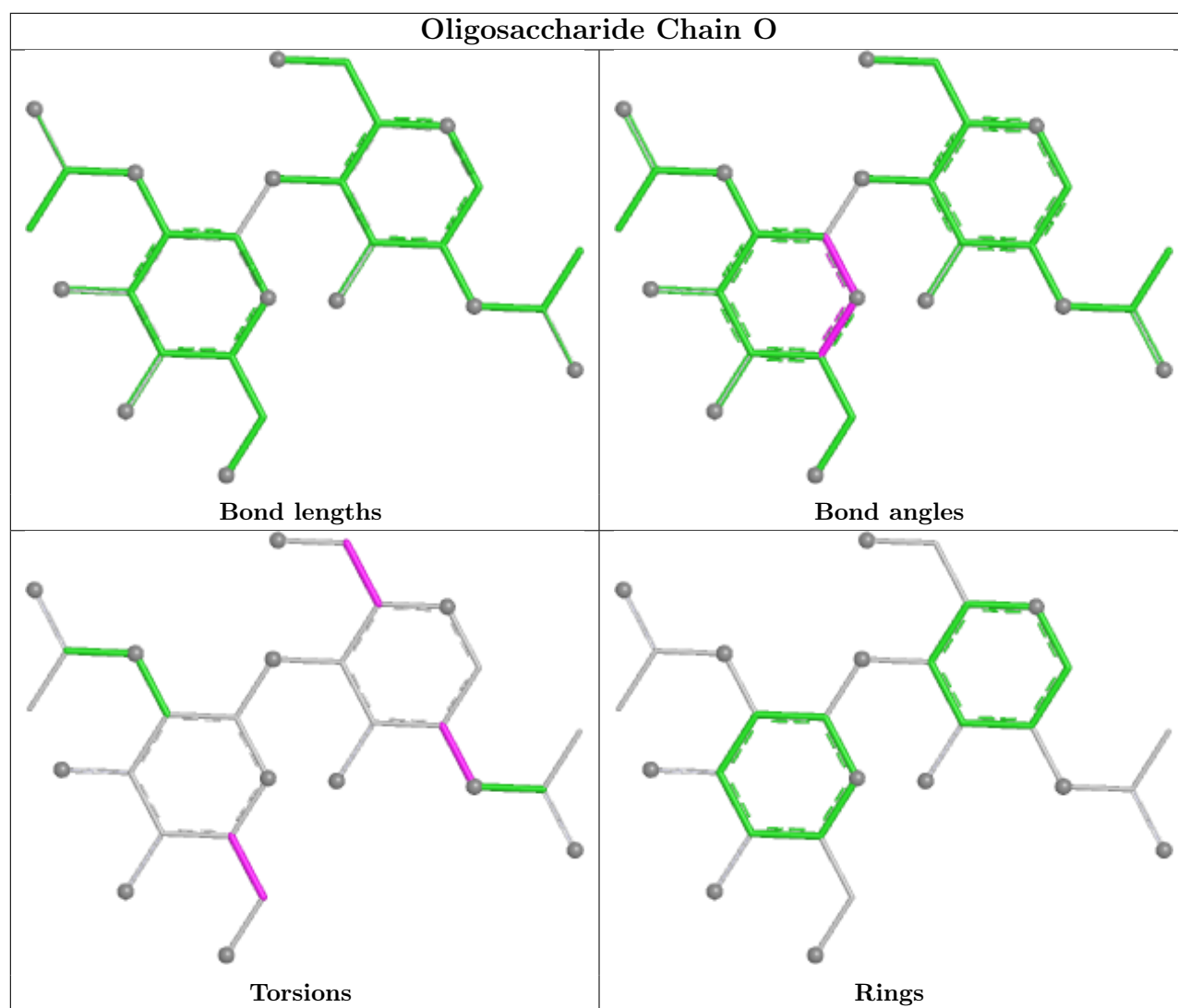


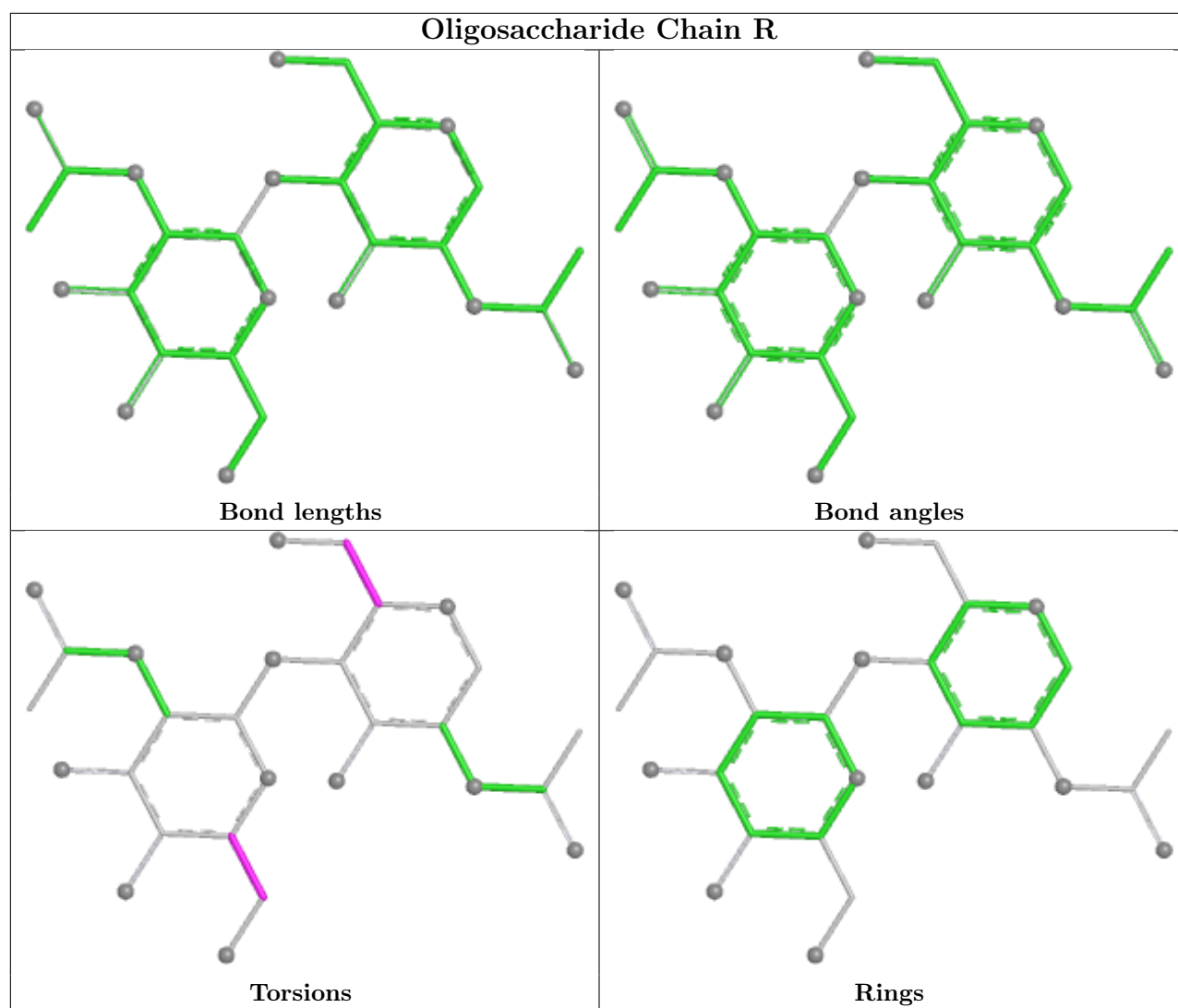


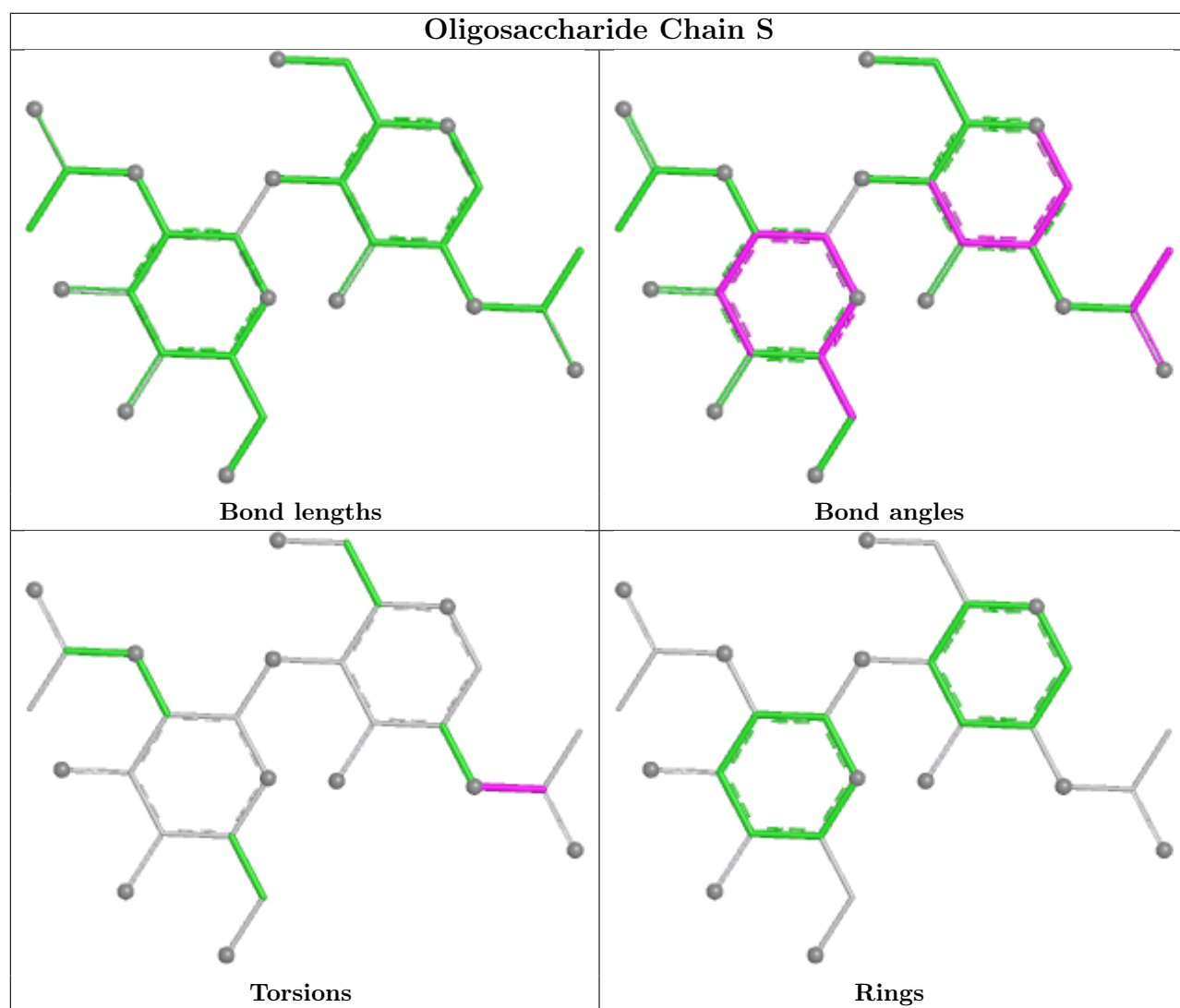


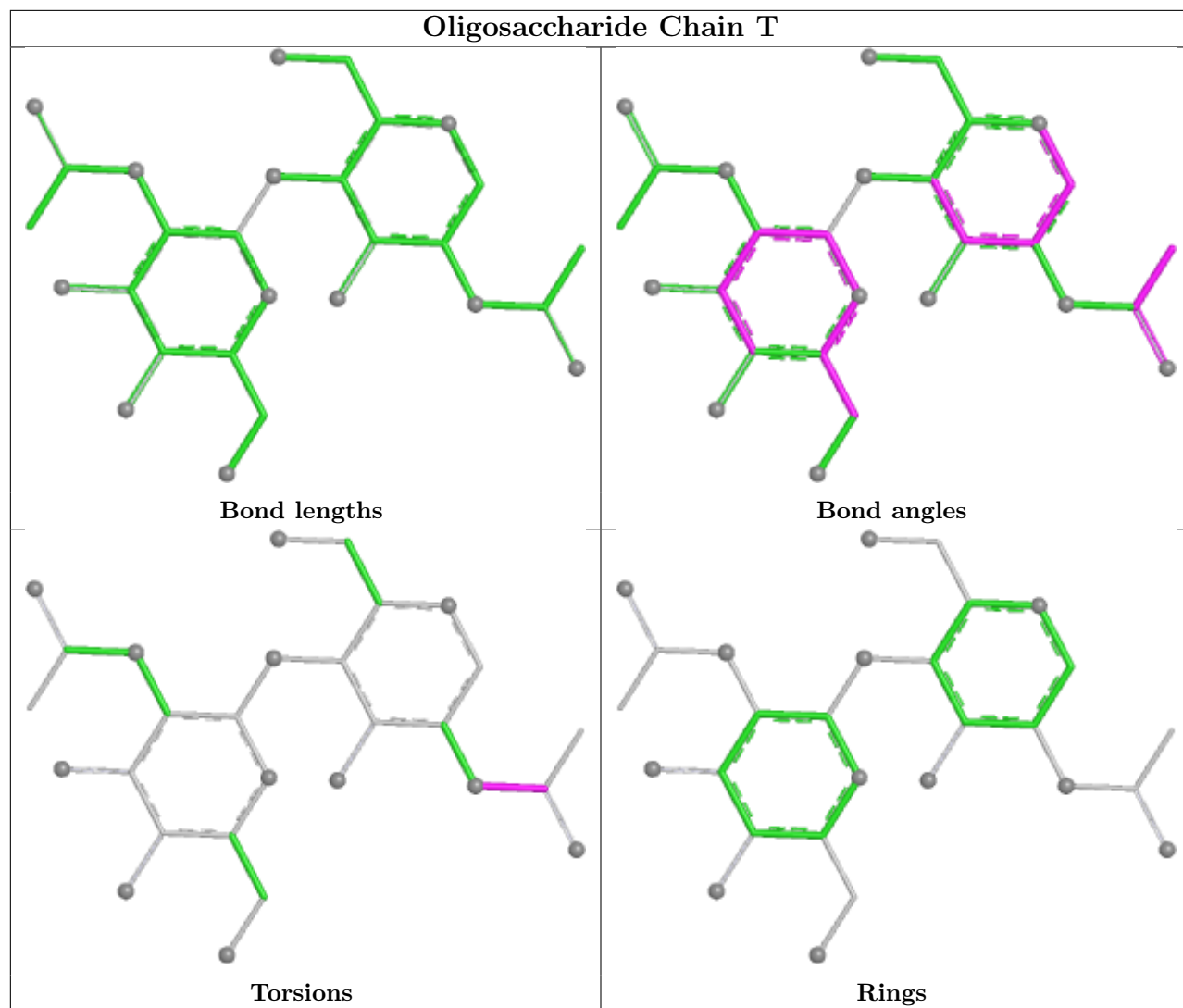


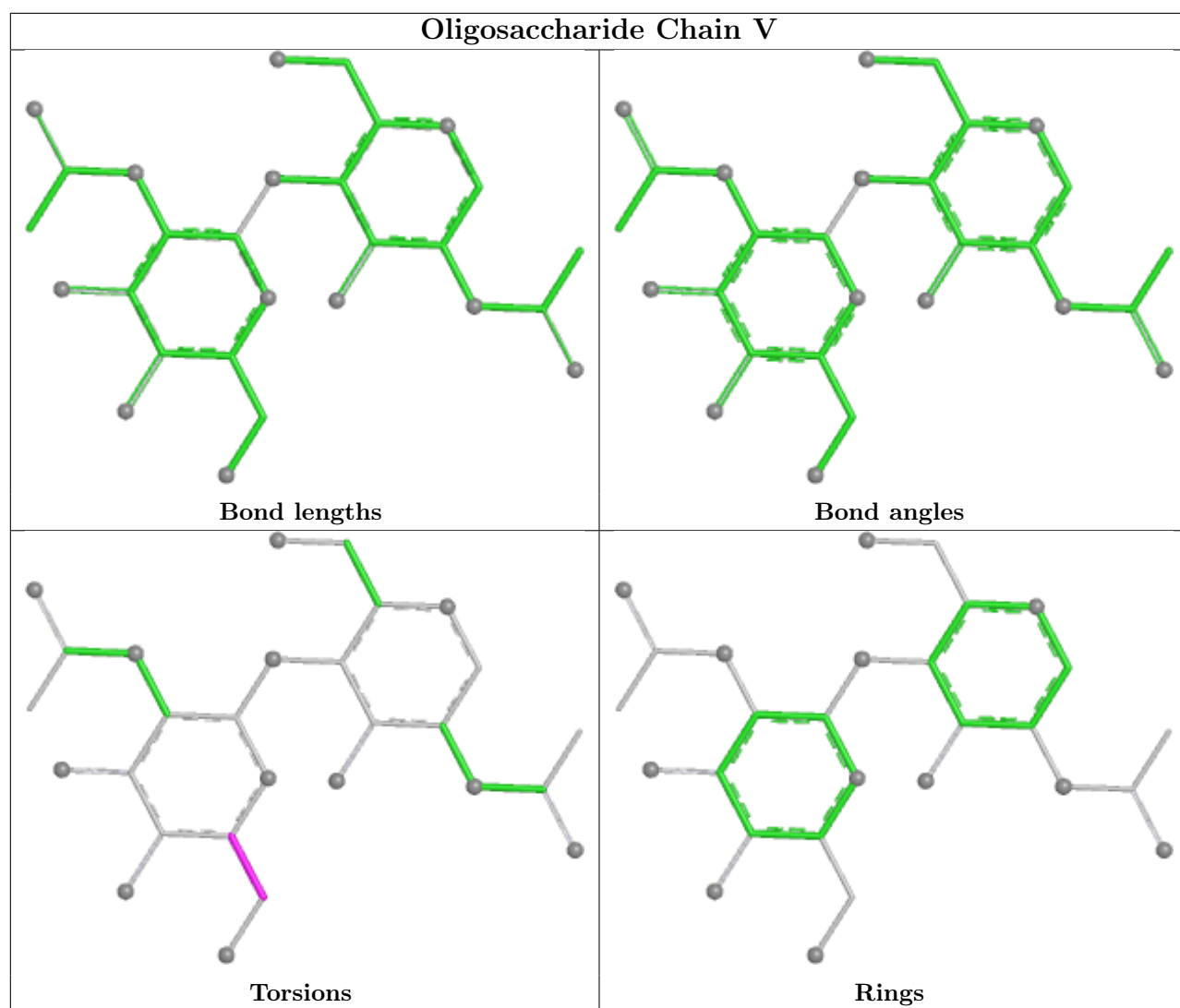


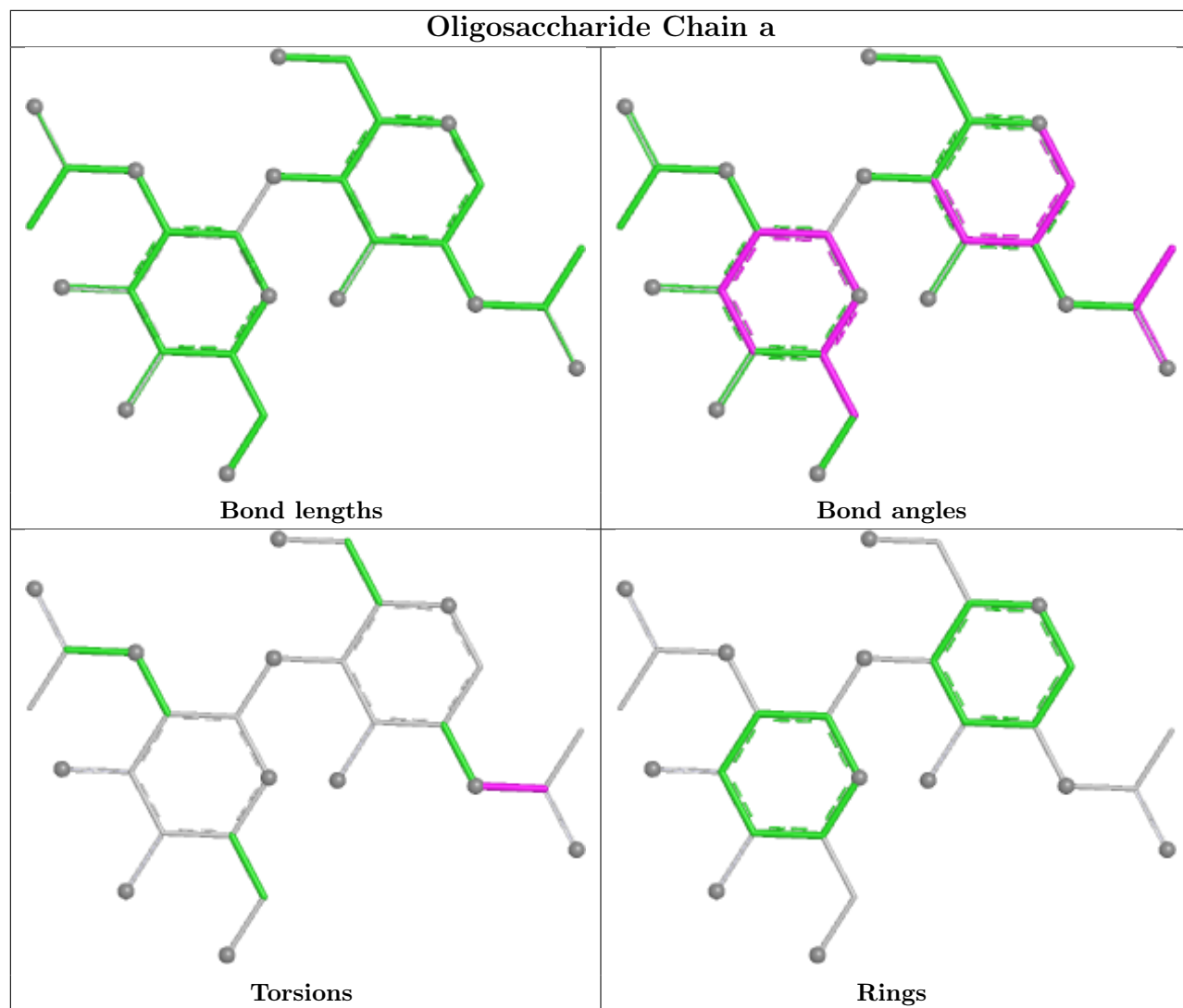


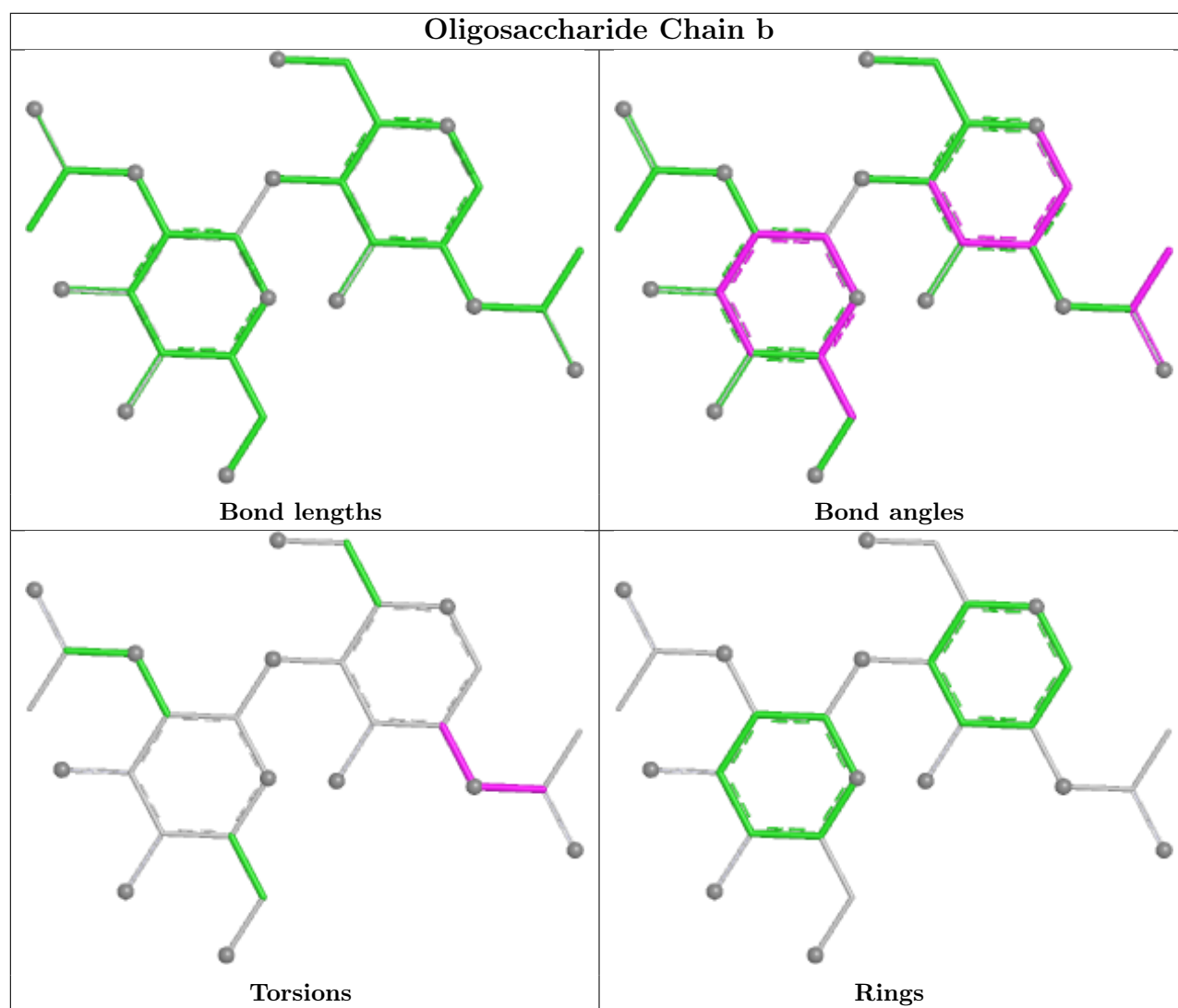


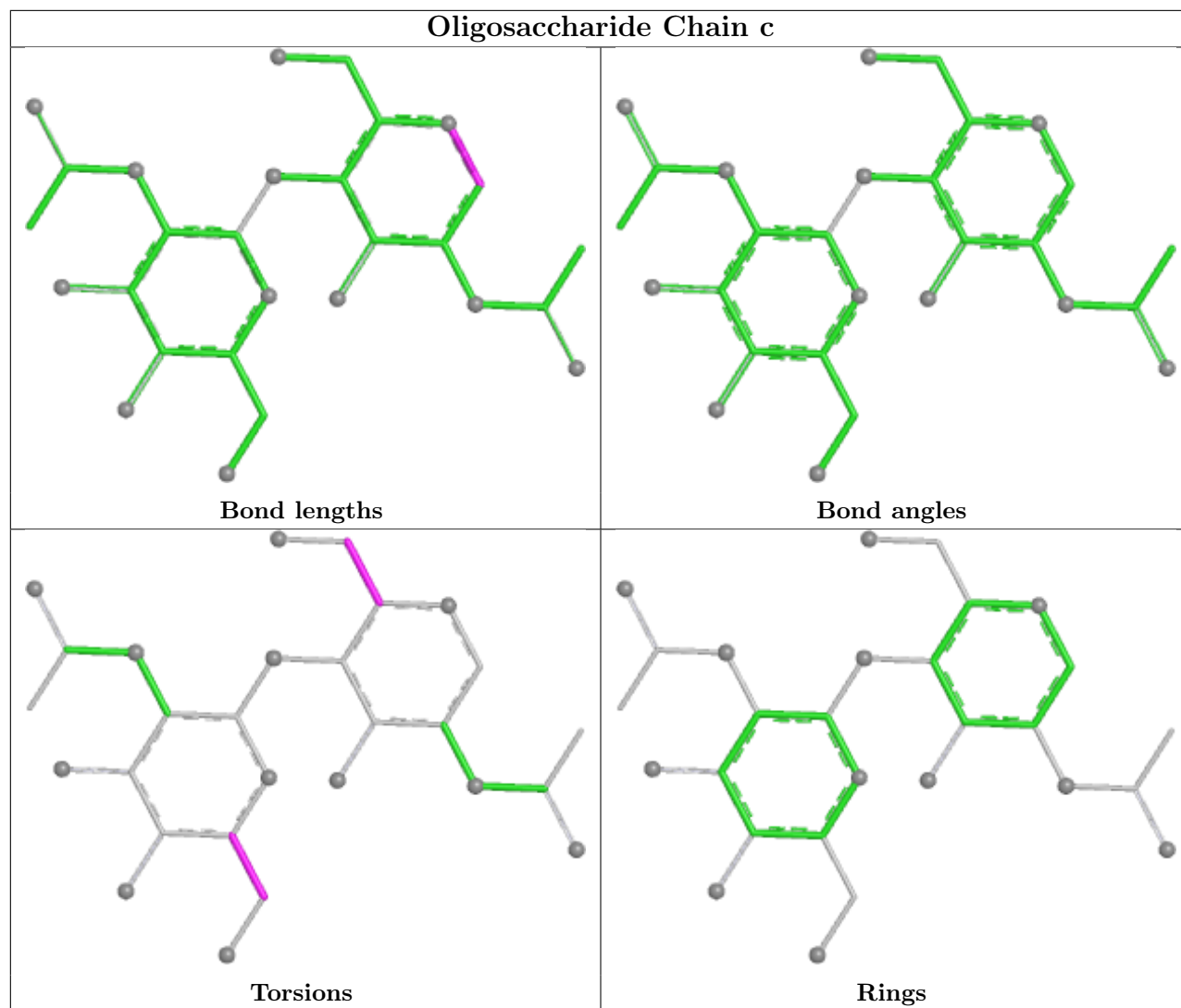


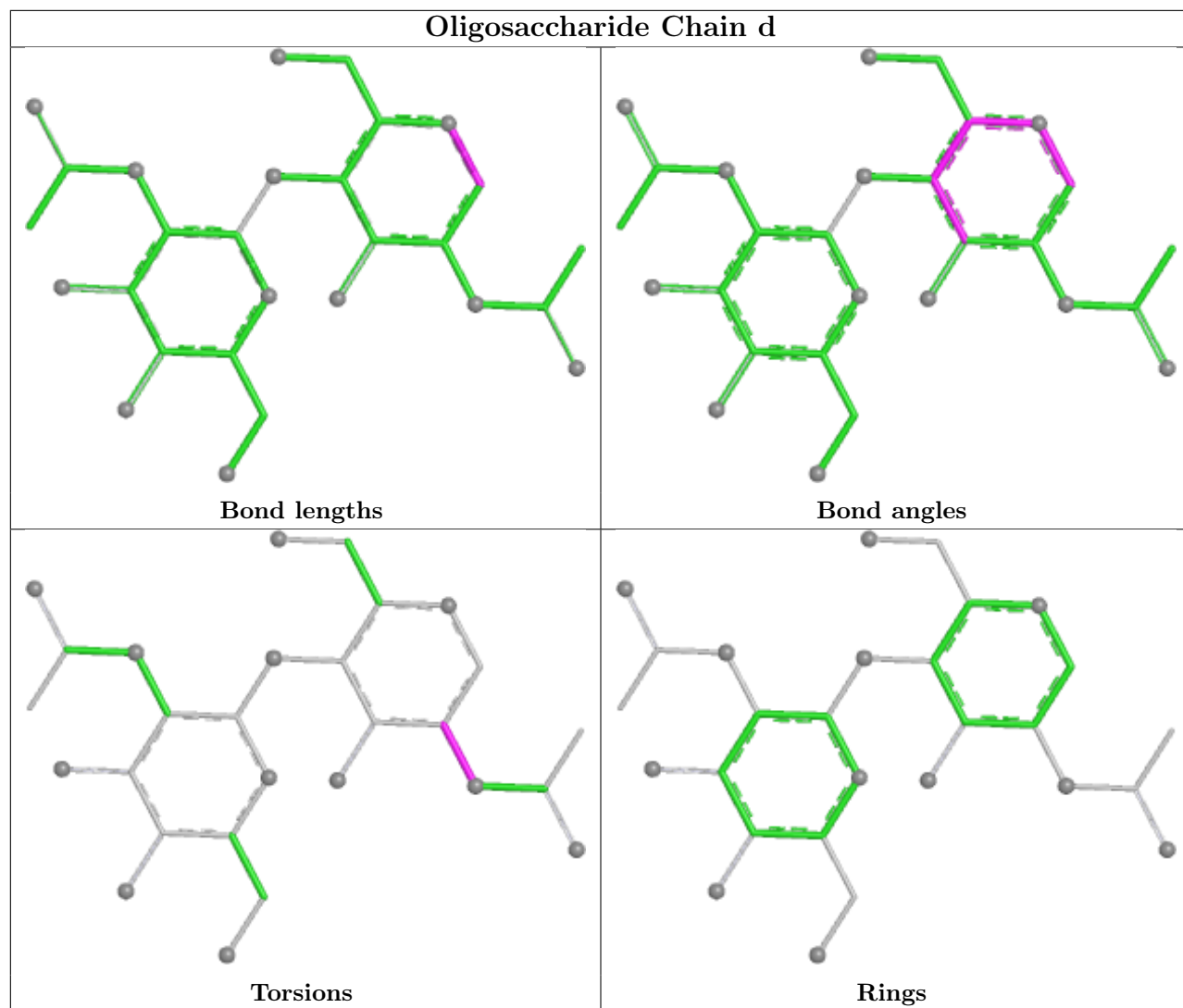


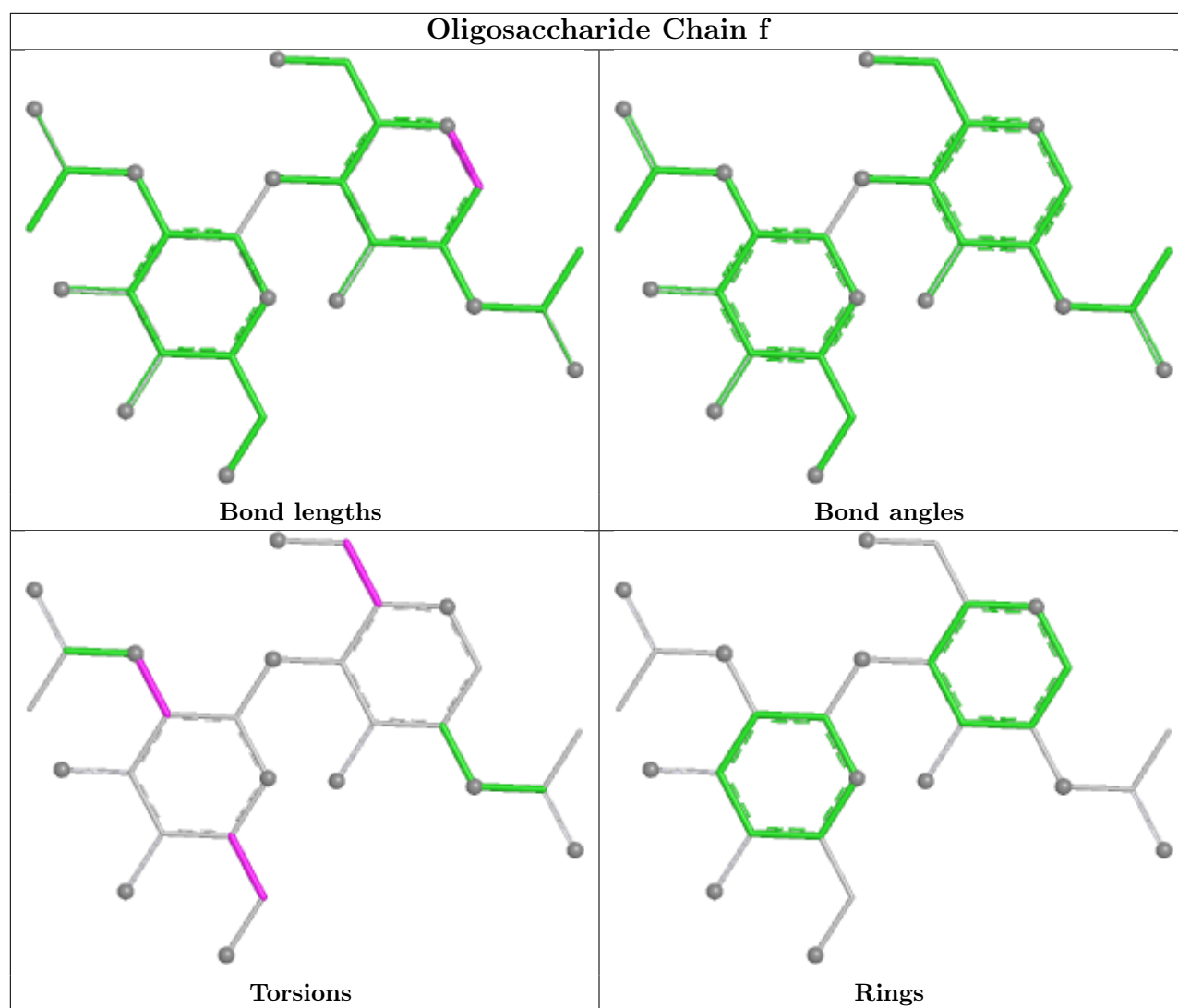


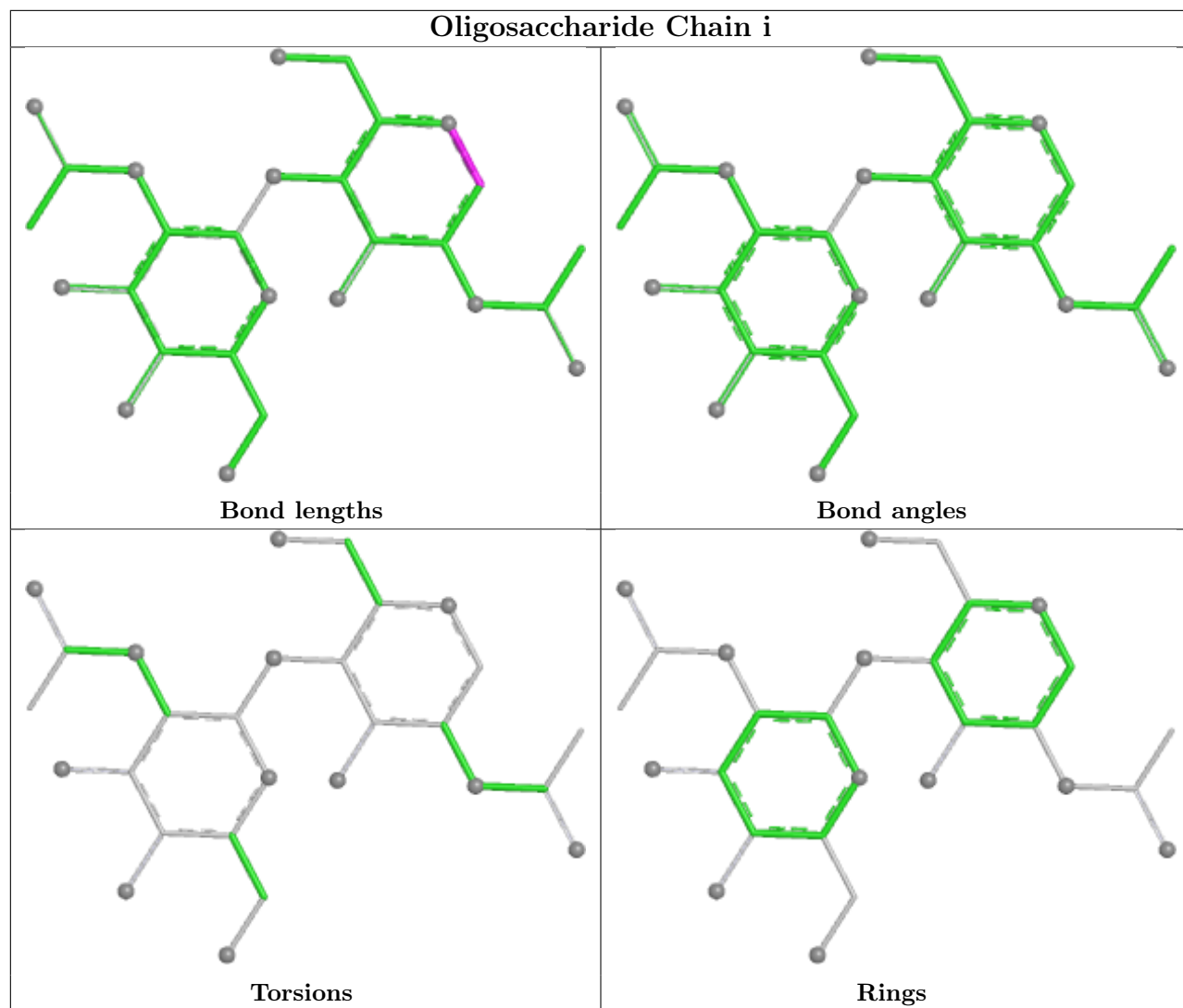


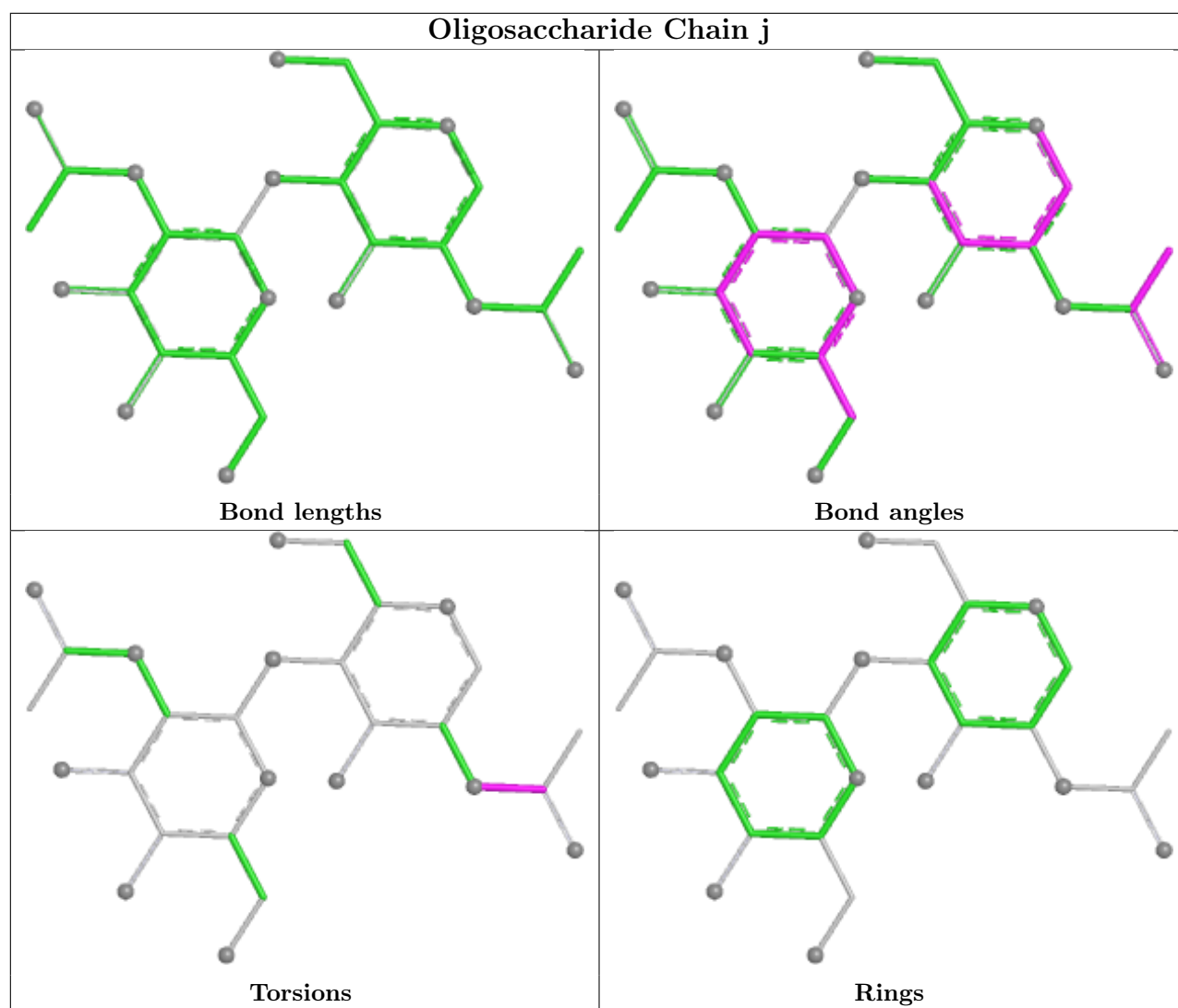


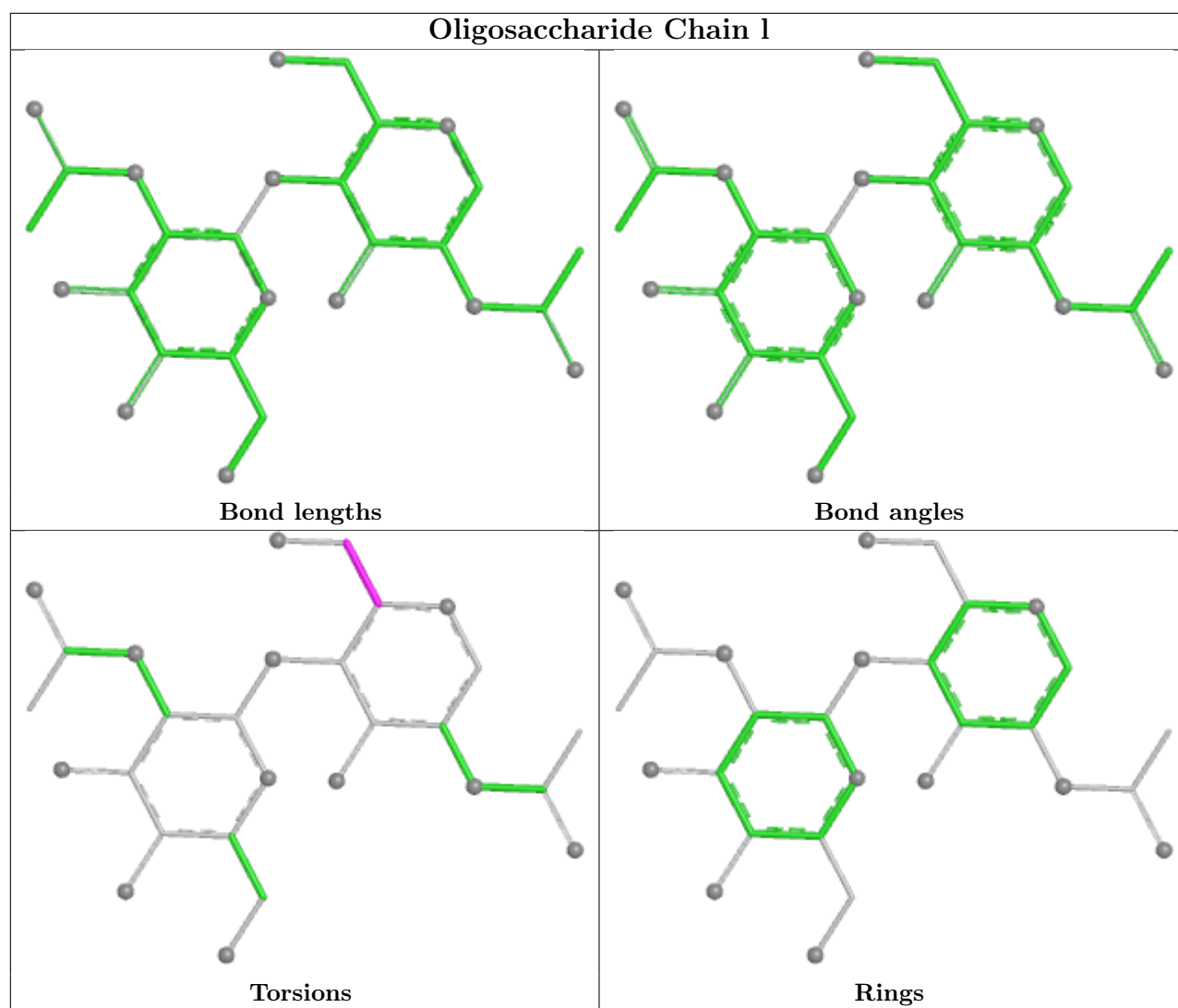


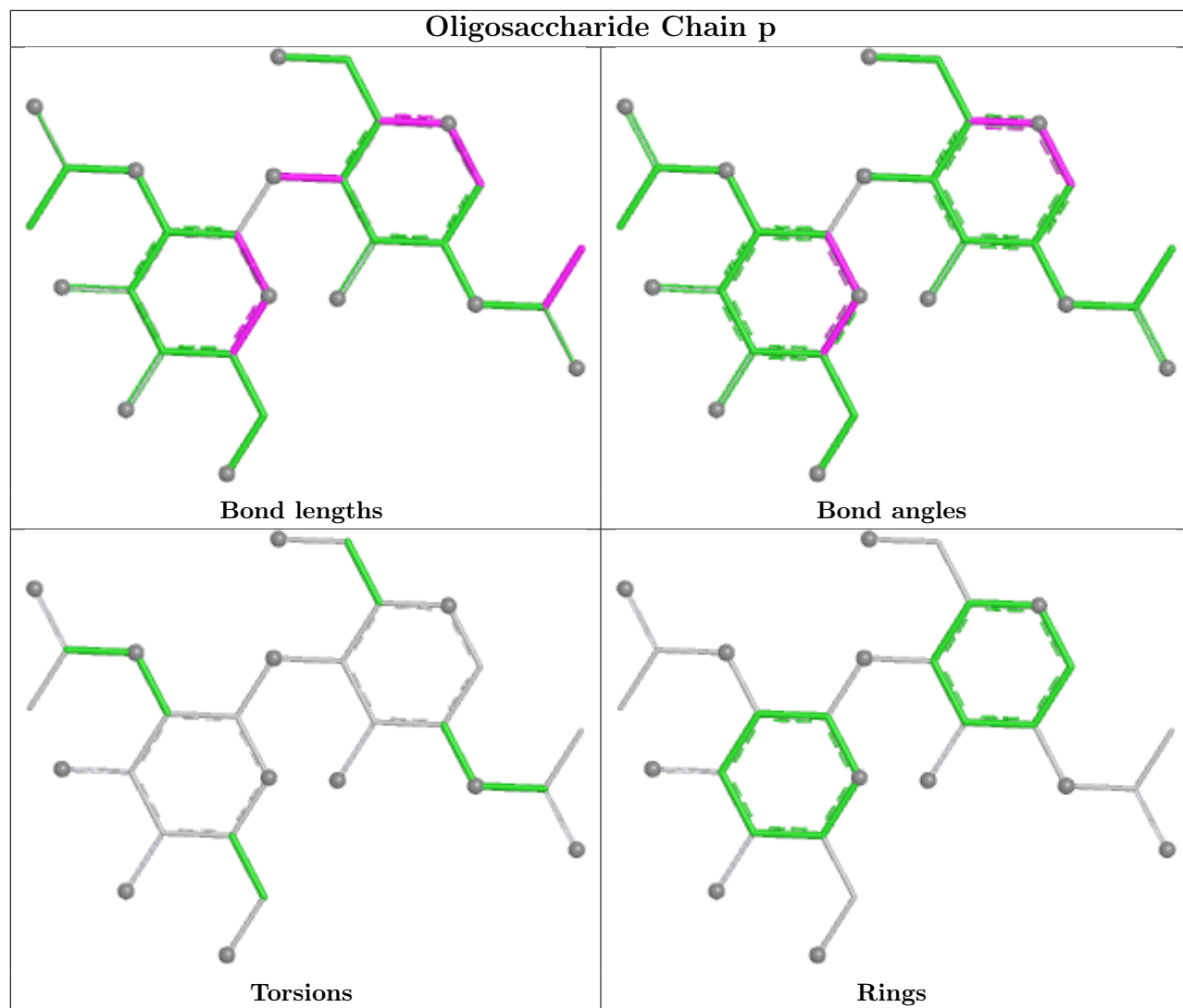


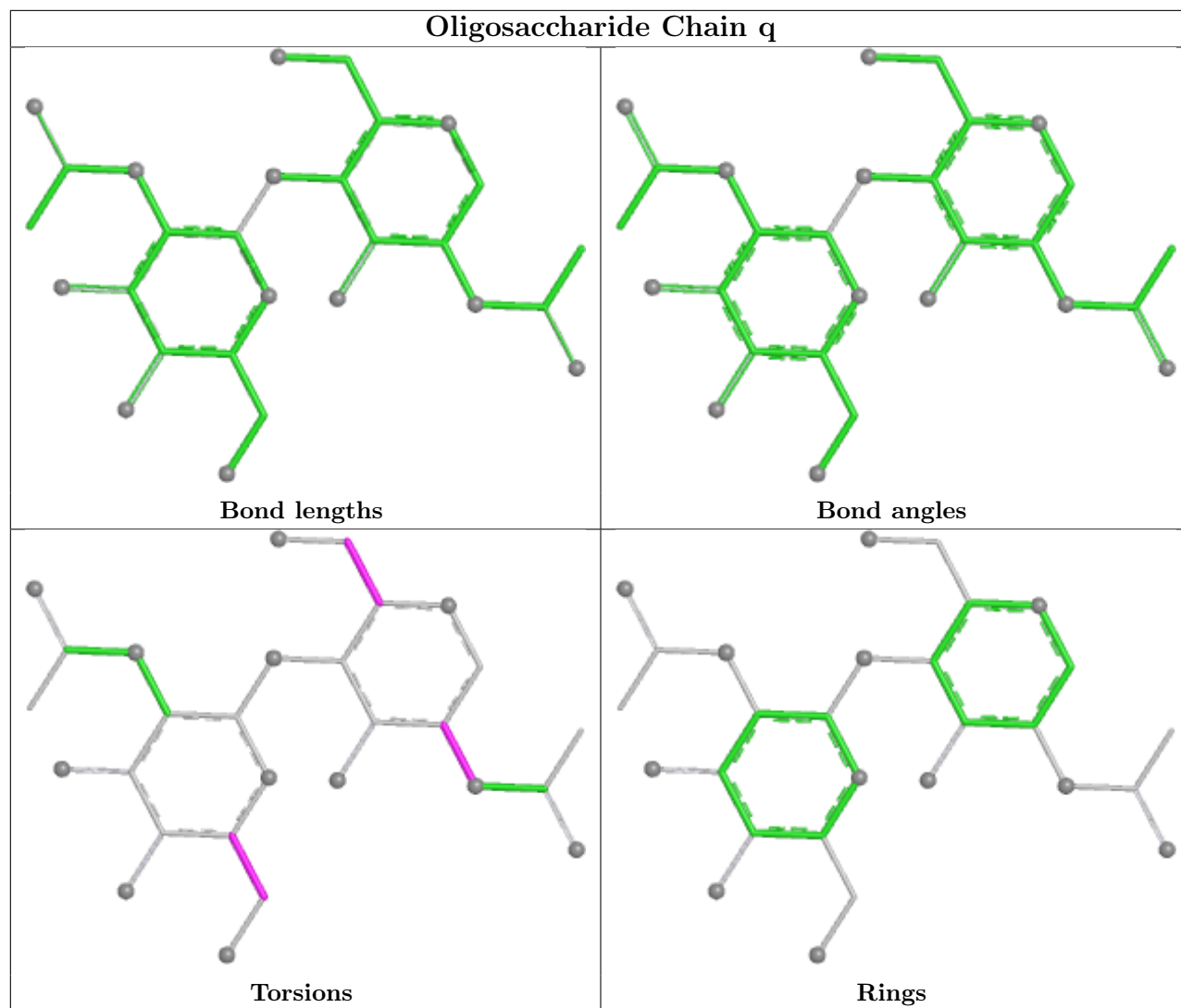


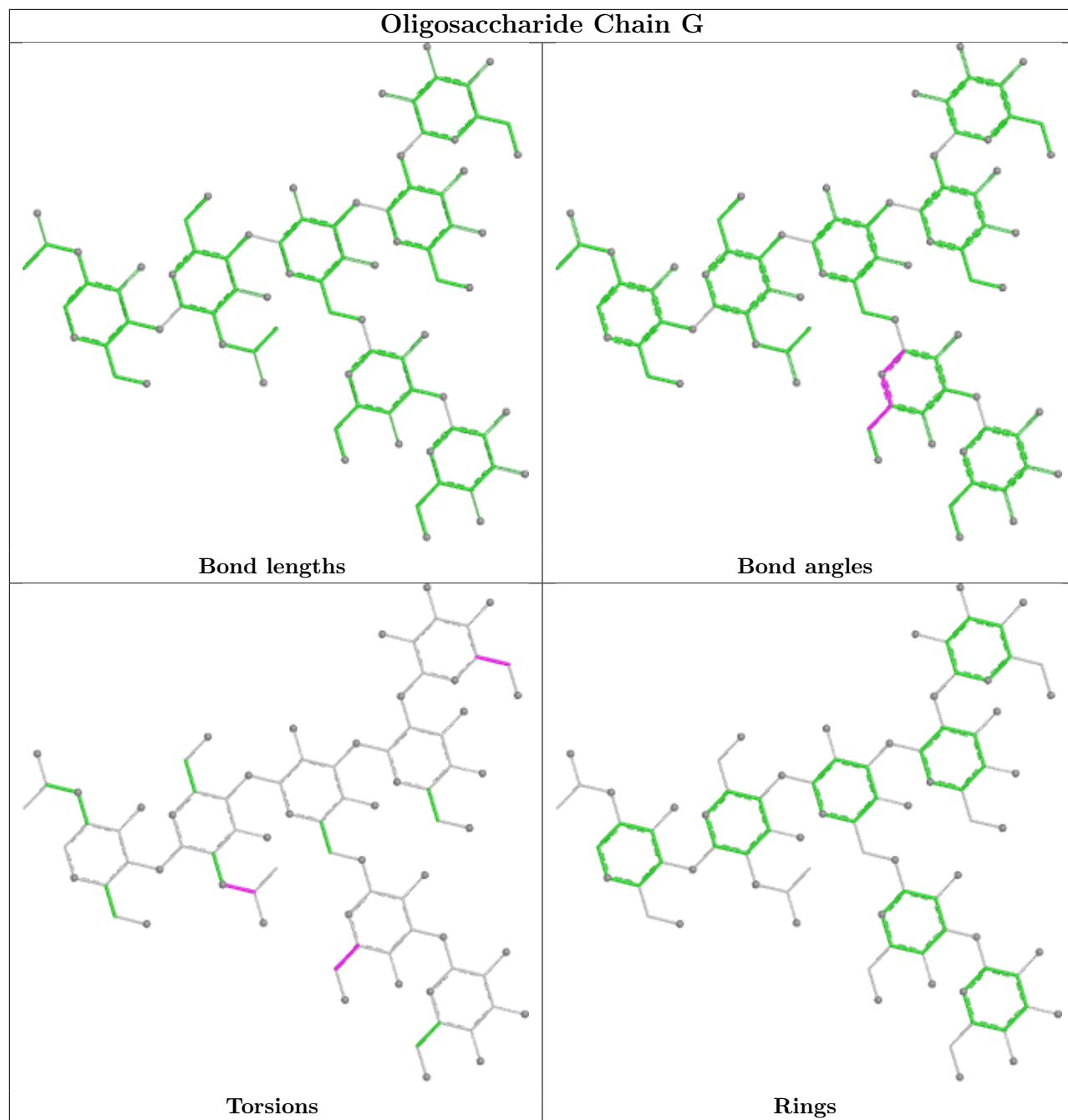


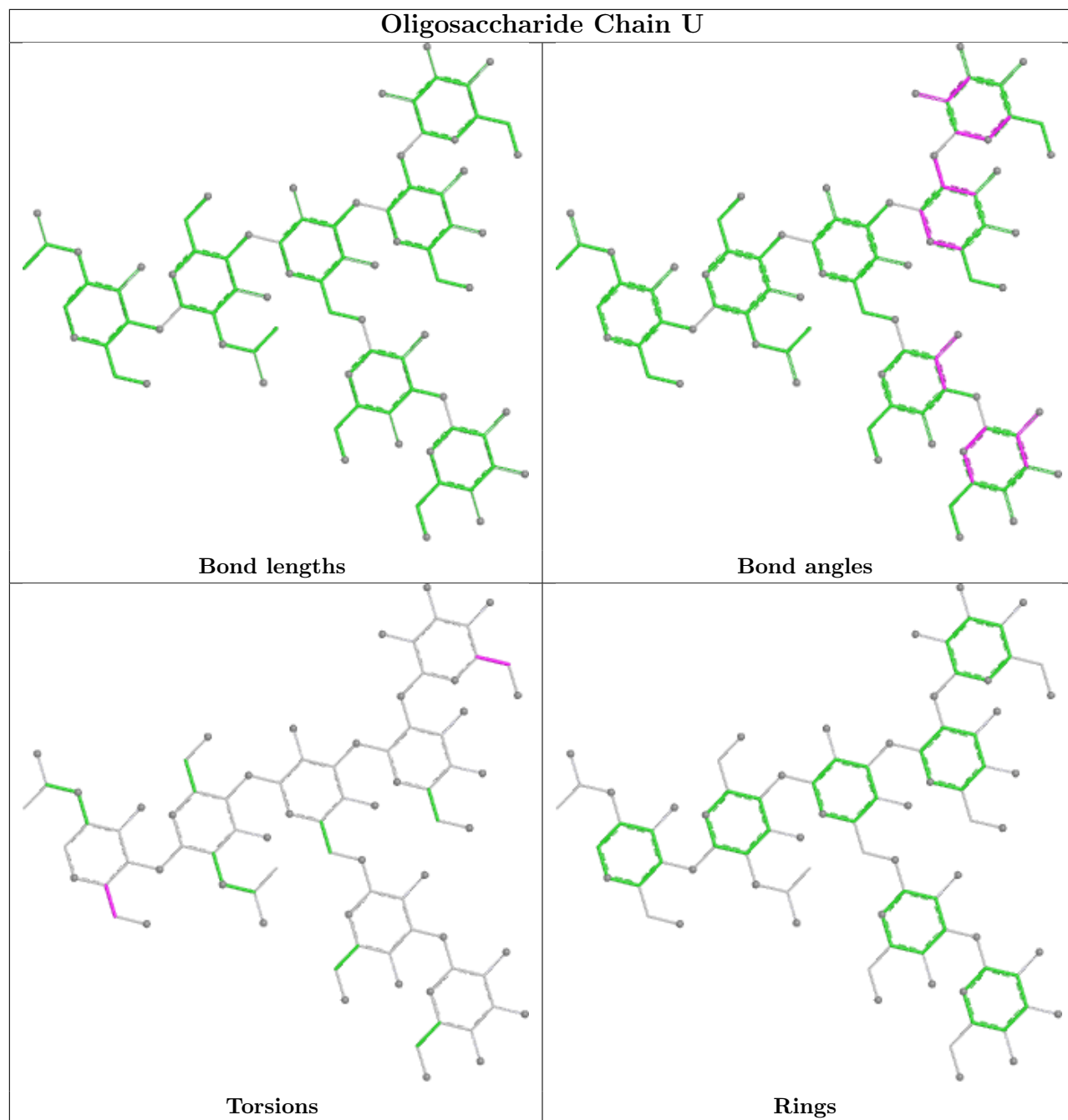


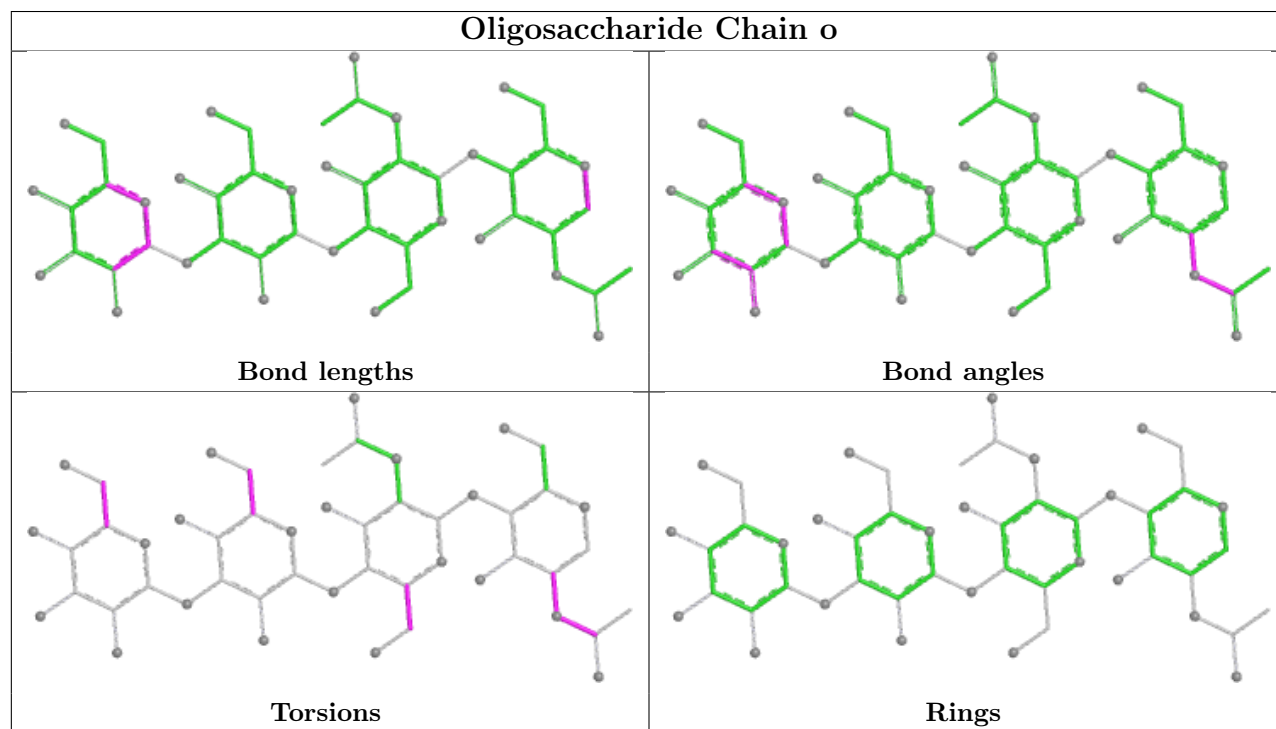
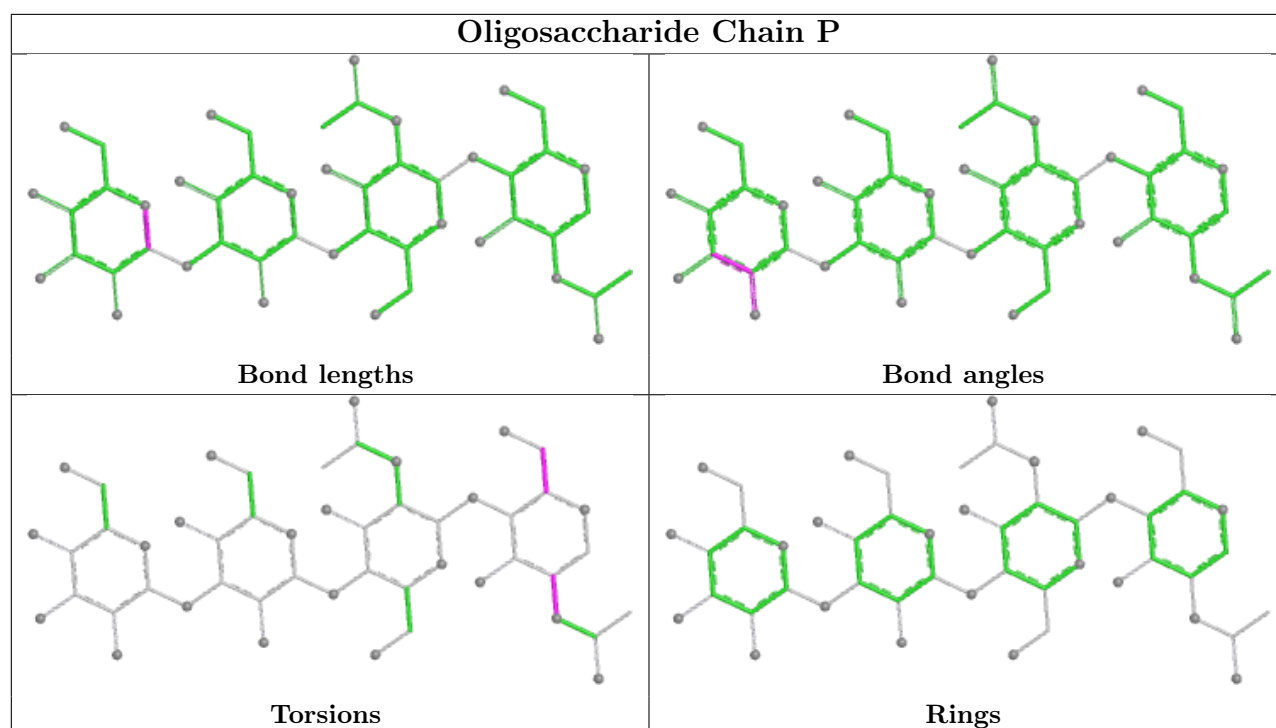


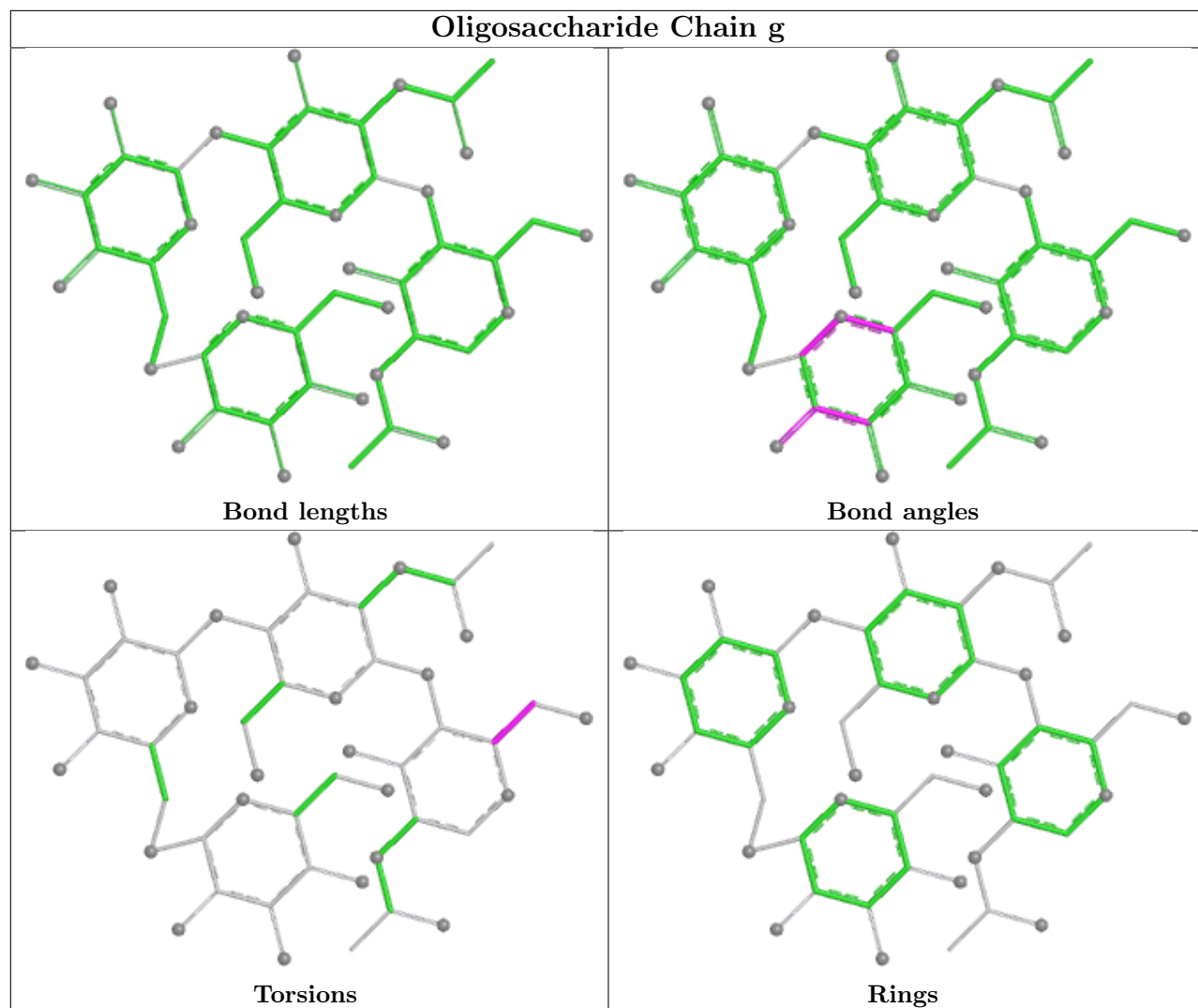


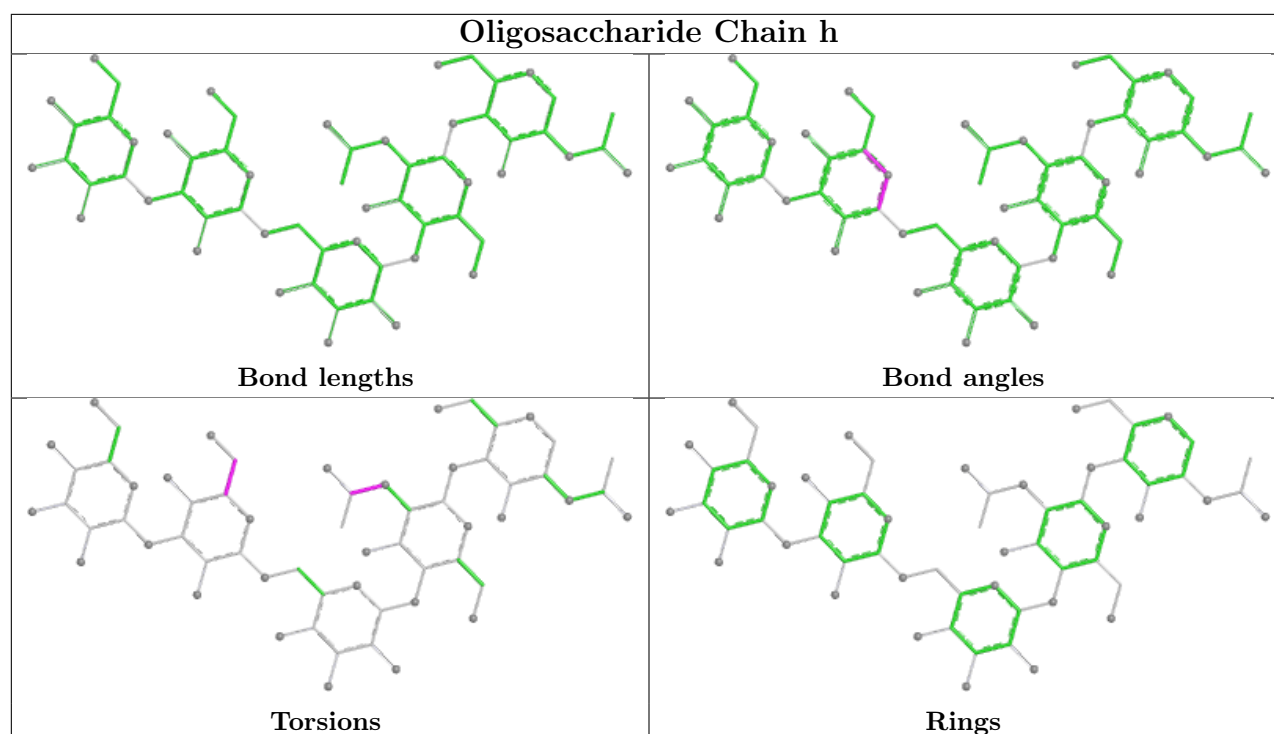












5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
8	NAG	B	901	1	14,14,15	0.28	0	17,19,21	0.61	0
9	83G	A	904	-	33,33,33	2.22	8 (24%)	44,47,47	3.20	11 (25%)
8	NAG	A	903	1	14,14,15	0.40	0	17,19,21	1.10	1 (5%)
9	83G	B	903	-	33,33,33	2.25	10 (30%)	44,47,47	3.11	15 (34%)
8	NAG	B	902	1	14,14,15	0.21	0	17,19,21	0.54	0
8	NAG	A	902	1	14,14,15	0.41	0	17,19,21	0.76	0
8	NAG	C	902	1	14,14,15	0.50	0	17,19,21	2.26	3 (17%)
8	NAG	C	901	1	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
8	NAG	A	901	1	14,14,15	0.32	0	17,19,21	0.52	0
9	83G	C	903	-	33,33,33	2.23	10 (30%)	44,47,47	3.23	13 (29%)

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
8	NAG	B	901	1	-	2/6/23/26	0/1/1/1
9	83G	A	904	-	-	6/22/35/35	0/4/4/4
8	NAG	A	903	1	-	3/6/23/26	0/1/1/1
9	83G	B	903	-	-	2/22/35/35	0/4/4/4
8	NAG	B	902	1	-	2/6/23/26	0/1/1/1
8	NAG	A	902	1	-	1/6/23/26	0/1/1/1
8	NAG	C	902	1	-	1/6/23/26	0/1/1/1
8	NAG	C	901	1	-	1/6/23/26	0/1/1/1
8	NAG	A	901	1	-	2/6/23/26	0/1/1/1
9	83G	C	903	-	-	6/22/35/35	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	903	83G	C14-N16	6.68	1.44	1.34
9	A	904	83G	C14-N16	6.11	1.43	1.34
9	C	903	83G	C14-N16	6.00	1.43	1.34
9	B	903	83G	C23-N19	5.57	1.46	1.34
9	C	903	83G	C23-N19	5.22	1.45	1.34
9	A	904	83G	C23-N19	5.18	1.45	1.34
9	A	904	83G	C08-C11	-4.63	1.35	1.45
9	C	903	83G	C08-C11	-4.60	1.35	1.45
9	B	903	83G	C08-C11	-4.51	1.35	1.45
9	C	903	83G	C08-C07	-3.50	1.36	1.41
9	B	903	83G	C11-C12	3.50	1.52	1.45
9	C	903	83G	C18-N19	-3.30	1.41	1.47
9	A	904	83G	C18-N19	-3.28	1.41	1.47
9	A	904	83G	C08-C07	-3.24	1.36	1.41
9	A	904	83G	C11-C12	3.12	1.51	1.45
9	B	903	83G	C08-C07	-3.10	1.36	1.41
9	C	903	83G	C11-C12	3.02	1.51	1.45
9	B	903	83G	C18-N19	-2.63	1.42	1.47
9	C	903	83G	O13-C12	-2.50	1.17	1.23
9	A	904	83G	O15-C14	-2.46	1.18	1.23
9	C	903	83G	O15-C14	-2.44	1.18	1.23
9	C	903	83G	C04-C03	-2.28	1.34	1.39
9	B	903	83G	O15-C14	-2.25	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	904	83G	O13-C12	-2.23	1.18	1.23
9	B	903	83G	O13-C12	-2.20	1.18	1.23
9	B	903	83G	O24-C23	-2.07	1.18	1.22
9	B	903	83G	C04-C03	-2.05	1.35	1.39
9	C	903	83G	O24-C23	-2.02	1.18	1.22

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	904	83G	C10-C11-C12	-11.13	100.85	126.74
9	C	903	83G	C10-C11-C12	-10.91	101.37	126.74
9	B	903	83G	C10-C11-C12	-10.68	101.89	126.74
9	C	903	83G	C11-C10-N09	-9.96	103.47	110.22
9	B	903	83G	C11-C10-N09	-9.86	103.54	110.22
9	A	904	83G	C11-C10-N09	-9.66	103.68	110.22
9	A	904	83G	C08-C11-C10	7.65	114.68	106.10
9	C	903	83G	C08-C11-C10	7.64	114.67	106.10
8	C	901	NAG	O5-C1-C2	-7.54	99.62	111.29
8	C	902	NAG	O5-C1-C2	-7.43	99.79	111.29
9	B	903	83G	C08-C11-C10	7.18	114.15	106.10
9	B	903	83G	C08-C07-N06	-7.03	119.15	126.64
9	C	903	83G	C08-C07-N06	-6.80	119.39	126.64
9	A	904	83G	C08-C07-N06	-6.73	119.47	126.64
9	C	903	83G	O02-C03-C08	5.14	123.13	115.84
9	A	904	83G	O02-C03-C08	4.92	122.81	115.84
9	C	903	83G	C21-C20-N19	4.88	116.56	110.99
9	A	904	83G	C18-C17-N16	4.62	118.67	110.33
9	A	904	83G	O02-C03-C04	-3.92	117.70	124.30
9	B	903	83G	O02-C03-C08	3.87	121.33	115.84
9	A	904	83G	C01-O02-C03	-3.67	112.13	117.51
9	C	903	83G	O02-C03-C04	-3.63	118.18	124.30
9	C	903	83G	C04-C05-N06	-3.57	119.60	123.97
9	B	903	83G	C21-C20-N19	-3.49	107.00	110.99
9	C	903	83G	C18-C17-N16	-3.26	104.45	110.33
9	B	903	83G	C04-C05-N06	-3.08	120.20	123.97
9	A	904	83G	C04-C05-N06	-3.06	120.22	123.97
9	B	903	83G	N09-C07-N06	3.05	131.62	126.69
8	C	902	NAG	O7-C7-C8	-2.89	116.91	122.05
8	C	901	NAG	O7-C7-C8	-2.85	116.98	122.05
9	C	903	83G	C05-C04-C03	2.68	121.04	118.07
8	C	902	NAG	C4-C3-C2	-2.66	107.12	111.02
8	C	901	NAG	C4-C3-C2	-2.64	107.15	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	903	83G	N09-C07-N06	2.63	130.95	126.69
9	A	904	83G	N09-C07-N06	2.61	130.91	126.69
9	B	903	83G	C25-C23-N19	2.61	121.92	118.66
9	B	903	83G	O02-C03-C04	-2.56	119.98	124.30
9	A	904	83G	C21-C20-N19	-2.41	108.23	110.99
8	A	903	NAG	C2-N2-C7	2.33	126.02	122.90
9	B	903	83G	C18-C17-N16	2.29	114.47	110.33
9	B	903	83G	O24-C23-N19	-2.27	118.78	122.35
9	C	903	83G	C30-C25-C26	2.25	121.43	118.57
9	B	903	83G	C22-C21-N16	-2.18	108.07	111.55
9	C	903	83G	C01-O02-C03	-2.16	114.34	117.51
9	B	903	83G	C05-C04-C03	2.10	120.41	118.07
9	B	903	83G	C30-C25-C26	2.10	121.24	118.57

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	901	NAG	C8-C7-N2-C2
8	A	901	NAG	O7-C7-N2-C2
8	A	903	NAG	C8-C7-N2-C2
8	A	903	NAG	O7-C7-N2-C2
8	B	901	NAG	C8-C7-N2-C2
8	B	901	NAG	O7-C7-N2-C2
9	A	904	83G	C04-C03-O02-C01
9	C	903	83G	C04-C03-O02-C01
9	A	904	83G	C08-C03-O02-C01
8	B	902	NAG	C4-C5-C6-O6
9	C	903	83G	C08-C03-O02-C01
8	A	903	NAG	C3-C2-N2-C7
8	B	902	NAG	O5-C5-C6-O6
9	B	903	83G	C04-C03-O02-C01
9	B	903	83G	C08-C03-O02-C01
8	A	902	NAG	C1-C2-N2-C7
9	A	904	83G	C08-C11-C12-O13
9	C	903	83G	C08-C11-C12-O13
9	A	904	83G	C10-C11-C12-O13
9	C	903	83G	C10-C11-C12-O13
9	A	904	83G	C10-C11-C12-C14
9	A	904	83G	C08-C11-C12-C14
9	C	903	83G	C10-C11-C12-C14
9	C	903	83G	C08-C11-C12-C14

Continued on next page...

Continued from previous page...

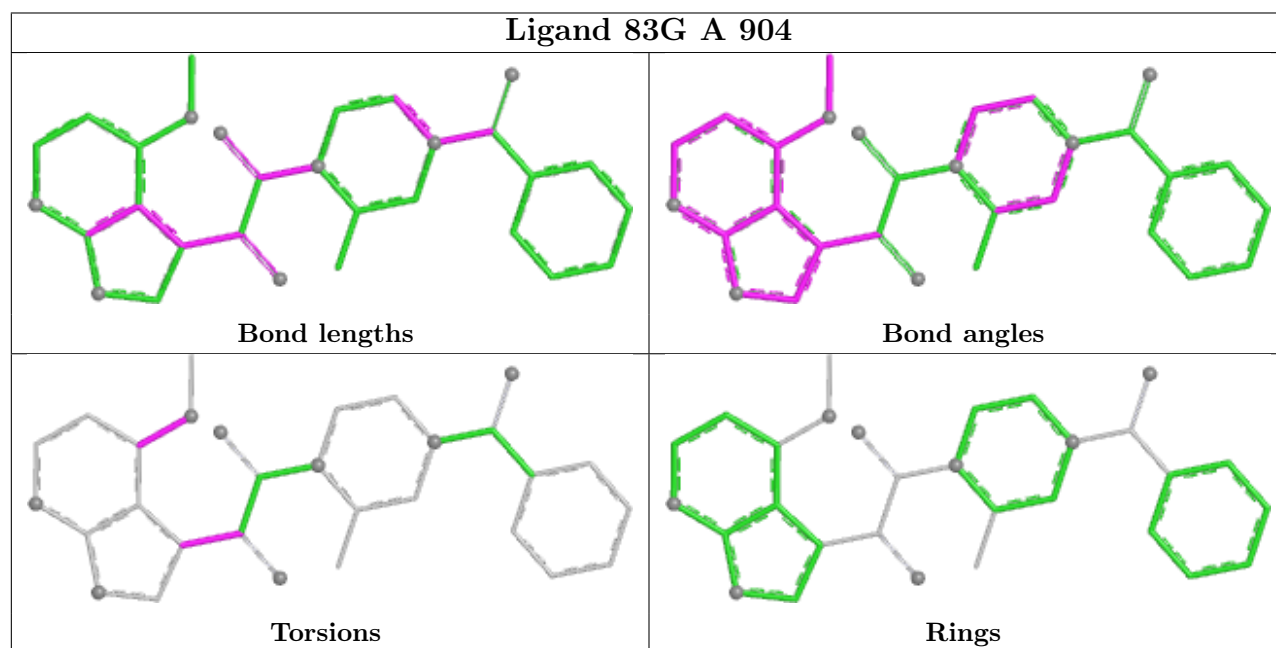
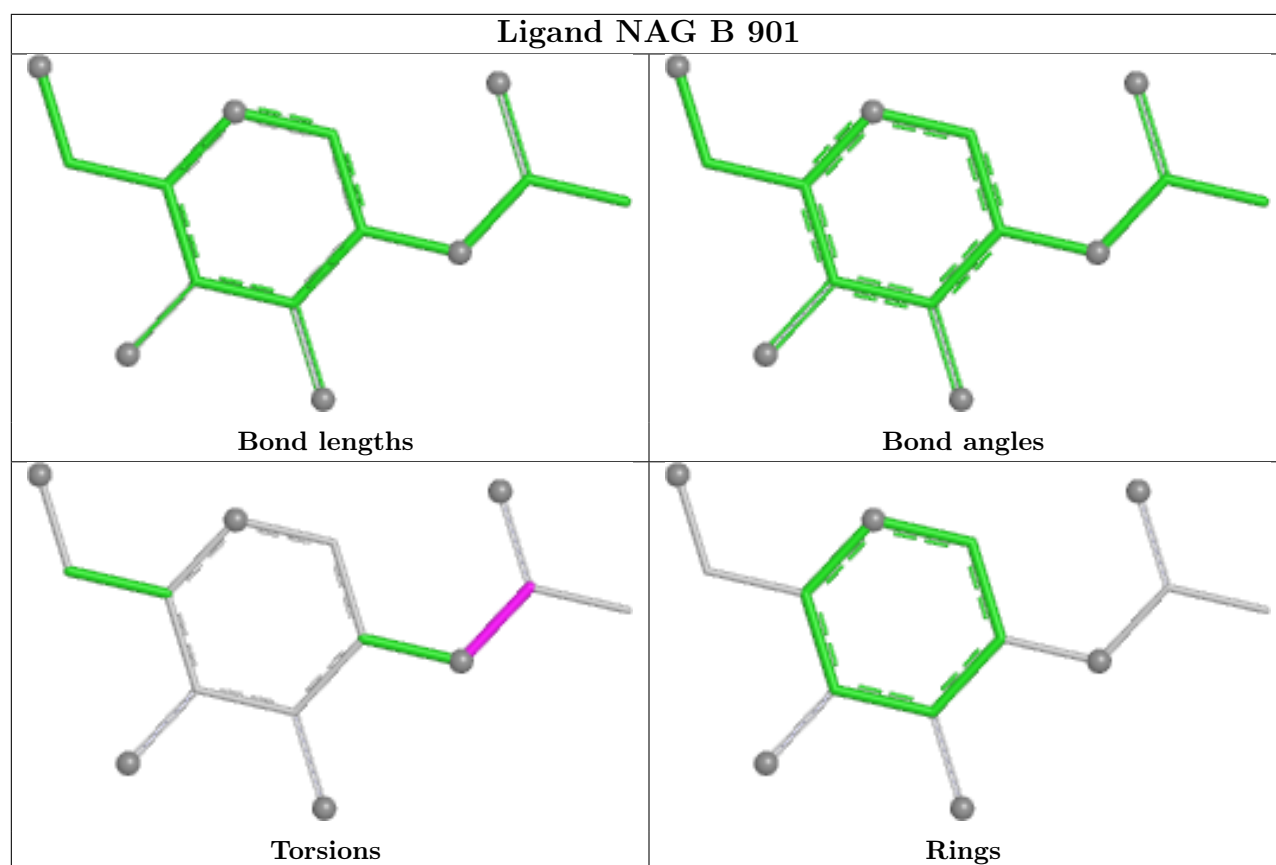
Mol	Chain	Res	Type	Atoms
8	C	901	NAG	O7-C7-N2-C2
8	C	902	NAG	O7-C7-N2-C2

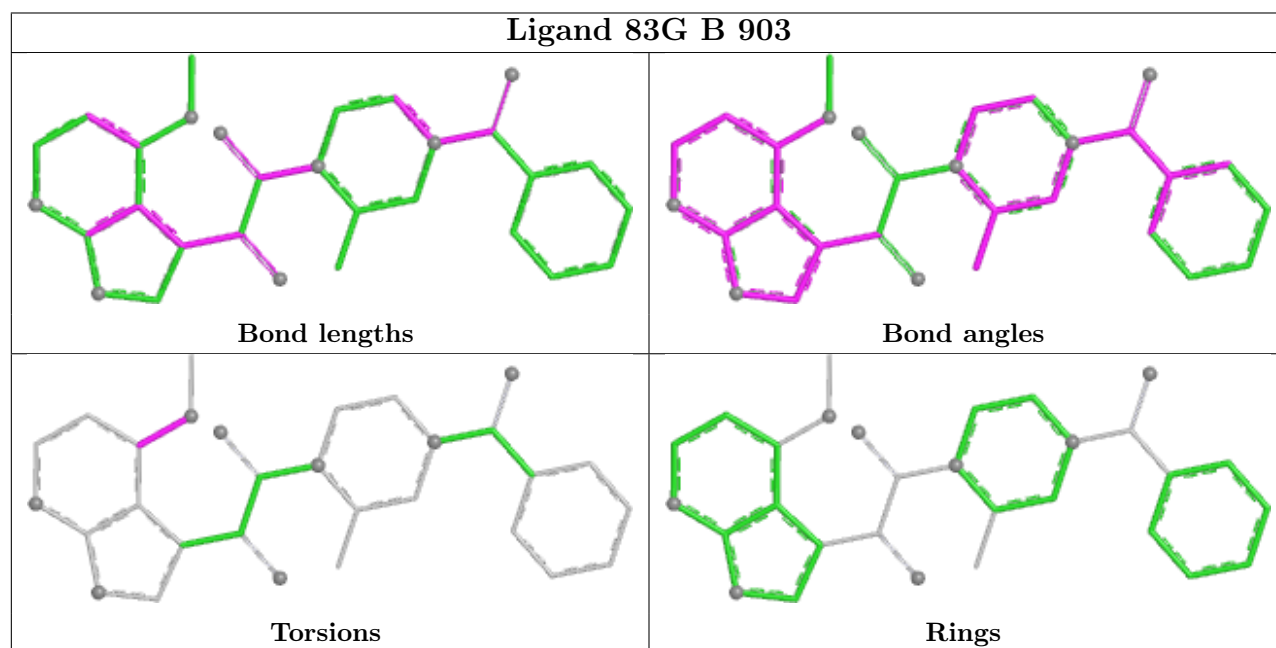
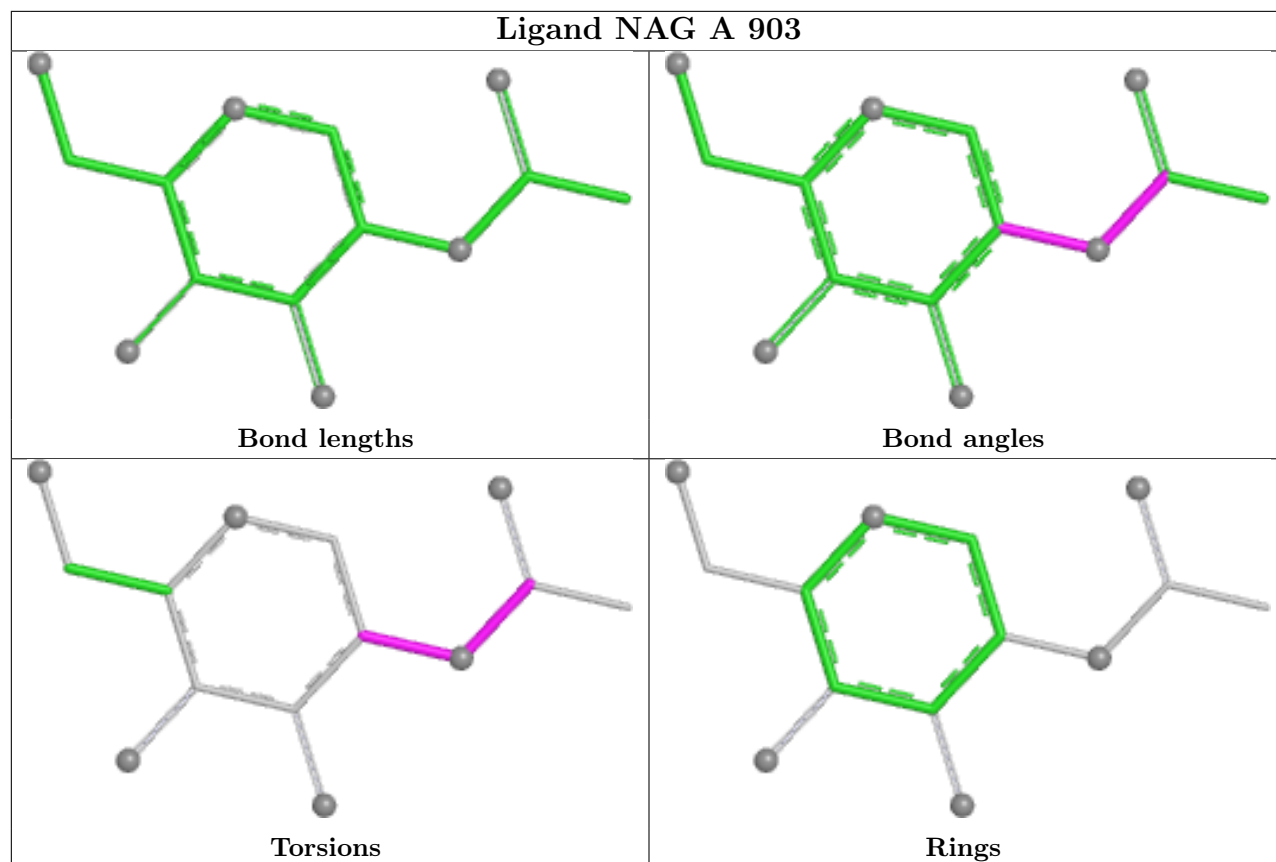
There are no ring outliers.

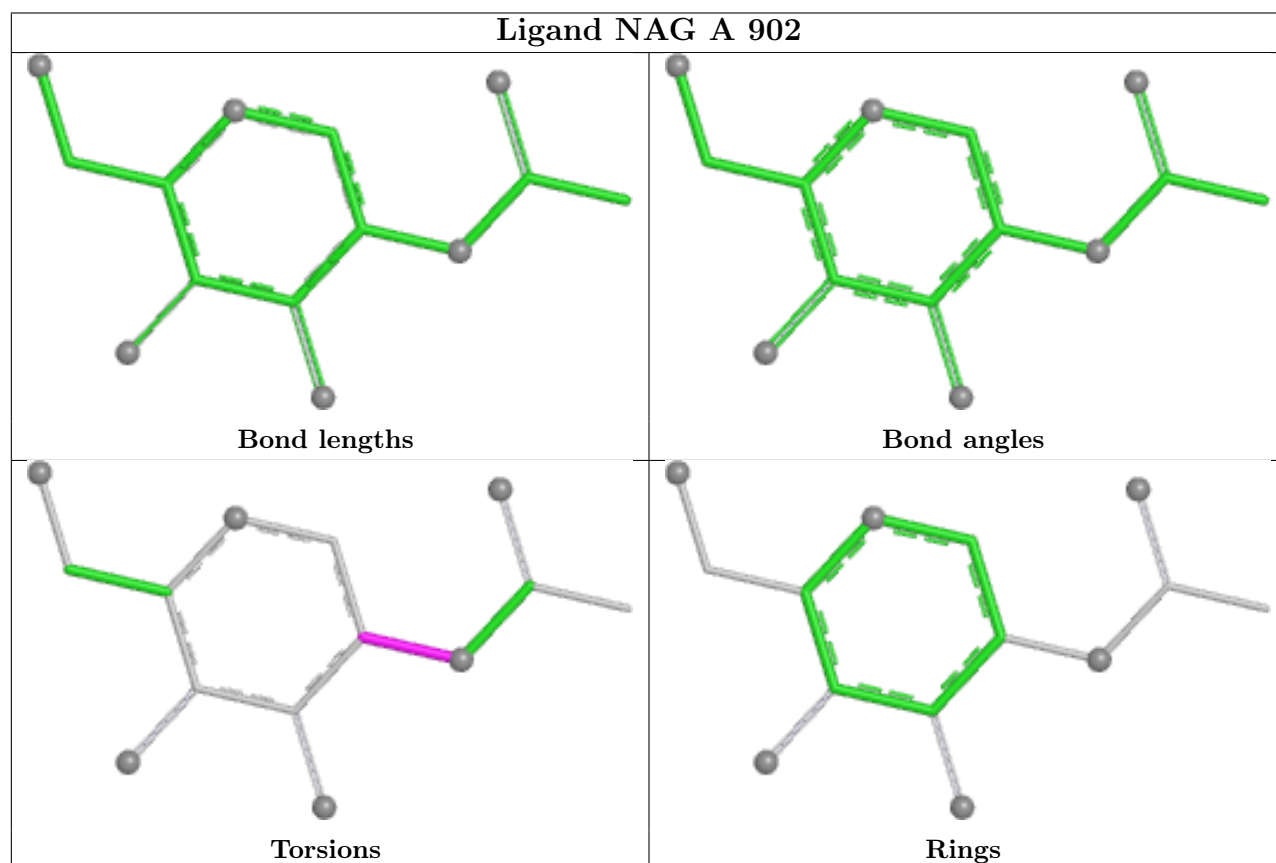
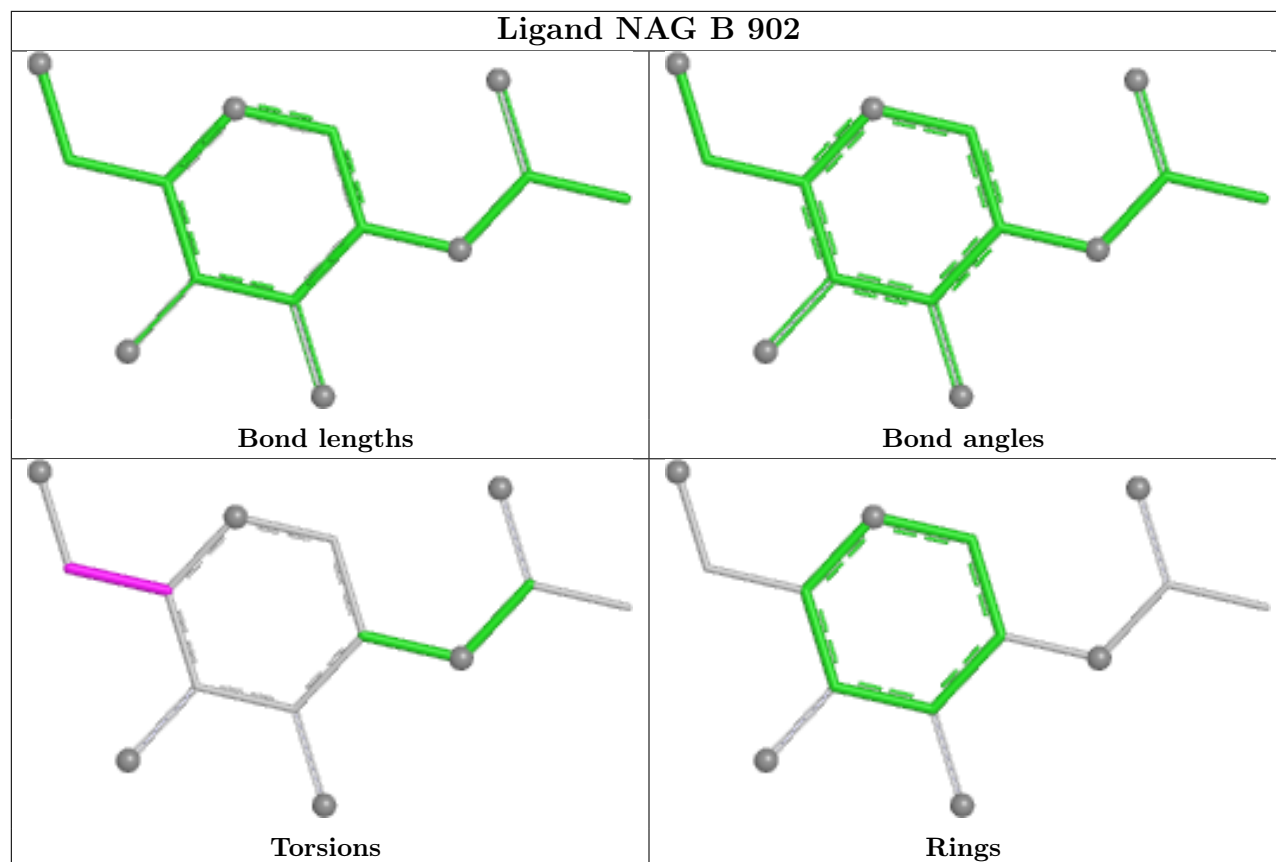
3 monomers are involved in 14 short contacts:

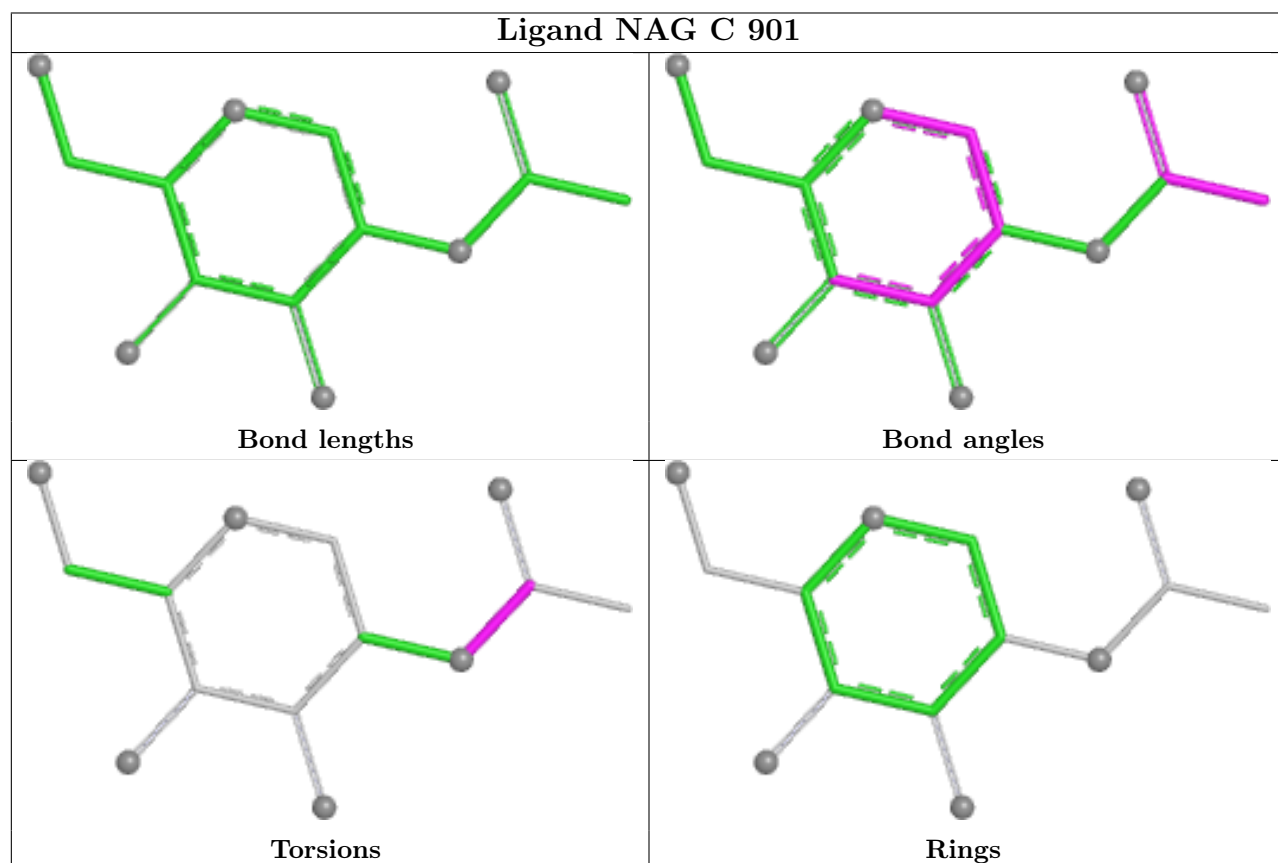
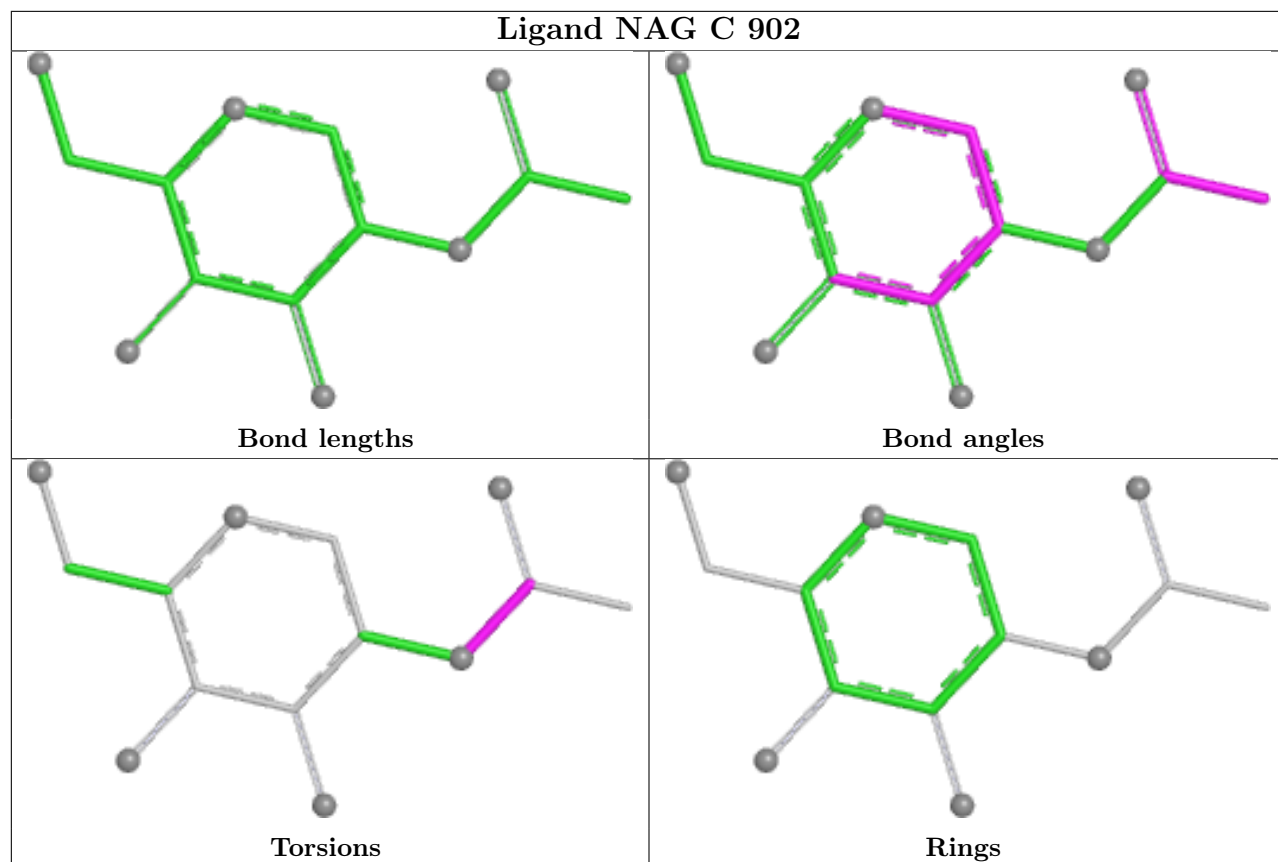
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	901	NAG	4	0
8	A	901	NAG	9	0
9	C	903	83G	1	0

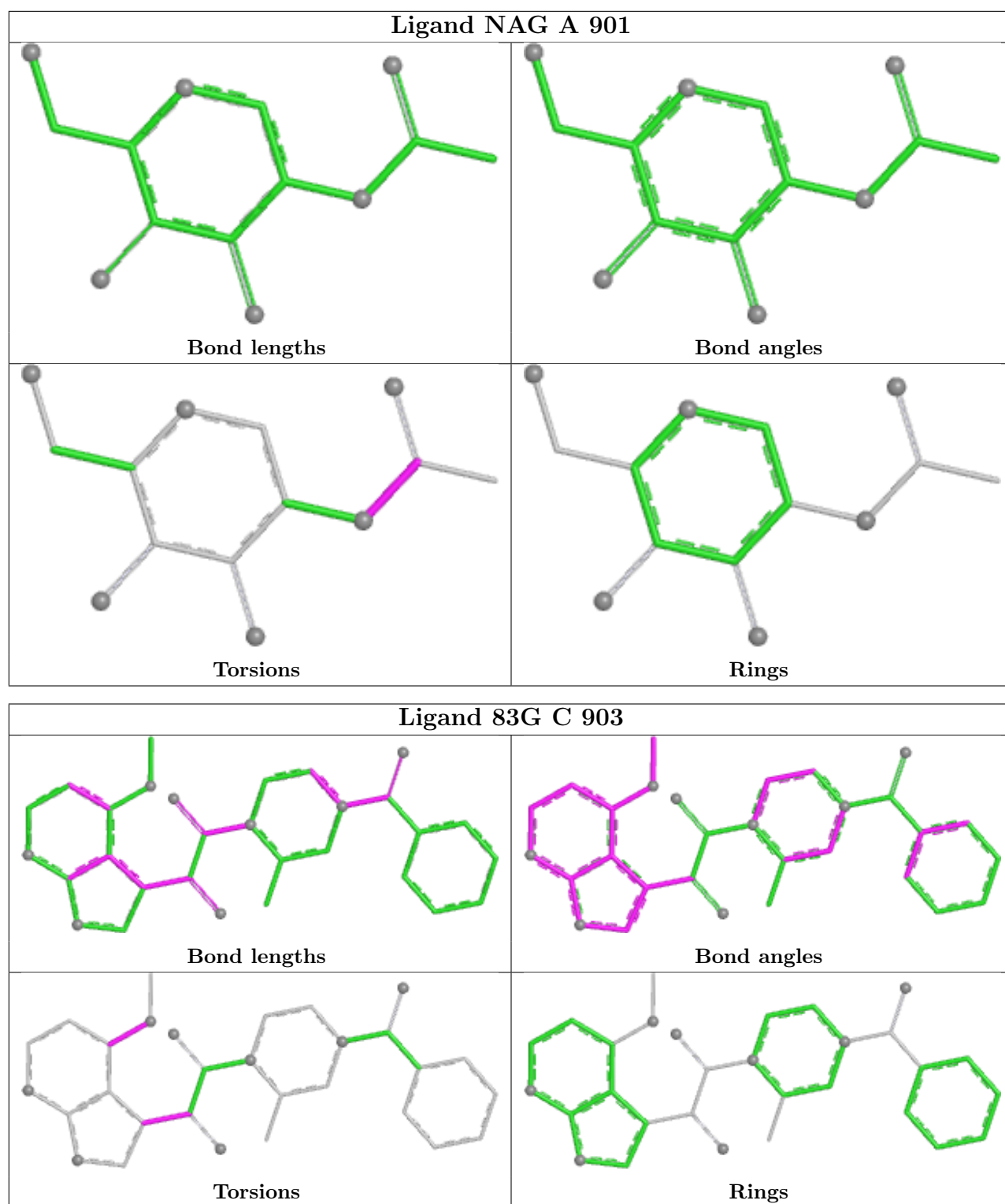
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

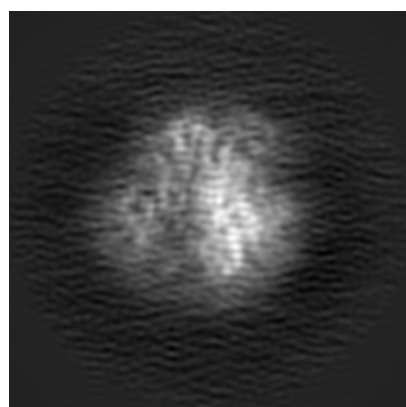
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23861. These allow visual inspection of the internal detail of the map and identification of artifacts.

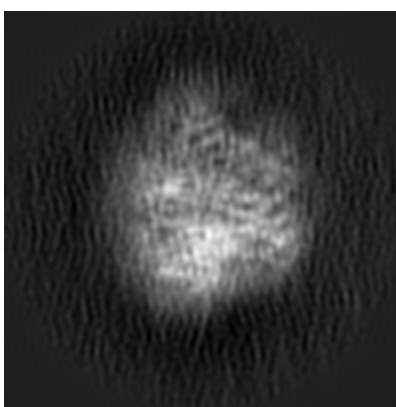
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

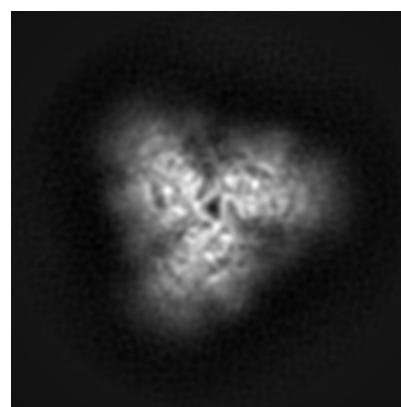
6.1.1 Primary map



X



Y

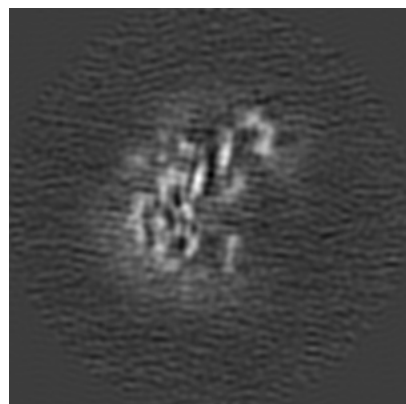


Z

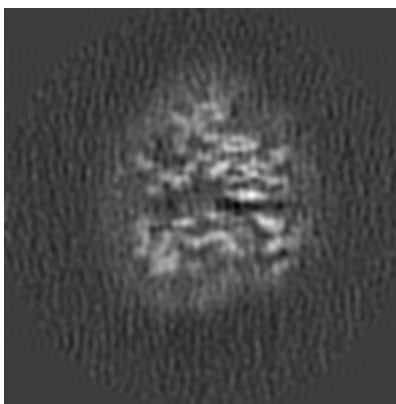
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

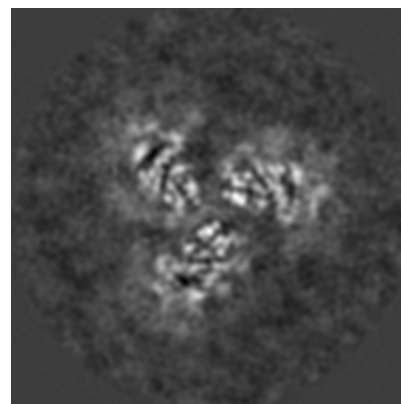
6.2.1 Primary map



X Index: 168



Y Index: 168

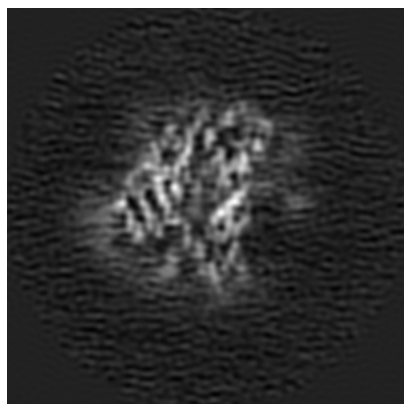


Z Index: 168

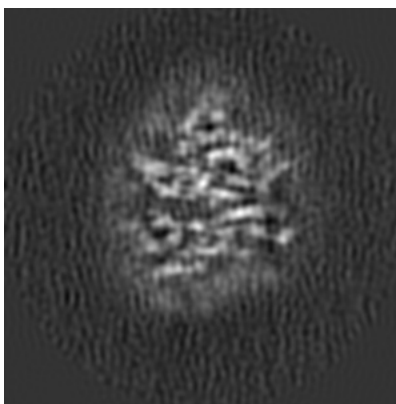
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

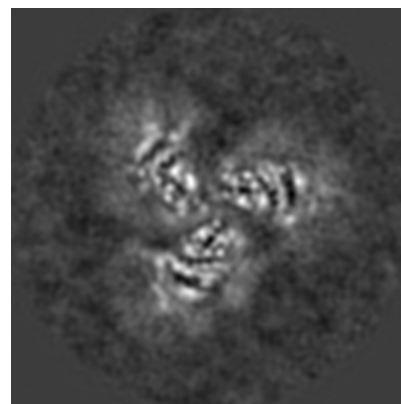
6.3.1 Primary map



X Index: 151



Y Index: 177

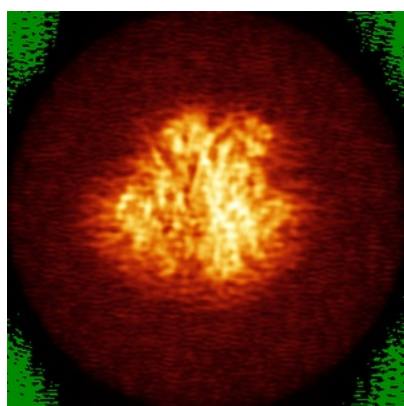


Z Index: 172

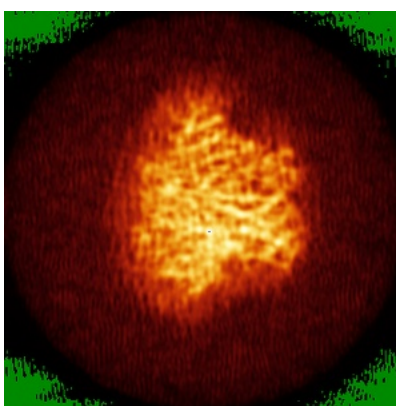
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

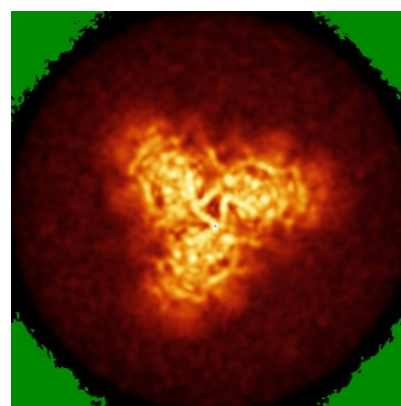
6.4.1 Primary map



X



Y

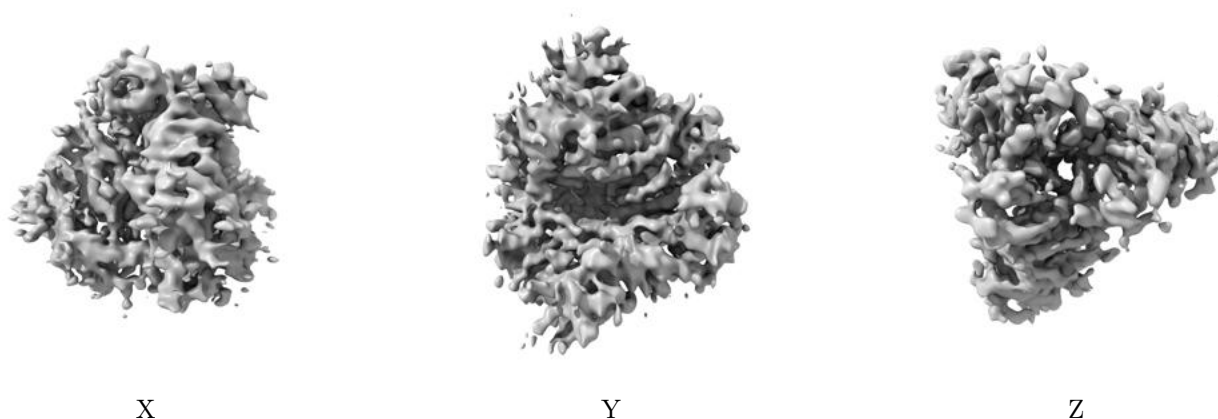


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

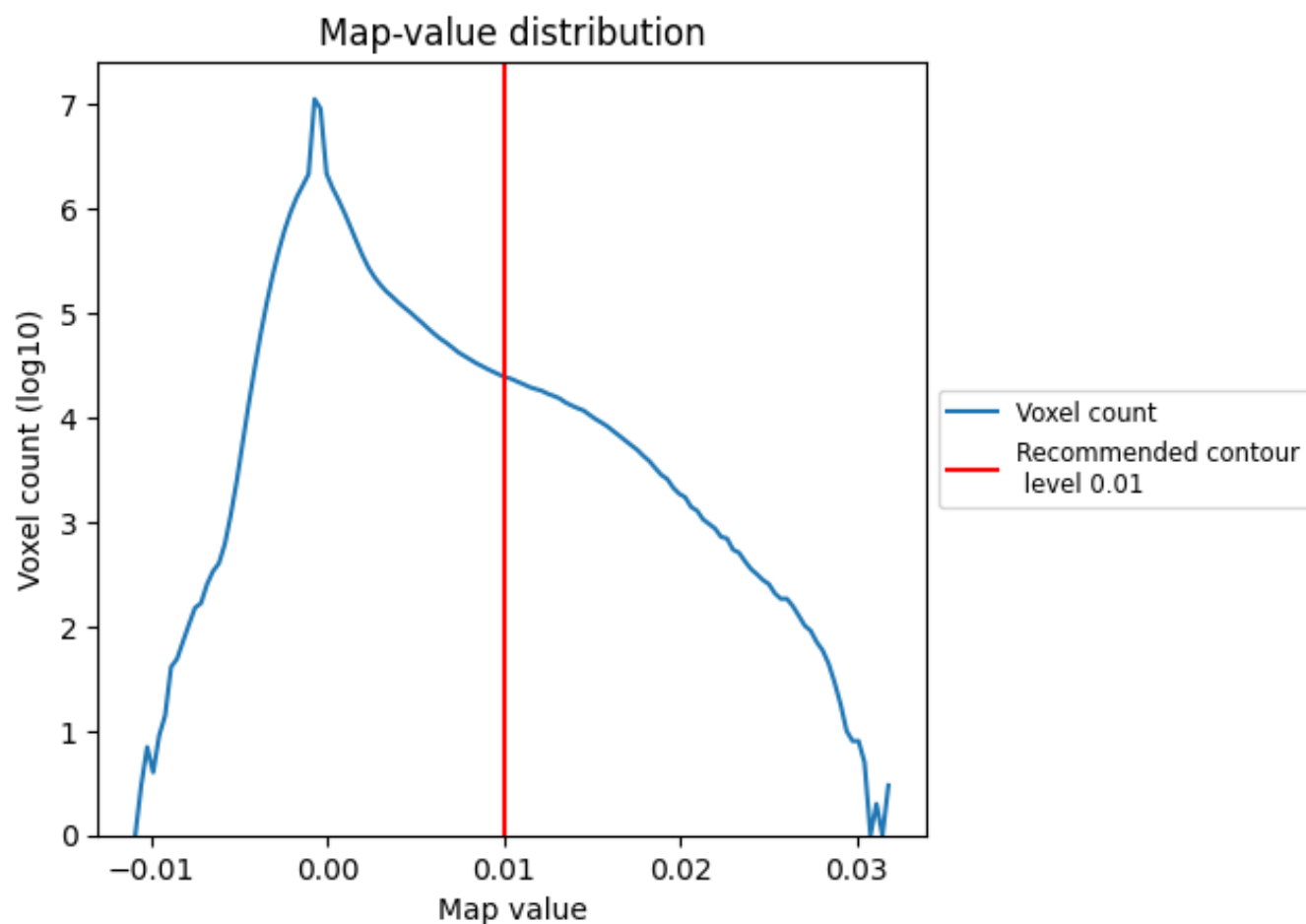
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

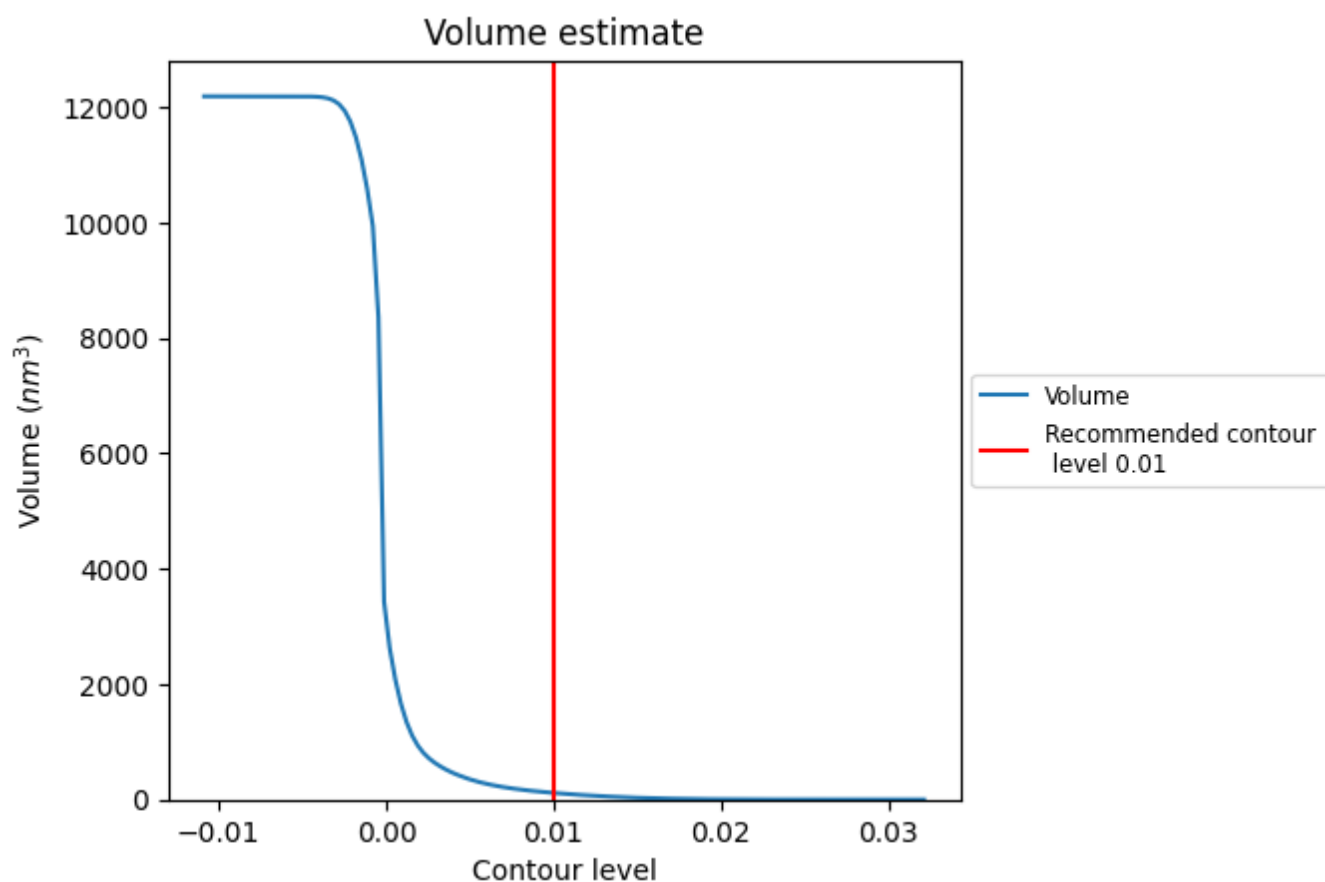
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

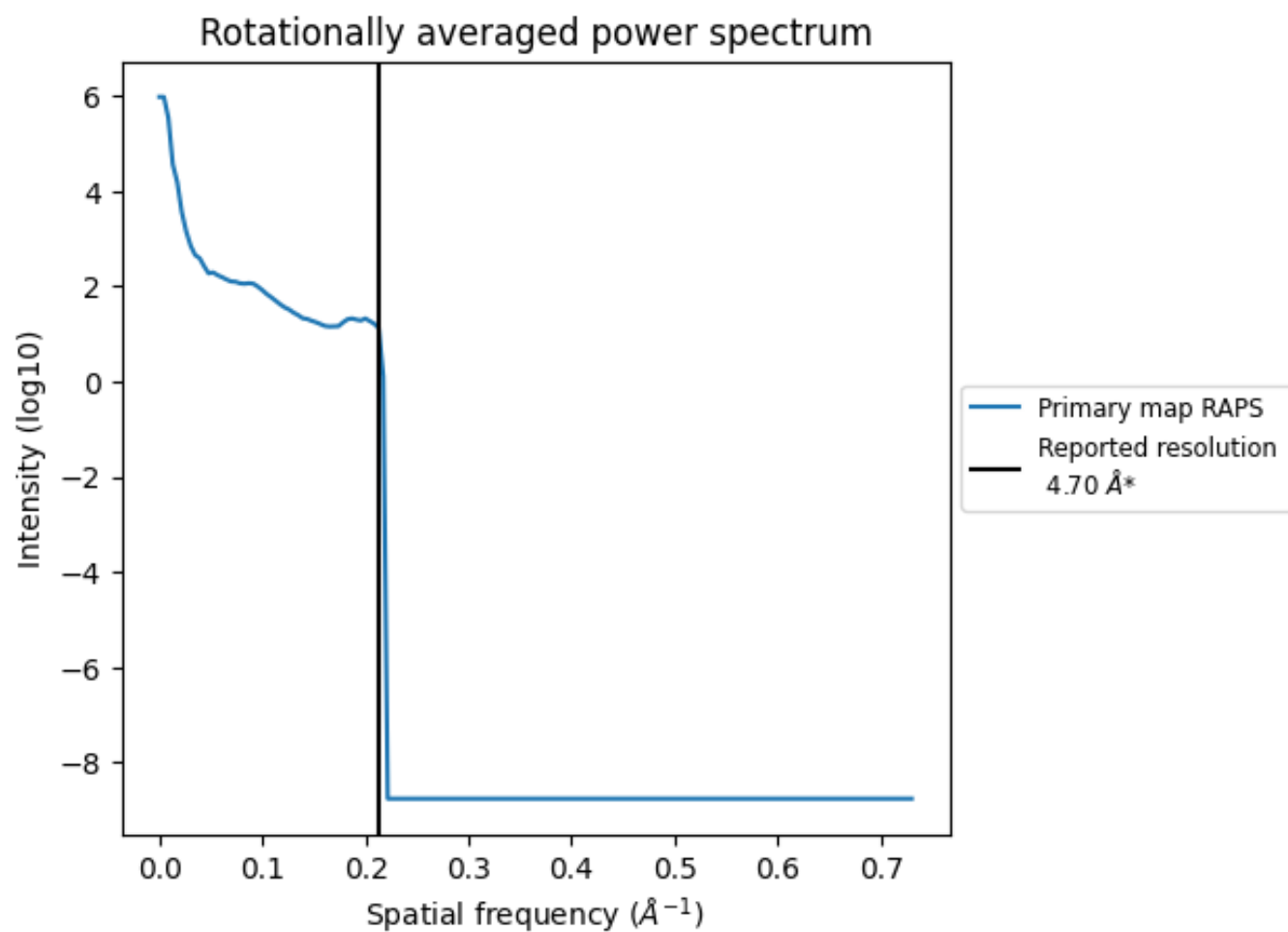
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

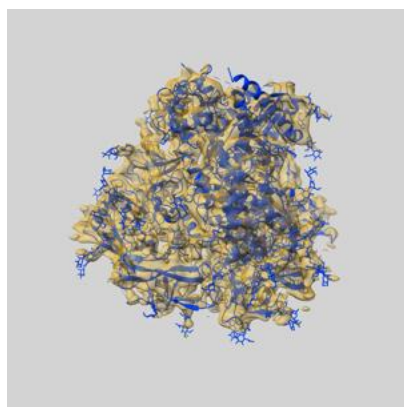
8 Fourier-Shell correlation ⓘ

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

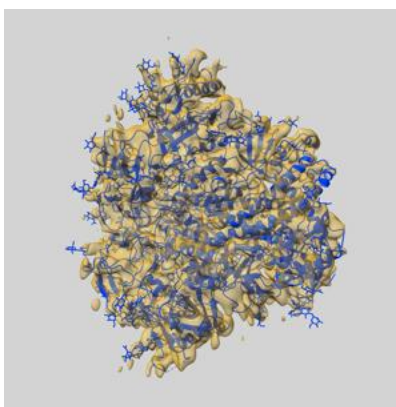
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23861 and PDB model 7N6W. Per-residue inclusion information can be found in section [3](#) on page [13](#).

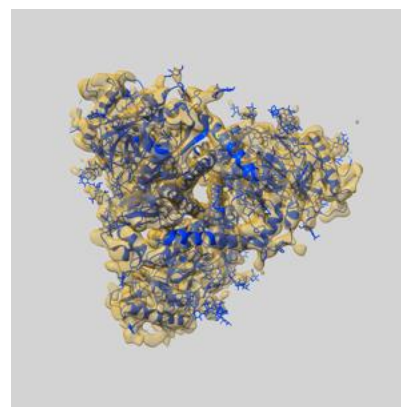
9.1 Map-model overlay [i](#)



X



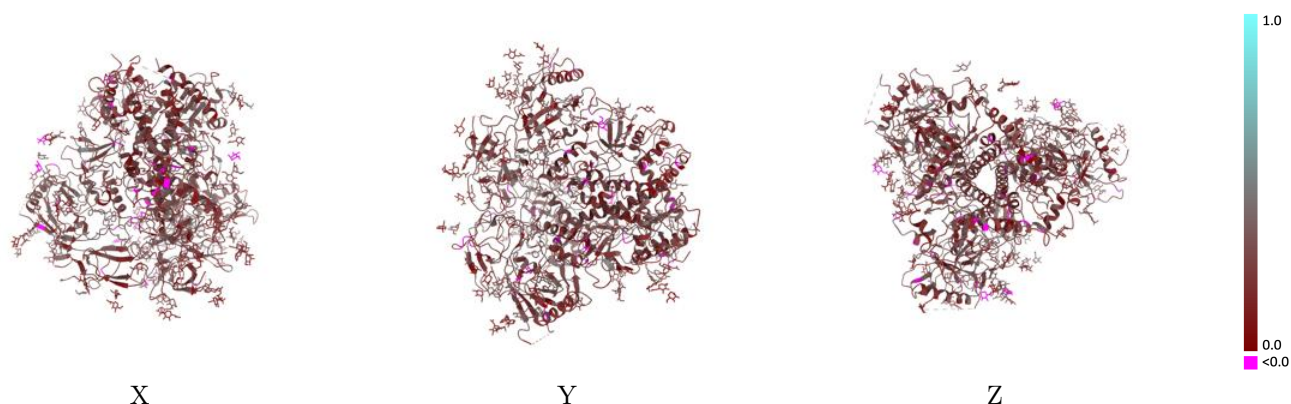
Y



Z

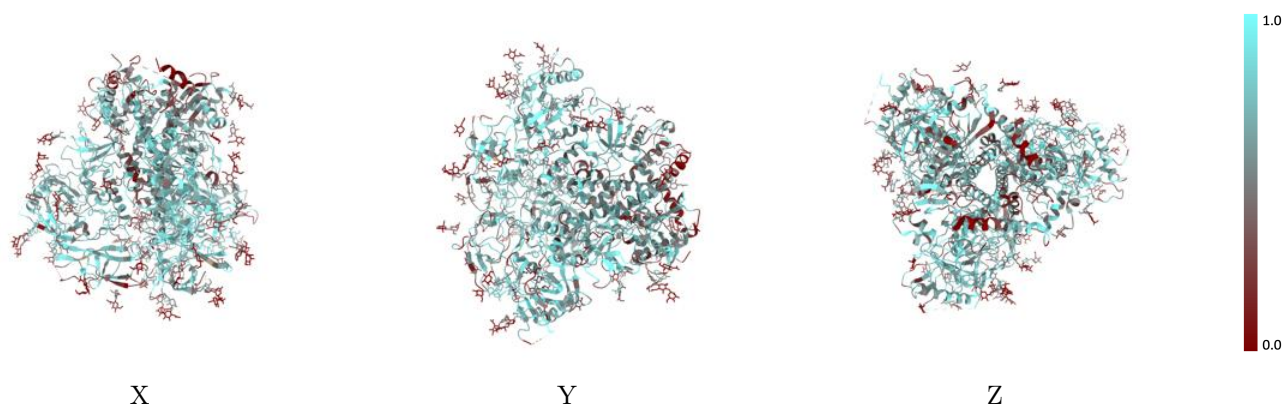
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



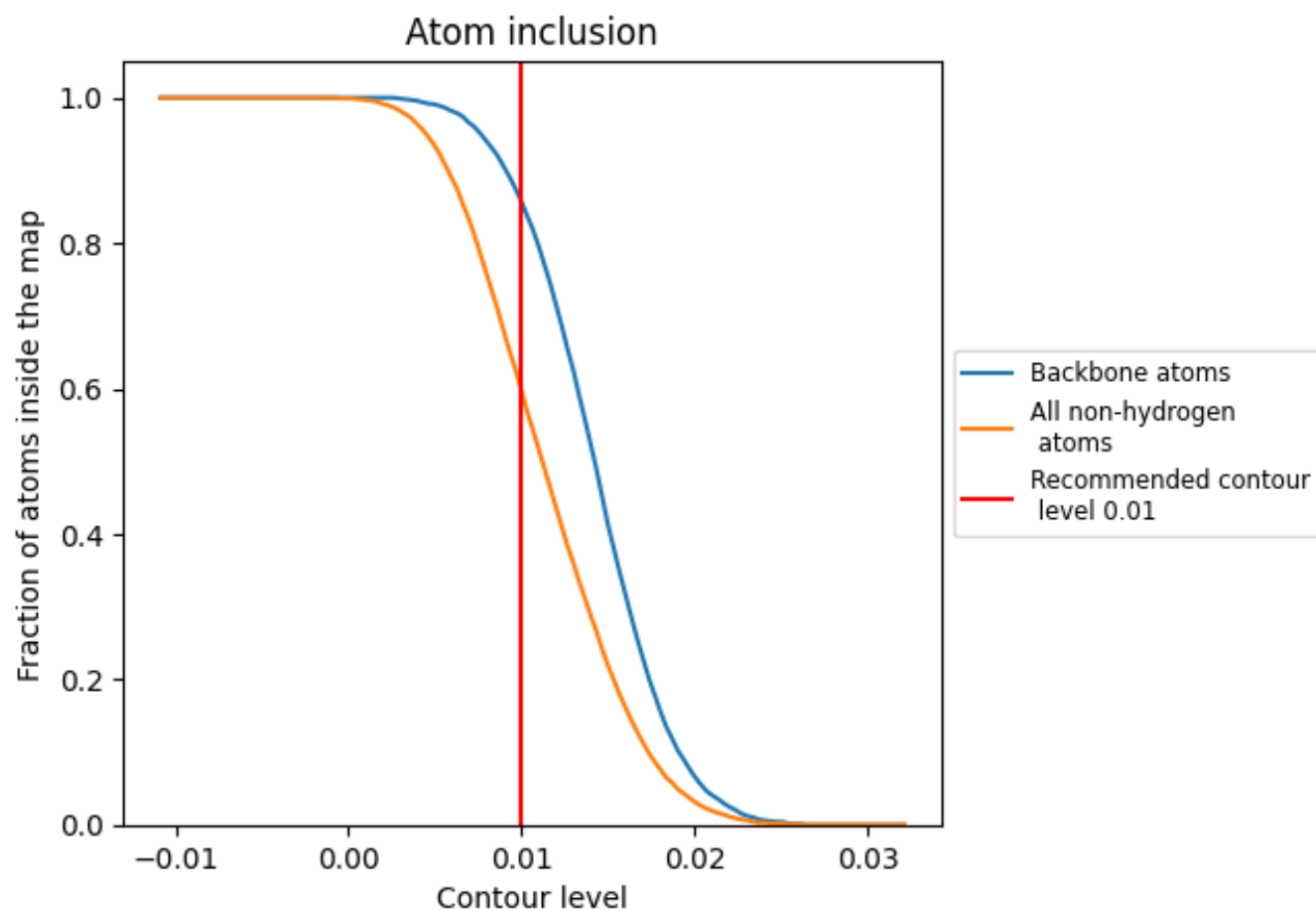
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.5970	 0.2490
A	 0.6280	 0.2520
B	 0.6060	 0.2500
C	 0.6460	 0.2510
D	 0.2310	 0.1980
E	 0.2500	 0.1770
F	 0.4100	 0.3070
G	 0.4700	 0.2780
H	 0.2140	 0.3000
I	 0.5360	 0.3370
J	 0.1430	 0.2020
K	 0.3850	 0.2340
L	 0.2860	 0.1720
M	 0.4100	 0.3140
N	 0.3590	 0.2090
O	 0.3210	 0.1950
P	 0.2000	 0.2030
Q	 0.1790	 0.1840
R	 0.3210	 0.2380
S	 0.1430	 0.1950
T	 0.5000	 0.2720
U	 0.3730	 0.2290
V	 0.2500	 0.1640
W	 0.1030	 0.0600
X	 0.2560	 0.2050
Y	 0.3850	 0.2770
Z	 0.5380	 0.2790
a	 0.2860	 0.1720
b	 0.2860	 0.2390
c	 0.2140	 0.2230
d	 0.1430	 0.1450
e	 0.0770	 0.2170
f	 0.2860	 0.1270
g	 0.3400	 0.1870
h	 0.3280	 0.2020



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.3930	 0.3020
j	 0.4640	 0.3550
k	 0.3330	 0.1920
l	 0.3930	 0.2040
m	 0.3850	 0.2550
n	 0.3850	 0.2750
o	 0.3200	 0.2620
p	 0.3570	 0.2150
q	 0.0710	 0.1630