



# Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 04:25 pm GMT

PDB ID : 7Z3A  
EMDB ID : EMD-14474  
Title : AMC009 SOSIPv5.2 in complex with Fabs ACS101 and ACS124  
Authors : van Schooten, J.; Ward, A.  
Deposited on : 2022-03-02  
Resolution : 3.95 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

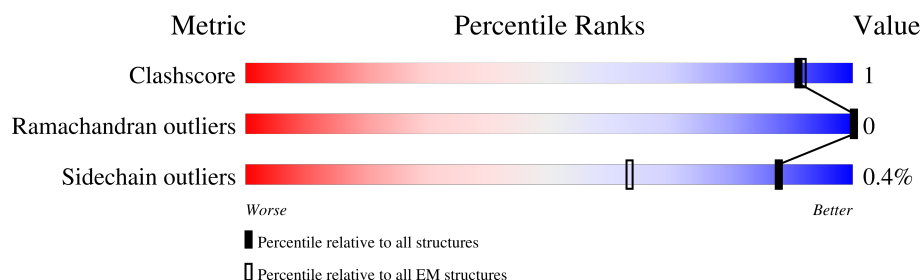
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.95 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	482	
1	C	482	
1	D	482	
2	B	154	
2	E	154	
2	F	154	
3	G	124	
3	M	124	

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Mol	Chain	Length	Quality of chain
4	I	108	
4	O	108	
5	H	126	
5	J	126	
5	K	126	
6	L	108	
6	N	108	
6	P	108	
7	2	2	
7	9	2	
7	AA	2	
7	Q	2	
7	W	2	
7	g	2	
7	l	2	
7	s	2	
7	u	2	
7	v	2	
8	0	3	
8	1	3	
8	3	3	
8	4	3	
8	5	3	
8	6	3	
8	7	3	

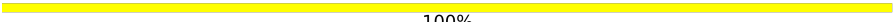




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Mol	Chain	Length	Quality of chain	
8	8	3	67%	100%
8	R	3	67%	100%
8	T	3	67%	100%
8	U	3		100%
8	V	3		100%
8	X	3	67%	100%
8	Y	3	33%	100%
8	Z	3	33%	100%
8	a	3	67%	100%
8	b	3	67%	100%
8	c	3	67%	100%
8	e	3	67%	100%
8	f	3	67%	100%
8	h	3	67%	100%
8	i	3	67%	100%
8	j	3		100%
8	k	3		100%
8	m	3	67%	100%
8	n	3	67%	100%
8	o	3		100%
8	p	3	67%	100%
8	q	3	67%	100%
8	r	3	67%	100%
8	t	3	67%	100%
8	w	3	67%	100%

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Mol	Chain	Length	Quality of chain
8	x	3	 100%
8	z	3	 67% 100%
9	S	5	 80% 100%
9	y	5	 60% 100%
10	d	3	 67% 100%

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 24000 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 AMC009 SOSIPv5.2 envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	429	Total	C	N	O	S	0	0
			3403	2149	598	629	27		
1	C	429	Total	C	N	O	S	0	0
			3403	2149	598	629	27		
1	D	429	Total	C	N	O	S	0	0
			3403	2149	598	629	27		

- Molecule 2 is a protein called AMC009 SOSIP.v5.2 envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	124	Total	C	N	O	S	0	0
			992	623	172	190	7		
2	E	113	Total	C	N	O	S	0	0
			898	566	158	167	7		
2	F	114	Total	C	N	O	S	0	0
			907	571	159	170	7		

- Molecule 3 is a protein called ACS124 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	123	Total	C	N	O	S	0	0
			969	618	164	183	4		
3	M	123	Total	C	N	O	S	0	0
			969	618	164	183	4		

- Molecule 4 is a protein called ACS124 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	108	Total	C	N	O	S	0	0
			820	510	142	165	3		
4	O	108	Total	C	N	O	S	0	0
			820	510	142	165	3		

- Molecule 5 is a protein called ACS101 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	125	Total	C	N	O	S	0	0
			990	630	171	186	3		
5	J	125	Total	C	N	O	S	0	0
			990	630	171	186	3		
5	K	125	Total	C	N	O	S	0	0
			990	630	171	186	3		

- Molecule 6 is a protein called ACS101 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	106	Total	C	N	O	S	0	0
			795	502	130	160	3		
6	N	106	Total	C	N	O	S	0	0
			795	502	130	160	3		
6	P	106	Total	C	N	O	S	0	0
			795	502	130	160	3		

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



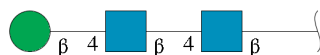
Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		
7	l	2	Total	C	N	O	0	0
			28	16	2	10		
7	s	2	Total	C	N	O	0	0
			28	16	2	10		
7	u	2	Total	C	N	O	0	0
			28	16	2	10		
7	v	2	Total	C	N	O	0	0
			28	16	2	10		
7	2	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	9	2	Total	C	N	O	0	0
			28	16	2	10		
7	AA	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 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
8	R	3	Total	C	N	O	0	0
			39	22	2	15		
8	T	3	Total	C	N	O	0	0
			39	22	2	15		
8	U	3	Total	C	N	O	0	0
			39	22	2	15		
8	V	3	Total	C	N	O	0	0
			39	22	2	15		
8	X	3	Total	C	N	O	0	0
			39	22	2	15		
8	Y	3	Total	C	N	O	0	0
			39	22	2	15		
8	Z	3	Total	C	N	O	0	0
			39	22	2	15		
8	a	3	Total	C	N	O	0	0
			39	22	2	15		
8	b	3	Total	C	N	O	0	0
			39	22	2	15		
8	c	3	Total	C	N	O	0	0
			39	22	2	15		
8	e	3	Total	C	N	O	0	0
			39	22	2	15		
8	f	3	Total	C	N	O	0	0
			39	22	2	15		
8	h	3	Total	C	N	O	0	0
			39	22	2	15		
8	i	3	Total	C	N	O	0	0
			39	22	2	15		
8	j	3	Total	C	N	O	0	0
			39	22	2	15		

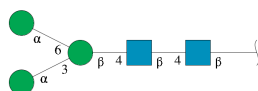
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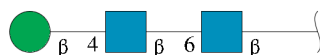
Mol	Chain	Residues	Atoms				AltConf	Trace
8	k	3	Total	C	N	O	0	0
			39	22	2	15		
8	m	3	Total	C	N	O	0	0
			39	22	2	15		
8	n	3	Total	C	N	O	0	0
			39	22	2	15		
8	o	3	Total	C	N	O	0	0
			39	22	2	15		
8	p	3	Total	C	N	O	0	0
			39	22	2	15		
8	q	3	Total	C	N	O	0	0
			39	22	2	15		
8	r	3	Total	C	N	O	0	0
			39	22	2	15		
8	t	3	Total	C	N	O	0	0
			39	22	2	15		
8	w	3	Total	C	N	O	0	0
			39	22	2	15		
8	x	3	Total	C	N	O	0	0
			39	22	2	15		
8	z	3	Total	C	N	O	0	0
			39	22	2	15		
8	0	3	Total	C	N	O	0	0
			39	22	2	15		
8	1	3	Total	C	N	O	0	0
			39	22	2	15		
8	3	3	Total	C	N	O	0	0
			39	22	2	15		
8	4	3	Total	C	N	O	0	0
			39	22	2	15		
8	5	3	Total	C	N	O	0	0
			39	22	2	15		
8	6	3	Total	C	N	O	0	0
			39	22	2	15		
8	7	3	Total	C	N	O	0	0
			39	22	2	15		
8	8	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 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.



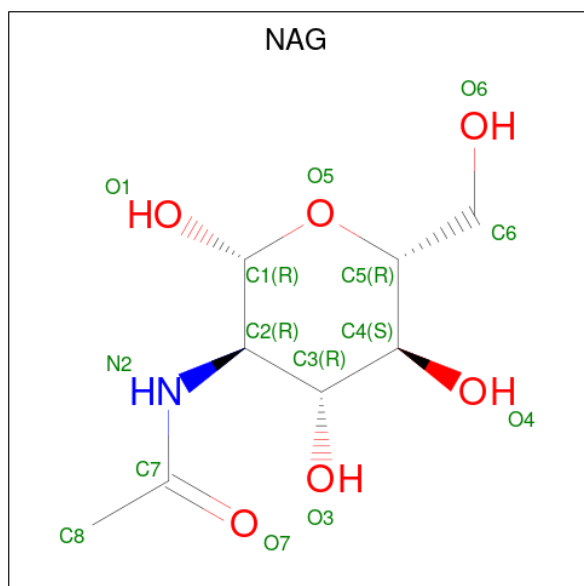
Mol	Chain	Residues	Atoms				AltConf	Trace
9	S	5	Total	C	N	O	0	0
			61	34	2	25		
9	y	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
10	d	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

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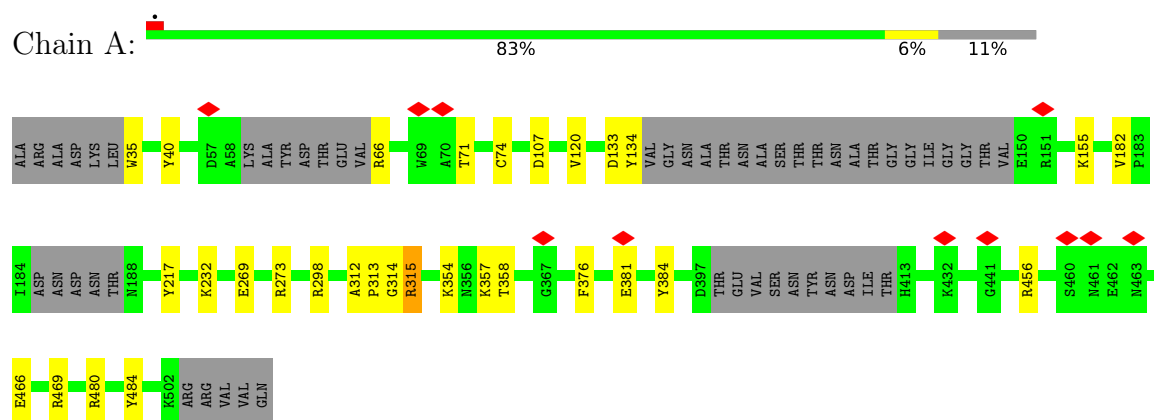
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Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total 14	C 8	N 1	O 5	0
11	A	1	Total 14	C 8	N 1	O 5	0
11	A	1	Total 14	C 8	N 1	O 5	0
11	A	1	Total 14	C 8	N 1	O 5	0
11	B	1	Total 14	C 8	N 1	O 5	0
11	B	1	Total 14	C 8	N 1	O 5	0
11	B	1	Total 14	C 8	N 1	O 5	0
11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

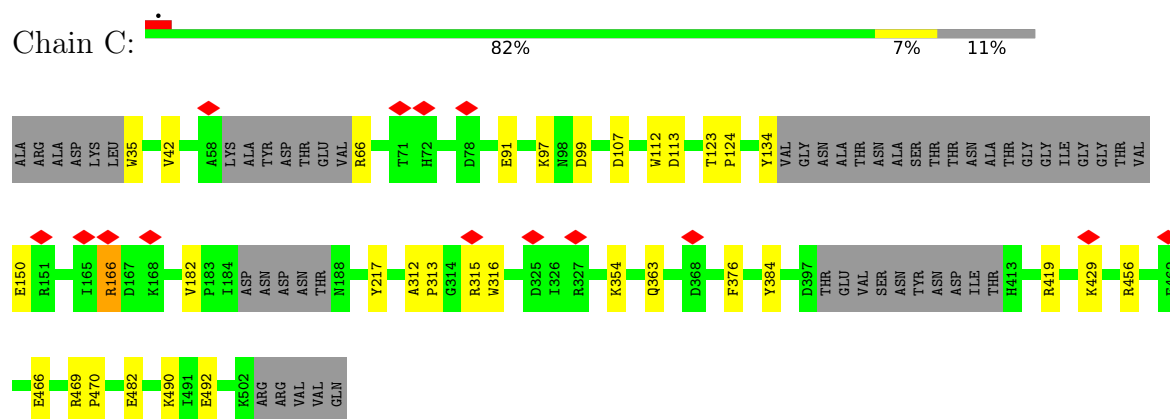
### 3 Residue-property plots

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

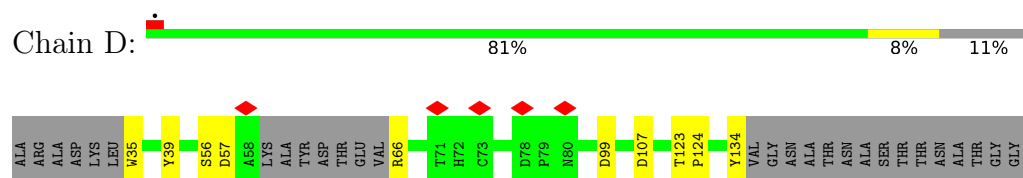
- Molecule 1: AMC009 SOSIPv5.2 envelope glycoprotein gp120

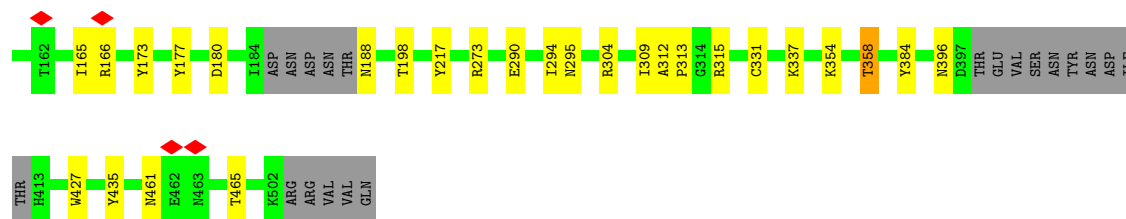


- Molecule 1: AMC009 SOSIPv5.2 envelope glycoprotein gp120

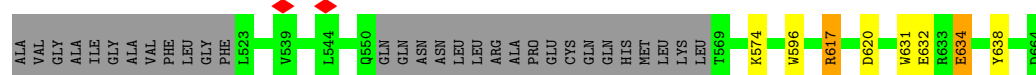
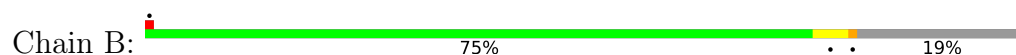


- Molecule 1: AMC009 SOSIPv5.2 envelope glycoprotein gp120

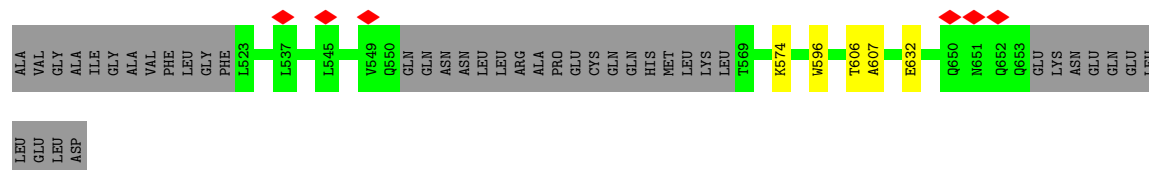




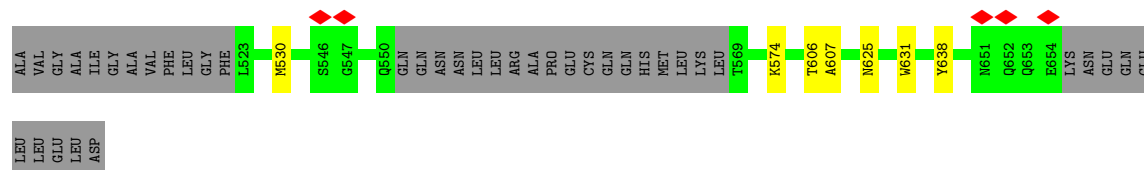
- Molecule 2: AMC009 SOSIP.v5.2 envelope glycoprotein gp41



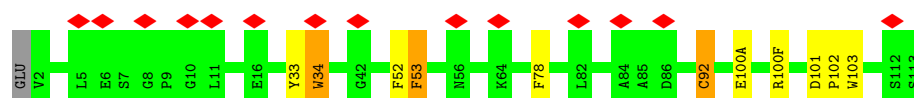
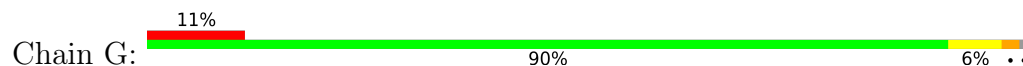
- Molecule 2: AMC009 SOSIP.v5.2 envelope glycoprotein gp41



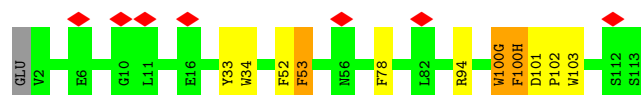
- Molecule 2: AMC009 SOSIP.v5.2 envelope glycoprotein gp41



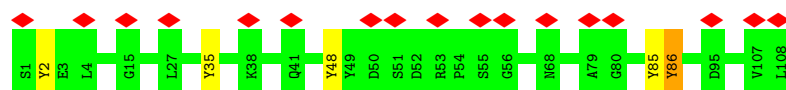
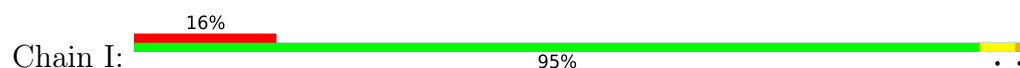
- Molecule 3: ACS124 heavy chain



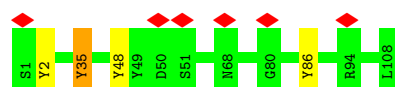
- Molecule 3: ACS124 heavy chain



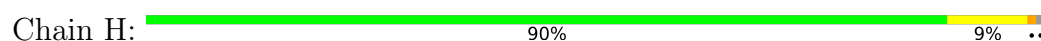
- Molecule 4: ACS124 light chain



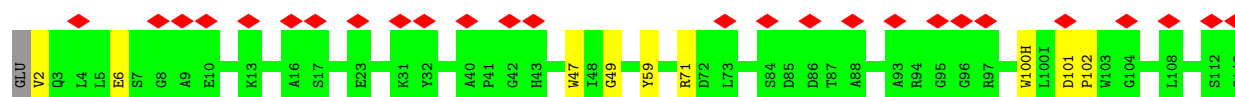
- Molecule 4: ACS124 light chain



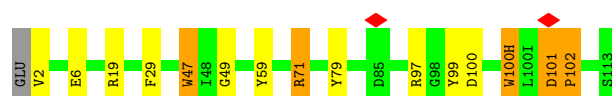
- Molecule 5: ACS101 heavy chain



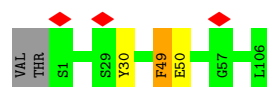
- Molecule 5: ACS101 heavy chain



- Molecule 5: ACS101 heavy chain

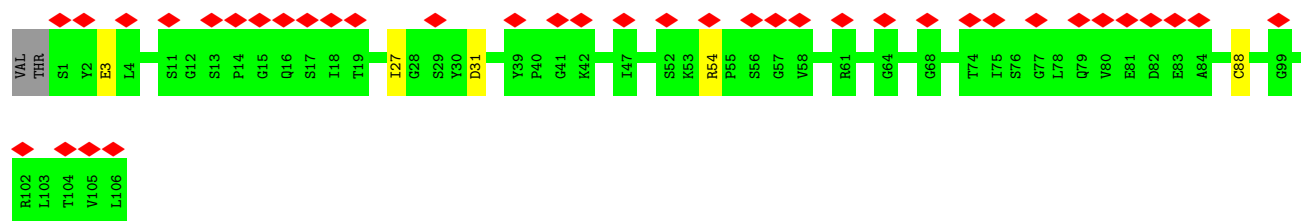


- Molecule 6: ACS101 light chain



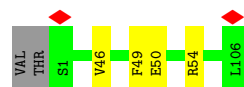
- Molecule 6: ACS101 light chain





- Molecule 6: ACS101 light chain

Chain P: 94%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l: 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose







- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



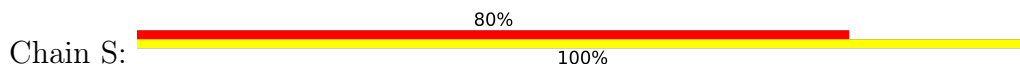
- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 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



- Molecule 9: 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

nose



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	95062	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.860	Depositor
Minimum map value	-0.373	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.2	Depositor
Map size ( $\text{\AA}$ )	345.0, 345.0, 345.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.15, 1.15, 1.15	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, 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	1.16	13/3476 (0.4%)	0.95	10/4718 (0.2%)
1	C	1.15	19/3476 (0.5%)	0.94	6/4718 (0.1%)
1	D	1.17	15/3476 (0.4%)	0.92	7/4718 (0.1%)
2	B	1.32	5/1008 (0.5%)	0.90	1/1367 (0.1%)
2	E	1.20	2/914 (0.2%)	0.89	0/1241
2	F	1.22	1/923 (0.1%)	0.86	2/1253 (0.2%)
3	G	1.35	8/994 (0.8%)	0.98	2/1355 (0.1%)
3	M	1.37	11/994 (1.1%)	0.94	0/1355
4	I	1.18	6/839 (0.7%)	0.97	2/1143 (0.2%)
4	O	1.22	3/839 (0.4%)	0.93	2/1143 (0.2%)
5	H	1.36	7/1018 (0.7%)	1.01	2/1387 (0.1%)
5	J	1.18	4/1018 (0.4%)	0.99	0/1387
5	K	1.31	9/1018 (0.9%)	1.04	4/1387 (0.3%)
6	L	1.14	1/813 (0.1%)	0.98	2/1103 (0.2%)
6	N	1.10	3/813 (0.4%)	1.01	1/1103 (0.1%)
6	P	1.11	0/813	0.97	1/1103 (0.1%)
All	All	1.21	107/22432 (0.5%)	0.95	42/30481 (0.1%)

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	48	TYR	CB-CG	-11.48	1.34	1.51
3	G	92	CYS	CB-SG	-10.80	1.63	1.82
3	M	78	PHE	CB-CG	-8.92	1.36	1.51
1	A	376	PHE	CB-CG	-8.75	1.36	1.51
3	M	53	PHE	CB-CG	-8.30	1.37	1.51
3	G	53	PHE	CB-CG	-8.05	1.37	1.51
6	L	49	PHE	CB-CG	-8.04	1.37	1.51
1	A	134	TYR	CG-CD1	7.97	1.49	1.39
1	D	134	TYR	CE1-CZ	7.96	1.49	1.38
4	I	48	TYR	CB-CG	-7.96	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	134	TYR	CG-CD1	7.93	1.49	1.39
1	A	134	TYR	CG-CD2	7.85	1.49	1.39
1	D	427	TRP	CB-CG	-7.85	1.36	1.50
1	C	134	TYR	CE1-CZ	7.69	1.48	1.38
1	D	134	TYR	CG-CD2	7.67	1.49	1.39
5	J	59	TYR	CB-CG	-7.44	1.40	1.51
1	A	134	TYR	CE2-CZ	7.21	1.48	1.38
1	A	134	TYR	CE1-CZ	7.18	1.47	1.38
1	D	134	TYR	CG-CD1	7.08	1.48	1.39
1	C	134	TYR	CG-CD2	6.97	1.48	1.39
1	C	134	TYR	CE2-CZ	6.89	1.47	1.38
6	N	3	GLU	CG-CD	-6.84	1.41	1.51
1	C	384	TYR	CB-CG	-6.57	1.41	1.51
6	N	88	CYS	CB-SG	-6.54	1.71	1.82
1	C	134	TYR	CD1-CE1	6.48	1.49	1.39
1	D	134	TYR	CE2-CZ	6.42	1.47	1.38
3	M	34	TRP	CB-CG	-6.42	1.38	1.50
2	B	596	TRP	CB-CG	-6.39	1.38	1.50
1	D	150	GLU	CB-CG	6.36	1.64	1.52
5	H	6	GLU	CD-OE1	-6.28	1.18	1.25
3	G	34	TRP	CZ3-CH2	-6.27	1.30	1.40
5	K	79	TYR	CB-CG	-6.27	1.42	1.51
5	K	99	TYR	CD1-CE1	-6.27	1.29	1.39
5	K	100(H)	TRP	CB-CG	-6.23	1.39	1.50
1	A	35	TRP	CZ2-CH2	6.12	1.49	1.37
1	A	466	GLU	CD-OE2	-6.11	1.19	1.25
1	C	134	TYR	CB-CG	6.08	1.60	1.51
1	C	217	TYR	CB-CG	-6.07	1.42	1.51
1	D	435	TYR	CG-CD1	-6.06	1.31	1.39
4	I	86	TYR	CB-CG	-6.03	1.42	1.51
3	G	78	PHE	CB-CG	-6.03	1.41	1.51
5	J	100(H)	TRP	CB-CG	-6.02	1.39	1.50
3	M	103	TRP	NE1-CE2	-6.01	1.29	1.37
1	D	35	TRP	CZ2-CH2	5.91	1.48	1.37
1	A	182	VAL	CB-CG2	-5.90	1.40	1.52
4	O	35	TYR	CB-CG	-5.88	1.42	1.51
5	H	100(A)	GLU	CD-OE1	-5.85	1.19	1.25
4	I	48	TYR	CD2-CE2	-5.85	1.30	1.39
2	B	634	GLU	CD-OE1	-5.81	1.19	1.25
2	F	631	TRP	CB-CG	-5.80	1.39	1.50
5	H	79	TYR	CB-CG	-5.79	1.43	1.51
5	J	6	GLU	CG-CD	-5.78	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	35	TRP	CZ2-CH2	5.76	1.48	1.37
1	C	35	TRP	CD2-CE3	5.76	1.49	1.40
5	K	59	TYR	CB-CG	-5.67	1.43	1.51
3	M	100(G)	TRP	CD2-CE2	-5.67	1.34	1.41
1	C	182	VAL	CB-CG2	-5.66	1.41	1.52
1	C	150	GLU	CB-CG	5.65	1.62	1.52
1	A	66	ARG	NE-CZ	5.62	1.40	1.33
3	M	100(H)	PHE	CB-CG	5.62	1.60	1.51
1	D	66	ARG	NE-CZ	5.58	1.40	1.33
3	M	78	PHE	CD2-CE2	-5.58	1.28	1.39
3	M	33	TYR	CE1-CZ	-5.54	1.31	1.38
1	A	35	TRP	CD2-CE3	5.53	1.48	1.40
4	I	48	TYR	CE2-CZ	-5.53	1.31	1.38
3	G	103	TRP	NE1-CE2	-5.52	1.30	1.37
2	B	638	TYR	CB-CG	-5.47	1.43	1.51
1	D	435	TYR	CB-CG	-5.44	1.43	1.51
1	A	217	TYR	CB-CG	-5.40	1.43	1.51
4	O	48	TYR	CD2-CE2	-5.39	1.31	1.39
1	D	39	TYR	CB-CG	-5.37	1.43	1.51
1	D	435	TYR	CD1-CE1	-5.37	1.31	1.39
5	K	29	PHE	CB-CG	-5.36	1.42	1.51
3	G	34	TRP	CB-CG	-5.36	1.40	1.50
5	K	102	PRO	N-CD	-5.35	1.40	1.47
3	M	33	TYR	CB-CG	-5.34	1.43	1.51
1	C	66	ARG	NE-CZ	5.31	1.40	1.33
3	G	100(A)	GLU	CD-OE2	-5.29	1.19	1.25
5	K	2	VAL	CB-CG2	5.29	1.64	1.52
4	I	2	TYR	CB-CG	-5.28	1.43	1.51
6	N	3	GLU	CD-OE2	-5.28	1.19	1.25
1	D	384	TYR	CB-CG	-5.27	1.43	1.51
3	G	103	TRP	CZ3-CH2	-5.22	1.31	1.40
3	M	103	TRP	CZ3-CH2	-5.22	1.31	1.40
2	E	596	TRP	CB-CG	-5.22	1.40	1.50
1	C	466	GLU	CD-OE1	-5.21	1.20	1.25
5	H	99	TYR	CB-CG	-5.21	1.43	1.51
5	K	6	GLU	CD-OE1	-5.21	1.20	1.25
2	B	632	GLU	CD-OE1	-5.20	1.20	1.25
2	E	632	GLU	CD-OE2	-5.19	1.20	1.25
2	B	631	TRP	CB-CG	-5.18	1.41	1.50
1	D	35	TRP	CD2-CE3	5.18	1.48	1.40
5	H	29	PHE	CB-CG	-5.17	1.42	1.51
1	C	376	PHE	CB-CG	-5.17	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	GLU	CD-OE2	-5.16	1.20	1.25
1	A	484	TYR	CB-CG	-5.15	1.44	1.51
3	M	33	TYR	CG-CD1	-5.15	1.32	1.39
1	C	91	GLU	CD-OE1	-5.13	1.20	1.25
1	C	42	VAL	CB-CG1	-5.09	1.42	1.52
1	D	188	ASN	CB-CG	5.09	1.62	1.51
4	I	48	TYR	CG-CD1	-5.09	1.32	1.39
5	K	47	TRP	CZ3-CH2	-5.09	1.31	1.40
1	C	112	TRP	CB-CG	-5.06	1.41	1.50
5	H	47	TRP	CZ3-CH2	-5.05	1.31	1.40
1	C	482	GLU	CD-OE2	-5.03	1.20	1.25
5	H	103	TRP	CB-CG	-5.02	1.41	1.50
5	J	2	VAL	CB-CG1	5.01	1.63	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	66	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	A	273	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	D	273	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	C	166	ARG	NE-CZ-NH2	-8.51	116.05	120.30
3	G	100(F)	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	469	ARG	NE-CZ-NH2	-8.09	116.25	120.30
2	B	617	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	D	304	ARG	NE-CZ-NH2	-7.32	116.64	120.30
6	P	54	ARG	NE-CZ-NH2	-7.27	116.67	120.30
6	N	54	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	217	TYR	CB-CG-CD2	-7.16	116.70	121.00
5	K	97	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	C	217	TYR	CB-CG-CD1	-6.95	116.83	121.00
4	I	48	TYR	CB-CG-CD2	-6.81	116.92	121.00
1	A	40	TYR	CB-CG-CD1	-6.48	117.11	121.00
6	L	49	PHE	CB-CG-CD1	-6.29	116.39	120.80
1	C	166	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	456	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	C	419	ARG	NE-CZ-NH2	-6.16	117.22	120.30
4	O	2	TYR	CB-CG-CD1	-6.09	117.34	121.00
5	H	66	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	480	ARG	NE-CZ-NH1	5.79	123.19	120.30
3	G	33	TYR	CB-CG-CD2	-5.77	117.53	121.00
1	A	273	ARG	NE-CZ-NH1	5.76	123.18	120.30
6	L	30	TYR	CB-CG-CD2	-5.58	117.65	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	638	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	A	384	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	D	177	TYR	CB-CG-CD2	-5.44	117.74	121.00
4	O	48	TYR	CB-CG-CD2	-5.40	117.76	121.00
4	I	85	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	C	469	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	F	530	MET	CG-SD-CE	5.33	108.73	100.20
1	A	298	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	D	173	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	D	66	ARG	NE-CZ-NH1	5.22	122.91	120.30
5	K	101	ASP	CB-CG-OD2	5.21	122.99	118.30
5	K	19	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	217	TYR	CB-CG-CD1	-5.16	117.91	121.00
5	K	71	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	C	456	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	D	180	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	66	ARG	NE-CZ-NH1	5.07	122.83	120.30

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	3403	0	3351	8	0
1	C	3403	0	3352	12	0
1	D	3403	0	3351	15	0
2	B	992	0	967	4	0
2	E	898	0	879	2	0
2	F	907	0	885	2	0
3	G	969	0	948	3	0
3	M	969	0	948	7	0
4	I	820	0	788	1	0
4	O	820	0	788	3	0
5	H	990	0	942	2	0
5	J	990	0	942	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	990	0	942	9	0
6	L	795	0	773	1	0
6	N	795	0	773	1	0
6	P	795	0	773	5	0
7	2	28	0	25	0	0
7	9	28	0	25	0	0
7	AA	28	0	25	0	0
7	Q	28	0	25	0	0
7	W	28	0	25	0	0
7	g	28	0	25	0	0
7	l	28	0	25	0	0
7	s	28	0	25	0	0
7	u	28	0	25	0	0
7	v	28	0	25	0	0
8	0	39	0	34	0	0
8	1	39	0	34	0	0
8	3	39	0	34	0	0
8	4	39	0	34	0	0
8	5	39	0	34	0	0
8	6	39	0	34	0	0
8	7	39	0	34	0	0
8	8	39	0	34	0	0
8	R	39	0	34	0	0
8	T	39	0	34	0	0
8	U	39	0	34	0	0
8	V	39	0	33	0	0
8	X	39	0	34	0	0
8	Y	39	0	34	0	0
8	Z	39	0	34	0	0
8	a	39	0	34	0	0
8	b	39	0	34	0	0
8	c	39	0	34	0	0
8	e	39	0	34	0	0
8	f	39	0	34	0	0
8	h	39	0	34	0	0
8	i	39	0	34	0	0
8	j	39	0	34	0	0
8	k	39	0	34	0	0
8	m	39	0	34	0	0
8	n	39	0	34	0	0
8	o	39	0	34	0	0
8	p	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	q	39	0	34	0	0
8	r	39	0	34	0	0
8	t	39	0	34	0	0
8	w	39	0	34	0	0
8	x	39	0	34	0	0
8	z	39	0	34	0	0
9	S	61	0	52	0	0
9	y	61	0	52	0	0
10	d	39	0	34	0	0
11	A	70	0	65	0	0
11	B	42	0	39	2	0
11	C	42	0	39	0	0
11	D	84	0	78	0	0
11	E	28	0	26	0	0
11	F	28	0	26	0	0
All	All	24000	0	23218	67	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 1.

All (67) 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)
5:K:101:ASP:OD1	6:P:46:VAL:HG21	1.43	1.17
5:K:101:ASP:OD1	6:P:46:VAL:CG2	1.98	1.10
1:D:358:THR:HG23	1:D:396:ASN:HB3	1.59	0.82
5:K:100(H):TRP:NE1	5:K:101:ASP:OD2	2.12	0.82
1:C:312:ALA:HB3	1:C:315:ARG:HB3	1.74	0.69
1:A:120:VAL:HG22	1:A:315:ARG:HG3	1.76	0.67
5:K:101:ASP:HB2	5:K:102:PRO:HD3	1.75	0.67
1:C:312:ALA:HB1	1:C:313:PRO:HD2	1.77	0.67
1:C:166:ARG:NH2	1:C:313:PRO:HB3	2.10	0.66
2:B:634:GLU:O	11:B:702:NAG:H83	1.99	0.62
1:D:312:ALA:HB3	1:D:315:ARG:HB2	1.86	0.57
1:A:107:ASP:OD1	2:B:574:LYS:NZ	2.40	0.55
5:K:101:ASP:OD1	6:P:46:VAL:CB	2.53	0.55
4:O:35:TYR:CE1	4:O:86:TYR:HB2	2.42	0.55
1:C:312:ALA:HB3	1:C:315:ARG:CB	2.37	0.54
1:D:107:ASP:OD1	2:F:574:LYS:NZ	2.42	0.53
5:K:100(H):TRP:CD1	5:K:101:ASP:OD2	2.62	0.53
5:K:101:ASP:OD1	6:P:46:VAL:HG23	2.02	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:620:ASP:N	2:B:620:ASP:OD1	2.43	0.51
1:C:107:ASP:OD1	2:E:574:LYS:NZ	2.44	0.50
1:A:232:LYS:NZ	1:A:269:GLU:OE2	2.45	0.50
1:A:312:ALA:HB1	1:A:313:PRO:HD2	1.95	0.49
5:J:101:ASP:HB3	5:J:102:PRO:HD3	1.95	0.49
1:C:490:LYS:NZ	1:C:492:GLU:OE2	2.44	0.48
4:I:35:TYR:CZ	4:I:86:TYR:HB2	2.49	0.48
3:M:100(G):TRP:CG	3:M:100(G):TRP:O	2.66	0.48
3:M:101:ASP:HB2	3:M:102:PRO:HD3	1.97	0.47
1:D:123:THR:N	1:D:124:PRO:CD	2.78	0.47
1:D:290:GLU:OE2	1:D:337:LYS:NZ	2.46	0.46
1:C:363:GLN:O	1:C:470:PRO:HD2	2.15	0.46
1:C:97:LYS:NZ	5:K:100:ASP:O	2.49	0.46
2:B:617:ARG:HB2	11:B:701:NAG:H81	1.98	0.46
2:F:606:THR:OG1	2:F:607:ALA:N	2.48	0.46
3:G:34:TRP:CH2	3:G:92:CYS:SG	3.09	0.45
1:C:123:THR:N	1:C:124:PRO:CD	2.80	0.45
1:D:165:ILE:HG12	1:D:313:PRO:HA	1.99	0.45
1:D:309:ILE:HG13	1:D:312:ALA:H	1.82	0.45
1:A:357:LYS:HB3	1:A:358:THR:H	1.70	0.45
2:E:606:THR:OG1	2:E:607:ALA:N	2.50	0.44
6:L:49:PHE:O	6:L:50:GLU:C	2.56	0.44
4:O:35:TYR:CZ	4:O:86:TYR:HB2	2.52	0.44
6:P:49:PHE:O	6:P:50:GLU:C	2.55	0.44
1:A:71:THR:HB	1:A:74:CYS:HB2	2.00	0.44
1:C:315:ARG:C	1:C:316:TRP:CD1	2.91	0.44
3:M:100(G):TRP:NE1	4:O:35:TYR:CD1	2.86	0.44
1:A:314:GLY:H	1:D:198:THR:HA	1.82	0.43
1:D:358:THR:HB	1:D:465:THR:HG23	2.00	0.43
3:M:100(G):TRP:O	3:M:100(H):PHE:CB	2.64	0.43
1:D:461:ASN:OD1	1:D:461:ASN:N	2.50	0.43
3:G:101:ASP:HB2	3:G:102:PRO:HD3	2.00	0.43
5:H:101:ASP:HB2	5:H:102:PRO:HD3	2.00	0.43
1:D:165:ILE:O	1:D:166:ARG:HB2	2.19	0.43
3:M:52:PHE:CG	3:M:53:PHE:N	2.87	0.42
5:H:47:TRP:CZ2	5:H:49:GLY:HA2	2.55	0.41
1:D:294:ILE:HD11	1:D:331:CYS:HB3	2.01	0.41
5:K:47:TRP:CZ2	5:K:49:GLY:HA2	2.55	0.41
1:C:113:ASP:OD2	1:C:429:LYS:NZ	2.53	0.41
1:D:56:SER:O	1:D:57:ASP:C	2.56	0.41
1:D:99:ASP:OD1	1:D:99:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:100(G):TRP:O	3:M:100(H):PHE:HB2	2.21	0.41
1:A:133:ASP:OD1	1:A:155:LYS:NZ	2.46	0.41
6:N:27:ILE:O	6:N:31:ASP:N	2.54	0.41
1:C:99:ASP:OD1	1:C:99:ASP:N	2.50	0.40
1:D:165:ILE:CG1	1:D:313:PRO:HA	2.51	0.40
3:M:94:ARG:HB3	3:M:102:PRO:HG2	2.04	0.40
3:G:52:PHE:CG	3:G:53:PHE:N	2.89	0.40
5:J:47:TRP:CZ2	5:J:49:GLY:HA2	2.56	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	419/482 (87%)	410 (98%)	9 (2%)	0	100	100
1	C	419/482 (87%)	404 (96%)	15 (4%)	0	100	100
1	D	419/482 (87%)	408 (97%)	11 (3%)	0	100	100
2	B	120/154 (78%)	118 (98%)	2 (2%)	0	100	100
2	E	109/154 (71%)	106 (97%)	3 (3%)	0	100	100
2	F	110/154 (71%)	108 (98%)	2 (2%)	0	100	100
3	G	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
3	M	121/124 (98%)	115 (95%)	6 (5%)	0	100	100
4	I	106/108 (98%)	106 (100%)	0	0	100	100
4	O	106/108 (98%)	106 (100%)	0	0	100	100
5	H	123/126 (98%)	119 (97%)	4 (3%)	0	100	100
5	J	123/126 (98%)	119 (97%)	4 (3%)	0	100	100
5	K	123/126 (98%)	120 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	L	104/108 (96%)	99 (95%)	5 (5%)	0	100	100
6	N	104/108 (96%)	101 (97%)	3 (3%)	0	100	100
6	P	104/108 (96%)	102 (98%)	2 (2%)	0	100	100
All	All	2731/3074 (89%)	2658 (97%)	73 (3%)	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	387/429 (90%)	385 (100%)	2 (0%)	86	89
1	C	387/429 (90%)	386 (100%)	1 (0%)	91	92
1	D	387/429 (90%)	384 (99%)	3 (1%)	79	84
2	B	107/130 (82%)	107 (100%)	0	100	100
2	E	96/130 (74%)	96 (100%)	0	100	100
2	F	97/130 (75%)	96 (99%)	1 (1%)	73	81
3	G	109/110 (99%)	109 (100%)	0	100	100
3	M	109/110 (99%)	109 (100%)	0	100	100
4	I	91/91 (100%)	91 (100%)	0	100	100
4	O	91/91 (100%)	91 (100%)	0	100	100
5	H	103/104 (99%)	102 (99%)	1 (1%)	73	81
5	J	103/104 (99%)	102 (99%)	1 (1%)	73	81
5	K	103/104 (99%)	102 (99%)	1 (1%)	73	81
6	L	89/91 (98%)	89 (100%)	0	100	100
6	N	89/91 (98%)	89 (100%)	0	100	100
6	P	89/91 (98%)	89 (100%)	0	100	100
All	All	2437/2664 (92%)	2427 (100%)	10 (0%)	88	91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	ARG
1	A	354	LYS
1	C	354	LYS
1	D	295	ASN
1	D	354	LYS
1	D	358	THR
2	F	625	ASN
5	H	71	ARG
5	J	71	ARG
5	K	71	ARG

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

### 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 ⓘ

135 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	$\# Z  > 2$
8	NAG	0	1	8,1	14,14,15	2.24	6 (42%)	17,19,21	1.36	3 (17%)
8	NAG	0	2	8	14,14,15	1.99	4 (28%)	17,19,21	1.02	1 (5%)
8	BMA	0	3	8	11,11,12	1.94	4 (36%)	15,15,17	0.75	0
8	NAG	1	1	8,1	14,14,15	1.92	6 (42%)	17,19,21	1.46	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	1	2	8	14,14,15	1.85	5 (35%)	17,19,21	1.06	2 (11%)
8	BMA	1	3	8	11,11,12	1.92	5 (45%)	15,15,17	0.79	1 (6%)
7	NAG	2	1	1,7	14,14,15	2.00	5 (35%)	17,19,21	1.23	2 (11%)
7	NAG	2	2	7	14,14,15	2.19	6 (42%)	17,19,21	1.11	2 (11%)
8	NAG	3	1	8,1	14,14,15	2.16	5 (35%)	17,19,21	1.71	4 (23%)
8	NAG	3	2	8	14,14,15	2.21	7 (50%)	17,19,21	1.21	3 (17%)
8	BMA	3	3	8	11,11,12	2.05	6 (54%)	15,15,17	0.70	0
8	NAG	4	1	8,1	14,14,15	1.96	5 (35%)	17,19,21	1.08	1 (5%)
8	NAG	4	2	8	14,14,15	1.99	5 (35%)	17,19,21	0.98	1 (5%)
8	BMA	4	3	8	11,11,12	1.97	6 (54%)	15,15,17	0.68	0
8	NAG	5	1	8,1	14,14,15	1.90	5 (35%)	17,19,21	1.14	1 (5%)
8	NAG	5	2	8	14,14,15	2.00	6 (42%)	17,19,21	0.96	1 (5%)
8	BMA	5	3	8	11,11,12	1.98	6 (54%)	15,15,17	0.77	0
8	NAG	6	1	8,1	14,14,15	2.15	5 (35%)	17,19,21	1.24	2 (11%)
8	NAG	6	2	8	14,14,15	2.31	7 (50%)	17,19,21	1.31	3 (17%)
8	BMA	6	3	8	11,11,12	2.01	6 (54%)	15,15,17	0.72	0
8	NAG	7	1	8,1	14,14,15	2.07	6 (42%)	17,19,21	1.01	1 (5%)
8	NAG	7	2	8	14,14,15	2.03	5 (35%)	17,19,21	0.92	1 (5%)
8	BMA	7	3	8	11,11,12	2.01	6 (54%)	15,15,17	0.79	0
8	NAG	8	1	8,1	14,14,15	0.56	0	17,19,21	1.24	2 (11%)
8	NAG	8	2	8	14,14,15	0.31	0	17,19,21	1.47	3 (17%)
8	BMA	8	3	8	11,11,12	0.20	0	15,15,17	0.86	1 (6%)
7	NAG	9	1	2,7	14,14,15	2.26	4 (28%)	17,19,21	1.16	1 (5%)
7	NAG	9	2	7	14,14,15	2.18	7 (50%)	17,19,21	0.88	2 (11%)
7	NAG	AA	1	2,7	14,14,15	2.16	7 (50%)	17,19,21	1.24	2 (11%)
7	NAG	AA	2	7	14,14,15	2.22	7 (50%)	17,19,21	0.87	1 (5%)
7	NAG	Q	1	1,7	14,14,15	2.24	6 (42%)	17,19,21	1.16	1 (5%)
7	NAG	Q	2	7	14,14,15	2.02	7 (50%)	17,19,21	0.89	1 (5%)
8	NAG	R	1	8,1	14,14,15	2.18	7 (50%)	17,19,21	1.51	3 (17%)
8	NAG	R	2	8	14,14,15	2.01	5 (35%)	17,19,21	1.11	2 (11%)
8	BMA	R	3	8	11,11,12	2.03	6 (54%)	15,15,17	0.77	0
9	NAG	S	1	9,1	14,14,15	2.03	5 (35%)	17,19,21	0.97	0
9	NAG	S	2	9	14,14,15	1.96	5 (35%)	17,19,21	1.00	1 (5%)
9	BMA	S	3	9	11,11,12	1.60	3 (27%)	15,15,17	0.90	1 (6%)
9	MAN	S	4	9	11,11,12	2.04	5 (45%)	15,15,17	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	S	5	9	11,11,12	1.88	5 (45%)	15,15,17	0.85	0
8	NAG	T	1	8,1	14,14,15	1.89	5 (35%)	17,19,21	1.10	1 (5%)
8	NAG	T	2	8	14,14,15	2.02	6 (42%)	17,19,21	0.98	1 (5%)
8	BMA	T	3	8	11,11,12	2.00	6 (54%)	15,15,17	0.68	0
8	NAG	U	1	8,1	14,14,15	2.07	5 (35%)	17,19,21	1.15	1 (5%)
8	NAG	U	2	8	14,14,15	2.09	6 (42%)	17,19,21	1.32	3 (17%)
8	BMA	U	3	8	11,11,12	2.05	4 (36%)	15,15,17	0.70	0
8	NAG	V	1	8,1	14,14,15	2.12	6 (42%)	17,19,21	0.95	1 (5%)
8	NAG	V	2	8	14,14,15	1.85	5 (35%)	17,19,21	12.05	4 (23%)
8	BMA	V	3	8	11,11,12	1.91	5 (45%)	15,15,17	0.82	0
7	NAG	W	1	1,7	14,14,15	1.88	5 (35%)	17,19,21	1.26	2 (11%)
7	NAG	W	2	7	14,14,15	2.02	5 (35%)	17,19,21	0.92	1 (5%)
8	NAG	X	1	8,1	14,14,15	1.94	7 (50%)	17,19,21	1.26	2 (11%)
8	NAG	X	2	8	14,14,15	2.09	5 (35%)	17,19,21	0.92	1 (5%)
8	BMA	X	3	8	11,11,12	2.03	6 (54%)	15,15,17	0.68	0
8	NAG	Y	1	8,1	14,14,15	1.98	6 (42%)	17,19,21	1.08	1 (5%)
8	NAG	Y	2	8	14,14,15	1.94	5 (35%)	17,19,21	0.99	2 (11%)
8	BMA	Y	3	8	11,11,12	1.98	6 (54%)	15,15,17	0.78	0
8	NAG	Z	1	8,1	14,14,15	1.93	4 (28%)	17,19,21	0.97	0
8	NAG	Z	2	8	14,14,15	1.96	6 (42%)	17,19,21	0.93	1 (5%)
8	BMA	Z	3	8	11,11,12	1.98	6 (54%)	15,15,17	0.77	0
8	NAG	a	1	8,1	14,14,15	2.14	5 (35%)	17,19,21	1.15	2 (11%)
8	NAG	a	2	8	14,14,15	2.33	7 (50%)	17,19,21	1.24	2 (11%)
8	BMA	a	3	8	11,11,12	2.06	6 (54%)	15,15,17	0.67	0
8	NAG	b	1	8,1	14,14,15	2.08	4 (28%)	17,19,21	0.93	1 (5%)
8	NAG	b	2	8	14,14,15	1.98	5 (35%)	17,19,21	0.95	1 (5%)
8	BMA	b	3	8	11,11,12	2.02	6 (54%)	15,15,17	0.72	0
8	NAG	c	1	8,1	14,14,15	2.05	5 (35%)	17,19,21	1.13	1 (5%)
8	NAG	c	2	8	14,14,15	2.33	6 (42%)	17,19,21	1.11	2 (11%)
8	BMA	c	3	8	11,11,12	2.06	6 (54%)	15,15,17	0.67	0
10	NAG	d	1	10,1	14,14,15	2.04	4 (28%)	17,19,21	1.10	2 (11%)
10	NAG	d	2	10	14,14,15	2.17	8 (57%)	17,19,21	1.30	3 (17%)
10	BMA	d	3	10	11,11,12	1.99	6 (54%)	15,15,17	0.73	0
8	NAG	e	1	8,2	14,14,15	2.11	6 (42%)	17,19,21	1.70	4 (23%)
8	NAG	e	2	8	14,14,15	2.09	6 (42%)	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BMA	e	3	8	11,11,12	2.03	6 (54%)	15,15,17	0.67	0
8	NAG	f	1	8,1	14,14,15	2.03	6 (42%)	17,19,21	1.08	1 (5%)
8	NAG	f	2	8	14,14,15	2.03	7 (50%)	17,19,21	1.27	1 (5%)
8	BMA	f	3	8	11,11,12	1.99	6 (54%)	15,15,17	0.73	0
7	NAG	g	1	1,7	14,14,15	2.25	6 (42%)	17,19,21	0.83	0
7	NAG	g	2	7	14,14,15	1.91	6 (42%)	17,19,21	0.96	2 (11%)
8	NAG	h	1	8,1	14,14,15	1.99	5 (35%)	17,19,21	1.21	3 (17%)
8	NAG	h	2	8	14,14,15	2.00	6 (42%)	17,19,21	0.97	1 (5%)
8	BMA	h	3	8	11,11,12	2.04	6 (54%)	15,15,17	0.67	0
8	NAG	i	1	8,1	14,14,15	2.08	6 (42%)	17,19,21	1.40	3 (17%)
8	NAG	i	2	8	14,14,15	2.12	6 (42%)	17,19,21	1.23	4 (23%)
8	BMA	i	3	8	11,11,12	2.01	6 (54%)	15,15,17	0.69	0
8	NAG	j	1	8,1	14,14,15	2.18	7 (50%)	17,19,21	1.30	3 (17%)
8	NAG	j	2	8	14,14,15	1.94	4 (28%)	17,19,21	1.03	1 (5%)
8	BMA	j	3	8	11,11,12	1.99	4 (36%)	15,15,17	0.79	0
8	NAG	k	1	8,1	14,14,15	1.95	6 (42%)	17,19,21	1.21	2 (11%)
8	NAG	k	2	8	14,14,15	1.88	6 (42%)	17,19,21	1.08	1 (5%)
8	BMA	k	3	8	11,11,12	1.99	5 (45%)	15,15,17	0.71	0
7	NAG	l	1	1,7	14,14,15	1.93	5 (35%)	17,19,21	1.34	4 (23%)
7	NAG	l	2	7	14,14,15	1.94	6 (42%)	17,19,21	0.87	1 (5%)
8	NAG	m	1	8,1	14,14,15	1.99	6 (42%)	17,19,21	1.13	2 (11%)
8	NAG	m	2	8	14,14,15	2.03	5 (35%)	17,19,21	0.87	1 (5%)
8	BMA	m	3	8	11,11,12	2.01	6 (54%)	15,15,17	0.77	0
8	NAG	n	1	8,1	14,14,15	2.30	6 (42%)	17,19,21	1.58	4 (23%)
8	NAG	n	2	8	14,14,15	2.14	6 (42%)	17,19,21	1.07	1 (5%)
8	BMA	n	3	8	11,11,12	2.10	6 (54%)	15,15,17	0.71	0
8	NAG	o	1	8,1	14,14,15	2.04	6 (42%)	17,19,21	1.32	3 (17%)
8	NAG	o	2	8	14,14,15	2.11	7 (50%)	17,19,21	1.23	4 (23%)
8	BMA	o	3	8	11,11,12	2.01	6 (54%)	15,15,17	0.73	0
8	NAG	p	1	8,1	14,14,15	2.02	5 (35%)	17,19,21	1.07	0
8	NAG	p	2	8	14,14,15	2.31	7 (50%)	17,19,21	1.31	4 (23%)
8	BMA	p	3	8	11,11,12	2.03	6 (54%)	15,15,17	0.71	0
8	NAG	q	1	8,1	14,14,15	2.03	7 (50%)	17,19,21	1.12	2 (11%)
8	NAG	q	2	8	14,14,15	2.18	7 (50%)	17,19,21	0.94	0
8	BMA	q	3	8	11,11,12	2.03	6 (54%)	15,15,17	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	r	1	8,1	14,14,15	2.14	5 (35%)	17,19,21	1.06	1 (5%)
8	NAG	r	2	8	14,14,15	2.01	6 (42%)	17,19,21	1.02	2 (11%)
8	BMA	r	3	8	11,11,12	2.02	6 (54%)	15,15,17	0.67	0
7	NAG	s	1	1,7	14,14,15	2.11	5 (35%)	17,19,21	1.11	0
7	NAG	s	2	7	14,14,15	1.99	4 (28%)	17,19,21	0.85	1 (5%)
8	NAG	t	1	8,1	14,14,15	2.06	5 (35%)	17,19,21	1.09	2 (11%)
8	NAG	t	2	8	14,14,15	2.14	6 (42%)	17,19,21	1.30	4 (23%)
8	BMA	t	3	8	11,11,12	2.09	6 (54%)	15,15,17	0.73	0
7	NAG	u	1	2,7	14,14,15	2.20	7 (50%)	17,19,21	1.50	3 (17%)
7	NAG	u	2	7	14,14,15	2.16	7 (50%)	17,19,21	0.92	1 (5%)
7	NAG	v	1	2,7	14,14,15	2.29	6 (42%)	17,19,21	1.04	1 (5%)
7	NAG	v	2	7	14,14,15	1.98	6 (42%)	17,19,21	0.87	1 (5%)
8	NAG	w	1	8,1	14,14,15	1.94	5 (35%)	17,19,21	1.08	1 (5%)
8	NAG	w	2	8	14,14,15	2.02	6 (42%)	17,19,21	1.00	2 (11%)
8	BMA	w	3	8	11,11,12	2.00	6 (54%)	15,15,17	0.67	0
8	NAG	x	1	8,1	14,14,15	2.28	6 (42%)	17,19,21	1.31	1 (5%)
8	NAG	x	2	8	14,14,15	2.11	6 (42%)	17,19,21	1.22	3 (17%)
8	BMA	x	3	8	11,11,12	2.03	6 (54%)	15,15,17	0.69	0
9	NAG	y	1	9,1	14,14,15	2.20	6 (42%)	17,19,21	1.19	2 (11%)
9	NAG	y	2	9	14,14,15	2.17	7 (50%)	17,19,21	1.73	4 (23%)
9	BMA	y	3	9	11,11,12	1.44	3 (27%)	15,15,17	0.69	0
9	MAN	y	4	9	11,11,12	1.97	6 (54%)	15,15,17	0.69	0
9	MAN	y	5	9	11,11,12	1.93	5 (45%)	15,15,17	0.75	0
8	NAG	z	1	8,1	14,14,15	2.12	5 (35%)	17,19,21	1.07	2 (11%)
8	NAG	z	2	8	14,14,15	2.19	6 (42%)	17,19,21	1.05	1 (5%)
8	BMA	z	3	8	11,11,12	2.02	6 (54%)	15,15,17	0.68	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
8	NAG	0	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	0	2	8	-	0/6/23/26	0/1/1/1
8	BMA	0	3	8	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	1	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	1	2	8	-	0/6/23/26	0/1/1/1
8	BMA	1	3	8	-	0/2/19/22	0/1/1/1
7	NAG	2	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	2	2	7	-	0/6/23/26	0/1/1/1
8	NAG	3	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	3	2	8	-	0/6/23/26	0/1/1/1
8	BMA	3	3	8	-	0/2/19/22	0/1/1/1
8	NAG	4	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	4	2	8	-	0/6/23/26	0/1/1/1
8	BMA	4	3	8	-	0/2/19/22	0/1/1/1
8	NAG	5	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	5	2	8	-	0/6/23/26	0/1/1/1
8	BMA	5	3	8	-	1/2/19/22	0/1/1/1
8	NAG	6	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	6	2	8	-	0/6/23/26	0/1/1/1
8	BMA	6	3	8	-	1/2/19/22	0/1/1/1
8	NAG	7	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	7	2	8	-	0/6/23/26	0/1/1/1
8	BMA	7	3	8	-	1/2/19/22	0/1/1/1
8	NAG	8	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	8	2	8	-	3/6/23/26	0/1/1/1
8	BMA	8	3	8	-	1/2/19/22	0/1/1/1
7	NAG	9	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	9	2	7	-	0/6/23/26	0/1/1/1
7	NAG	AA	1	2,7	-	1/6/23/26	0/1/1/1
7	NAG	AA	2	7	-	0/6/23/26	0/1/1/1
7	NAG	Q	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
8	NAG	R	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	R	2	8	-	0/6/23/26	0/1/1/1
8	BMA	R	3	8	-	1/2/19/22	0/1/1/1
9	NAG	S	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	S	2	9	-	0/6/23/26	0/1/1/1
9	BMA	S	3	9	-	0/2/19/22	0/1/1/1
9	MAN	S	4	9	-	1/2/19/22	0/1/1/1
9	MAN	S	5	9	-	1/2/19/22	0/1/1/1
8	NAG	T	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	T	2	8	-	0/6/23/26	0/1/1/1
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
8	NAG	U	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	U	2	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	U	3	8	-	0/2/19/22	0/1/1/1
8	NAG	V	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	V	2	8	-	2/6/23/26	0/1/1/1
8	BMA	V	3	8	-	1/2/19/22	0/1/1/1
7	NAG	W	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
8	NAG	X	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	X	2	8	-	0/6/23/26	0/1/1/1
8	BMA	X	3	8	-	0/2/19/22	0/1/1/1
8	NAG	Y	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	1/2/19/22	0/1/1/1
8	NAG	Z	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Z	3	8	-	1/2/19/22	0/1/1/1
8	NAG	a	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	0/6/23/26	0/1/1/1
8	BMA	a	3	8	-	0/2/19/22	0/1/1/1
8	NAG	b	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	0/6/23/26	0/1/1/1
8	BMA	b	3	8	-	1/2/19/22	0/1/1/1
8	NAG	c	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	c	2	8	-	0/6/23/26	0/1/1/1
8	BMA	c	3	8	-	0/2/19/22	0/1/1/1
10	NAG	d	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	d	2	10	-	0/6/23/26	0/1/1/1
10	BMA	d	3	10	-	0/2/19/22	0/1/1/1
8	NAG	e	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	0/6/23/26	0/1/1/1
8	BMA	e	3	8	-	0/2/19/22	0/1/1/1
8	NAG	f	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	f	2	8	-	0/6/23/26	0/1/1/1
8	BMA	f	3	8	-	1/2/19/22	0/1/1/1
7	NAG	g	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	g	2	7	-	0/6/23/26	0/1/1/1
8	NAG	h	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	h	2	8	-	0/6/23/26	0/1/1/1
8	BMA	h	3	8	-	0/2/19/22	0/1/1/1
8	NAG	i	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	i	2	8	-	0/6/23/26	0/1/1/1
8	BMA	i	3	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	j	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	j	2	8	-	0/6/23/26	0/1/1/1
8	BMA	j	3	8	-	1/2/19/22	0/1/1/1
8	NAG	k	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	k	2	8	-	0/6/23/26	0/1/1/1
8	BMA	k	3	8	-	1/2/19/22	0/1/1/1
7	NAG	l	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	l	2	7	-	0/6/23/26	0/1/1/1
8	NAG	m	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	m	2	8	-	0/6/23/26	0/1/1/1
8	BMA	m	3	8	-	1/2/19/22	0/1/1/1
8	NAG	n	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	n	2	8	-	0/6/23/26	0/1/1/1
8	BMA	n	3	8	-	0/2/19/22	0/1/1/1
8	NAG	o	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	o	2	8	-	0/6/23/26	0/1/1/1
8	BMA	o	3	8	-	1/2/19/22	0/1/1/1
8	NAG	p	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	p	2	8	-	0/6/23/26	0/1/1/1
8	BMA	p	3	8	-	1/2/19/22	0/1/1/1
8	NAG	q	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	q	2	8	-	0/6/23/26	0/1/1/1
8	BMA	q	3	8	-	1/2/19/22	0/1/1/1
8	NAG	r	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	r	2	8	-	0/6/23/26	0/1/1/1
8	BMA	r	3	8	-	0/2/19/22	0/1/1/1
7	NAG	s	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	s	2	7	-	0/6/23/26	0/1/1/1
8	NAG	t	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	t	2	8	-	0/6/23/26	0/1/1/1
8	BMA	t	3	8	-	1/2/19/22	0/1/1/1
7	NAG	u	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	u	2	7	-	0/6/23/26	0/1/1/1
7	NAG	v	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	v	2	7	-	0/6/23/26	0/1/1/1
8	NAG	w	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	w	2	8	-	0/6/23/26	0/1/1/1
8	BMA	w	3	8	-	0/2/19/22	0/1/1/1
8	NAG	x	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	x	2	8	-	0/6/23/26	0/1/1/1
8	BMA	x	3	8	-	1/2/19/22	0/1/1/1
9	NAG	y	1	9,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	y	2	9	-	1/6/23/26	0/1/1/1
9	BMA	y	3	9	-	2/2/19/22	0/1/1/1
9	MAN	y	4	9	-	0/2/19/22	0/1/1/1
9	MAN	y	5	9	-	0/2/19/22	0/1/1/1
8	NAG	z	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	z	2	8	-	0/6/23/26	0/1/1/1
8	BMA	z	3	8	-	0/2/19/22	0/1/1/1

All (750) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	c	2	NAG	C1-C2	5.95	1.61	1.52
7	g	1	NAG	C1-C2	5.91	1.61	1.52
8	p	2	NAG	C1-C2	5.76	1.60	1.52
7	9	1	NAG	C1-C2	5.73	1.60	1.52
8	a	2	NAG	C1-C2	5.71	1.60	1.52
7	2	2	NAG	C1-C2	5.70	1.60	1.52
8	x	1	NAG	C1-C2	5.66	1.60	1.52
7	AA	2	NAG	C1-C2	5.65	1.60	1.52
8	6	2	NAG	C1-C2	5.60	1.60	1.52
8	n	1	NAG	C1-C2	5.57	1.60	1.52
7	u	1	NAG	C1-C2	5.56	1.60	1.52
7	v	1	NAG	C1-C2	5.55	1.60	1.52
8	3	1	NAG	C1-C2	5.55	1.60	1.52
7	Q	1	NAG	C1-C2	5.31	1.60	1.52
7	s	1	NAG	C1-C2	5.23	1.60	1.52
8	o	1	NAG	C1-C2	5.22	1.60	1.52
8	r	1	NAG	C1-C2	5.19	1.60	1.52
8	6	1	NAG	C1-C2	5.19	1.60	1.52
7	9	2	NAG	C1-C2	5.18	1.60	1.52
7	u	2	NAG	C1-C2	5.17	1.60	1.52
9	y	1	NAG	C1-C2	5.15	1.60	1.52
8	V	1	NAG	C1-C2	5.12	1.60	1.52
8	z	1	NAG	C1-C2	5.12	1.60	1.52
8	X	2	NAG	C1-C2	5.08	1.59	1.52
8	b	1	NAG	C1-C2	5.03	1.59	1.52
8	R	1	NAG	C1-C2	5.02	1.59	1.52
7	W	2	NAG	C1-C2	5.02	1.59	1.52
7	AA	1	NAG	C1-C2	4.99	1.59	1.52
10	d	1	NAG	C1-C2	4.99	1.59	1.52
8	a	1	NAG	C1-C2	4.97	1.59	1.52
8	3	2	NAG	C1-C2	4.95	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	z	2	NAG	C1-C2	4.93	1.59	1.52
8	x	2	NAG	C1-C2	4.91	1.59	1.52
8	m	1	NAG	C1-C2	4.87	1.59	1.52
8	i	1	NAG	C1-C2	4.87	1.59	1.52
8	e	2	NAG	C1-C2	4.86	1.59	1.52
8	7	1	NAG	C1-C2	4.85	1.59	1.52
8	w	1	NAG	C1-C2	4.83	1.59	1.52
7	l	1	NAG	C1-C2	4.82	1.59	1.52
8	j	1	NAG	C1-C2	4.81	1.59	1.52
8	Y	1	NAG	C1-C2	4.78	1.59	1.52
8	i	2	NAG	C1-C2	4.78	1.59	1.52
8	4	1	NAG	C1-C2	4.77	1.59	1.52
8	7	2	NAG	C1-C2	4.76	1.59	1.52
8	t	2	NAG	C1-C2	4.74	1.59	1.52
8	0	1	NAG	C1-C2	4.74	1.59	1.52
7	s	2	NAG	C1-C2	4.72	1.59	1.52
8	U	1	NAG	C1-C2	4.69	1.59	1.52
9	y	2	NAG	C1-C2	4.68	1.59	1.52
8	c	1	NAG	C1-C2	4.68	1.59	1.52
8	Z	1	NAG	C1-C2	4.67	1.59	1.52
8	5	1	NAG	C1-C2	4.65	1.59	1.52
8	4	2	NAG	C1-C2	4.64	1.59	1.52
8	T	1	NAG	C1-C2	4.63	1.59	1.52
8	0	2	NAG	C1-C2	4.61	1.59	1.52
8	t	1	NAG	C1-C2	4.60	1.59	1.52
9	S	1	NAG	C1-C2	4.60	1.59	1.52
8	o	2	NAG	C1-C2	4.59	1.59	1.52
8	h	1	NAG	C1-C2	4.58	1.59	1.52
7	W	1	NAG	C1-C2	4.55	1.59	1.52
8	q	2	NAG	C1-C2	4.54	1.59	1.52
8	k	1	NAG	C1-C2	4.52	1.59	1.52
8	w	2	NAG	C1-C2	4.51	1.59	1.52
7	Q	2	NAG	C1-C2	4.51	1.59	1.52
8	T	2	NAG	C1-C2	4.51	1.59	1.52
8	m	2	NAG	C1-C2	4.49	1.59	1.52
7	2	1	NAG	C1-C2	4.45	1.59	1.52
8	f	1	NAG	C1-C2	4.44	1.59	1.52
8	h	2	NAG	C1-C2	4.43	1.59	1.52
8	p	1	NAG	C1-C2	4.43	1.59	1.52
8	5	2	NAG	C1-C2	4.43	1.59	1.52
7	l	2	NAG	C1-C2	4.42	1.58	1.52
8	n	2	NAG	C1-C2	4.42	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	l	2	NAG	C1-C2	4.41	1.58	1.52
10	d	2	NAG	C1-C2	4.39	1.58	1.52
8	j	2	NAG	C1-C2	4.37	1.58	1.52
8	e	1	NAG	C1-C2	4.36	1.58	1.52
8	X	1	NAG	C1-C2	4.36	1.58	1.52
8	q	1	NAG	C1-C2	4.35	1.58	1.52
8	R	2	NAG	C1-C2	4.30	1.58	1.52
7	v	2	NAG	C1-C2	4.29	1.58	1.52
8	Y	2	NAG	C1-C2	4.26	1.58	1.52
8	r	2	NAG	C1-C2	4.24	1.58	1.52
7	g	2	NAG	C1-C2	4.22	1.58	1.52
8	Z	2	NAG	C1-C2	4.22	1.58	1.52
8	l	1	NAG	C1-C2	4.21	1.58	1.52
8	f	2	NAG	C1-C2	4.20	1.58	1.52
8	b	2	NAG	C1-C2	4.19	1.58	1.52
9	S	2	NAG	C1-C2	4.16	1.58	1.52
8	U	2	NAG	C1-C2	4.14	1.58	1.52
8	k	2	NAG	C1-C2	4.06	1.58	1.52
8	V	2	NAG	C1-C2	3.91	1.58	1.52
8	0	1	NAG	O5-C5	3.88	1.51	1.43
8	n	3	BMA	C2-C3	3.56	1.57	1.52
8	U	3	BMA	C2-C3	3.53	1.57	1.52
8	p	1	NAG	O5-C5	3.52	1.50	1.43
8	j	1	NAG	O5-C5	3.49	1.50	1.43
9	S	4	MAN	C2-C3	3.45	1.57	1.52
7	Q	1	NAG	O5-C5	3.44	1.50	1.43
8	c	3	BMA	C2-C3	3.40	1.57	1.52
8	R	3	BMA	C2-C3	3.39	1.57	1.52
8	q	2	NAG	O5-C5	3.38	1.50	1.43
8	b	1	NAG	O5-C5	3.38	1.50	1.43
8	a	1	NAG	O5-C5	3.37	1.50	1.43
8	j	3	BMA	C2-C3	3.36	1.57	1.52
9	S	1	NAG	O5-C5	3.36	1.50	1.43
8	3	3	BMA	C2-C3	3.36	1.57	1.52
10	d	3	BMA	C2-C3	3.36	1.57	1.52
7	9	2	NAG	O5-C5	3.35	1.50	1.43
9	y	2	NAG	O5-C5	3.34	1.50	1.43
8	a	3	BMA	C2-C3	3.34	1.57	1.52
8	m	3	BMA	C2-C3	3.34	1.57	1.52
7	9	1	NAG	O5-C5	3.34	1.50	1.43
8	Y	3	BMA	C2-C3	3.33	1.57	1.52
8	t	3	BMA	C2-C3	3.33	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	0	3	BMA	C2-C3	3.32	1.57	1.52
8	7	3	BMA	C2-C3	3.32	1.57	1.52
8	X	3	BMA	C2-C3	3.31	1.57	1.52
8	T	3	BMA	C2-C3	3.31	1.57	1.52
8	f	3	BMA	C2-C3	3.30	1.57	1.52
8	o	3	BMA	C2-C3	3.30	1.57	1.52
8	Z	3	BMA	C2-C3	3.30	1.57	1.52
8	r	3	BMA	C2-C3	3.29	1.57	1.52
8	5	3	BMA	C2-C3	3.28	1.57	1.52
8	h	3	BMA	O5-C5	3.28	1.50	1.43
8	U	1	NAG	O5-C5	3.28	1.50	1.43
8	z	1	NAG	O5-C5	3.27	1.50	1.43
10	d	1	NAG	O5-C5	3.27	1.50	1.43
8	c	3	BMA	O5-C5	3.26	1.50	1.43
8	q	3	BMA	C2-C3	3.26	1.57	1.52
8	t	3	BMA	O5-C5	3.26	1.50	1.43
9	y	5	MAN	C2-C3	3.26	1.57	1.52
8	e	3	BMA	C2-C3	3.25	1.57	1.52
8	n	3	BMA	O5-C5	3.25	1.50	1.43
9	y	1	NAG	O5-C5	3.25	1.50	1.43
8	i	3	BMA	C2-C3	3.24	1.57	1.52
8	6	3	BMA	C2-C3	3.24	1.57	1.52
8	r	3	BMA	O5-C5	3.24	1.50	1.43
8	x	3	BMA	C2-C3	3.23	1.57	1.52
8	h	3	BMA	C2-C3	3.23	1.57	1.52
8	z	3	BMA	C2-C3	3.23	1.57	1.52
8	l	3	BMA	C2-C3	3.23	1.57	1.52
8	a	3	BMA	O5-C5	3.23	1.50	1.43
8	e	3	BMA	O5-C5	3.22	1.50	1.43
9	y	4	MAN	C2-C3	3.22	1.57	1.52
7	Q	2	NAG	O5-C5	3.20	1.49	1.43
8	p	3	BMA	C2-C3	3.19	1.57	1.52
8	4	3	BMA	C2-C3	3.19	1.57	1.52
8	X	3	BMA	O5-C5	3.19	1.49	1.43
8	b	3	BMA	C2-C3	3.19	1.57	1.52
8	x	3	BMA	O5-C5	3.18	1.49	1.43
7	v	1	NAG	O5-C5	3.18	1.49	1.43
8	c	1	NAG	O5-C5	3.17	1.49	1.43
8	z	3	BMA	O5-C5	3.17	1.49	1.43
7	AA	1	NAG	O5-C5	3.17	1.49	1.43
8	i	3	BMA	O5-C5	3.16	1.49	1.43
8	r	1	NAG	O5-C5	3.16	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	V	3	BMA	C2-C3	3.15	1.57	1.52
8	U	3	BMA	O5-C5	3.15	1.49	1.43
8	q	3	BMA	O5-C5	3.15	1.49	1.43
8	n	3	BMA	C1-C2	3.15	1.59	1.52
8	w	3	BMA	C2-C3	3.14	1.57	1.52
9	S	4	MAN	O5-C5	3.14	1.49	1.43
8	6	2	NAG	O5-C5	3.14	1.49	1.43
8	t	2	NAG	O5-C5	3.13	1.49	1.43
8	p	3	BMA	O5-C5	3.13	1.49	1.43
9	y	4	MAN	O5-C5	3.12	1.49	1.43
8	e	2	NAG	O5-C5	3.12	1.49	1.43
8	U	3	BMA	C1-C2	3.12	1.59	1.52
7	v	2	NAG	O5-C5	3.12	1.49	1.43
7	u	2	NAG	O5-C5	3.11	1.49	1.43
7	s	2	NAG	O5-C5	3.11	1.49	1.43
8	6	1	NAG	O5-C5	3.11	1.49	1.43
8	q	1	NAG	O5-C5	3.10	1.49	1.43
7	g	1	NAG	O5-C5	3.10	1.49	1.43
8	c	2	NAG	O5-C5	3.10	1.49	1.43
8	3	3	BMA	O5-C5	3.10	1.49	1.43
8	n	1	NAG	C4-C5	3.10	1.59	1.53
8	U	2	NAG	O5-C5	3.09	1.49	1.43
9	S	5	MAN	C2-C3	3.09	1.57	1.52
8	f	1	NAG	O5-C5	3.08	1.49	1.43
8	x	1	NAG	O5-C5	3.08	1.49	1.43
9	y	5	MAN	O5-C5	3.07	1.49	1.43
8	k	3	BMA	C1-C2	3.07	1.59	1.52
8	b	3	BMA	O5-C5	3.06	1.49	1.43
8	T	3	BMA	O5-C5	3.06	1.49	1.43
8	w	3	BMA	O5-C5	3.06	1.49	1.43
8	o	3	BMA	O5-C5	3.06	1.49	1.43
8	t	1	NAG	O5-C5	3.06	1.49	1.43
8	V	1	NAG	O5-C5	3.05	1.49	1.43
8	q	3	BMA	C1-C2	3.05	1.59	1.52
8	m	2	NAG	O5-C5	3.05	1.49	1.43
8	p	2	NAG	O5-C5	3.05	1.49	1.43
9	S	2	NAG	O5-C5	3.05	1.49	1.43
8	k	3	BMA	C2-C3	3.04	1.57	1.52
8	k	3	BMA	O5-C5	3.04	1.49	1.43
8	3	3	BMA	C1-C2	3.04	1.59	1.52
8	z	3	BMA	C1-C2	3.04	1.59	1.52
8	7	3	BMA	O5-C5	3.04	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	j	2	NAG	O5-C5	3.04	1.49	1.43
8	b	2	NAG	O5-C5	3.04	1.49	1.43
8	p	3	BMA	C1-C2	3.03	1.59	1.52
8	R	3	BMA	O5-C5	3.02	1.49	1.43
8	3	2	NAG	O5-C5	3.02	1.49	1.43
10	d	2	NAG	C4-C5	3.02	1.59	1.53
8	a	2	NAG	O5-C5	3.02	1.49	1.43
7	2	2	NAG	O5-C5	3.02	1.49	1.43
10	d	3	BMA	O5-C5	3.01	1.49	1.43
8	f	3	BMA	O5-C5	3.01	1.49	1.43
8	e	1	NAG	C4-C5	3.01	1.59	1.53
8	4	3	BMA	O5-C5	3.01	1.49	1.43
8	z	2	NAG	O5-C5	3.01	1.49	1.43
8	n	2	NAG	O5-C5	3.00	1.49	1.43
8	t	3	BMA	C1-C2	3.00	1.59	1.52
8	0	3	BMA	O5-C5	2.99	1.49	1.43
7	2	1	NAG	O5-C5	2.99	1.49	1.43
8	Y	3	BMA	O5-C5	2.99	1.49	1.43
8	j	3	BMA	O5-C5	2.99	1.49	1.43
8	6	3	BMA	O5-C5	2.99	1.49	1.43
8	0	2	NAG	O5-C5	2.99	1.49	1.43
8	1	3	BMA	O5-C5	2.99	1.49	1.43
8	a	3	BMA	C1-C2	2.98	1.59	1.52
7	l	2	NAG	O5-C5	2.97	1.49	1.43
9	S	5	MAN	O5-C5	2.97	1.49	1.43
7	AA	2	NAG	O5-C5	2.97	1.49	1.43
8	Z	3	BMA	O5-C5	2.96	1.49	1.43
8	x	2	NAG	O5-C5	2.96	1.49	1.43
8	c	3	BMA	C1-C2	2.95	1.58	1.52
8	n	2	NAG	C4-C5	2.95	1.59	1.53
8	V	2	NAG	O5-C5	2.95	1.49	1.43
8	m	3	BMA	O5-C5	2.95	1.49	1.43
8	w	2	NAG	O5-C5	2.94	1.49	1.43
8	i	3	BMA	C1-C2	2.94	1.58	1.52
7	g	2	NAG	O5-C5	2.93	1.49	1.43
8	Z	2	NAG	O5-C5	2.93	1.49	1.43
8	h	2	NAG	O5-C5	2.92	1.49	1.43
8	5	3	BMA	O5-C5	2.92	1.49	1.43
8	R	2	NAG	O5-C5	2.92	1.49	1.43
8	R	1	NAG	O5-C5	2.91	1.49	1.43
8	5	2	NAG	O5-C5	2.91	1.49	1.43
8	Z	1	NAG	O5-C5	2.90	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	NAG	O5-C5	2.89	1.49	1.43
8	b	3	BMA	C1-C2	2.88	1.58	1.52
8	6	3	BMA	C1-C2	2.88	1.58	1.52
8	Y	2	NAG	O5-C5	2.88	1.49	1.43
8	o	3	BMA	C1-C2	2.88	1.58	1.52
8	r	3	BMA	C1-C2	2.88	1.58	1.52
7	s	1	NAG	O5-C5	2.87	1.49	1.43
8	h	3	BMA	C1-C2	2.87	1.58	1.52
8	X	3	BMA	C1-C2	2.87	1.58	1.52
8	m	3	BMA	C1-C2	2.87	1.58	1.52
8	e	3	BMA	C1-C2	2.86	1.58	1.52
8	7	2	NAG	O5-C5	2.86	1.49	1.43
8	x	3	BMA	C1-C2	2.86	1.58	1.52
8	n	1	NAG	O4-C4	2.85	1.49	1.43
8	j	3	BMA	C1-C2	2.85	1.58	1.52
7	W	2	NAG	O5-C5	2.85	1.49	1.43
8	i	2	NAG	O5-C5	2.85	1.49	1.43
8	7	3	BMA	C1-C2	2.84	1.58	1.52
8	o	2	NAG	O5-C5	2.84	1.49	1.43
10	d	3	BMA	C1-C2	2.84	1.58	1.52
8	U	2	NAG	C4-C5	2.84	1.59	1.53
10	d	2	NAG	O5-C5	2.83	1.49	1.43
8	z	2	NAG	C4-C5	2.83	1.59	1.53
8	3	1	NAG	C4-C5	2.83	1.59	1.53
8	w	3	BMA	C1-C2	2.82	1.58	1.52
8	5	3	BMA	C1-C2	2.82	1.58	1.52
8	6	2	NAG	C4-C3	2.82	1.59	1.52
8	T	3	BMA	C1-C2	2.82	1.58	1.52
8	4	2	NAG	O5-C5	2.81	1.49	1.43
8	V	3	BMA	C1-C2	2.81	1.58	1.52
7	u	1	NAG	C4-C5	2.80	1.58	1.53
8	0	1	NAG	O5-C1	2.80	1.48	1.43
8	T	2	NAG	O5-C5	2.79	1.49	1.43
8	7	1	NAG	O5-C5	2.79	1.49	1.43
8	Z	3	BMA	C1-C2	2.79	1.58	1.52
8	r	2	NAG	O5-C5	2.79	1.49	1.43
8	4	3	BMA	C1-C2	2.78	1.58	1.52
8	R	3	BMA	C1-C2	2.78	1.58	1.52
8	0	3	BMA	C1-C2	2.78	1.58	1.52
8	a	1	NAG	O5-C1	2.78	1.48	1.43
8	t	2	NAG	C3-C2	2.77	1.58	1.52
8	U	2	NAG	O4-C4	2.76	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	k	1	NAG	O5-C5	2.76	1.49	1.43
10	d	1	NAG	O5-C1	2.75	1.48	1.43
8	3	2	NAG	C4-C5	2.75	1.58	1.53
8	X	2	NAG	O5-C5	2.75	1.49	1.43
8	h	1	NAG	O5-C5	2.75	1.49	1.43
8	i	2	NAG	C3-C2	2.74	1.58	1.52
8	3	1	NAG	O5-C5	2.74	1.49	1.43
8	V	3	BMA	O5-C5	2.74	1.49	1.43
8	a	2	NAG	C4-C5	2.73	1.58	1.53
7	Q	1	NAG	O5-C1	2.73	1.48	1.43
8	f	2	NAG	C4-C3	2.73	1.59	1.52
8	f	2	NAG	O5-C5	2.73	1.49	1.43
7	9	1	NAG	O5-C1	2.73	1.48	1.43
8	U	2	NAG	C3-C2	2.73	1.58	1.52
8	f	3	BMA	C1-C2	2.72	1.58	1.52
8	1	3	BMA	C1-C2	2.72	1.58	1.52
7	u	1	NAG	O5-C5	2.72	1.48	1.43
8	R	2	NAG	C3-C2	2.72	1.58	1.52
8	U	1	NAG	O5-C1	2.72	1.48	1.43
8	Y	3	BMA	C1-C2	2.71	1.58	1.52
8	i	2	NAG	C4-C5	2.70	1.58	1.53
8	c	2	NAG	C3-C2	2.70	1.58	1.52
8	w	1	NAG	O5-C5	2.69	1.48	1.43
8	n	2	NAG	C4-C3	2.68	1.59	1.52
8	e	2	NAG	C4-C5	2.68	1.58	1.53
8	n	2	NAG	C3-C2	2.68	1.58	1.52
9	S	4	MAN	C1-C2	2.68	1.58	1.52
8	1	1	NAG	O5-C5	2.67	1.48	1.43
8	6	1	NAG	O5-C1	2.67	1.48	1.43
8	R	1	NAG	C4-C5	2.66	1.58	1.53
8	r	2	NAG	C4-C5	2.66	1.58	1.53
8	x	1	NAG	C4-C5	2.66	1.58	1.53
7	Q	1	NAG	C4-C5	2.66	1.58	1.53
8	q	2	NAG	C4-C5	2.65	1.58	1.53
7	v	1	NAG	O5-C1	2.64	1.47	1.43
9	y	4	MAN	C1-C2	2.64	1.58	1.52
9	y	2	NAG	C4-C5	2.64	1.58	1.53
8	0	2	NAG	C4-C5	2.64	1.58	1.53
7	v	2	NAG	C3-C2	2.63	1.58	1.52
7	AA	2	NAG	C3-C2	2.63	1.58	1.52
7	W	2	NAG	C3-C2	2.63	1.58	1.52
8	0	1	NAG	C4-C5	2.63	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	2	NAG	C4-C3	2.62	1.59	1.52
8	m	3	BMA	C4-C5	2.62	1.58	1.53
8	k	2	NAG	C4-C5	2.62	1.58	1.53
8	c	1	NAG	O5-C1	2.62	1.47	1.43
8	p	2	NAG	C4-C3	2.61	1.59	1.52
8	o	2	NAG	C3-C2	2.61	1.58	1.52
8	X	2	NAG	C3-C2	2.60	1.58	1.52
8	i	1	NAG	C4-C5	2.60	1.58	1.53
8	f	1	NAG	O5-C1	2.59	1.47	1.43
8	e	1	NAG	C2-N2	2.59	1.50	1.46
8	x	2	NAG	C3-C2	2.59	1.58	1.52
8	p	2	NAG	C3-C2	2.59	1.58	1.52
8	e	1	NAG	C4-C3	2.59	1.58	1.52
8	7	2	NAG	C3-C2	2.58	1.58	1.52
8	b	3	BMA	C4-C5	2.58	1.58	1.53
8	Y	1	NAG	O5-C5	2.58	1.48	1.43
8	o	2	NAG	C4-C5	2.58	1.58	1.53
10	d	2	NAG	C3-C2	2.58	1.58	1.52
8	p	2	NAG	C4-C5	2.58	1.58	1.53
8	j	1	NAG	C4-C5	2.57	1.58	1.53
7	2	1	NAG	O5-C1	2.57	1.47	1.43
8	p	1	NAG	O5-C1	2.57	1.47	1.43
8	q	1	NAG	O5-C1	2.57	1.47	1.43
8	a	2	NAG	C4-C3	2.57	1.58	1.52
7	2	2	NAG	C3-C2	2.57	1.58	1.52
8	4	2	NAG	C3-C2	2.57	1.58	1.52
8	t	3	BMA	C4-C5	2.56	1.58	1.53
9	y	1	NAG	C4-C3	2.56	1.58	1.52
8	p	3	BMA	C4-C5	2.55	1.58	1.53
7	v	1	NAG	C4-C5	2.55	1.58	1.53
8	6	2	NAG	C4-C5	2.55	1.58	1.53
8	4	1	NAG	O5-C5	2.54	1.48	1.43
8	z	2	NAG	C3-C2	2.54	1.57	1.52
9	S	4	MAN	O5-C1	2.54	1.47	1.43
7	u	2	NAG	C3-C2	2.54	1.57	1.52
8	o	1	NAG	O5-C5	2.54	1.48	1.43
8	V	1	NAG	O5-C1	2.54	1.47	1.43
8	q	1	NAG	C4-C5	2.54	1.58	1.53
8	j	3	BMA	C4-C5	2.53	1.58	1.53
8	V	2	NAG	C4-C5	2.53	1.58	1.53
8	U	1	NAG	C4-C5	2.53	1.58	1.53
8	T	2	NAG	C3-C2	2.53	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	x	1	NAG	O5-C1	2.53	1.47	1.43
8	6	3	BMA	C4-C5	2.53	1.58	1.53
8	b	1	NAG	C4-C5	2.52	1.58	1.53
8	f	2	NAG	C4-C5	2.52	1.58	1.53
8	k	2	NAG	O5-C5	2.52	1.48	1.43
8	5	3	BMA	C4-C5	2.52	1.58	1.53
8	r	1	NAG	O5-C1	2.52	1.47	1.43
8	m	2	NAG	C3-C2	2.52	1.57	1.52
7	g	2	NAG	C3-C2	2.52	1.57	1.52
8	3	2	NAG	C3-C2	2.52	1.57	1.52
9	S	1	NAG	O5-C1	2.52	1.47	1.43
8	t	1	NAG	C4-C5	2.52	1.58	1.53
8	n	1	NAG	O5-C5	2.51	1.48	1.43
8	f	3	BMA	C4-C5	2.51	1.58	1.53
9	y	2	NAG	C2-N2	2.51	1.50	1.46
8	a	2	NAG	C3-C2	2.50	1.57	1.52
8	k	3	BMA	C4-C5	2.50	1.58	1.53
8	q	3	BMA	C4-C5	2.50	1.58	1.53
8	r	2	NAG	C3-C2	2.49	1.57	1.52
8	Z	3	BMA	C4-C5	2.49	1.58	1.53
8	X	1	NAG	C4-C3	2.49	1.58	1.52
8	z	2	NAG	C4-C3	2.49	1.58	1.52
8	o	2	NAG	C4-C3	2.49	1.58	1.52
8	q	2	NAG	O5-C1	2.49	1.47	1.43
8	7	3	BMA	C4-C5	2.49	1.58	1.53
8	b	2	NAG	C4-C5	2.49	1.58	1.53
8	w	1	NAG	C4-C5	2.48	1.58	1.53
8	3	3	BMA	C4-C5	2.48	1.58	1.53
8	R	2	NAG	C4-C5	2.48	1.58	1.53
8	Z	1	NAG	C4-C5	2.48	1.58	1.53
9	S	3	BMA	C2-C3	2.47	1.56	1.52
8	e	1	NAG	O5-C5	2.47	1.48	1.43
8	3	2	NAG	C4-C3	2.47	1.58	1.52
7	g	1	NAG	O5-C1	2.47	1.47	1.43
9	y	1	NAG	C4-C5	2.47	1.58	1.53
7	u	2	NAG	C2-N2	2.47	1.50	1.46
8	n	1	NAG	C3-C2	2.47	1.57	1.52
7	9	1	NAG	C4-C5	2.47	1.58	1.53
10	d	1	NAG	C4-C5	2.47	1.58	1.53
8	w	3	BMA	O5-C1	2.47	1.47	1.43
8	R	3	BMA	C4-C5	2.47	1.58	1.53
8	o	3	BMA	C4-C5	2.47	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	d	2	NAG	C4-C3	2.46	1.58	1.52
9	S	2	NAG	C3-C2	2.46	1.57	1.52
9	S	3	BMA	O5-C5	2.46	1.48	1.43
8	x	3	BMA	C4-C5	2.46	1.58	1.53
8	0	1	NAG	C4-C3	2.46	1.58	1.52
7	W	1	NAG	C3-C2	2.45	1.57	1.52
7	AA	1	NAG	C4-C3	2.45	1.58	1.52
7	s	1	NAG	O5-C1	2.45	1.47	1.43
8	V	1	NAG	C4-C5	2.45	1.58	1.53
7	s	2	NAG	C3-C2	2.44	1.57	1.52
8	V	3	BMA	C4-C5	2.44	1.58	1.53
8	6	2	NAG	C3-C2	2.44	1.57	1.52
9	y	4	MAN	C4-C5	2.44	1.58	1.53
7	l	2	NAG	C3-C2	2.44	1.57	1.52
8	0	3	BMA	C4-C5	2.44	1.58	1.53
8	Z	2	NAG	C4-C5	2.44	1.58	1.53
8	X	2	NAG	C4-C5	2.44	1.58	1.53
9	S	5	MAN	C4-C5	2.43	1.58	1.53
8	t	2	NAG	C4-C3	2.43	1.58	1.52
8	U	2	NAG	C4-C3	2.43	1.58	1.52
8	X	3	BMA	C4-C5	2.43	1.58	1.53
8	a	3	BMA	C4-C5	2.43	1.58	1.53
8	h	2	NAG	C4-C5	2.43	1.58	1.53
7	9	2	NAG	C3-C2	2.43	1.57	1.52
9	y	5	MAN	C4-C5	2.43	1.58	1.53
8	h	1	NAG	O5-C1	2.43	1.47	1.43
8	f	2	NAG	C3-C2	2.43	1.57	1.52
8	w	2	NAG	C3-C2	2.43	1.57	1.52
8	m	1	NAG	C3-C2	2.43	1.57	1.52
8	j	2	NAG	C4-C5	2.43	1.58	1.53
8	5	2	NAG	C3-C2	2.42	1.57	1.52
8	Y	3	BMA	C4-C5	2.42	1.58	1.53
8	j	1	NAG	C4-C3	2.42	1.58	1.52
7	Q	2	NAG	C4-C5	2.42	1.58	1.53
8	e	1	NAG	C3-C2	2.42	1.57	1.52
8	x	2	NAG	C4-C5	2.42	1.58	1.53
8	5	1	NAG	C4-C5	2.42	1.58	1.53
8	t	3	BMA	O5-C1	2.42	1.47	1.43
7	W	1	NAG	C4-C3	2.41	1.58	1.52
8	e	3	BMA	C4-C5	2.41	1.58	1.53
8	j	2	NAG	C3-C2	2.41	1.57	1.52
8	r	3	BMA	C4-C5	2.41	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	y	5	MAN	C1-C2	2.41	1.57	1.52
8	l	1	NAG	C4-C5	2.41	1.58	1.53
8	R	1	NAG	C3-C2	2.41	1.57	1.52
7	9	2	NAG	C4-C5	2.41	1.58	1.53
9	y	1	NAG	C3-C2	2.40	1.57	1.52
9	S	4	MAN	C4-C5	2.40	1.58	1.53
8	c	2	NAG	C4-C5	2.40	1.58	1.53
8	h	2	NAG	C3-C2	2.40	1.57	1.52
8	h	1	NAG	C4-C5	2.40	1.58	1.53
8	5	1	NAG	O5-C5	2.40	1.48	1.43
8	b	2	NAG	C3-C2	2.40	1.57	1.52
8	h	3	BMA	C4-C5	2.39	1.58	1.53
8	n	3	BMA	C4-C5	2.39	1.58	1.53
9	y	3	BMA	C1-C2	2.39	1.57	1.52
7	Q	2	NAG	C3-C2	2.39	1.57	1.52
8	t	1	NAG	C3-C2	2.39	1.57	1.52
7	Q	1	NAG	C3-C2	2.39	1.57	1.52
9	S	3	BMA	C1-C2	2.39	1.57	1.52
8	q	2	NAG	C3-C2	2.39	1.57	1.52
8	c	1	NAG	C4-C5	2.39	1.58	1.53
7	v	1	NAG	C4-C3	2.39	1.58	1.52
8	R	3	BMA	O5-C1	2.39	1.47	1.43
8	r	2	NAG	C4-C3	2.39	1.58	1.52
9	S	5	MAN	C1-C2	2.38	1.57	1.52
7	AA	1	NAG	O5-C1	2.38	1.47	1.43
8	7	2	NAG	C4-C5	2.38	1.58	1.53
8	T	2	NAG	C4-C5	2.38	1.58	1.53
7	9	2	NAG	C2-N2	2.38	1.50	1.46
10	d	2	NAG	C2-N2	2.37	1.50	1.46
7	AA	1	NAG	C4-C5	2.37	1.58	1.53
8	p	1	NAG	C4-C5	2.37	1.58	1.53
8	z	3	BMA	C4-C5	2.37	1.58	1.53
8	x	3	BMA	O5-C1	2.37	1.47	1.43
9	S	2	NAG	C4-C5	2.37	1.58	1.53
8	n	1	NAG	C4-C3	2.37	1.58	1.52
8	T	2	NAG	C2-N2	2.37	1.50	1.46
8	R	1	NAG	C4-C3	2.37	1.58	1.52
7	g	1	NAG	C4-C5	2.37	1.58	1.53
8	Y	2	NAG	C3-C2	2.36	1.57	1.52
8	w	2	NAG	C4-C5	2.36	1.58	1.53
8	t	1	NAG	O5-C1	2.36	1.47	1.43
7	s	1	NAG	C4-C5	2.36	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	c	3	BMA	C4-C5	2.36	1.58	1.53
9	S	1	NAG	C4-C5	2.35	1.58	1.53
8	T	3	BMA	C4-C5	2.35	1.58	1.53
8	5	2	NAG	C4-C5	2.35	1.58	1.53
8	6	1	NAG	C4-C5	2.35	1.58	1.53
9	y	2	NAG	C3-C2	2.35	1.57	1.52
8	k	1	NAG	C4-C5	2.35	1.58	1.53
8	k	2	NAG	C3-C2	2.34	1.57	1.52
8	b	1	NAG	O5-C1	2.34	1.47	1.43
7	2	1	NAG	C4-C5	2.34	1.58	1.53
8	1	3	BMA	C4-C5	2.34	1.58	1.53
8	1	2	NAG	C3-C2	2.34	1.57	1.52
8	U	3	BMA	C4-C5	2.34	1.58	1.53
10	d	3	BMA	C4-C5	2.34	1.58	1.53
9	y	3	BMA	C2-C3	2.34	1.56	1.52
7	g	2	NAG	C4-C5	2.34	1.58	1.53
8	n	2	NAG	C2-N2	2.34	1.50	1.46
8	R	1	NAG	O5-C1	2.34	1.47	1.43
8	4	3	BMA	C4-C5	2.34	1.58	1.53
8	r	1	NAG	C4-C5	2.33	1.58	1.53
8	i	3	BMA	C4-C5	2.33	1.57	1.53
7	v	2	NAG	C4-C5	2.33	1.57	1.53
8	t	2	NAG	C4-C5	2.33	1.57	1.53
8	z	1	NAG	O5-C1	2.33	1.47	1.43
8	w	2	NAG	C4-C3	2.33	1.58	1.52
8	f	1	NAG	C4-C5	2.32	1.57	1.53
8	Z	2	NAG	C3-C2	2.32	1.57	1.52
8	R	2	NAG	C4-C3	2.32	1.58	1.52
7	s	1	NAG	C3-C2	2.32	1.57	1.52
7	AA	2	NAG	C2-N2	2.32	1.50	1.46
8	h	3	BMA	O5-C1	2.32	1.47	1.43
8	T	1	NAG	C3-C2	2.32	1.57	1.52
8	q	2	NAG	C4-C3	2.31	1.58	1.52
8	c	1	NAG	C4-C3	2.31	1.58	1.52
8	w	3	BMA	C4-C5	2.31	1.57	1.53
8	c	2	NAG	C4-C3	2.31	1.58	1.52
8	i	1	NAG	C4-C3	2.31	1.58	1.52
8	4	2	NAG	C4-C5	2.30	1.57	1.53
7	AA	2	NAG	C4-C5	2.30	1.57	1.53
8	m	2	NAG	C4-C3	2.30	1.58	1.52
8	7	1	NAG	O5-C1	2.30	1.47	1.43
8	Y	2	NAG	C4-C5	2.30	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	x	2	NAG	C2-N2	2.30	1.50	1.46
8	z	1	NAG	C4-C5	2.29	1.57	1.53
8	b	3	BMA	O5-C1	2.29	1.47	1.43
8	r	2	NAG	C2-N2	2.29	1.50	1.46
8	3	1	NAG	C3-C2	2.29	1.57	1.52
8	T	1	NAG	O5-C5	2.29	1.48	1.43
8	7	1	NAG	C3-C2	2.29	1.57	1.52
8	4	1	NAG	C3-C2	2.29	1.57	1.52
8	a	1	NAG	C4-C5	2.29	1.57	1.53
7	2	2	NAG	C4-C5	2.29	1.57	1.53
8	j	1	NAG	O5-C1	2.28	1.47	1.43
10	d	2	NAG	O5-C1	2.28	1.47	1.43
8	3	2	NAG	C2-N2	2.28	1.50	1.46
7	l	1	NAG	O5-C5	2.28	1.48	1.43
8	T	3	BMA	O5-C1	2.27	1.47	1.43
9	S	2	NAG	C4-C3	2.26	1.58	1.52
8	3	1	NAG	C4-C3	2.26	1.58	1.52
8	j	1	NAG	C3-C2	2.26	1.57	1.52
8	Y	2	NAG	C4-C3	2.26	1.58	1.52
8	V	1	NAG	C3-C2	2.25	1.57	1.52
8	4	3	BMA	O5-C1	2.25	1.47	1.43
9	y	1	NAG	O5-C1	2.25	1.47	1.43
8	a	1	NAG	C4-C3	2.25	1.58	1.52
8	e	2	NAG	C3-C2	2.25	1.57	1.52
7	u	2	NAG	O5-C1	2.25	1.47	1.43
8	q	2	NAG	O4-C4	2.25	1.48	1.43
8	l	2	NAG	C4-C3	2.24	1.58	1.52
8	X	1	NAG	C3-C2	2.24	1.57	1.52
8	c	2	NAG	C2-N2	2.24	1.50	1.46
8	h	1	NAG	C3-C2	2.24	1.57	1.52
8	6	3	BMA	O5-C1	2.24	1.47	1.43
8	e	3	BMA	O5-C1	2.24	1.47	1.43
8	r	1	NAG	C4-C3	2.24	1.58	1.52
8	X	1	NAG	C2-N2	2.24	1.50	1.46
8	l	1	NAG	C3-C2	2.23	1.57	1.52
7	l	2	NAG	C4-C5	2.23	1.57	1.53
7	u	2	NAG	C4-C5	2.23	1.57	1.53
8	z	2	NAG	O4-C4	2.23	1.48	1.43
8	7	1	NAG	C4-C5	2.23	1.57	1.53
7	s	2	NAG	C4-C5	2.23	1.57	1.53
8	6	1	NAG	C4-C3	2.22	1.58	1.52
8	m	2	NAG	C4-C5	2.22	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	NAG	O4-C4	2.22	1.48	1.43
7	g	1	NAG	C3-C2	2.22	1.57	1.52
8	i	3	BMA	O5-C1	2.22	1.47	1.43
8	Y	1	NAG	C4-C5	2.22	1.57	1.53
8	a	3	BMA	O5-C1	2.21	1.47	1.43
7	Q	2	NAG	C2-N2	2.21	1.50	1.46
8	4	2	NAG	C4-C3	2.21	1.58	1.52
8	k	1	NAG	O5-C1	2.21	1.47	1.43
8	f	1	NAG	C3-C2	2.21	1.57	1.52
7	l	1	NAG	C3-C2	2.21	1.57	1.52
7	2	1	NAG	C4-C3	2.21	1.58	1.52
8	5	2	NAG	C4-C3	2.21	1.58	1.52
7	l	1	NAG	C4-C3	2.21	1.57	1.52
7	9	2	NAG	C4-C3	2.20	1.57	1.52
8	a	2	NAG	O4-C4	2.20	1.48	1.43
8	1	1	NAG	C4-C3	2.20	1.57	1.52
8	m	1	NAG	O5-C5	2.20	1.47	1.43
8	5	2	NAG	C2-N2	2.20	1.50	1.46
8	j	1	NAG	O4-C4	2.20	1.48	1.43
8	o	1	NAG	C4-C3	2.19	1.57	1.52
8	o	3	BMA	O5-C1	2.19	1.47	1.43
7	u	1	NAG	C3-C2	2.19	1.57	1.52
8	k	1	NAG	C4-C3	2.19	1.57	1.52
8	o	1	NAG	C4-C5	2.19	1.57	1.53
8	f	3	BMA	O5-C1	2.19	1.47	1.43
8	7	3	BMA	O5-C1	2.19	1.47	1.43
8	Z	2	NAG	C4-C3	2.19	1.57	1.52
9	y	5	MAN	C4-C3	2.19	1.57	1.52
8	c	3	BMA	O5-C1	2.19	1.47	1.43
8	Y	1	NAG	O5-C1	2.18	1.47	1.43
8	i	1	NAG	C3-C2	2.18	1.57	1.52
8	b	2	NAG	C4-C3	2.18	1.57	1.52
8	m	1	NAG	C4-C3	2.17	1.57	1.52
8	1	2	NAG	C4-C5	2.17	1.57	1.53
8	X	1	NAG	C4-C5	2.17	1.57	1.53
8	X	1	NAG	O5-C5	2.17	1.47	1.43
7	l	1	NAG	C4-C5	2.17	1.57	1.53
8	3	3	BMA	O5-C1	2.17	1.47	1.43
8	a	2	NAG	C2-N2	2.17	1.50	1.46
8	w	2	NAG	C2-N2	2.16	1.50	1.46
8	q	1	NAG	C4-C3	2.16	1.57	1.52
7	2	2	NAG	C2-N2	2.16	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2	2	NAG	C4-C3	2.16	1.57	1.52
7	v	2	NAG	C2-N2	2.16	1.50	1.46
8	e	2	NAG	C4-C3	2.16	1.57	1.52
8	x	2	NAG	C4-C3	2.16	1.57	1.52
8	0	2	NAG	C3-C2	2.16	1.57	1.52
8	X	3	BMA	O5-C1	2.16	1.47	1.43
8	Z	2	NAG	C2-N2	2.16	1.50	1.46
7	u	2	NAG	C4-C3	2.16	1.57	1.52
8	p	3	BMA	O5-C1	2.16	1.47	1.43
8	k	3	BMA	O5-C1	2.16	1.47	1.43
8	Y	1	NAG	C3-C2	2.16	1.57	1.52
7	AA	2	NAG	C4-C3	2.15	1.57	1.52
9	y	2	NAG	O5-C1	2.15	1.47	1.43
8	6	2	NAG	O4-C4	2.15	1.48	1.43
8	o	1	NAG	C2-N2	2.15	1.50	1.46
8	1	2	NAG	O5-C5	2.15	1.47	1.43
8	7	1	NAG	C4-C3	2.15	1.57	1.52
8	x	1	NAG	C3-C2	2.14	1.57	1.52
8	X	2	NAG	C4-C3	2.14	1.57	1.52
8	X	1	NAG	O5-C1	2.14	1.47	1.43
8	5	3	BMA	O5-C1	2.14	1.47	1.43
8	5	1	NAG	C3-C2	2.14	1.57	1.52
8	p	2	NAG	C2-N2	2.14	1.50	1.46
8	T	1	NAG	C4-C3	2.14	1.57	1.52
8	V	2	NAG	C4-C3	2.14	1.57	1.52
7	u	1	NAG	C4-C3	2.14	1.57	1.52
7	v	1	NAG	O4-C4	2.13	1.48	1.43
10	d	2	NAG	O4-C4	2.13	1.48	1.43
8	p	2	NAG	O4-C4	2.13	1.48	1.43
8	h	2	NAG	C2-N2	2.13	1.49	1.46
7	g	2	NAG	C4-C3	2.13	1.57	1.52
8	U	1	NAG	C4-C3	2.13	1.57	1.52
9	y	4	MAN	O5-C1	2.13	1.47	1.43
8	1	3	BMA	C4-C3	2.13	1.57	1.52
8	z	3	BMA	O5-C1	2.12	1.47	1.43
8	k	2	NAG	C4-C3	2.12	1.57	1.52
7	W	1	NAG	C4-C5	2.12	1.57	1.53
8	m	1	NAG	C4-C5	2.12	1.57	1.53
8	R	1	NAG	C2-N2	2.12	1.49	1.46
8	Y	3	BMA	C4-C3	2.12	1.57	1.52
8	o	2	NAG	O4-C4	2.12	1.48	1.43
8	x	1	NAG	O4-C4	2.12	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	9	2	NAG	O5-C1	2.11	1.47	1.43
7	Q	2	NAG	C4-C3	2.11	1.57	1.52
7	l	2	NAG	C2-N2	2.11	1.49	1.46
7	g	1	NAG	C4-C3	2.11	1.57	1.52
8	0	1	NAG	O4-C4	2.11	1.47	1.43
8	T	2	NAG	C4-C3	2.11	1.57	1.52
8	e	3	BMA	C4-C3	2.11	1.57	1.52
8	X	3	BMA	C4-C3	2.11	1.57	1.52
8	Y	3	BMA	O5-C1	2.11	1.47	1.43
7	W	2	NAG	C4-C5	2.10	1.57	1.53
10	d	3	BMA	C4-C3	2.10	1.57	1.52
8	r	3	BMA	O5-C1	2.10	1.47	1.43
8	V	1	NAG	C4-C3	2.10	1.57	1.52
8	z	1	NAG	C4-C3	2.10	1.57	1.52
8	3	3	BMA	C4-C3	2.10	1.57	1.52
8	t	2	NAG	O5-C1	2.10	1.47	1.43
8	n	3	BMA	O5-C1	2.10	1.47	1.43
8	V	2	NAG	C3-C2	2.10	1.57	1.52
8	q	3	BMA	O5-C1	2.10	1.47	1.43
8	f	1	NAG	C4-C3	2.10	1.57	1.52
8	6	2	NAG	C2-N2	2.10	1.49	1.46
8	m	3	BMA	C4-C3	2.09	1.57	1.52
8	4	1	NAG	C4-C5	2.09	1.57	1.53
8	Z	1	NAG	O5-C1	2.09	1.47	1.43
8	m	1	NAG	C2-N2	2.09	1.49	1.46
8	o	2	NAG	C2-N2	2.09	1.49	1.46
8	c	3	BMA	C4-C3	2.09	1.57	1.52
8	f	2	NAG	C2-N2	2.09	1.49	1.46
8	7	2	NAG	C4-C3	2.09	1.57	1.52
8	Z	3	BMA	O5-C1	2.09	1.47	1.43
8	a	3	BMA	C4-C3	2.09	1.57	1.52
8	o	1	NAG	C3-C2	2.08	1.56	1.52
8	q	1	NAG	C3-C2	2.08	1.56	1.52
8	i	2	NAG	O4-C4	2.08	1.47	1.43
9	y	3	BMA	O5-C5	2.07	1.47	1.43
7	Q	1	NAG	C4-C3	2.07	1.57	1.52
8	n	3	BMA	C4-C3	2.07	1.57	1.52
8	3	2	NAG	O5-C1	2.07	1.47	1.43
8	e	2	NAG	C2-N2	2.07	1.49	1.46
8	6	3	BMA	C4-C3	2.07	1.57	1.52
7	AA	1	NAG	C2-N2	2.07	1.49	1.46
8	4	3	BMA	C4-C3	2.07	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	7	3	BMA	C4-C3	2.07	1.57	1.52
8	f	2	NAG	O4-C4	2.07	1.47	1.43
8	o	3	BMA	C4-C3	2.06	1.57	1.52
8	f	3	BMA	C4-C3	2.06	1.57	1.52
8	4	1	NAG	C4-C3	2.06	1.57	1.52
7	AA	2	NAG	O5-C1	2.06	1.47	1.43
9	y	4	MAN	C4-C3	2.06	1.57	1.52
8	5	3	BMA	C4-C3	2.06	1.57	1.52
7	Q	2	NAG	O5-C1	2.06	1.47	1.43
8	Y	1	NAG	C4-C3	2.06	1.57	1.52
8	w	3	BMA	C4-C3	2.05	1.57	1.52
8	T	1	NAG	C4-C5	2.05	1.57	1.53
8	1	1	NAG	O5-C1	2.05	1.47	1.43
8	Z	3	BMA	C4-C3	2.05	1.57	1.52
7	g	2	NAG	C2-N2	2.05	1.49	1.46
7	u	1	NAG	C2-N2	2.05	1.49	1.46
10	d	3	BMA	O5-C1	2.04	1.47	1.43
8	R	3	BMA	C4-C3	2.04	1.57	1.52
8	5	1	NAG	C4-C3	2.04	1.57	1.52
8	r	3	BMA	C4-C3	2.04	1.57	1.52
8	h	2	NAG	C4-C3	2.04	1.57	1.52
8	p	1	NAG	C4-C3	2.04	1.57	1.52
9	S	5	MAN	C4-C3	2.04	1.57	1.52
8	k	1	NAG	C3-C2	2.04	1.56	1.52
7	v	2	NAG	C4-C3	2.04	1.57	1.52
9	S	1	NAG	C3-C2	2.04	1.56	1.52
8	q	1	NAG	C2-N2	2.03	1.49	1.46
8	x	3	BMA	C4-C3	2.03	1.57	1.52
8	w	1	NAG	O5-C1	2.03	1.47	1.43
7	u	1	NAG	O5-C1	2.03	1.47	1.43
8	m	3	BMA	O5-C1	2.03	1.47	1.43
8	i	3	BMA	C4-C3	2.03	1.57	1.52
8	V	3	BMA	C4-C3	2.03	1.57	1.52
8	T	3	BMA	C4-C3	2.03	1.57	1.52
8	b	3	BMA	C4-C3	2.03	1.57	1.52
7	AA	1	NAG	C3-C2	2.02	1.56	1.52
9	y	2	NAG	C4-C3	2.02	1.57	1.52
8	q	3	BMA	C4-C3	2.02	1.57	1.52
8	p	3	BMA	C4-C3	2.02	1.57	1.52
8	z	3	BMA	C4-C3	2.02	1.57	1.52
7	W	2	NAG	C4-C3	2.02	1.57	1.52
8	w	1	NAG	C3-C2	2.01	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	3	BMA	C4-C3	2.01	1.57	1.52
7	W	1	NAG	O5-C5	2.00	1.47	1.43
8	t	3	BMA	C4-C3	2.00	1.57	1.52
7	l	2	NAG	C4-C3	2.00	1.57	1.52
8	k	2	NAG	C2-N2	2.00	1.49	1.46

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	2	NAG	C8-C7-N2	27.73	163.04	116.10
8	V	2	NAG	C2-N2-C7	26.61	160.79	122.90
8	V	2	NAG	O7-C7-N2	-25.05	75.90	121.95
8	V	2	NAG	O7-C7-C8	-18.80	87.14	122.06
8	3	1	NAG	O4-C4-C3	-4.87	99.10	110.35
9	y	2	NAG	O4-C4-C5	4.24	119.82	109.30
8	e	1	NAG	O4-C4-C3	-4.09	100.89	110.35
8	n	1	NAG	O4-C4-C5	3.92	119.03	109.30
7	u	1	NAG	O4-C4-C3	-3.90	101.33	110.35
8	1	1	NAG	O4-C4-C5	-3.90	99.62	109.30
8	R	1	NAG	C8-C7-N2	3.66	122.29	116.10
8	x	1	NAG	O4-C4-C5	3.53	118.07	109.30
8	f	2	NAG	O4-C4-C3	3.22	117.79	110.35
9	y	2	NAG	C8-C7-N2	3.22	121.54	116.10
8	o	1	NAG	C8-C7-N2	3.20	121.52	116.10
8	8	1	NAG	O4-C4-C5	-3.18	101.40	109.30
8	6	2	NAG	O4-C4-C3	3.16	117.66	110.35
8	e	1	NAG	O5-C5-C6	-3.15	102.26	107.20
7	2	2	NAG	C8-C7-N2	3.09	121.33	116.10
8	x	2	NAG	C8-C7-N2	3.07	121.30	116.10
8	0	1	NAG	C1-C2-N2	3.06	115.72	110.49
8	R	1	NAG	O7-C7-C8	-3.04	116.41	122.06
8	a	2	NAG	C8-C7-N2	3.04	121.24	116.10
8	8	1	NAG	O3-C3-C2	-3.03	103.19	109.47
10	d	2	NAG	O4-C4-C5	3.01	116.78	109.30
8	c	2	NAG	C8-C7-N2	2.99	121.17	116.10
8	6	2	NAG	C8-C7-N2	2.94	121.08	116.10
8	e	1	NAG	C8-C7-N2	2.93	121.06	116.10
8	p	2	NAG	C8-C7-N2	2.90	121.01	116.10
7	Q	1	NAG	O4-C4-C3	-2.89	103.68	110.35
8	r	1	NAG	C8-C7-N2	2.88	120.98	116.10
8	q	1	NAG	C8-C7-N2	2.87	120.95	116.10
8	1	1	NAG	C8-C7-N2	2.84	120.90	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	NAG	O4-C4-C3	-2.82	103.82	110.35
7	l	1	NAG	C8-C7-N2	2.77	120.79	116.10
8	8	3	BMA	C1-O5-C5	2.75	115.92	112.19
8	8	2	NAG	C1-O5-C5	2.75	115.92	112.19
8	k	1	NAG	O4-C4-C5	-2.71	102.56	109.30
7	u	1	NAG	O5-C5-C6	-2.71	102.95	107.20
8	X	1	NAG	C1-C2-N2	-2.70	105.88	110.49
8	w	2	NAG	C8-C7-N2	2.67	120.62	116.10
8	U	2	NAG	O4-C4-C3	2.67	116.51	110.35
9	y	2	NAG	C1-O5-C5	2.67	115.80	112.19
8	5	2	NAG	C8-C7-N2	2.66	120.61	116.10
8	h	1	NAG	C8-C7-N2	2.66	120.60	116.10
8	Y	1	NAG	C8-C7-N2	2.64	120.57	116.10
8	R	2	NAG	C8-C7-N2	2.64	120.56	116.10
8	o	2	NAG	C8-C7-N2	2.63	120.56	116.10
7	9	1	NAG	O4-C4-C5	-2.62	102.79	109.30
8	3	1	NAG	C1-C2-N2	-2.61	106.03	110.49
8	R	1	NAG	O4-C4-C5	-2.61	102.82	109.30
9	y	1	NAG	O4-C4-C5	-2.61	102.83	109.30
7	AA	1	NAG	C8-C7-N2	2.59	120.48	116.10
8	4	1	NAG	C8-C7-N2	2.57	120.44	116.10
8	1	2	NAG	C1-O5-C5	2.56	115.66	112.19
8	3	1	NAG	O5-C5-C6	-2.55	103.20	107.20
9	y	2	NAG	O7-C7-C8	-2.55	117.33	122.06
8	m	1	NAG	C8-C7-N2	2.54	120.40	116.10
8	w	1	NAG	O4-C4-C3	-2.52	104.52	110.35
8	U	2	NAG	C8-C7-N2	2.52	120.37	116.10
8	t	2	NAG	C1-O5-C5	2.52	115.61	112.19
8	U	1	NAG	O4-C4-C3	-2.50	104.56	110.35
8	Z	2	NAG	C8-C7-N2	2.50	120.33	116.10
8	8	2	NAG	O4-C4-C5	-2.48	103.14	109.30
8	V	1	NAG	C8-C7-N2	2.48	120.29	116.10
8	c	2	NAG	O7-C7-C8	-2.48	117.46	122.06
8	i	1	NAG	O5-C5-C6	-2.46	103.34	107.20
8	t	1	NAG	C8-C7-N2	2.46	120.26	116.10
8	6	1	NAG	C8-C7-N2	2.45	120.24	116.10
8	t	2	NAG	O4-C4-C3	2.45	116.00	110.35
8	0	2	NAG	C8-C7-N2	2.44	120.22	116.10
8	o	1	NAG	O5-C5-C6	-2.43	103.39	107.20
8	f	1	NAG	C8-C7-N2	2.43	120.22	116.10
8	8	2	NAG	O3-C3-C2	-2.43	104.43	109.47
9	y	1	NAG	C8-C7-N2	2.43	120.21	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	u	2	NAG	C8-C7-N2	2.43	120.20	116.10
8	Y	2	NAG	C8-C7-N2	2.40	120.16	116.10
7	9	2	NAG	C8-C7-N2	2.39	120.14	116.10
8	T	1	NAG	C8-C7-N2	2.38	120.12	116.10
8	3	2	NAG	C8-C7-N2	2.38	120.12	116.10
9	S	3	BMA	O3-C3-C4	2.37	115.84	110.35
8	a	2	NAG	O7-C7-C8	-2.37	117.66	122.06
8	j	2	NAG	C8-C7-N2	2.36	120.10	116.10
8	n	1	NAG	C1-C2-N2	-2.36	106.46	110.49
7	AA	2	NAG	C8-C7-N2	2.36	120.09	116.10
8	p	2	NAG	O7-C7-C8	-2.36	117.68	122.06
8	4	2	NAG	C8-C7-N2	2.35	120.08	116.10
10	d	1	NAG	C1-O5-C5	2.33	115.35	112.19
8	T	2	NAG	C8-C7-N2	2.32	120.03	116.10
8	z	2	NAG	C8-C7-N2	2.32	120.02	116.10
7	2	2	NAG	O7-C7-C8	-2.29	117.80	122.06
10	d	2	NAG	C8-C7-N2	2.29	119.98	116.10
7	l	1	NAG	C1-O5-C5	2.29	115.29	112.19
7	2	1	NAG	O7-C7-C8	-2.28	117.82	122.06
8	3	2	NAG	O4-C4-C5	2.27	114.94	109.30
8	m	1	NAG	C1-O5-C5	2.27	115.27	112.19
7	v	1	NAG	C8-C7-N2	2.26	119.93	116.10
8	t	2	NAG	O4-C4-C5	2.25	114.89	109.30
7	Q	2	NAG	C8-C7-N2	2.25	119.91	116.10
8	6	2	NAG	O7-C7-C8	-2.24	117.89	122.06
7	AA	1	NAG	O7-C7-C8	-2.24	117.90	122.06
8	3	1	NAG	C2-N2-C7	2.24	126.09	122.90
8	t	1	NAG	O4-C4-C5	-2.23	103.75	109.30
8	a	1	NAG	C8-C7-N2	2.23	119.88	116.10
9	S	2	NAG	C8-C7-N2	2.22	119.86	116.10
8	r	2	NAG	C8-C7-N2	2.22	119.86	116.10
7	2	1	NAG	C8-C7-N2	2.21	119.85	116.10
8	x	2	NAG	C1-O5-C5	2.21	115.18	112.19
8	j	1	NAG	O4-C4-C5	2.20	114.77	109.30
8	X	1	NAG	C8-C7-N2	2.20	119.82	116.10
8	k	2	NAG	C8-C7-N2	2.19	119.81	116.10
8	U	2	NAG	O7-C7-C8	-2.19	117.99	122.06
8	h	2	NAG	C8-C7-N2	2.19	119.80	116.10
8	x	2	NAG	O7-C7-C8	-2.18	118.00	122.06
8	n	1	NAG	O5-C5-C6	-2.18	103.79	107.20
7	l	1	NAG	O5-C5-C6	-2.18	103.79	107.20
8	o	1	NAG	O7-C7-C8	-2.18	118.01	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	z	1	NAG	C8-C7-N2	2.17	119.78	116.10
8	n	1	NAG	O4-C4-C3	-2.17	105.32	110.35
8	i	2	NAG	O4-C4-C5	2.17	114.69	109.30
7	W	2	NAG	C8-C7-N2	2.17	119.77	116.10
8	k	1	NAG	C8-C7-N2	2.17	119.77	116.10
7	u	1	NAG	C8-C7-N2	2.16	119.76	116.10
8	m	2	NAG	C8-C7-N2	2.15	119.75	116.10
8	i	1	NAG	C8-C7-N2	2.15	119.74	116.10
8	i	2	NAG	O4-C4-C3	2.15	115.32	110.35
7	l	2	NAG	C8-C7-N2	2.14	119.73	116.10
7	9	2	NAG	O7-C7-C8	-2.14	118.09	122.06
8	a	1	NAG	O7-C7-C8	-2.14	118.09	122.06
8	w	2	NAG	O7-C7-C8	-2.14	118.09	122.06
8	l	2	NAG	C8-C7-N2	2.14	119.72	116.10
8	q	1	NAG	O7-C7-C8	-2.13	118.09	122.06
8	i	2	NAG	C8-C7-N2	2.13	119.71	116.10
8	z	1	NAG	O4-C4-C3	-2.13	105.42	110.35
8	e	2	NAG	C8-C7-N2	2.13	119.70	116.10
8	0	1	NAG	O4-C4-C3	2.13	115.26	110.35
8	7	2	NAG	C8-C7-N2	2.12	119.69	116.10
8	b	2	NAG	C8-C7-N2	2.12	119.68	116.10
10	d	1	NAG	O5-C1-C2	-2.12	107.95	111.29
7	g	2	NAG	C1-O5-C5	2.11	115.05	112.19
8	j	1	NAG	C8-C7-N2	2.11	119.66	116.10
8	e	1	NAG	O7-C7-C8	-2.10	118.15	122.06
8	o	2	NAG	O4-C4-C5	2.10	114.50	109.30
8	n	2	NAG	C8-C7-N2	2.09	119.64	116.10
7	v	2	NAG	C8-C7-N2	2.09	119.63	116.10
8	1	3	BMA	C1-O5-C5	2.08	115.01	112.19
7	W	1	NAG	C1-O5-C5	2.08	115.01	112.19
8	6	1	NAG	C1-O5-C5	2.07	115.00	112.19
8	3	2	NAG	O7-C7-C8	-2.07	118.21	122.06
8	7	1	NAG	C8-C7-N2	2.07	119.60	116.10
8	o	2	NAG	C1-O5-C5	2.06	114.99	112.19
7	W	1	NAG	C1-C2-N2	-2.06	106.97	110.49
8	o	2	NAG	O7-C7-C8	-2.06	118.24	122.06
7	g	2	NAG	C8-C7-N2	2.05	119.57	116.10
8	X	2	NAG	C8-C7-N2	2.04	119.56	116.10
8	0	1	NAG	O4-C4-C5	2.04	114.37	109.30
8	h	1	NAG	O7-C7-C8	-2.04	118.27	122.06
7	l	1	NAG	O7-C7-C8	-2.04	118.27	122.06
8	p	2	NAG	O4-C4-C5	2.04	114.36	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	2	NAG	O7-C7-C8	-2.04	118.28	122.06
8	p	2	NAG	C1-O5-C5	2.03	114.95	112.19
7	s	2	NAG	C8-C7-N2	2.03	119.54	116.10
8	c	1	NAG	O7-C7-C8	-2.03	118.28	122.06
8	t	2	NAG	C8-C7-N2	2.03	119.54	116.10
8	h	1	NAG	O5-C1-C2	-2.02	108.09	111.29
8	5	1	NAG	C1-C2-N2	-2.02	107.04	110.49
8	r	2	NAG	C1-O5-C5	2.01	114.92	112.19
8	i	2	NAG	C1-O5-C5	2.01	114.92	112.19
8	b	1	NAG	C8-C7-N2	2.01	119.50	116.10
8	Y	2	NAG	O7-C7-C8	-2.00	118.33	122.06
8	j	1	NAG	C1-C2-N2	2.00	113.91	110.49
10	d	2	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	8	1	NAG	C8-C7-N2-C2
8	8	1	NAG	O7-C7-N2-C2
8	8	2	NAG	C8-C7-N2-C2
8	8	2	NAG	O7-C7-N2-C2
8	p	1	NAG	O5-C5-C6-O6
10	d	1	NAG	O5-C5-C6-O6
8	n	1	NAG	C4-C5-C6-O6
10	d	1	NAG	C4-C5-C6-O6
8	V	2	NAG	O7-C7-N2-C2
9	y	3	BMA	O5-C5-C6-O6
7	2	1	NAG	O5-C5-C6-O6
8	n	1	NAG	O5-C5-C6-O6
8	c	1	NAG	O5-C5-C6-O6
8	0	1	NAG	C4-C5-C6-O6
8	8	2	NAG	C1-C2-N2-C7
8	f	3	BMA	O5-C5-C6-O6
8	t	3	BMA	O5-C5-C6-O6
8	6	3	BMA	O5-C5-C6-O6
8	V	3	BMA	O5-C5-C6-O6
8	p	1	NAG	C4-C5-C6-O6
8	b	3	BMA	O5-C5-C6-O6
8	p	3	BMA	O5-C5-C6-O6
8	0	1	NAG	O5-C5-C6-O6
8	8	3	BMA	O5-C5-C6-O6

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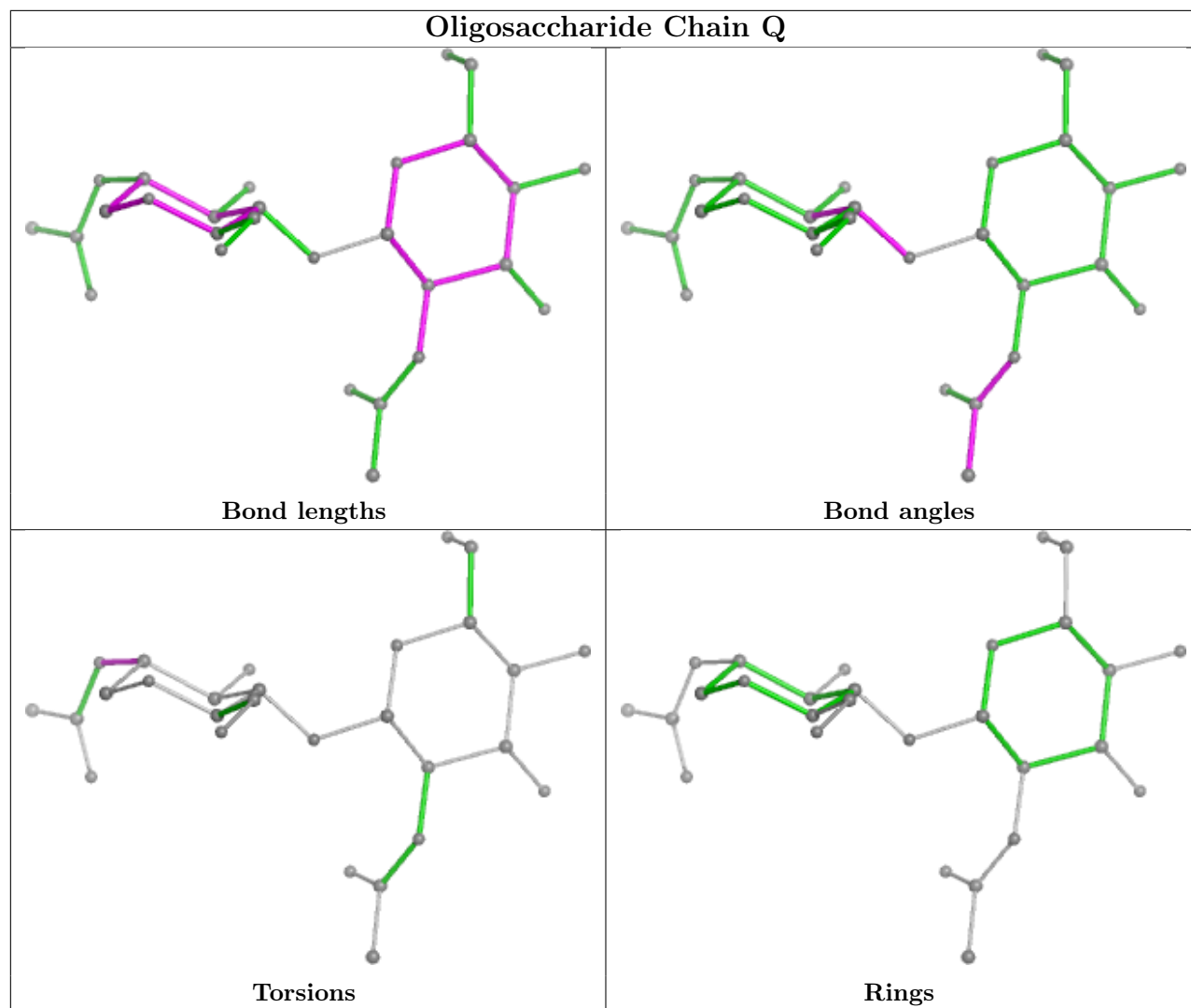
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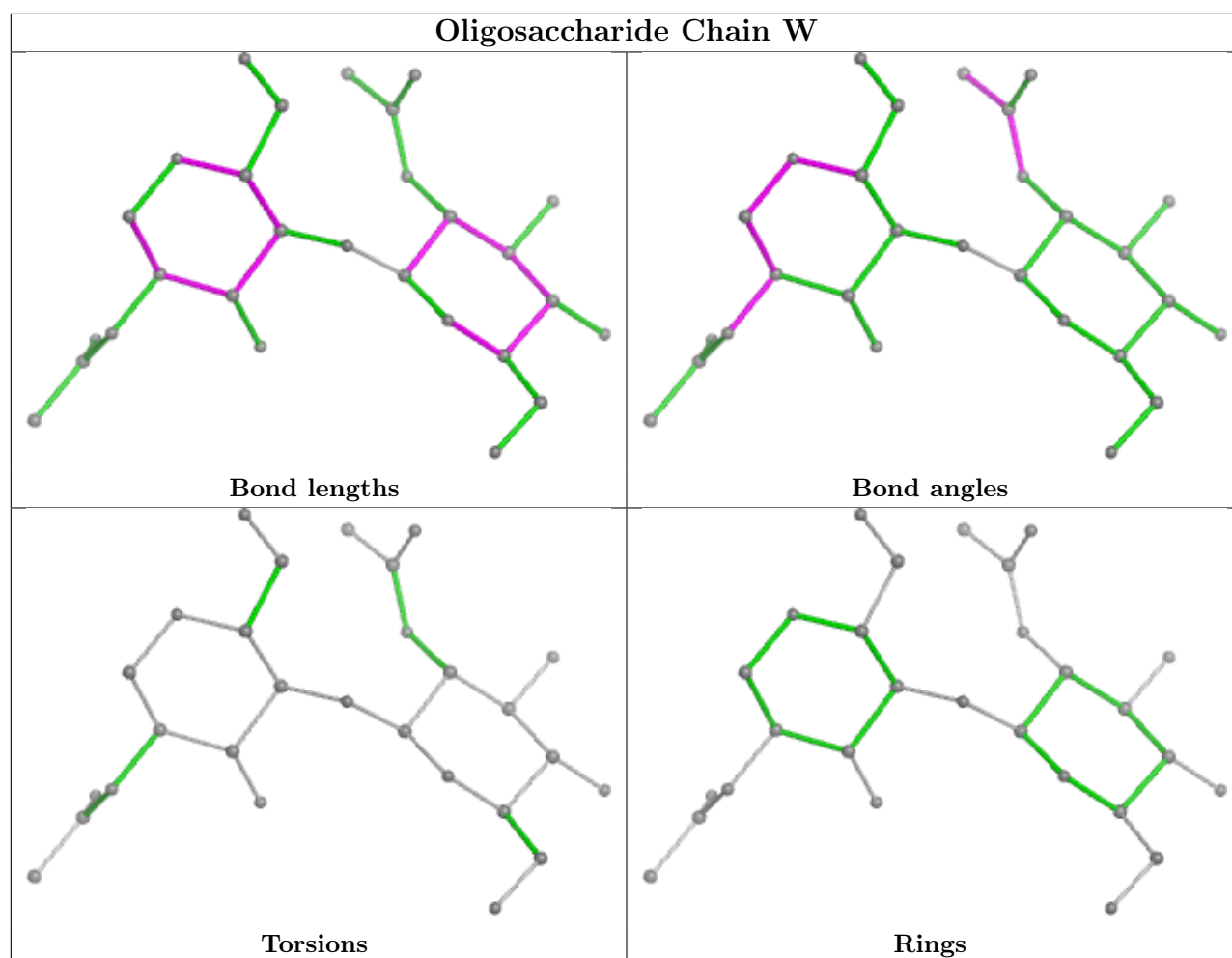
Mol	Chain	Res	Type	Atoms
8	m	3	BMA	O5-C5-C6-O6
8	q	3	BMA	O5-C5-C6-O6
8	Z	3	BMA	O5-C5-C6-O6
8	Y	3	BMA	O5-C5-C6-O6
8	0	3	BMA	O5-C5-C6-O6
8	7	3	BMA	O5-C5-C6-O6
9	S	4	MAN	O5-C5-C6-O6
8	R	3	BMA	O5-C5-C6-O6
8	k	3	BMA	O5-C5-C6-O6
8	o	3	BMA	O5-C5-C6-O6
8	5	3	BMA	O5-C5-C6-O6
8	x	3	BMA	O5-C5-C6-O6
9	y	3	BMA	C4-C5-C6-O6
9	S	5	MAN	O5-C5-C6-O6
8	j	3	BMA	O5-C5-C6-O6
9	y	2	NAG	O5-C5-C6-O6
7	2	1	NAG	C4-C5-C6-O6
8	V	2	NAG	C1-C2-N2-C7
8	c	1	NAG	C4-C5-C6-O6
8	0	1	NAG	C1-C2-N2-C7
7	Q	1	NAG	C3-C2-N2-C7
8	j	1	NAG	C3-C2-N2-C7
7	AA	1	NAG	C4-C5-C6-O6
8	j	1	NAG	C1-C2-N2-C7
8	0	1	NAG	C3-C2-N2-C7

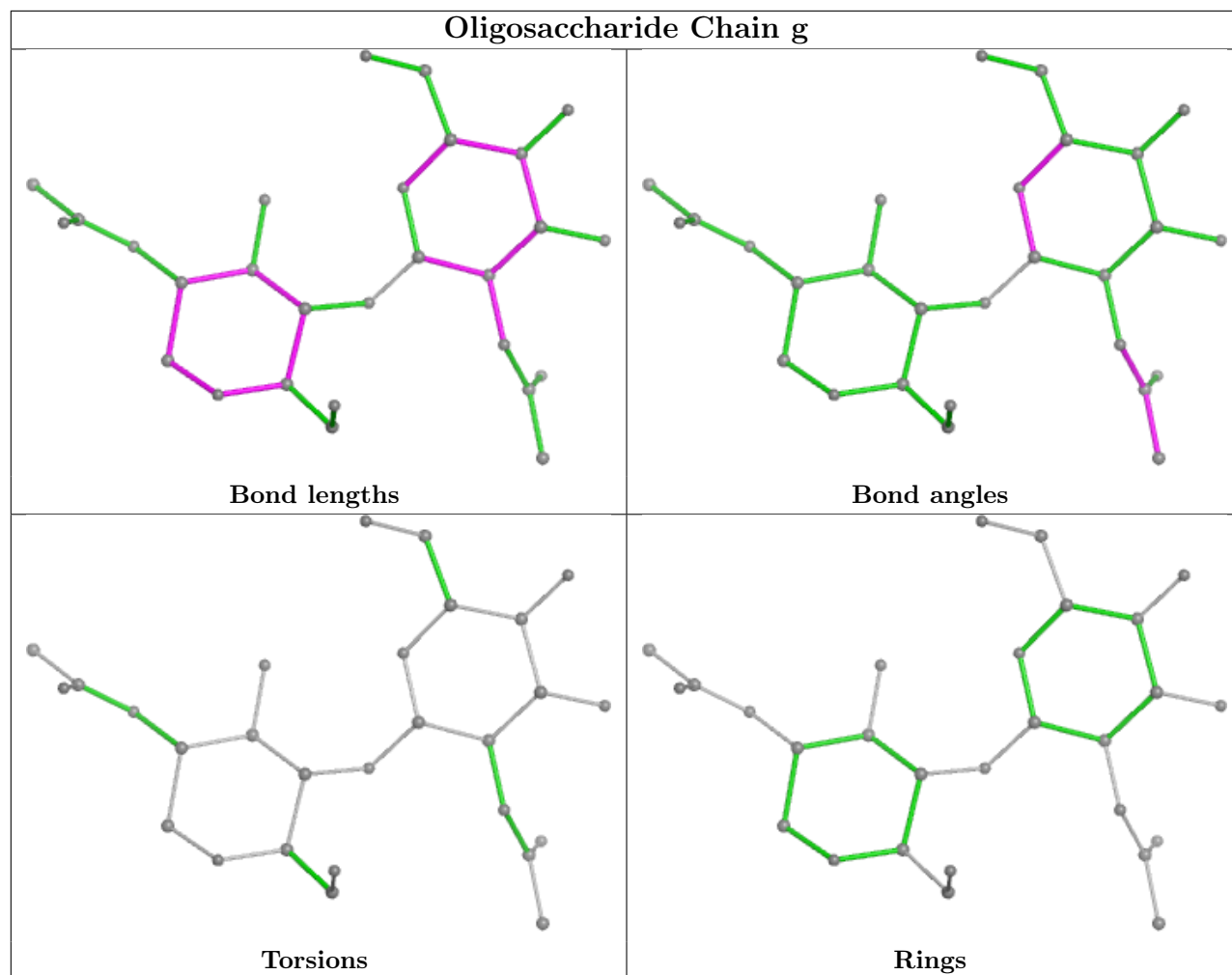
There are no ring outliers.

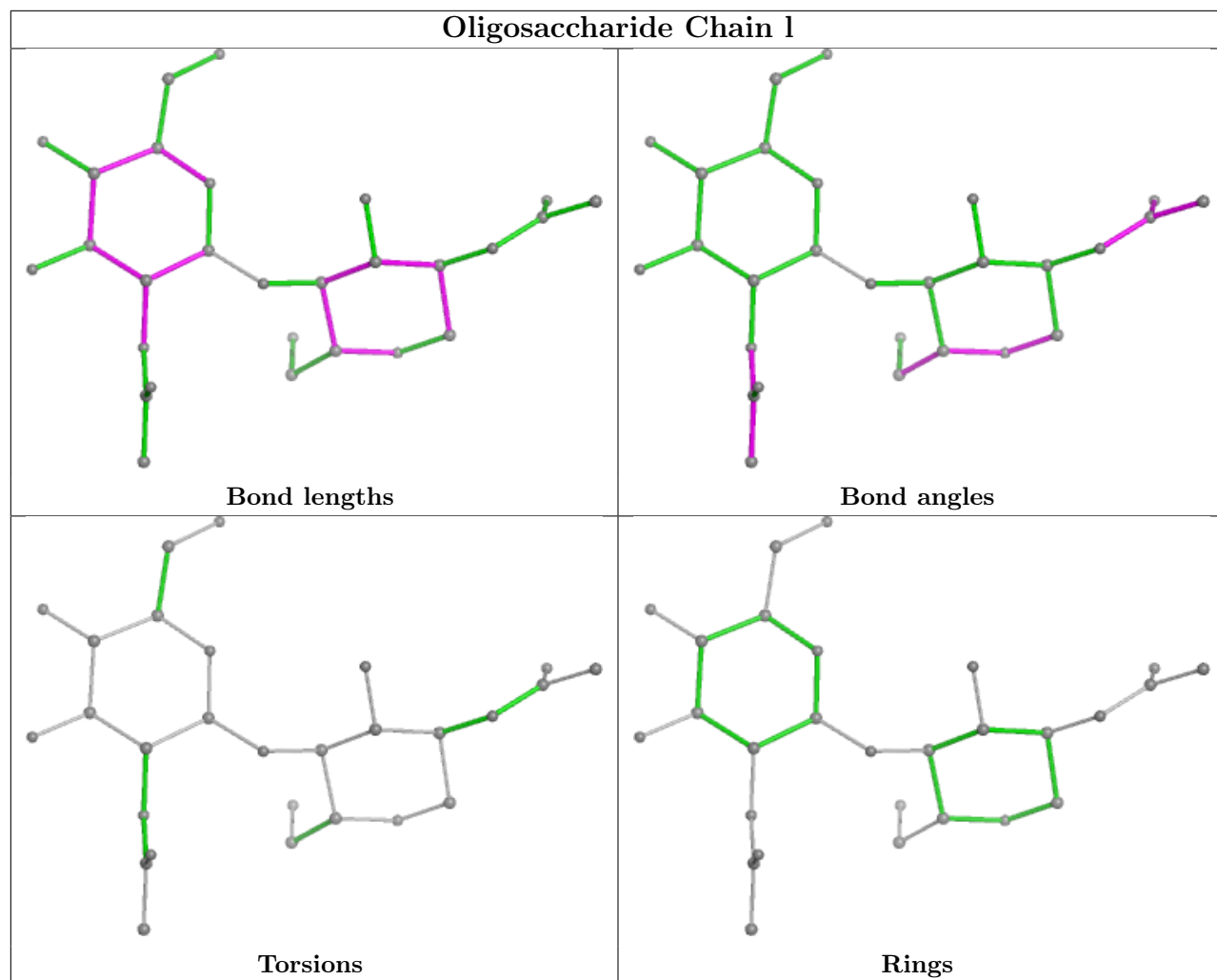
No monomer is involved in short contacts.

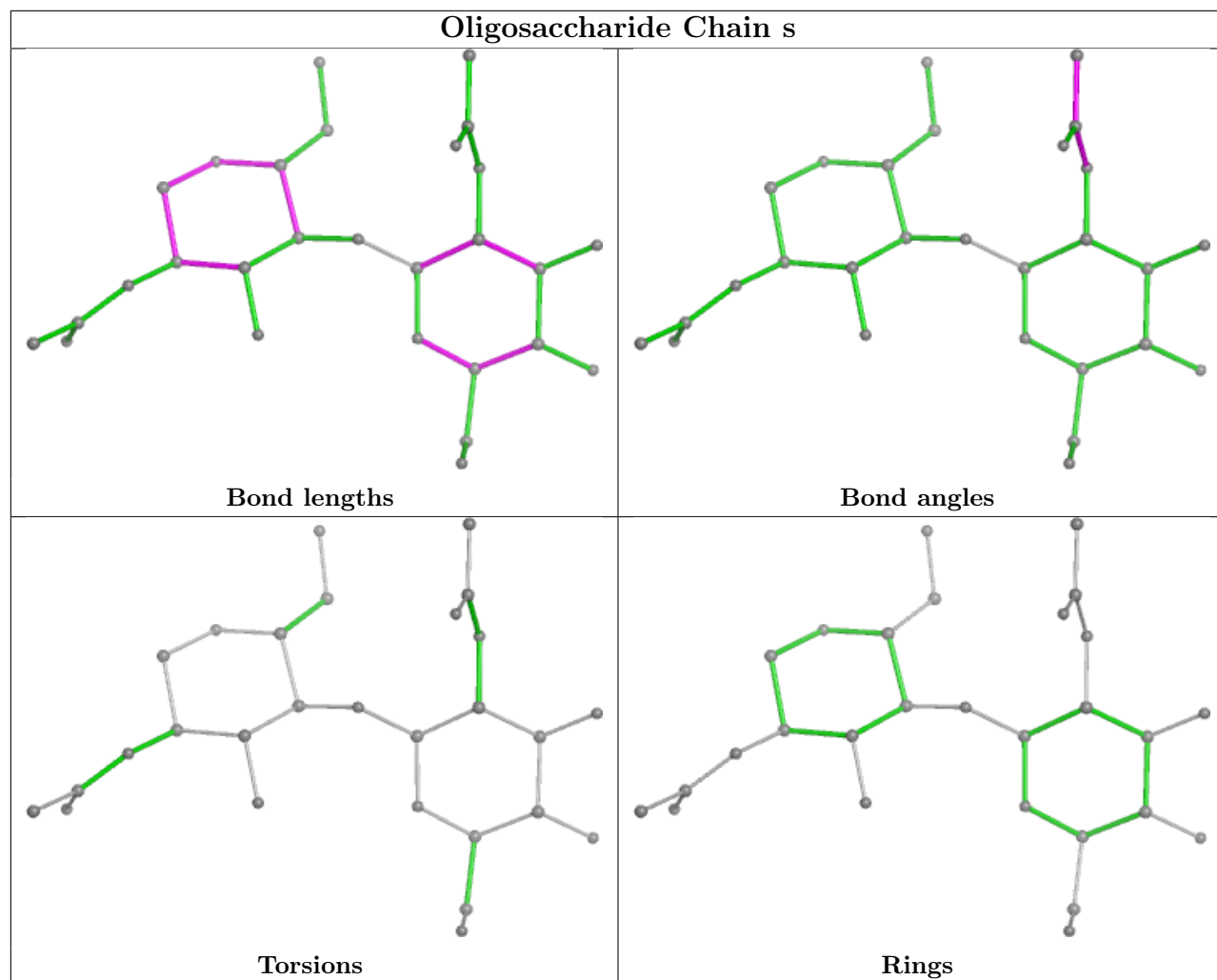
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

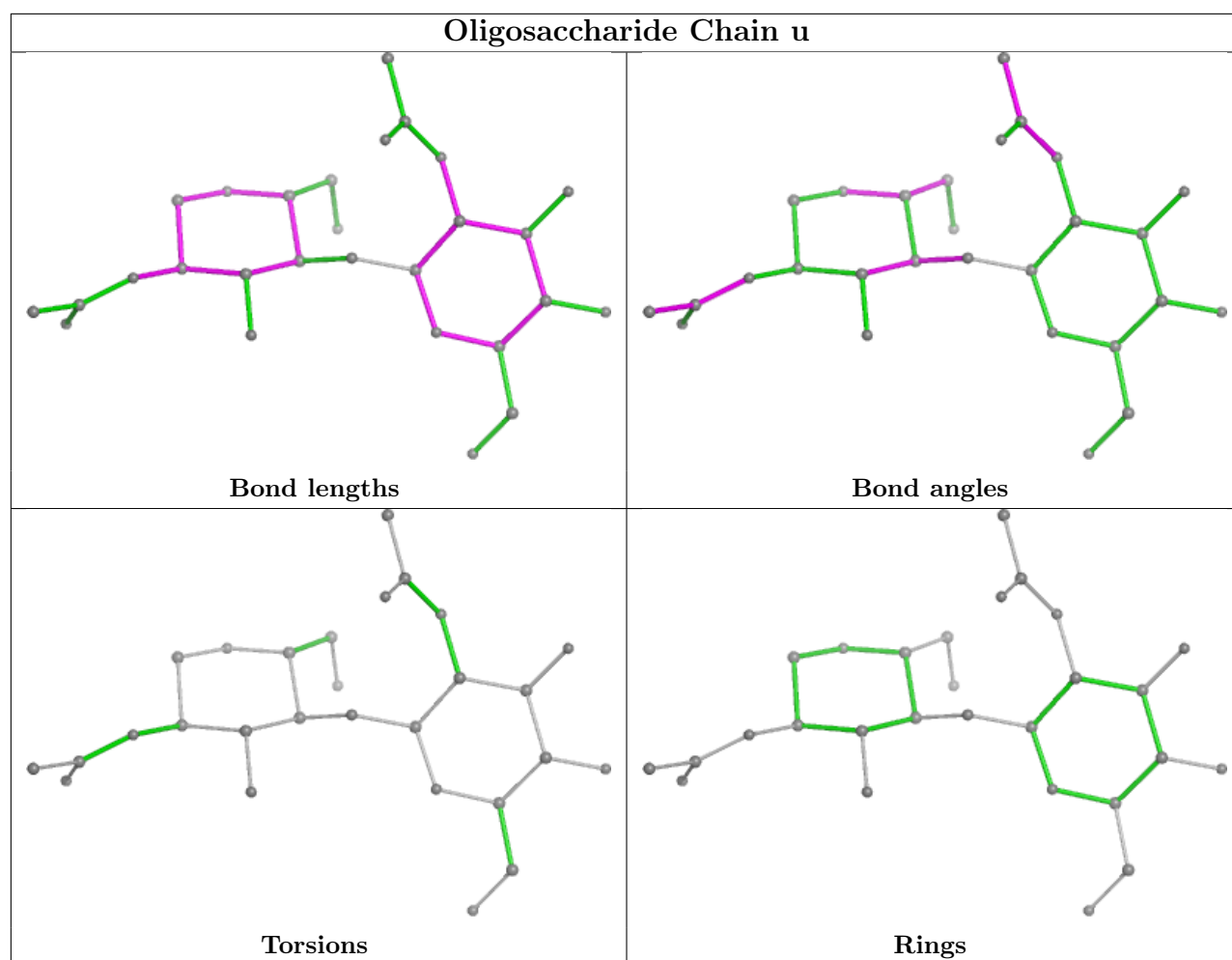




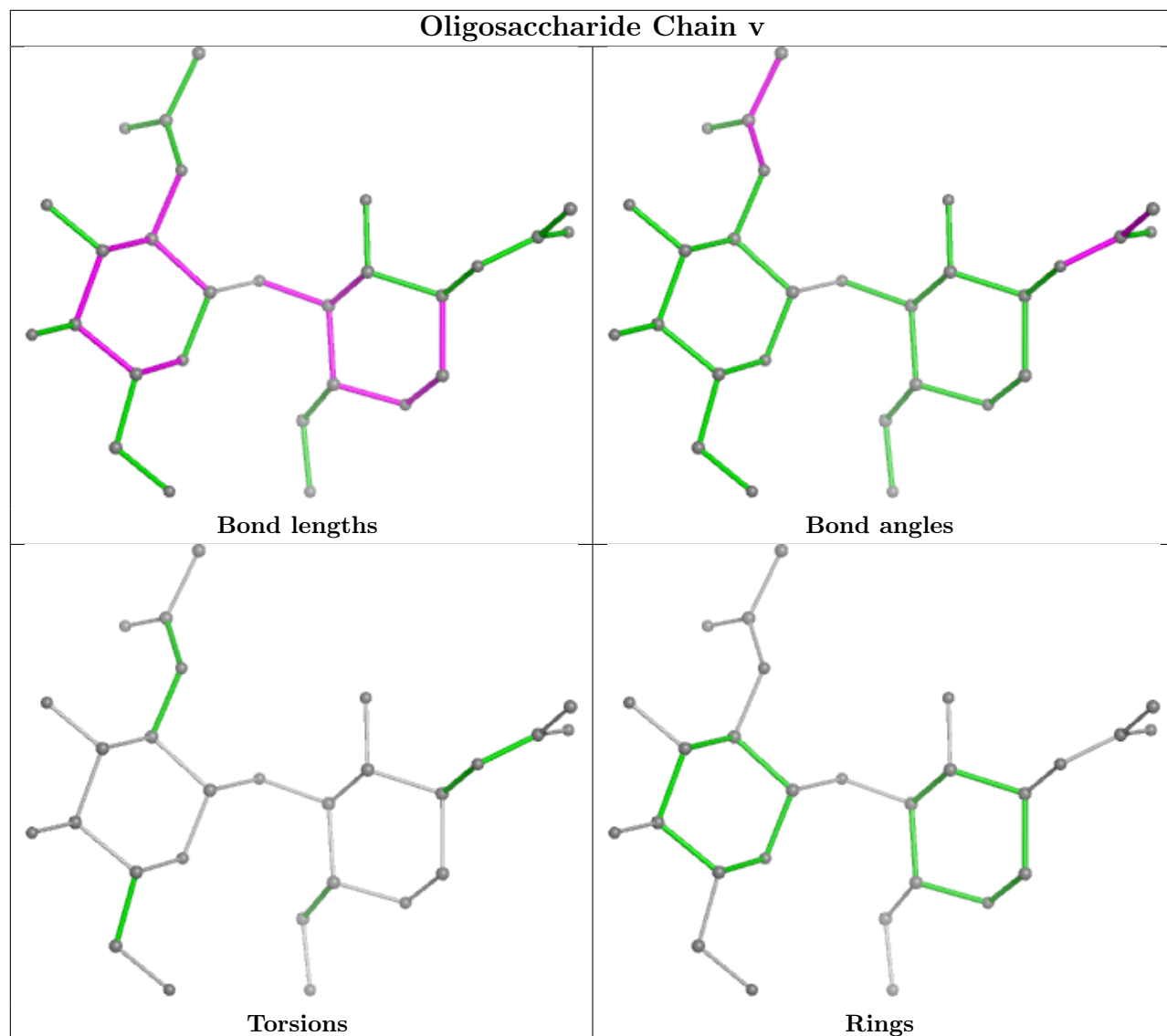


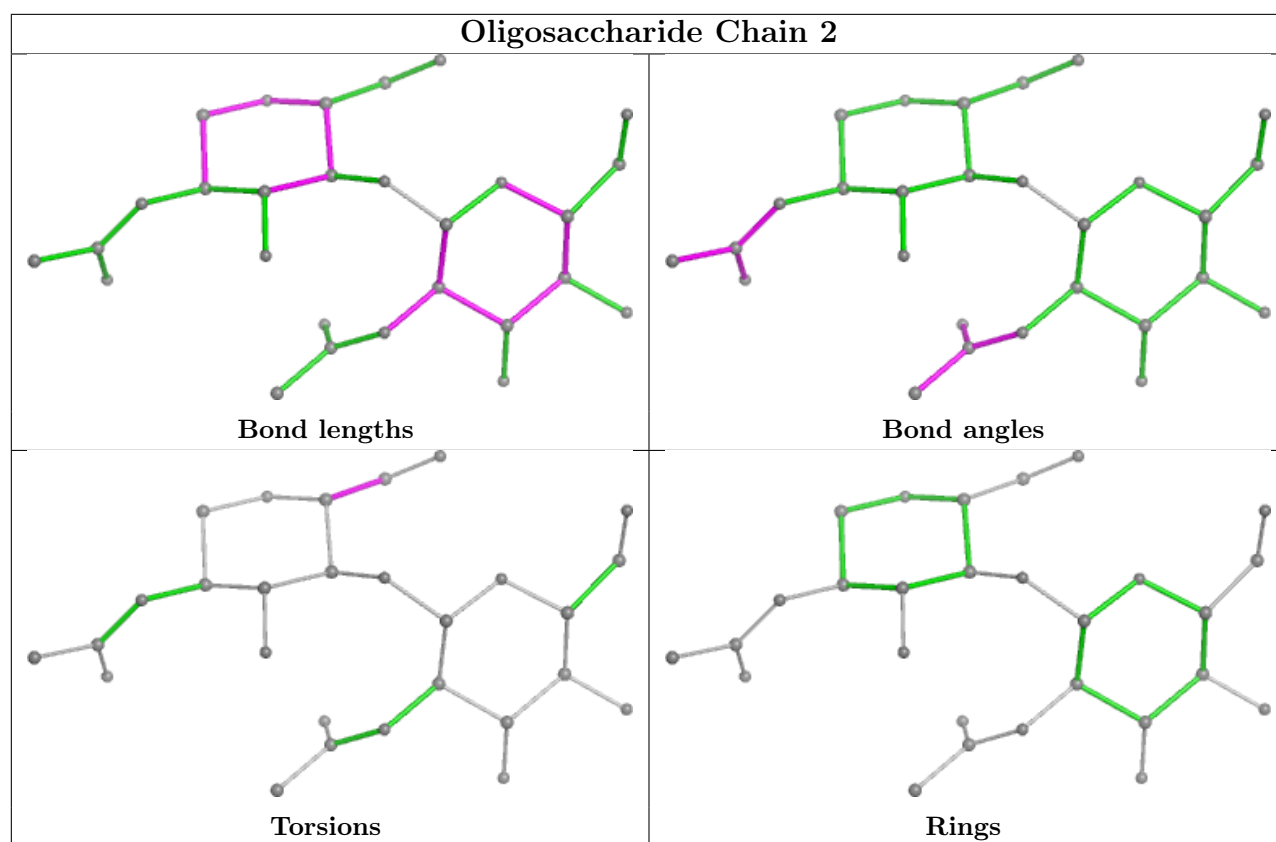


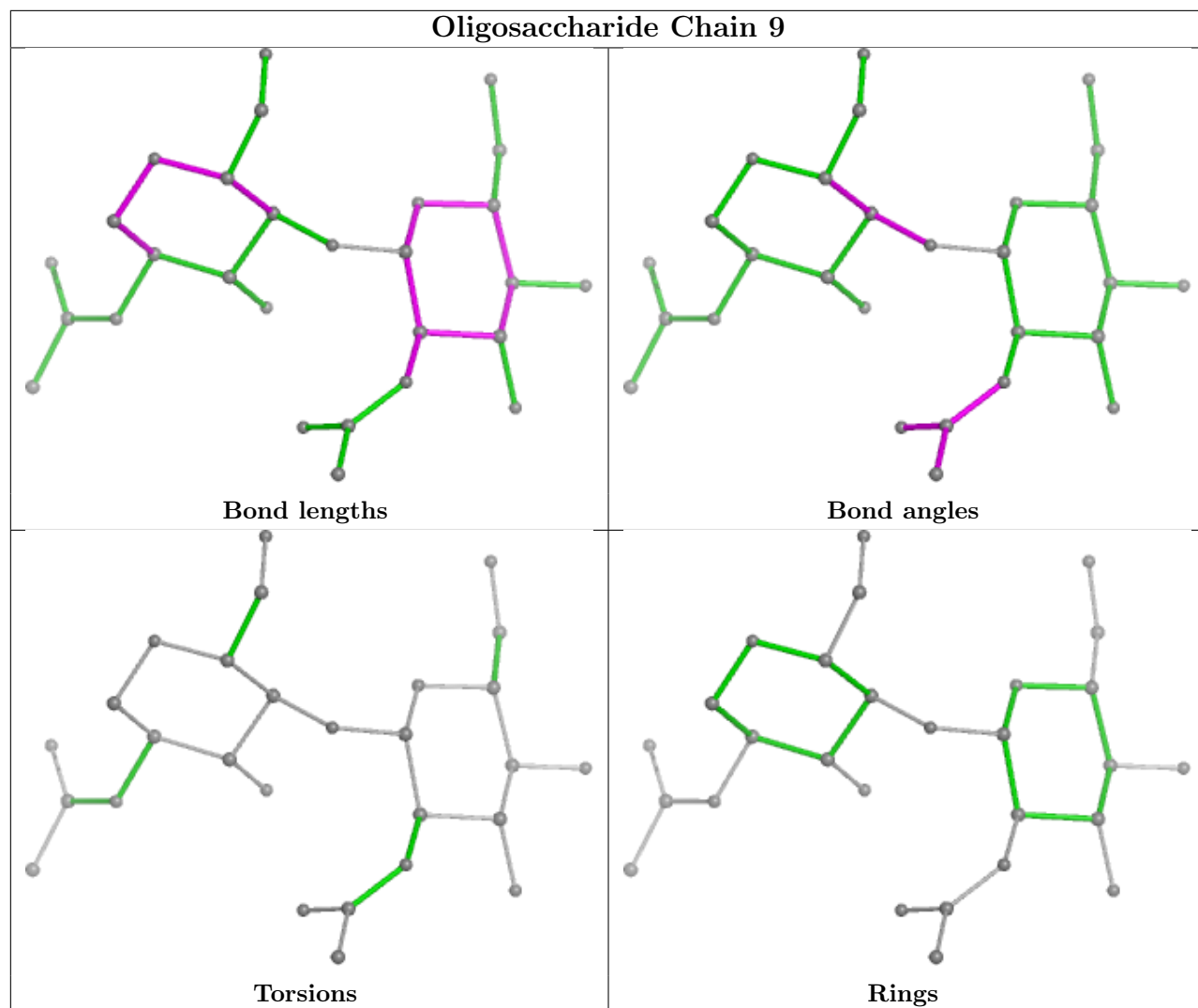


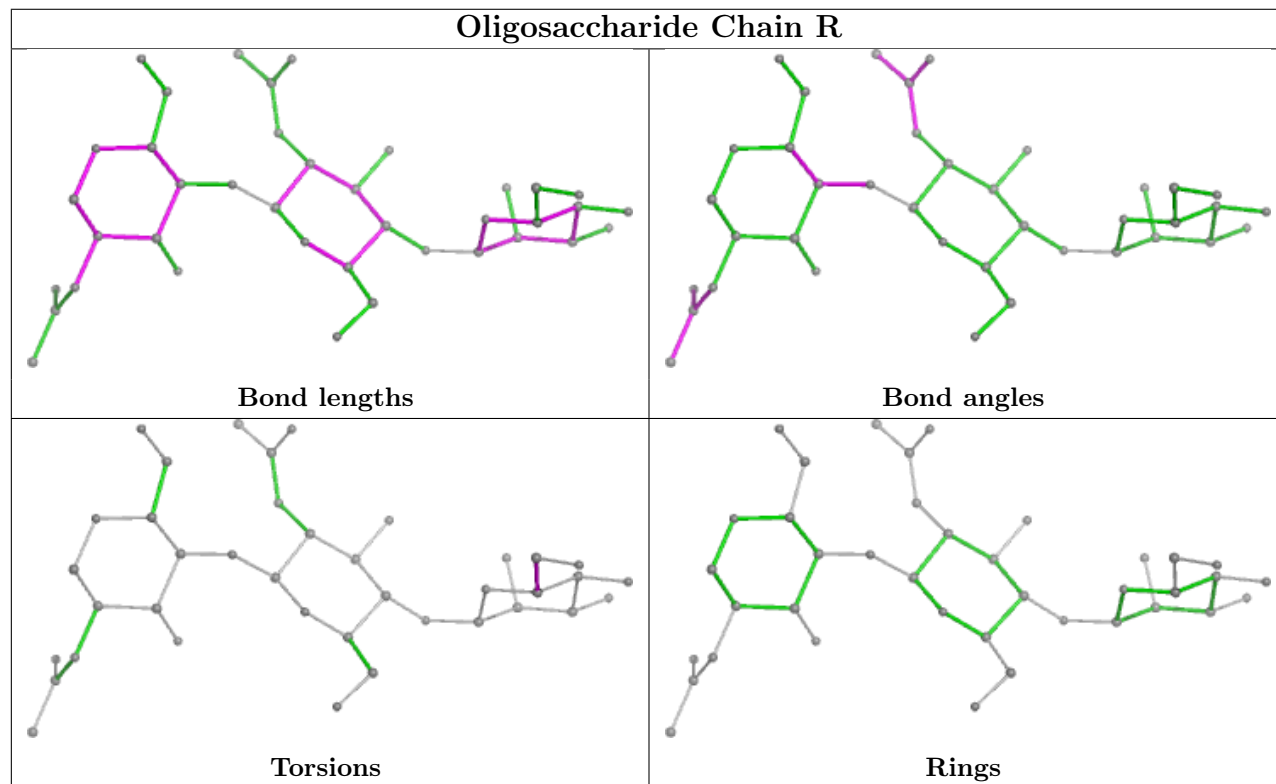
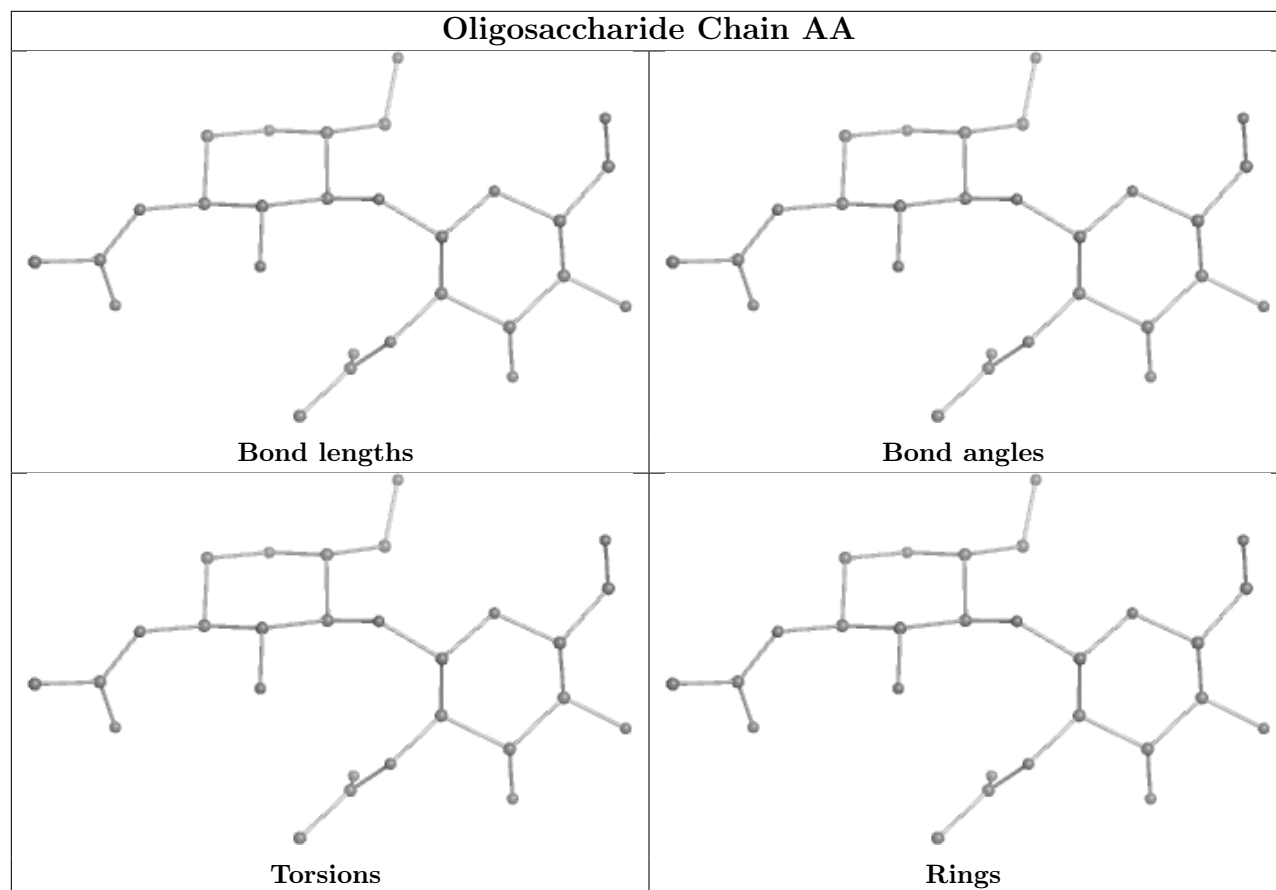


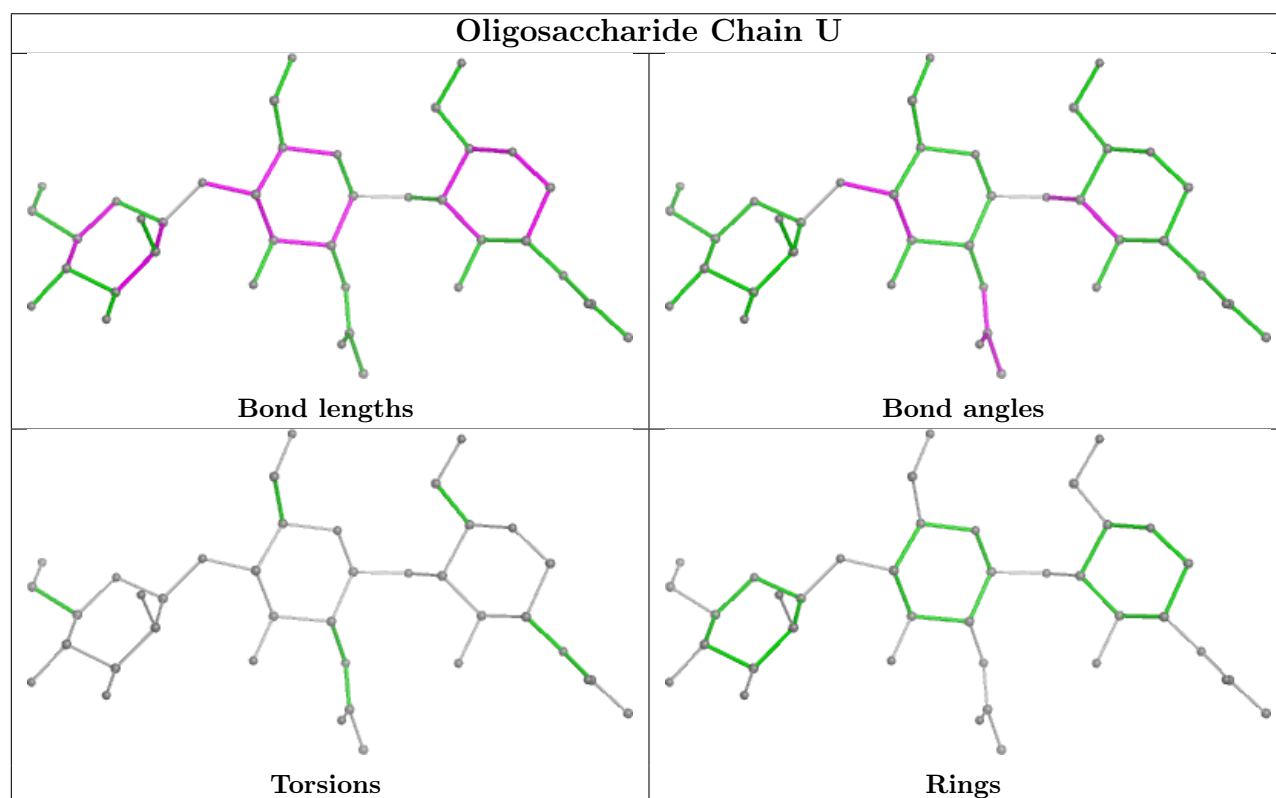
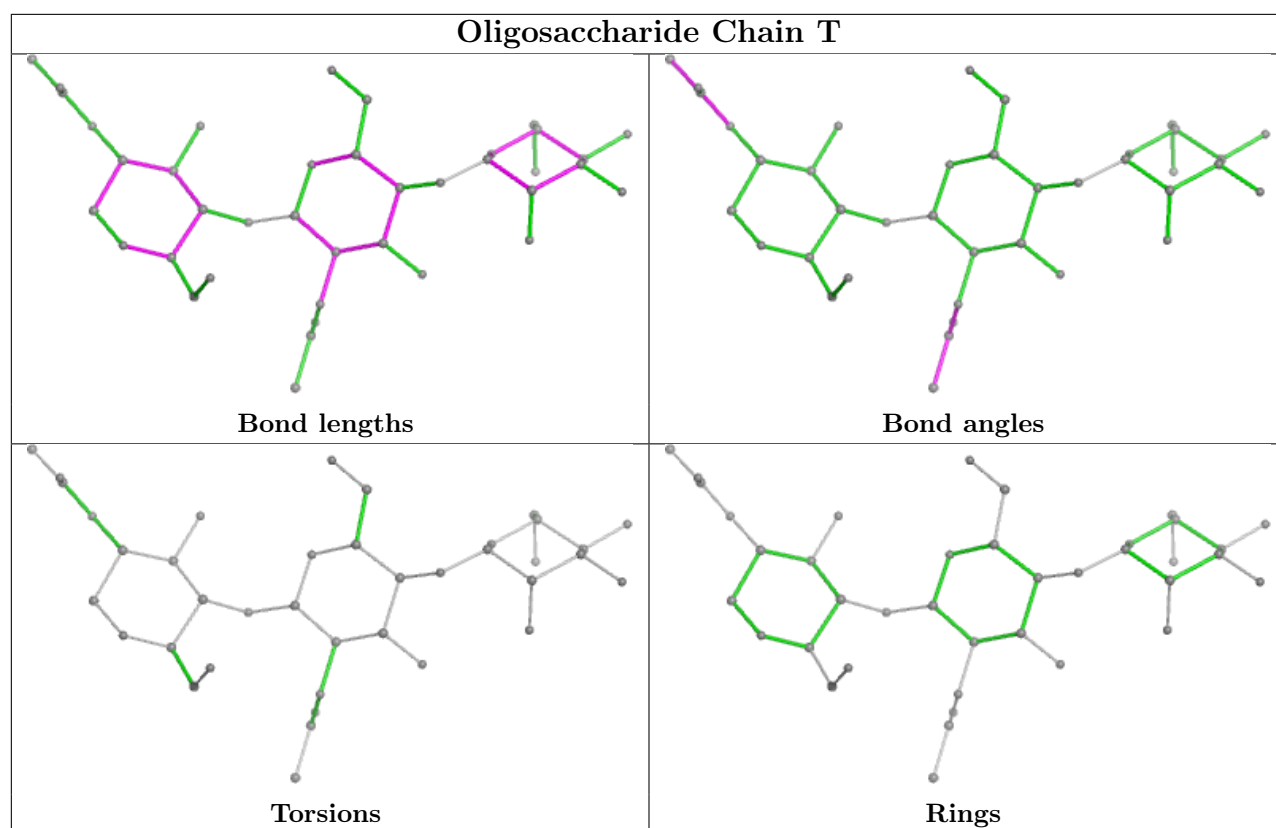




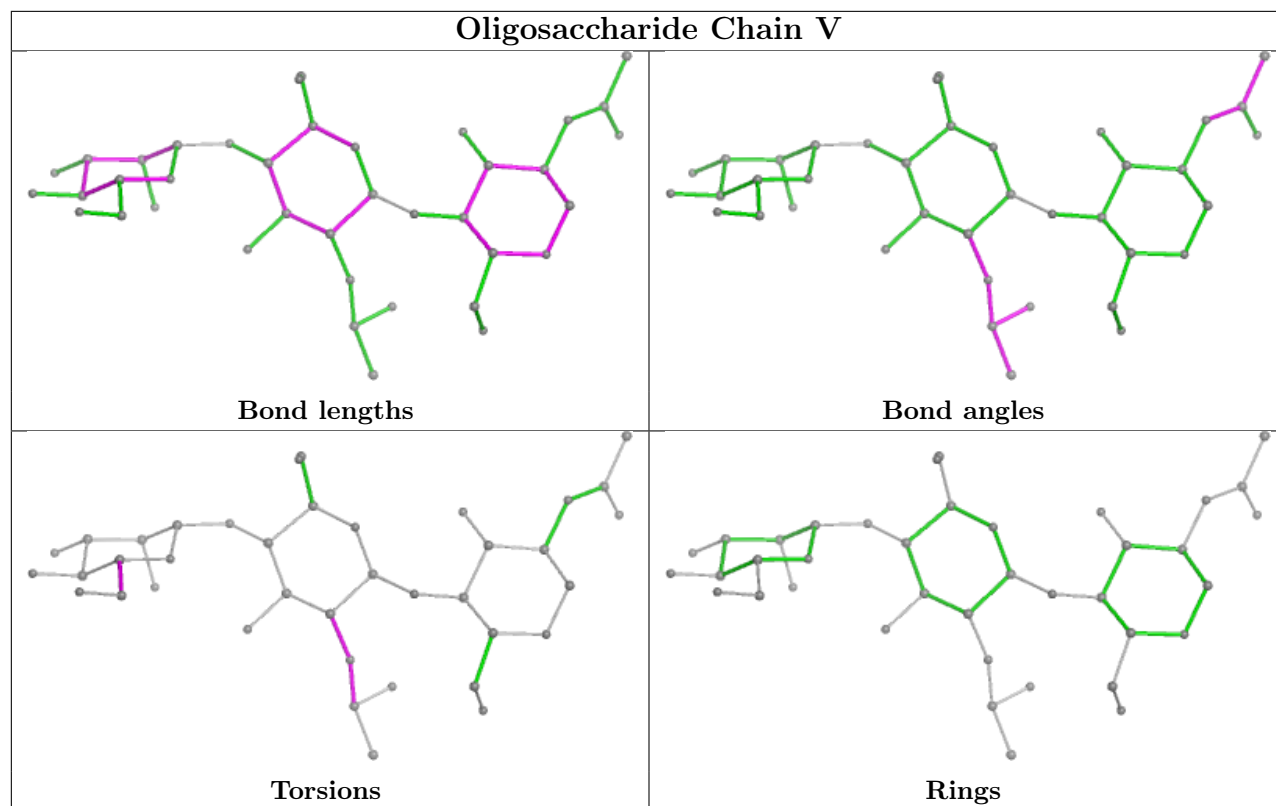




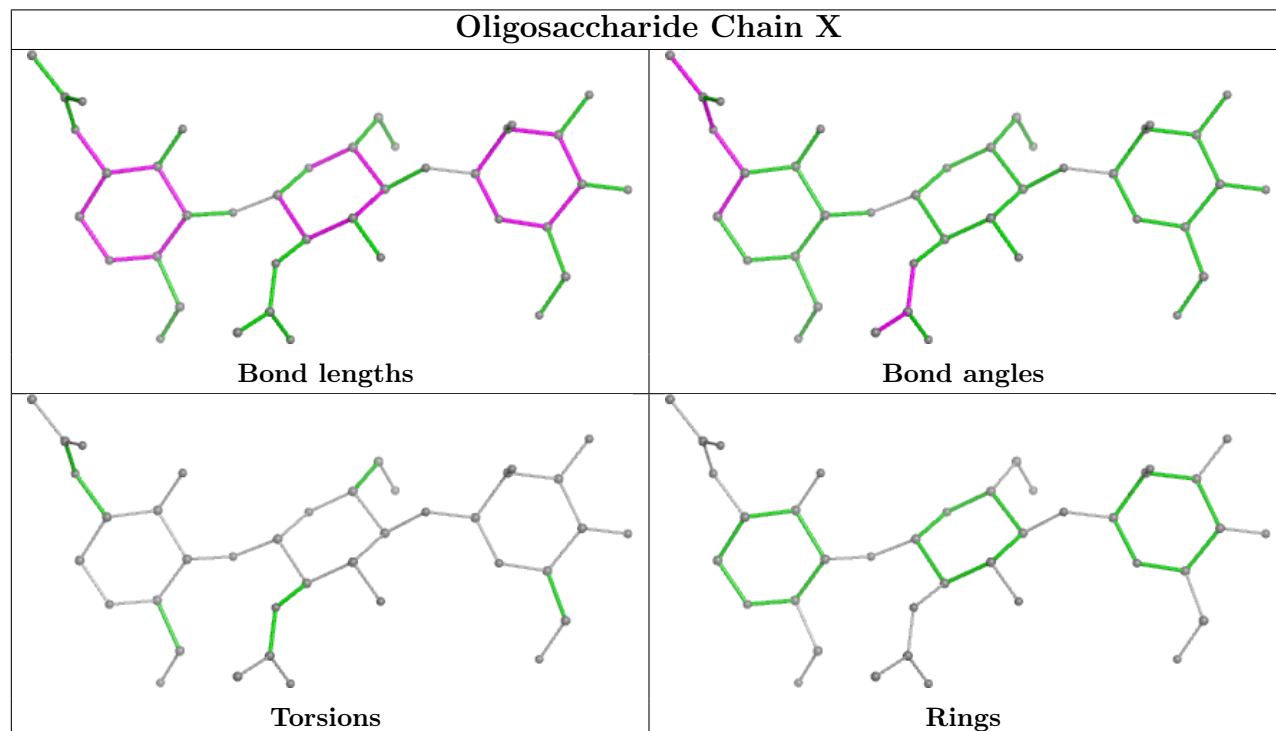


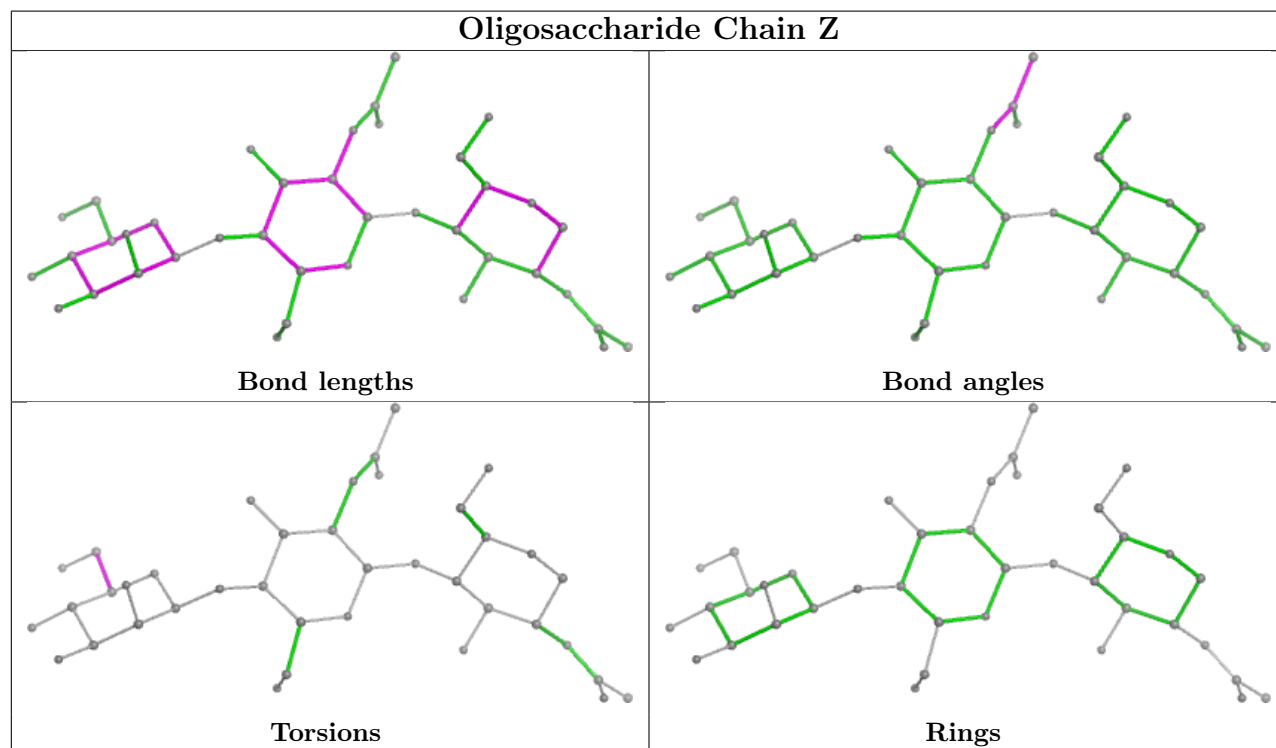
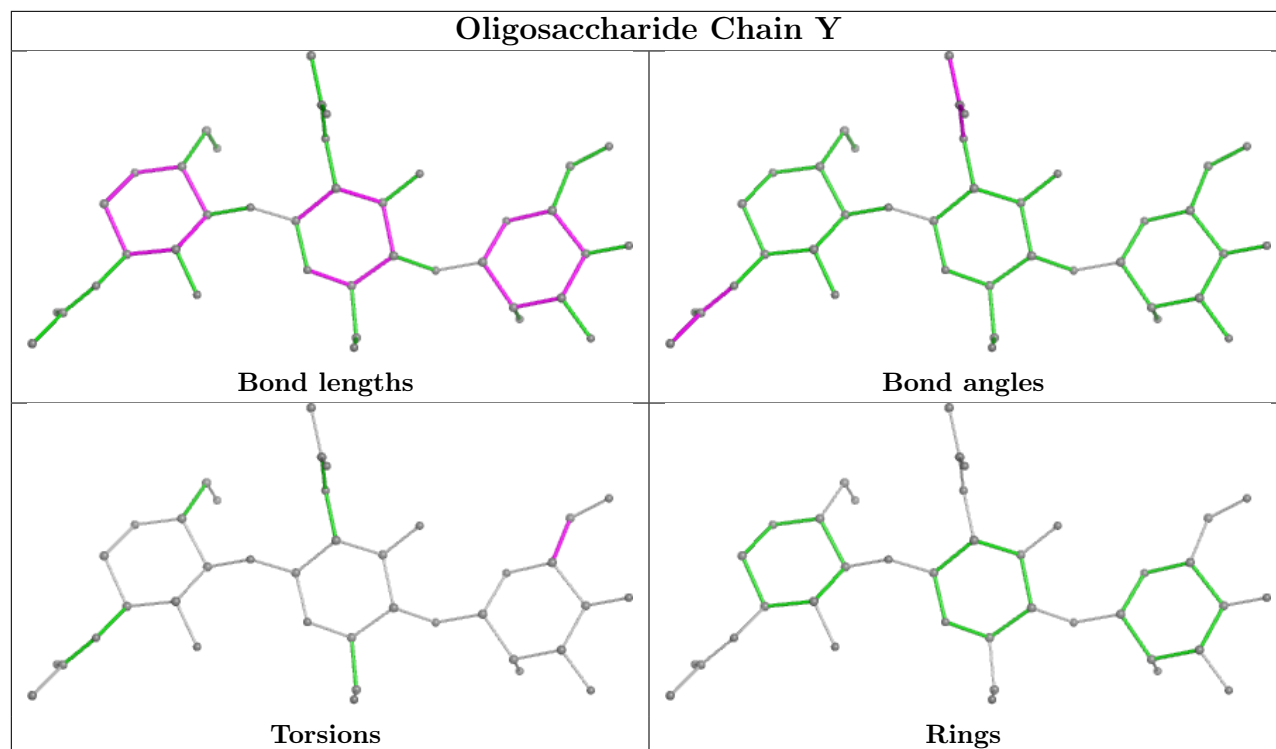


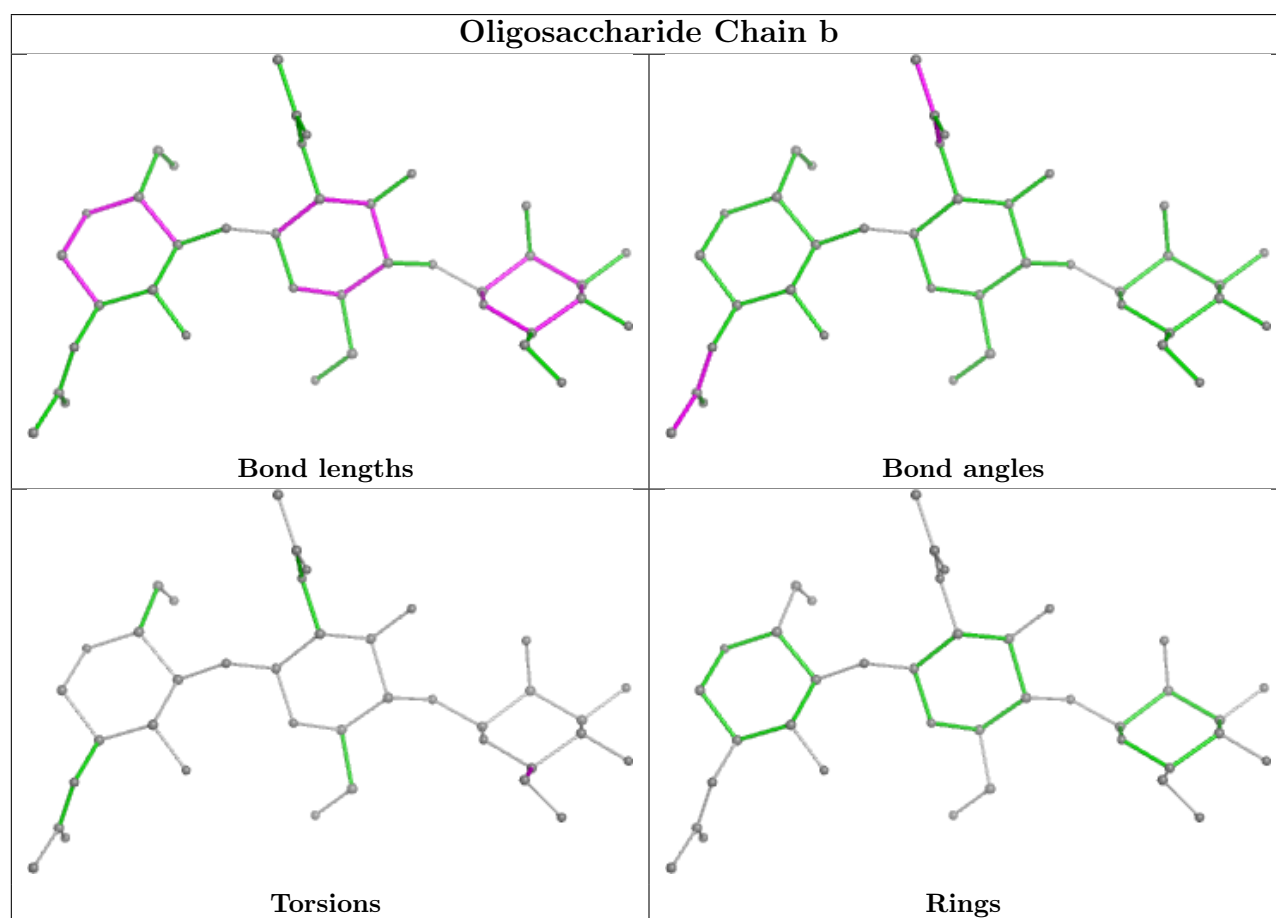
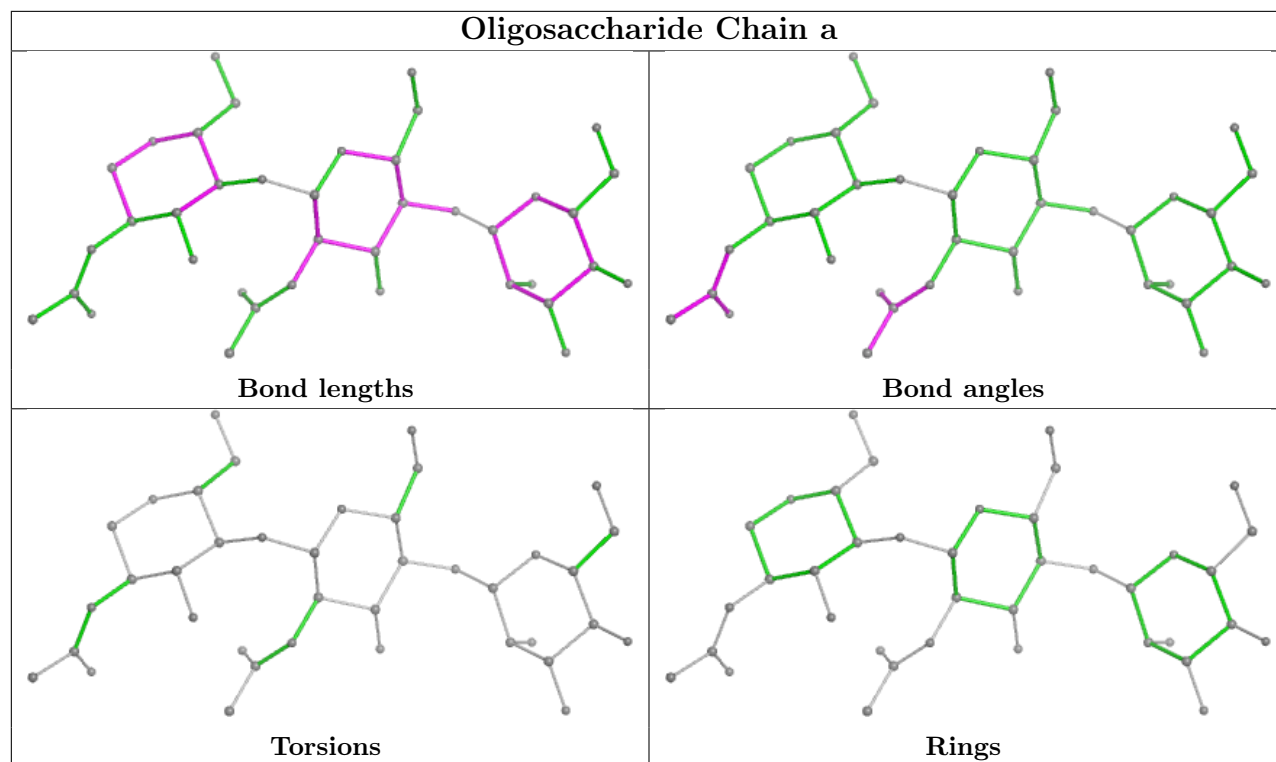
## Oligosaccharide Chain V



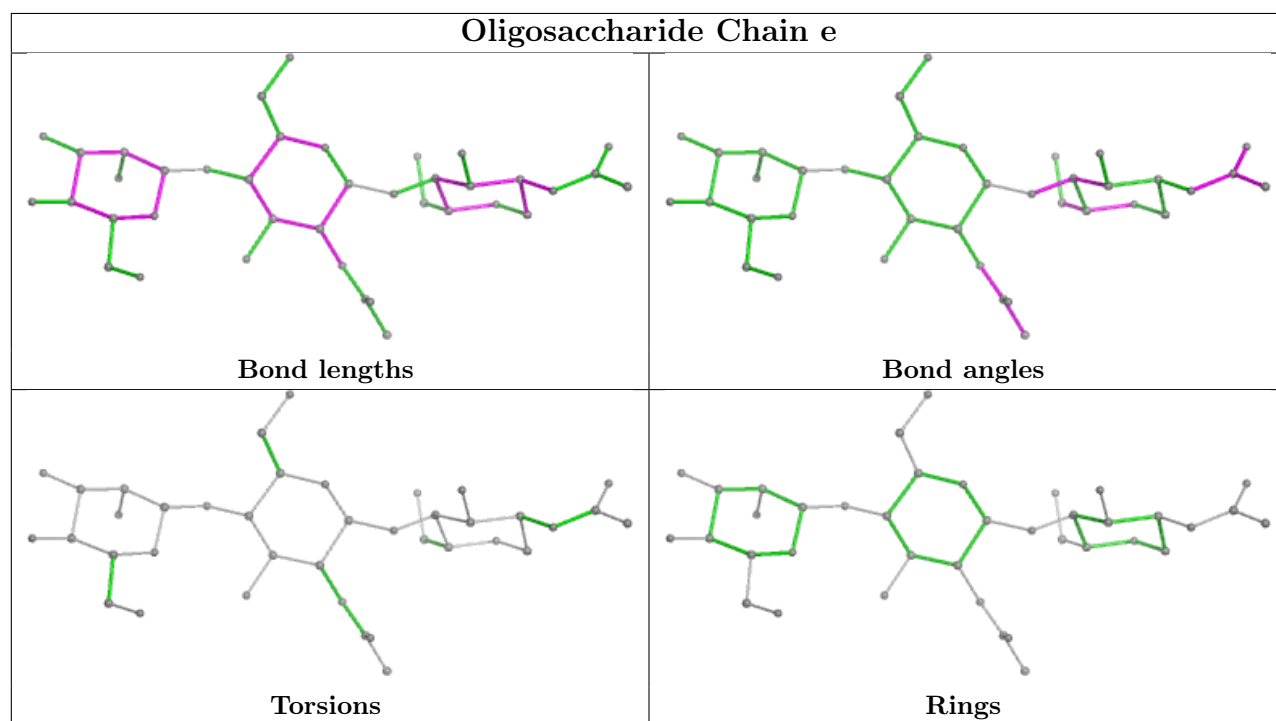
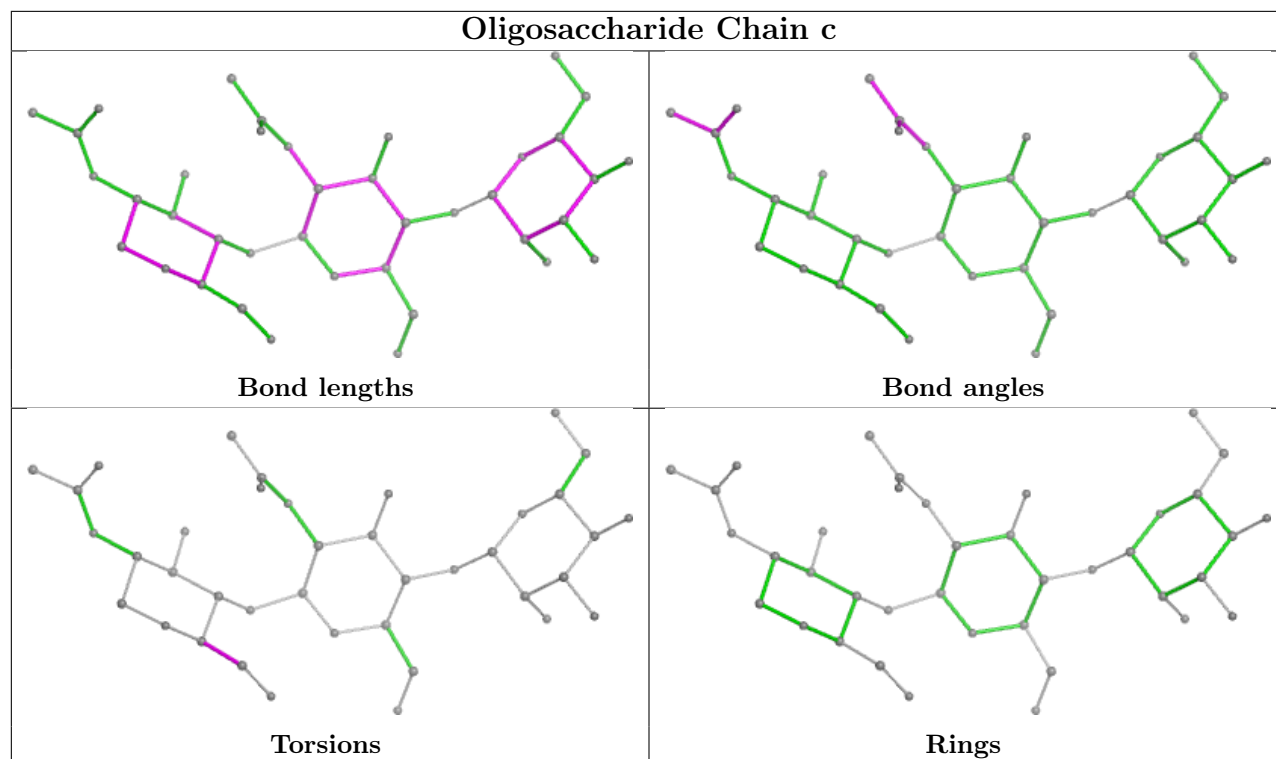
## Oligosaccharide Chain X

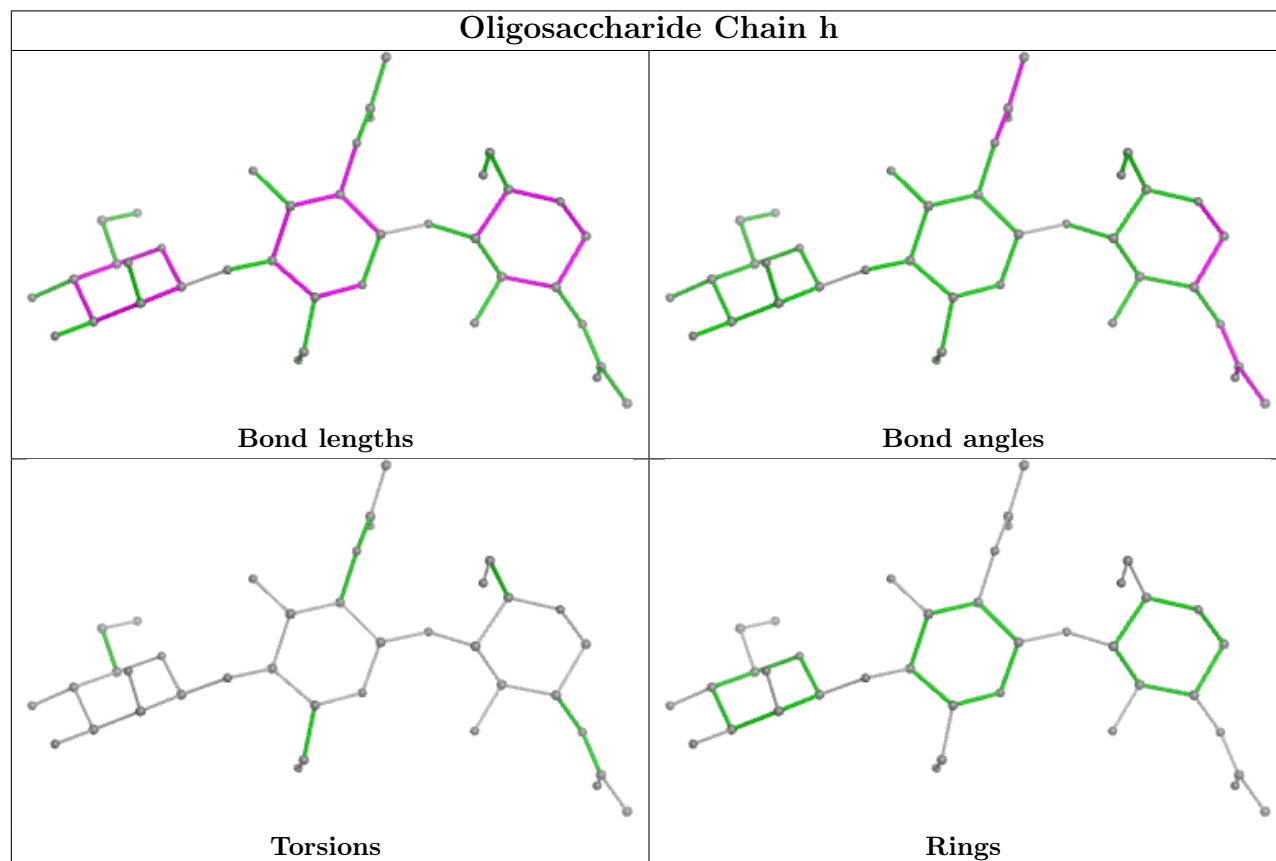
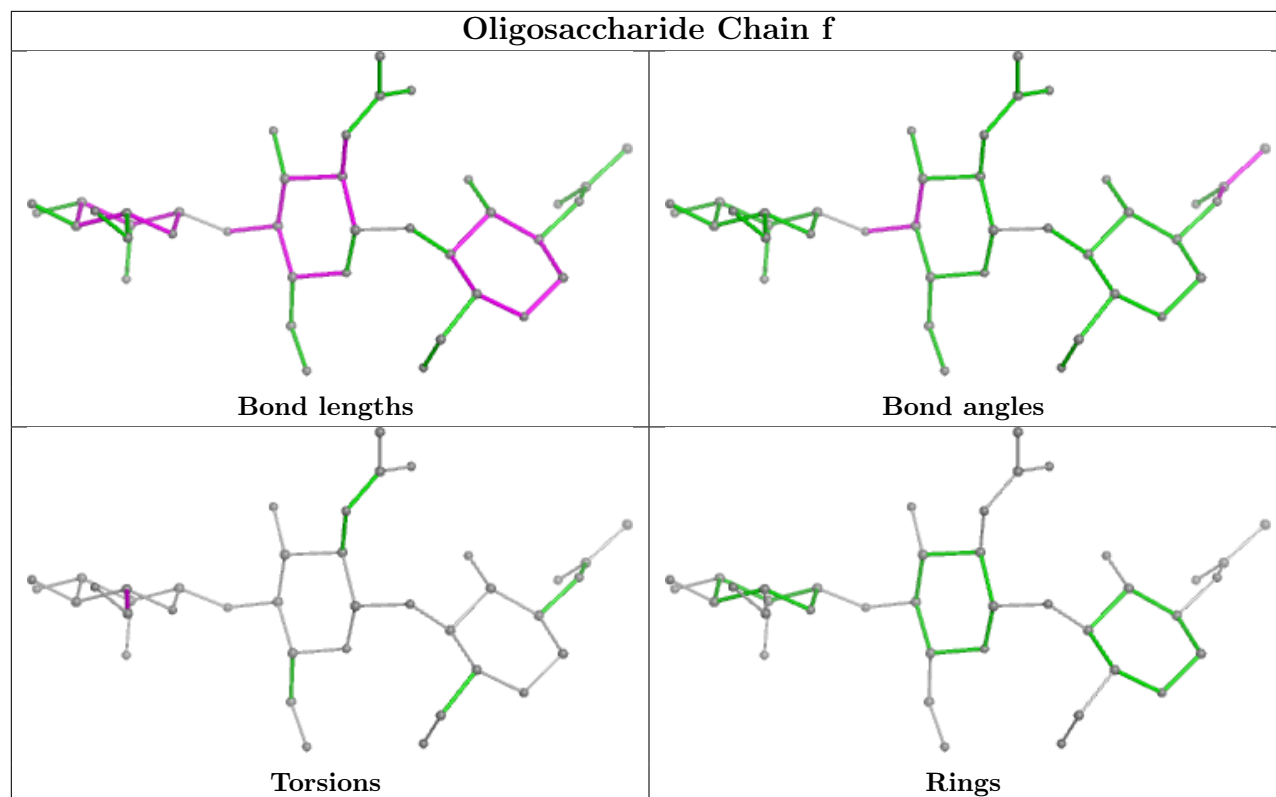


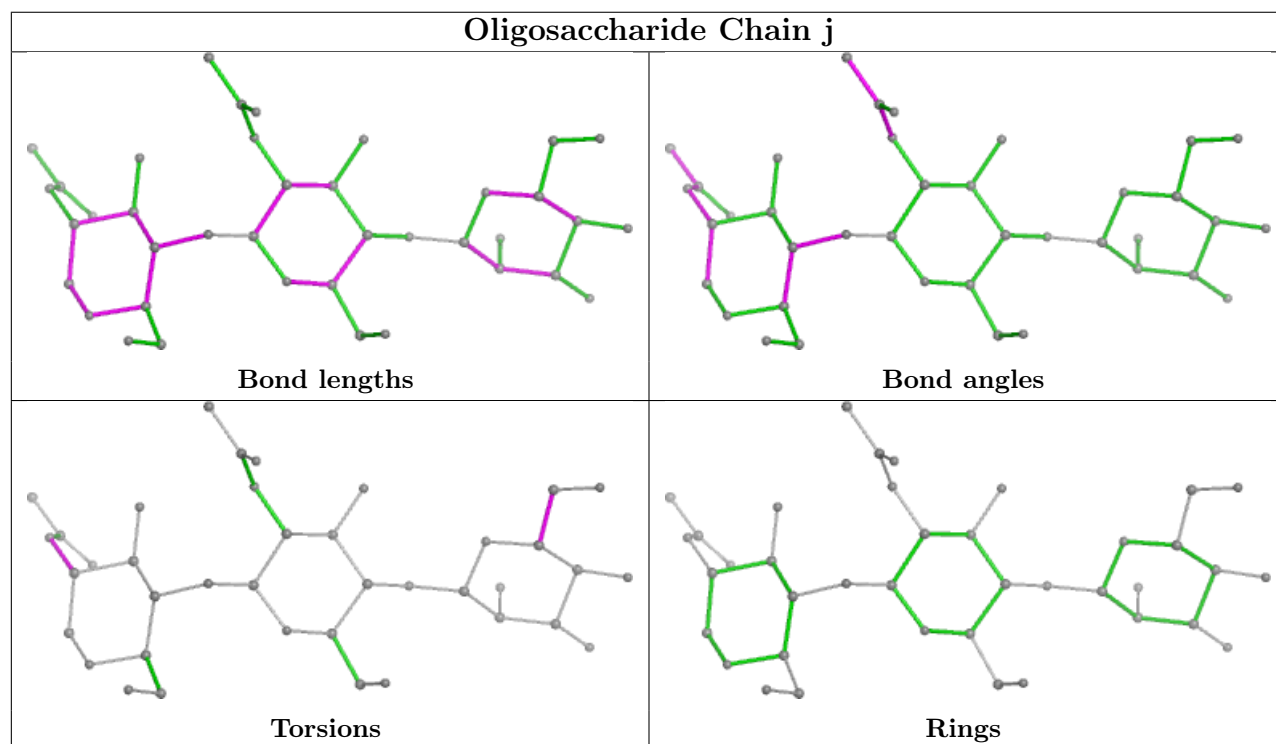
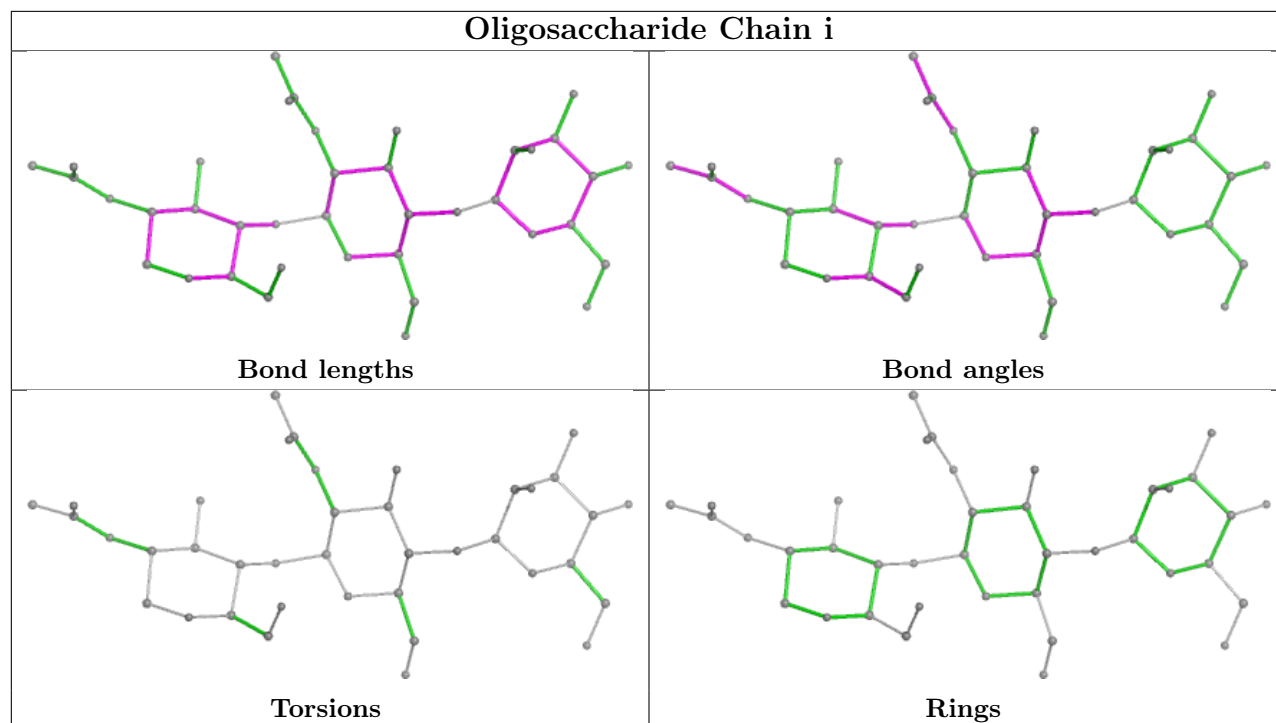


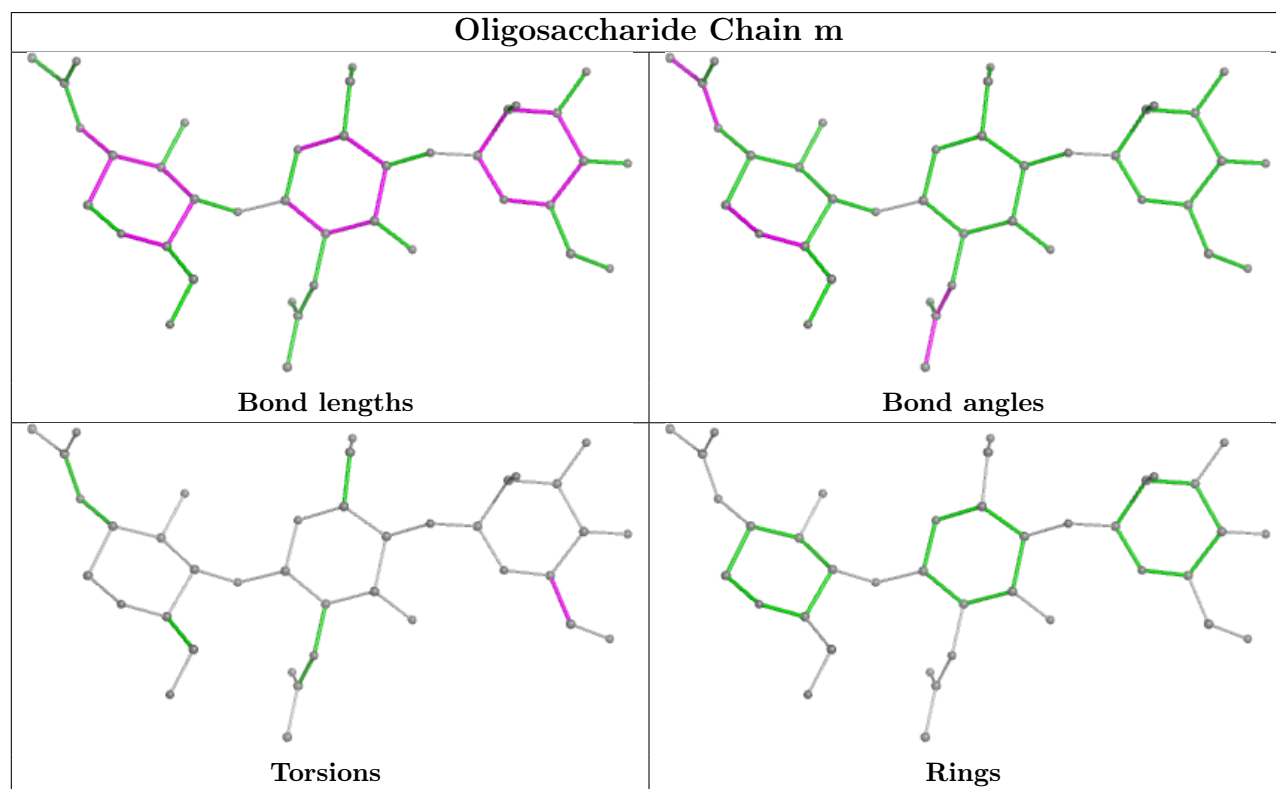
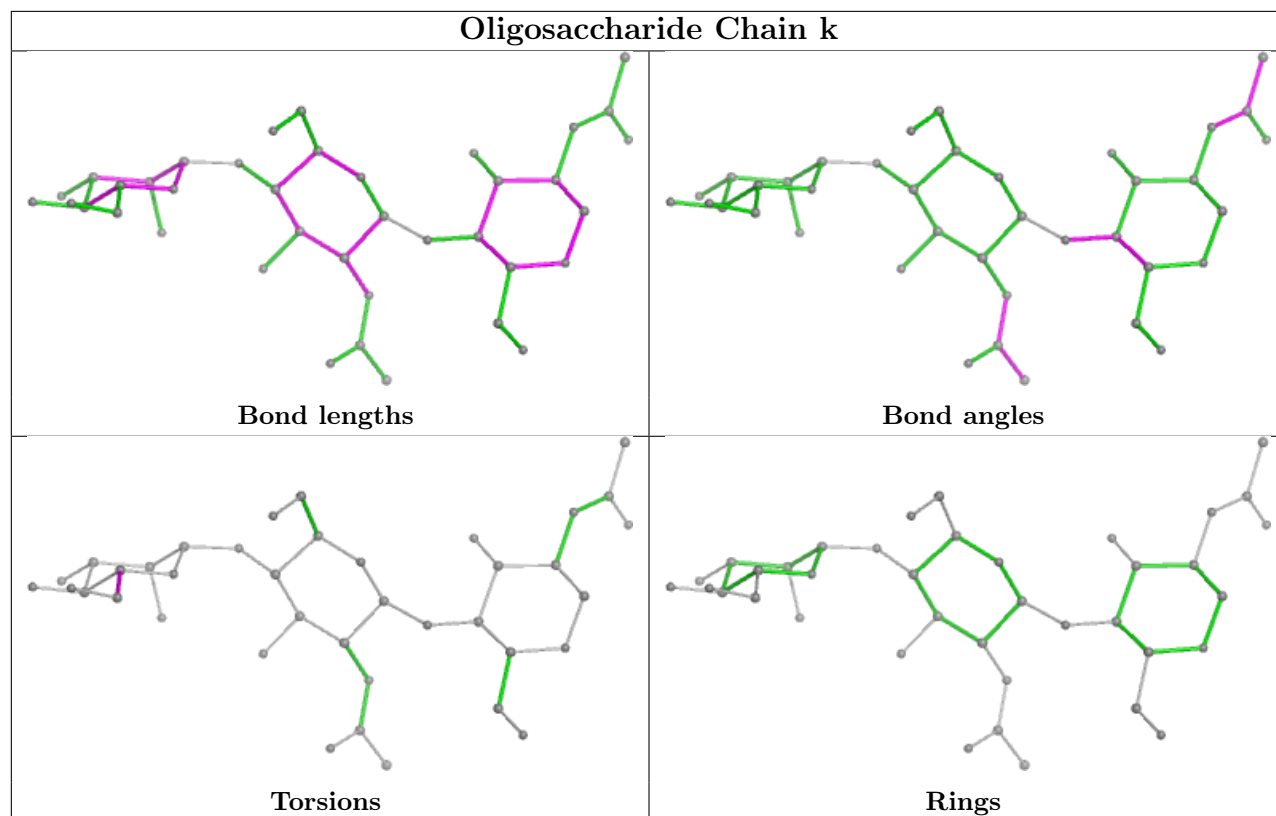


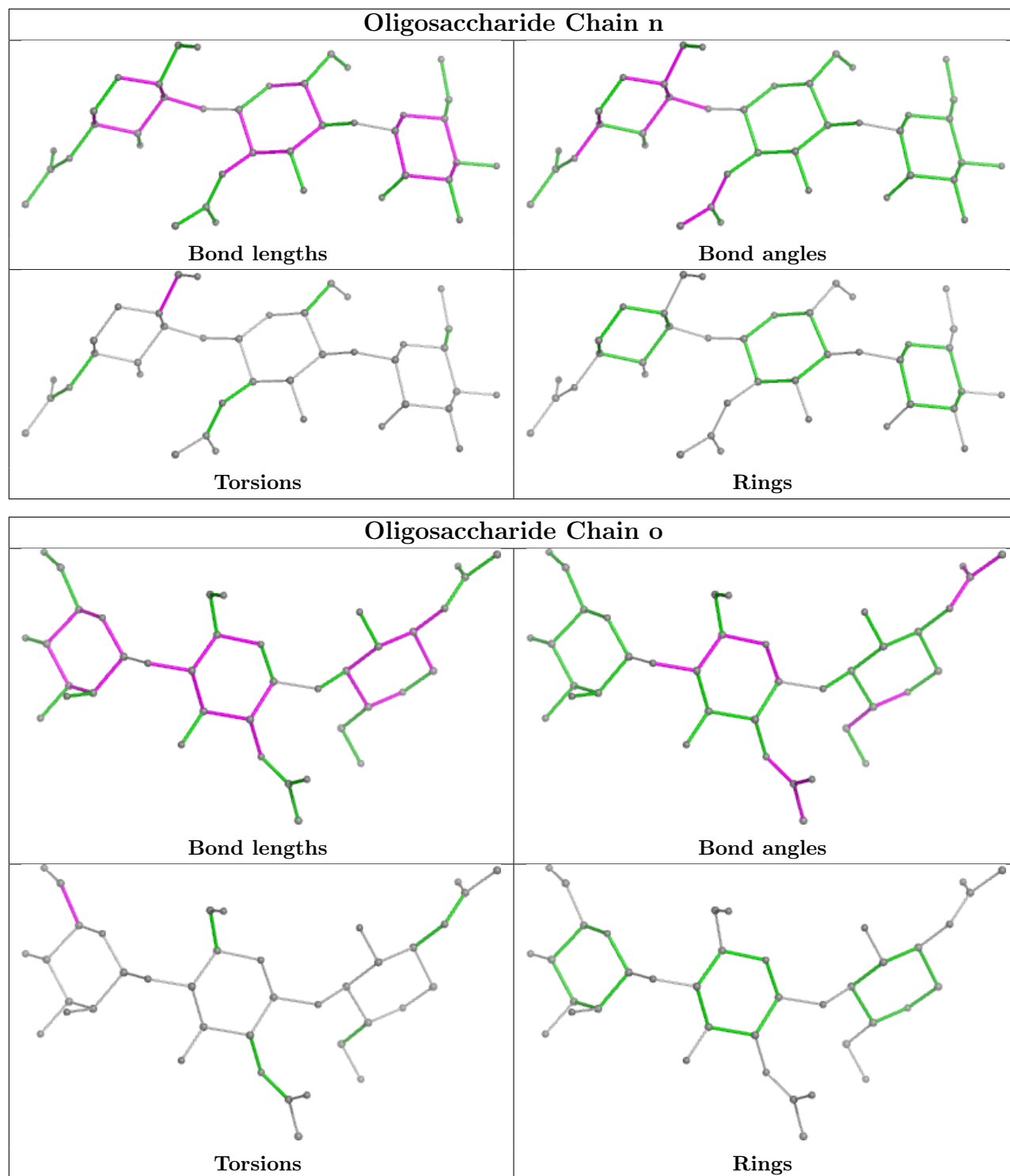


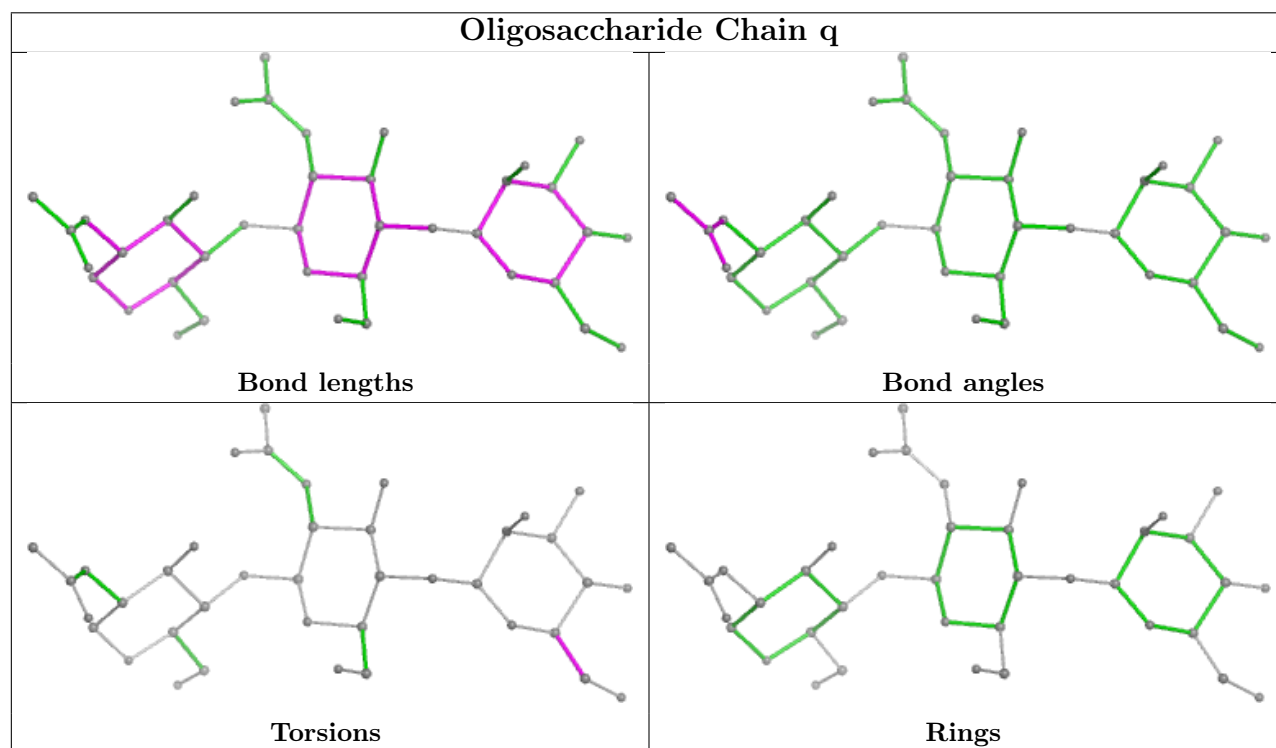
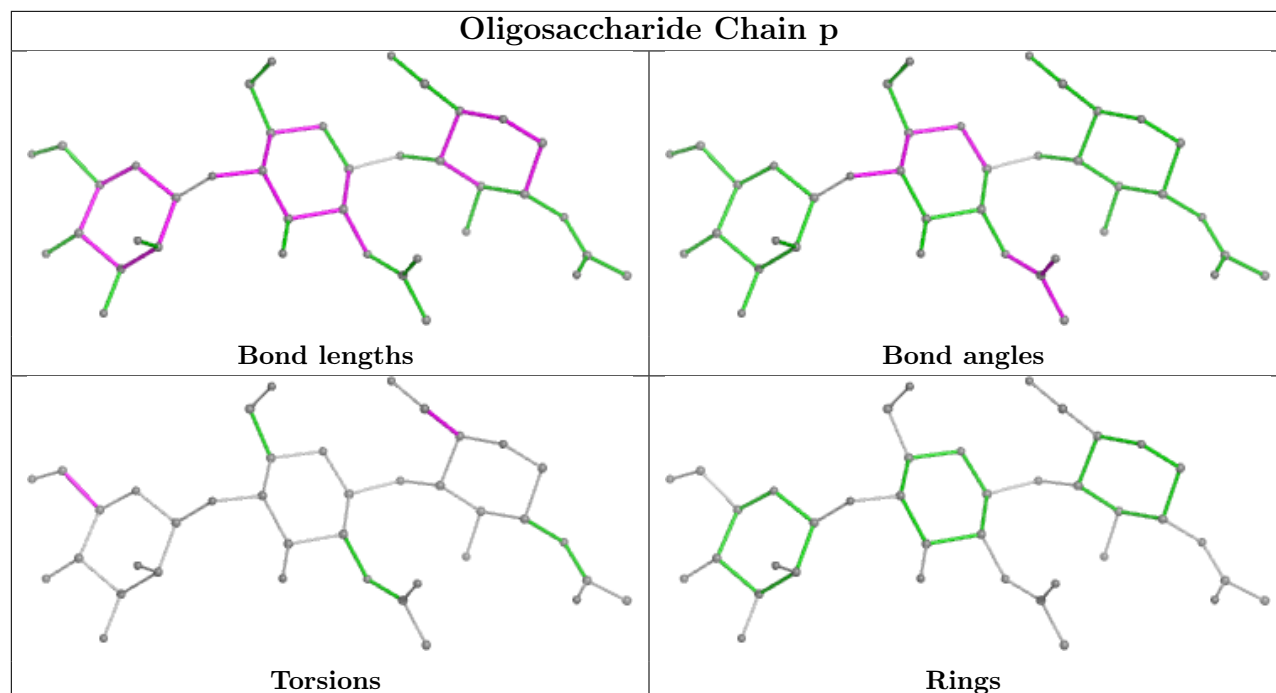


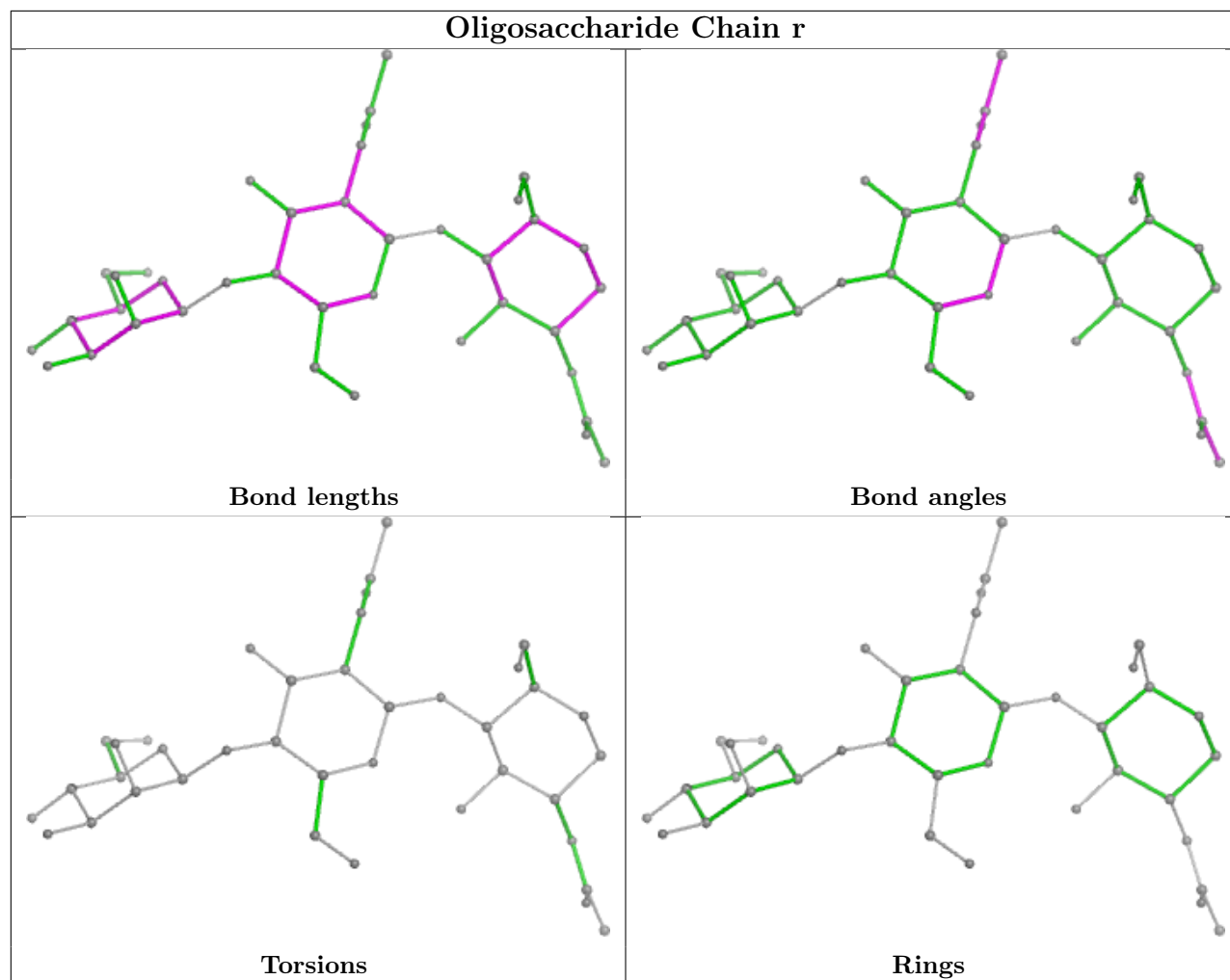


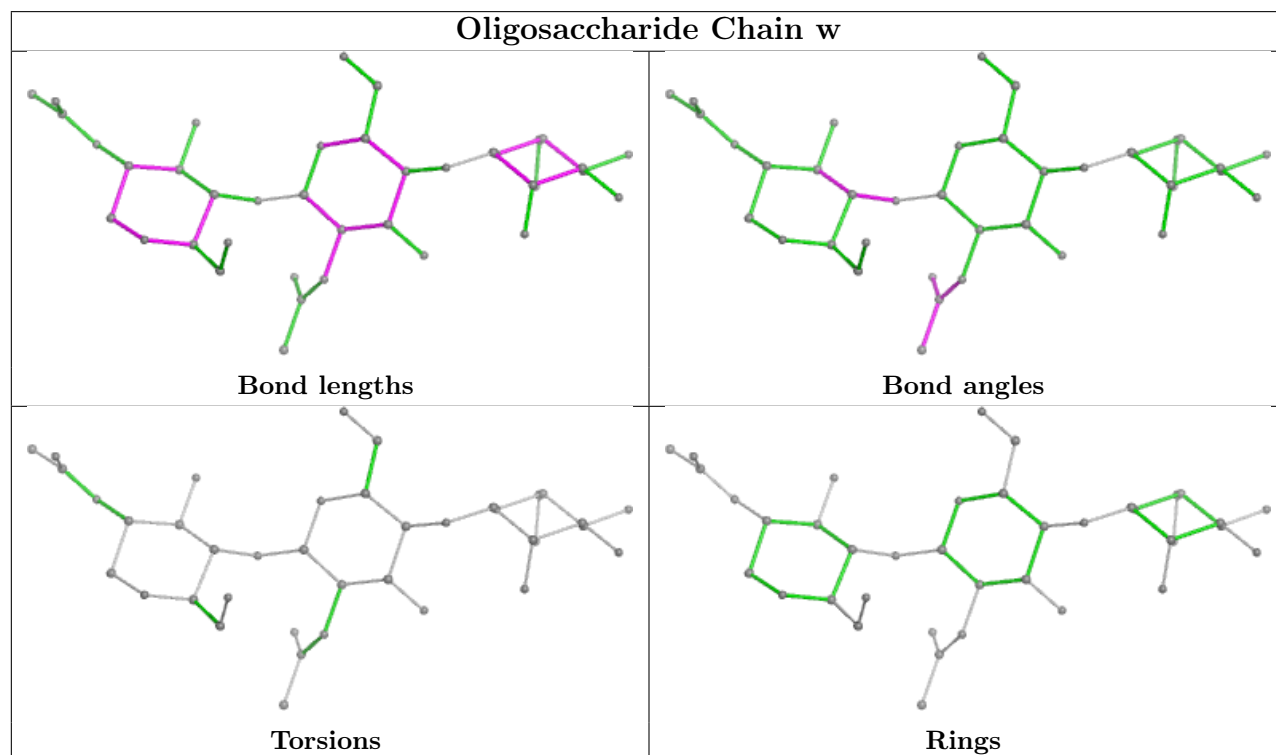
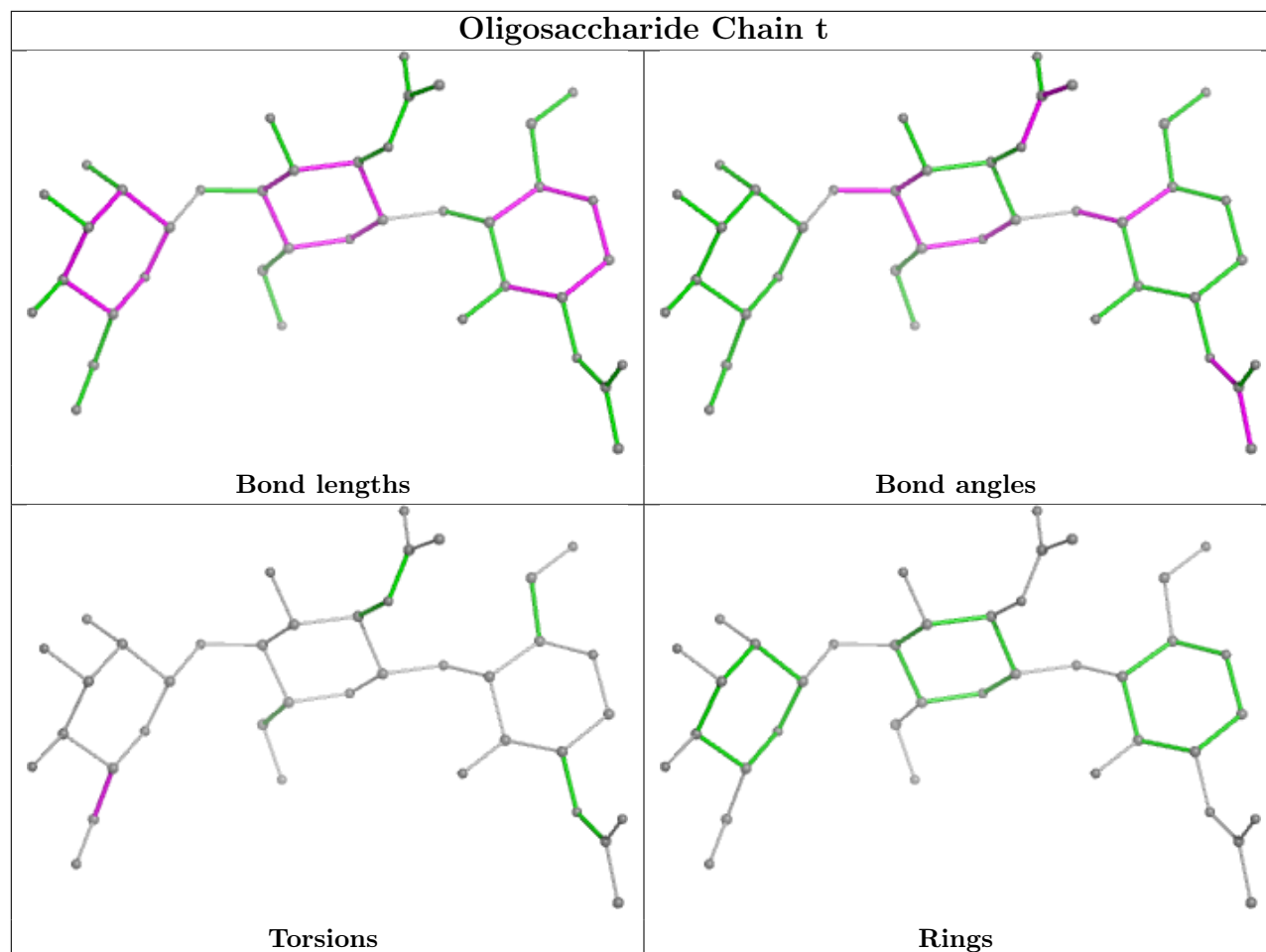




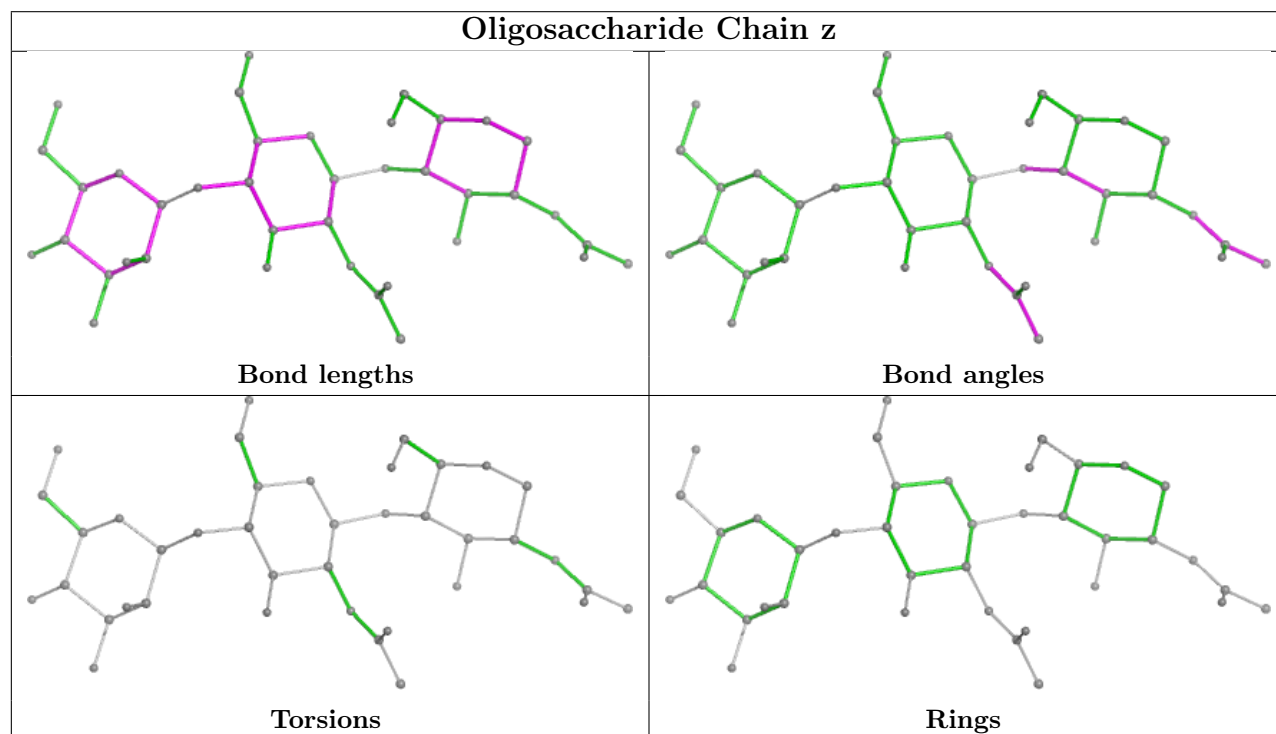
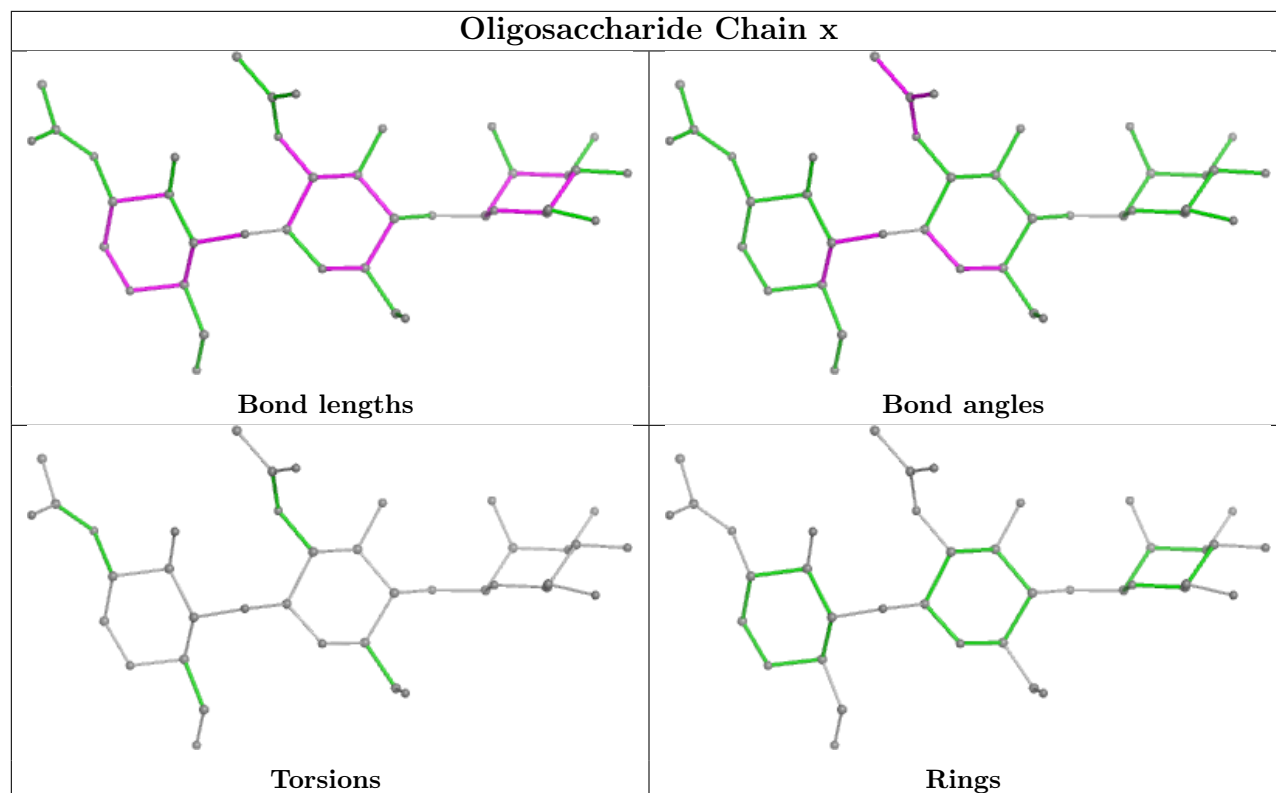


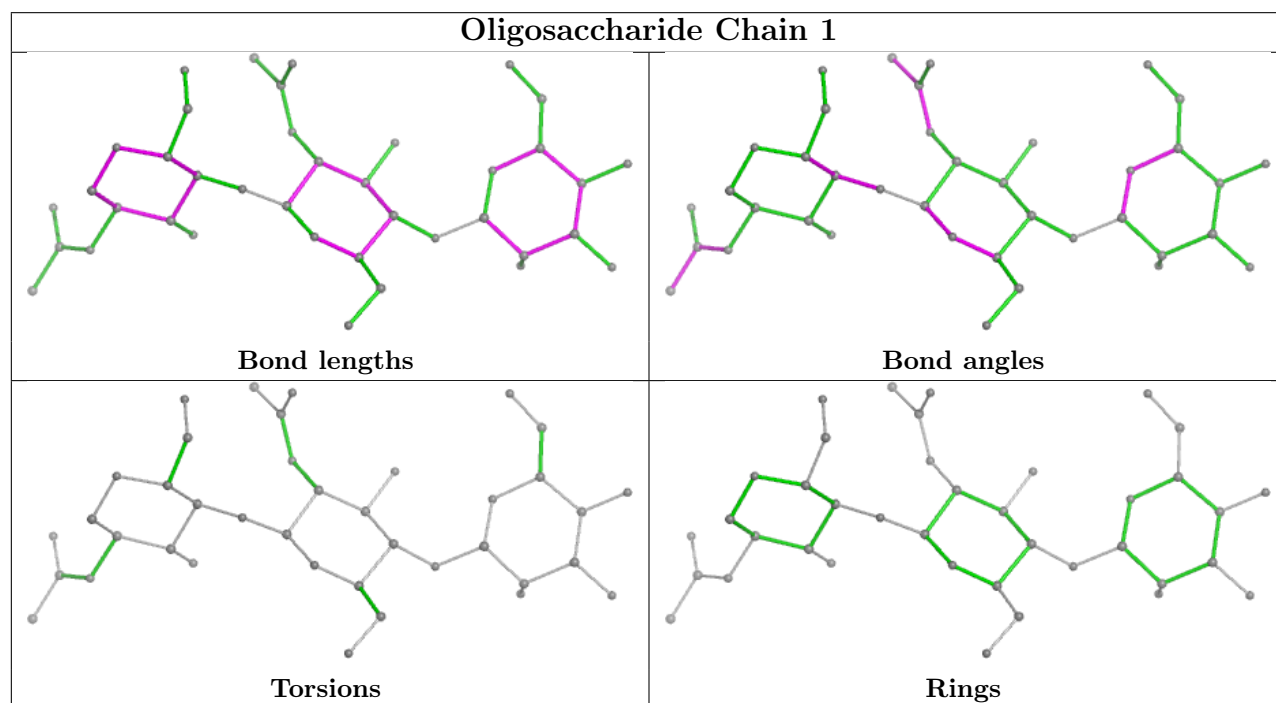
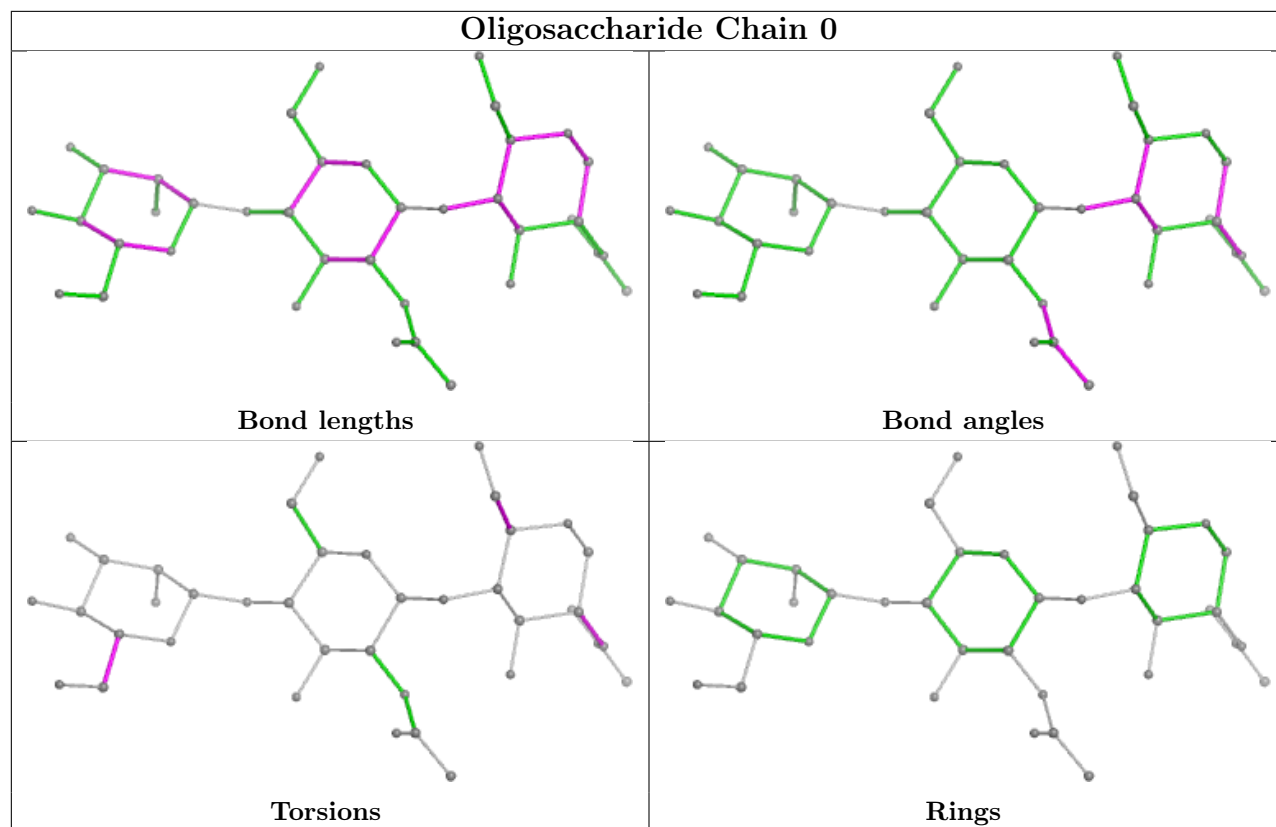




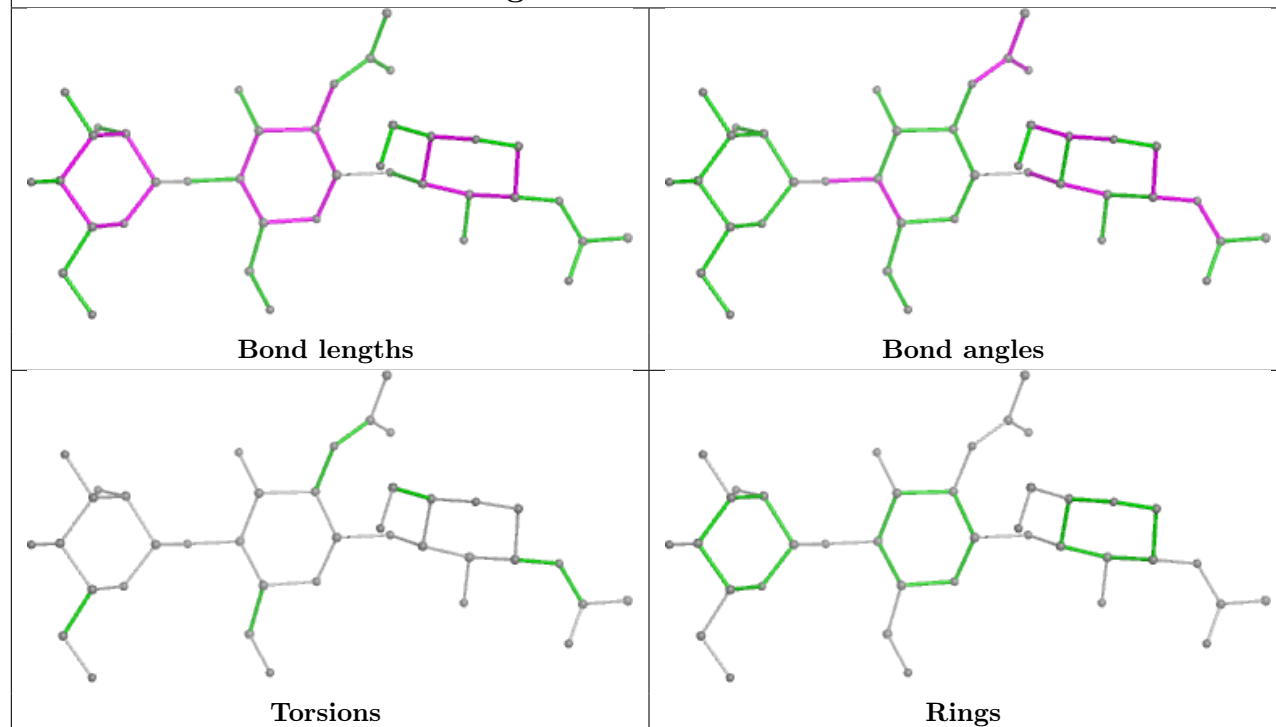




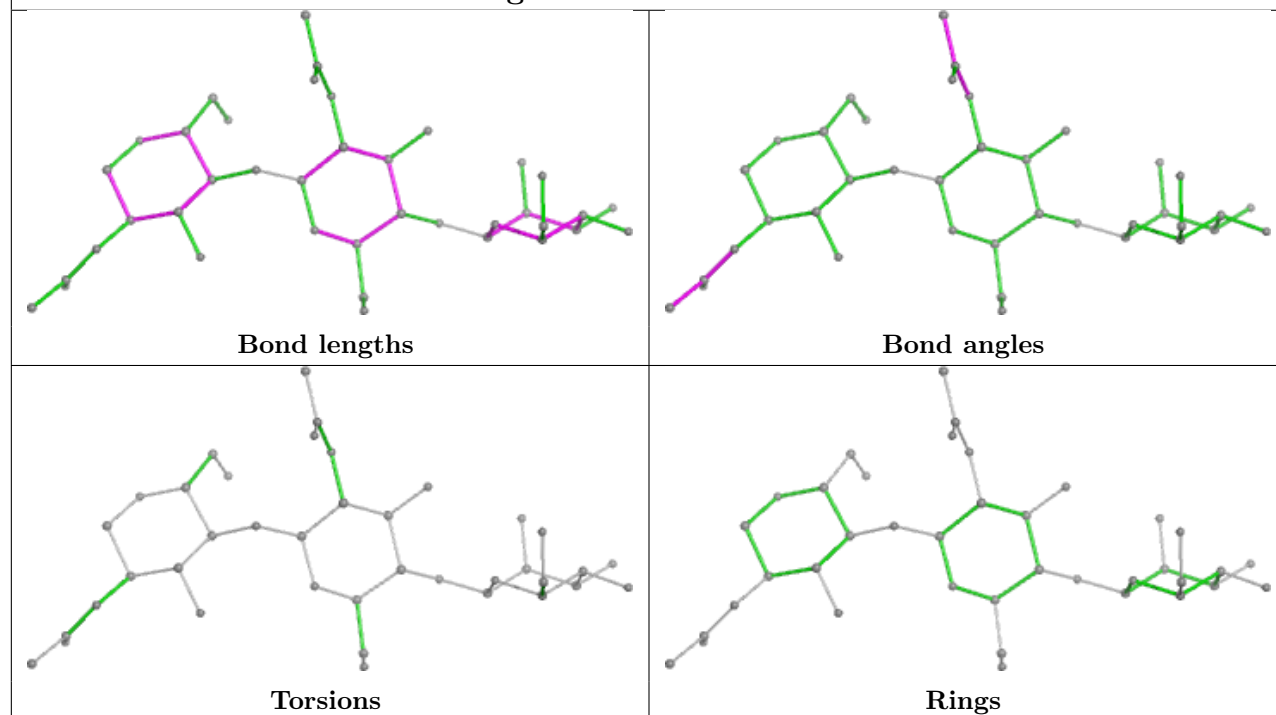




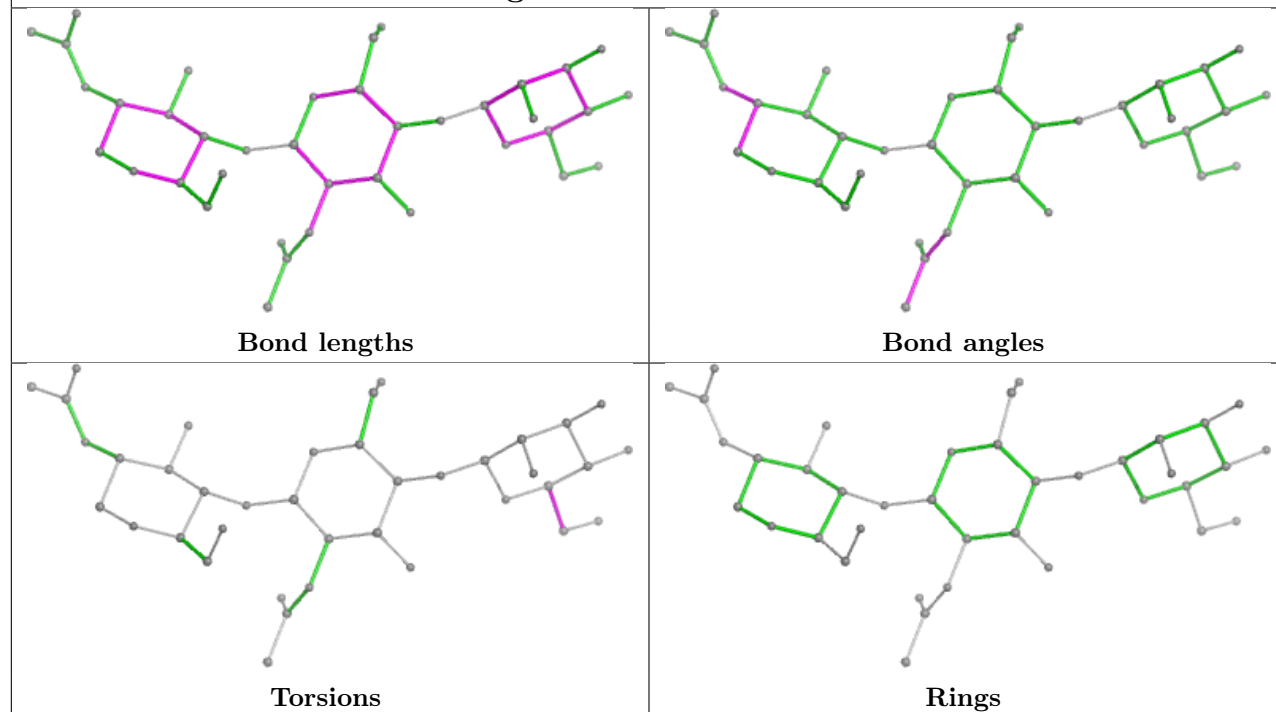
## Oligosaccharide Chain 3



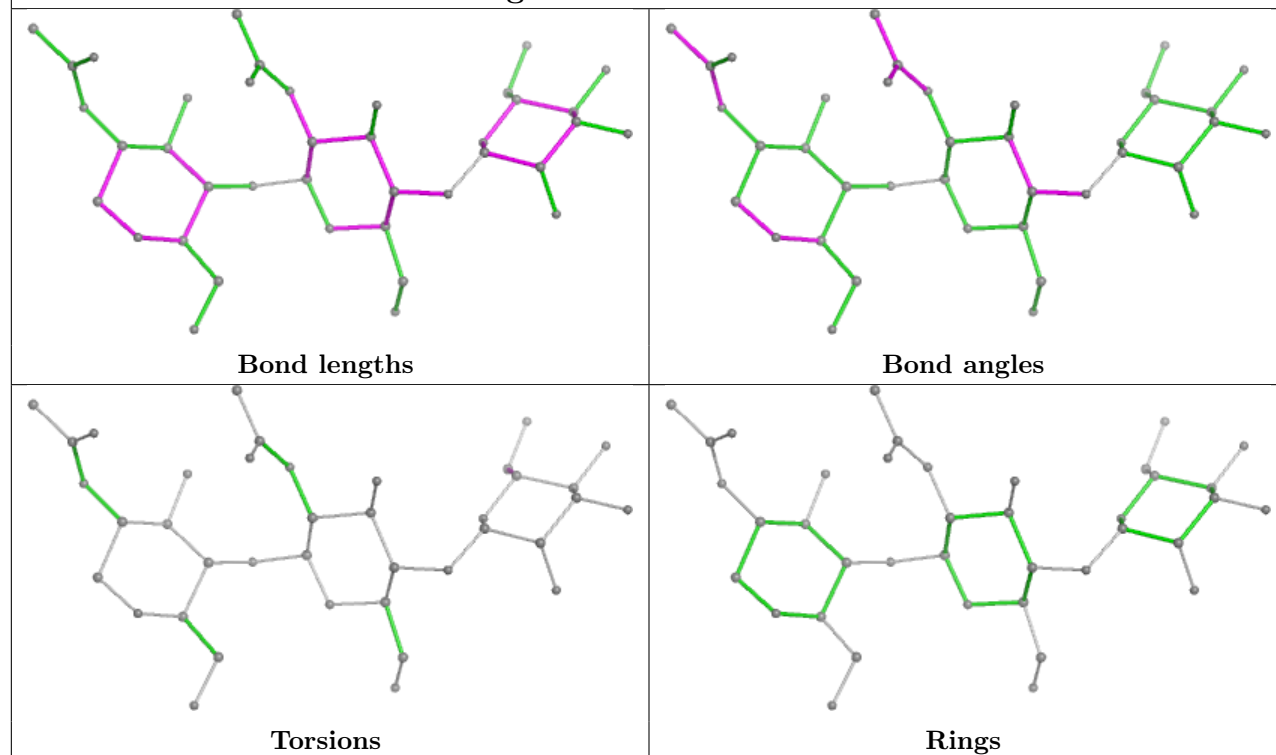
## Oligosaccharide Chain 4



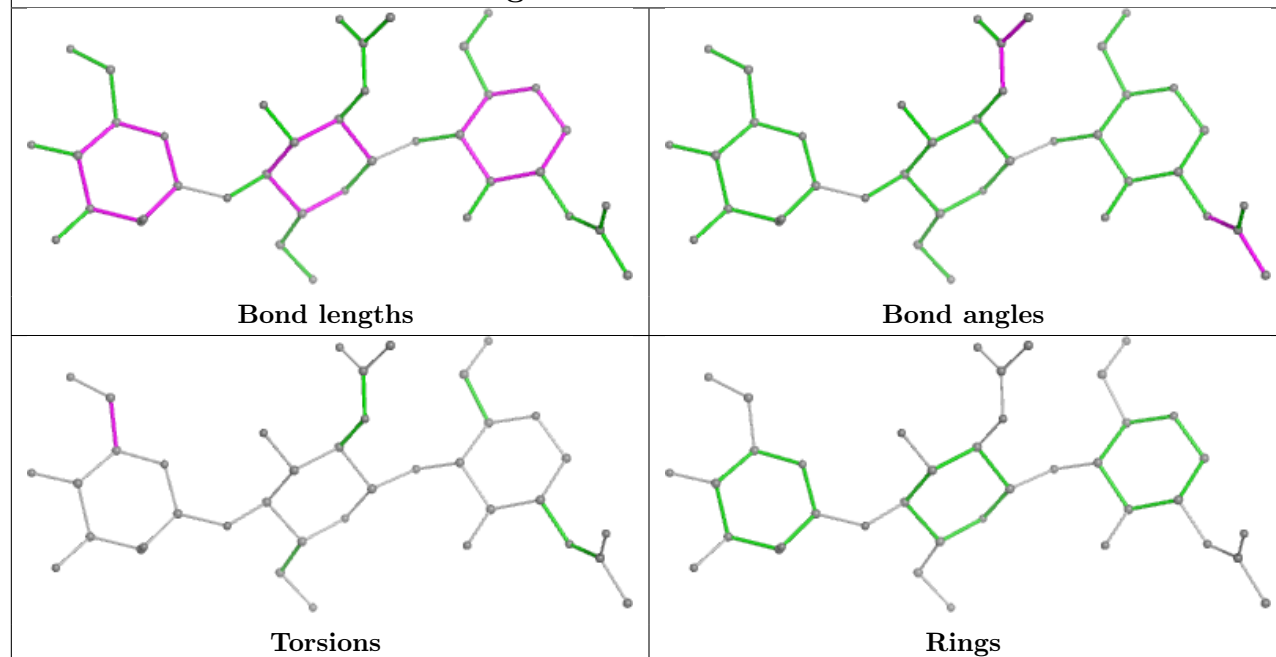
## Oligosaccharide Chain 5



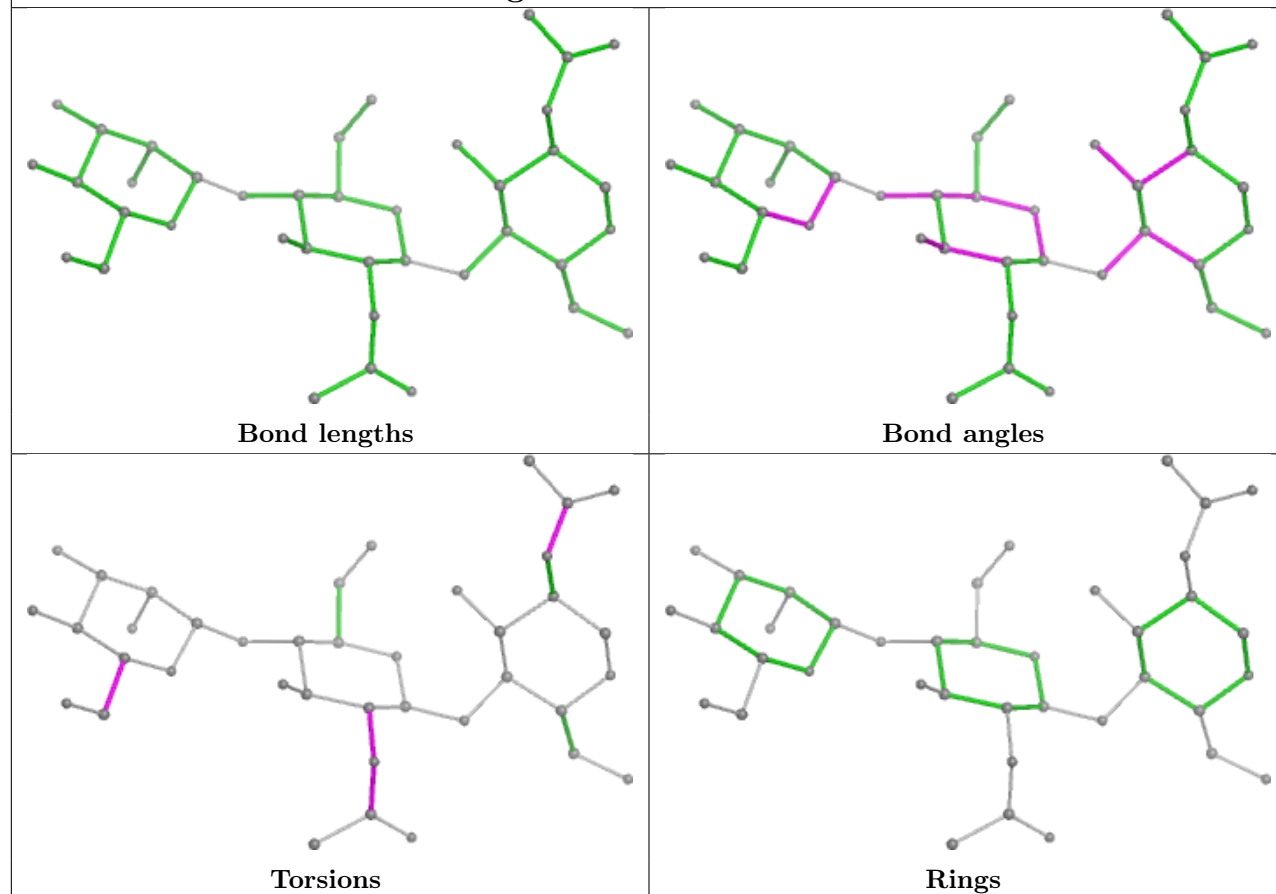
## Oligosaccharide Chain 6

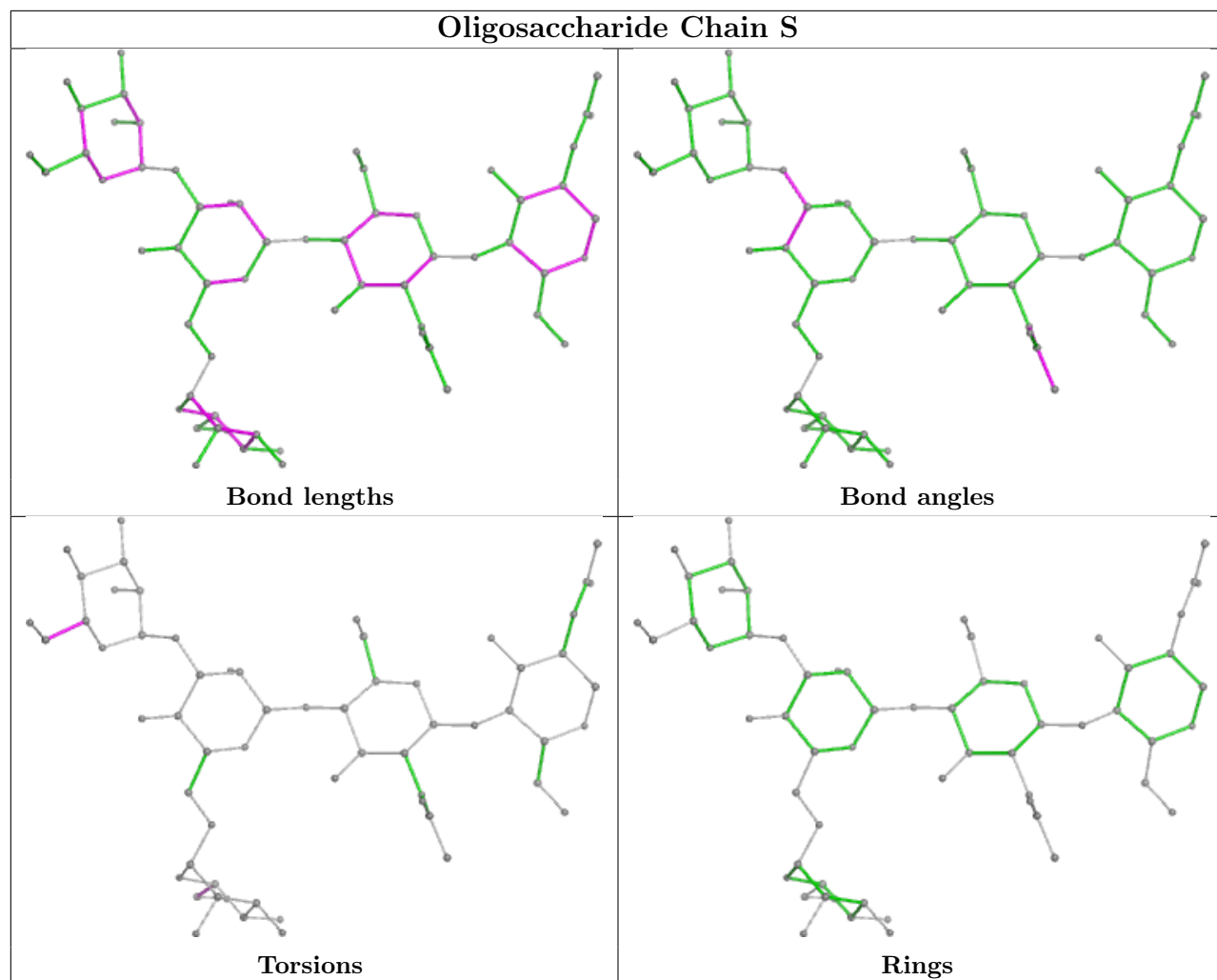


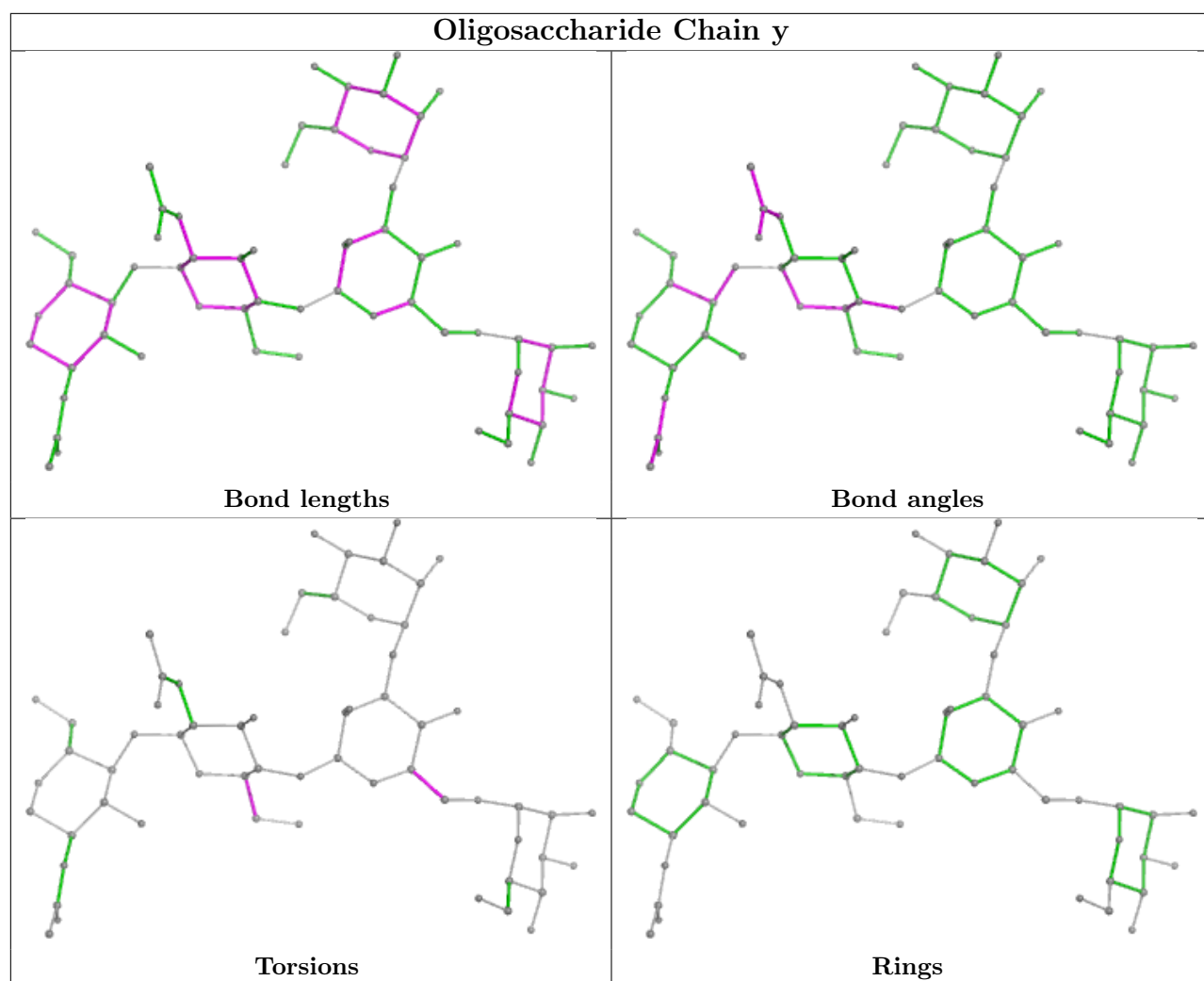
## Oligosaccharide Chain 7

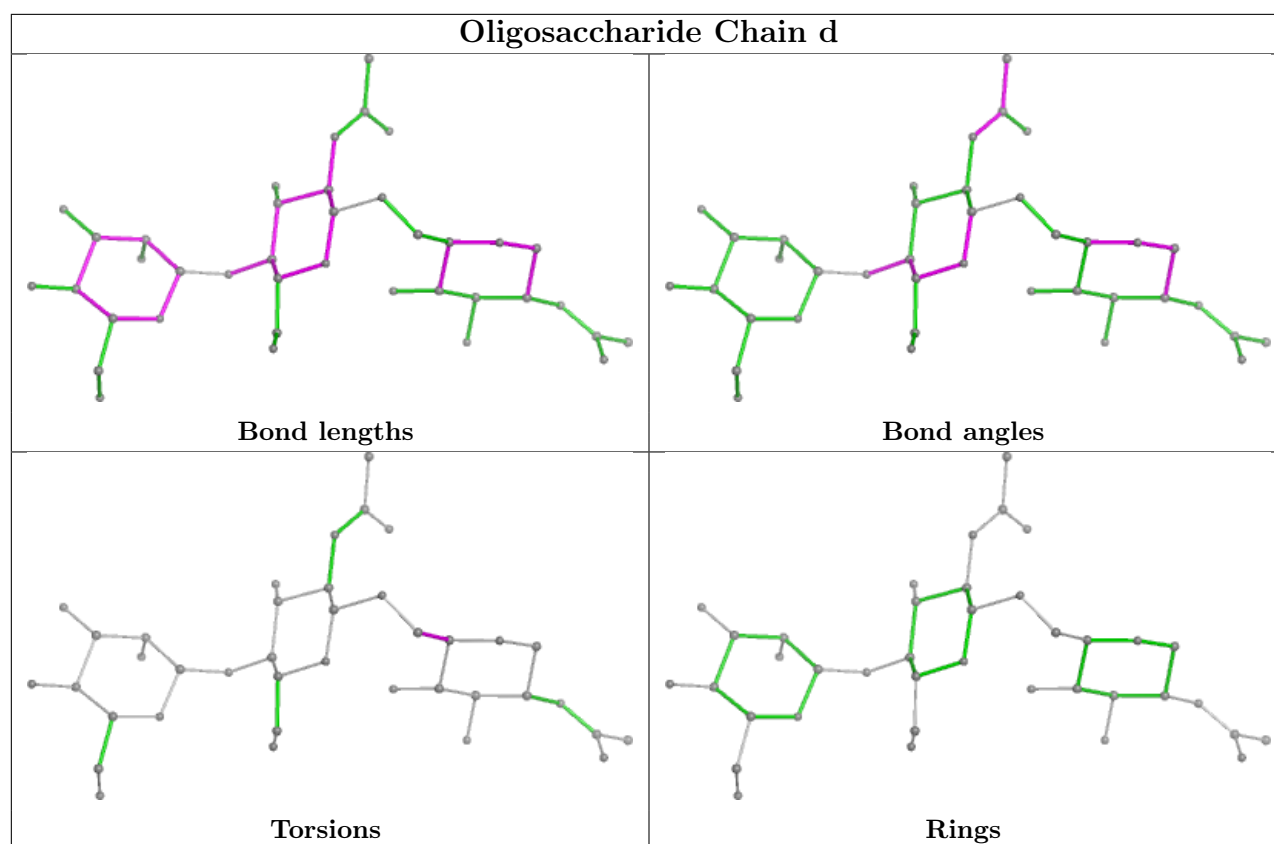


## Oligosaccharide Chain 8









## 5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
11	NAG	E	701	2	14,14,15	2.23	5 (35%)	17,19,21	0.87	1 (5%)
11	NAG	D	602	1	14,14,15	2.05	5 (35%)	17,19,21	0.96	0
11	NAG	B	703	2	14,14,15	2.25	5 (35%)	17,19,21	1.08	1 (5%)
11	NAG	A	602	1	14,14,15	2.10	5 (35%)	17,19,21	0.92	0
11	NAG	D	601	1	14,14,15	2.02	5 (35%)	17,19,21	1.06	1 (5%)
11	NAG	D	603	1	14,14,15	2.01	6 (42%)	17,19,21	1.02	1 (5%)
11	NAG	B	701	2	14,14,15	2.14	6 (42%)	17,19,21	0.94	0
11	NAG	A	604	1	14,14,15	2.21	7 (50%)	17,19,21	0.92	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	F	702	2	14,14,15	2.24	7 (50%)	17,19,21	1.10	2 (11%)
11	NAG	B	702	2	14,14,15	2.34	6 (42%)	17,19,21	1.48	5 (29%)
11	NAG	E	702	2	14,14,15	2.11	7 (50%)	17,19,21	1.05	1 (5%)
11	NAG	D	606	1	14,14,15	0.34	0	17,19,21	0.65	0
11	NAG	C	601	1	14,14,15	2.09	5 (35%)	17,19,21	0.90	0
11	NAG	A	605	1	14,14,15	2.39	6 (42%)	17,19,21	1.80	4 (23%)
11	NAG	D	605	1	14,14,15	2.10	5 (35%)	17,19,21	0.93	0
11	NAG	A	603	1	14,14,15	2.00	5 (35%)	17,19,21	1.02	2 (11%)
11	NAG	D	604	1	14,14,15	2.19	7 (50%)	17,19,21	1.18	2 (11%)
11	NAG	C	602	1	14,14,15	2.27	7 (50%)	17,19,21	1.27	3 (17%)
11	NAG	A	601	1	14,14,15	2.20	6 (42%)	17,19,21	1.34	4 (23%)
11	NAG	F	701	2	14,14,15	2.21	6 (42%)	17,19,21	0.91	0
11	NAG	C	603	1	14,14,15	1.96	6 (42%)	17,19,21	1.58	2 (11%)

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
11	NAG	E	701	2	-	0/6/23/26	0/1/1/1
11	NAG	D	602	1	-	0/6/23/26	0/1/1/1
11	NAG	B	703	2	-	0/6/23/26	0/1/1/1
11	NAG	A	602	1	-	1/6/23/26	0/1/1/1
11	NAG	D	601	1	-	0/6/23/26	0/1/1/1
11	NAG	D	603	1	-	0/6/23/26	0/1/1/1
11	NAG	B	701	2	-	0/6/23/26	0/1/1/1
11	NAG	A	604	1	-	1/6/23/26	0/1/1/1
11	NAG	F	702	2	-	0/6/23/26	0/1/1/1
11	NAG	B	702	2	-	0/6/23/26	0/1/1/1
11	NAG	E	702	2	-	0/6/23/26	0/1/1/1
11	NAG	D	606	1	-	2/6/23/26	0/1/1/1
11	NAG	C	601	1	-	1/6/23/26	0/1/1/1
11	NAG	A	605	1	-	1/6/23/26	0/1/1/1
11	NAG	D	605	1	-	0/6/23/26	0/1/1/1
11	NAG	A	603	1	-	0/6/23/26	0/1/1/1
11	NAG	D	604	1	-	2/6/23/26	0/1/1/1
11	NAG	C	602	1	-	1/6/23/26	0/1/1/1
11	NAG	A	601	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	F	701	2	-	0/6/23/26	0/1/1/1
11	NAG	C	603	1	-	1/6/23/26	0/1/1/1

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	605	NAG	C1-C2	6.22	1.61	1.52
11	B	703	NAG	C1-C2	6.09	1.61	1.52
11	C	602	NAG	C1-C2	5.65	1.60	1.52
11	F	702	NAG	C1-C2	5.65	1.60	1.52
11	F	701	NAG	C1-C2	5.62	1.60	1.52
11	D	605	NAG	C1-C2	5.57	1.60	1.52
11	E	701	NAG	C1-C2	5.57	1.60	1.52
11	A	601	NAG	C1-C2	5.51	1.60	1.52
11	C	601	NAG	C1-C2	5.31	1.60	1.52
11	B	701	NAG	C1-C2	5.24	1.60	1.52
11	A	602	NAG	C1-C2	5.23	1.60	1.52
11	D	602	NAG	C1-C2	5.20	1.60	1.52
11	B	702	NAG	C1-C2	5.17	1.60	1.52
11	A	604	NAG	C1-C2	5.07	1.59	1.52
11	D	603	NAG	C1-C2	4.83	1.59	1.52
11	D	601	NAG	C1-C2	4.83	1.59	1.52
11	E	702	NAG	C1-C2	4.82	1.59	1.52
11	D	604	NAG	C1-C2	4.78	1.59	1.52
11	A	603	NAG	C1-C2	4.54	1.59	1.52
11	B	702	NAG	O5-C5	4.01	1.51	1.43
11	C	603	NAG	C1-C2	3.89	1.58	1.52
11	C	603	NAG	O5-C5	3.50	1.50	1.43
11	D	604	NAG	O5-C5	3.46	1.50	1.43
11	A	604	NAG	O5-C5	3.33	1.50	1.43
11	B	701	NAG	O5-C5	3.28	1.50	1.43
11	A	601	NAG	O5-C5	3.28	1.50	1.43
11	D	601	NAG	O5-C5	3.28	1.50	1.43
11	E	702	NAG	O5-C5	3.28	1.50	1.43
11	C	602	NAG	O5-C5	3.26	1.50	1.43
11	D	603	NAG	O5-C5	3.24	1.50	1.43
11	A	605	NAG	C2-N2	3.20	1.51	1.46
11	E	701	NAG	O5-C5	3.16	1.49	1.43
11	A	603	NAG	O5-C5	3.14	1.49	1.43
11	A	602	NAG	O5-C5	3.13	1.49	1.43
11	B	702	NAG	O5-C1	3.08	1.48	1.43
11	D	605	NAG	O5-C5	3.05	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	701	NAG	O5-C5	3.03	1.49	1.43
11	B	703	NAG	O5-C5	3.02	1.49	1.43
11	F	702	NAG	C3-C2	3.02	1.58	1.52
11	C	601	NAG	O5-C5	3.01	1.49	1.43
11	B	702	NAG	C4-C5	2.99	1.59	1.53
11	A	604	NAG	O5-C1	2.96	1.48	1.43
11	A	605	NAG	O5-C1	2.93	1.48	1.43
11	D	602	NAG	O5-C5	2.93	1.49	1.43
11	A	605	NAG	O5-C5	2.87	1.49	1.43
11	F	701	NAG	O5-C1	2.79	1.48	1.43
11	E	702	NAG	O5-C1	2.78	1.48	1.43
11	C	603	NAG	C3-C2	2.76	1.58	1.52
11	C	601	NAG	O5-C1	2.76	1.48	1.43
11	E	701	NAG	C3-C2	2.75	1.58	1.52
11	E	701	NAG	O5-C1	2.75	1.48	1.43
11	A	602	NAG	O5-C1	2.74	1.48	1.43
11	B	703	NAG	O5-C1	2.73	1.48	1.43
11	F	702	NAG	O5-C5	2.73	1.49	1.43
11	D	604	NAG	O5-C1	2.71	1.48	1.43
11	A	603	NAG	O5-C1	2.70	1.48	1.43
11	B	701	NAG	O5-C1	2.68	1.48	1.43
11	C	602	NAG	O5-C1	2.64	1.47	1.43
11	D	602	NAG	O5-C1	2.64	1.47	1.43
11	D	604	NAG	C3-C2	2.64	1.58	1.52
11	F	702	NAG	O5-C1	2.60	1.47	1.43
11	D	604	NAG	C4-C5	2.59	1.58	1.53
11	A	601	NAG	C4-C5	2.59	1.58	1.53
11	A	601	NAG	O5-C1	2.52	1.47	1.43
11	C	602	NAG	C2-N2	2.51	1.50	1.46
11	A	601	NAG	C3-C2	2.43	1.57	1.52
11	F	701	NAG	C3-C2	2.41	1.57	1.52
11	E	702	NAG	C4-C5	2.39	1.58	1.53
11	A	604	NAG	C2-N2	2.39	1.50	1.46
11	D	603	NAG	C4-C5	2.39	1.58	1.53
11	A	604	NAG	C3-C2	2.35	1.57	1.52
11	A	604	NAG	C4-C5	2.34	1.58	1.53
11	D	605	NAG	O5-C1	2.34	1.47	1.43
11	C	603	NAG	C2-N2	2.34	1.50	1.46
11	A	602	NAG	C3-C2	2.32	1.57	1.52
11	C	602	NAG	C4-C5	2.32	1.57	1.53
11	D	601	NAG	C4-C5	2.32	1.57	1.53
11	B	702	NAG	C4-C3	2.32	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	603	NAG	C4-C5	2.31	1.57	1.53
11	D	602	NAG	C3-C2	2.31	1.57	1.52
11	D	604	NAG	C4-C3	2.30	1.58	1.52
11	B	701	NAG	C3-C2	2.29	1.57	1.52
11	C	601	NAG	C3-C2	2.29	1.57	1.52
11	D	603	NAG	C3-C2	2.28	1.57	1.52
11	B	701	NAG	C4-C5	2.27	1.57	1.53
11	D	604	NAG	C2-N2	2.25	1.50	1.46
11	F	701	NAG	C4-C5	2.25	1.57	1.53
11	C	602	NAG	C3-C2	2.24	1.57	1.52
11	F	702	NAG	C2-N2	2.24	1.50	1.46
11	C	602	NAG	C4-C3	2.21	1.58	1.52
11	E	702	NAG	C4-C3	2.20	1.57	1.52
11	D	603	NAG	O5-C1	2.19	1.47	1.43
11	D	605	NAG	C3-C2	2.18	1.57	1.52
11	D	601	NAG	C3-C2	2.18	1.57	1.52
11	D	601	NAG	O5-C1	2.18	1.47	1.43
11	E	702	NAG	C3-C2	2.16	1.57	1.52
11	B	703	NAG	C3-C2	2.16	1.57	1.52
11	E	702	NAG	C2-N2	2.14	1.50	1.46
11	C	603	NAG	C4-C5	2.13	1.57	1.53
11	B	701	NAG	C4-C3	2.11	1.57	1.52
11	A	605	NAG	C3-C2	2.11	1.57	1.52
11	D	605	NAG	C4-C5	2.10	1.57	1.53
11	A	602	NAG	C4-C5	2.10	1.57	1.53
11	A	605	NAG	C4-C5	2.10	1.57	1.53
11	C	603	NAG	O5-C1	2.09	1.47	1.43
11	C	601	NAG	C4-C5	2.08	1.57	1.53
11	B	703	NAG	C4-C5	2.07	1.57	1.53
11	A	604	NAG	C4-C3	2.06	1.57	1.52
11	E	701	NAG	C4-C5	2.06	1.57	1.53
11	A	601	NAG	C4-C3	2.06	1.57	1.52
11	F	701	NAG	C4-C3	2.05	1.57	1.52
11	F	702	NAG	C4-C5	2.04	1.57	1.53
11	D	603	NAG	C4-C3	2.04	1.57	1.52
11	A	603	NAG	C2-N2	2.03	1.49	1.46
11	B	702	NAG	C3-C2	2.03	1.56	1.52
11	F	702	NAG	C4-C3	2.02	1.57	1.52
11	D	602	NAG	C4-C5	2.00	1.57	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	603	NAG	C2-N2-C7	4.59	129.44	122.90
11	A	605	NAG	C2-N2-C7	4.50	129.31	122.90
11	A	605	NAG	C1-C2-N2	3.87	117.09	110.49
11	B	702	NAG	O7-C7-C8	-3.05	116.39	122.06
11	B	702	NAG	C8-C7-N2	3.03	121.23	116.10
11	D	604	NAG	C2-N2-C7	2.81	126.90	122.90
11	C	602	NAG	C8-C7-N2	2.78	120.81	116.10
11	A	605	NAG	O7-C7-C8	-2.77	116.91	122.06
11	E	702	NAG	C8-C7-N2	2.65	120.59	116.10
11	B	703	NAG	C8-C7-N2	2.64	120.56	116.10
11	D	601	NAG	C8-C7-N2	2.59	120.48	116.10
11	A	605	NAG	C8-C7-N2	2.52	120.36	116.10
11	F	702	NAG	C8-C7-N2	2.51	120.35	116.10
11	C	602	NAG	O7-C7-C8	-2.38	117.63	122.06
11	B	702	NAG	C4-C3-C2	-2.35	107.57	111.02
11	A	603	NAG	C8-C7-N2	2.34	120.06	116.10
11	B	702	NAG	O3-C3-C4	2.33	115.74	110.35
11	A	603	NAG	C1-C2-N2	-2.32	106.52	110.49
11	A	601	NAG	O5-C1-C2	-2.32	107.63	111.29
11	F	702	NAG	C1-O5-C5	2.31	115.32	112.19
11	A	601	NAG	O5-C5-C6	-2.28	103.63	107.20
11	C	602	NAG	C2-N2-C7	2.25	126.11	122.90
11	E	701	NAG	C8-C7-N2	2.22	119.86	116.10
11	A	601	NAG	C4-C3-C2	-2.18	107.82	111.02
11	D	604	NAG	C8-C7-N2	2.16	119.76	116.10
11	A	601	NAG	C2-N2-C7	2.16	125.97	122.90
11	C	603	NAG	O7-C7-C8	-2.10	118.16	122.06
11	D	603	NAG	C8-C7-N2	2.06	119.59	116.10
11	B	702	NAG	O5-C1-C2	-2.02	108.10	111.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	605	NAG	C1-C2-N2-C7
11	C	603	NAG	C3-C2-N2-C7
11	D	606	NAG	C8-C7-N2-C2
11	D	606	NAG	O7-C7-N2-C2
11	C	601	NAG	O5-C5-C6-O6
11	A	604	NAG	O5-C5-C6-O6
11	D	604	NAG	O5-C5-C6-O6
11	A	602	NAG	O5-C5-C6-O6
11	A	601	NAG	O5-C5-C6-O6

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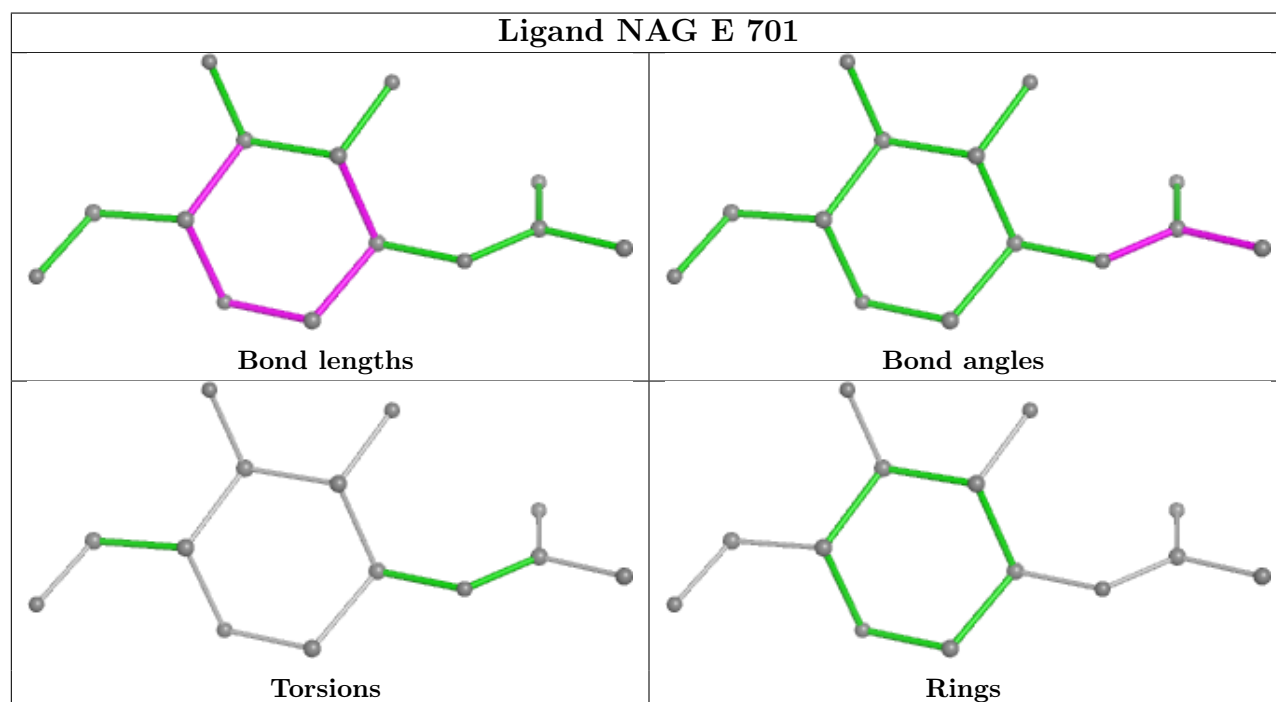
Mol	Chain	Res	Type	Atoms
11	C	602	NAG	C1-C2-N2-C7
11	D	604	NAG	C3-C2-N2-C7
11	A	601	NAG	C3-C2-N2-C7

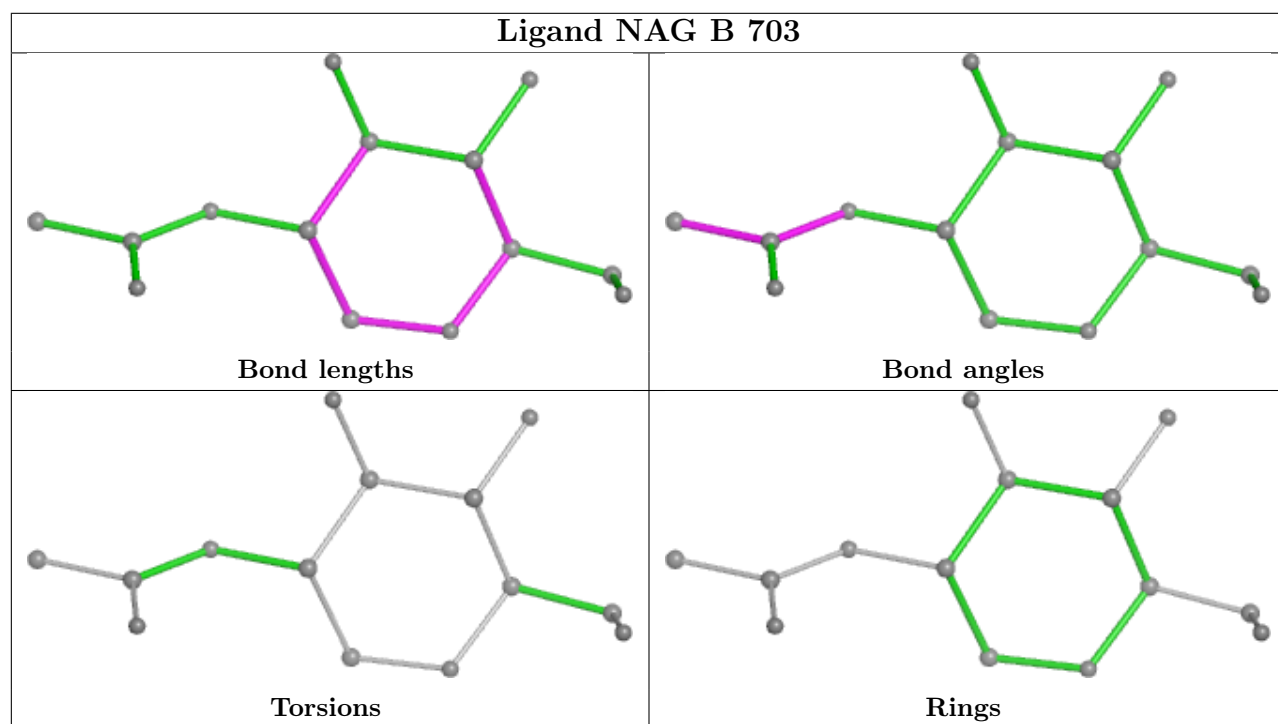
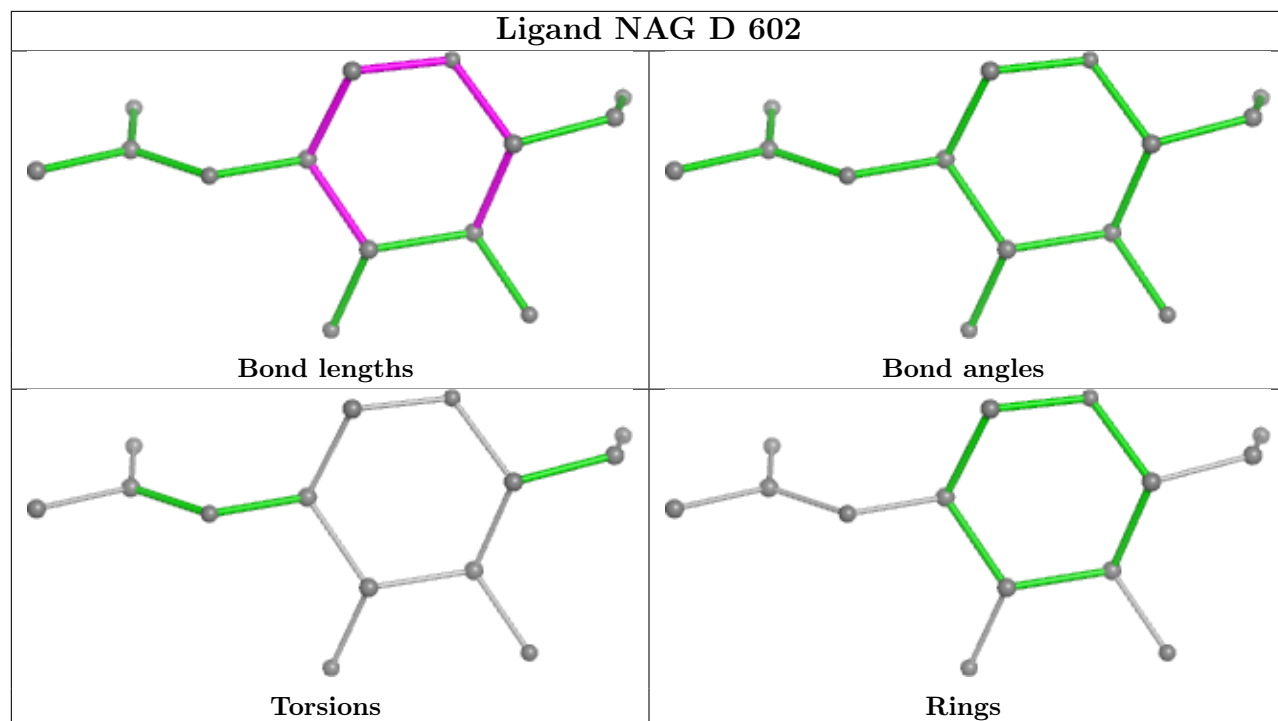
There are no ring outliers.

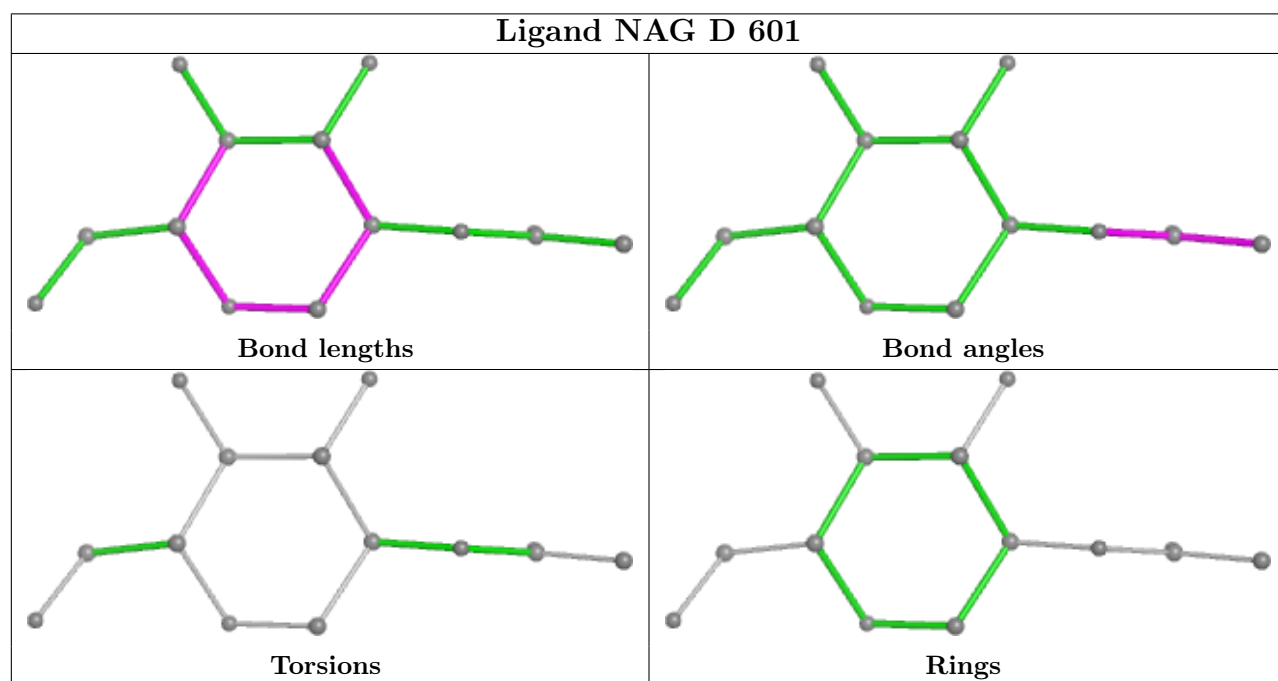
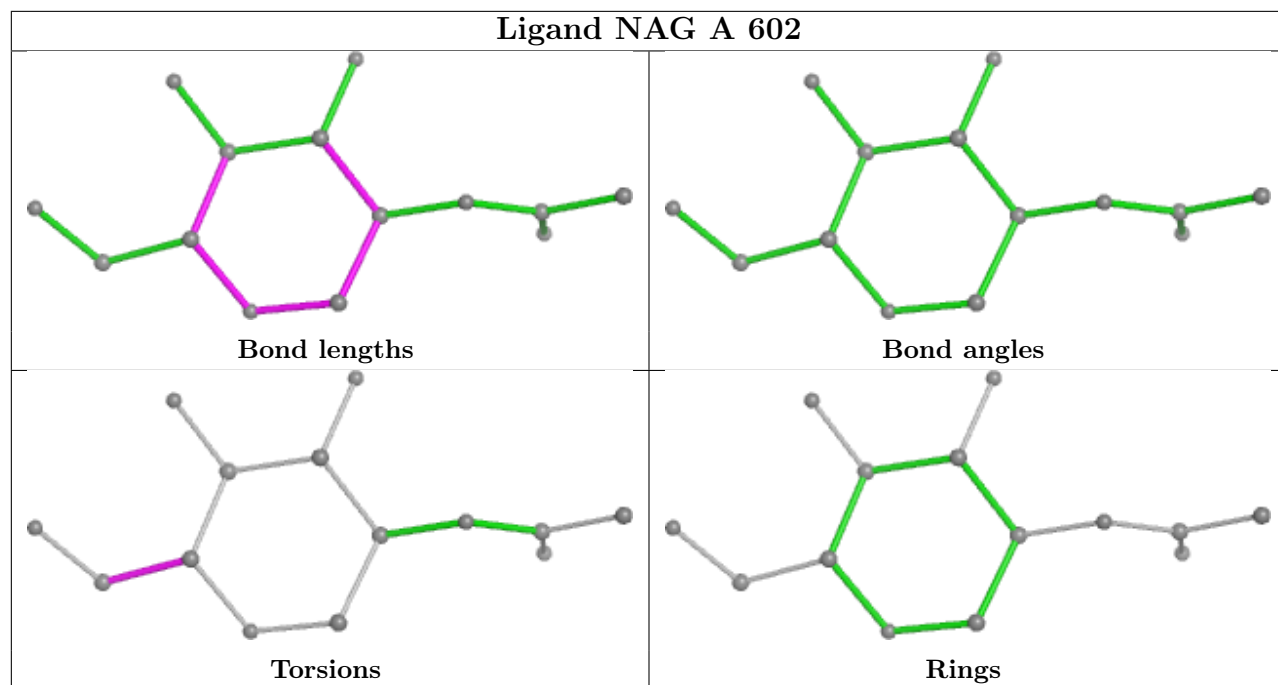
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	701	NAG	1	0
11	B	702	NAG	1	0

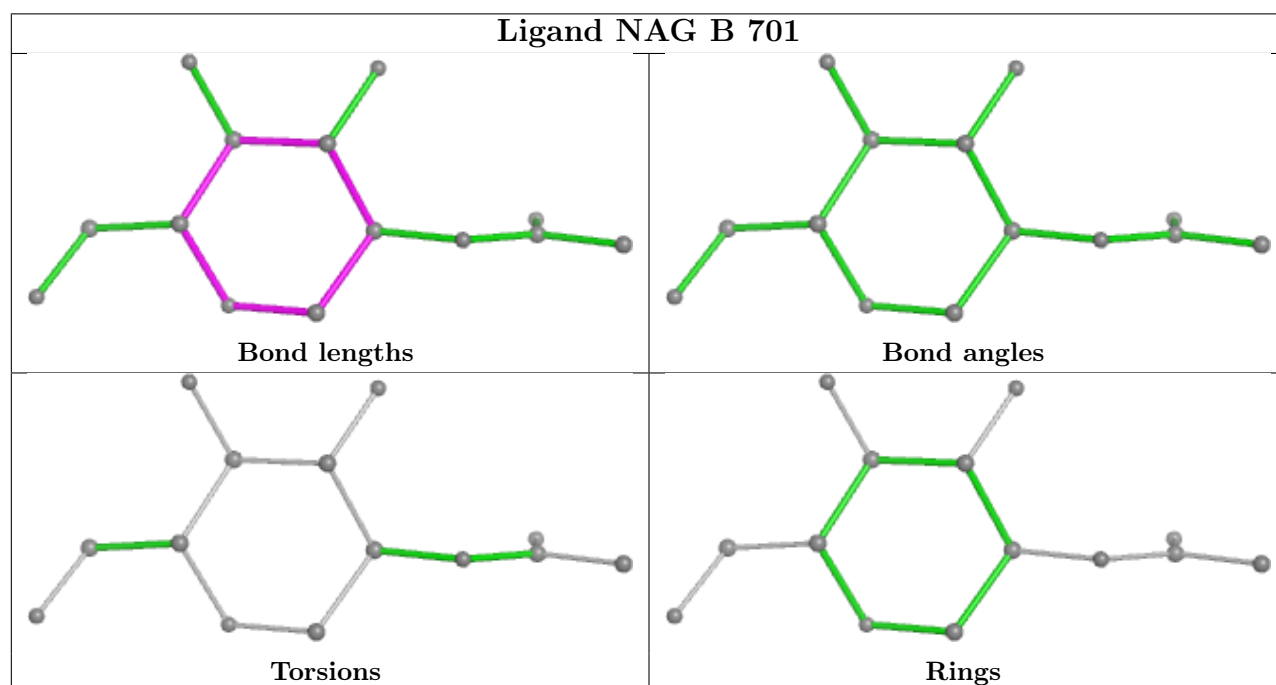
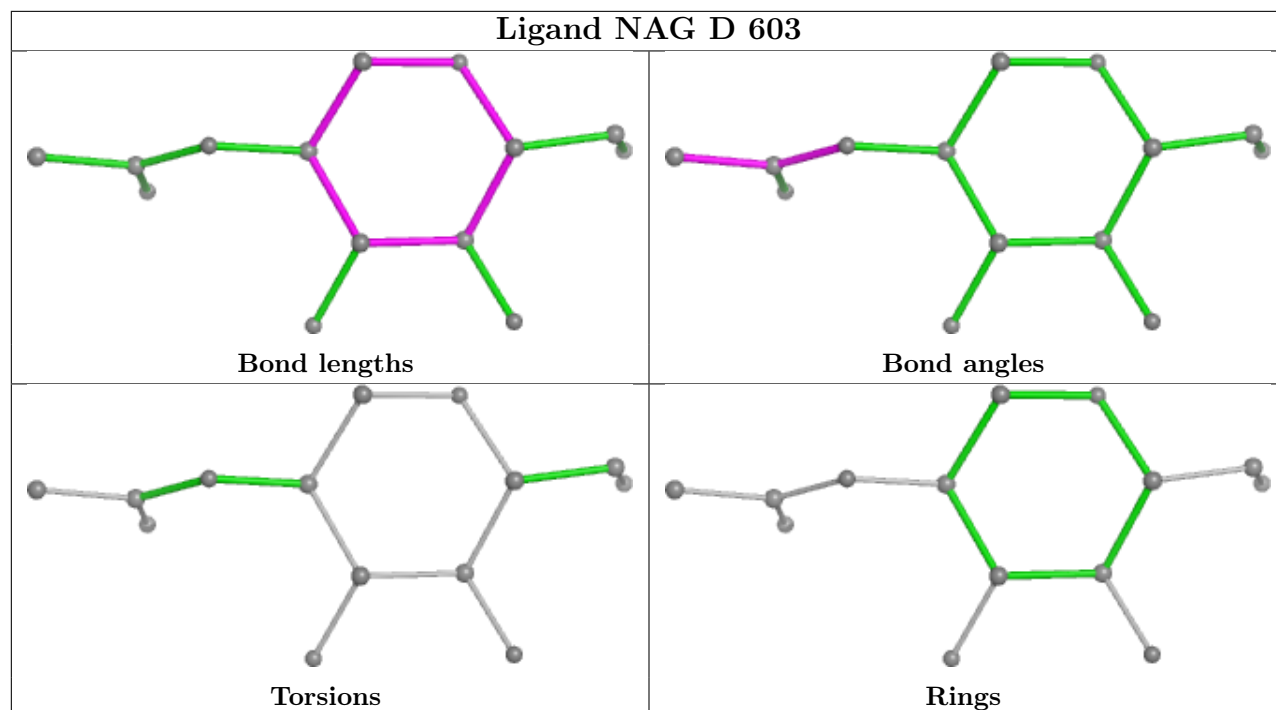
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

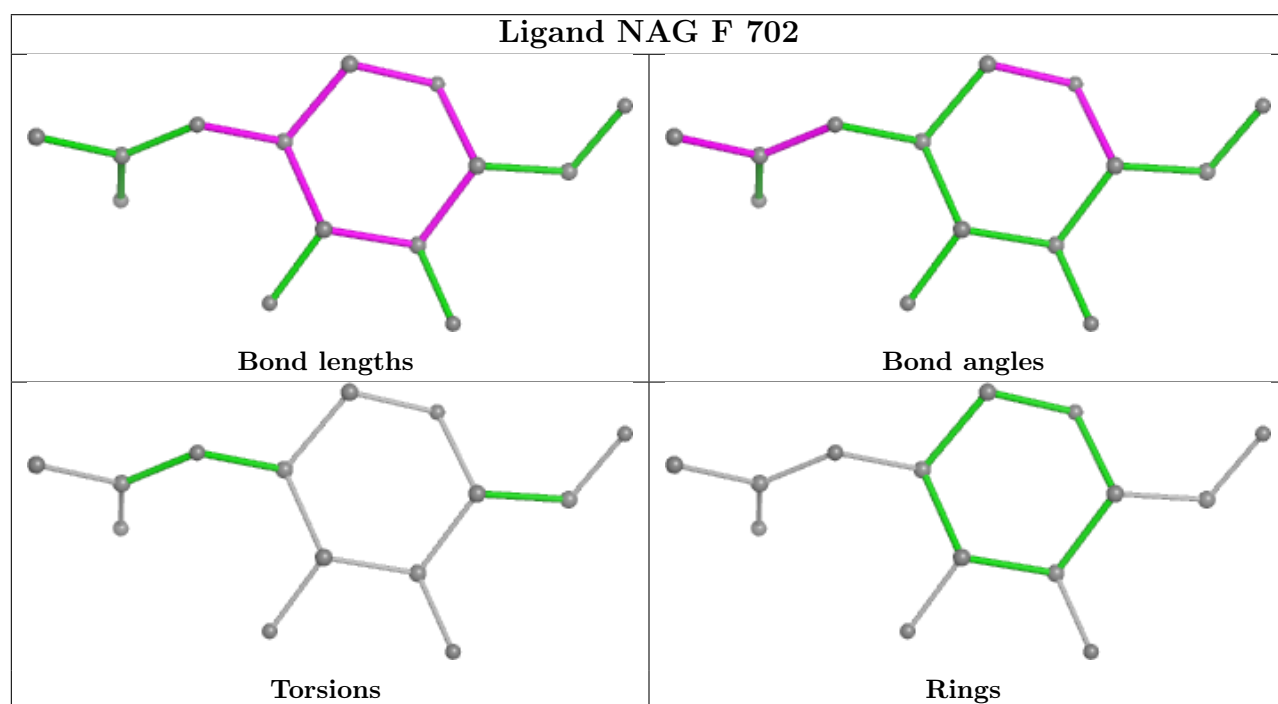
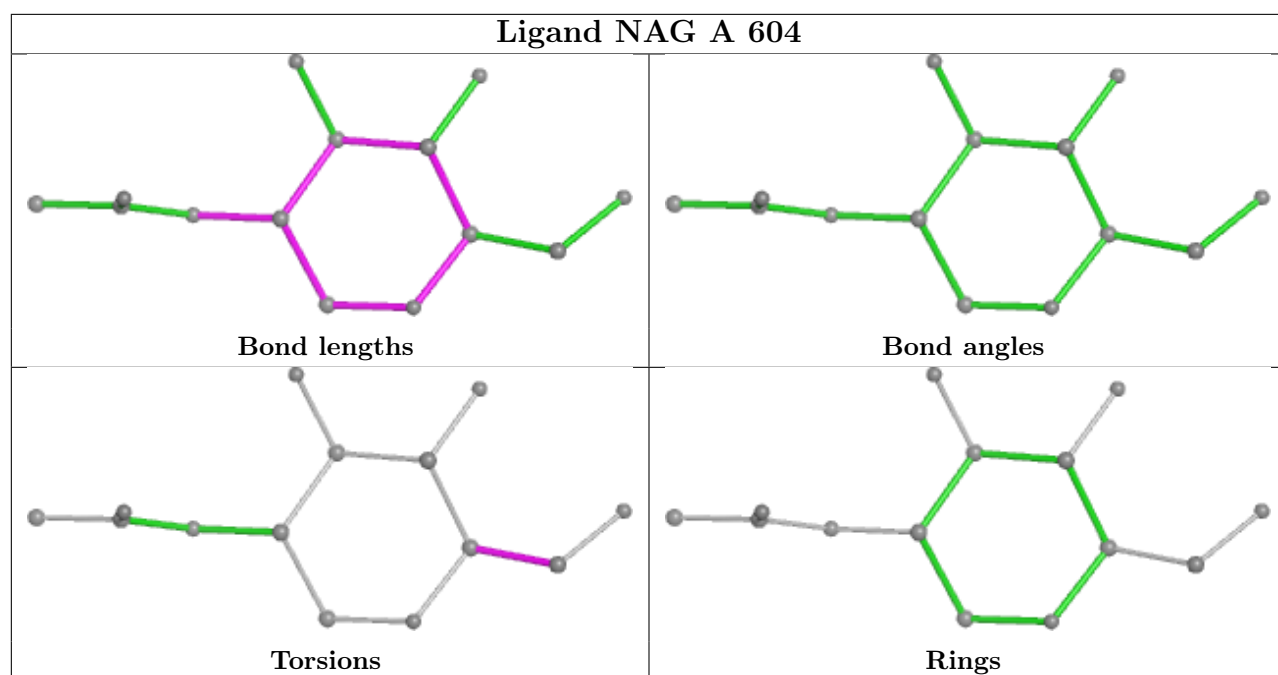


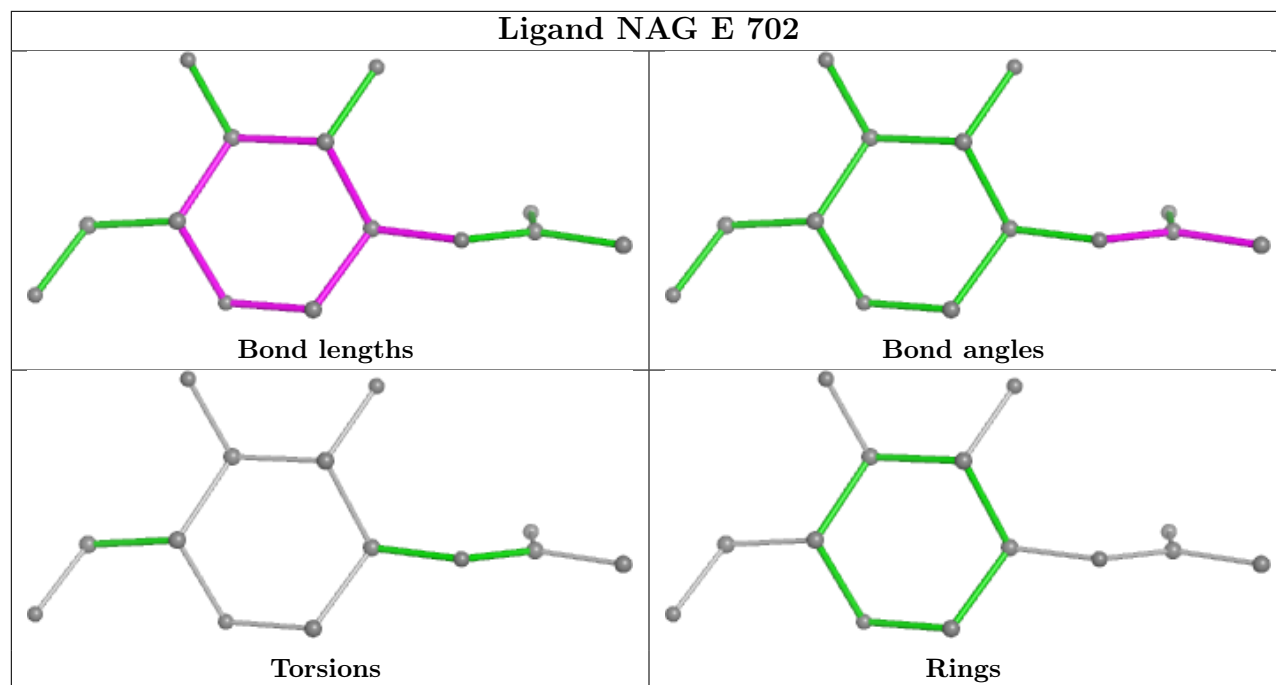
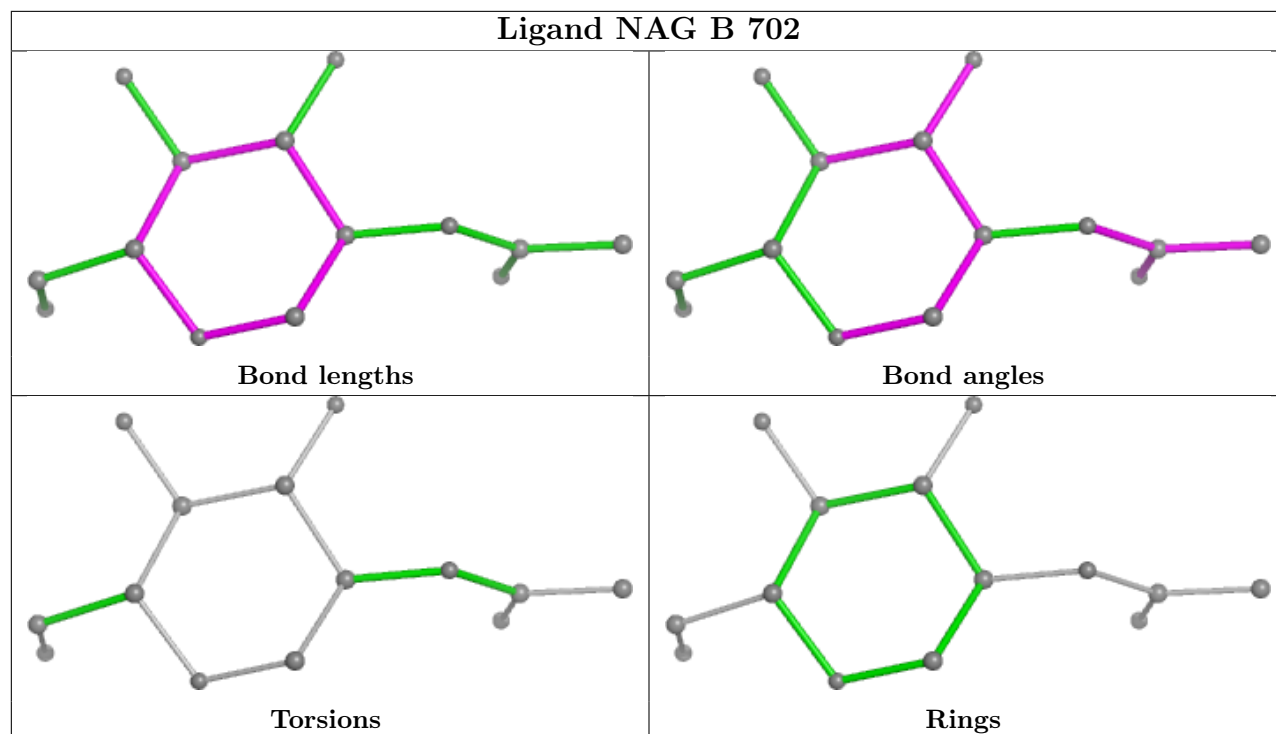


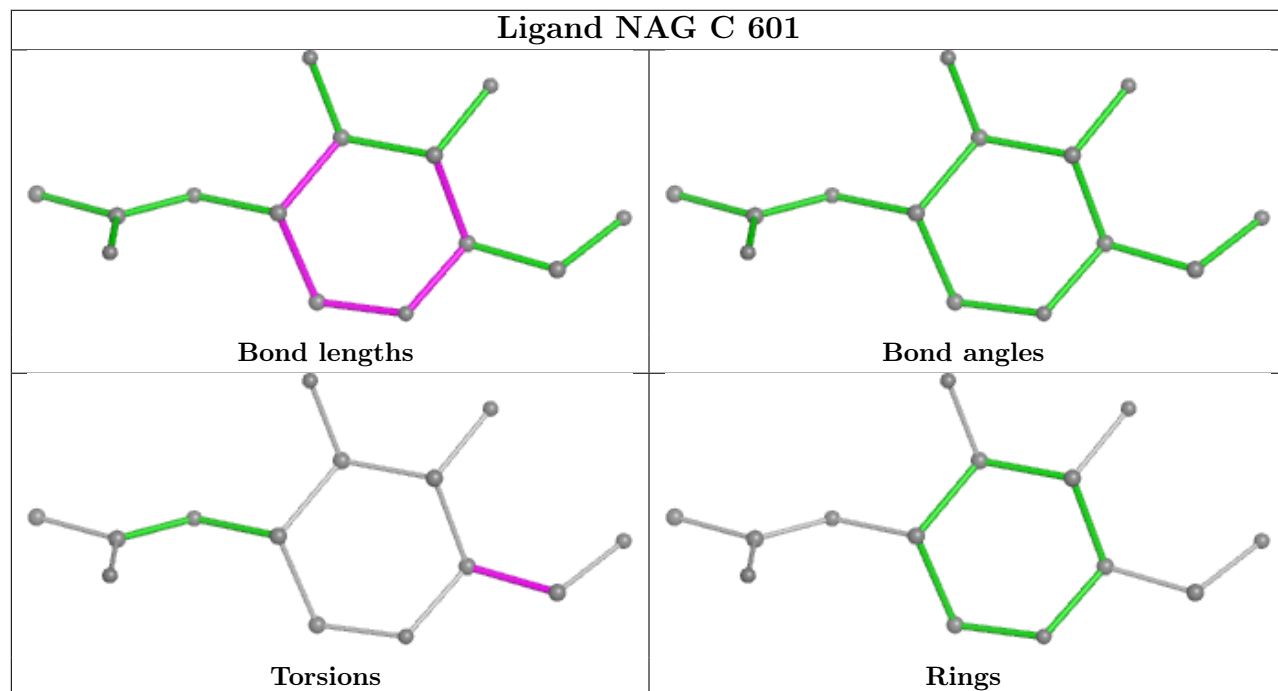
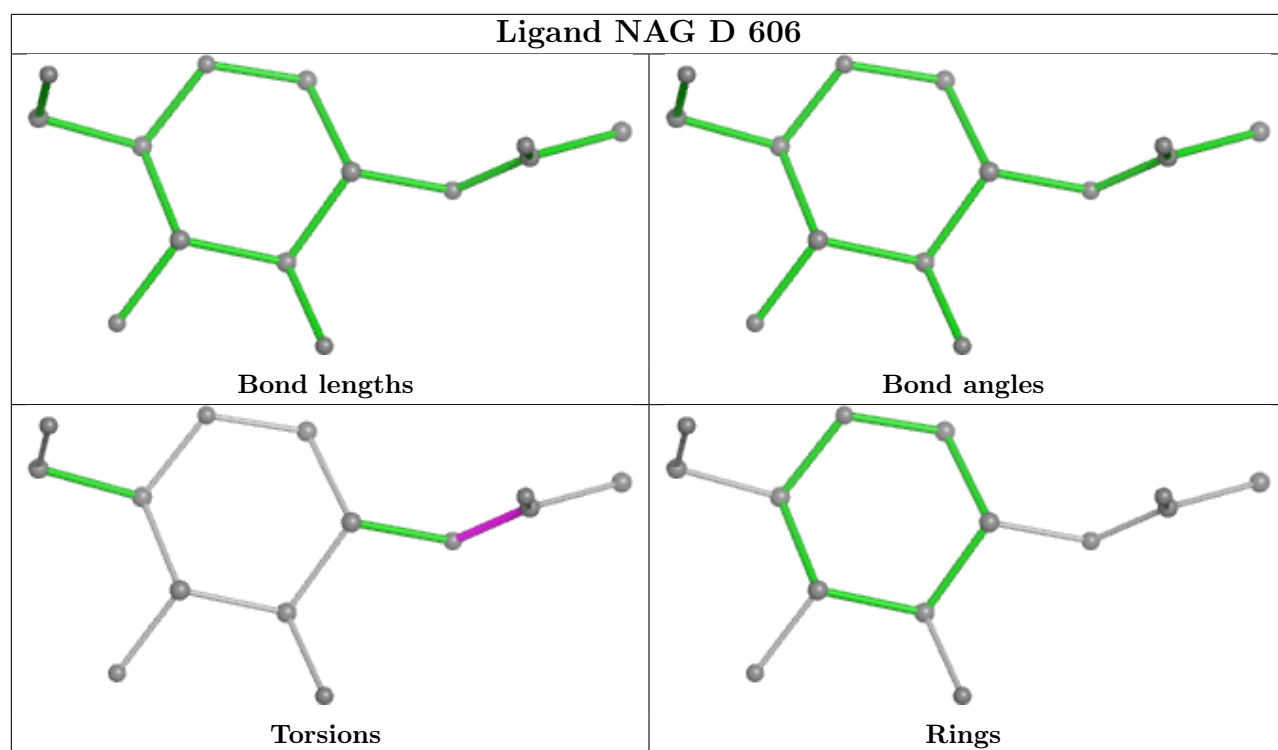


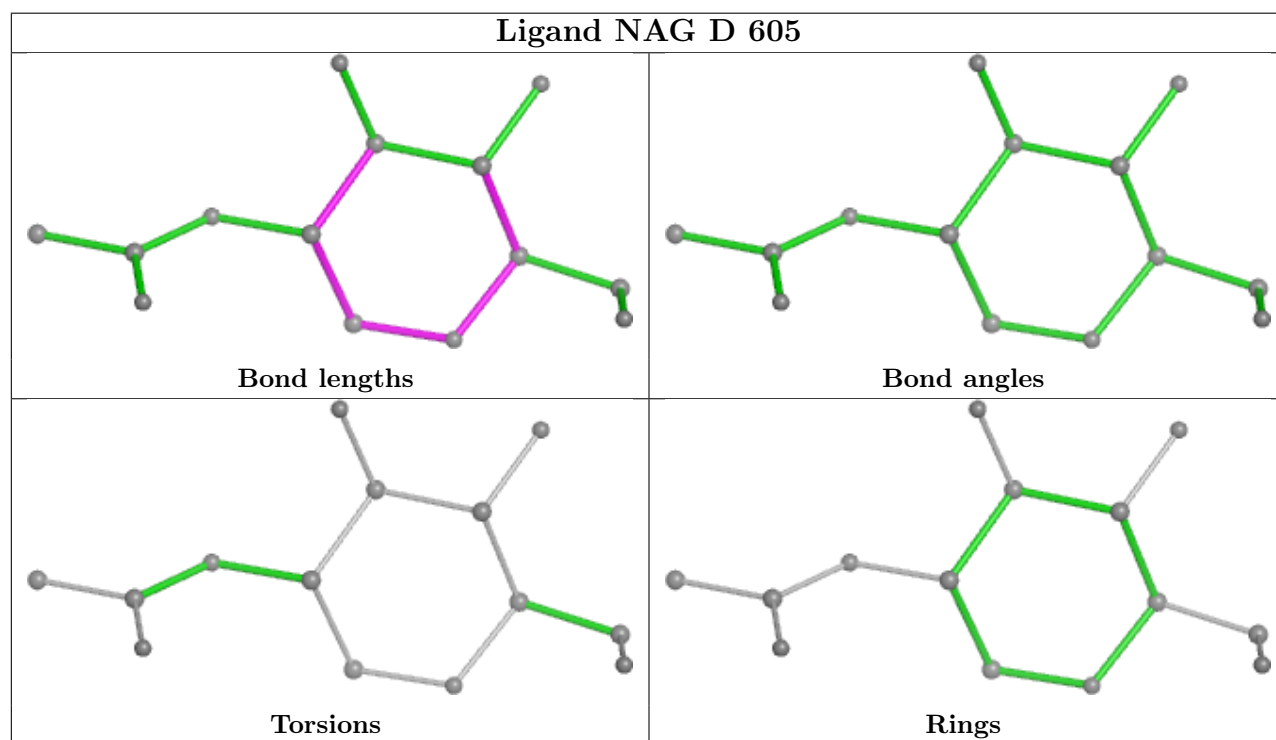
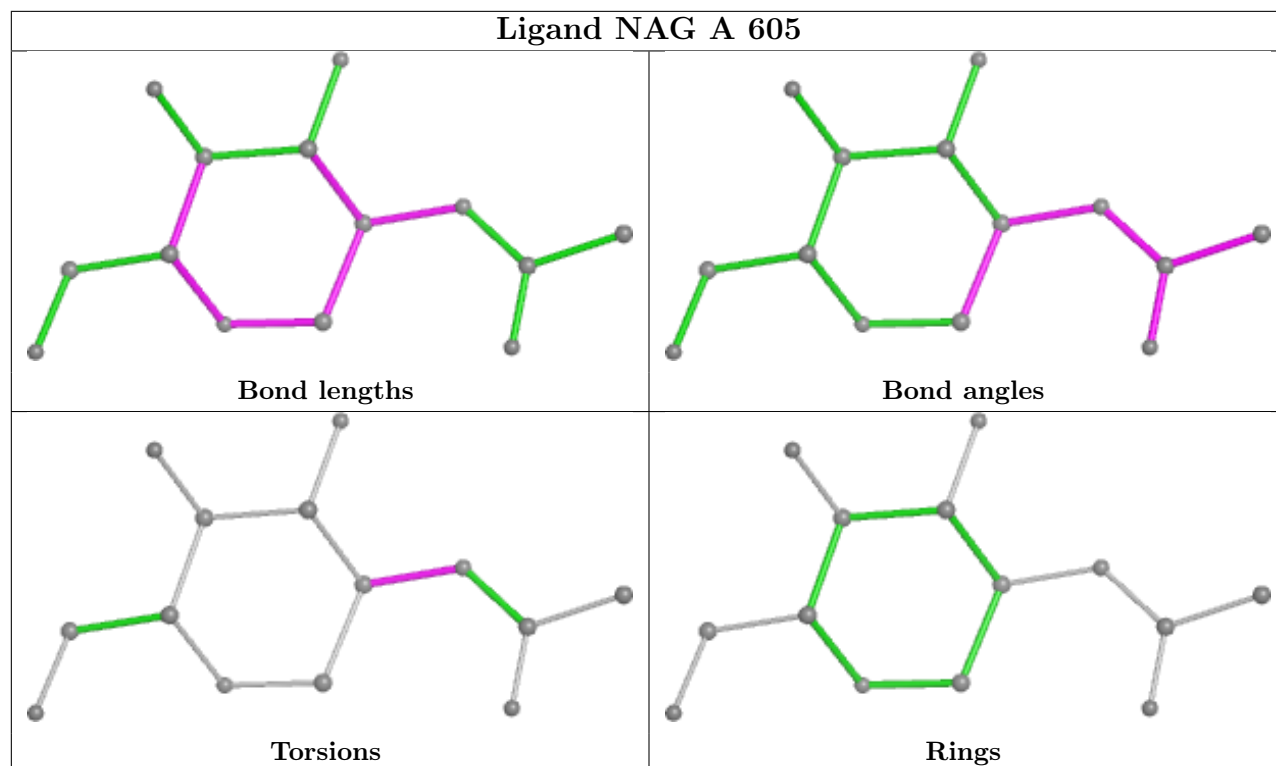


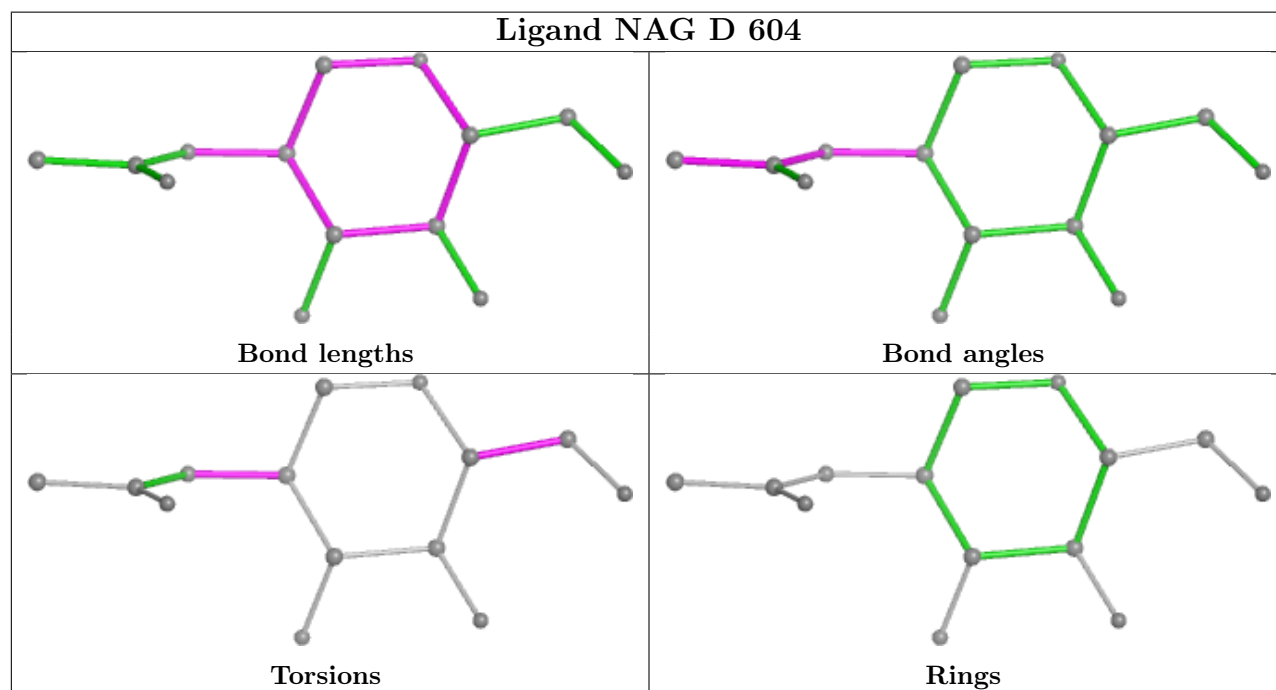
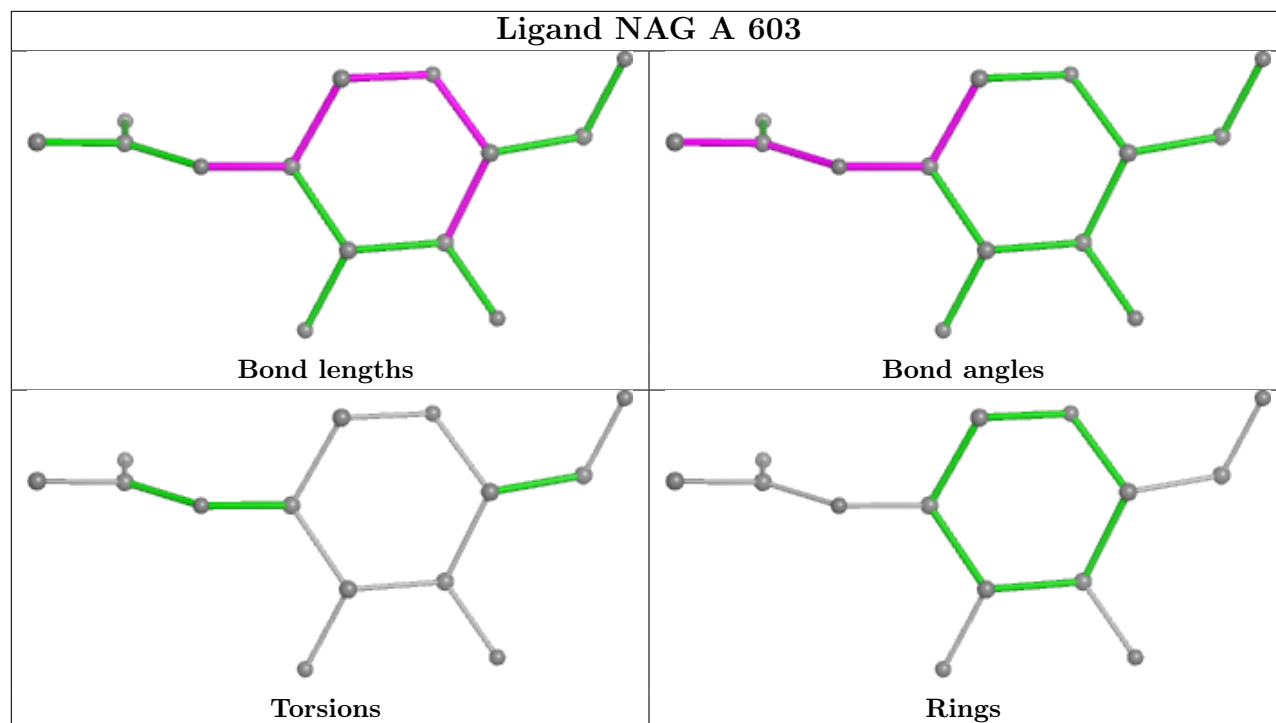


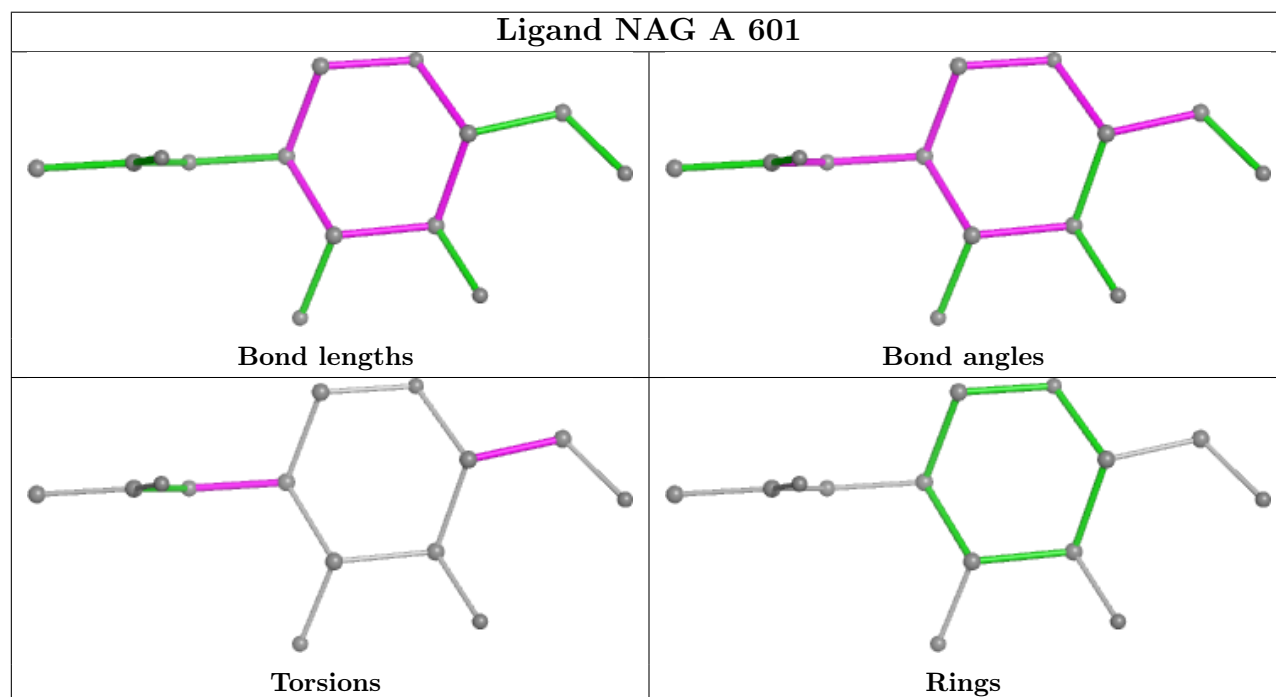
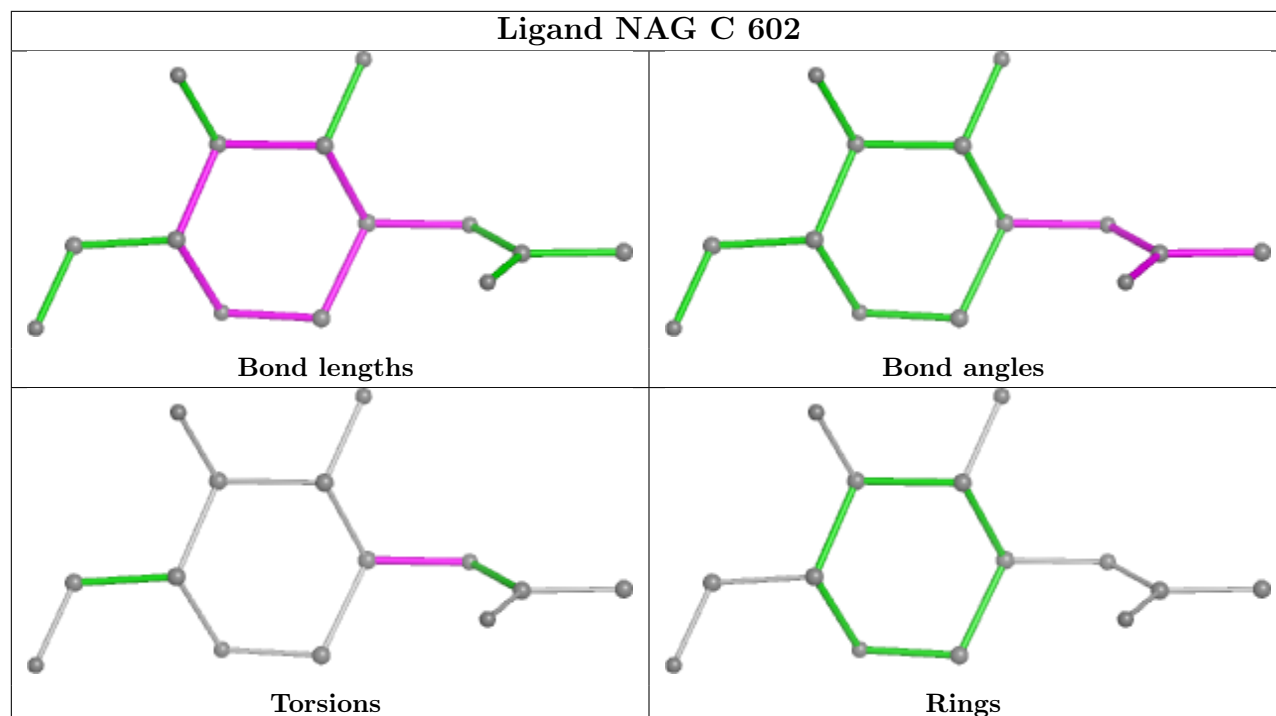


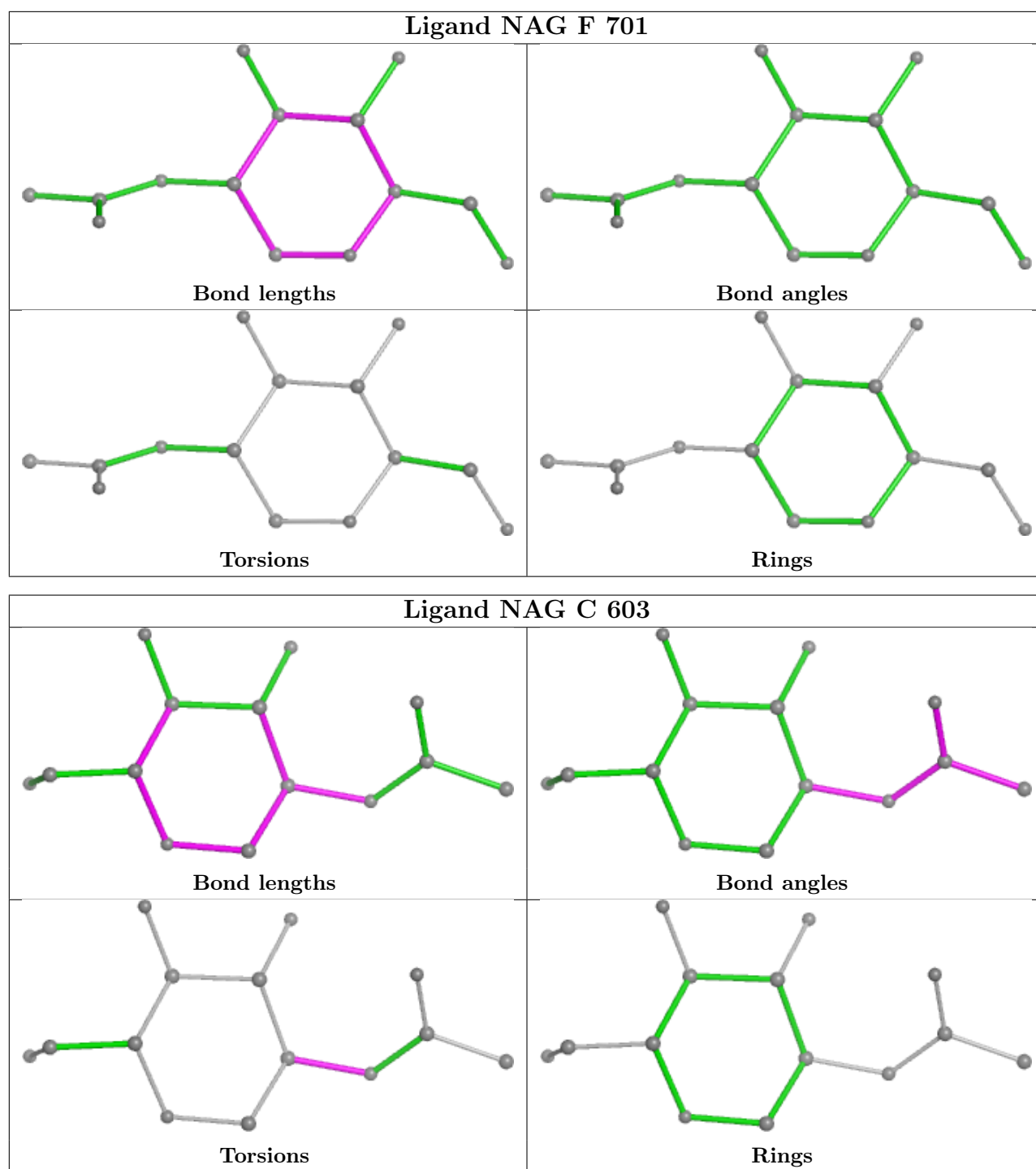












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



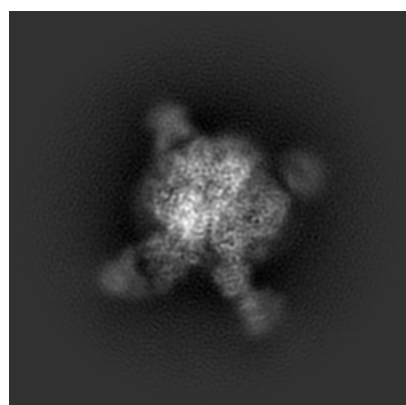
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14474. These allow visual inspection of the internal detail of the map and identification of artifacts.

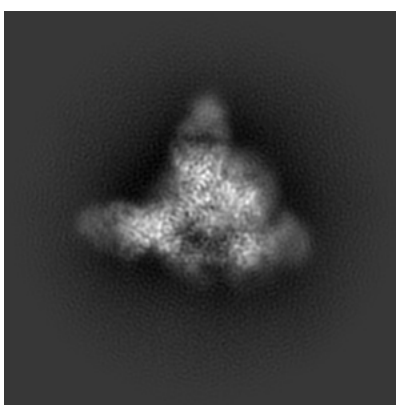
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

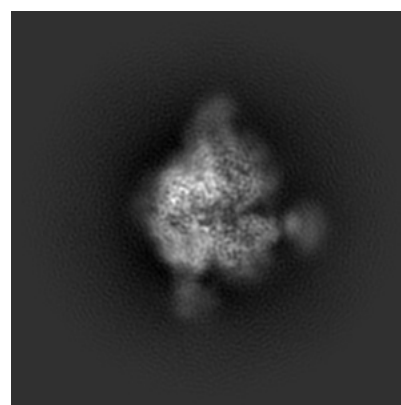
#### 6.1.1 Primary map



X



Y

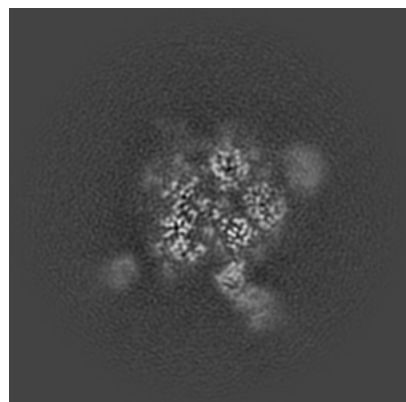


Z

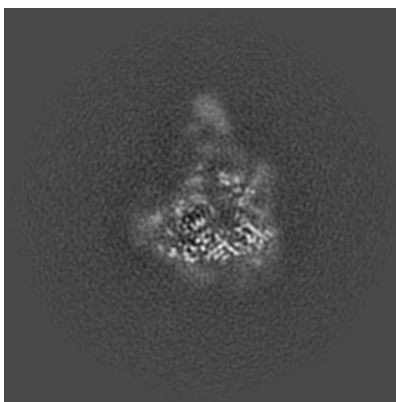
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

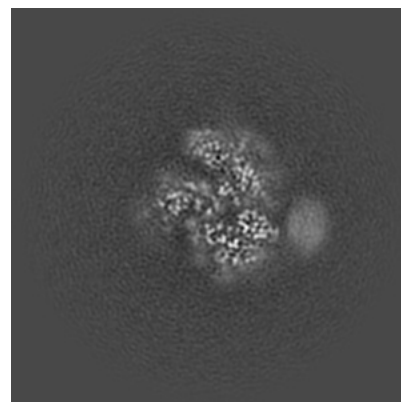
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

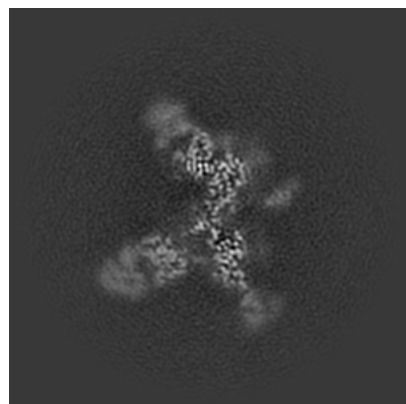


Z Index: 150

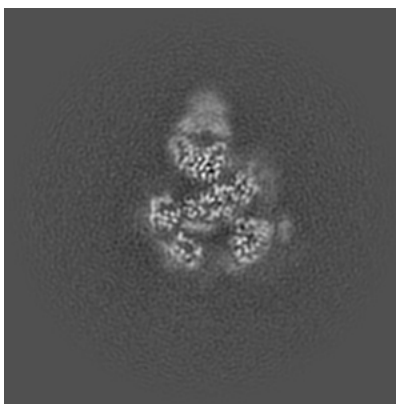
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

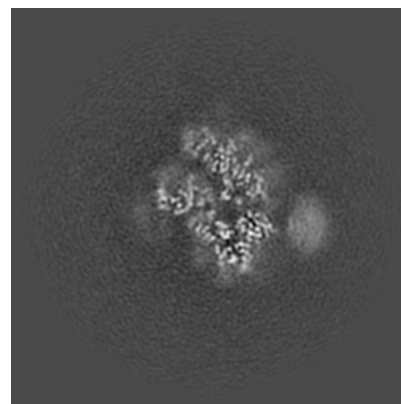
### 6.3.1 Primary map



X Index: 131



Y Index: 137

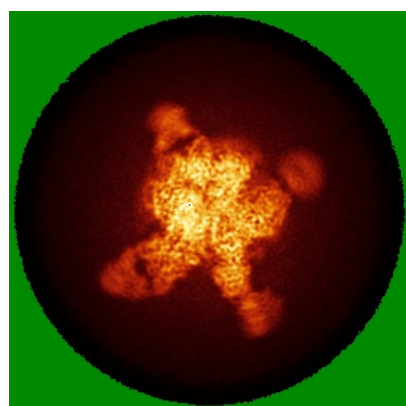


Z Index: 153

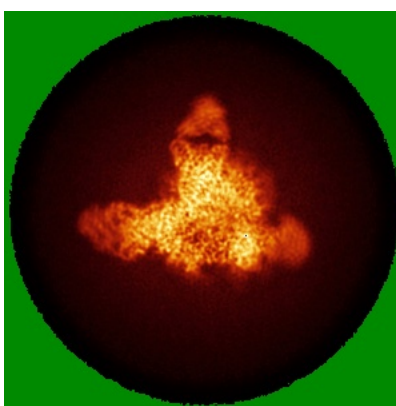
The images above show the largest variance slices of the map in three orthogonal directions.

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

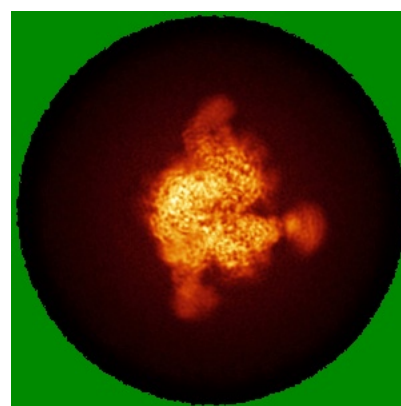
### 6.4.1 Primary map



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 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

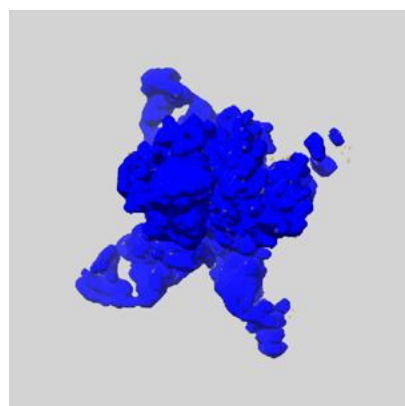
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

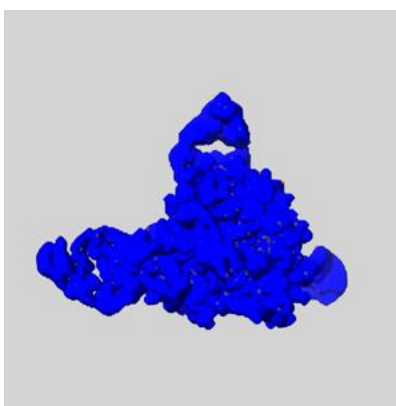
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

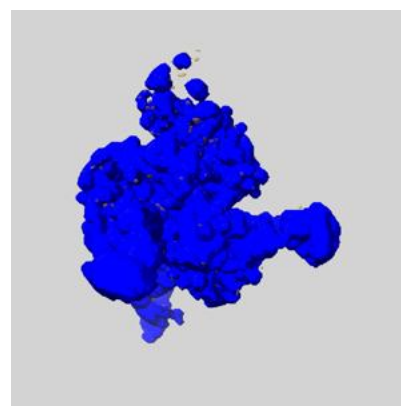
### 6.6.1 emd\_14474\_msk\_1.map [i](#)



X



Y

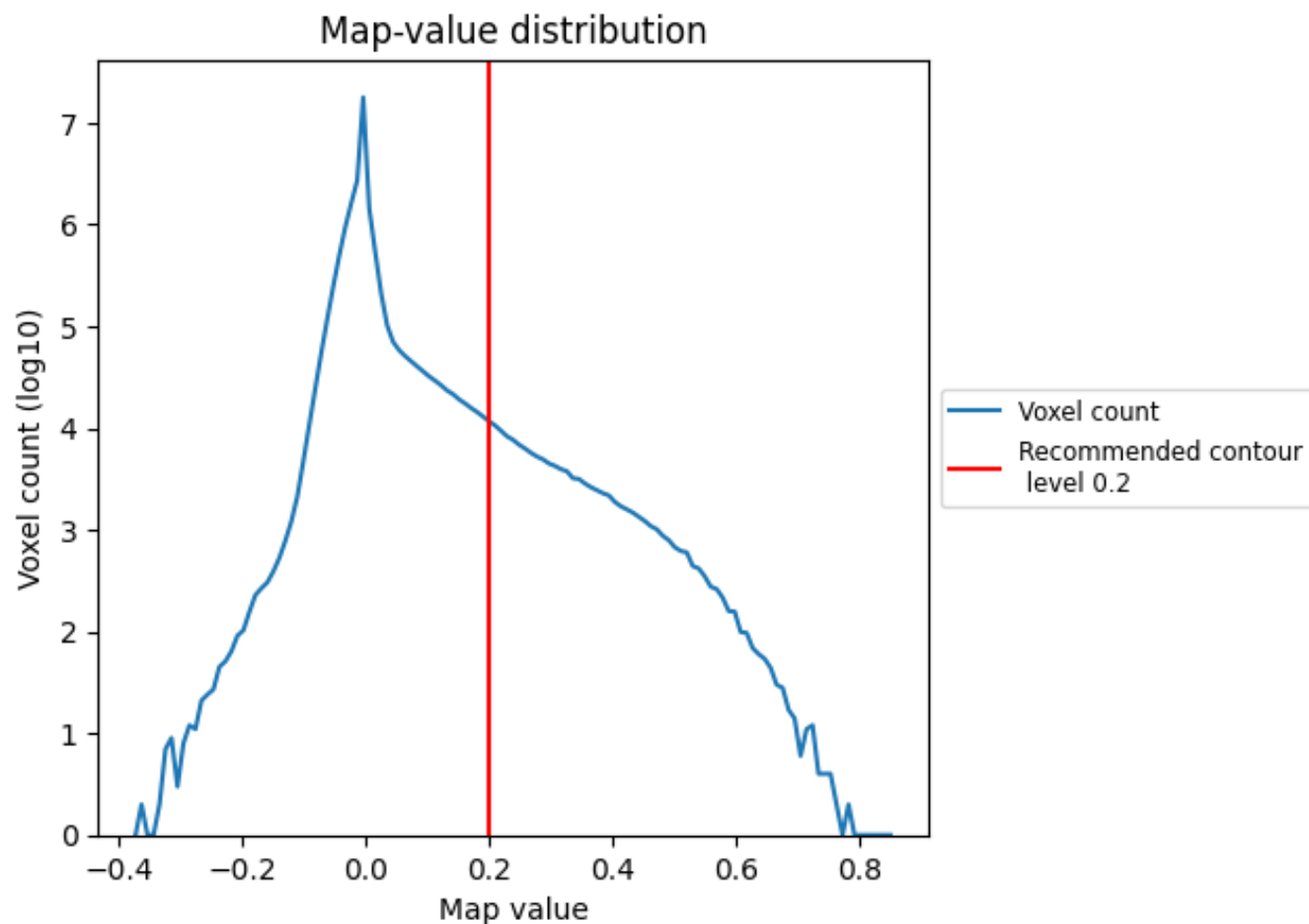


Z

## 7 Map analysis [i](#)

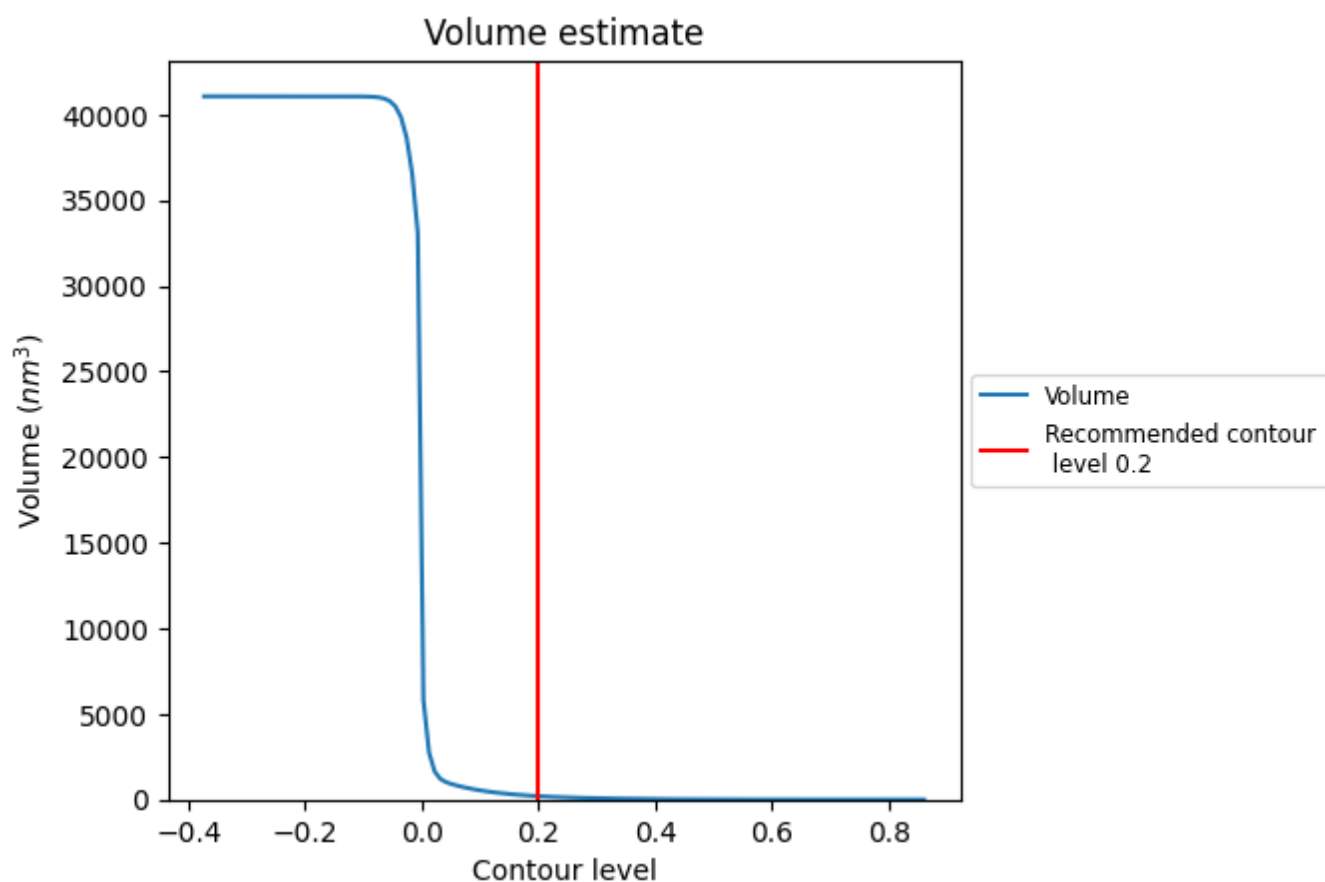
This section contains the results of statistical analysis of the map.

### 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.

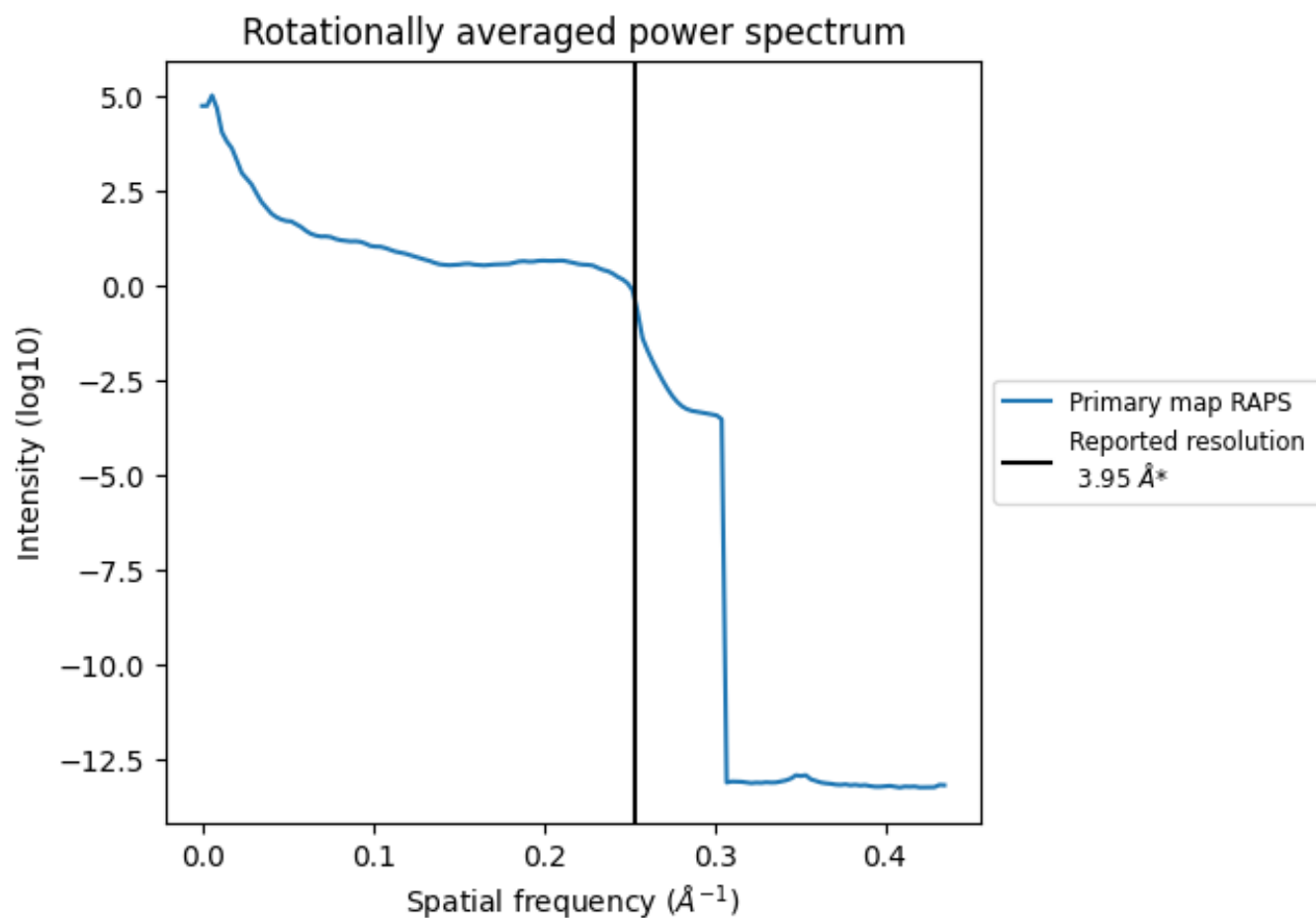
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm<sup>3</sup>; this corresponds to an approximate mass of 178 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 ⓘ

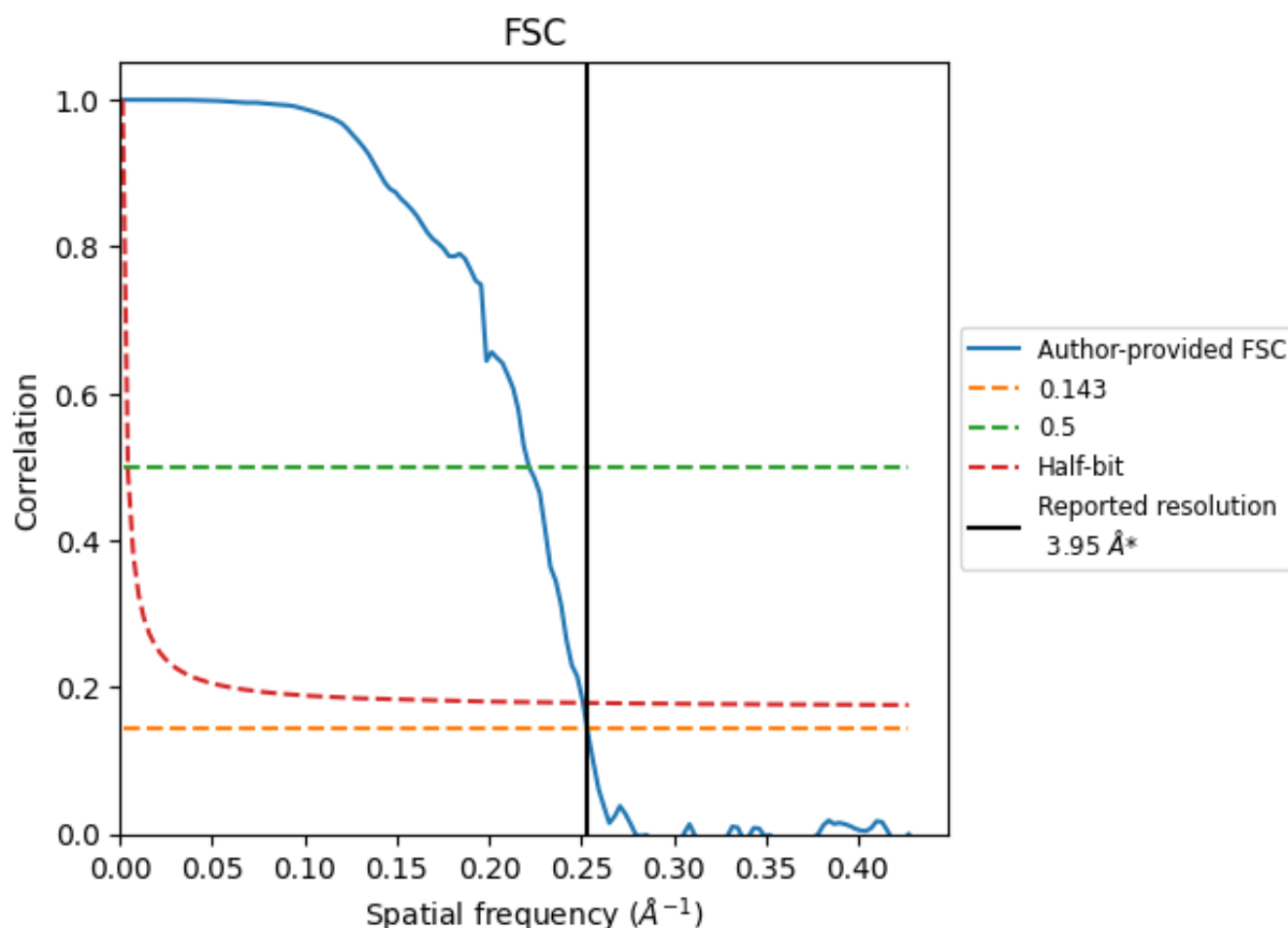


\*Reported resolution corresponds to spatial frequency of 0.253 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.253 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

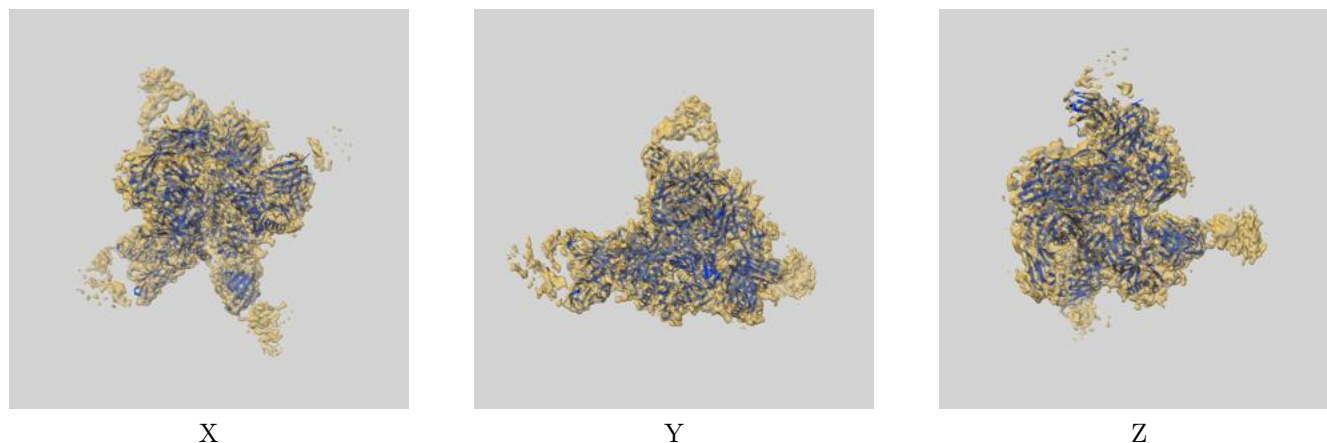
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.95	-	-
Author-provided FSC curve	3.95	4.51	3.98
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

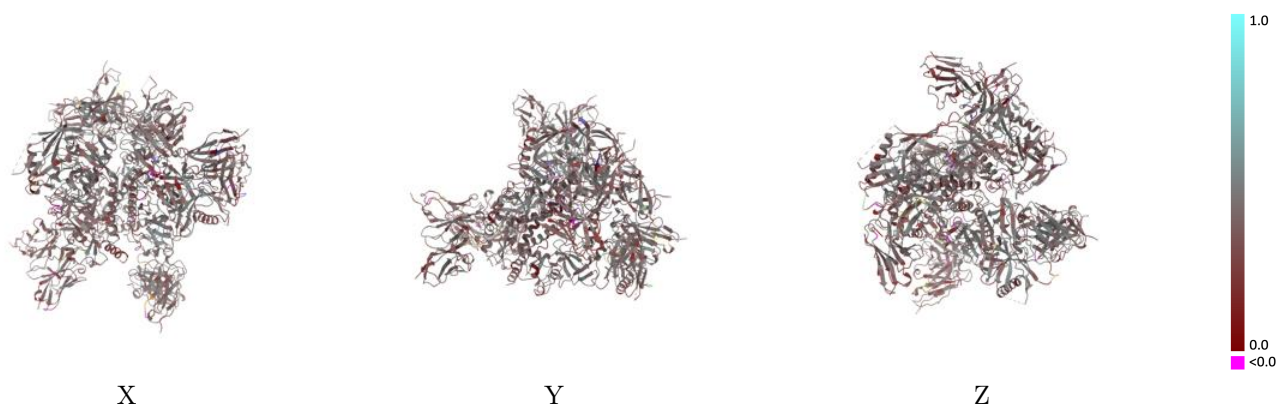
This section contains information regarding the fit between EMDB map EMD-14474 and PDB model 7Z3A. Per-residue inclusion information can be found in section [3](#) on page [12](#).

### 9.1 Map-model overlay [i](#)



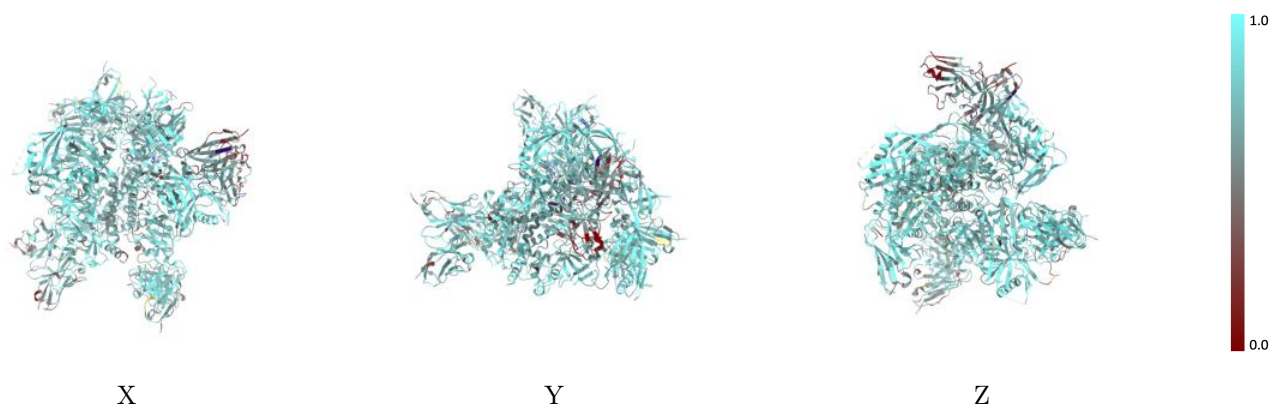
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



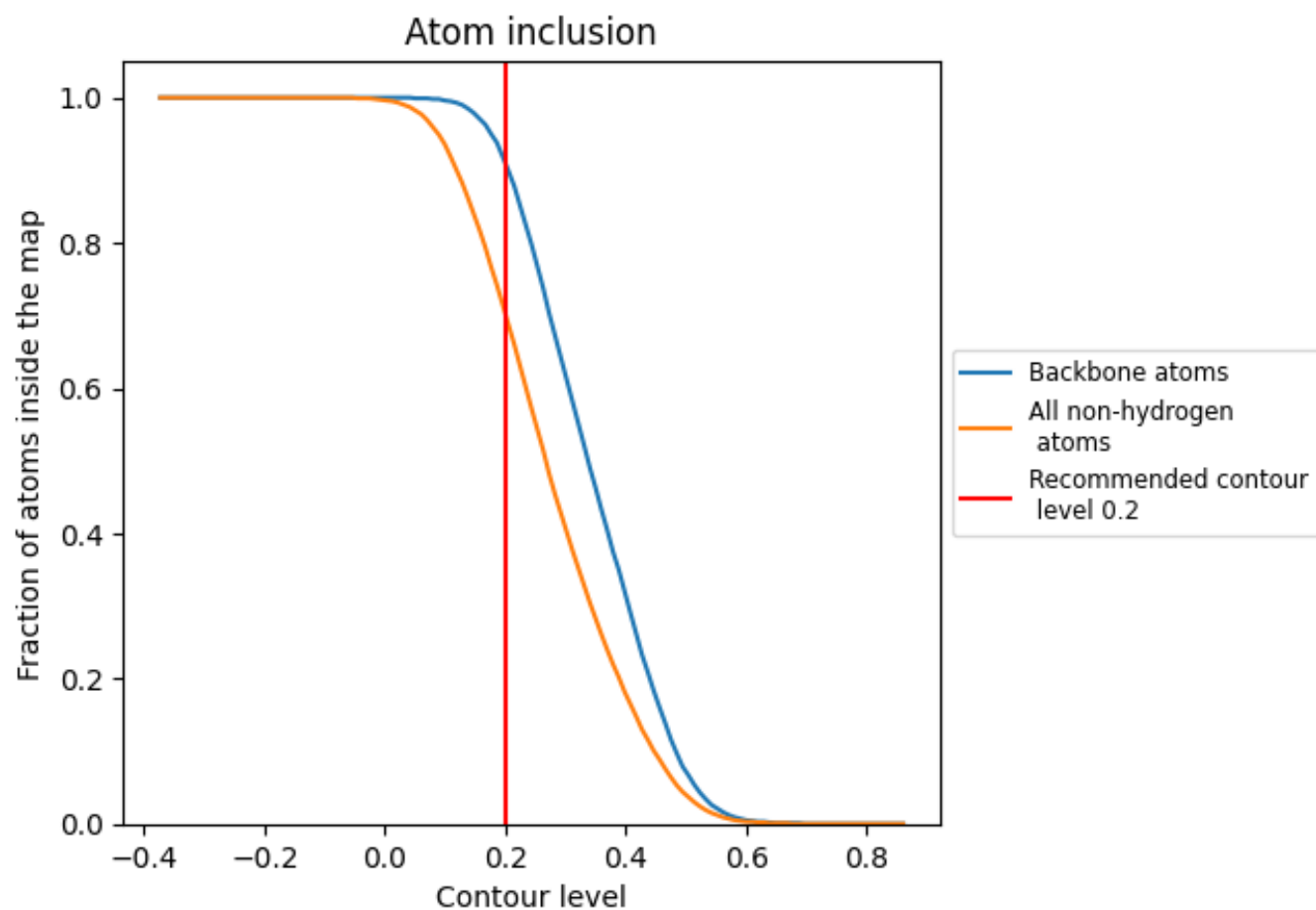
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 70% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7020	 0.3680
0	 0.7440	 0.3360
1	 0.7180	 0.3470
2	 0.4290	 0.2480
3	 0.1540	 0.1290
4	 0.5640	 0.3230
5	 0.5380	 0.3430
6	 0.4360	 0.3370
7	 0.2050	 0.2350
8	 0.2560	 0.3710
9	 0.0360	 0.2780
A	 0.7550	 0.3850
AA	 0.2500	 0.2050
B	 0.7230	 0.3530
C	 0.7550	 0.3840
D	 0.7710	 0.4030
E	 0.7270	 0.3310
F	 0.7100	 0.3310
G	 0.6570	 0.3140
H	 0.8110	 0.4210
I	 0.6300	 0.3110
J	 0.5760	 0.3810
K	 0.7820	 0.4080
L	 0.7610	 0.3670
M	 0.7280	 0.3700
N	 0.4870	 0.3170
O	 0.6960	 0.3660
P	 0.7480	 0.3460
Q	 0.3210	 0.2640
R	 0.2820	 0.3760
S	 0.2620	 0.3050
T	 0.3590	 0.3220
U	 0.6670	 0.3800
V	 0.5380	 0.2810
W	 0.5000	 0.2830



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Chain	Atom inclusion	Q-score
X	 0.2820	 0.3460
Y	 0.5900	 0.3680
Z	 0.5380	 0.4100
a	 0.3080	 0.2520
b	 0.3080	 0.3060
c	 0.2310	 0.2950
d	 0.4360	 0.2990
e	 0.2310	 0.2270
f	 0.2820	 0.4110
g	 0.1790	 0.1630
h	 0.4620	 0.3810
i	 0.3590	 0.3830
j	 0.7950	 0.3700
k	 0.6670	 0.3030
l	 0.5710	 0.3060
m	 0.3080	 0.2840
n	 0.2310	 0.2270
o	 0.6150	 0.3090
p	 0.4100	 0.3190
q	 0.3330	 0.2220
r	 0.2310	 0.2940
s	 0.2500	 0.2750
t	 0.3850	 0.3420
u	 0.1070	 0.1460
v	 0.2860	 0.3900
w	 0.3330	 0.3650
x	 0.5640	 0.3660
y	 0.2790	 0.3250
z	 0.3590	 0.3240