



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 10:29 AM EDT

PDB ID : 7LUA
EMDB ID : EMD-23519
Title : Cryo-EM structure of DH898.1 Fab-dimer bound near the CD4 binding site of HIV-1 Env CH848 SOSIP trimer
Authors : Manne, K.; Edwards, R.J.; Acharya, P.
Deposited on : 2021-02-21
Resolution : 4.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
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

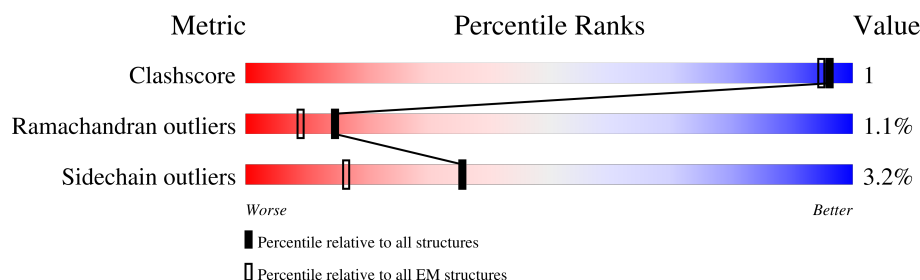
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	466	<div> <div>35%</div> <div>94%</div> <div>6%</div> </div>
1	c	466	<div> <div>41%</div> <div>94%</div> <div>6%</div> </div>
1	e	466	<div> <div>19%</div> <div>95%</div> <div>5%</div> </div>
2	b	146	<div> <div>19%</div> <div>84%</div> <div>14%</div> </div>
2	d	146	<div> <div>14%</div> <div>82%</div> <div>14%</div> </div>
2	f	146	<div> <div>13%</div> <div>83%</div> <div>14%</div> </div>
3	g	218	<div> <div>72%</div> <div>91%</div> <div>9%</div> </div>
3	j	218	<div> <div>71%</div> <div>94%</div> <div>6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	h	219	<div>55%</div> <div>91%</div> <div>9%</div>
4	i	219	<div>54%</div> <div>91%</div> <div>8%</div>
5	A	3	<div>67%</div> <div>100%</div>
5	C	3	<div>67%</div> <div>100%</div>
5	E	3	<div>67%</div> <div>100%</div>
5	F	3	<div>67%</div> <div>100%</div>
5	H	3	<div>67%</div> <div>100%</div>
5	I	3	<div>67%</div> <div>100%</div>
5	K	3	<div>100%</div>
5	L	3	<div>100%</div>
5	O	3	<div>100%</div>
5	P	3	<div>100%</div>
5	R	3	<div>100%</div>
5	T	3	<div>33%</div> <div>67%</div> <div>33%</div> <div>67%</div>
5	U	3	<div>100%</div>
5	W	3	<div>67%</div> <div>100%</div>
5	X	3	<div>67%</div> <div>100%</div>
5	Z	3	<div>100%</div>
5	k	3	<div>67%</div> <div>100%</div>
5	l	3	<div>100%</div>
5	m	3	<div>100%</div>
5	o	3	<div>67%</div> <div>100%</div>
5	q	3	<div>67%</div> <div>100%</div>
5	r	3	<div>100%</div>
5	t	3	<div>100%</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	u	3	100%
5	w	3	100%
5	x	3	100%
6	B	2	50%
6	G	2	50%
6	J	2	100%
6	Q	2	100%
6	V	2	100%
6	Y	2	100%
6	n	2	50%
6	s	2	100%
6	v	2	100%
7	D	5	60%
7	N	5	100%
7	S	5	60%
7	p	5	60%
8	M	6	17%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 44233 atoms, of which 21843 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 CH848 SOSIP gp120.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	a	466	Total	C	H	N	O	S	0	0
			7192	2277	3551	634	701	29		
1	c	466	Total	C	H	N	O	S	0	0
			7192	2277	3551	634	701	29		
1	e	466	Total	C	H	N	O	S	0	0
			7195	2277	3554	634	701	29		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	31	ALA	-	expression tag	UNP A0A1W6IPB2
a	32	GLU	-	expression tag	UNP A0A1W6IPB2
a	33	ASN	-	expression tag	UNP A0A1W6IPB2
a	201	CYS	VAL	conflict	UNP A0A1W6IPB2
a	433	CYS	ALA	conflict	UNP A0A1W6IPB2
a	490	LYS	GLU	conflict	UNP A0A1W6IPB2
a	492	GLU	GLN	conflict	UNP A0A1W6IPB2
a	496	VAL	ILE	conflict	UNP A0A1W6IPB2
a	500	ARG	GLY	conflict	UNP A0A1W6IPB2
a	501	CYS	ALA	conflict	UNP A0A1W6IPB2
a	506E	GLY	GLU	conflict	UNP A0A1W6IPB2
c	31	ALA	-	expression tag	UNP A0A1W6IPB2
c	32	GLU	-	expression tag	UNP A0A1W6IPB2
c	33	ASN	-	expression tag	UNP A0A1W6IPB2
c	201	CYS	VAL	conflict	UNP A0A1W6IPB2
c	433	CYS	ALA	conflict	UNP A0A1W6IPB2
c	490	LYS	GLU	conflict	UNP A0A1W6IPB2
c	492	GLU	GLN	conflict	UNP A0A1W6IPB2
c	496	VAL	ILE	conflict	UNP A0A1W6IPB2
c	500	ARG	GLY	conflict	UNP A0A1W6IPB2
c	501	CYS	ALA	conflict	UNP A0A1W6IPB2
c	506E	GLY	GLU	conflict	UNP A0A1W6IPB2
e	31	ALA	-	expression tag	UNP A0A1W6IPB2
e	32	GLU	-	expression tag	UNP A0A1W6IPB2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
e	33	ASN	-	expression tag	UNP A0A1W6IPB2
e	201	CYS	VAL	conflict	UNP A0A1W6IPB2
e	433	CYS	ALA	conflict	UNP A0A1W6IPB2
e	490	LYS	GLU	conflict	UNP A0A1W6IPB2
e	492	GLU	GLN	conflict	UNP A0A1W6IPB2
e	496	VAL	ILE	conflict	UNP A0A1W6IPB2
e	500	ARG	GLY	conflict	UNP A0A1W6IPB2
e	501	CYS	ALA	conflict	UNP A0A1W6IPB2
e	506E	GLY	GLU	conflict	UNP A0A1W6IPB2

- Molecule 2 is a protein called Env polyprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	b	126	Total	C	H	N	O	S	0	0
			1985	634	982	172	191	6		
2	d	126	Total	C	H	N	O	S	0	0
			1985	634	982	172	191	6		
2	f	126	Total	C	H	N	O	S	0	0
			1985	634	982	172	191	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	547	PRO	ILE	conflict	UNP A0A6H1VEB8
b	593	CYS	THR	conflict	UNP A0A6H1VEB8
d	547	PRO	ILE	conflict	UNP A0A6H1VEB8
d	593	CYS	THR	conflict	UNP A0A6H1VEB8
f	547	PRO	ILE	conflict	UNP A0A6H1VEB8
f	593	CYS	THR	conflict	UNP A0A6H1VEB8

- Molecule 3 is a protein called DH898.1 light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	g	218	Total	C	H	N	O	S	0	0
			3275	1044	1616	281	329	5		
3	j	218	Total	C	H	N	O	S	0	0
			3275	1044	1616	281	329	5		

- Molecule 4 is a protein called DH898.1 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	h	219	Total	C	H	N	O	S	0	0
			3295	1053	1635	275	325	7		
4	i	219	Total	C	H	N	O	S	0	0
			3296	1053	1636	275	325	7		

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



Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	C	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	E	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	F	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	H	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	I	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	K	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	L	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	O	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	P	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	R	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	T	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	U	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	W	3	Total	C	H	N	O		0	0
			76	22	37	2	15			
5	X	3	Total	C	H	N	O		0	0
			76	22	37	2	15			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Z	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	k	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	l	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	m	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	o	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	q	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	r	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	t	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	u	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	w	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
5	x	3	Total	C	H	N	O	0	0
			76	22	37	2	15		

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



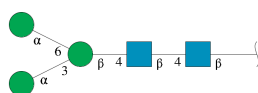
Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
6	G	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
6	J	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
6	Q	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
6	V	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
6	Y	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

Continued on next page...

Continued from previous page...

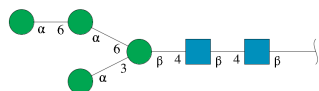
Mol	Chain	Residues	Atoms					AltConf	Trace
6	n	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
6	s	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
6	v	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
7	N	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
7	S	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
7	p	5	Total	C	H	N	O	0	0
			118	34	57	2	25		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	6	Total	C	H	N	O	0	0
			139	40	67	2	30		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					AltConf
9	a	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	a	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	a	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	a	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	b	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	b	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	c	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	c	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	c	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	d	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	d	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	e	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	e	1	Total	C	H	N	O	0
			28	8	14	1	5	

Continued on next page...

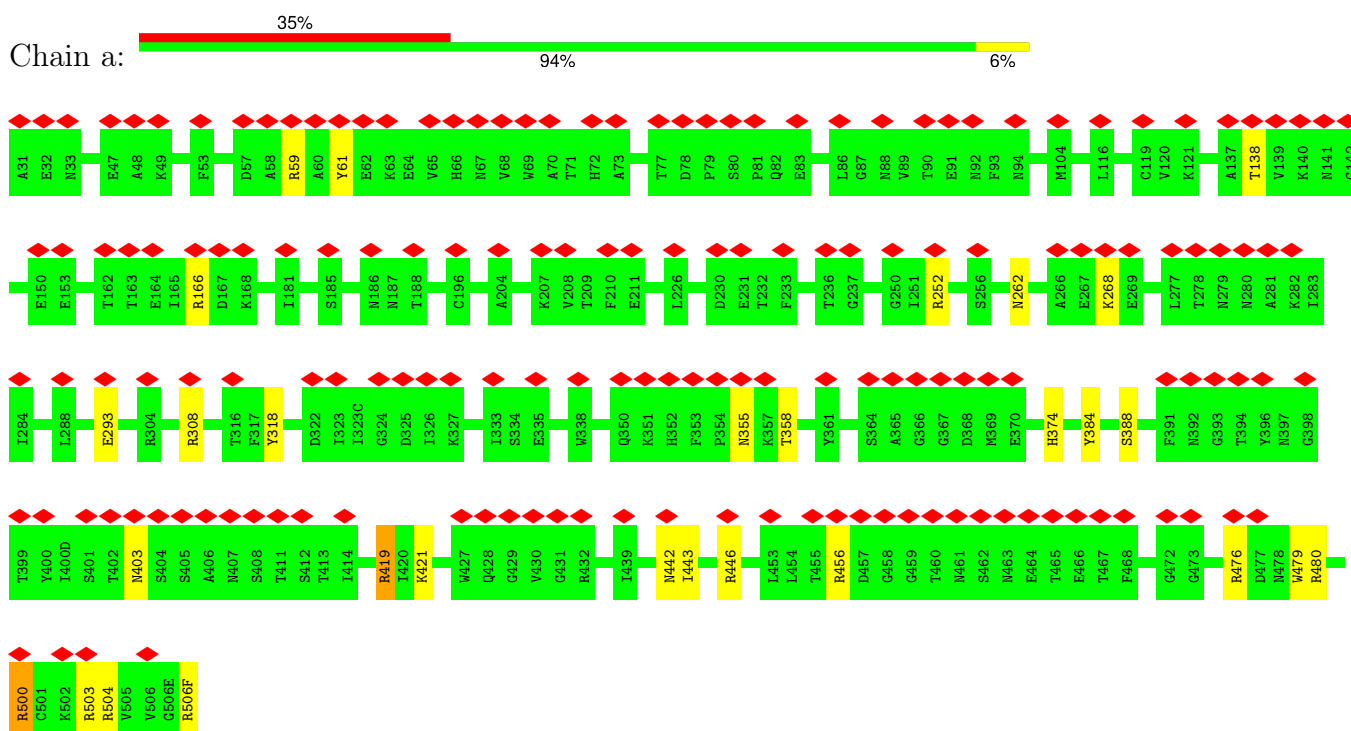
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
9	e	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	f	1	Total	C	H	N	O	0
			28	8	14	1	5	
9	f	1	Total	C	H	N	O	0
			28	8	14	1	5	

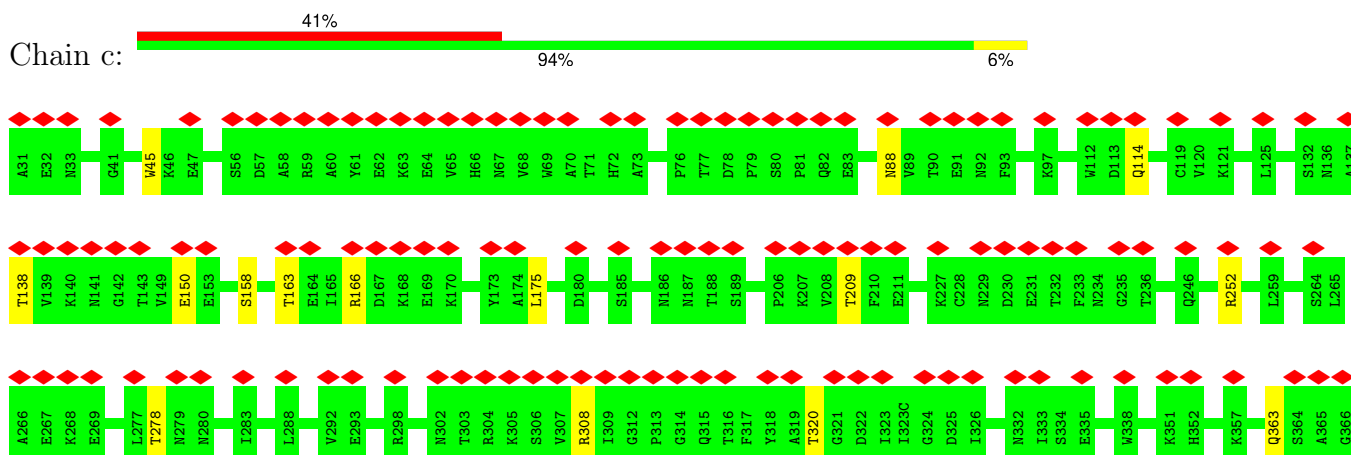
3 Residue-property plots

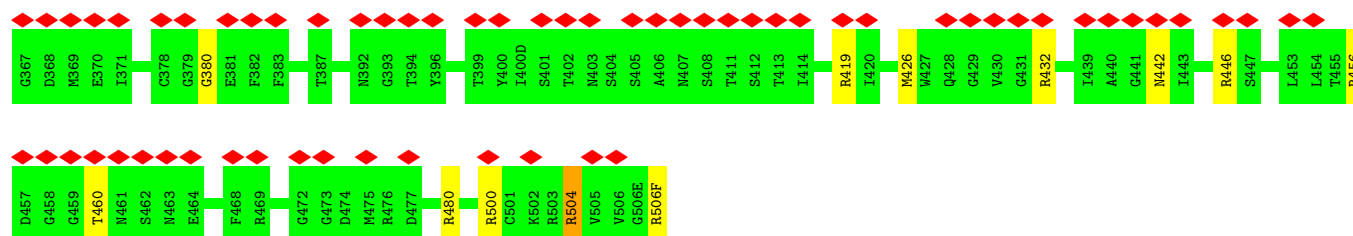
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: CH848 SOSIP gp120

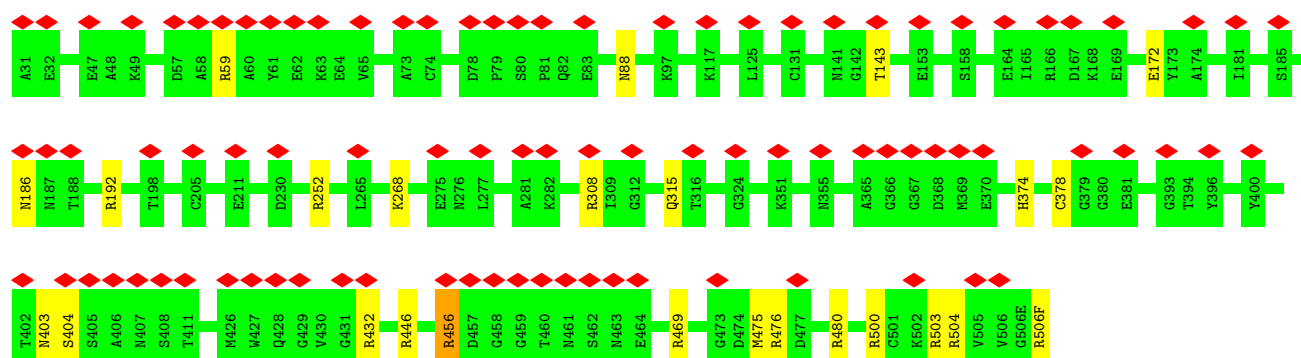


• Molecule 1: CH848 SOSIP gp120

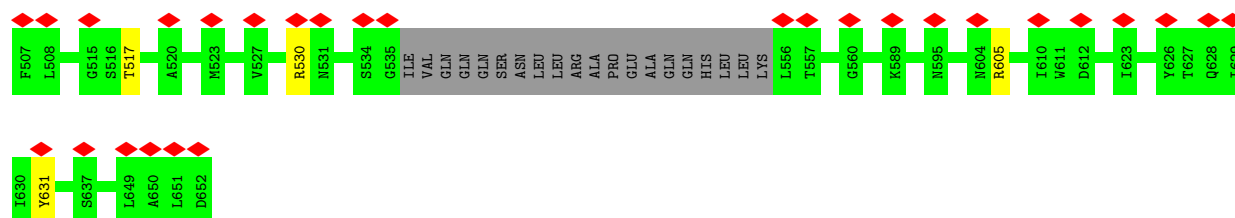
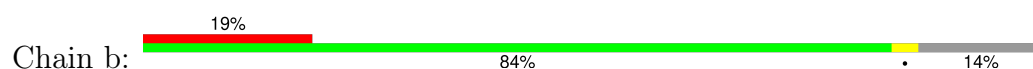




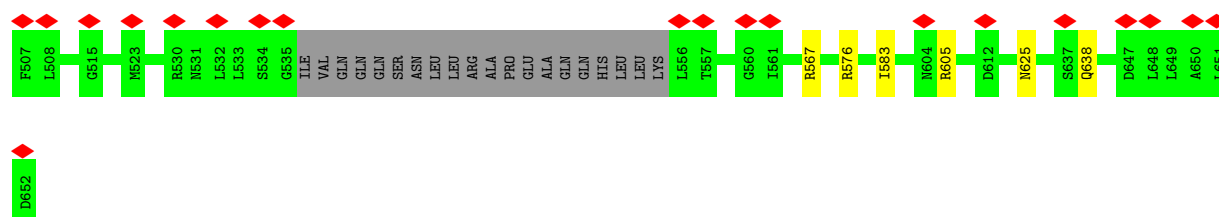
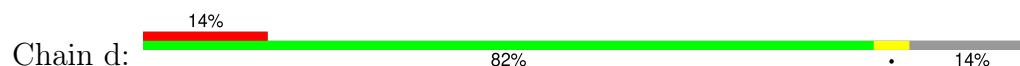
• Molecule 1: CH848 SOSIP gp120



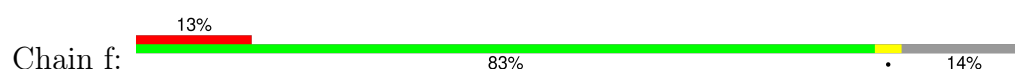
• Molecule 2: Env polyprotein

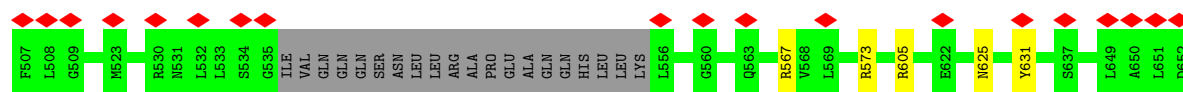


• Molecule 2: Env polyprotein

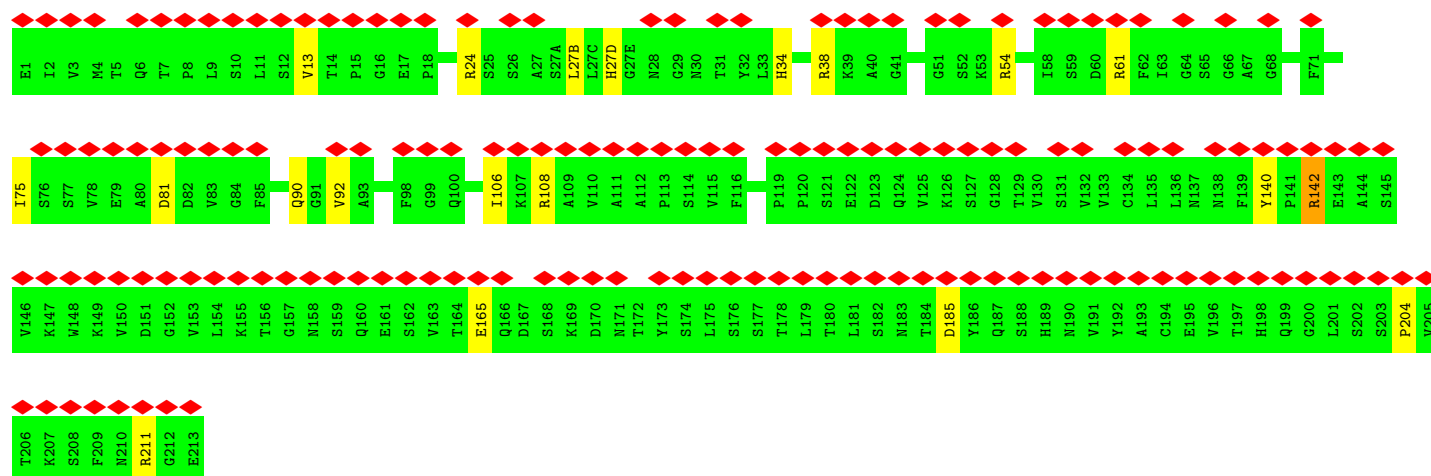
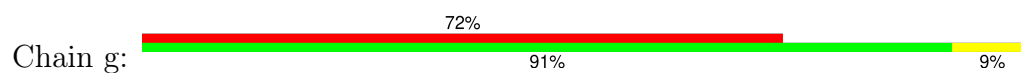


• Molecule 2: Env polyprotein

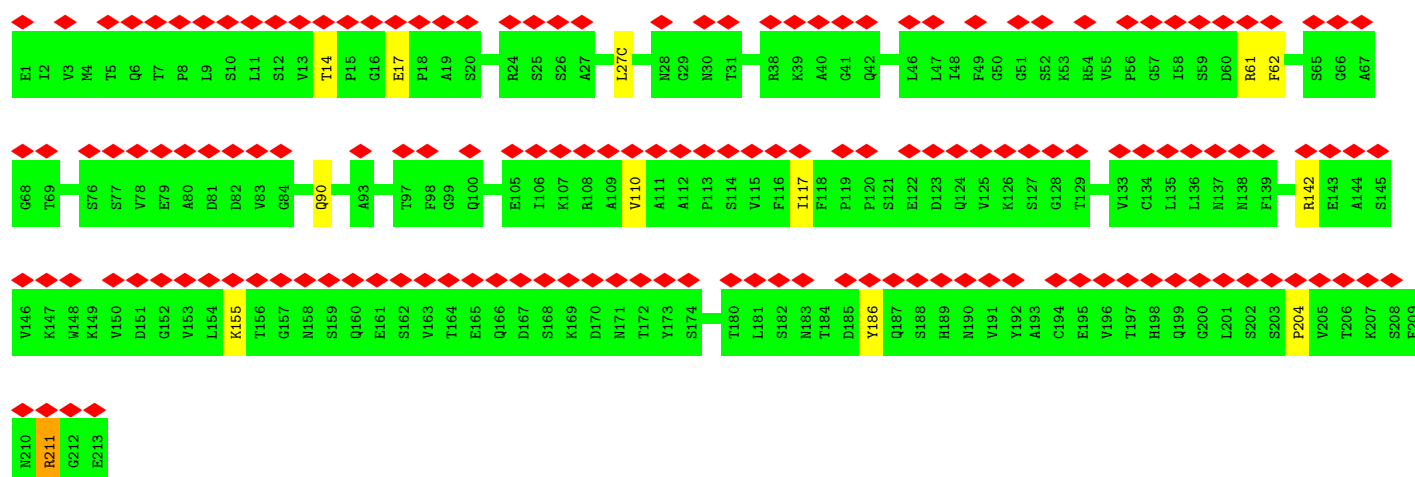
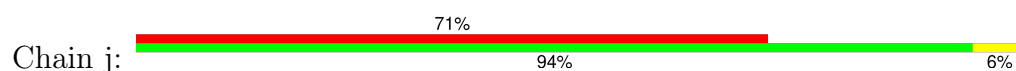




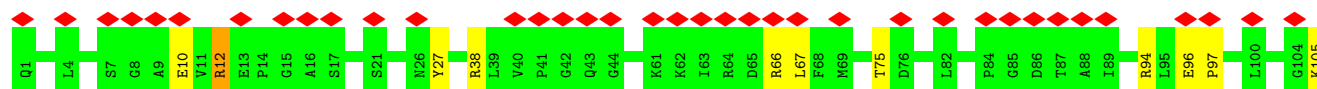
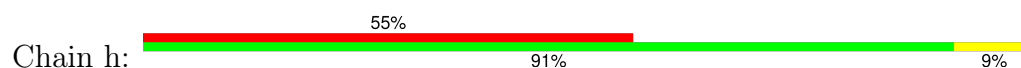
• Molecule 3: DH898.1 light chain

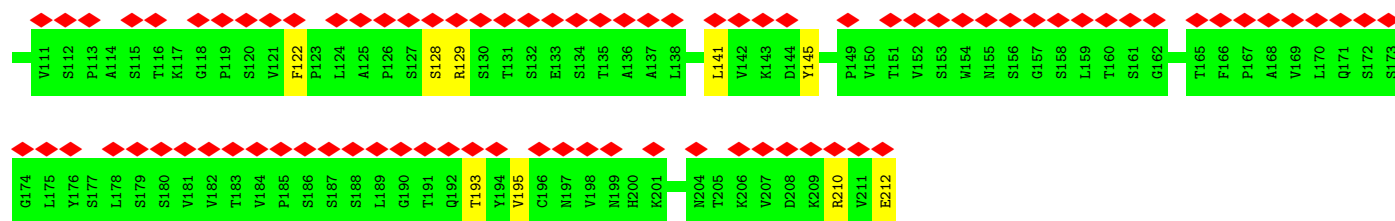


• Molecule 3: DH898.1 light chain

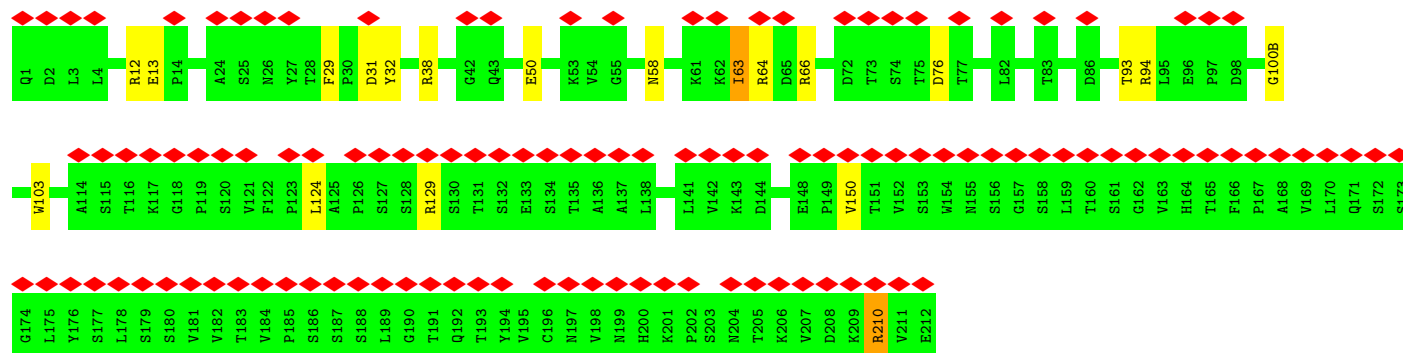
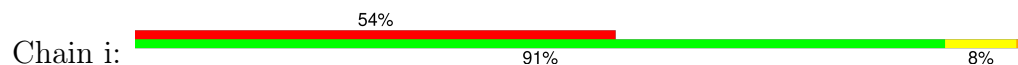


• Molecule 4: DH898.1 heavy chain





• Molecule 4: DH898.1 heavy chain



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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





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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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





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



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



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



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



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



- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose

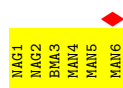
se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



• Molecule 8: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.910	Depositor
Minimum map value	-0.540	Depositor
Average map value	0.027	Depositor
Map value standard deviation	0.115	Depositor
Recommended contour level	0.816	Depositor
Map size (Å)	273.02298, 273.02298, 273.02298	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066496, 1.066496, 1.066496	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	0.64	0/3718	1.04	13/5058 (0.3%)
1	c	0.63	0/3718	1.03	11/5058 (0.2%)
1	e	0.63	0/3718	1.02	15/5058 (0.3%)
2	b	0.60	0/1021	1.06	3/1383 (0.2%)
2	d	0.59	0/1021	1.02	3/1383 (0.2%)
2	f	0.62	0/1021	1.02	3/1383 (0.2%)
3	g	0.66	0/1697	1.08	6/2306 (0.3%)
3	j	0.66	0/1697	1.03	1/2306 (0.0%)
4	h	0.64	0/1703	1.12	6/2329 (0.3%)
4	i	0.65	0/1703	1.10	5/2329 (0.2%)
All	All	0.64	0/21017	1.05	66/28593 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	3
1	c	0	1
2	f	0	1
3	g	0	1
3	j	0	1
4	h	0	4
4	i	0	2
All	All	0	13

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	480	ARG	NE-CZ-NH1	8.96	124.78	120.30
3	g	61	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	e	480	ARG	NE-CZ-NH1	8.13	124.36	120.30
2	d	605	ARG	NE-CZ-NH1	8.02	124.31	120.30
4	h	210	ARG	NE-CZ-NH1	7.97	124.29	120.30
4	i	94	ARG	NE-CZ-NH1	7.92	124.26	120.30
4	h	38	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	c	456	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	c	480	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	a	166	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	f	567	ARG	NE-CZ-NH1	7.12	123.86	120.30
4	h	12	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	a	456	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	a	252	ARG	NE-CZ-NH1	6.91	123.75	120.30
3	j	211	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	c	456	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	c	308	ARG	NE-CZ-NH1	6.55	123.58	120.30
2	b	605	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	c	419	ARG	NE-CZ-NH1	6.48	123.54	120.30
3	g	54	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	a	446	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	e	469	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	a	419	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	a	61	TYR	CB-CG-CD2	-6.23	117.26	121.00
3	g	142	ARG	NE-CZ-NH1	6.18	123.39	120.30
4	i	66	ARG	NE-CZ-NH1	6.15	123.38	120.30
4	i	12	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	e	469	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	c	446	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	c	506(F)	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	e	456	ARG	NE-CZ-NH1	5.93	123.27	120.30
4	h	66	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	c	252	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	e	500	ARG	NE-CZ-NH1	5.80	123.20	120.30
3	g	38	ARG	NE-CZ-NH1	5.71	123.15	120.30
2	f	605	ARG	NE-CZ-NH1	5.70	123.15	120.30
4	i	64	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	e	308	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	d	567	ARG	NE-CZ-NH1	5.64	123.12	120.30
4	h	12	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	e	506(F)	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	a	476	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	a	500	ARG	NE-CZ-NH1	5.54	123.07	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	446	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	c	500	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	b	530	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	e	59	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	e	192	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	e	504	ARG	NE-CZ-NH1	5.43	123.01	120.30
2	d	576	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	e	432	ARG	NE-CZ-NH1	5.37	122.98	120.30
4	h	129	ARG	NE-CZ-NH1	5.36	122.98	120.30
3	g	24	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	c	166	ARG	NE-CZ-NH1	5.31	122.95	120.30
3	g	108	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	a	506(F)	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	e	252	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	c	432	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	b	631	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	e	476	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	a	308	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	e	503	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	a	503	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	f	631	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	a	59	ARG	NE-CZ-NH1	5.03	122.82	120.30
4	i	38	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	318	TYR	Sidechain
1	a	374	HIS	Sidechain
1	a	384	TYR	Sidechain
1	c	504	ARG	Sidechain
2	f	573	ARG	Sidechain
3	g	140	TYR	Sidechain
4	h	122	PHE	Sidechain
4	h	145	TYR	Sidechain
4	h	27	TYR	Sidechain
4	h	94	ARG	Sidechain
4	i	210	ARG	Sidechain
4	i	32	TYR	Sidechain
3	j	186	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3641	3551	3547	0	0
1	c	3641	3551	3547	0	0
1	e	3641	3554	3551	0	0
2	b	1003	982	978	0	0
2	d	1003	982	978	0	0
2	f	1003	982	978	0	0
3	g	1659	1616	1615	0	0
3	j	1659	1616	1615	0	0
4	h	1660	1635	1635	0	0
4	i	1660	1636	1635	0	0
5	A	39	37	34	0	0
5	C	39	37	34	0	0
5	E	39	37	34	0	0
5	F	39	37	34	0	0
5	H	39	37	34	0	0
5	I	39	37	34	0	0
5	K	39	37	34	0	0
5	L	39	37	34	0	0
5	O	39	37	34	0	0
5	P	39	37	34	0	0
5	R	39	37	34	1	0
5	T	39	37	34	0	0
5	U	39	37	34	0	0
5	W	39	37	34	0	0
5	X	39	37	34	0	0
5	Z	39	37	34	0	0
5	k	39	37	34	0	0
5	l	39	37	34	0	0
5	m	39	37	34	0	0
5	o	39	37	34	0	0
5	q	39	37	34	0	0
5	r	39	37	34	0	0
5	t	39	37	34	0	0
5	u	39	37	34	0	0
5	w	39	37	34	0	0
5	x	39	37	34	0	0
6	B	28	27	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	28	27	25	0	0
6	J	28	27	25	0	0
6	Q	28	27	25	0	0
6	V	28	27	25	0	0
6	Y	28	27	25	0	0
6	n	28	27	25	0	0
6	s	28	27	25	0	0
6	v	28	27	25	0	0
7	D	61	57	52	0	0
7	N	61	57	52	0	0
7	S	61	57	52	0	0
7	p	61	57	52	0	0
8	M	72	67	61	0	0
9	a	56	56	52	0	0
9	b	28	28	26	0	0
9	c	56	56	52	0	0
9	d	28	28	26	0	0
9	e	42	42	39	0	0
9	f	28	28	26	0	0
All	All	22390	21843	21678	1	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 (1) 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:R:1:NAG:H4	5:R:2:NAG:H2	3.60	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	464/466 (100%)	419 (90%)	38 (8%)	7 (2%)	8	39
1	c	464/466 (100%)	416 (90%)	42 (9%)	6 (1%)	10	42
1	e	464/466 (100%)	421 (91%)	40 (9%)	3 (1%)	22	60
2	b	122/146 (84%)	110 (90%)	12 (10%)	0	100	100
2	d	122/146 (84%)	113 (93%)	9 (7%)	0	100	100
2	f	122/146 (84%)	109 (89%)	13 (11%)	0	100	100
3	g	216/218 (99%)	190 (88%)	23 (11%)	3 (1%)	9	40
3	j	216/218 (99%)	196 (91%)	18 (8%)	2 (1%)	14	51
4	h	217/219 (99%)	190 (88%)	24 (11%)	3 (1%)	9	40
4	i	217/219 (99%)	192 (88%)	20 (9%)	5 (2%)	5	28
All	All	2624/2710 (97%)	2356 (90%)	239 (9%)	29 (1%)	15	46

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	443	ILE
3	g	92	VAL
4	h	96	GLU
1	a	355	ASN
1	a	358	THR
1	c	88	ASN
1	c	138	THR
4	h	97	PRO
4	i	124	LEU
1	a	138	THR
1	c	163	THR
1	e	403	ASN
3	g	211	ARG
4	h	128	SER
1	e	404	SER
1	a	403	ASN
1	a	500	ARG
1	c	426	MET
1	c	460	THR
1	e	88	ASN
4	i	29	PHE
4	i	76	ASP
1	a	262	ASN
4	i	100(B)	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	j	110	VAL
1	c	380	GLY
3	j	204	PRO
3	g	204	PRO
4	i	63	ILE

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	413/413 (100%)	405 (98%)	8 (2%)	52	70
1	c	413/413 (100%)	402 (97%)	11 (3%)	40	60
1	e	413/413 (100%)	404 (98%)	9 (2%)	47	66
2	b	108/126 (86%)	107 (99%)	1 (1%)	75	83
2	d	108/126 (86%)	105 (97%)	3 (3%)	38	59
2	f	108/126 (86%)	107 (99%)	1 (1%)	75	83
3	g	187/187 (100%)	176 (94%)	11 (6%)	16	38
3	j	187/187 (100%)	177 (95%)	10 (5%)	19	41
4	h	190/190 (100%)	181 (95%)	9 (5%)	22	45
4	i	190/190 (100%)	180 (95%)	10 (5%)	19	41
All	All	2317/2371 (98%)	2244 (97%)	73 (3%)	36	54

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	268	LYS
1	a	293	GLU
1	a	388	SER
1	a	419	ARG
1	a	421	LYS
1	a	442	ASN
1	a	479	TRP
1	a	504	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	517	THR
1	c	45	TRP
1	c	114	GLN
1	c	150	GLU
1	c	158	SER
1	c	175	LEU
1	c	209	THR
1	c	278	THR
1	c	320	THR
1	c	363	GLN
1	c	442	ASN
1	c	504	ARG
2	d	583	ILE
2	d	625	ASN
2	d	638	GLN
1	e	143	THR
1	e	172	GLU
1	e	186	ASN
1	e	268	LYS
1	e	315	GLN
1	e	374	HIS
1	e	378	CYS
1	e	456	ARG
1	e	475	MET
2	f	625	ASN
3	g	13	VAL
3	g	27(B)	LEU
3	g	27(D)	HIS
3	g	34	HIS
3	g	75	ILE
3	g	81	ASP
3	g	90	GLN
3	g	106	ILE
3	g	142	ARG
3	g	165	GLU
3	g	185	ASP
4	h	10	GLU
4	h	12	ARG
4	h	67	LEU
4	h	75	THR
4	h	105	LYS
4	h	141	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	h	193	THR
4	h	195	VAL
4	h	212	GLU
4	i	13	GLU
4	i	31	ASP
4	i	50	GLU
4	i	58	ASN
4	i	63	ILE
4	i	93	THR
4	i	103	TRP
4	i	129	ARG
4	i	150	VAL
4	i	210	ARG
3	j	14	THR
3	j	17	GLU
3	j	27(C)	LEU
3	j	61	ARG
3	j	62	PHE
3	j	90	GLN
3	j	117	ILE
3	j	142	ARG
3	j	155	LYS
3	j	211	ARG

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

Mol	Chain	Res	Type
1	e	374	HIS

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 ⓘ

122 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	$\# Z > 2$
5	NAG	A	1	5	14,14,15	1.22	3 (21%)	17,19,21	1.24	1 (5%)
5	NAG	A	2	5	14,14,15	1.31	2 (14%)	17,19,21	1.03	1 (5%)
5	BMA	A	3	5	11,11,12	1.27	1 (9%)	15,15,17	0.99	1 (6%)
6	NAG	B	1	1,6	14,14,15	1.16	2 (14%)	17,19,21	0.95	1 (5%)
6	NAG	B	2	6	14,14,15	1.29	3 (21%)	17,19,21	0.75	0
5	NAG	C	1	5	14,14,15	1.08	0	17,19,21	0.80	1 (5%)
5	NAG	C	2	5	14,14,15	1.17	1 (7%)	17,19,21	0.83	1 (5%)
5	BMA	C	3	5	11,11,12	1.33	2 (18%)	15,15,17	0.87	1 (6%)
7	NAG	D	1	1,7	14,14,15	1.03	1 (7%)	17,19,21	0.90	0
7	NAG	D	2	7	14,14,15	1.04	1 (7%)	17,19,21	0.92	1 (5%)
7	BMA	D	3	7	11,11,12	1.38	2 (18%)	15,15,17	1.24	1 (6%)
7	MAN	D	4	7	11,11,12	1.22	1 (9%)	15,15,17	1.02	1 (6%)
7	MAN	D	5	7	11,11,12	1.28	1 (9%)	15,15,17	0.77	1 (6%)
5	NAG	E	1	1,5	14,14,15	1.05	1 (7%)	17,19,21	0.95	1 (5%)
5	NAG	E	2	5	14,14,15	1.28	2 (14%)	17,19,21	0.75	0
5	BMA	E	3	5	11,11,12	1.27	1 (9%)	15,15,17	1.00	1 (6%)
5	NAG	F	1	1,5	14,14,15	1.15	2 (14%)	17,19,21	1.98	5 (29%)
5	NAG	F	2	5	14,14,15	1.36	2 (14%)	17,19,21	0.95	1 (5%)
5	BMA	F	3	5	11,11,12	1.34	2 (18%)	15,15,17	0.85	1 (6%)
6	NAG	G	1	1,6	14,14,15	0.98	0	17,19,21	0.91	1 (5%)
6	NAG	G	2	6	14,14,15	1.18	1 (7%)	17,19,21	0.80	0
5	NAG	H	1	1,5	14,14,15	0.85	0	17,19,21	1.17	2 (11%)
5	NAG	H	2	5	14,14,15	1.03	1 (7%)	17,19,21	1.08	2 (11%)
5	BMA	H	3	5	11,11,12	1.11	1 (9%)	15,15,17	0.89	1 (6%)
5	NAG	I	1	1,5	14,14,15	1.10	2 (14%)	17,19,21	1.10	2 (11%)
5	NAG	I	2	5	14,14,15	1.35	3 (21%)	17,19,21	1.40	2 (11%)
5	BMA	I	3	5	11,11,12	1.42	2 (18%)	15,15,17	0.99	1 (6%)
6	NAG	J	1	1,6	14,14,15	1.13	1 (7%)	17,19,21	1.16	2 (11%)
6	NAG	J	2	6	14,14,15	1.18	2 (14%)	17,19,21	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	K	1	1,5	14,14,15	1.08	1 (7%)	17,19,21	0.83	0
5	NAG	K	2	5	14,14,15	1.36	2 (14%)	17,19,21	0.86	0
5	BMA	K	3	5	11,11,12	1.33	1 (9%)	15,15,17	0.98	1 (6%)
5	NAG	L	1	1,5	14,14,15	1.11	2 (14%)	17,19,21	1.01	1 (5%)
5	NAG	L	2	5	14,14,15	1.29	2 (14%)	17,19,21	1.18	1 (5%)
5	BMA	L	3	5	11,11,12	1.34	2 (18%)	15,15,17	0.79	0
8	NAG	M	1	8	14,14,15	1.04	1 (7%)	17,19,21	0.99	2 (11%)
8	NAG	M	2	8	14,14,15	1.14	2 (14%)	17,19,21	1.03	1 (5%)
8	BMA	M	3	8	11,11,12	1.32	2 (18%)	15,15,17	1.34	1 (6%)
8	MAN	M	4	8	11,11,12	1.20	1 (9%)	15,15,17	1.08	1 (6%)
8	MAN	M	5	8	11,11,12	1.25	2 (18%)	15,15,17	1.24	1 (6%)
8	MAN	M	6	8	11,11,12	1.20	1 (9%)	15,15,17	1.25	1 (6%)
7	NAG	N	1	1,7	14,14,15	1.11	1 (7%)	17,19,21	0.90	0
7	NAG	N	2	7	14,14,15	1.33	3 (21%)	17,19,21	0.72	1 (5%)
7	BMA	N	3	7	11,11,12	1.48	3 (27%)	15,15,17	1.25	1 (6%)
7	MAN	N	4	7	11,11,12	1.22	1 (9%)	15,15,17	1.02	2 (13%)
7	MAN	N	5	7	11,11,12	1.34	2 (18%)	15,15,17	1.01	1 (6%)
5	NAG	O	1	1,5	14,14,15	1.13	1 (7%)	17,19,21	0.93	0
5	NAG	O	2	5	14,14,15	1.36	2 (14%)	17,19,21	0.78	0
5	BMA	O	3	5	11,11,12	1.20	2 (18%)	15,15,17	1.10	1 (6%)
5	NAG	P	1	1,5	14,14,15	1.07	2 (14%)	17,19,21	0.92	1 (5%)
5	NAG	P	2	5	14,14,15	1.12	1 (7%)	17,19,21	1.09	2 (11%)
5	BMA	P	3	5	11,11,12	1.18	1 (9%)	15,15,17	0.87	1 (6%)
6	NAG	Q	1	1,6	14,14,15	1.00	1 (7%)	17,19,21	0.96	0
6	NAG	Q	2	6	14,14,15	1.00	1 (7%)	17,19,21	0.93	1 (5%)
5	NAG	R	1	1,5	14,14,15	1.14	2 (14%)	17,19,21	1.30	3 (17%)
5	NAG	R	2	5	14,14,15	1.41	2 (14%)	17,19,21	0.81	1 (5%)
5	BMA	R	3	5	11,11,12	1.21	1 (9%)	15,15,17	1.03	2 (13%)
7	NAG	S	1	1,7	14,14,15	1.07	1 (7%)	17,19,21	0.91	1 (5%)
7	NAG	S	2	7	14,14,15	1.18	1 (7%)	17,19,21	0.91	0
7	BMA	S	3	7	11,11,12	1.27	2 (18%)	15,15,17	1.35	1 (6%)
7	MAN	S	4	7	11,11,12	1.21	1 (9%)	15,15,17	0.76	0
7	MAN	S	5	7	11,11,12	1.24	1 (9%)	15,15,17	1.07	1 (6%)
5	NAG	T	1	1,5	14,14,15	1.03	0	17,19,21	0.87	0
5	NAG	T	2	5	14,14,15	1.32	3 (21%)	17,19,21	0.70	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	T	3	5	11,11,12	1.21	2 (18%)	15,15,17	1.20	1 (6%)
5	NAG	U	1	1,5	14,14,15	1.40	4 (28%)	17,19,21	1.72	3 (17%)
5	NAG	U	2	5	14,14,15	1.49	4 (28%)	17,19,21	1.25	1 (5%)
5	BMA	U	3	5	11,11,12	1.31	2 (18%)	15,15,17	0.86	0
6	NAG	V	1	1,6	14,14,15	1.16	2 (14%)	17,19,21	1.11	1 (5%)
6	NAG	V	2	6	14,14,15	1.14	1 (7%)	17,19,21	0.79	0
5	NAG	W	1	1,5	14,14,15	0.97	0	17,19,21	0.88	1 (5%)
5	NAG	W	2	5	14,14,15	1.08	1 (7%)	17,19,21	0.82	0
5	BMA	W	3	5	11,11,12	1.09	1 (9%)	15,15,17	1.24	1 (6%)
5	NAG	X	1	1,5	14,14,15	1.09	1 (7%)	17,19,21	1.03	2 (11%)
5	NAG	X	2	5	14,14,15	1.38	4 (28%)	17,19,21	1.24	2 (11%)
5	BMA	X	3	5	11,11,12	1.30	2 (18%)	15,15,17	1.00	1 (6%)
6	NAG	Y	1	1,6	14,14,15	1.19	2 (14%)	17,19,21	0.76	0
6	NAG	Y	2	6	14,14,15	1.21	2 (14%)	17,19,21	1.06	1 (5%)
5	NAG	Z	1	1,5	14,14,15	1.21	2 (14%)	17,19,21	1.29	3 (17%)
5	NAG	Z	2	5	14,14,15	1.40	3 (21%)	17,19,21	1.01	1 (5%)
5	BMA	Z	3	5	11,11,12	1.34	2 (18%)	15,15,17	1.01	1 (6%)
5	NAG	k	1	1,5	14,14,15	1.17	2 (14%)	17,19,21	1.35	2 (11%)
5	NAG	k	2	5	14,14,15	1.38	3 (21%)	17,19,21	0.86	1 (5%)
5	BMA	k	3	5	11,11,12	1.20	2 (18%)	15,15,17	0.93	1 (6%)
5	NAG	l	1	1,5	14,14,15	1.23	2 (14%)	17,19,21	0.62	0
5	NAG	l	2	5	14,14,15	1.48	3 (21%)	17,19,21	0.96	0
5	BMA	l	3	5	11,11,12	1.29	2 (18%)	15,15,17	0.55	0
5	NAG	m	1	1,5	14,14,15	1.28	2 (14%)	17,19,21	1.37	3 (17%)
5	NAG	m	2	5	14,14,15	1.27	2 (14%)	17,19,21	1.20	2 (11%)
5	BMA	m	3	5	11,11,12	1.29	2 (18%)	15,15,17	1.03	1 (6%)
6	NAG	n	1	1,6	14,14,15	1.03	2 (14%)	17,19,21	1.25	2 (11%)
6	NAG	n	2	6	14,14,15	1.15	1 (7%)	17,19,21	0.73	0
5	NAG	o	1	1,5	14,14,15	1.14	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	o	2	5	14,14,15	1.30	2 (14%)	17,19,21	0.68	0
5	BMA	o	3	5	11,11,12	1.09	1 (9%)	15,15,17	0.81	1 (6%)
7	NAG	p	1	1,7	14,14,15	1.01	0	17,19,21	0.92	1 (5%)
7	NAG	p	2	7	14,14,15	1.06	1 (7%)	17,19,21	1.21	2 (11%)
7	BMA	p	3	7	11,11,12	1.31	2 (18%)	15,15,17	1.27	1 (6%)
7	MAN	p	4	7	11,11,12	1.28	2 (18%)	15,15,17	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	p	5	7	11,11,12	1.37	2 (18%)	15,15,17	1.24	1 (6%)
5	NAG	q	1	1,5	14,14,15	1.03	1 (7%)	17,19,21	1.12	2 (11%)
5	NAG	q	2	5	14,14,15	1.34	3 (21%)	17,19,21	0.87	1 (5%)
5	BMA	q	3	5	11,11,12	1.25	1 (9%)	15,15,17	0.76	0
5	NAG	r	1	1,5	14,14,15	1.31	2 (14%)	17,19,21	1.66	3 (17%)
5	NAG	r	2	5	14,14,15	1.45	4 (28%)	17,19,21	1.36	1 (5%)
5	BMA	r	3	5	11,11,12	1.37	2 (18%)	15,15,17	0.88	0
6	NAG	s	1	1,6	14,14,15	1.33	3 (21%)	17,19,21	1.70	5 (29%)
6	NAG	s	2	6	14,14,15	1.10	0	17,19,21	0.93	1 (5%)
5	NAG	t	1	1,5	14,14,15	1.11	2 (14%)	17,19,21	1.52	4 (23%)
5	NAG	t	2	5	14,14,15	1.29	2 (14%)	17,19,21	0.70	0
5	BMA	t	3	5	11,11,12	1.34	2 (18%)	15,15,17	0.88	1 (6%)
5	NAG	u	1	1,5	14,14,15	1.20	3 (21%)	17,19,21	1.20	2 (11%)
5	NAG	u	2	5	14,14,15	1.23	2 (14%)	17,19,21	1.12	1 (5%)
5	BMA	u	3	5	11,11,12	1.29	2 (18%)	15,15,17	1.07	1 (6%)
6	NAG	v	1	1,6	14,14,15	1.23	2 (14%)	17,19,21	1.16	2 (11%)
6	NAG	v	2	6	14,14,15	1.23	1 (7%)	17,19,21	1.36	1 (5%)
5	NAG	w	1	1,5	14,14,15	1.18	1 (7%)	17,19,21	0.65	0
5	NAG	w	2	5	14,14,15	1.44	4 (28%)	17,19,21	0.78	0
5	BMA	w	3	5	11,11,12	1.12	1 (9%)	15,15,17	1.11	1 (6%)
5	NAG	x	1	1,5	14,14,15	1.34	2 (14%)	17,19,21	1.13	2 (11%)
5	NAG	x	2	5	14,14,15	1.38	2 (14%)	17,19,21	1.14	1 (5%)
5	BMA	x	3	5	11,11,12	1.26	1 (9%)	15,15,17	0.86	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1	5	-	0/6/23/26	0/1/1/1
5	NAG	A	2	5	-	2/6/23/26	0/1/1/1
5	BMA	A	3	5	-	0/2/19/22	0/1/1/1
6	NAG	B	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	2	6	-	1/6/23/26	0/1/1/1
5	NAG	C	1	5	-	1/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
7	NAG	D	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	2	7	-	0/6/23/26	0/1/1/1
7	BMA	D	3	7	-	0/2/19/22	0/1/1/1
7	MAN	D	4	7	-	0/2/19/22	0/1/1/1
7	MAN	D	5	7	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	1/2/19/22	0/1/1/1
6	NAG	G	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	1/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	NAG	L	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
5	BMA	L	3	5	-	0/2/19/22	0/1/1/1
8	NAG	M	1	8	-	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	MAN	M	4	8	-	0/2/19/22	0/1/1/1
8	MAN	M	5	8	-	0/2/19/22	0/1/1/1
8	MAN	M	6	8	-	0/2/19/22	0/1/1/1
7	NAG	N	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
7	MAN	N	4	7	-	0/2/19/22	0/1/1/1
7	MAN	N	5	7	-	0/2/19/22	0/1/1/1
5	NAG	O	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	m	2	5	-	2/6/23/26	0/1/1/1
5	BMA	m	3	5	-	0/2/19/22	0/1/1/1
6	NAG	n	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	n	2	6	-	1/6/23/26	0/1/1/1
5	NAG	o	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	o	2	5	-	0/6/23/26	0/1/1/1
5	BMA	o	3	5	-	0/2/19/22	0/1/1/1
7	NAG	p	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	p	2	7	-	0/6/23/26	0/1/1/1
7	BMA	p	3	7	-	0/2/19/22	0/1/1/1
7	MAN	p	4	7	-	0/2/19/22	0/1/1/1
7	MAN	p	5	7	-	0/2/19/22	0/1/1/1
5	NAG	q	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	q	2	5	-	0/6/23/26	0/1/1/1
5	BMA	q	3	5	-	0/2/19/22	0/1/1/1
5	NAG	r	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	r	2	5	-	0/6/23/26	0/1/1/1
5	BMA	r	3	5	-	1/2/19/22	0/1/1/1
6	NAG	s	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	s	2	6	-	1/6/23/26	0/1/1/1
5	NAG	t	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	t	2	5	-	1/6/23/26	0/1/1/1
5	BMA	t	3	5	-	1/2/19/22	0/1/1/1
5	NAG	u	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	u	2	5	-	0/6/23/26	0/1/1/1
5	BMA	u	3	5	-	0/2/19/22	0/1/1/1
6	NAG	v	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	v	2	6	-	2/6/23/26	0/1/1/1
5	NAG	w	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	w	2	5	-	2/6/23/26	0/1/1/1
5	BMA	w	3	5	-	0/2/19/22	0/1/1/1
5	NAG	x	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	x	2	5	-	0/6/23/26	0/1/1/1
5	BMA	x	3	5	-	0/2/19/22	0/1/1/1

All (209) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	3	BMA	O5-C5	3.27	1.49	1.43
5	r	3	BMA	O5-C5	3.18	1.49	1.43
5	U	2	NAG	C1-C2	3.16	1.56	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Z	3	BMA	O5-C5	3.12	1.49	1.43
5	L	3	BMA	O5-C5	3.05	1.49	1.43
5	C	3	BMA	O5-C5	3.05	1.49	1.43
5	R	2	NAG	O5-C5	3.04	1.49	1.43
6	B	1	NAG	O5-C5	3.02	1.49	1.43
7	p	5	MAN	O5-C5	2.99	1.49	1.43
5	q	2	NAG	O5-C5	2.98	1.49	1.43
5	l	2	NAG	O5-C5	2.98	1.49	1.43
5	Z	2	NAG	O5-C5	2.96	1.49	1.43
5	r	2	NAG	C1-C2	2.96	1.56	1.52
5	K	2	NAG	O5-C5	2.94	1.49	1.43
7	N	3	BMA	O5-C5	2.94	1.49	1.43
7	D	5	MAN	O5-C5	2.94	1.49	1.43
5	A	3	BMA	O5-C5	2.94	1.49	1.43
5	w	2	NAG	O5-C5	2.92	1.49	1.43
5	E	3	BMA	O5-C5	2.90	1.49	1.43
7	N	2	NAG	O5-C5	2.89	1.49	1.43
5	m	3	BMA	O5-C5	2.89	1.49	1.43
5	l	3	BMA	O5-C5	2.88	1.49	1.43
5	x	1	NAG	O5-C5	2.88	1.49	1.43
7	S	5	MAN	O5-C5	2.87	1.49	1.43
5	o	2	NAG	O5-C5	2.83	1.48	1.43
5	t	3	BMA	O5-C5	2.83	1.48	1.43
6	J	2	NAG	O5-C5	2.83	1.48	1.43
8	M	6	MAN	O5-C5	2.82	1.48	1.43
5	A	2	NAG	C1-C2	2.80	1.56	1.52
5	k	1	NAG	O5-C5	2.79	1.48	1.43
5	I	2	NAG	O5-C5	2.79	1.48	1.43
5	k	3	BMA	O5-C5	2.79	1.48	1.43
5	Z	1	NAG	O5-C5	2.78	1.48	1.43
5	F	3	BMA	O5-C5	2.78	1.48	1.43
6	G	2	NAG	O5-C5	2.77	1.48	1.43
7	N	5	MAN	O5-C5	2.76	1.48	1.43
5	u	3	BMA	O5-C5	2.76	1.48	1.43
5	x	2	NAG	O5-C5	2.75	1.48	1.43
5	U	3	BMA	O5-C5	2.75	1.48	1.43
5	k	2	NAG	O5-C5	2.74	1.48	1.43
5	X	3	BMA	O5-C5	2.74	1.48	1.43
7	p	4	MAN	O5-C5	2.73	1.48	1.43
7	S	4	MAN	O5-C5	2.72	1.48	1.43
7	N	4	MAN	O5-C5	2.70	1.48	1.43
5	F	2	NAG	O4-C4	2.70	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	3	BMA	O5-C5	2.69	1.48	1.43
8	M	2	NAG	O5-C5	2.67	1.48	1.43
8	M	5	MAN	O5-C5	2.67	1.48	1.43
6	v	2	NAG	O5-C5	2.66	1.48	1.43
8	M	3	BMA	O5-C5	2.66	1.48	1.43
5	X	2	NAG	O5-C5	2.65	1.48	1.43
5	T	2	NAG	O5-C5	2.65	1.48	1.43
5	x	2	NAG	O4-C4	2.64	1.49	1.43
7	D	4	MAN	O5-C5	2.63	1.48	1.43
5	F	2	NAG	O5-C5	2.63	1.48	1.43
7	D	1	NAG	O5-C5	2.62	1.48	1.43
6	V	2	NAG	O5-C5	2.62	1.48	1.43
7	D	3	BMA	O5-C5	2.61	1.48	1.43
5	I	3	BMA	O5-C1	2.61	1.48	1.43
5	l	2	NAG	O5-C1	2.60	1.48	1.43
7	D	3	BMA	O3-C3	2.58	1.49	1.43
5	E	2	NAG	O5-C5	2.58	1.48	1.43
5	o	2	NAG	O4-C4	2.58	1.49	1.43
5	U	1	NAG	C1-C2	2.58	1.55	1.52
5	E	1	NAG	O5-C5	2.57	1.48	1.43
6	B	2	NAG	O5-C5	2.57	1.48	1.43
5	K	3	BMA	O5-C5	2.57	1.48	1.43
5	O	3	BMA	O5-C5	2.57	1.48	1.43
5	u	2	NAG	O5-C5	2.55	1.48	1.43
8	M	5	MAN	O5-C1	2.55	1.48	1.43
5	q	3	BMA	O5-C5	2.55	1.48	1.43
5	t	2	NAG	O5-C5	2.55	1.48	1.43
5	U	2	NAG	O4-C4	2.54	1.49	1.43
5	r	2	NAG	O4-C4	2.53	1.49	1.43
5	A	1	NAG	O5-C5	2.53	1.48	1.43
7	N	5	MAN	O5-C1	2.52	1.47	1.43
6	n	2	NAG	O5-C5	2.50	1.48	1.43
7	D	2	NAG	O5-C5	2.50	1.48	1.43
5	k	2	NAG	O4-C4	2.49	1.49	1.43
5	I	2	NAG	O4-C4	2.49	1.49	1.43
5	T	3	BMA	O5-C5	2.48	1.48	1.43
5	L	2	NAG	O5-C5	2.48	1.48	1.43
6	v	1	NAG	O5-C5	2.47	1.48	1.43
5	u	1	NAG	O5-C5	2.46	1.48	1.43
6	J	1	NAG	O5-C5	2.46	1.48	1.43
5	t	2	NAG	O4-C4	2.44	1.49	1.43
7	S	3	BMA	O3-C3	2.44	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	o	3	BMA	O5-C5	2.43	1.48	1.43
5	A	1	NAG	O5-C1	2.43	1.47	1.43
7	p	3	BMA	O3-C3	2.43	1.49	1.43
5	R	2	NAG	O4-C4	2.43	1.49	1.43
5	C	2	NAG	O4-C4	2.42	1.49	1.43
5	O	2	NAG	O5-C5	2.42	1.48	1.43
5	F	1	NAG	O4-C4	2.42	1.49	1.43
5	O	2	NAG	O4-C4	2.42	1.48	1.43
6	s	1	NAG	C1-C2	2.41	1.55	1.52
5	r	2	NAG	O5-C5	2.41	1.48	1.43
6	Y	2	NAG	O5-C5	2.41	1.48	1.43
7	S	2	NAG	O5-C5	2.41	1.48	1.43
5	x	3	BMA	O5-C5	2.40	1.48	1.43
8	M	4	MAN	O5-C5	2.40	1.48	1.43
6	Y	1	NAG	C1-C2	2.40	1.55	1.52
5	w	1	NAG	O5-C5	2.40	1.48	1.43
7	N	3	BMA	O3-C3	2.39	1.48	1.43
5	L	2	NAG	O4-C4	2.39	1.48	1.43
5	q	1	NAG	O5-C5	2.39	1.48	1.43
7	S	1	NAG	O5-C5	2.38	1.48	1.43
5	U	1	NAG	O5-C1	2.38	1.47	1.43
5	P	3	BMA	O5-C5	2.37	1.48	1.43
5	t	3	BMA	O5-C1	2.36	1.47	1.43
5	L	1	NAG	O4-C4	2.36	1.48	1.43
5	K	2	NAG	O4-C4	2.36	1.48	1.43
5	m	1	NAG	O5-C5	2.36	1.48	1.43
8	M	3	BMA	O3-C3	2.36	1.48	1.43
5	X	2	NAG	O4-C4	2.35	1.48	1.43
5	m	2	NAG	O5-C5	2.34	1.48	1.43
5	F	3	BMA	O5-C1	2.34	1.47	1.43
5	U	1	NAG	O4-C4	2.33	1.48	1.43
5	Z	1	NAG	O4-C4	2.33	1.48	1.43
5	T	2	NAG	O4-C4	2.32	1.48	1.43
7	p	5	MAN	O5-C1	2.30	1.47	1.43
5	x	1	NAG	O4-C4	2.30	1.48	1.43
5	u	1	NAG	C1-C2	2.29	1.55	1.52
5	U	3	BMA	O5-C1	2.29	1.47	1.43
5	w	2	NAG	O4-C4	2.29	1.48	1.43
7	N	3	BMA	O5-C1	2.28	1.47	1.43
5	C	3	BMA	O5-C1	2.28	1.47	1.43
5	L	1	NAG	O5-C5	2.28	1.47	1.43
5	I	1	NAG	O5-C5	2.27	1.47	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	1	NAG	O5-C5	2.26	1.47	1.43
5	L	3	BMA	O5-C1	2.25	1.47	1.43
5	H	3	BMA	O5-C5	2.25	1.47	1.43
5	Z	2	NAG	O4-C4	2.24	1.48	1.43
5	u	3	BMA	O5-C1	2.24	1.47	1.43
5	r	1	NAG	O4-C4	2.23	1.48	1.43
5	l	1	NAG	O5-C5	2.23	1.47	1.43
5	r	1	NAG	C1-C2	2.23	1.55	1.52
5	P	1	NAG	O5-C5	2.23	1.47	1.43
6	V	1	NAG	C1-C2	2.23	1.55	1.52
5	l	2	NAG	O4-C4	2.22	1.48	1.43
6	v	1	NAG	O4-C4	2.20	1.48	1.43
5	A	2	NAG	O5-C5	2.19	1.47	1.43
5	t	1	NAG	O5-C5	2.19	1.47	1.43
6	B	2	NAG	C1-C2	2.19	1.55	1.52
5	o	1	NAG	C1-C2	2.18	1.55	1.52
5	k	2	NAG	C1-C2	2.18	1.55	1.52
5	w	3	BMA	O5-C5	2.18	1.47	1.43
6	s	1	NAG	O4-C4	2.18	1.48	1.43
5	E	2	NAG	O4-C4	2.17	1.48	1.43
5	m	1	NAG	O4-C4	2.17	1.48	1.43
8	M	1	NAG	O5-C5	2.17	1.47	1.43
6	B	1	NAG	O4-C4	2.17	1.48	1.43
7	N	2	NAG	O4-C4	2.16	1.48	1.43
5	u	2	NAG	O4-C4	2.16	1.48	1.43
6	n	1	NAG	O4-C4	2.16	1.48	1.43
7	S	3	BMA	O5-C5	2.15	1.47	1.43
5	R	1	NAG	O4-C4	2.15	1.48	1.43
5	k	1	NAG	O4-C4	2.15	1.48	1.43
5	m	3	BMA	O5-C1	2.15	1.47	1.43
7	p	2	NAG	O5-C5	2.14	1.47	1.43
5	X	2	NAG	C1-C2	2.14	1.55	1.52
7	N	1	NAG	O5-C5	2.14	1.47	1.43
5	Z	2	NAG	C1-C2	2.13	1.55	1.52
7	p	3	BMA	O5-C5	2.13	1.47	1.43
7	N	2	NAG	O5-C1	2.13	1.47	1.43
5	X	3	BMA	O5-C1	2.13	1.47	1.43
5	r	3	BMA	O5-C1	2.12	1.47	1.43
5	w	2	NAG	O5-C1	2.12	1.47	1.43
5	Z	3	BMA	O5-C1	2.12	1.47	1.43
5	H	2	NAG	O4-C4	2.12	1.48	1.43
6	s	1	NAG	O5-C5	2.11	1.47	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	1	NAG	O5-C5	2.11	1.47	1.43
5	r	2	NAG	O5-C1	2.11	1.47	1.43
6	V	1	NAG	O5-C5	2.10	1.47	1.43
5	I	1	NAG	O4-C4	2.10	1.48	1.43
5	O	1	NAG	O5-C5	2.09	1.47	1.43
5	m	2	NAG	O4-C4	2.09	1.48	1.43
5	q	2	NAG	O4-C4	2.09	1.48	1.43
5	u	1	NAG	O4-C4	2.08	1.48	1.43
5	R	1	NAG	O5-C5	2.08	1.47	1.43
6	Y	1	NAG	O5-C5	2.08	1.47	1.43
5	l	1	NAG	O4-C4	2.08	1.48	1.43
5	t	1	NAG	C1-C2	2.07	1.55	1.52
5	F	1	NAG	O5-C5	2.07	1.47	1.43
6	n	1	NAG	O5-C5	2.07	1.47	1.43
5	A	1	NAG	O4-C4	2.07	1.48	1.43
8	M	2	NAG	O5-C1	2.06	1.47	1.43
5	K	1	NAG	O5-C5	2.06	1.47	1.43
5	I	2	NAG	O5-C1	2.06	1.47	1.43
5	k	3	BMA	O5-C1	2.06	1.47	1.43
5	l	3	BMA	O5-C1	2.06	1.47	1.43
5	U	2	NAG	O5-C5	2.05	1.47	1.43
5	T	3	BMA	O5-C1	2.05	1.47	1.43
6	Y	2	NAG	O5-C1	2.05	1.47	1.43
5	w	2	NAG	C1-C2	2.04	1.55	1.52
5	W	3	BMA	O5-C5	2.04	1.47	1.43
5	P	2	NAG	O5-C5	2.04	1.47	1.43
5	q	2	NAG	O5-C1	2.04	1.47	1.43
5	U	1	NAG	O5-C5	2.04	1.47	1.43
5	O	3	BMA	O5-C1	2.03	1.47	1.43
5	U	2	NAG	O5-C1	2.03	1.47	1.43
5	P	1	NAG	O4-C4	2.03	1.48	1.43
6	Q	2	NAG	O5-C5	2.02	1.47	1.43
5	W	2	NAG	O5-C5	2.02	1.47	1.43
5	X	2	NAG	O5-C1	2.02	1.47	1.43
6	B	2	NAG	O5-C1	2.02	1.47	1.43
5	T	2	NAG	O5-C1	2.01	1.47	1.43
7	p	4	MAN	O5-C1	2.01	1.47	1.43
6	J	2	NAG	O5-C1	2.00	1.47	1.43

All (133) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	1	NAG	C1-O5-C5	5.37	119.39	112.19
5	r	1	NAG	C1-O5-C5	5.11	119.04	112.19
6	v	2	NAG	C1-O5-C5	5.07	118.99	112.19
5	A	1	NAG	C1-O5-C5	4.42	118.11	112.19
5	I	2	NAG	C1-O5-C5	4.41	118.10	112.19
7	p	5	MAN	C1-O5-C5	4.31	117.97	112.19
8	M	3	BMA	C1-O5-C5	4.26	117.90	112.19
5	F	1	NAG	C4-C3-C2	4.24	117.23	111.02
7	S	3	BMA	C1-O5-C5	4.16	117.76	112.19
5	r	2	NAG	C1-O5-C5	4.15	117.75	112.19
8	M	6	MAN	C1-O5-C5	4.10	117.68	112.19
8	M	5	MAN	C1-O5-C5	4.02	117.57	112.19
5	x	2	NAG	C1-O5-C5	3.98	117.52	112.19
7	D	3	BMA	C1-O5-C5	3.94	117.47	112.19
5	F	1	NAG	O4-C4-C3	-3.90	101.19	110.38
5	X	2	NAG	C1-O5-C5	3.87	117.37	112.19
6	s	1	NAG	C1-O5-C5	3.84	117.34	112.19
5	u	2	NAG	C1-O5-C5	3.77	117.24	112.19
5	F	1	NAG	C1-O5-C5	3.75	117.21	112.19
7	N	3	BMA	C1-O5-C5	3.74	117.20	112.19
5	U	2	NAG	C1-O5-C5	3.74	117.20	112.19
5	W	3	BMA	C1-O5-C5	3.67	117.11	112.19
5	L	2	NAG	C1-O5-C5	3.66	117.10	112.19
5	T	3	BMA	C1-O5-C5	3.62	117.04	112.19
7	p	3	BMA	C1-O5-C5	3.51	116.89	112.19
5	m	3	BMA	C1-O5-C5	3.49	116.87	112.19
5	u	3	BMA	C1-O5-C5	3.49	116.86	112.19
6	Y	2	NAG	C1-O5-C5	3.45	116.82	112.19
5	m	2	NAG	C1-O5-C5	3.44	116.79	112.19
5	t	1	NAG	C4-C3-C2	3.42	116.02	111.02
8	M	2	NAG	C1-O5-C5	3.41	116.76	112.19
5	A	3	BMA	C1-O5-C5	3.36	116.69	112.19
7	S	5	MAN	C1-O5-C5	3.24	116.53	112.19
7	p	2	NAG	C1-O5-C5	3.24	116.52	112.19
5	u	1	NAG	C4-C3-C2	-3.23	106.28	111.02
5	k	1	NAG	C4-C3-C2	-3.18	106.36	111.02
5	O	3	BMA	C1-O5-C5	3.15	116.41	112.19
5	I	3	BMA	C1-O5-C5	3.12	116.36	112.19
5	w	3	BMA	C1-O5-C5	3.05	116.28	112.19
5	E	3	BMA	C1-O5-C5	3.01	116.22	112.19
5	q	2	NAG	C1-O5-C5	2.97	116.17	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	1	NAG	O5-C5-C4	-2.97	103.61	110.83
5	I	2	NAG	O5-C1-C2	-2.96	106.71	111.29
5	Z	1	NAG	O4-C4-C3	-2.95	103.42	110.38
5	P	3	BMA	C1-O5-C5	2.95	116.14	112.19
8	M	1	NAG	C1-O5-C5	2.94	116.13	112.19
5	K	3	BMA	C1-O5-C5	2.93	116.11	112.19
5	R	1	NAG	C2-N2-C7	2.88	126.77	122.90
5	L	1	NAG	C1-O5-C5	2.88	116.04	112.19
5	o	1	NAG	O4-C4-C5	-2.84	102.33	109.32
5	k	1	NAG	C1-O5-C5	2.82	115.97	112.19
6	J	2	NAG	C1-O5-C5	2.82	115.96	112.19
5	m	1	NAG	O4-C4-C3	-2.80	103.77	110.38
5	q	1	NAG	O5-C1-C2	-2.79	106.97	111.29
5	R	1	NAG	O4-C4-C5	-2.79	102.45	109.32
6	s	1	NAG	O5-C5-C4	-2.79	104.04	110.83
5	X	3	BMA	C1-O5-C5	2.77	115.90	112.19
6	n	1	NAG	O5-C1-C2	-2.76	107.03	111.29
5	E	1	NAG	O5-C1-C2	-2.75	107.03	111.29
5	I	1	NAG	C4-C3-C2	-2.72	107.03	111.02
7	D	2	NAG	O5-C1-C2	-2.72	107.09	111.29
5	Z	2	NAG	O5-C1-C2	-2.72	107.09	111.29
5	t	1	NAG	O4-C4-C5	-2.70	102.67	109.32
5	R	1	NAG	C4-C3-C2	2.69	114.96	111.02
5	F	2	NAG	C3-C4-C5	2.68	115.10	110.23
5	x	3	BMA	C1-O5-C5	2.68	115.78	112.19
5	t	1	NAG	O5-C1-C2	-2.68	107.14	111.29
5	H	1	NAG	O5-C1-C2	-2.68	107.15	111.29
5	m	1	NAG	C1-O5-C5	-2.63	108.66	112.19
8	M	4	MAN	C1-O5-C5	2.62	115.70	112.19
6	s	1	NAG	O4-C4-C5	2.61	115.76	109.32
5	Z	1	NAG	C1-O5-C5	2.61	115.68	112.19
5	A	2	NAG	C1-O5-C5	2.61	115.68	112.19
6	s	1	NAG	C6-C5-C4	2.59	119.39	113.02
5	R	3	BMA	C1-O5-C5	2.59	115.66	112.19
5	k	3	BMA	C1-O5-C5	2.57	115.62	112.19
6	V	1	NAG	O4-C4-C3	-2.56	104.33	110.38
5	Z	3	BMA	C1-O5-C5	2.56	115.62	112.19
5	x	1	NAG	C1-O5-C5	2.54	115.59	112.19
5	H	2	NAG	C1-O5-C5	2.52	115.57	112.19
5	t	3	BMA	C1-O5-C5	2.52	115.56	112.19
5	k	2	NAG	C1-O5-C5	2.51	115.55	112.19
7	N	5	MAN	C1-O5-C5	2.51	115.55	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	1	NAG	O5-C1-C2	-2.51	107.41	111.29
5	r	1	NAG	O5-C5-C4	-2.47	104.82	110.83
6	Q	2	NAG	C1-O5-C5	2.45	115.47	112.19
7	D	4	MAN	C1-O5-C5	2.44	115.46	112.19
5	q	1	NAG	C1-C2-N2	2.42	114.25	110.43
5	X	1	NAG	O4-C4-C5	-2.42	103.35	109.32
7	D	5	MAN	C1-O5-C5	2.38	115.38	112.19
5	X	2	NAG	O5-C1-C2	-2.37	107.63	111.29
5	R	2	NAG	C4-C3-C2	-2.36	107.55	111.02
6	s	1	NAG	C4-C3-C2	-2.36	107.56	111.02
6	s	2	NAG	O5-C1-C2	-2.31	107.72	111.29
5	m	1	NAG	C4-C3-C2	2.31	114.40	111.02
5	o	3	BMA	C1-O5-C5	2.29	115.25	112.19
5	W	1	NAG	O5-C1-C2	-2.28	107.76	111.29
5	H	3	BMA	C1-O5-C5	2.28	115.24	112.19
7	p	1	NAG	C1-O5-C5	2.26	115.21	112.19
6	v	1	NAG	O4-C4-C5	2.26	114.88	109.32
6	G	1	NAG	C1-O5-C5	2.25	115.20	112.19
5	P	2	NAG	C1-C2-N2	2.23	113.95	110.43
5	H	2	NAG	O5-C1-C2	-2.23	107.85	111.29
5	T	2	NAG	C1-O5-C5	2.22	115.17	112.19
5	H	1	NAG	O4-C4-C5	-2.22	103.86	109.32
6	n	1	NAG	O4-C4-C5	-2.22	103.86	109.32
8	M	1	NAG	O4-C4-C5	-2.22	103.86	109.32
7	N	4	MAN	C1-O5-C5	2.21	115.15	112.19
5	I	1	NAG	O5-C1-C2	-2.20	107.88	111.29
5	F	3	BMA	C1-O5-C5	2.20	115.13	112.19
7	S	1	NAG	O4-C4-C3	-2.17	105.26	110.38
5	C	2	NAG	C1-O5-C5	2.16	115.08	112.19
5	P	2	NAG	O4-C4-C5	-2.15	104.03	109.32
6	v	1	NAG	O4-C4-C3	-2.14	105.32	110.38
5	r	1	NAG	C6-C5-C4	2.13	118.26	113.02
5	P	1	NAG	O4-C4-C3	-2.12	105.38	110.38
6	J	1	NAG	C1-C2-N2	2.12	113.78	110.43
5	U	1	NAG	O4-C4-C5	2.11	114.51	109.32
7	p	2	NAG	C4-C3-C2	-2.10	107.94	111.02
5	m	2	NAG	C2-N2-C7	2.10	125.71	122.90
5	t	1	NAG	O4-C4-C3	-2.10	105.44	110.38
5	Z	1	NAG	O5-C1-C2	-2.08	108.08	111.29
6	B	1	NAG	O4-C4-C3	-2.07	105.50	110.38
5	C	3	BMA	C1-O5-C5	2.06	114.95	112.19
5	u	1	NAG	O3-C3-C2	2.06	113.69	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	4	MAN	C1-C2-C3	2.06	112.65	109.64
5	C	1	NAG	O5-C5-C4	-2.06	105.82	110.83
5	X	1	NAG	O5-C1-C2	-2.06	108.11	111.29
7	N	2	NAG	C1-O5-C5	2.05	114.93	112.19
5	F	1	NAG	C1-C2-N2	-2.03	107.23	110.43
5	R	3	BMA	C1-C2-C3	2.03	112.59	109.64
5	x	1	NAG	C4-C3-C2	-2.01	108.08	111.02
5	F	1	NAG	C6-C5-C4	2.00	117.94	113.02

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1	NAG	C1-C2-N2-C7
5	E	1	NAG	C1-C2-N2-C7
5	l	2	NAG	C1-C2-N2-C7
5	o	1	NAG	C1-C2-N2-C7
5	t	1	NAG	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
5	t	1	NAG	C4-C5-C6-O6
6	s	1	NAG	O5-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
5	I	1	NAG	C8-C7-N2-C2
5	Z	1	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	W	3	BMA	O5-C5-C6-O6
6	s	2	NAG	O5-C5-C6-O6
5	U	3	BMA	O5-C5-C6-O6
5	t	3	BMA	O5-C5-C6-O6
5	r	3	BMA	O5-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
6	B	2	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
6	n	2	NAG	O5-C5-C6-O6
5	q	1	NAG	C3-C2-N2-C7
6	V	2	NAG	O5-C5-C6-O6
8	M	3	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

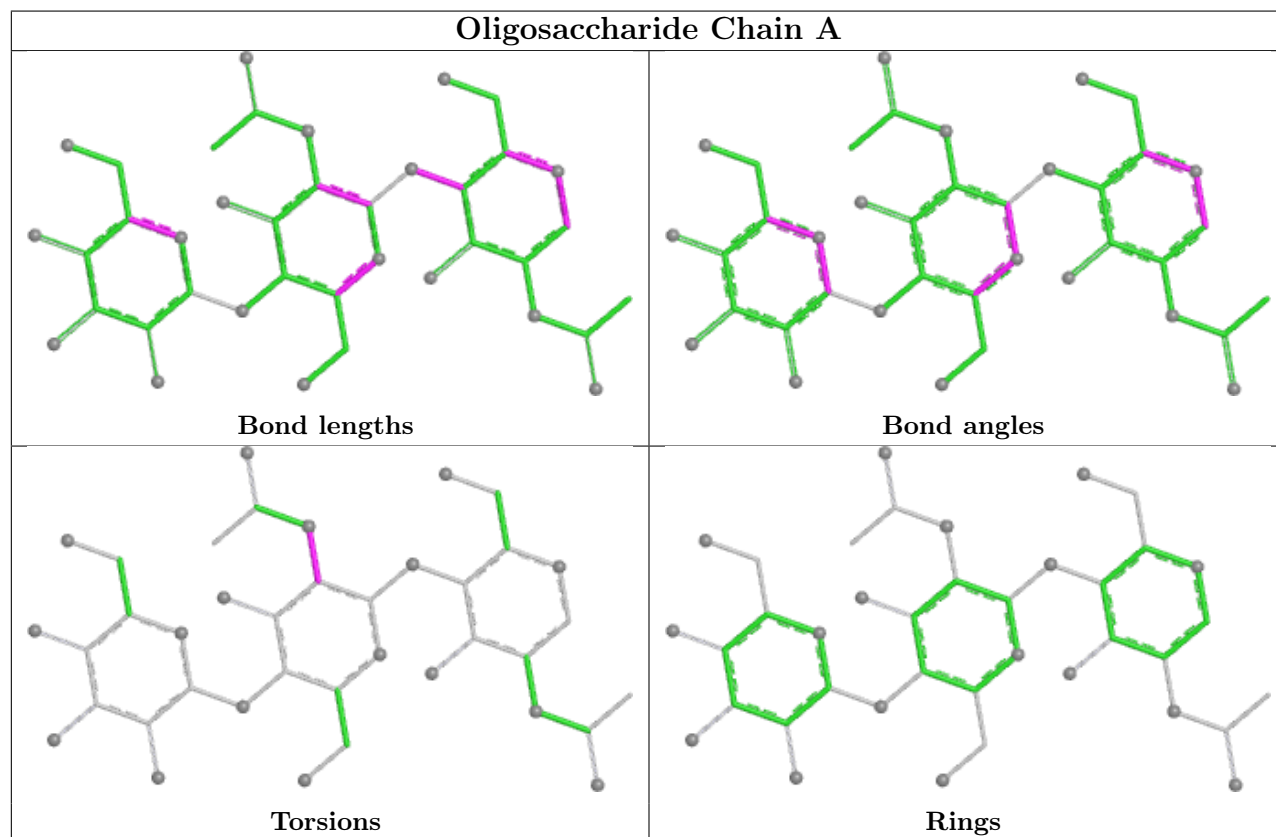
Mol	Chain	Res	Type	Atoms
5	P	2	NAG	O5-C5-C6-O6
6	s	1	NAG	C4-C5-C6-O6
5	A	2	NAG	C1-C2-N2-C7
5	K	2	NAG	C1-C2-N2-C7
5	O	2	NAG	C1-C2-N2-C7
5	R	1	NAG	C1-C2-N2-C7
5	Z	2	NAG	C1-C2-N2-C7
5	m	2	NAG	C1-C2-N2-C7
6	J	1	NAG	C1-C2-N2-C7
6	v	1	NAG	C1-C2-N2-C7
7	N	1	NAG	C1-C2-N2-C7
5	I	1	NAG	O7-C7-N2-C2
5	A	2	NAG	C3-C2-N2-C7
5	K	2	NAG	C3-C2-N2-C7
5	O	2	NAG	C3-C2-N2-C7
5	P	2	NAG	C3-C2-N2-C7
5	T	1	NAG	C3-C2-N2-C7
5	Z	2	NAG	C3-C2-N2-C7
6	Y	1	NAG	C3-C2-N2-C7
6	v	1	NAG	C3-C2-N2-C7
5	X	1	NAG	C8-C7-N2-C2
5	H	1	NAG	C4-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
6	v	1	NAG	C4-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	Z	1	NAG	C4-C5-C6-O6
5	P	2	NAG	C1-C2-N2-C7
5	T	1	NAG	C1-C2-N2-C7
5	w	2	NAG	C1-C2-N2-C7
6	Q	1	NAG	C1-C2-N2-C7
6	Y	1	NAG	C1-C2-N2-C7
7	p	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C3-C2-N2-C7
5	R	1	NAG	C3-C2-N2-C7
5	m	2	NAG	C3-C2-N2-C7
5	o	1	NAG	C3-C2-N2-C7
5	w	2	NAG	C3-C2-N2-C7
6	J	1	NAG	C3-C2-N2-C7
7	N	1	NAG	C3-C2-N2-C7
6	v	2	NAG	O5-C5-C6-O6
5	t	2	NAG	C8-C7-N2-C2
6	v	2	NAG	C4-C5-C6-O6

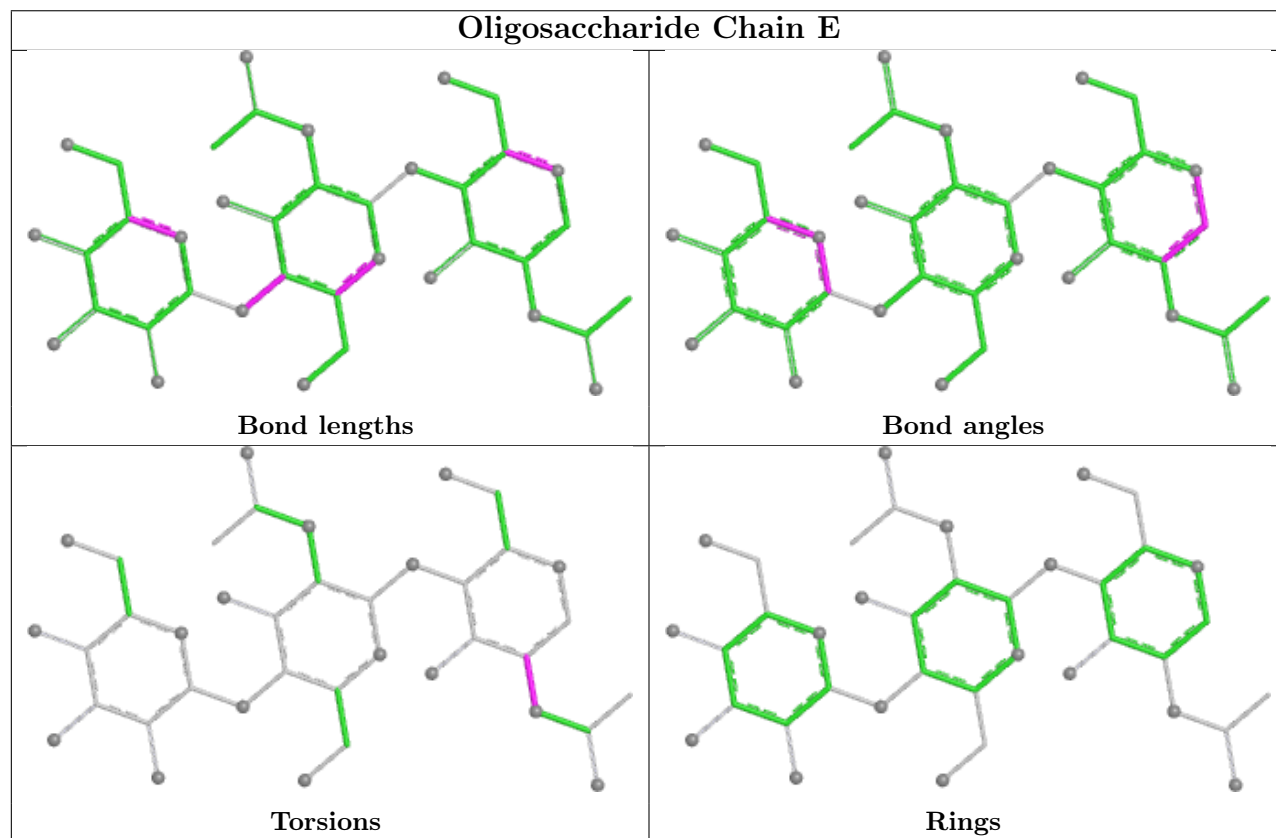
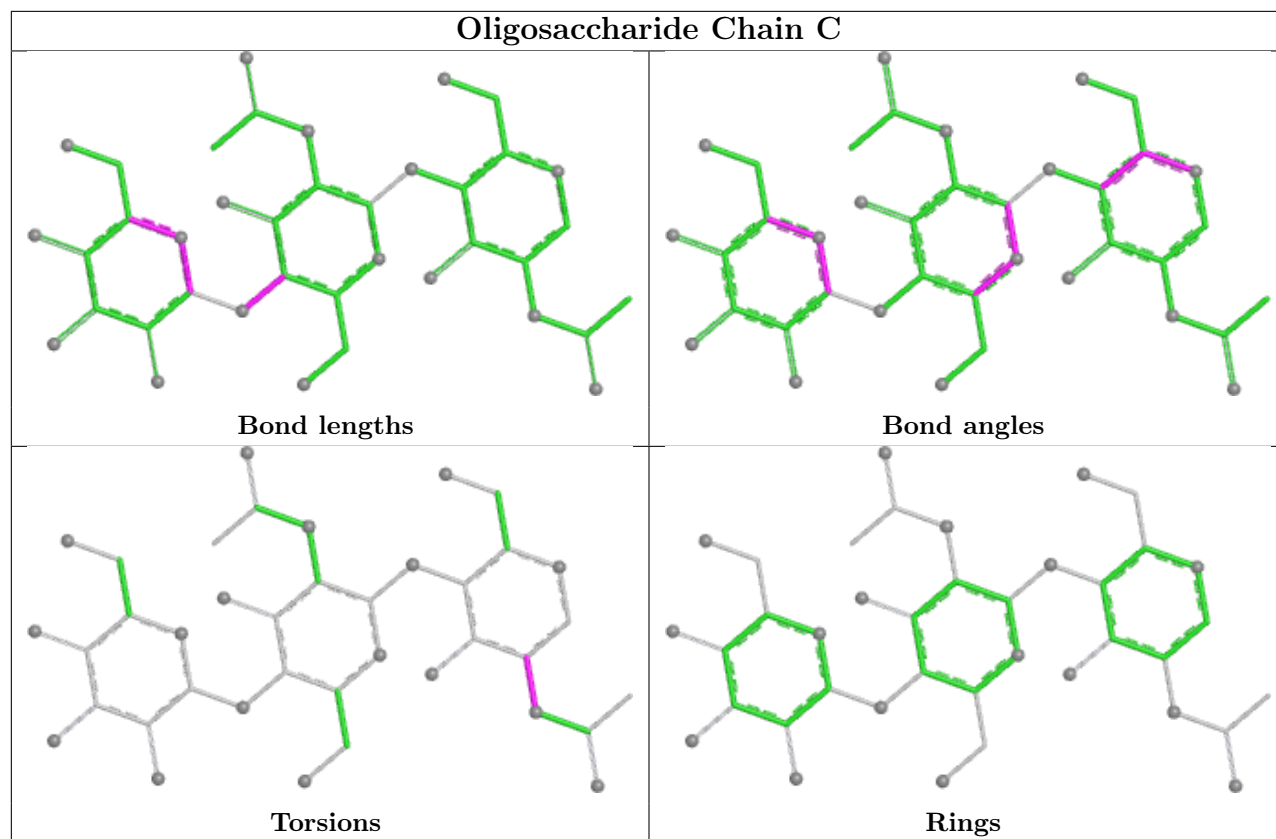
There are no ring outliers.

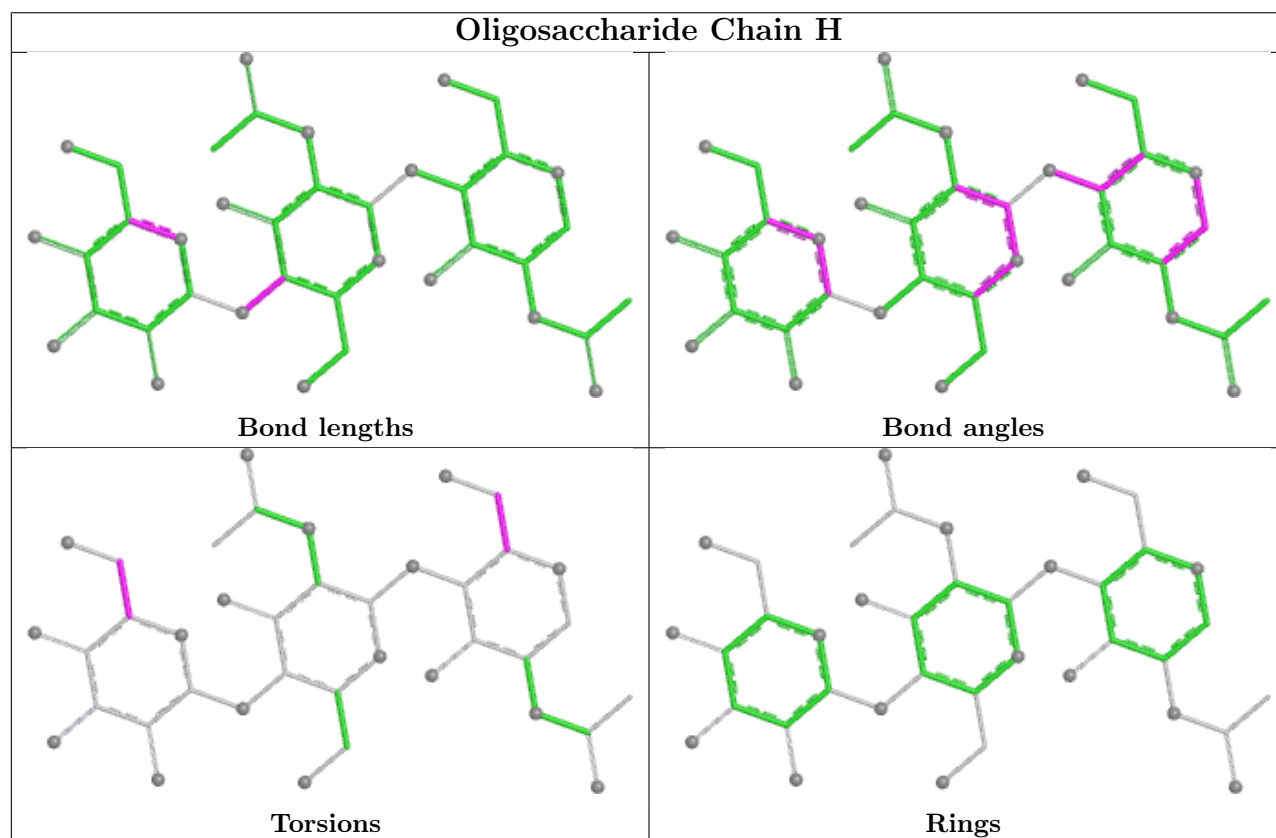
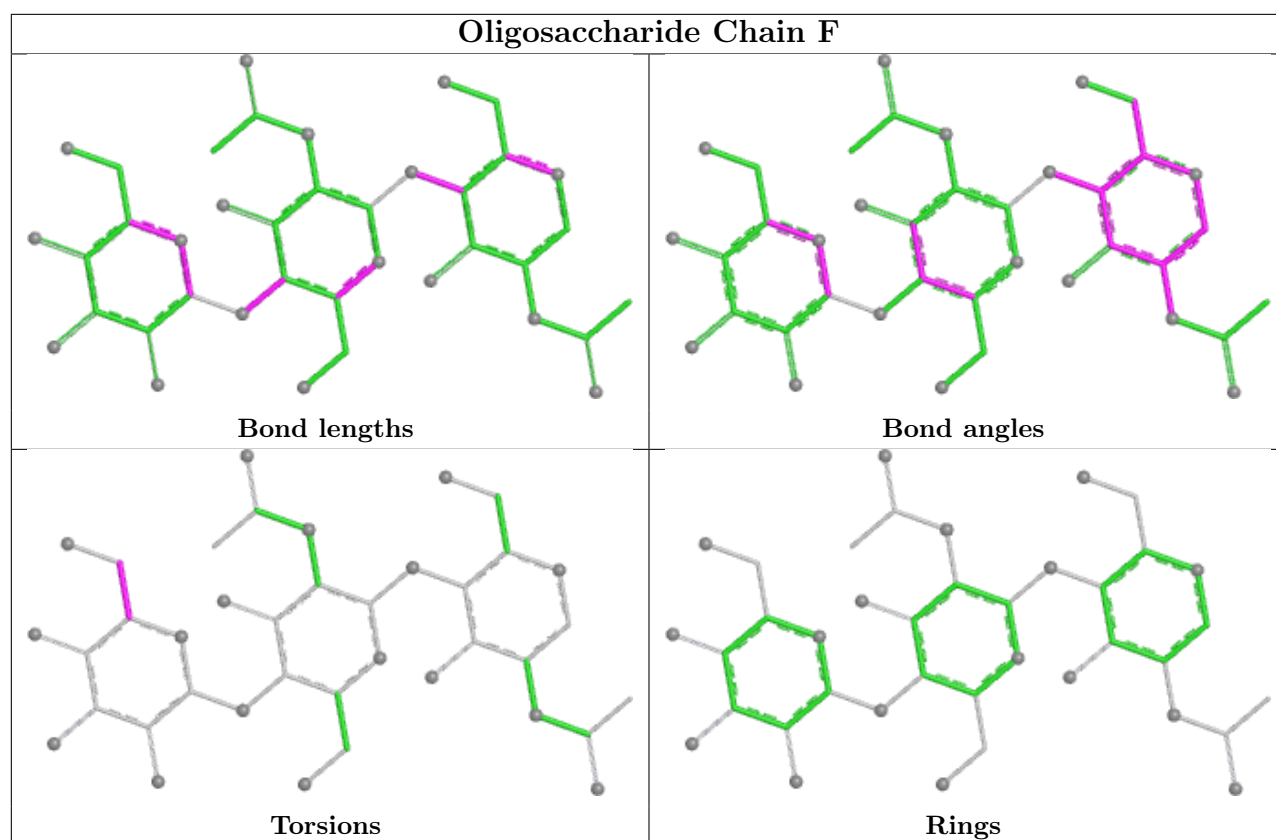
2 monomers are involved in 1 short contact:

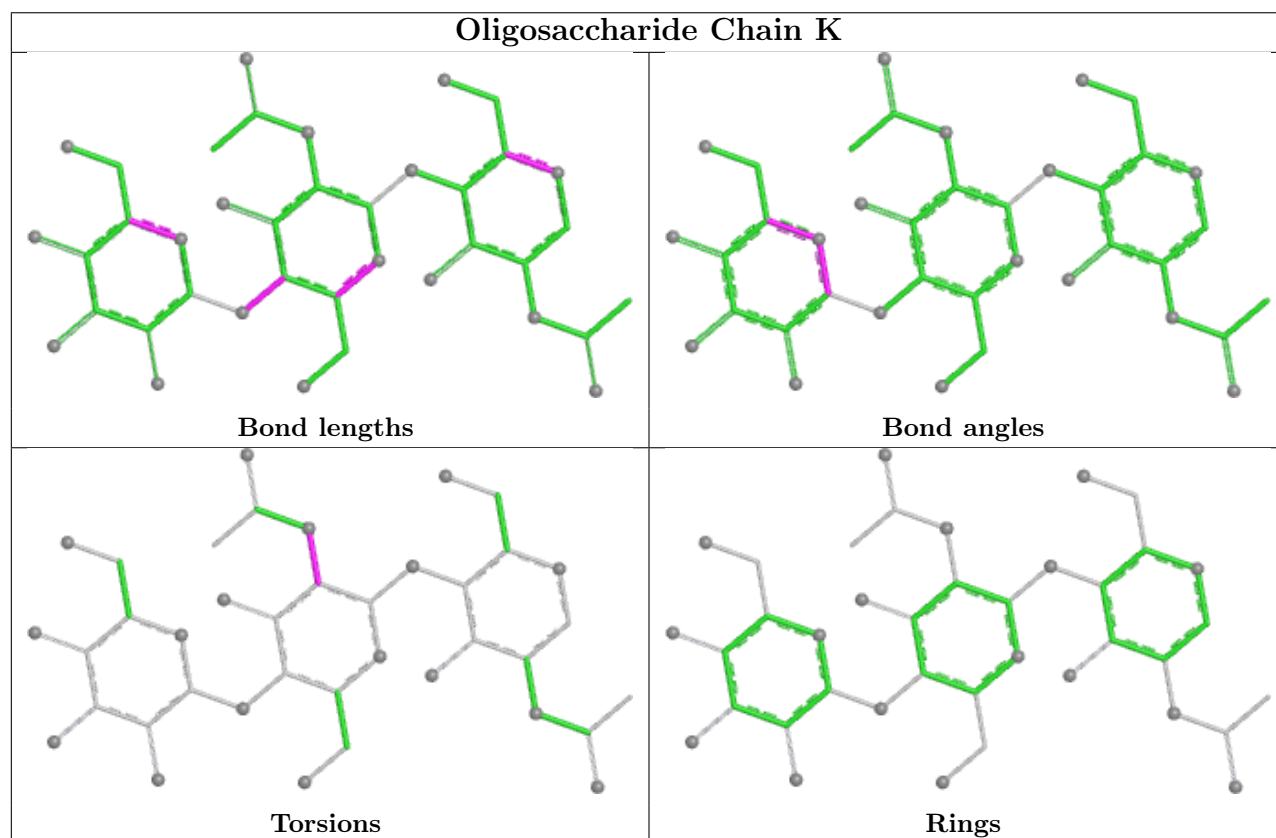
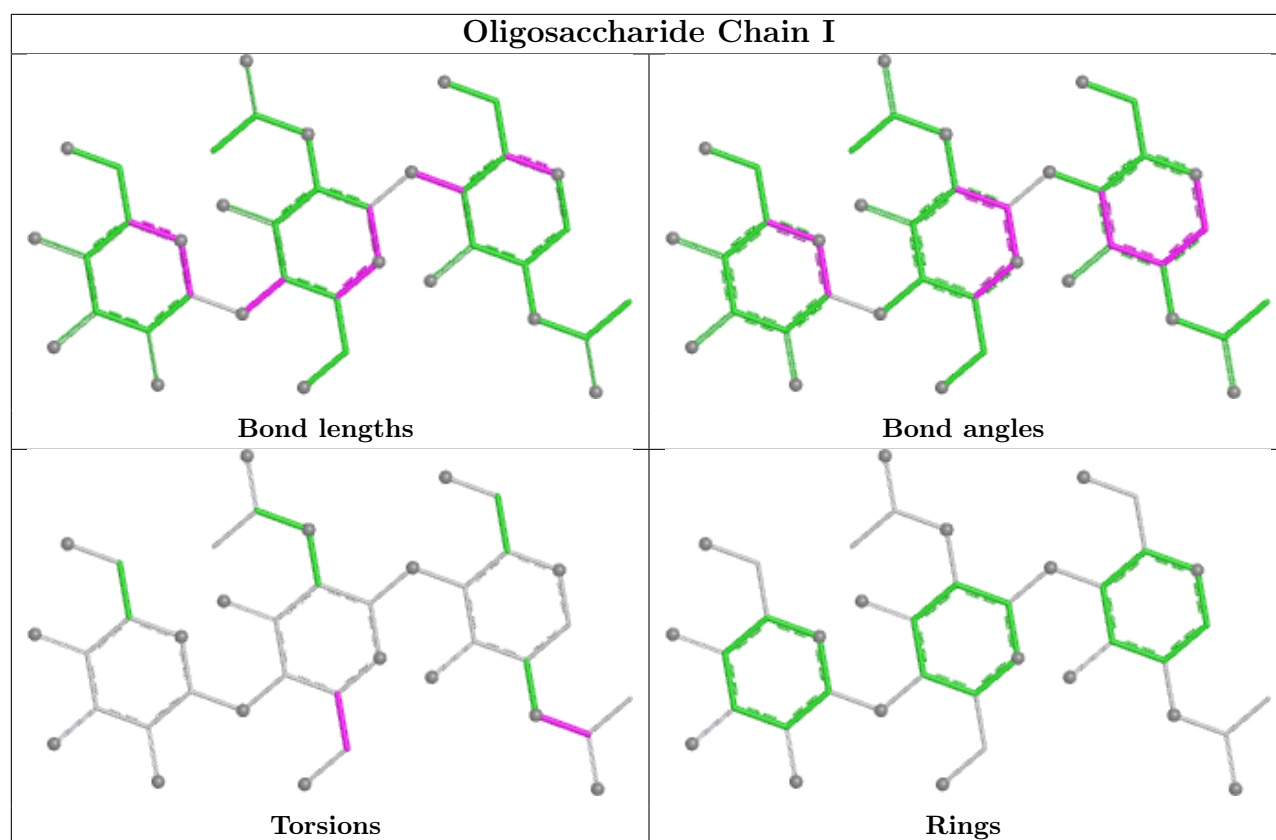
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	1	NAG	1	0
5	R	2	NAG	1	0

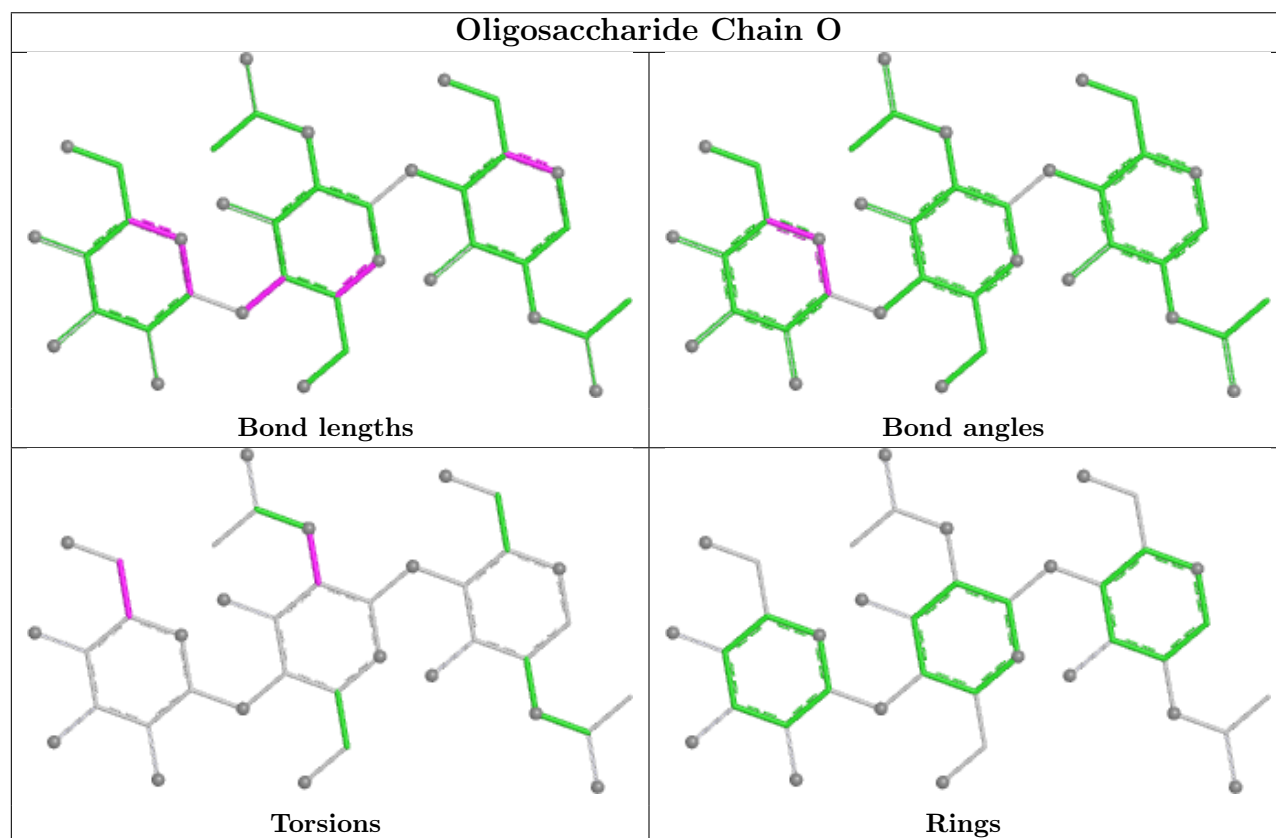
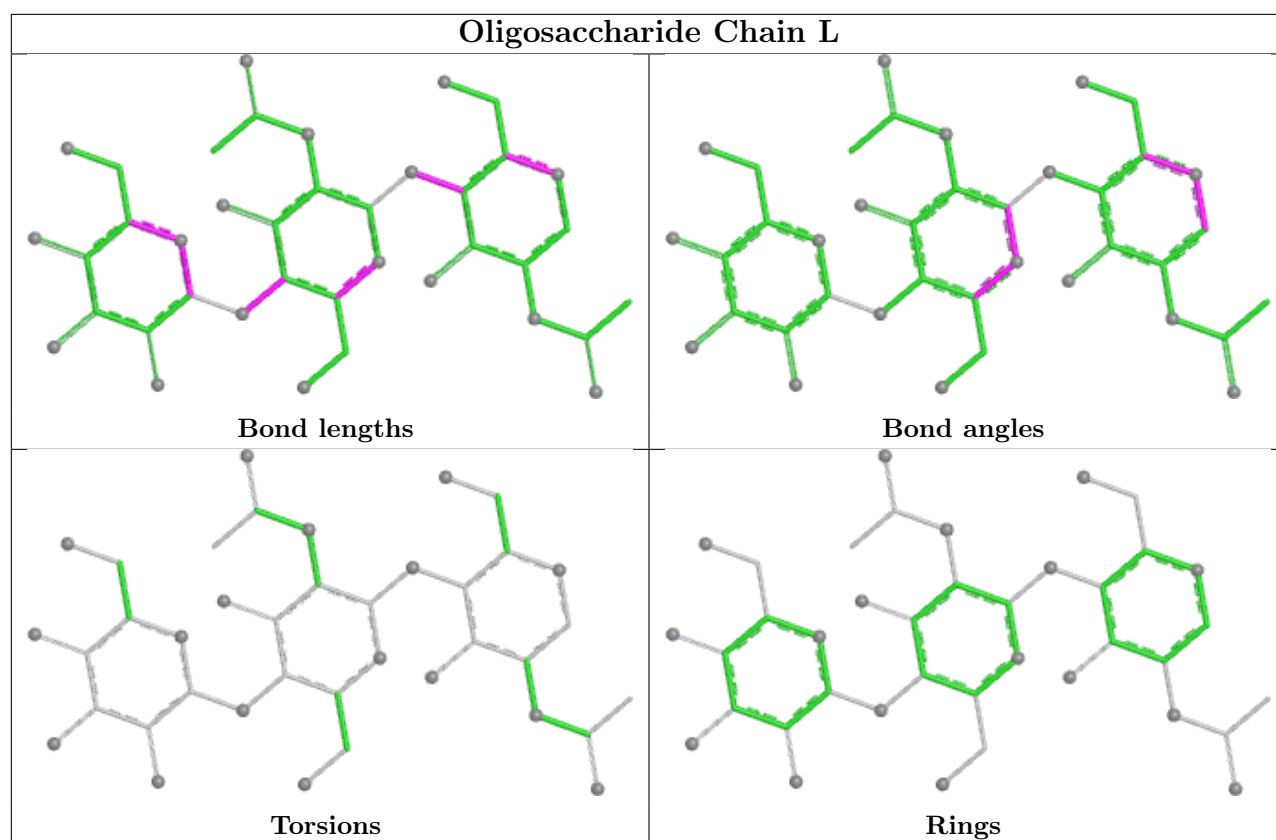
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

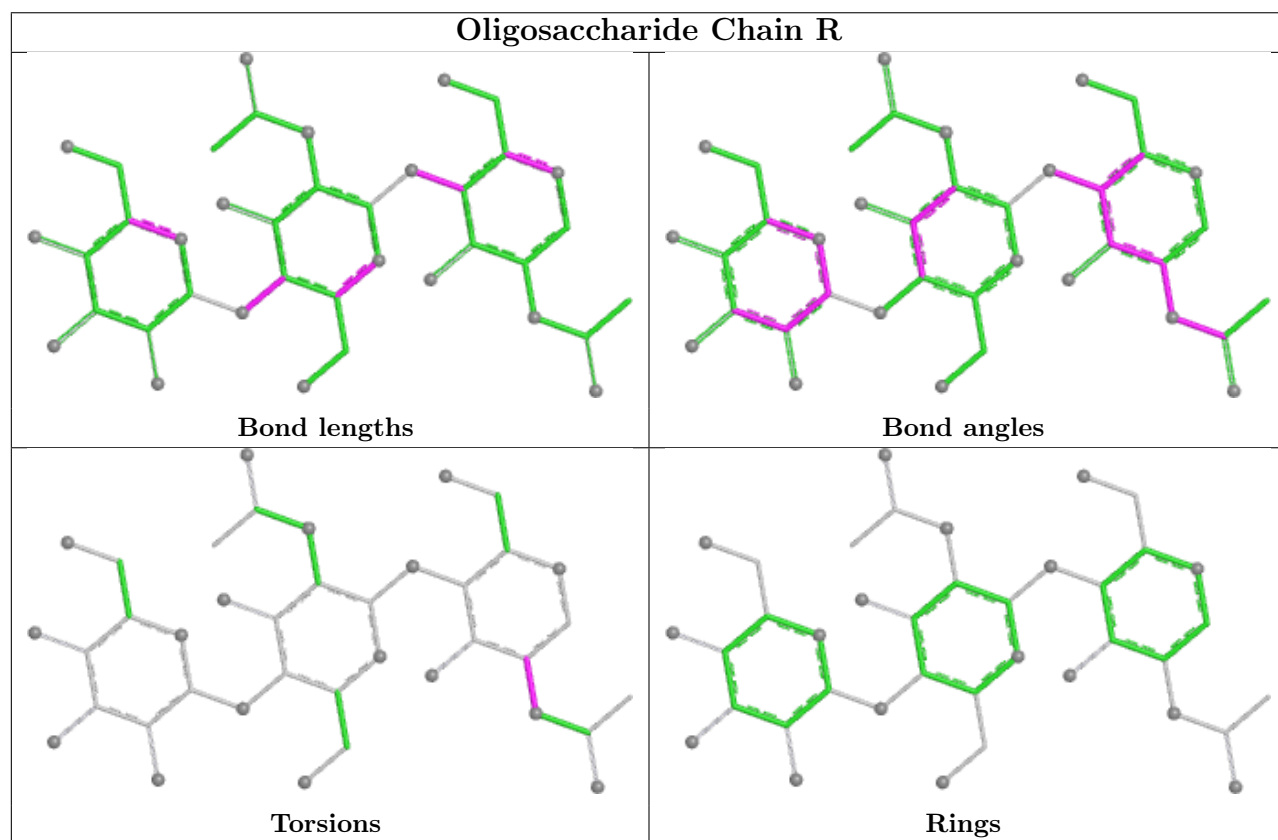
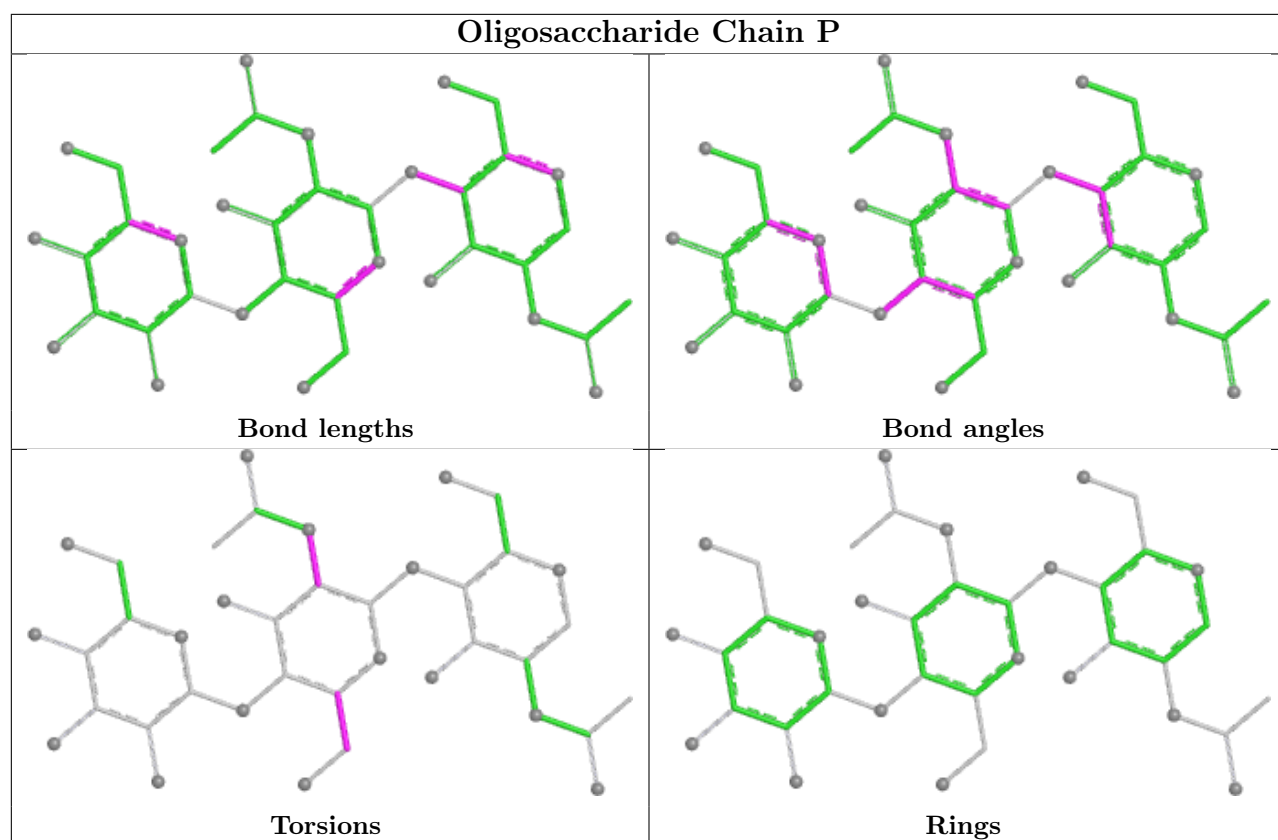


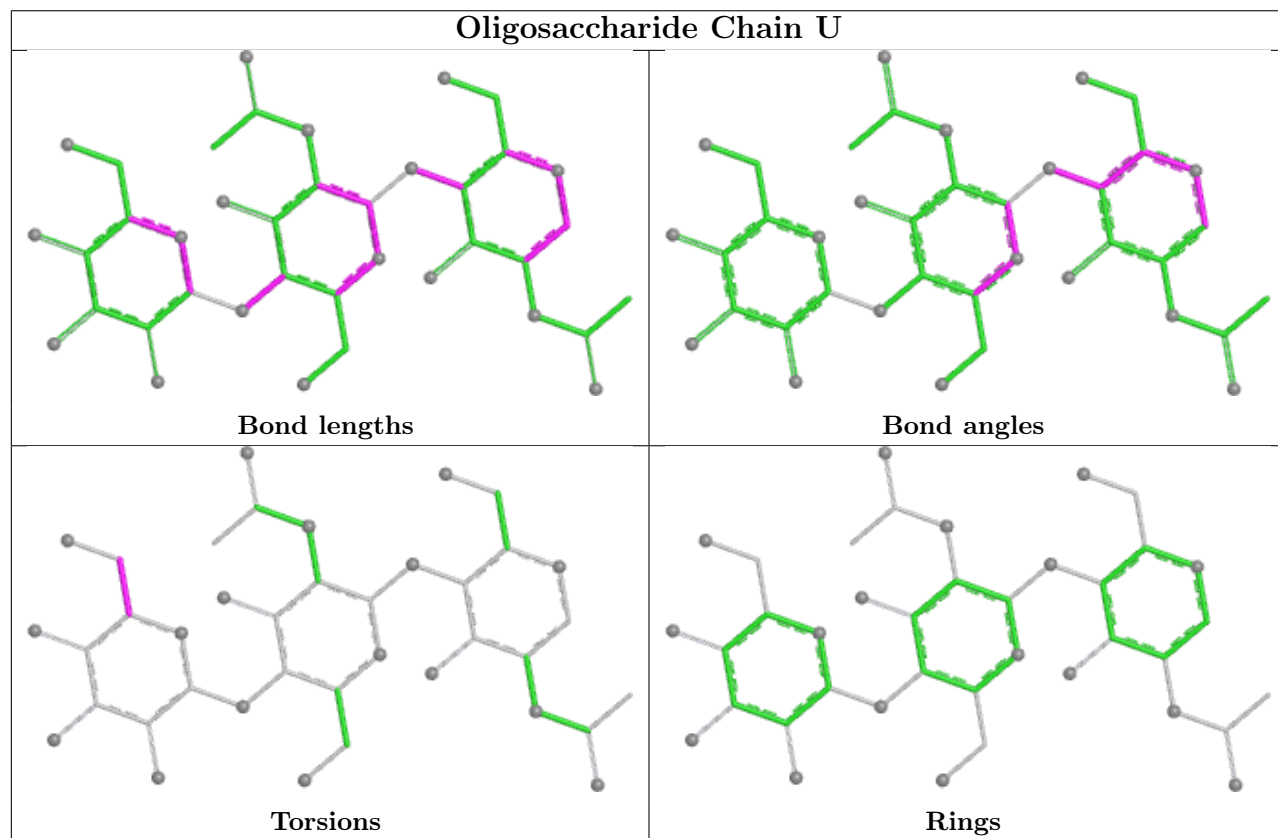
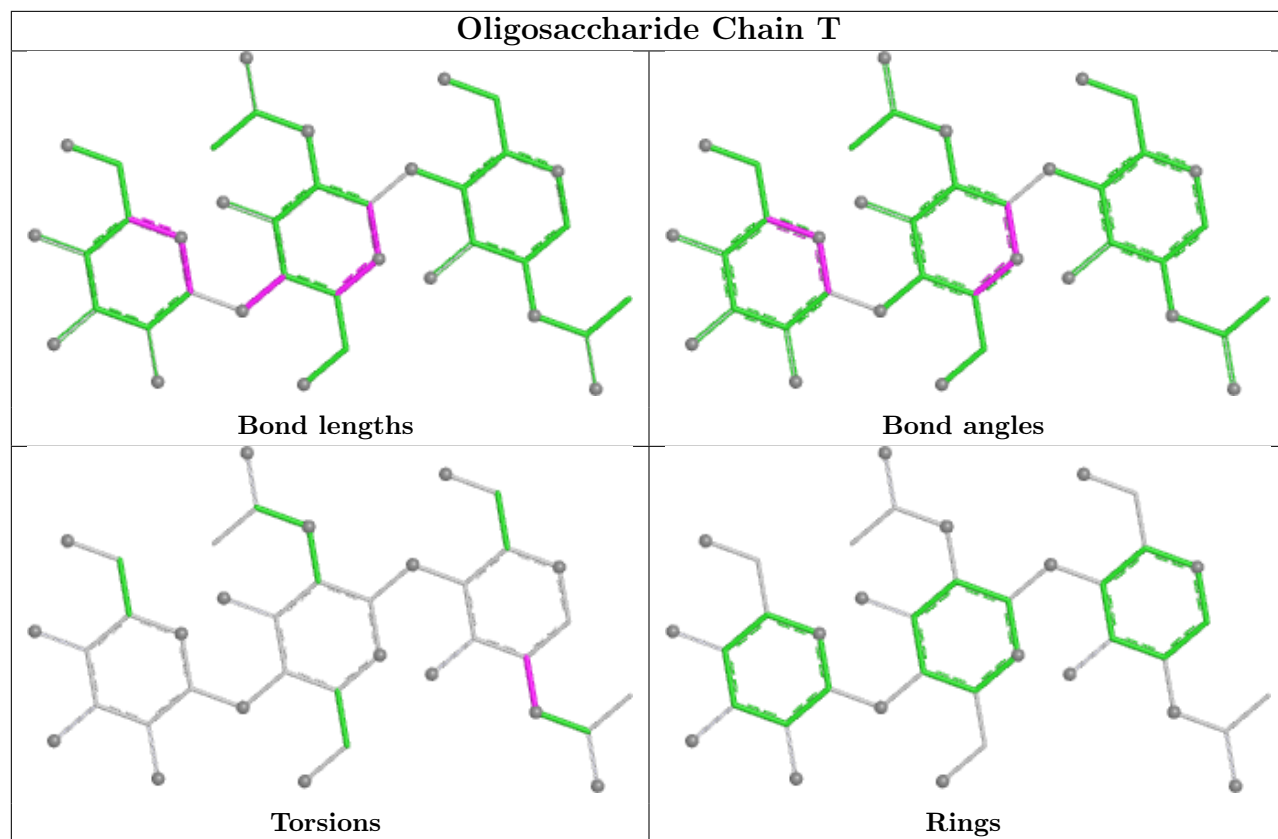


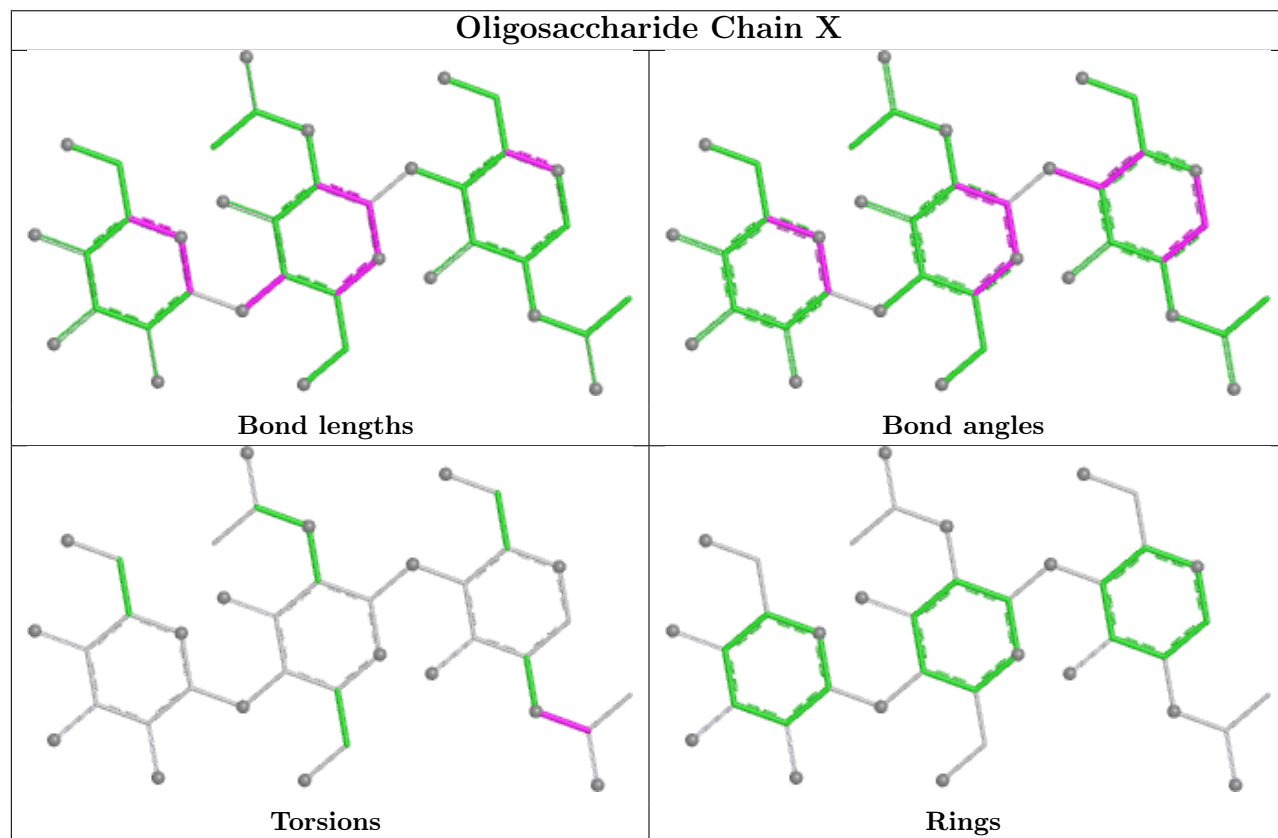
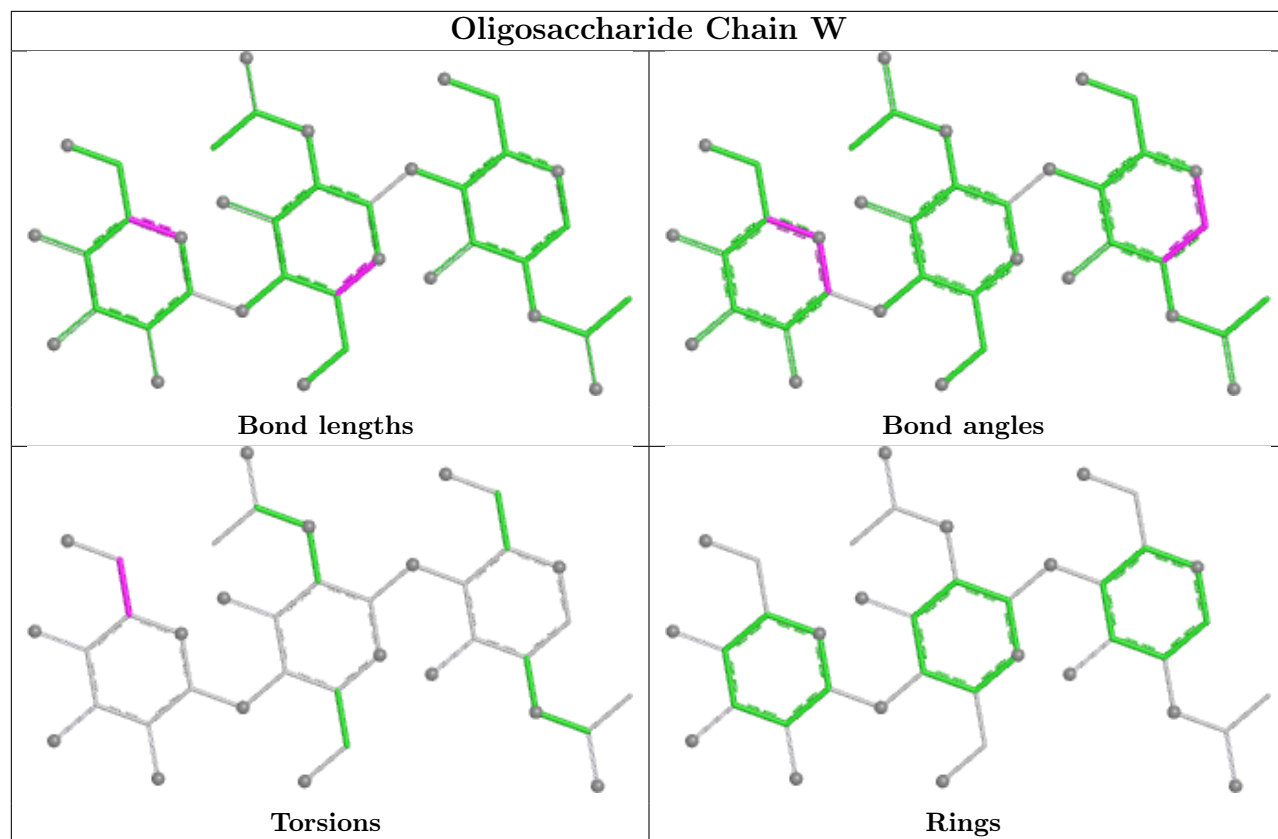


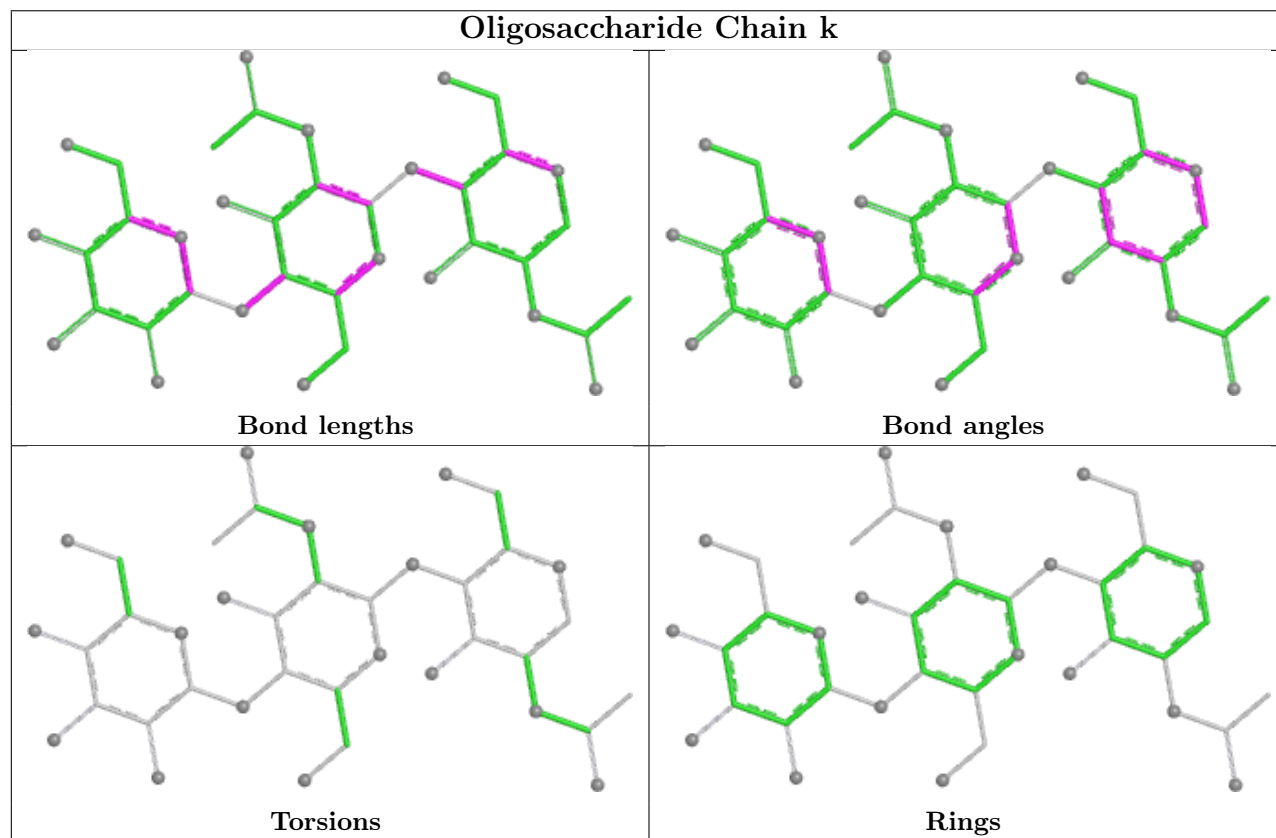
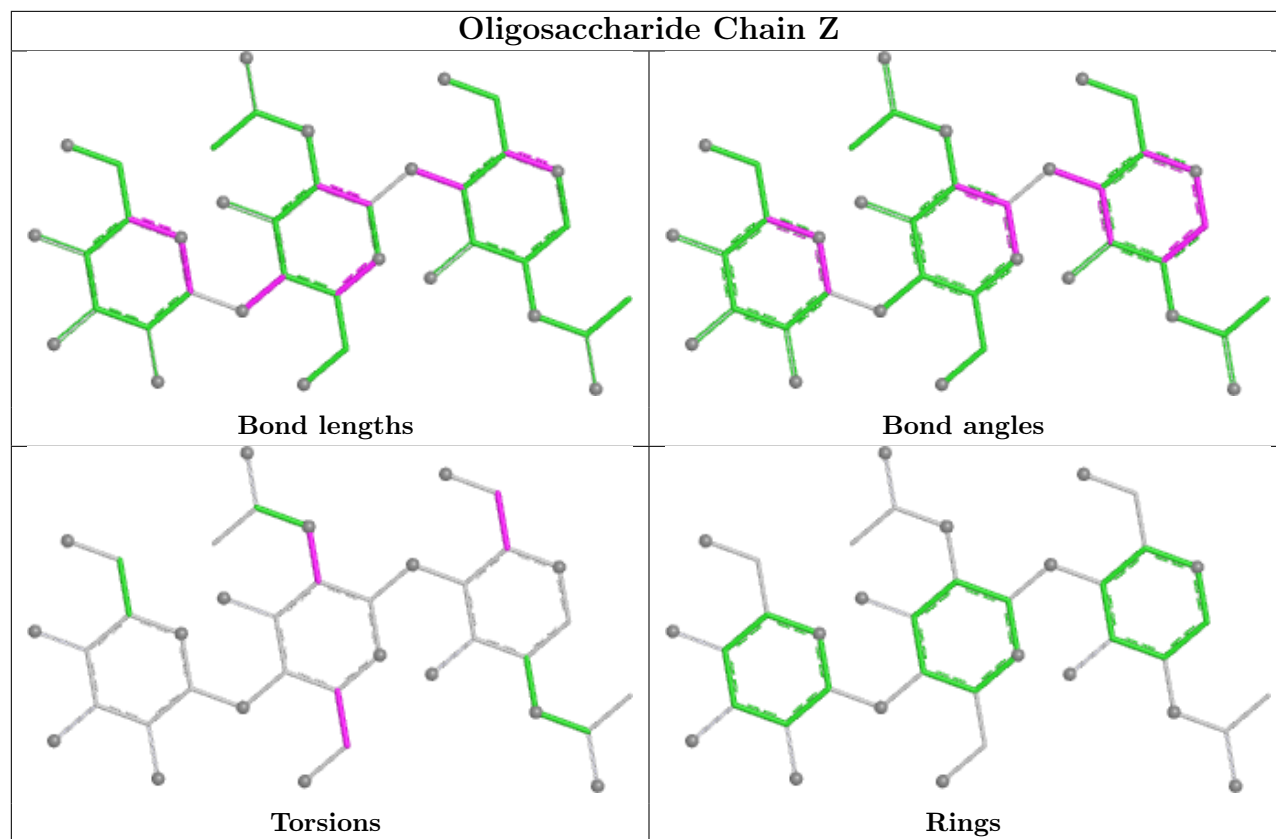


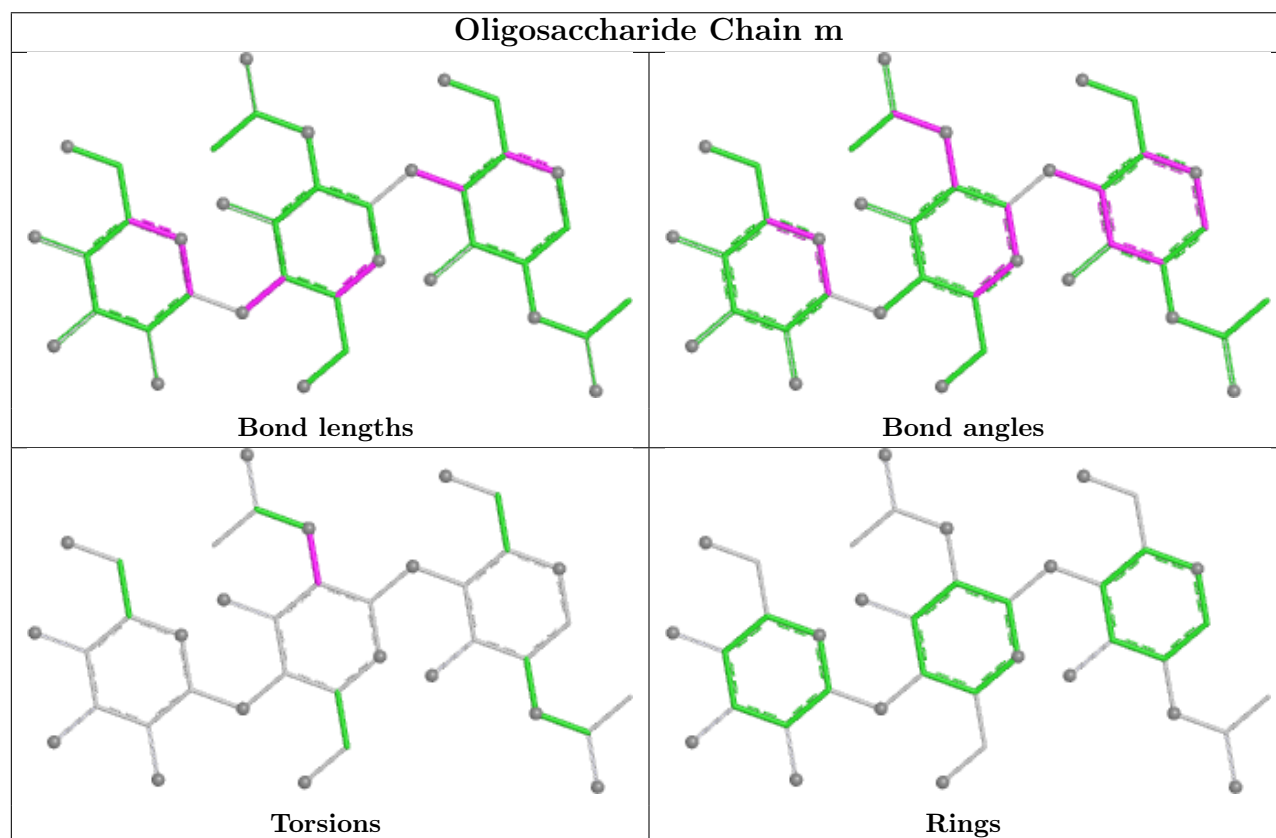
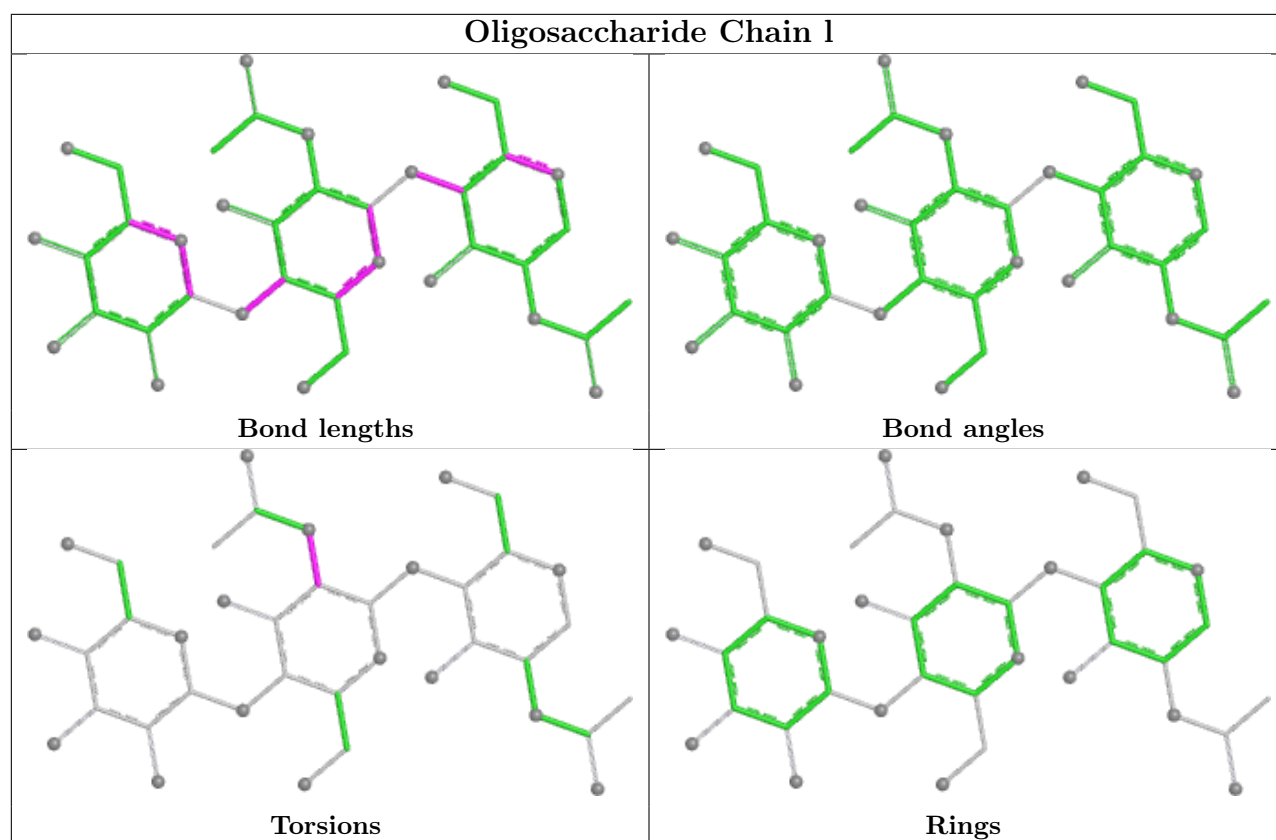


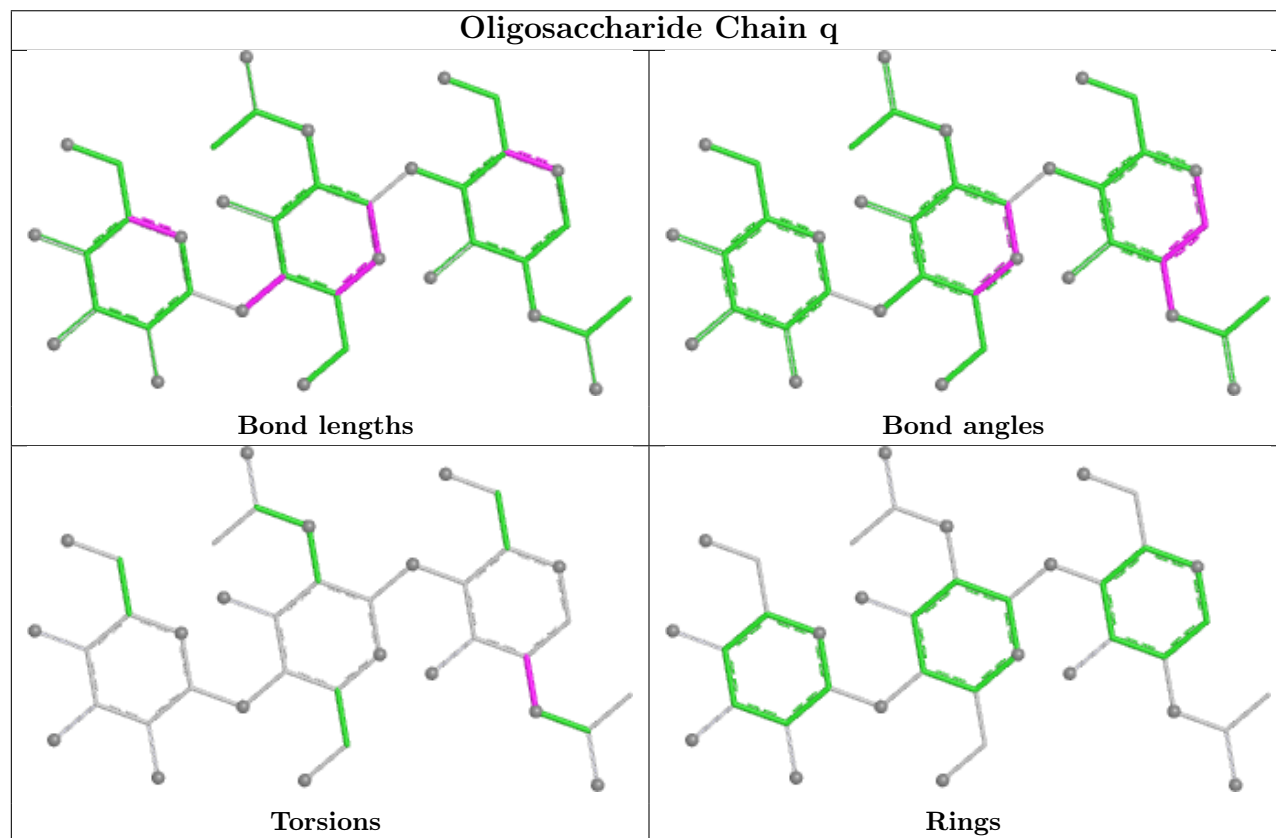
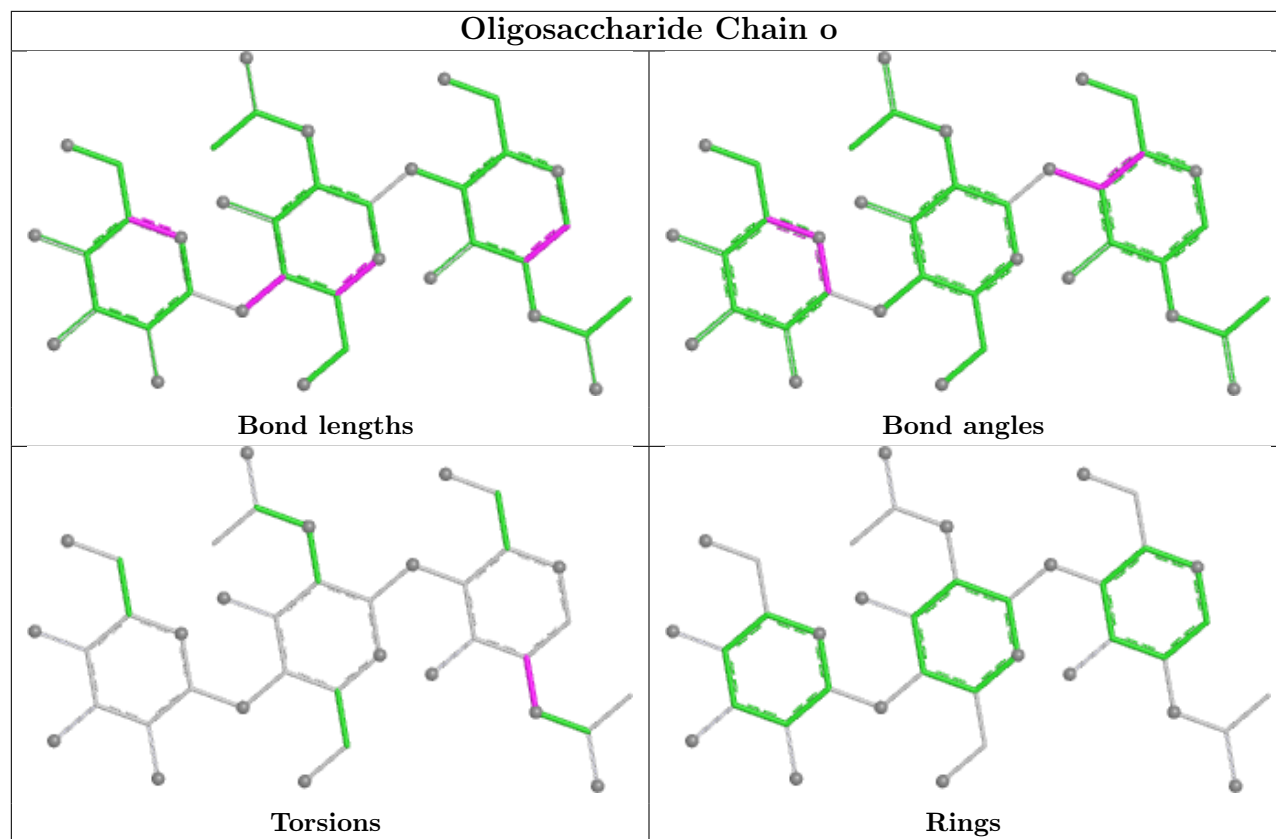


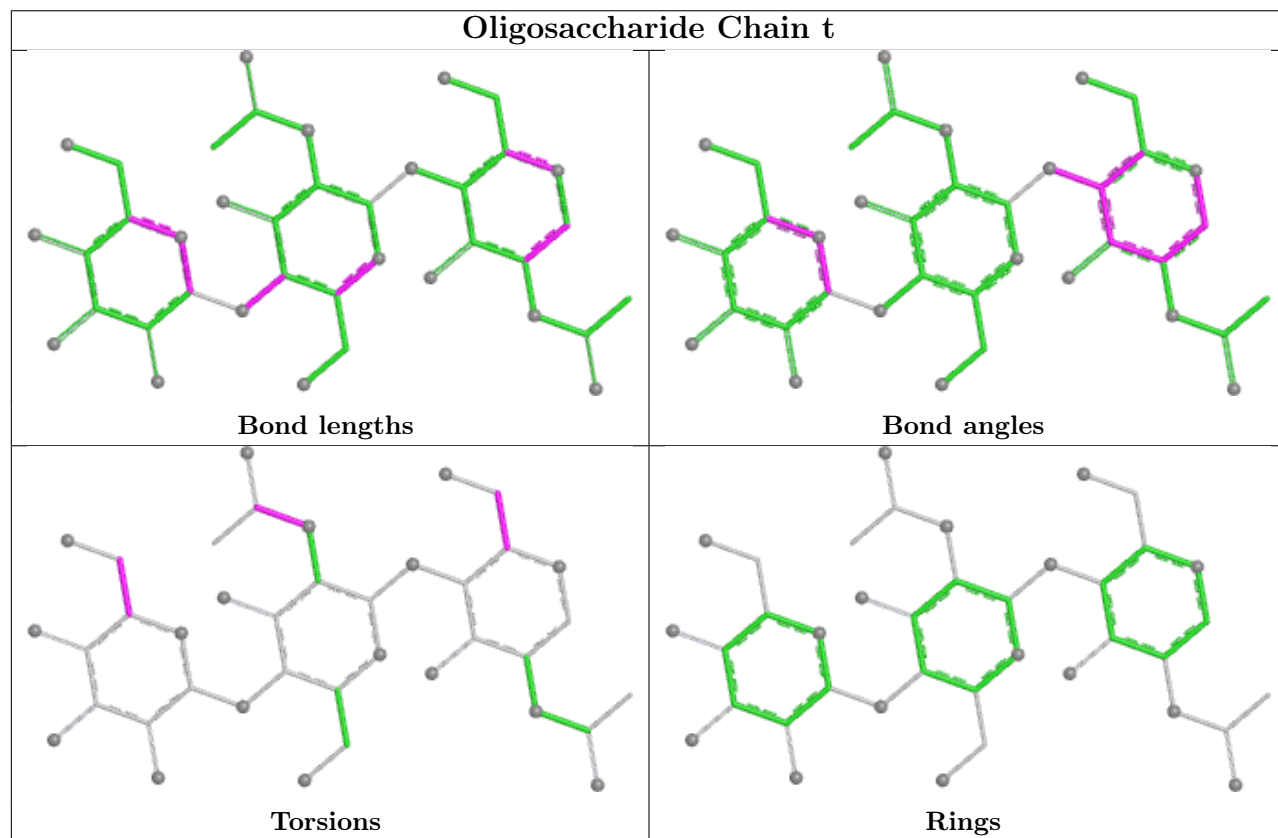
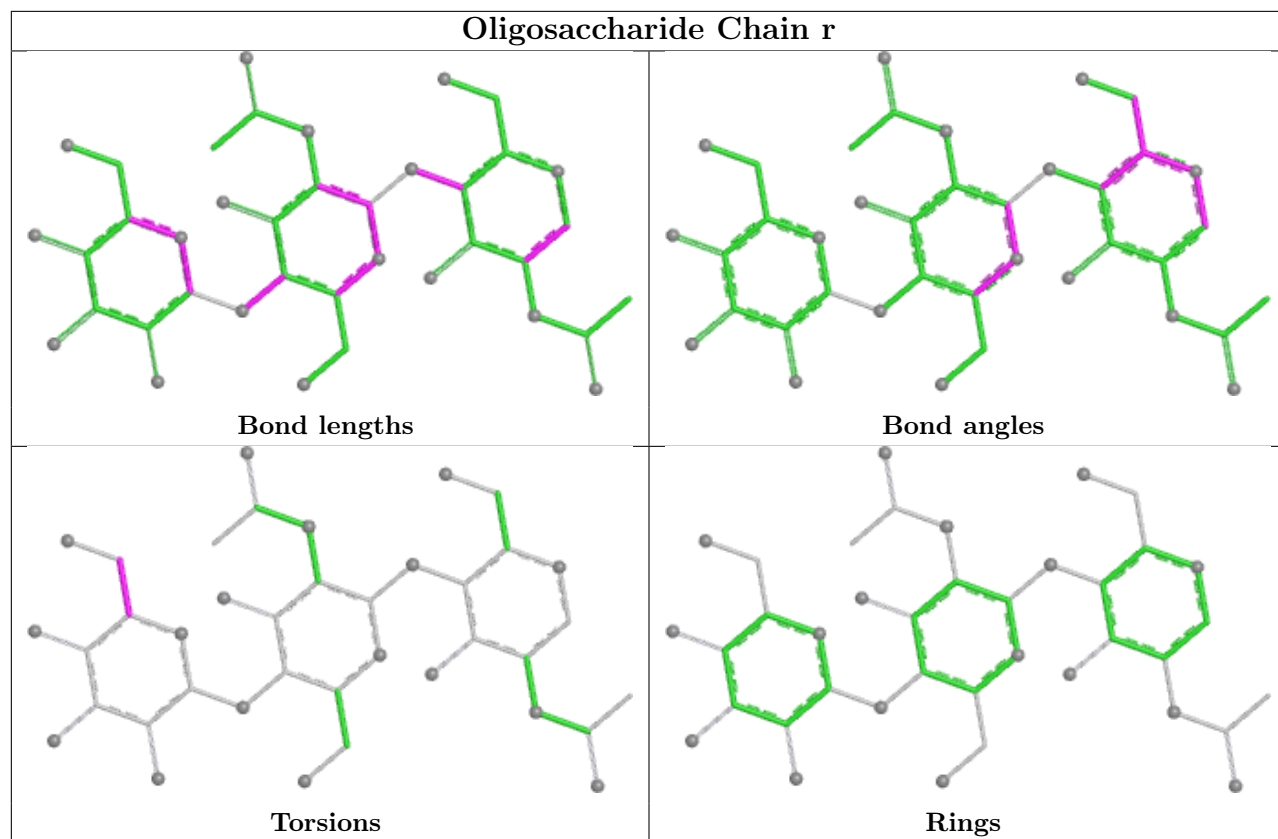


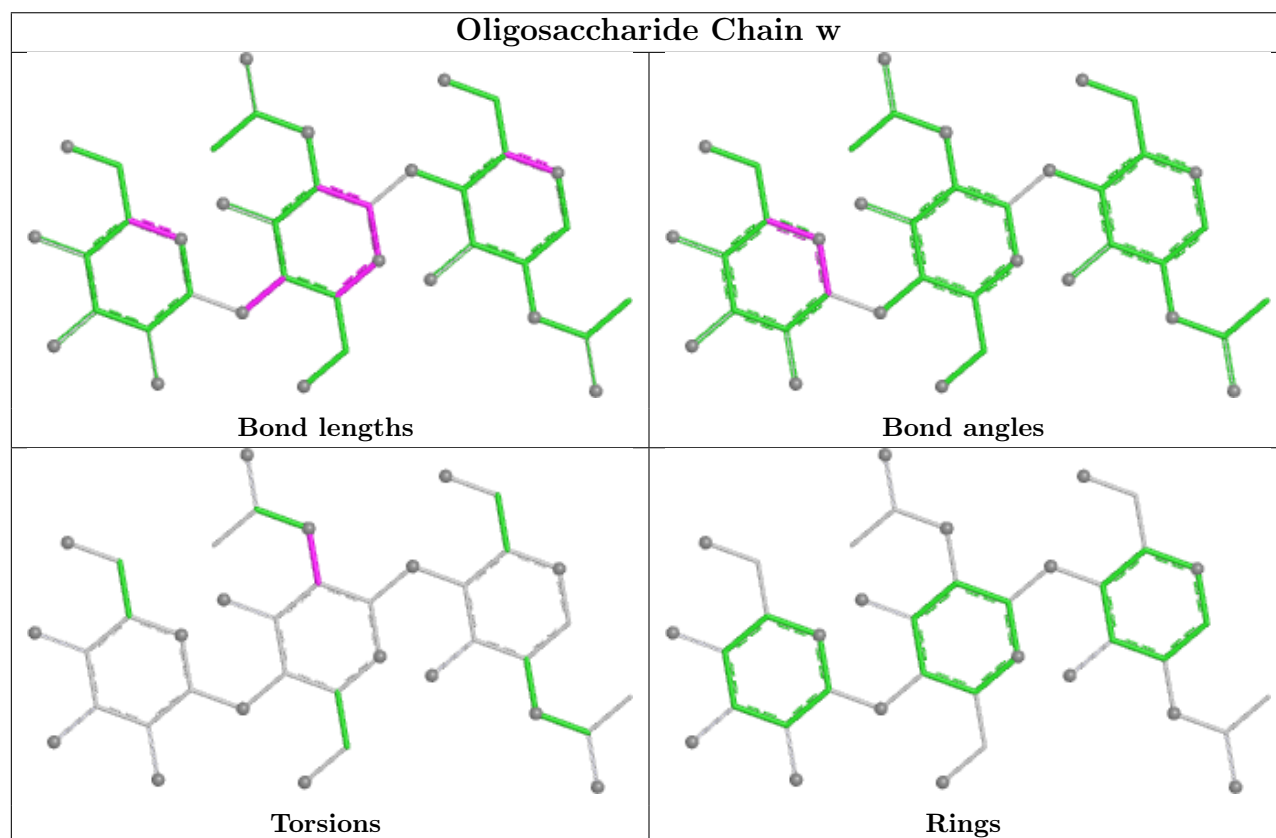
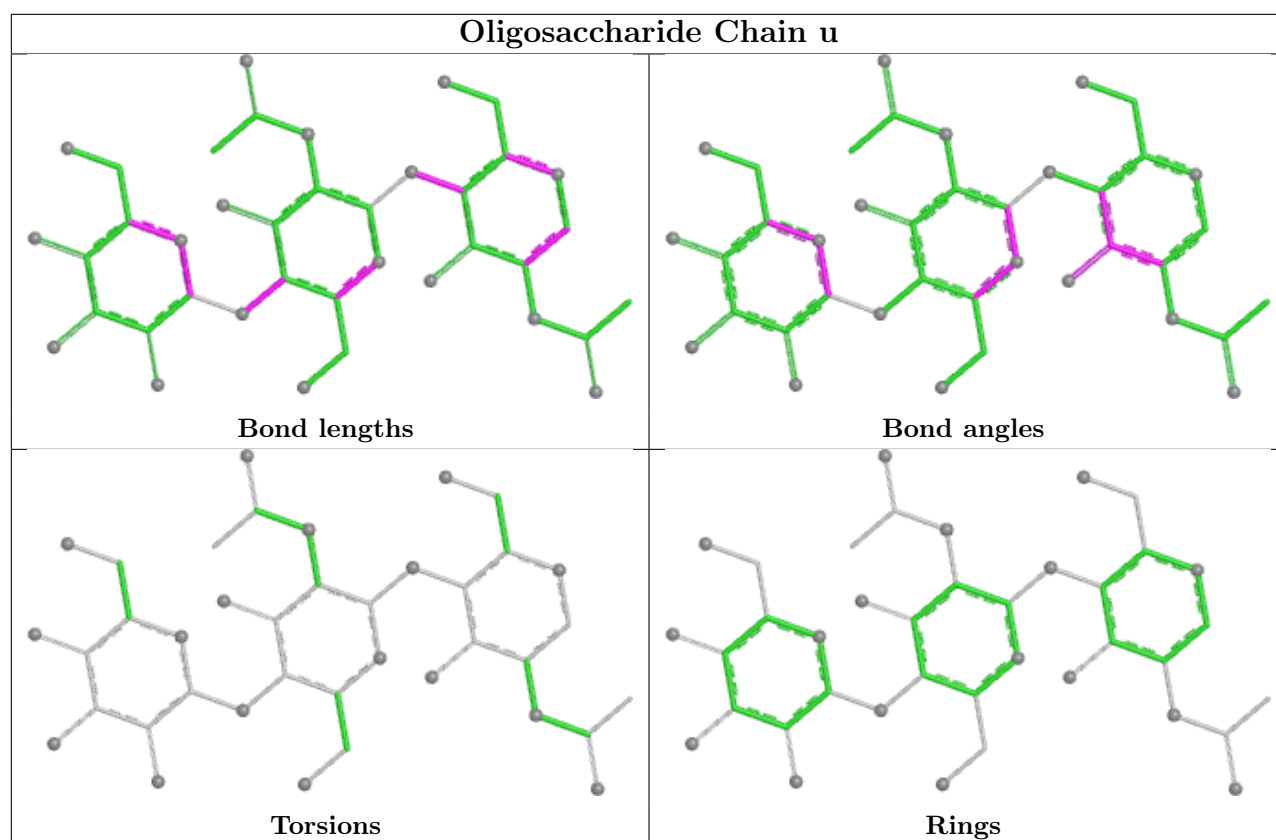


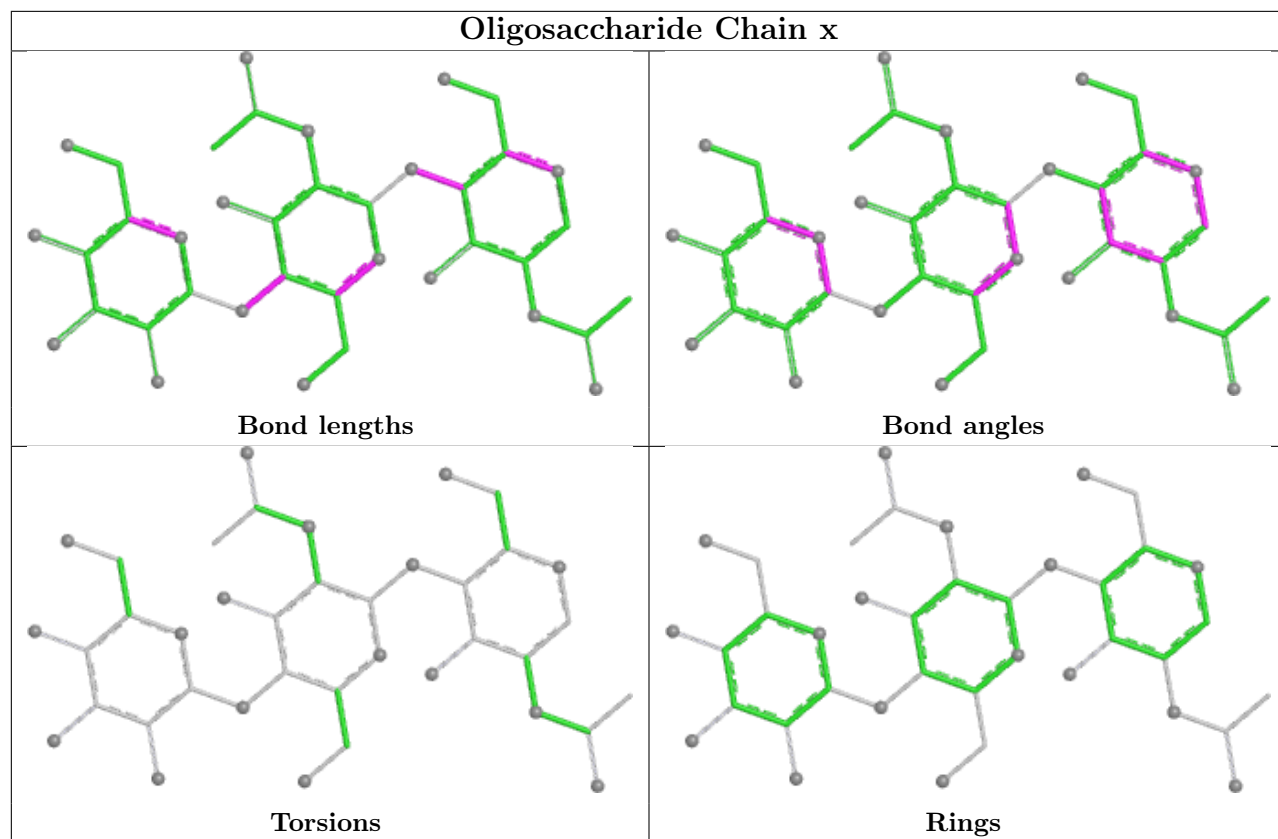


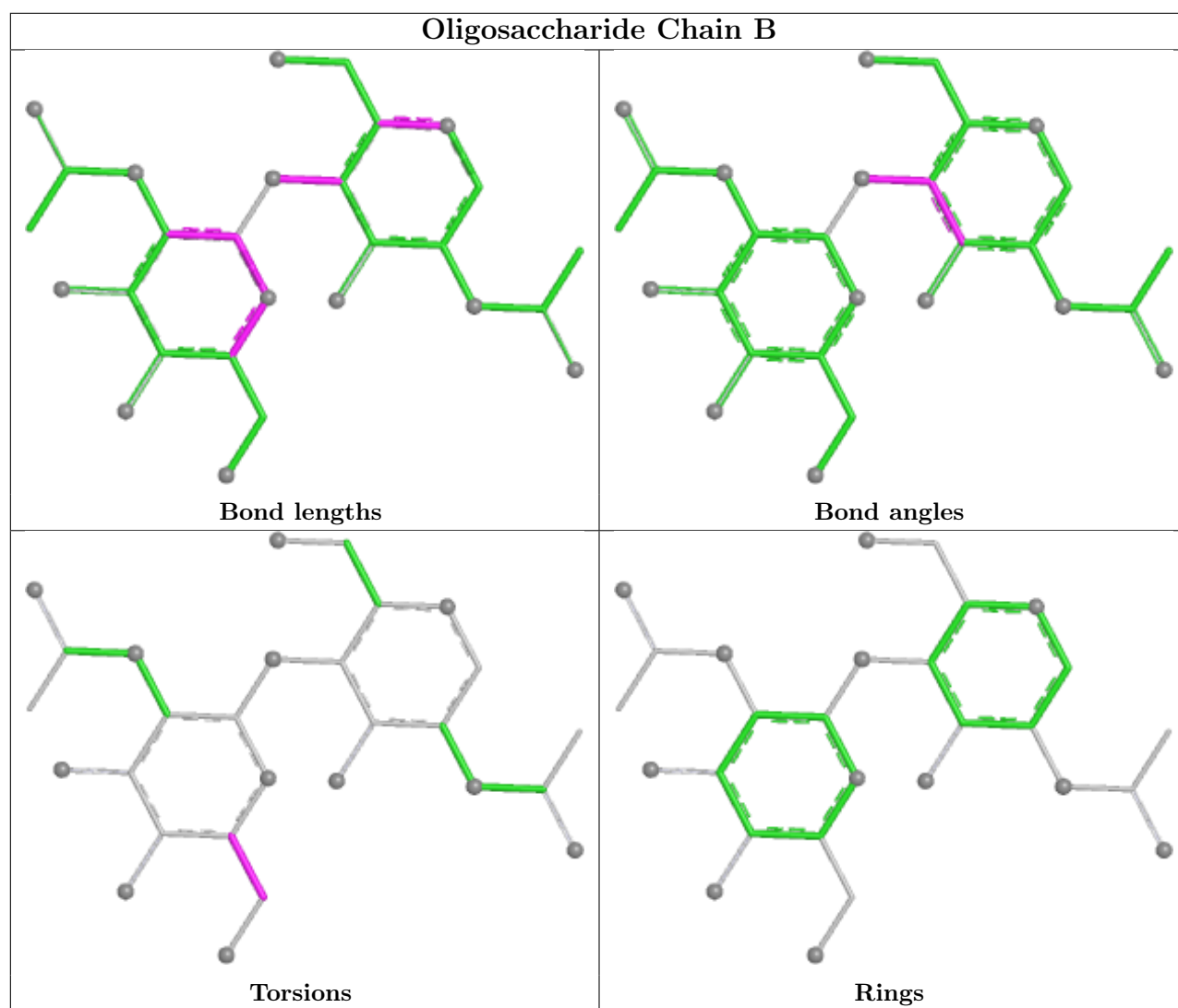


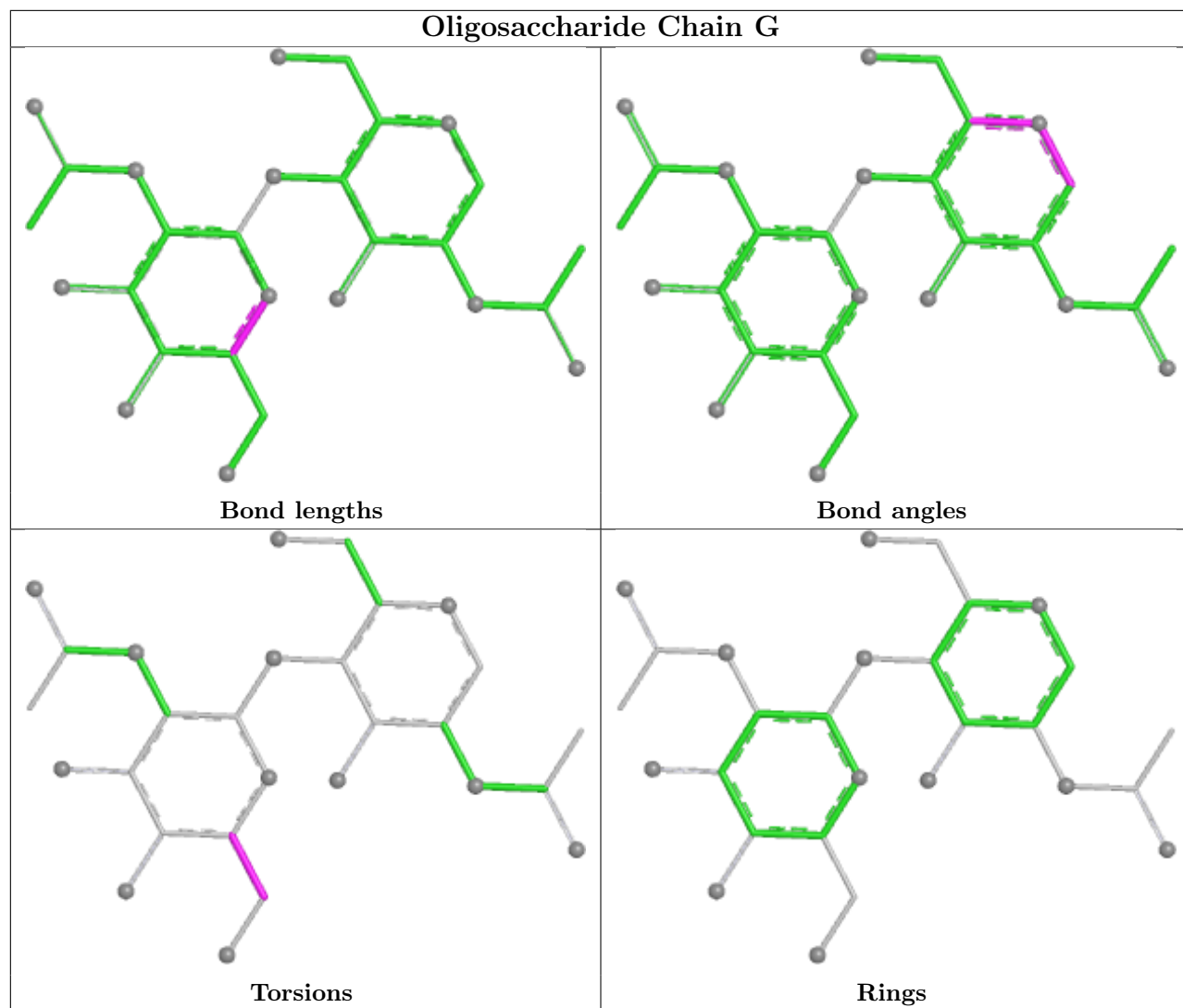


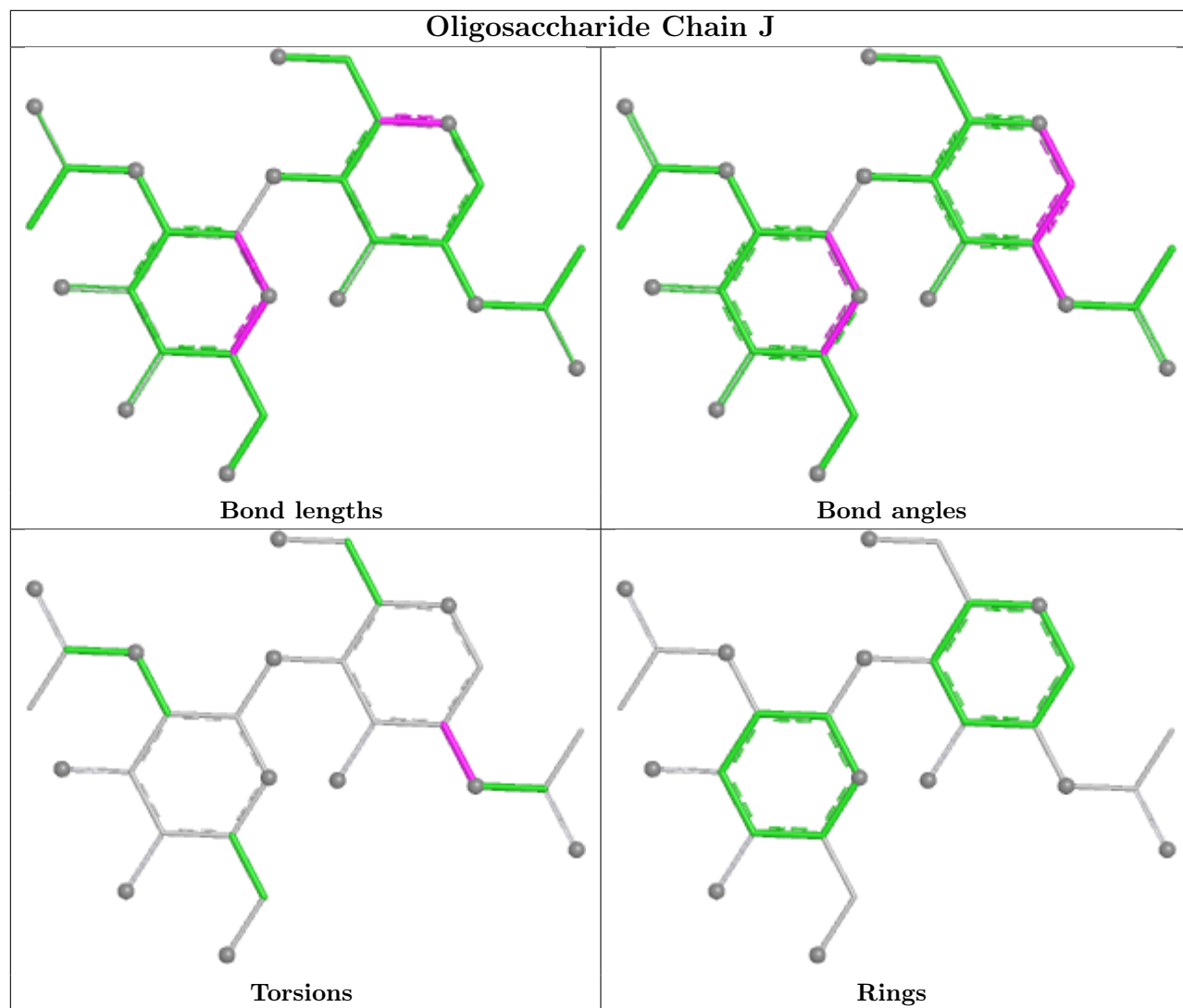


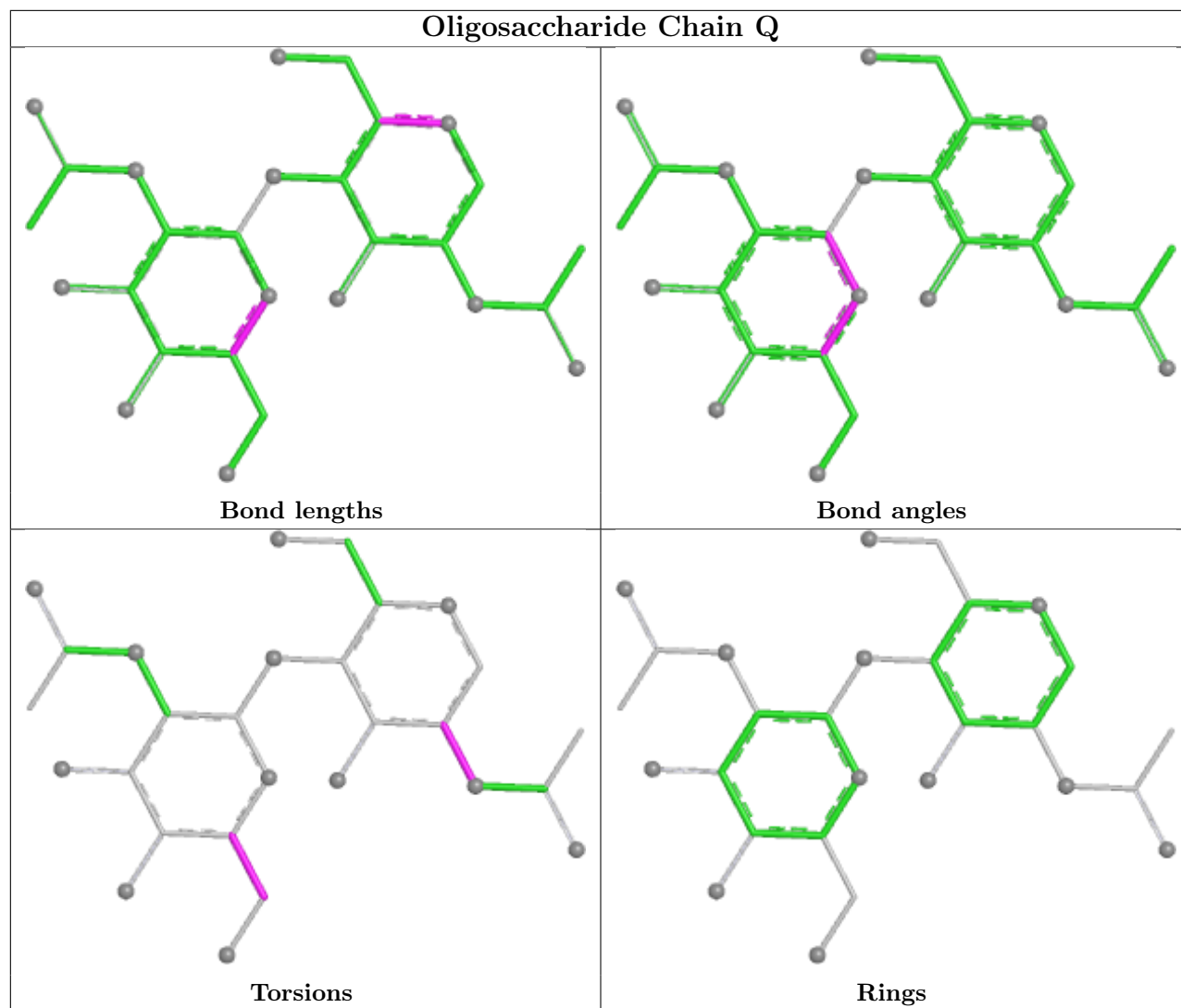


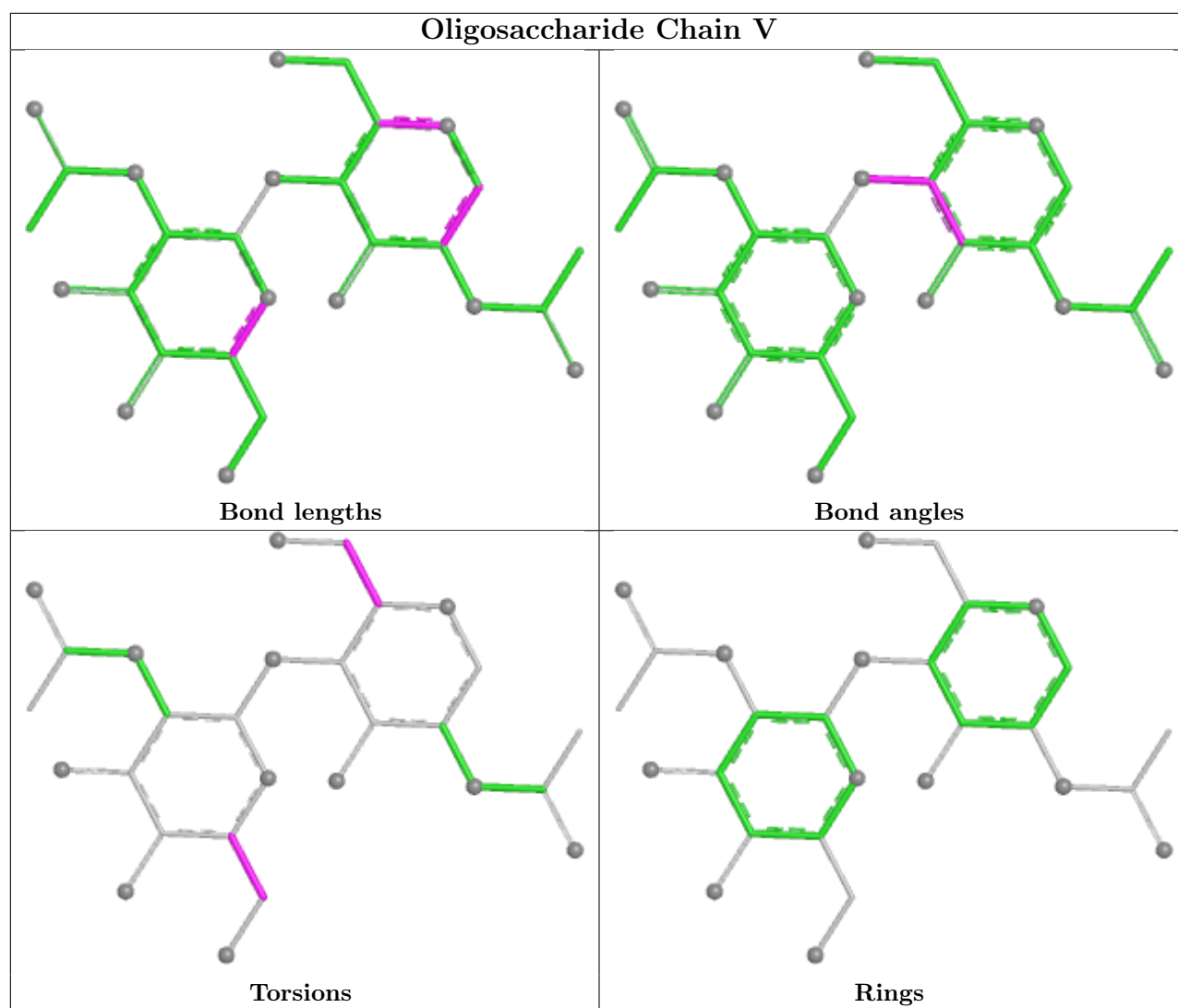


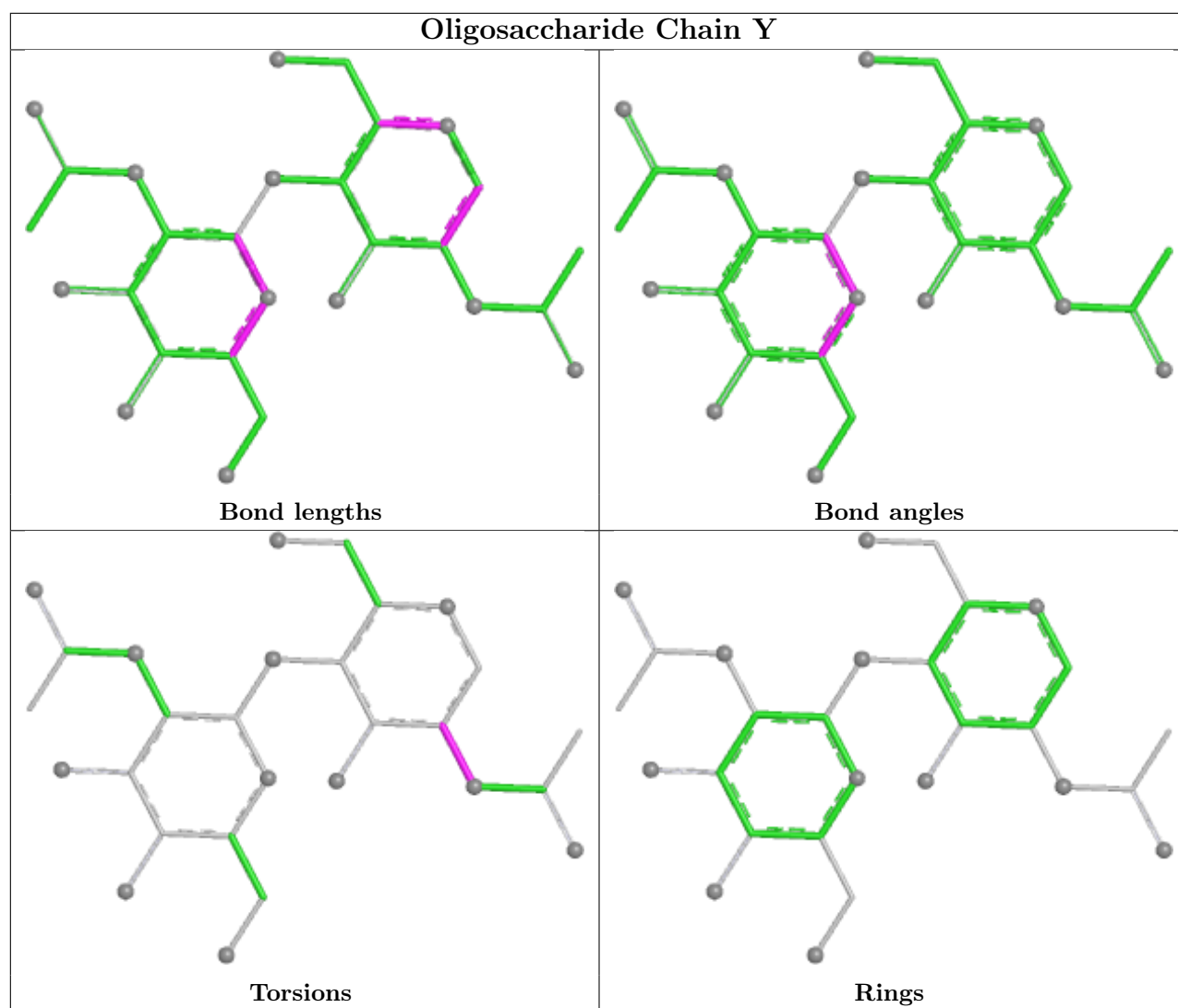


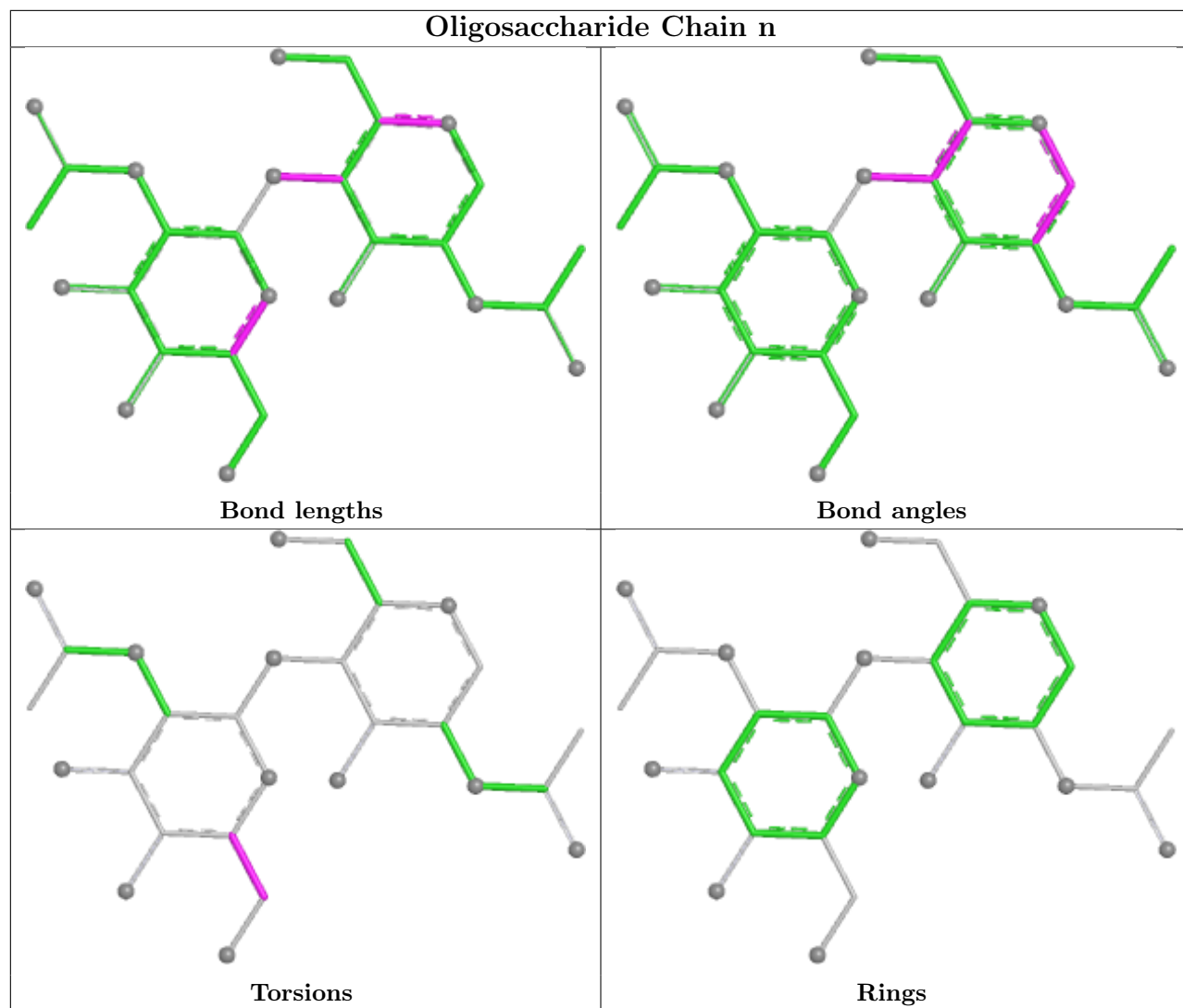


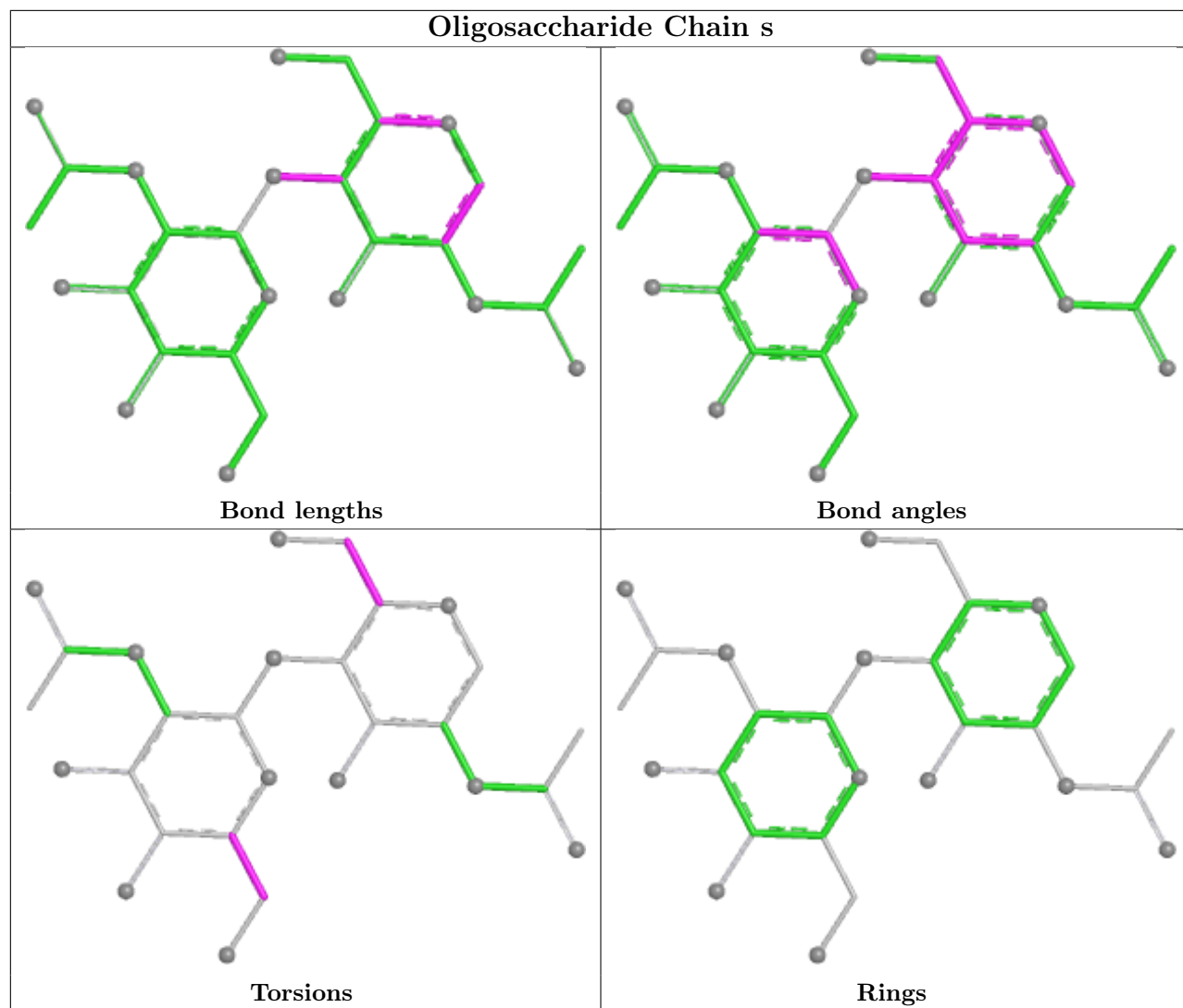


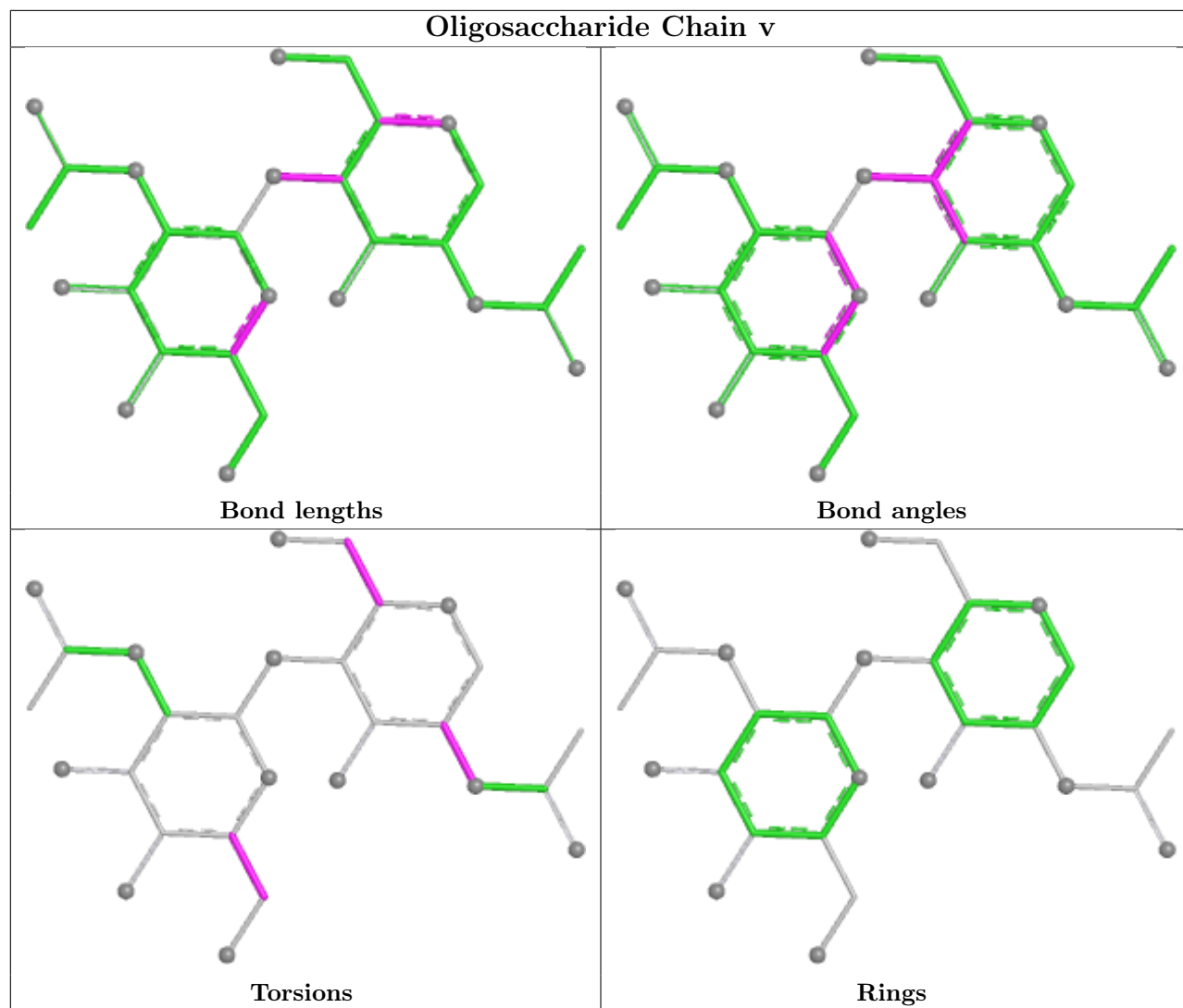


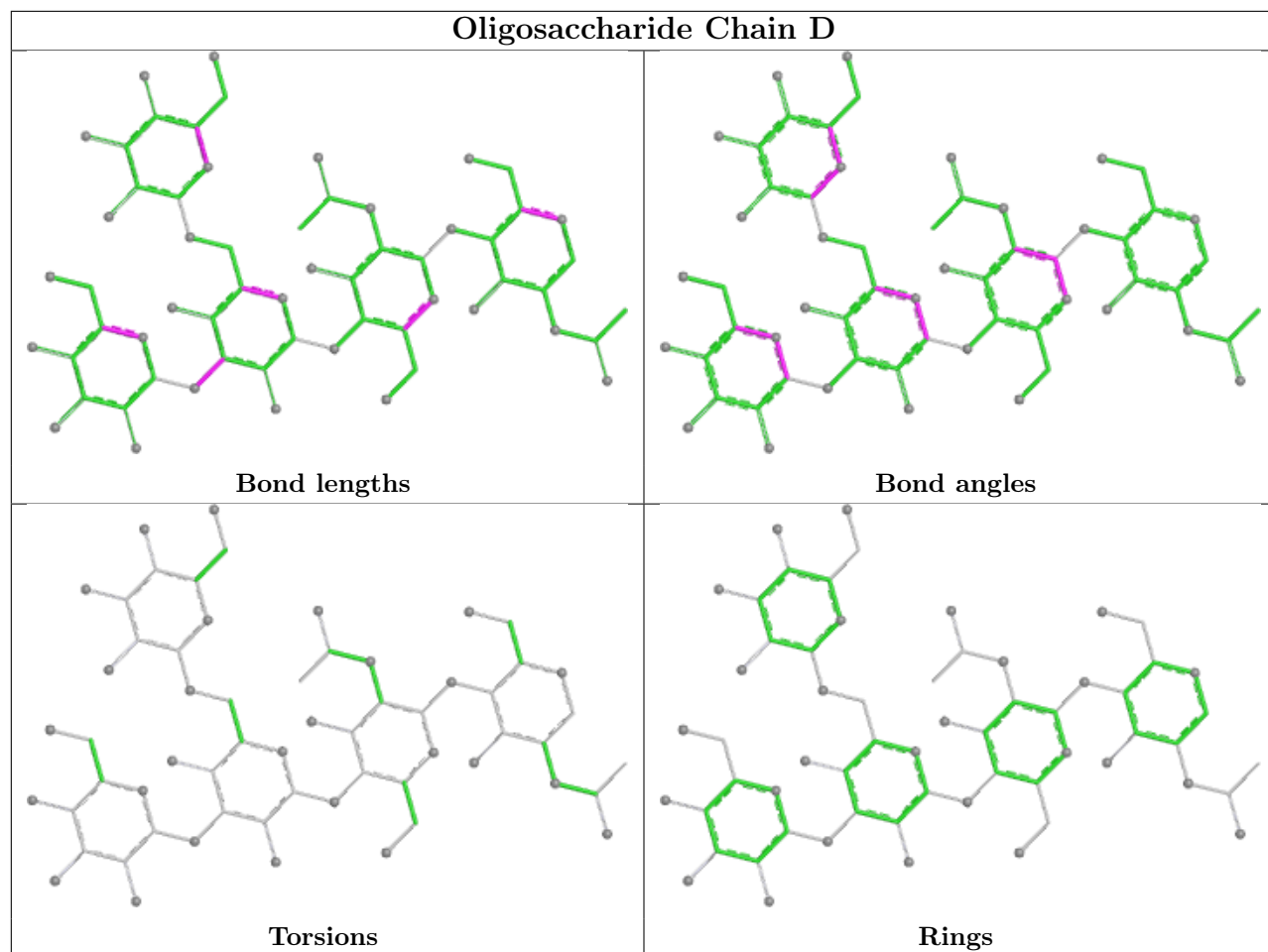


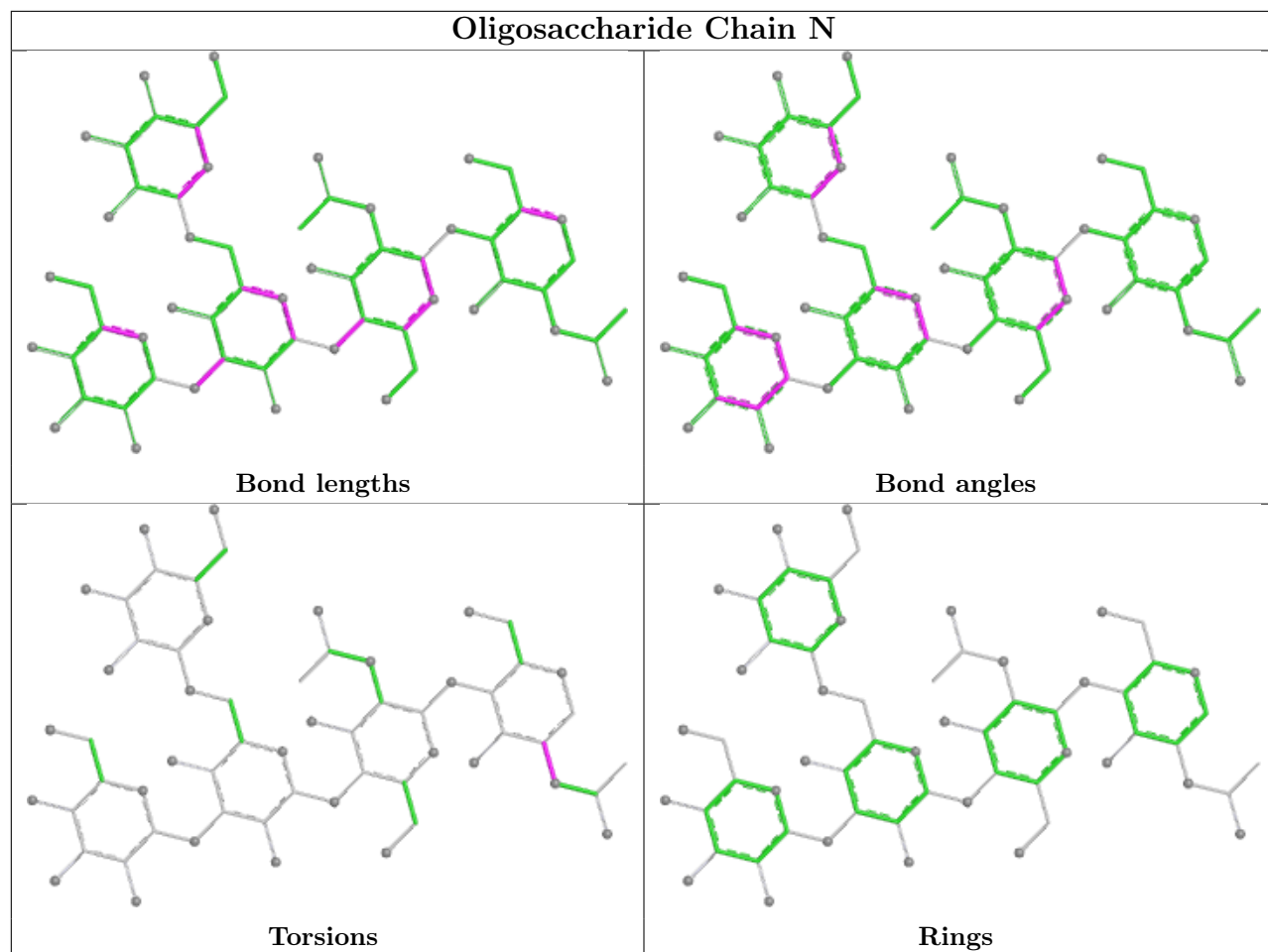


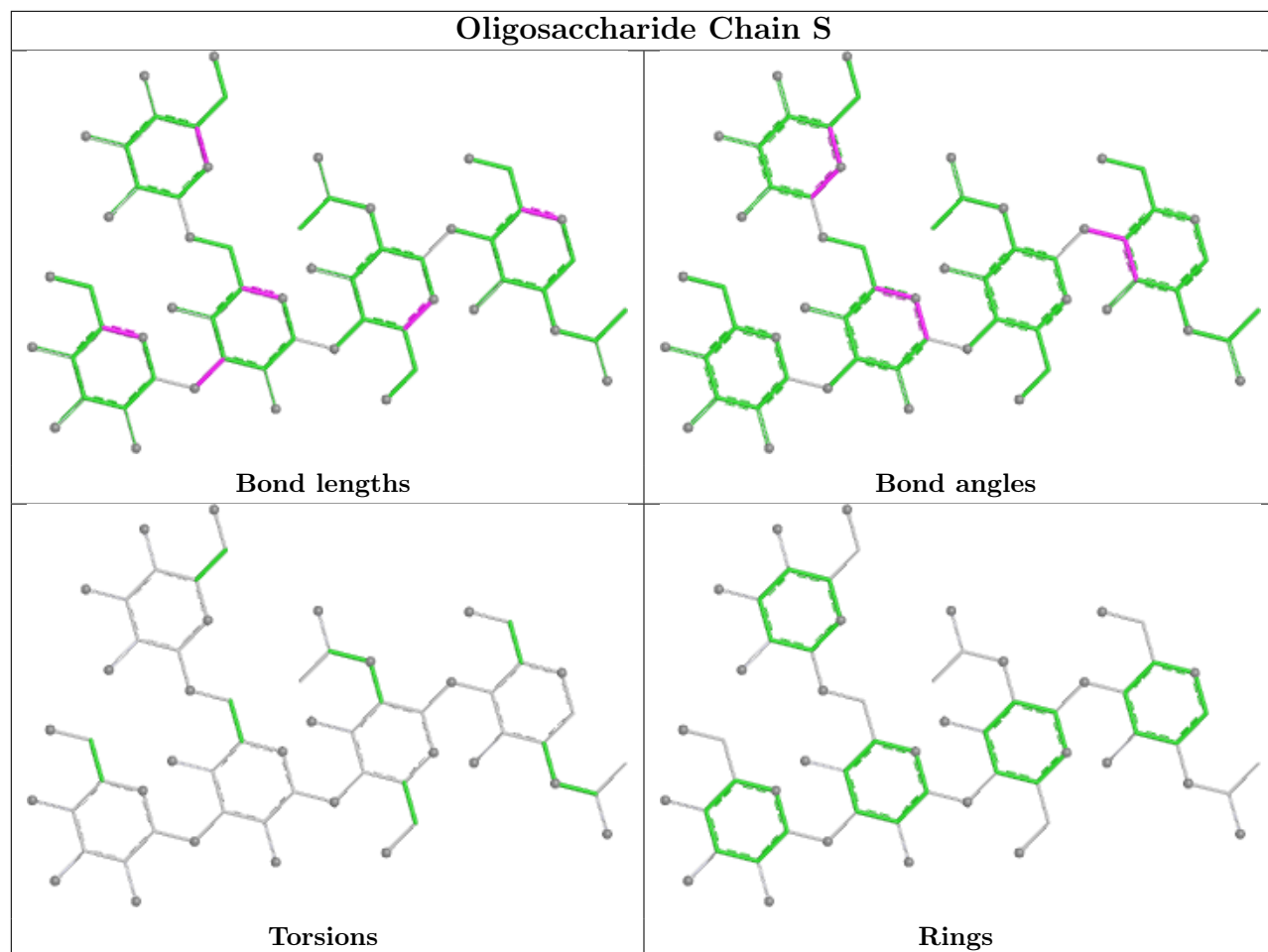


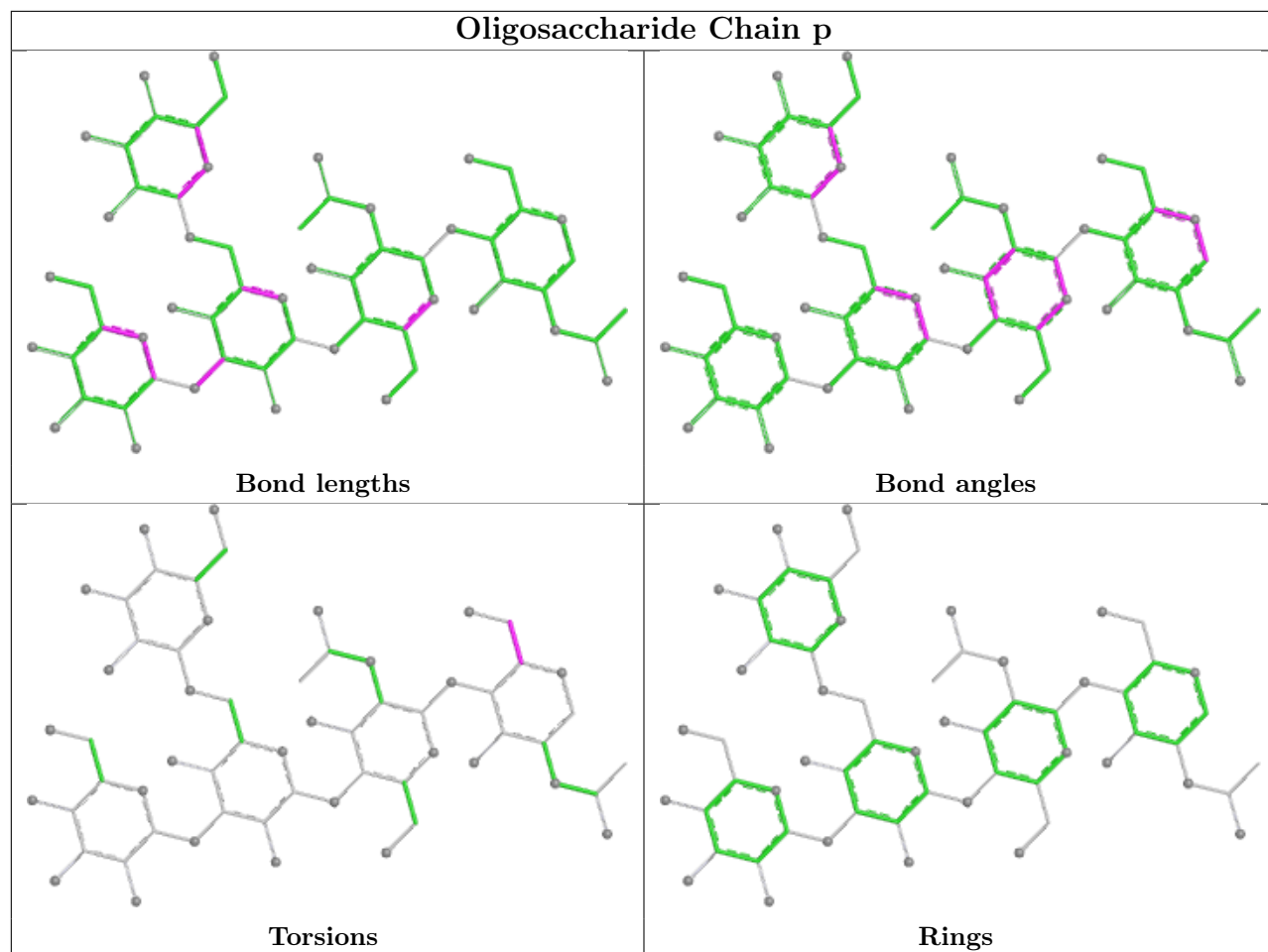


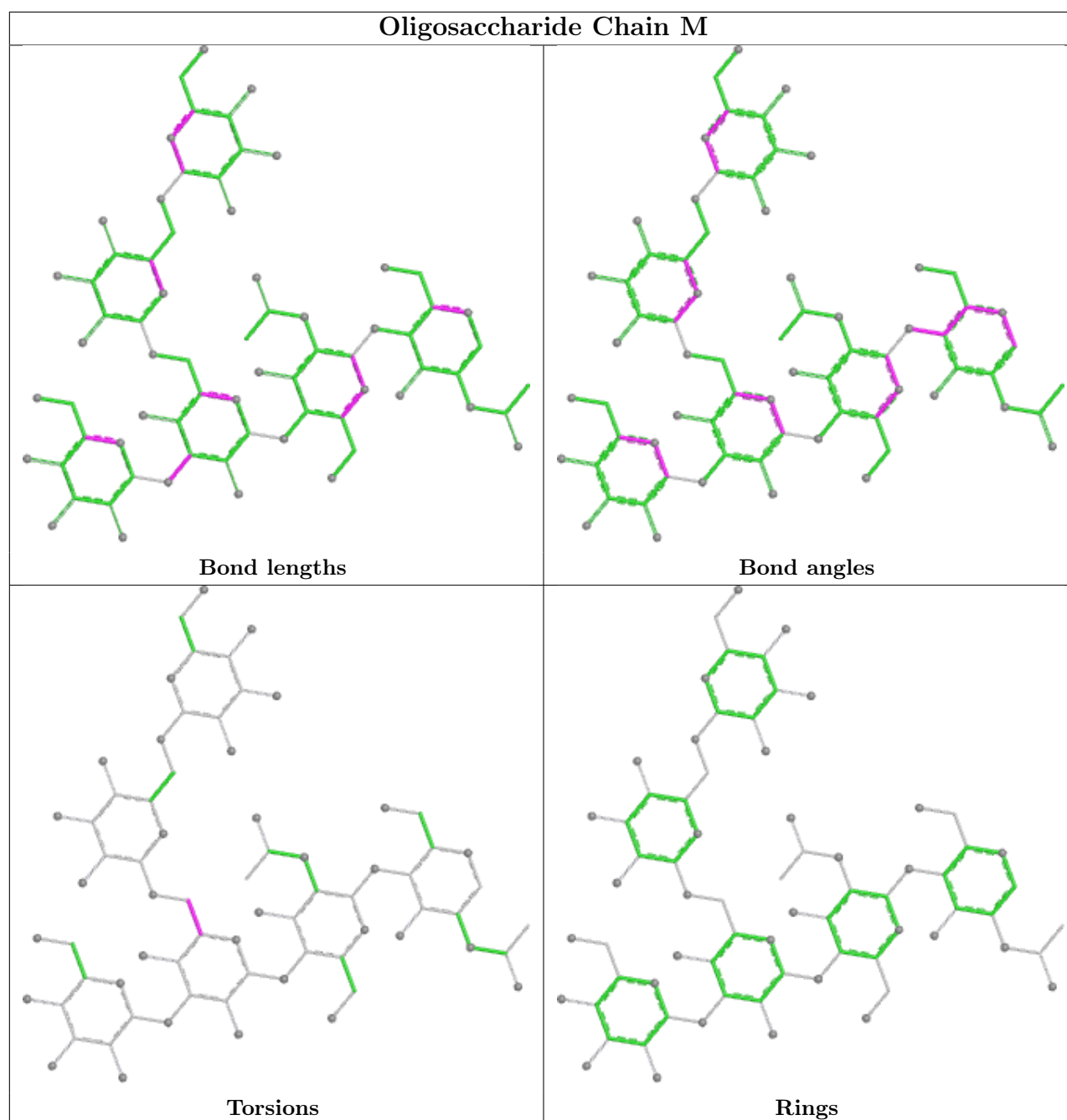












5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	a	602	1	14,14,15	1.08	1 (7%)	17,19,21	0.93	1 (5%)
9	NAG	e	601	1	14,14,15	1.23	2 (14%)	17,19,21	1.06	1 (5%)
9	NAG	a	601	1	14,14,15	1.24	2 (14%)	17,19,21	0.84	0
9	NAG	d	702	2	14,14,15	1.17	2 (14%)	17,19,21	0.81	1 (5%)
9	NAG	f	702	2	14,14,15	1.17	1 (7%)	17,19,21	0.76	1 (5%)
9	NAG	d	701	2	14,14,15	1.19	2 (14%)	17,19,21	0.94	1 (5%)
9	NAG	c	604	1	14,14,15	1.17	2 (14%)	17,19,21	0.90	0
9	NAG	b	701	2	14,14,15	1.10	1 (7%)	17,19,21	0.58	0
9	NAG	a	603	1	14,14,15	1.11	1 (7%)	17,19,21	0.63	0
9	NAG	b	702	2	14,14,15	1.12	2 (14%)	17,19,21	1.04	1 (5%)
9	NAG	a	604	1	14,14,15	1.28	3 (21%)	17,19,21	0.64	0
9	NAG	c	601	1	14,14,15	1.16	1 (7%)	17,19,21	0.75	0
9	NAG	e	602	1	14,14,15	1.12	1 (7%)	17,19,21	0.73	0
9	NAG	f	701	2	14,14,15	1.18	2 (14%)	17,19,21	0.84	1 (5%)
9	NAG	c	603	1	14,14,15	1.12	1 (7%)	17,19,21	0.91	1 (5%)
9	NAG	e	603	-	14,14,15	1.17	2 (14%)	17,19,21	0.73	0
9	NAG	c	602	1	14,14,15	1.25	2 (14%)	17,19,21	0.89	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
9	NAG	a	602	1	-	0/6/23/26	0/1/1/1
9	NAG	e	601	1	-	1/6/23/26	0/1/1/1
9	NAG	a	601	1	-	1/6/23/26	0/1/1/1
9	NAG	d	702	2	-	2/6/23/26	0/1/1/1
9	NAG	f	702	2	-	1/6/23/26	0/1/1/1
9	NAG	d	701	2	-	0/6/23/26	0/1/1/1
9	NAG	c	604	1	-	0/6/23/26	0/1/1/1
9	NAG	b	701	2	-	0/6/23/26	0/1/1/1
9	NAG	a	603	1	-	1/6/23/26	0/1/1/1
9	NAG	b	702	2	-	0/6/23/26	0/1/1/1
9	NAG	a	604	1	-	0/6/23/26	0/1/1/1
9	NAG	c	601	1	-	1/6/23/26	0/1/1/1
9	NAG	e	602	1	-	2/6/23/26	0/1/1/1
9	NAG	f	701	2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	c	603	1	-	1/6/23/26	0/1/1/1
9	NAG	e	603	-	-	0/6/23/26	0/1/1/1
9	NAG	c	602	1	-	1/6/23/26	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	c	602	NAG	O5-C5	3.12	1.49	1.43
9	e	602	NAG	O5-C5	2.94	1.49	1.43
9	f	702	NAG	O5-C5	2.78	1.48	1.43
9	e	601	NAG	O5-C5	2.77	1.48	1.43
9	c	603	NAG	O5-C5	2.73	1.48	1.43
9	a	604	NAG	O5-C5	2.72	1.48	1.43
9	a	603	NAG	O5-C5	2.71	1.48	1.43
9	a	604	NAG	C1-C2	2.65	1.56	1.52
9	e	603	NAG	O5-C5	2.65	1.48	1.43
9	d	701	NAG	O5-C5	2.64	1.48	1.43
9	f	701	NAG	O5-C5	2.64	1.48	1.43
9	c	604	NAG	C1-C2	2.64	1.55	1.52
9	a	602	NAG	O5-C5	2.63	1.48	1.43
9	a	601	NAG	O5-C5	2.61	1.48	1.43
9	e	603	NAG	O5-C1	2.50	1.47	1.43
9	b	701	NAG	O5-C5	2.49	1.48	1.43
9	d	702	NAG	O5-C5	2.48	1.48	1.43
9	c	601	NAG	O5-C5	2.33	1.48	1.43
9	e	601	NAG	O5-C1	2.23	1.47	1.43
9	c	604	NAG	O5-C5	2.23	1.47	1.43
9	a	604	NAG	O5-C1	2.22	1.47	1.43
9	a	601	NAG	C1-C2	2.20	1.55	1.52
9	d	701	NAG	C1-C2	2.16	1.55	1.52
9	b	702	NAG	O5-C5	2.14	1.47	1.43
9	b	702	NAG	C1-C2	2.06	1.55	1.52
9	d	702	NAG	C1-C2	2.06	1.55	1.52
9	c	602	NAG	C1-C2	2.05	1.55	1.52
9	f	701	NAG	C1-C2	2.05	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	602	NAG	C1-O5-C5	3.14	116.39	112.19
9	d	701	NAG	C1-O5-C5	2.84	115.99	112.19
9	c	603	NAG	C1-O5-C5	2.84	115.99	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	e	601	NAG	C1-O5-C5	2.64	115.72	112.19
9	f	701	NAG	C1-O5-C5	2.63	115.71	112.19
9	b	702	NAG	C4-C3-C2	2.57	114.78	111.02
9	f	702	NAG	C1-O5-C5	2.38	115.38	112.19
9	d	702	NAG	C1-O5-C5	2.02	114.90	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	e	601	NAG	O5-C5-C6-O6
9	a	601	NAG	O5-C5-C6-O6
9	c	601	NAG	O5-C5-C6-O6
9	e	602	NAG	C4-C5-C6-O6
9	e	602	NAG	O5-C5-C6-O6
9	d	702	NAG	C4-C5-C6-O6
9	d	702	NAG	O5-C5-C6-O6
9	c	602	NAG	C4-C5-C6-O6
9	c	603	NAG	C1-C2-N2-C7
9	f	702	NAG	C1-C2-N2-C7
9	a	603	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

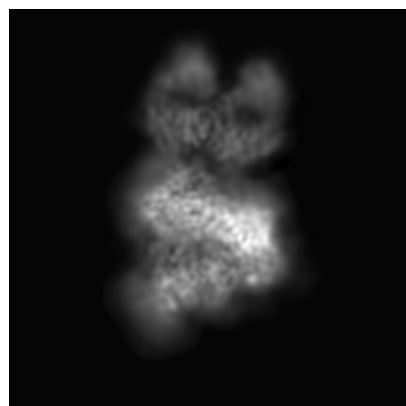
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23519. These allow visual inspection of the internal detail of the map and identification of artifacts.

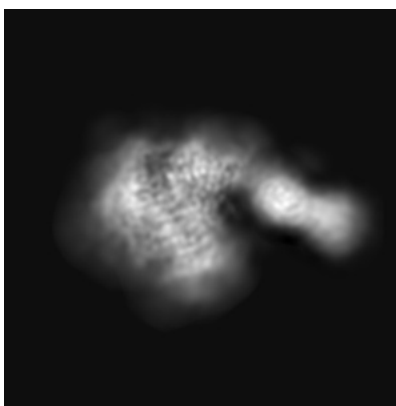
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

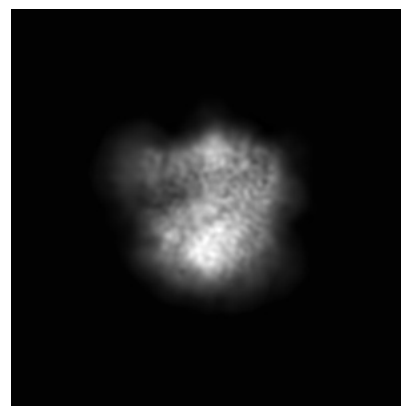
6.1.1 Primary map



X

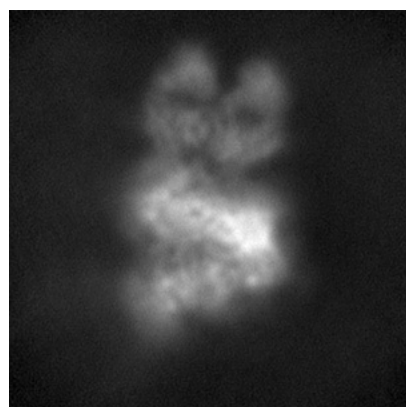


Y

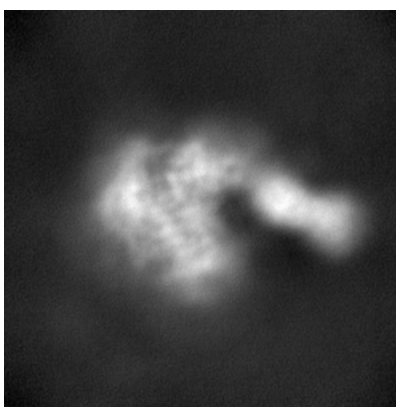


Z

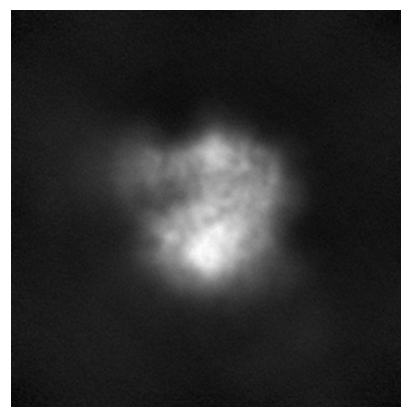
6.1.2 Raw map



X



Y

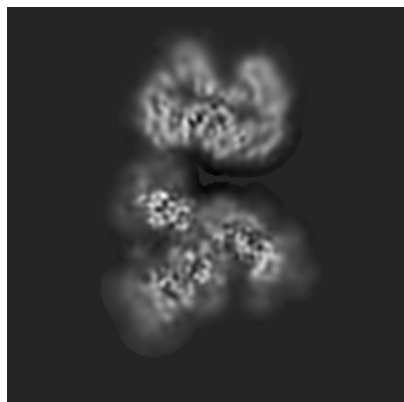


Z

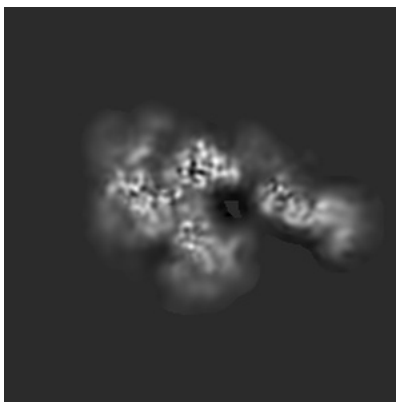
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

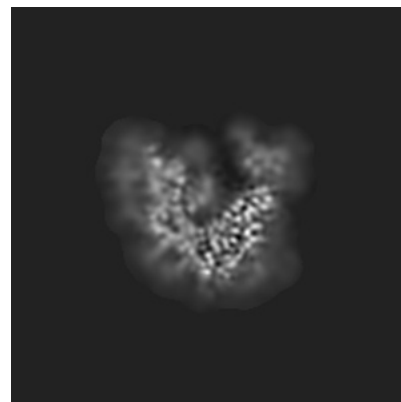
6.2.1 Primary map



X Index: 128

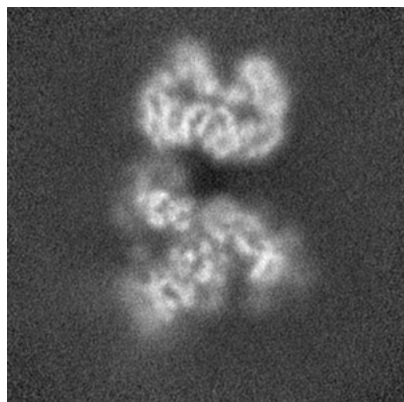


Y Index: 128

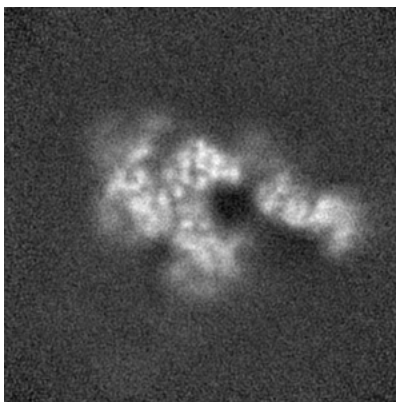


Z Index: 128

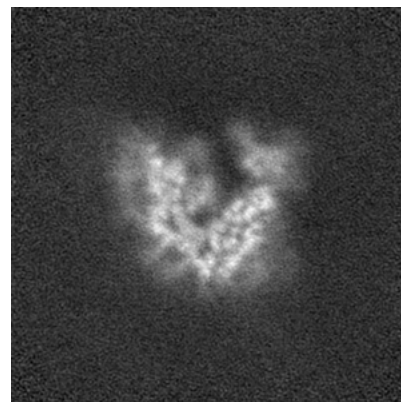
6.2.2 Raw map



X Index: 128



Y Index: 128

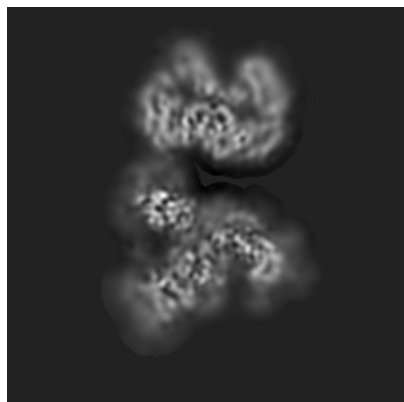


Z Index: 128

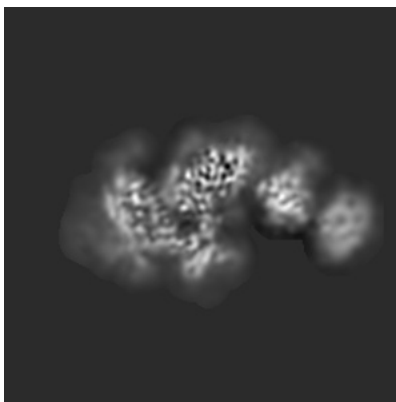
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

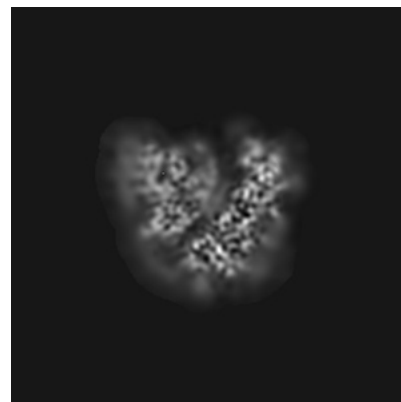
6.3.1 Primary map



X Index: 129

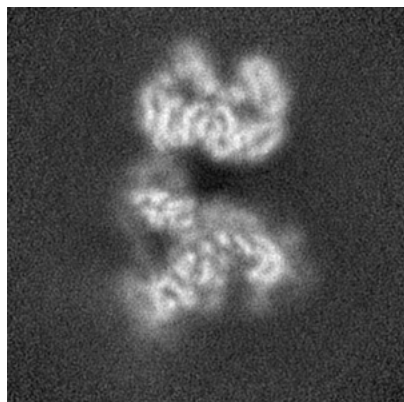


Y Index: 113

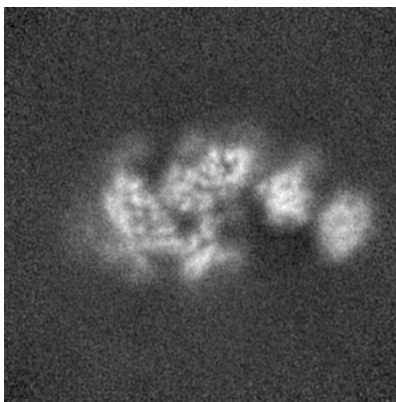


Z Index: 122

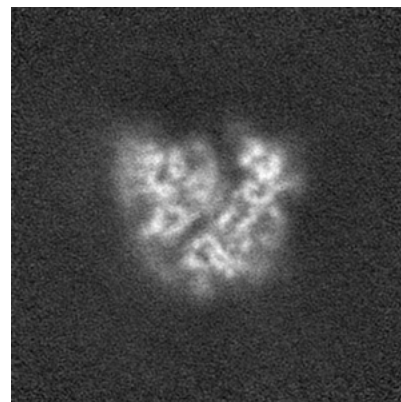
6.3.2 Raw map



X Index: 130



Y Index: 113

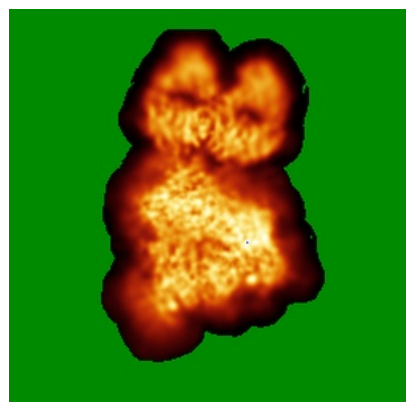


Z Index: 122

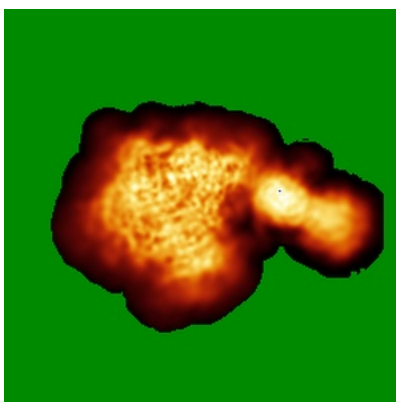
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

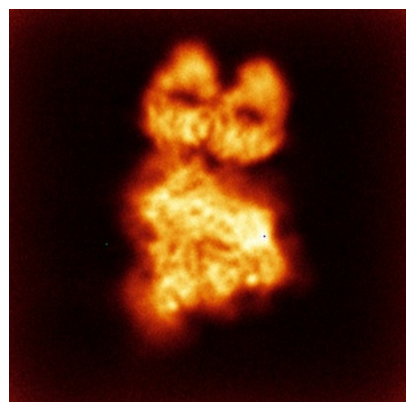


Y

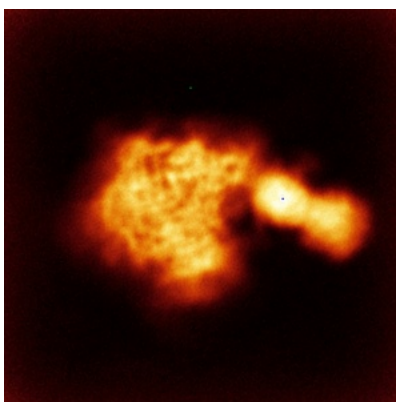


Z

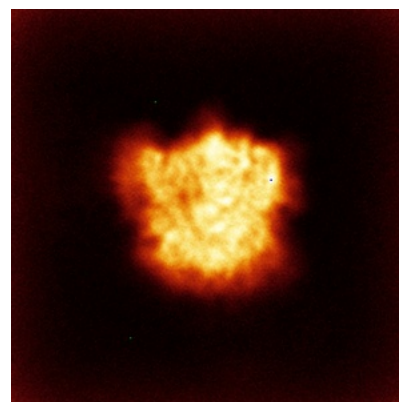
6.4.2 Raw map



X



Y

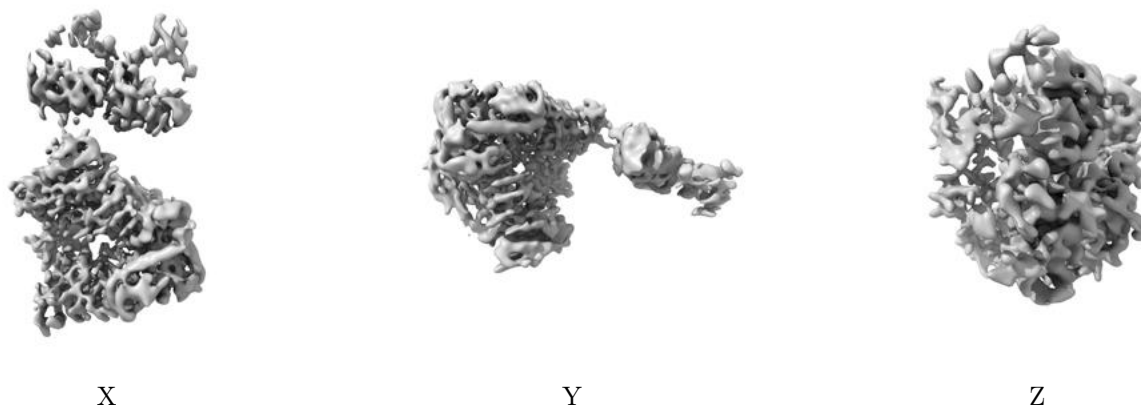


Z

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.

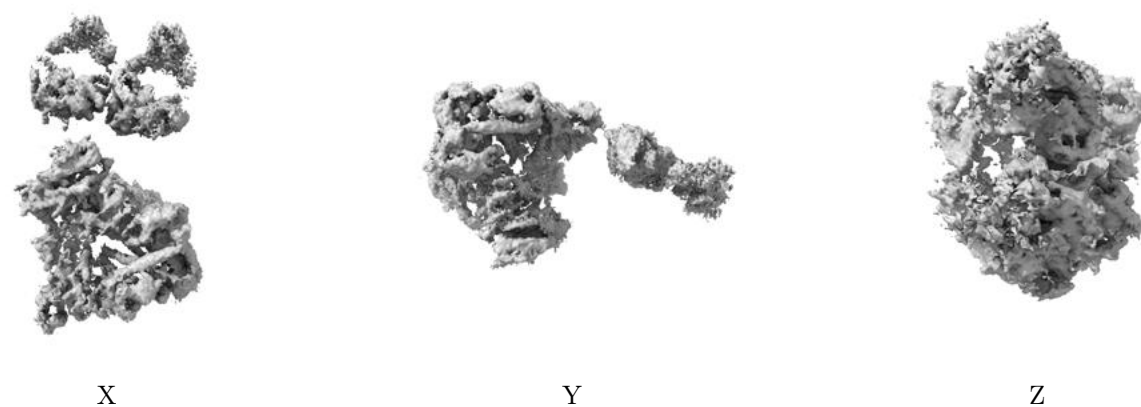
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.816. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

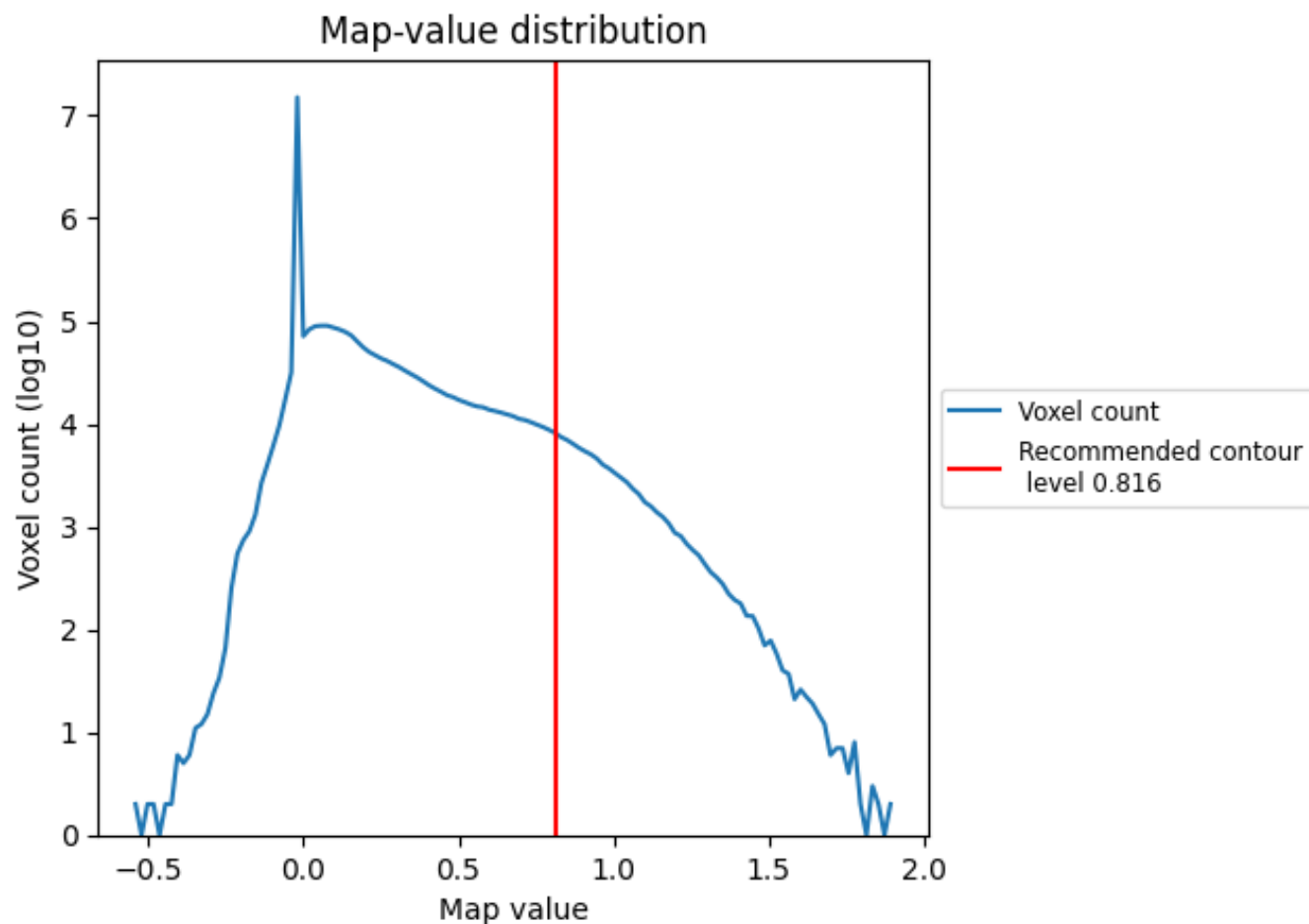
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

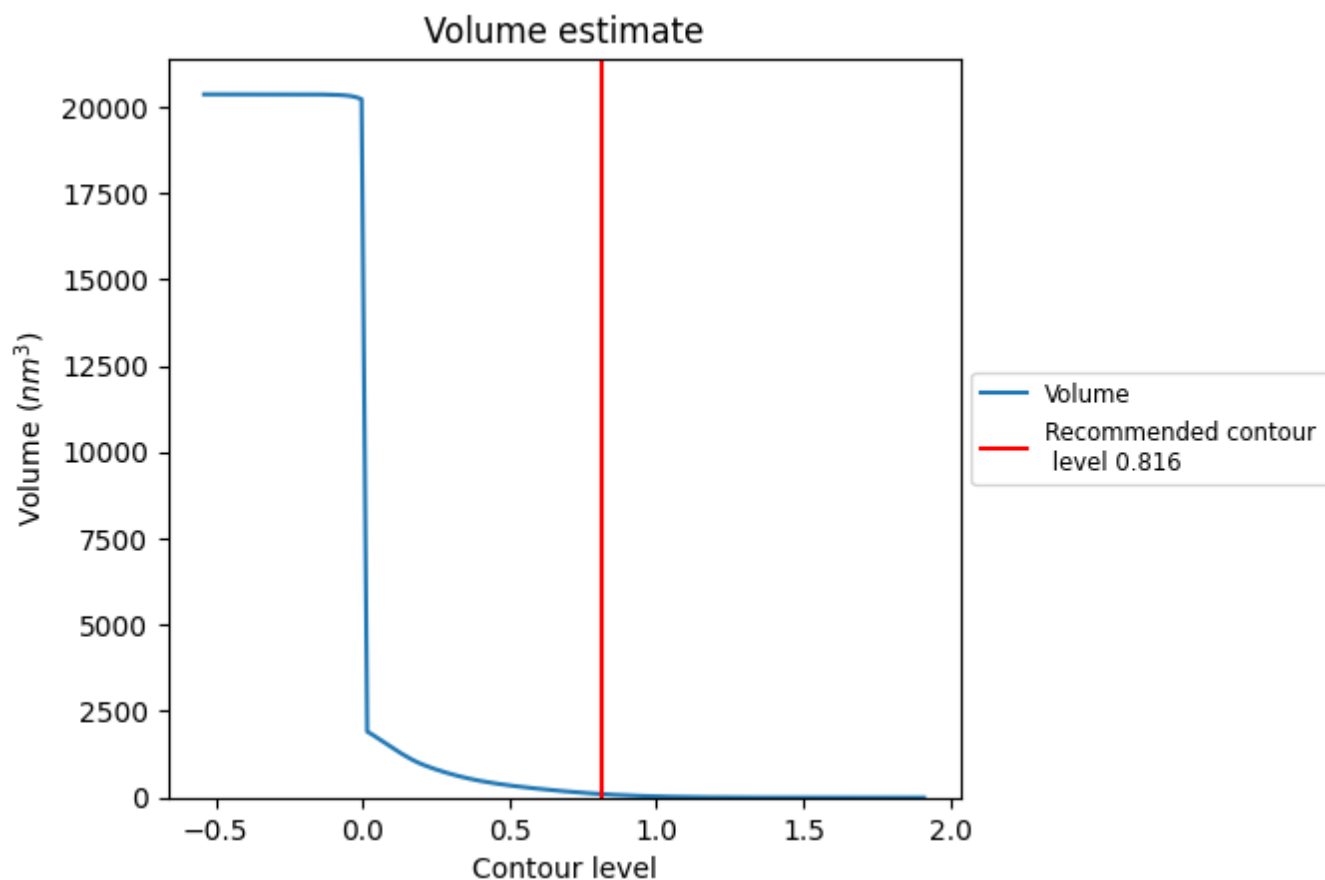
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

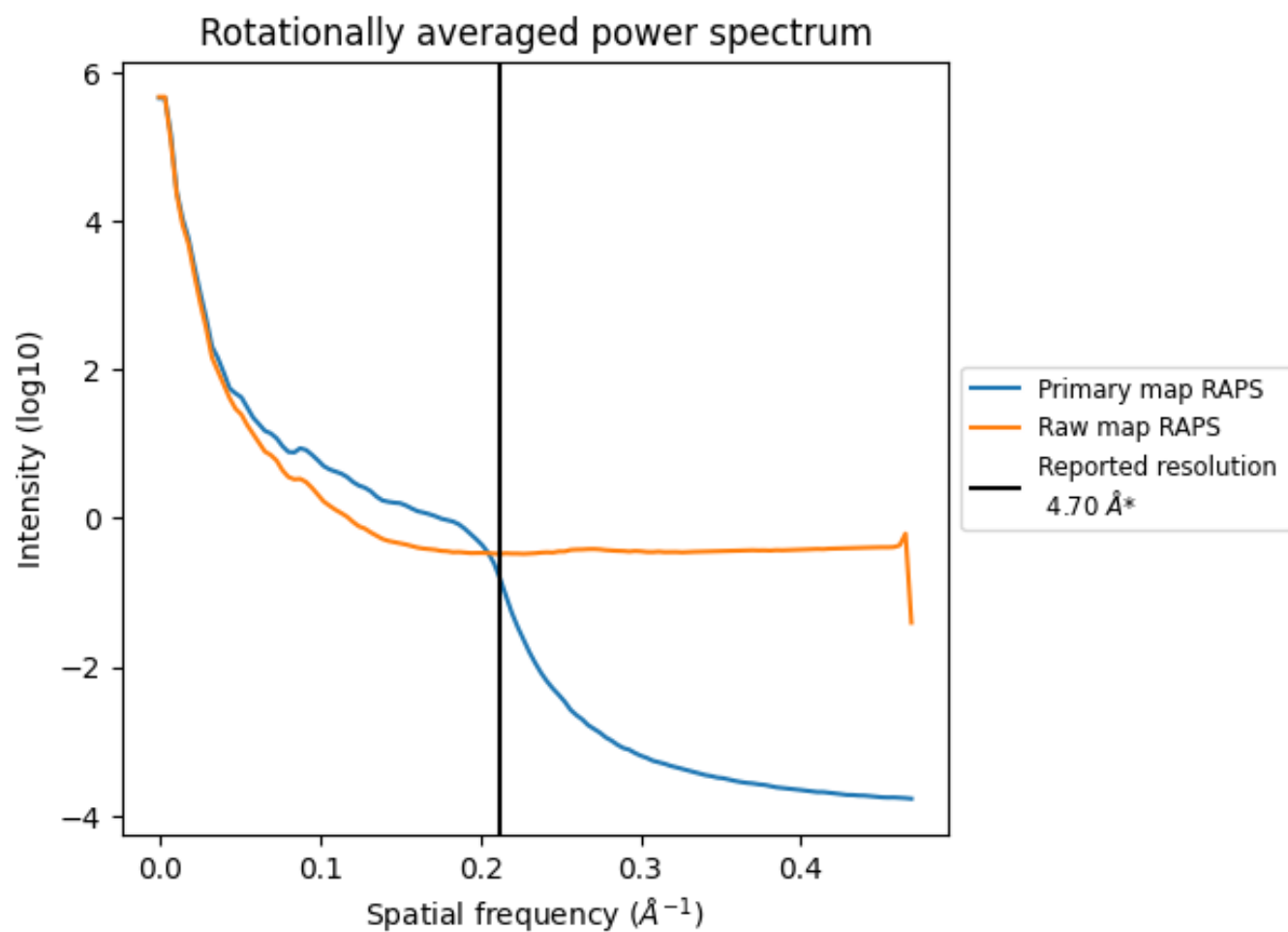
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm^3 ; this corresponds to an approximate mass of 90 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

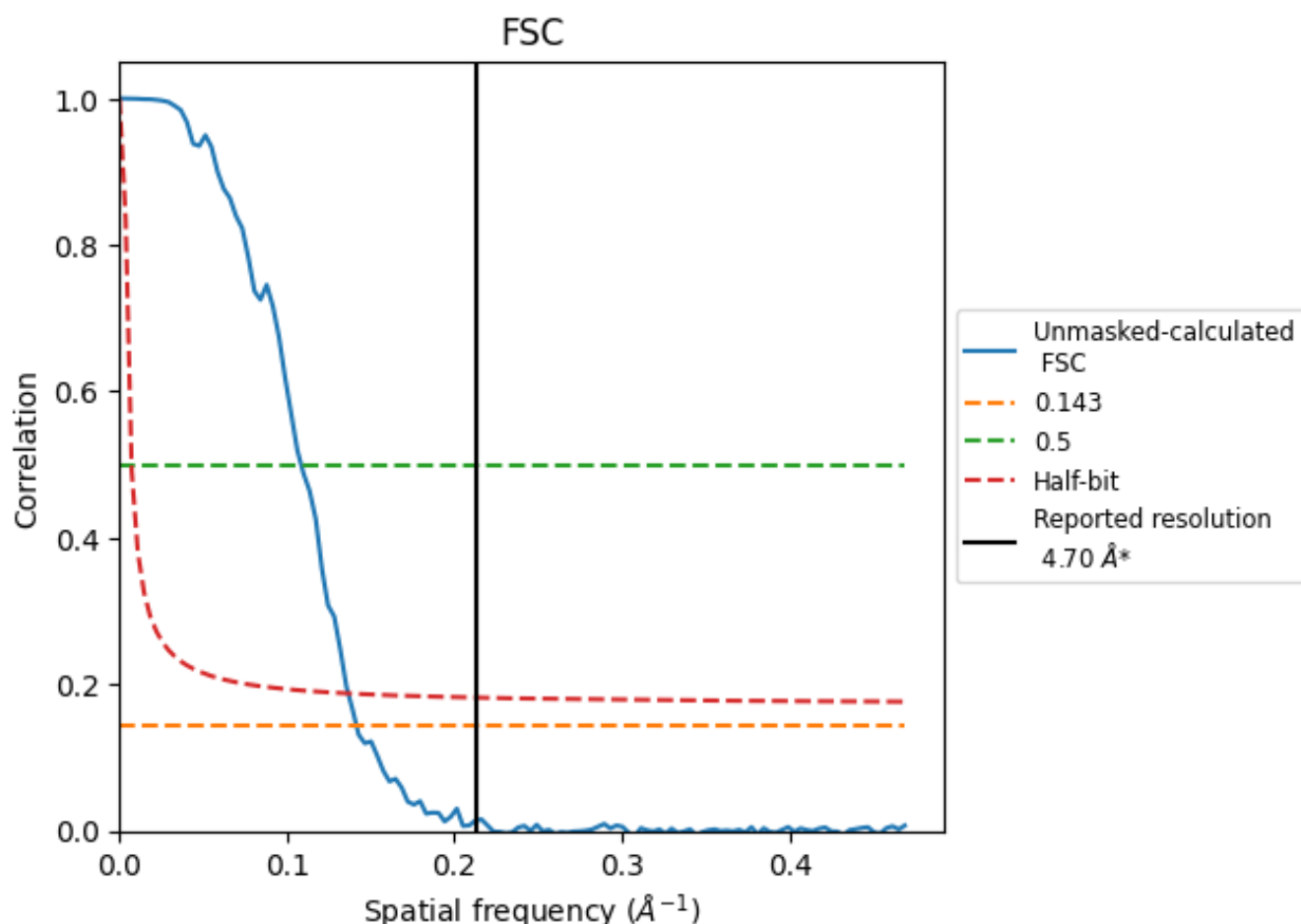


*Reported resolution corresponds to spatial frequency of 0.213 \AA^{-1}

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 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

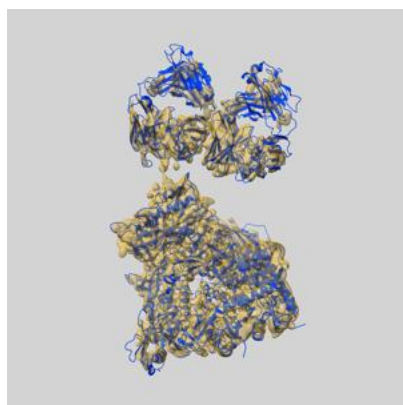
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.07	9.23	7.32

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.07 differs from the reported value 4.7 by more than 10 %

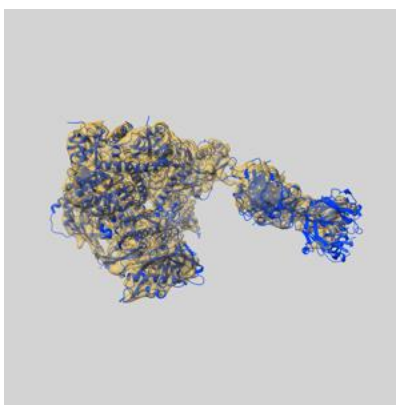
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23519 and PDB model 7LUA. Per-residue inclusion information can be found in section 3 on page 12.

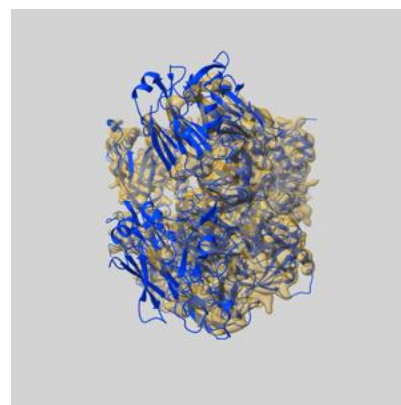
9.1 Map-model overlay [i](#)



X



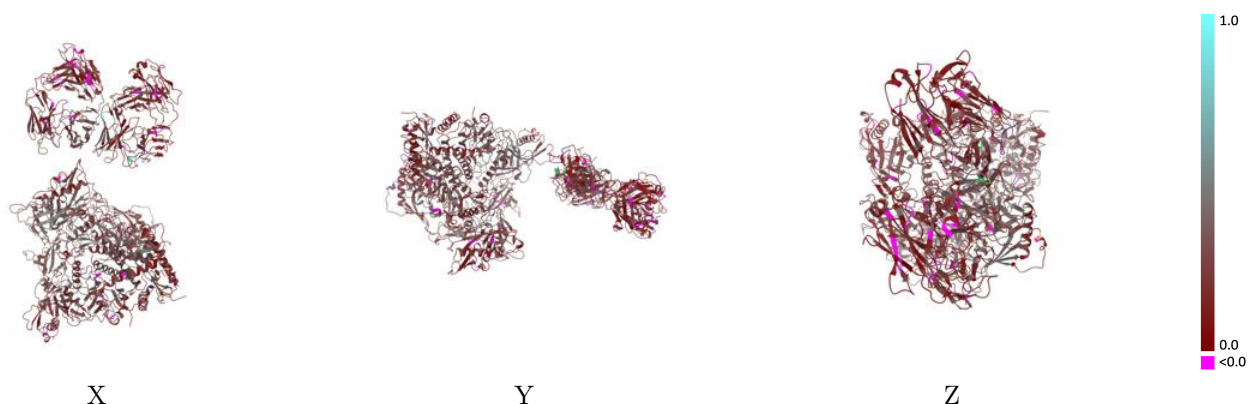
Y



Z

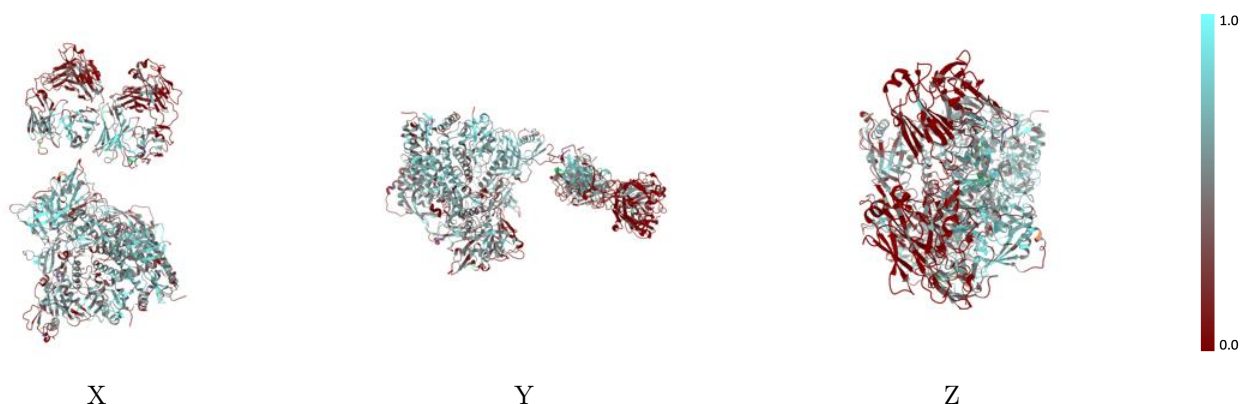
The images above show the 3D surface view of the map at the recommended contour level 0.816 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



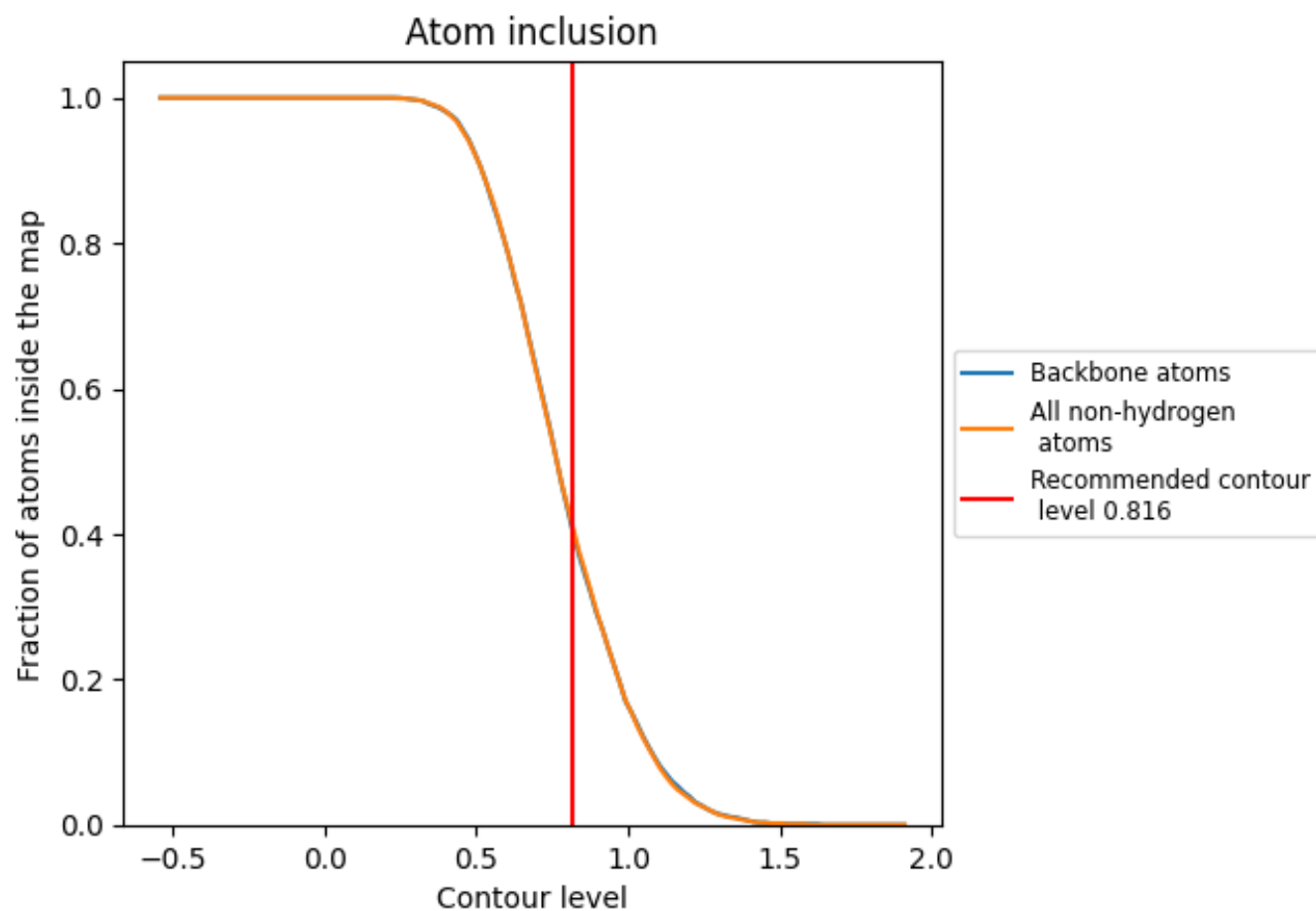
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.816).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 41% of all backbone atoms, 41% 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 (0.816) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4130	 0.2670
A	 0.2050	 0.3710
B	 0.2860	 0.3470
C	 0.3330	 0.2960
D	 0.3770	 0.4310
E	 0.3330	 0.3890
F	 0.1540	 0.3160
G	 0.2140	 0.3290
H	 0.3850	 0.4200
I	 0.2820	 0.3360
J	 0.0000	 0.3080
K	 0.0000	 0.3550
L	 0.0770	 0.3420
M	 0.4720	 0.4060
N	 0.0330	 0.3820
O	 0.0000	 0.2470
P	 0.0260	 0.3520
Q	 0.1790	 0.2520
R	 0.1030	 0.3270
S	 0.3110	 0.3900
T	 0.2310	 0.3590
U	 0.1030	 0.2990
V	 0.0000	 0.3500
W	 0.1540	 0.3580
X	 0.2050	 0.2210
Y	 0.0000	 0.3140
Z	 0.1030	 0.3590
a	 0.4610	 0.2700
b	 0.5520	 0.2780
c	 0.4190	 0.2610
d	 0.5490	 0.2770
e	 0.5960	 0.3450
f	 0.5720	 0.2940
g	 0.2250	 0.1780
h	 0.3800	 0.2250



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.3610	 0.2150
j	 0.2400	 0.1790
k	 0.1540	 0.3460
l	 0.0000	 0.2690
m	 0.0000	 0.3340
n	 0.2500	 0.2790
o	 0.2310	 0.3080
p	 0.2130	 0.3130
q	 0.1790	 0.3390
r	 0.0260	 0.3280
s	 0.0000	 0.2190
t	 0.1280	 0.3630
u	 0.1280	 0.3140
v	 0.0000	 0.3140
w	 0.0770	 0.3780
x	 0.0510	 0.3530