



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:14 PM UTC

PDB ID : 6DID / pdb_00006did
EMDB ID : EMD-7896
Title : HIV Env BG505 SOSIP with polyclonal Fabs from immunized rabbit #3417 post-boost#1
Authors : Turner, H.L.; Cottrell, C.A.; Oyen, D.; Wilson, I.A.; Ward, A.B.
Deposited on : 2018-05-23
Resolution : 4.71 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

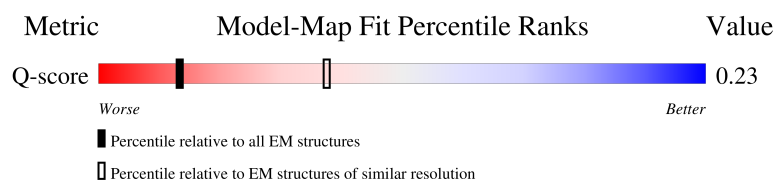
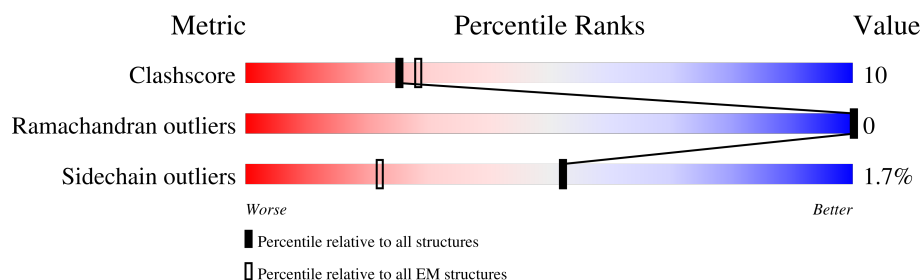
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.71 Å.

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



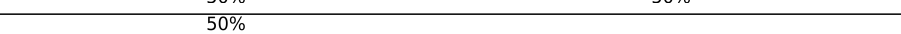
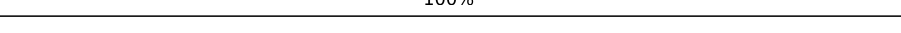
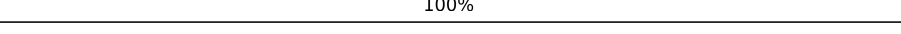
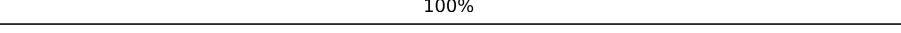
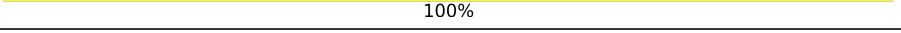
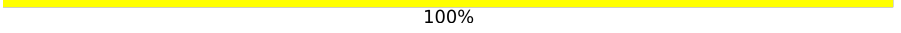
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1656 (4.21 - 5.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	481	
1	F	481	
1	G	481	
2	B	153	

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Mol	Chain	Length	Quality of chain
2	I	153	
2	J	153	
3	C	217	
3	E	217	
3	H	217	
4	D	214	
4	K	214	
4	L	214	
5	M	3	
5	Y	3	
5	k	3	
6	N	2	
6	O	2	
6	P	2	
6	S	2	
6	T	2	
6	U	2	
6	X	2	
6	Z	2	
6	a	2	
6	b	2	
6	e	2	
6	f	2	
6	g	2	
6	j	2	

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Mol	Chain	Length	Quality of chain
6	l	2	100%
6	m	2	50% 50%
6	n	2	100%
6	q	2	50% 50%
6	r	2	50% 100%
6	s	2	50% 50%
6	v	2	100%
7	Q	7	14% 100%
7	c	7	14% 100%
7	o	7	14% 100%
8	R	8	12% 88% 100%
8	d	8	12% 88% 100%
8	p	8	12% 88% 100%
9	V	6	17% 100%
9	h	6	17% 100%
9	t	6	17% 100%
10	W	4	25% 50% 25%
10	i	4	25% 50% 25%
10	u	4	25% 50% 25%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	S	1	-	-	X	-
6	NAG	e	1	-	-	X	-
6	NAG	q	1	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 34674 atoms, of which 9465 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	444	Total	C	N	O	S	0	0
			3493	2192	617	656	28		
1	F	444	Total	C	N	O	S	0	0
			3493	2192	617	656	28		
1	G	444	Total	C	N	O	S	0	0
			3493	2192	617	656	28		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
F	332	ASN	THR	conflict	UNP Q2N0S6
F	501	CYS	ALA	conflict	UNP Q2N0S6
F	509	ARG	-	expression tag	UNP Q2N0S6
F	510	ARG	-	expression tag	UNP Q2N0S6
F	511	ARG	-	expression tag	UNP Q2N0S6
F	512	ARG	-	expression tag	UNP Q2N0S6
F	513	ARG	-	expression tag	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		
2	I	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		
2	J	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S7
B	605	CYS	THR	conflict	UNP Q2N0S7
I	559	PRO	ILE	conflict	UNP Q2N0S7
I	605	CYS	THR	conflict	UNP Q2N0S7
J	559	PRO	ILE	conflict	UNP Q2N0S7
J	605	CYS	THR	conflict	UNP Q2N0S7

- Molecule 3 is a protein called Monoclonal antibody 10A light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	217	Total	C	H	N	O	S	7	0
			3258	1038	1596	272	343	9		
3	E	217	Total	C	H	N	O	S	7	0
			3258	1038	1596	272	343	9		
3	H	217	Total	C	H	N	O	S	7	0
			3258	1038	1596	272	343	9		

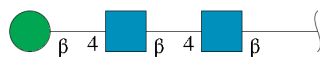
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	140	SER	THR	conflict	UNP P01840
E	140	SER	THR	conflict	UNP P01840
H	140	SER	THR	conflict	UNP P01840

- Molecule 4 is a protein called Monoclonal antibody 10A heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	213	Total	C	H	N	O	S	6	0
			3151	1001	1559	266	314	11		
4	K	213	Total	C	H	N	O	S	6	0
			3151	1001	1559	266	314	11		
4	L	213	Total	C	H	N	O	S	6	0
			3151	1001	1559	266	314	11		

- 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	M	3	Total	C	N	O	0	0
			39	22	2	15		
5	Y	3	Total	C	N	O	0	0
			39	22	2	15		
5	k	3	Total	C	N	O	0	0
			39	22	2	15		

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



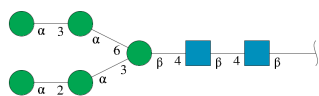
Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	O	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		
6	U	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		
6	Z	2	Total	C	N	O	0	0
			28	16	2	10		
6	a	2	Total	C	N	O	0	0
			28	16	2	10		
6	b	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	2	Total	C	N	O	0	0
			28	16	2	10		
6	f	2	Total	C	N	O	0	0
			28	16	2	10		
6	g	2	Total	C	N	O	0	0
			28	16	2	10		
6	j	2	Total	C	N	O	0	0
			28	16	2	10		
6	l	2	Total	C	N	O	0	0
			28	16	2	10		
6	m	2	Total	C	N	O	0	0
			28	16	2	10		
6	n	2	Total	C	N	O	0	0
			28	16	2	10		
6	q	2	Total	C	N	O	0	0
			28	16	2	10		
6	r	2	Total	C	N	O	0	0
			28	16	2	10		
6	s	2	Total	C	N	O	0	0
			28	16	2	10		
6	v	2	Total	C	N	O	0	0
			28	16	2	10		

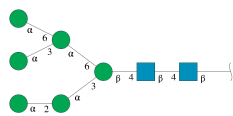
- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	7	Total	C	N	O	0	0
			83	46	2	35		
7	c	7	Total	C	N	O	0	0
			83	46	2	35		
7	o	7	Total	C	N	O	0	0
			83	46	2	35		

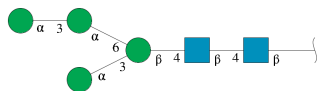
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2

-acetamido-2-deoxy-beta-D-glucopyranose.



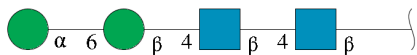
Mol	Chain	Residues	Atoms				AltConf	Trace
8	R	8	Total	C	N	O	0	0
			94	52	2	40		
8	d	8	Total	C	N	O	0	0
			94	52	2	40		
8	p	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
9	V	6	Total	C	N	O	0	0
			72	40	2	30		
9	h	6	Total	C	N	O	0	0
			72	40	2	30		
9	t	6	Total	C	N	O	0	0
			72	40	2	30		

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



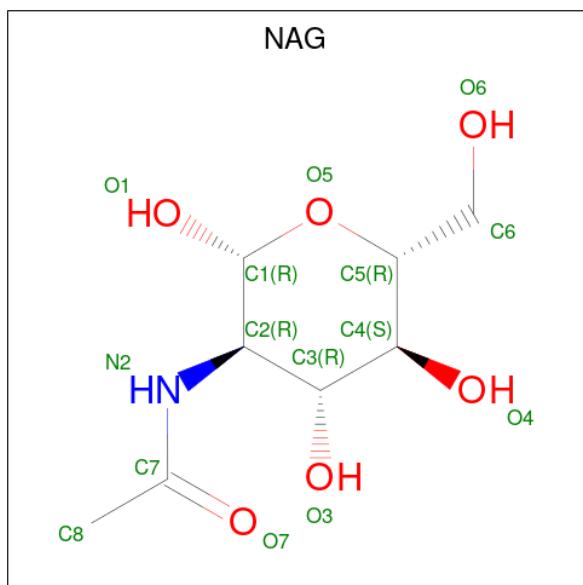
Mol	Chain	Residues	Atoms				AltConf	Trace
10	W	4	Total	C	N	O	0	0
			50	28	2	20		
10	i	4	Total	C	N	O	0	0
			50	28	2	20		

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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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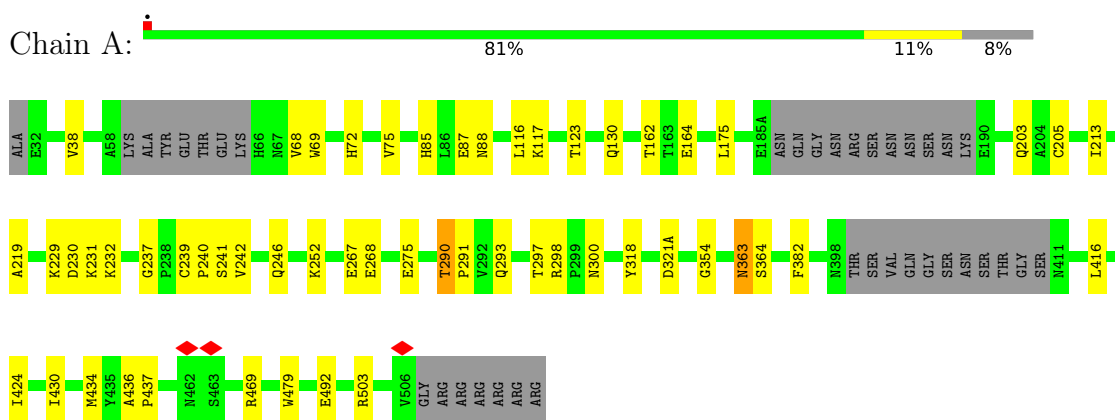
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Mol	Chain	Residues	Atoms				AltConf
11	F	1	Total 14	C 8	N 1	O 5	0
11	F	1	Total 14	C 8	N 1	O 5	0
11	I	1	Total 14	C 8	N 1	O 5	0
11	I	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	J	1	Total 14	C 8	N 1	O 5	0
11	J	1	Total 14	C 8	N 1	O 5	0

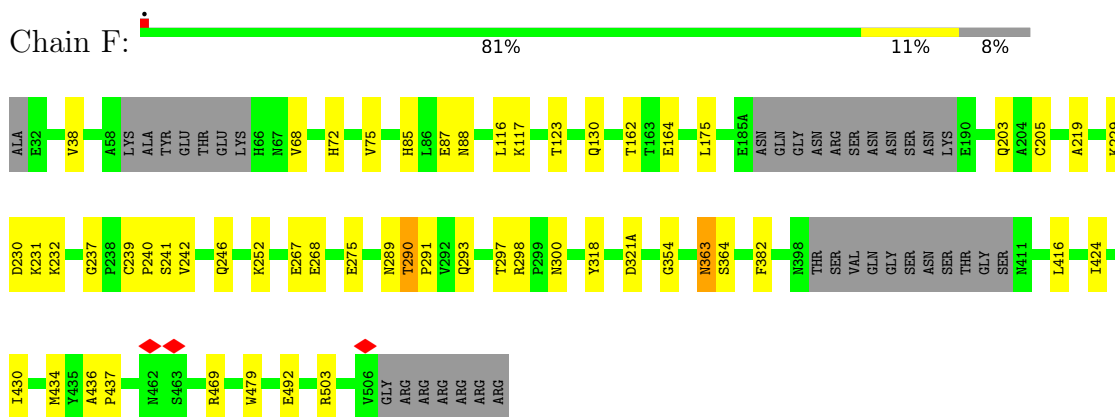
3 Residue-property plots

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.

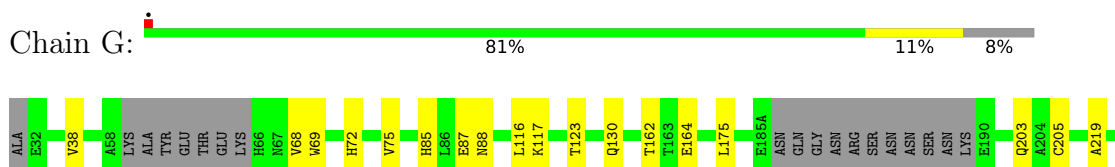
• Molecule 1: Envelope glycoprotein gp160

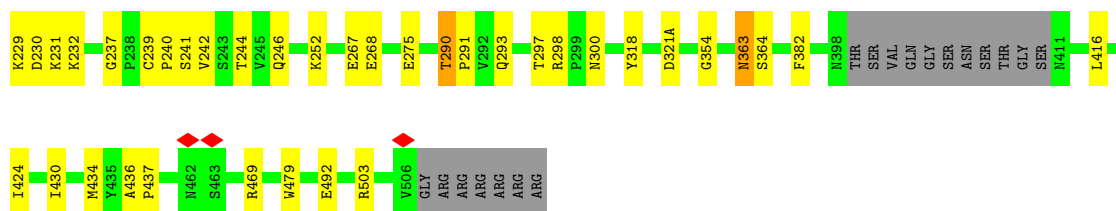


• Molecule 1: Envelope glycoprotein gp160



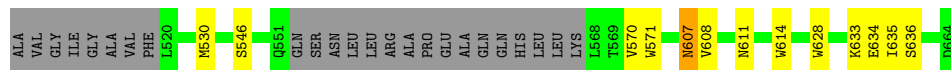
• Molecule 1: Envelope glycoprotein gp160





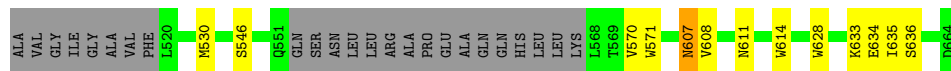
• Molecule 2: Envelope glycoprotein gp160

Chain B: 76% 8% 16%



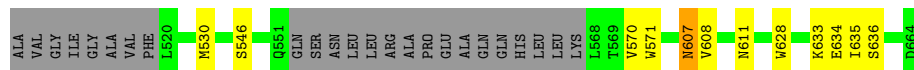
• Molecule 2: Envelope glycoprotein gp160

Chain I: 76% 8% 16%



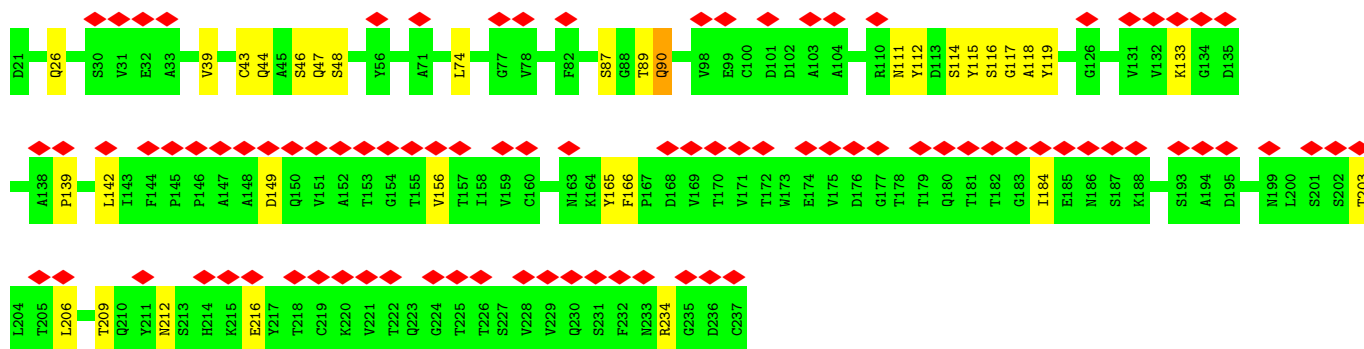
• Molecule 2: Envelope glycoprotein gp160

Chain J: 76% 7% 16%



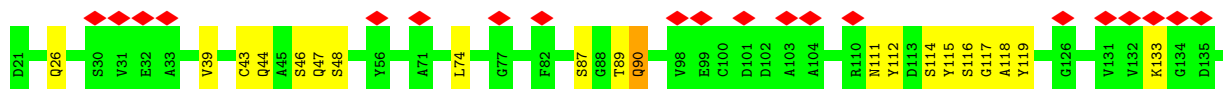
• Molecule 3: Monoclonal antibody 10A light chain

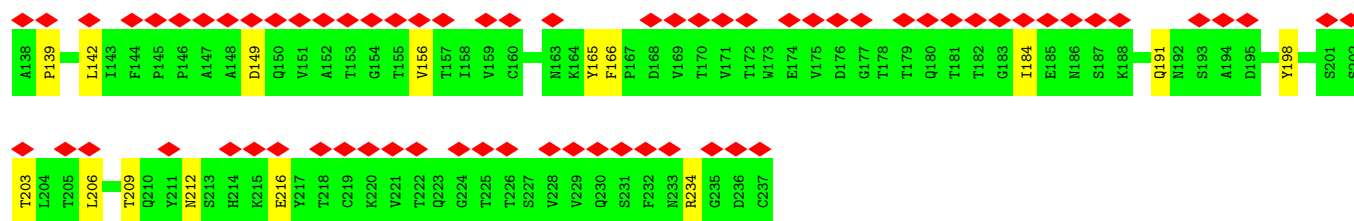
Chain C: 41% 85% 15%



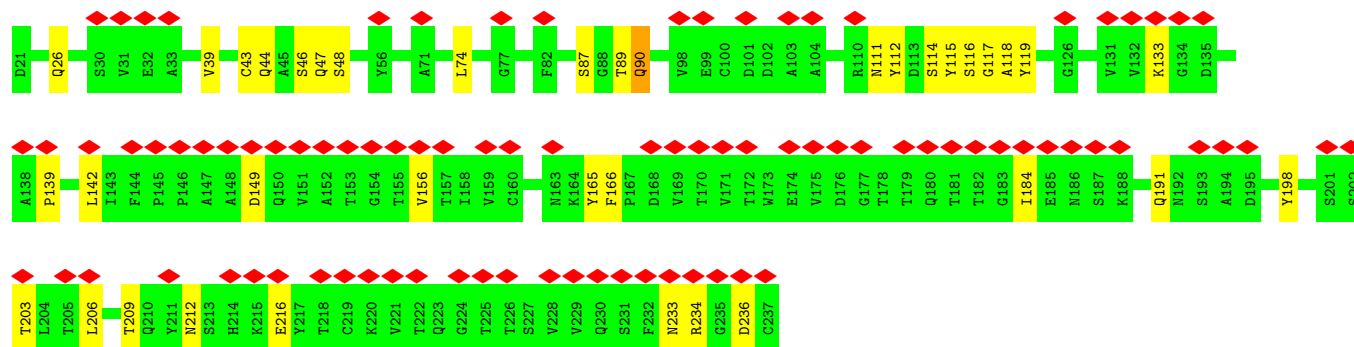
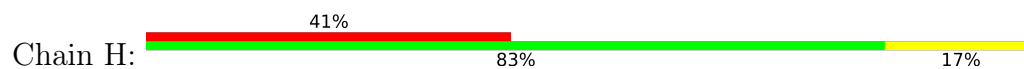
• Molecule 3: Monoclonal antibody 10A light chain

Chain E: 41% 84% 16%

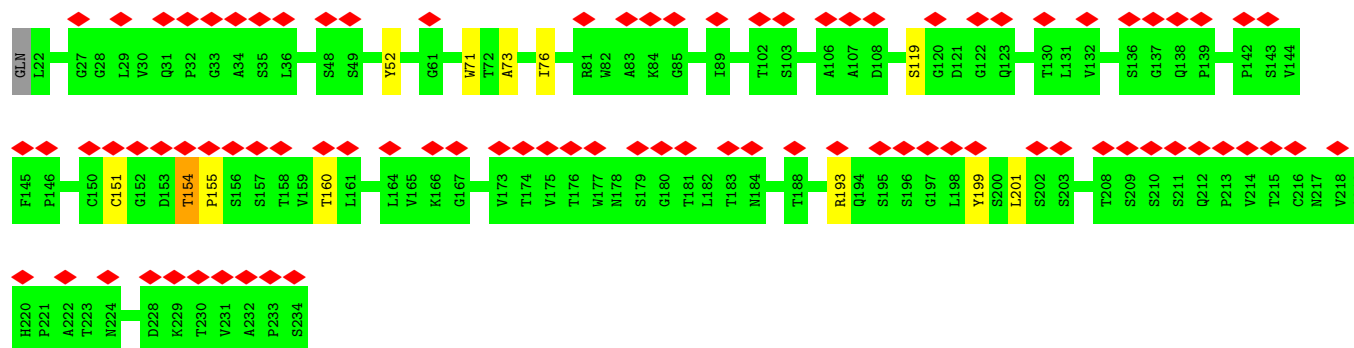
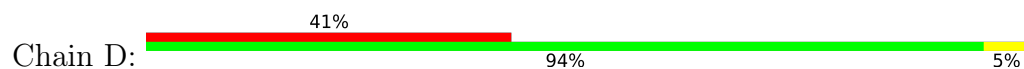




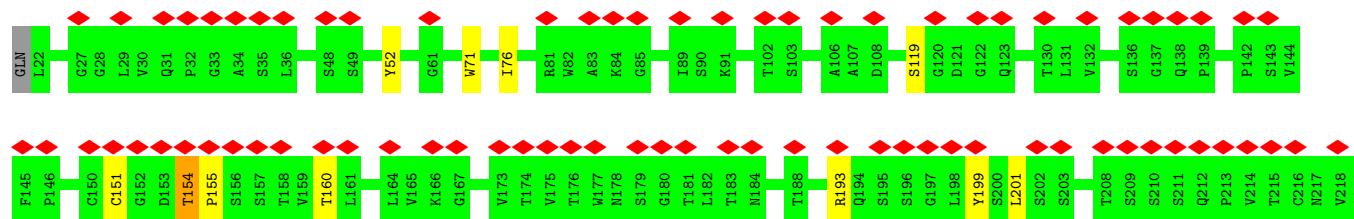
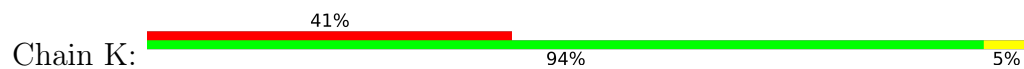
• Molecule 3: Monoclonal antibody 10A light chain

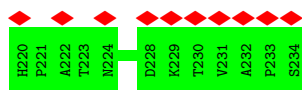


• Molecule 4: Monoclonal antibody 10A heavy chain



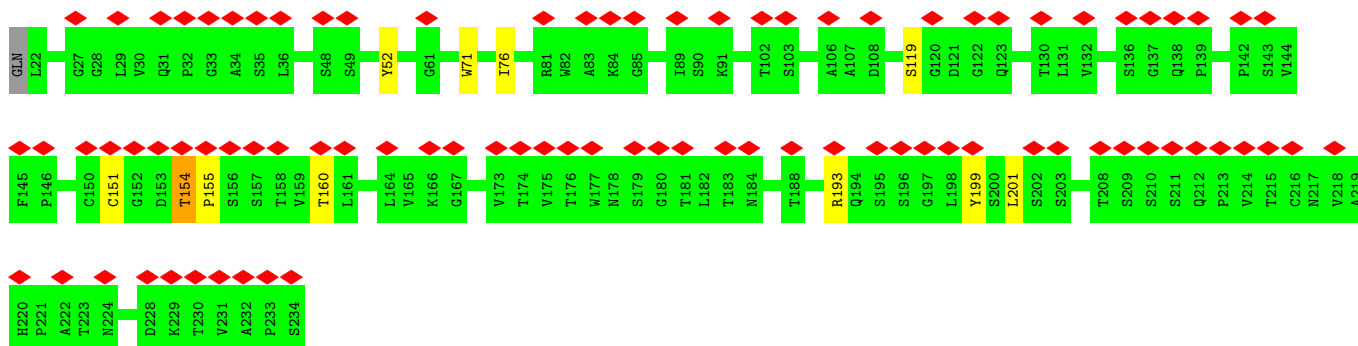
• Molecule 4: Monoclonal antibody 10A heavy chain





- Molecule 4: Monoclonal antibody 10A heavy chain

Chain L: 41% 94% 5%



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

Chain M: 33% 67% 67%



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

Chain Y: 33% 67% 67%



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

Chain k: 33% 67% 67%



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

Chain N: 100%

MAG1
MAG2

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

Chain O:  50% 50%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

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

Chain S:  50% 50%

MAG1
MAG2

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

Chain T:  50% 100%

MAG1
MAG2

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

Chain U:  50% 50%

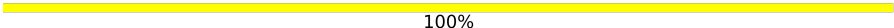
MAG1
MAG2

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

Chain X:  100%

MAG1
MAG2

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

Chain Z:  100%

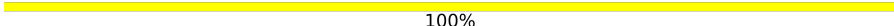
NAG1
NAG2

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

Chain a:  50% 50%

NAG1
NAG2

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

Chain b:  100%

NAG1
NAG2

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

Chain e:  50% 50%

NAG1
NAG2

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

Chain f:  50% 100%

♦
NAG1
NAG2

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

Chain g:  50% 50%

NAG1
NAG2

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

Chain j:  100%

NAG1
NAG2

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

Chain l:  100%

NAG1
NAG2

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

Chain m:  50% 50%

NAG1
NAG2

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

Chain n:  100%

NAG1
NAG2

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

Chain q:  50% 50%

NAG1
NAG2

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

Chain r:  50% 100%

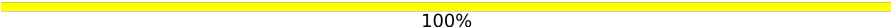

NAG1
NAG2

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

Chain s:  50% 50%

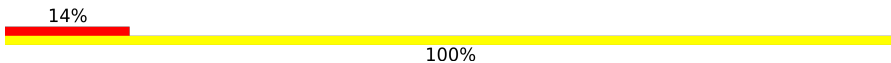


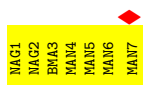
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:  100%

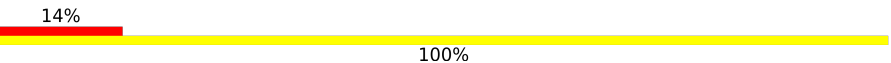


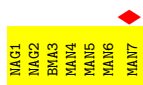
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  14% 100%

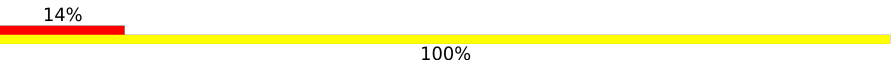


- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  14% 100%



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

Chain o:  14% 100%



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

Chain R:  12% 100% 88%



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



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



- Molecule 9: alpha-D-mannopyranose-(1-3)-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



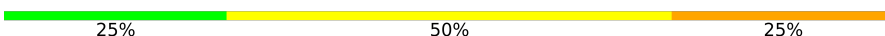
- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-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

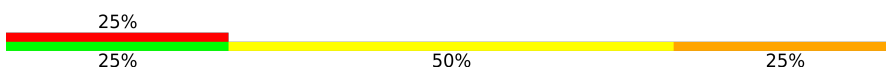


- Molecule 10: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 

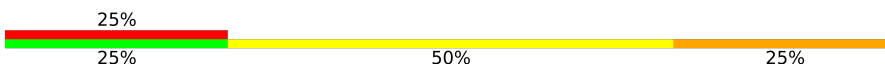


- Molecule 10: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i: 



- Molecule 10: 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

Chain u: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	161639	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 ($e^-/\text{\AA}^2$)	52.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.395	Depositor
Minimum map value	-0.402	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	345.0, 345.0, 345.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, NAG

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	0.97	0/3565	1.34	40/4842 (0.8%)
1	F	0.97	0/3565	1.34	40/4842 (0.8%)
1	G	0.97	0/3565	1.34	41/4842 (0.8%)
2	B	1.05	0/1041	1.16	7/1412 (0.5%)
2	I	1.05	0/1041	1.16	7/1412 (0.5%)
2	J	1.05	0/1041	1.16	7/1412 (0.5%)
3	C	0.44	0/1697	0.60	0/2319
3	E	0.44	0/1697	0.60	0/2319
3	H	0.44	0/1697	0.60	0/2319
4	D	0.48	0/1641	0.59	0/2249
4	K	0.48	0/1641	0.59	0/2249
4	L	0.48	0/1641	0.59	0/2249
All	All	0.81	0/23832	1.06	142/32466 (0.4%)

There are no bond length outliers.

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	LYS	CA-C-N	10.33	131.59	120.12
1	A	252	LYS	C-N-CA	10.33	131.59	120.12
1	G	252	LYS	CA-C-N	10.29	131.54	120.12
1	G	252	LYS	C-N-CA	10.29	131.54	120.12
1	F	252	LYS	CA-C-N	10.28	131.53	120.12
1	F	252	LYS	C-N-CA	10.28	131.53	120.12
1	F	239	CYS	CA-C-N	9.38	129.04	119.56
1	F	239	CYS	C-N-CA	9.38	129.04	119.56
1	A	239	CYS	CA-C-N	9.36	129.02	119.56
1	A	239	CYS	C-N-CA	9.36	129.02	119.56
1	G	239	CYS	CA-C-N	9.34	128.99	119.56
1	G	239	CYS	C-N-CA	9.34	128.99	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	ALA	CA-C-N	8.99	126.22	119.66
1	A	436	ALA	C-N-CA	8.99	126.22	119.66
1	F	436	ALA	CA-C-N	8.94	126.18	119.66
1	F	436	ALA	C-N-CA	8.94	126.18	119.66
1	G	436	ALA	CA-C-N	8.88	126.14	119.66
1	G	436	ALA	C-N-CA	8.88	126.14	119.66
1	G	237	GLY	CA-C-N	8.60	128.64	119.78
1	G	237	GLY	C-N-CA	8.60	128.64	119.78
1	A	237	GLY	CA-C-N	8.53	128.56	119.78
1	A	237	GLY	C-N-CA	8.53	128.56	119.78
1	F	237	GLY	CA-C-N	8.51	128.55	119.78
1	F	237	GLY	C-N-CA	8.51	128.55	119.78
1	A	298	ARG	CA-C-N	8.43	128.16	119.56
1	A	298	ARG	C-N-CA	8.43	128.16	119.56
1	G	298	ARG	CA-C-N	8.38	128.11	119.56
1	G	298	ARG	C-N-CA	8.38	128.11	119.56
1	F	298	ARG	CA-C-N	8.37	128.10	119.56
1	F	298	ARG	C-N-CA	8.37	128.10	119.56
2	I	608	VAL	CA-C-N	7.91	127.83	119.85
2	I	608	VAL	C-N-CA	7.91	127.83	119.85
2	B	608	VAL	CA-C-N	7.88	127.81	119.85
2	B	608	VAL	C-N-CA	7.88	127.81	119.85
2	J	608	VAL	CA-C-N	7.86	127.79	119.85
2	J	608	VAL	C-N-CA	7.86	127.79	119.85
1	G	416	LEU	CA-C-N	7.68	127.61	119.85
1	G	416	LEU	C-N-CA	7.68	127.61	119.85
1	F	416	LEU	CA-C-N	7.66	127.58	119.85
1	F	416	LEU	C-N-CA	7.66	127.58	119.85
1	A	416	LEU	CA-C-N	7.63	127.55	119.85
1	A	416	LEU	C-N-CA	7.63	127.55	119.85
1	G	219	ALA	CA-C-N	6.90	126.88	119.78
1	G	219	ALA	C-N-CA	6.90	126.88	119.78
1	G	205	CYS	CA-C-N	6.84	126.53	119.56
1	G	205	CYS	C-N-CA	6.84	126.53	119.56
1	A	219	ALA	CA-C-N	6.82	126.81	119.78
1	A	219	ALA	C-N-CA	6.82	126.81	119.78
1	F	219	ALA	CA-C-N	6.80	126.79	119.78
1	F	219	ALA	C-N-CA	6.80	126.79	119.78
1	F	205	CYS	CA-C-N	6.77	126.47	119.56
1	F	205	CYS	C-N-CA	6.77	126.47	119.56
1	F	492	GLU	CA-C-N	6.75	126.70	119.28
1	F	492	GLU	C-N-CA	6.75	126.70	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	492	GLU	CA-C-N	6.74	126.70	119.28
1	G	492	GLU	C-N-CA	6.74	126.70	119.28
1	A	205	CYS	CA-C-N	6.74	126.44	119.56
1	A	205	CYS	C-N-CA	6.74	126.44	119.56
1	A	492	GLU	CA-C-N	6.72	126.67	119.28
1	A	492	GLU	C-N-CA	6.72	126.67	119.28
1	G	437	PRO	CA-C-N	6.70	126.61	119.85
1	G	437	PRO	C-N-CA	6.70	126.61	119.85
1	G	38	VAL	N-CA-C	6.69	118.21	109.58
1	A	38	VAL	N-CA-C	6.67	118.19	109.58
1	F	437	PRO	CA-C-N	6.66	126.58	119.85
1	F	437	PRO	C-N-CA	6.66	126.58	119.85
1	A	437	PRO	CA-C-N	6.65	126.57	119.85
1	A	437	PRO	C-N-CA	6.65	126.57	119.85
1	F	38	VAL	N-CA-C	6.63	118.14	109.58
1	F	75	VAL	CA-C-N	6.61	126.53	119.85
1	F	75	VAL	C-N-CA	6.61	126.53	119.85
1	G	75	VAL	CA-C-N	6.55	126.53	119.78
1	G	75	VAL	C-N-CA	6.55	126.53	119.78
1	F	290	THR	CA-C-N	6.50	126.41	119.85
1	F	290	THR	C-N-CA	6.50	126.41	119.85
1	A	75	VAL	CA-C-N	6.49	126.47	119.78
1	A	75	VAL	C-N-CA	6.49	126.47	119.78
1	A	290	THR	CA-C-N	6.48	126.39	119.85
1	A	290	THR	C-N-CA	6.48	126.39	119.85
1	G	68	VAL	CB-CA-C	-6.44	103.44	112.14
1	A	68	VAL	CB-CA-C	-6.42	103.47	112.14
1	G	290	THR	CA-C-N	6.41	126.33	119.85
1	G	290	THR	C-N-CA	6.41	126.33	119.85
1	F	68	VAL	CB-CA-C	-6.39	103.52	112.14
1	G	275	GLU	CB-CA-C	-6.29	107.54	116.34
1	A	275	GLU	CB-CA-C	-6.24	107.60	116.34
1	F	275	GLU	CB-CA-C	-6.23	107.61	116.34
1	A	162	THR	N-CA-C	6.18	118.75	110.35
1	G	162	THR	N-CA-C	6.16	118.72	110.35
1	F	162	THR	N-CA-C	6.15	118.72	110.35
1	G	117	LYS	CA-C-N	6.10	125.72	119.56
1	G	117	LYS	C-N-CA	6.10	125.72	119.56
2	B	608	VAL	N-CA-C	6.09	113.92	107.76
1	A	117	LYS	CA-C-N	6.09	125.71	119.56
1	A	117	LYS	C-N-CA	6.09	125.71	119.56
2	J	608	VAL	N-CA-C	6.07	113.89	107.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	608	VAL	N-CA-C	6.06	113.88	107.76
1	F	117	LYS	CA-C-N	6.04	125.67	119.56
1	F	117	LYS	C-N-CA	6.04	125.67	119.56
1	F	469	ARG	CA-C-N	5.64	125.59	119.78
1	F	469	ARG	C-N-CA	5.64	125.59	119.78
2	B	546	SER	N-CA-C	5.63	118.44	110.50
2	J	546	SER	N-CA-C	5.62	118.43	110.50
2	I	546	SER	N-CA-C	5.62	118.42	110.50
1	A	469	ARG	CA-C-N	5.61	125.56	119.78
1	A	469	ARG	C-N-CA	5.61	125.56	119.78
1	G	469	ARG	CA-C-N	5.60	125.54	119.78
1	G	469	ARG	C-N-CA	5.60	125.54	119.78
1	F	382	PHE	CA-CB-CG	-5.51	108.29	113.80
1	G	382	PHE	CA-CB-CG	-5.50	108.30	113.80
1	A	382	PHE	CA-CB-CG	-5.49	108.31	113.80
1	A	354	GLY	N-CA-C	-5.38	105.19	112.14
2	B	607	ASN	CA-C-N	-5.37	118.73	122.59
2	B	607	ASN	C-N-CA	-5.37	118.73	122.59
1	G	354	GLY	N-CA-C	-5.37	105.22	112.14
1	F	354	GLY	N-CA-C	-5.35	105.24	112.14
2	J	607	ASN	CA-C-N	-5.33	118.76	122.59
2	J	607	ASN	C-N-CA	-5.33	118.76	122.59
1	A	424	ILE	N-CA-C	5.32	115.75	107.99
1	F	424	ILE	N-CA-C	5.26	115.68	107.99
2	I	607	ASN	CA-C-N	-5.26	118.80	122.59
2	I	607	ASN	C-N-CA	-5.26	118.80	122.59
1	F	242	VAL	N-CA-C	5.25	117.19	109.63
1	G	424	ILE	N-CA-C	5.24	115.65	107.99
1	A	242	VAL	N-CA-C	5.24	117.18	109.63
1	G	242	VAL	N-CA-C	5.22	117.15	109.63
1	A	300	ASN	CA-CB-CG	-5.18	107.42	112.60
1	G	300	ASN	CA-CB-CG	-5.16	107.44	112.60
1	F	300	ASN	CA-CB-CG	-5.13	107.47	112.60
2	J	636	SER	N-CA-C	5.09	118.96	112.34
1	G	123	THR	CA-C-N	5.07	124.73	119.56
1	G	123	THR	C-N-CA	5.07	124.73	119.56
2	B	636	SER	N-CA-C	5.05	118.90	112.34
1	A	318	TYR	CA-CB-CG	-5.04	104.82	113.90
1	A	123	THR	CA-C-N	5.04	124.70	119.56
1	A	123	THR	C-N-CA	5.04	124.70	119.56
1	F	318	TYR	CA-CB-CG	-5.03	104.84	113.90
1	G	318	TYR	CA-CB-CG	-5.03	104.85	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	123	THR	CA-C-N	5.02	124.68	119.56
1	F	123	THR	C-N-CA	5.02	124.68	119.56
2	I	636	SER	N-CA-C	5.02	118.86	112.34
1	G	244	THR	N-CA-C	5.00	116.79	109.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3493	0	3420	136	0
1	F	3493	0	3420	139	0
1	G	3493	0	3420	136	0
2	B	1024	0	1005	11	0
2	I	1024	0	1005	11	0
2	J	1024	0	1005	10	0
3	C	1662	1596	1588	81	0
3	E	1662	1596	1587	80	0
3	H	1662	1596	1587	80	0
4	D	1592	1559	1545	28	0
4	K	1592	1559	1545	26	0
4	L	1592	1559	1545	26	0
5	M	39	0	34	7	0
5	Y	39	0	34	7	0
5	k	39	0	34	7	0
6	N	28	0	25	6	0
6	O	28	0	25	6	0
6	P	28	0	25	0	0
6	S	28	0	25	13	0
6	T	28	0	25	1	0
6	U	28	0	25	5	0
6	X	28	0	25	2	0
6	Z	28	0	25	6	0
6	a	28	0	25	6	0
6	b	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	e	28	0	25	13	0
6	f	28	0	25	1	0
6	g	28	0	25	5	0
6	j	28	0	25	1	0
6	l	28	0	25	6	0
6	m	28	0	25	6	0
6	n	28	0	25	0	0
6	q	28	0	25	13	0
6	r	28	0	25	1	0
6	s	28	0	25	5	0
6	v	28	0	25	2	0
7	Q	83	0	70	0	0
7	c	83	0	70	0	0
7	o	83	0	70	0	0
8	R	94	0	79	0	0
8	d	94	0	79	0	0
8	p	94	0	79	0	0
9	V	72	0	61	1	0
9	h	72	0	61	1	0
9	t	72	0	61	1	0
10	W	50	0	43	1	0
10	i	50	0	43	1	0
10	u	50	0	43	1	0
11	A	70	0	65	0	0
11	B	28	0	26	6	0
11	F	70	0	65	0	0
11	G	70	0	65	0	0
11	I	28	0	26	6	0
11	J	28	0	26	6	0
All	All	25209	9465	24331	502	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 10.

All (502) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:LYS:NZ	4:D:52:TYR:CZ	1.74	1.53
1:G:231:LYS:NZ	4:K:52:TYR:CZ	1.78	1.50
1:A:231:LYS:NZ	4:L:52:TYR:CZ	1.77	1.50
1:F:232:LYS:HE3	4:D:119:SER:OG	1.20	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:ASN:OD1	3:C:47:GLN:HA	1.20	1.36
1:A:88:ASN:OD1	3:H:47:GLN:HA	1.22	1.30
1:A:232:LYS:HE3	4:L:119:SER:OG	1.19	1.27
1:G:88:ASN:OD1	3:E:47:GLN:HA	1.24	1.27
1:G:232:LYS:HE3	4:K:119:SER:OG	1.21	1.27
3:C:46:SER:O	5:Y:1:NAG:N2	1.66	1.26
3:E:46:SER:O	5:k:1:NAG:N2	1.69	1.23
3:H:46:SER:O	5:M:1:NAG:N2	1.71	1.22
1:F:88:ASN:OD1	3:C:47:GLN:CA	1.92	1.18
1:A:229:LYS:HZ1	3:H:115:TYR:HA	1.07	1.15
1:F:229:LYS:HZ1	3:C:115:TYR:HA	1.09	1.14
1:A:130:GLN:HG2	6:O:1:NAG:C8	1.79	1.13
1:A:88:ASN:OD1	3:H:47:GLN:CA	1.96	1.12
1:G:88:ASN:OD1	3:E:47:GLN:CA	1.97	1.12
1:F:130:GLN:HG2	6:a:1:NAG:C8	1.79	1.11
1:F:268:GLU:O	4:D:71:TRP:NE1	1.83	1.10
1:F:232:LYS:CE	4:D:119:SER:OG	1.99	1.10
1:G:130:GLN:HG2	6:m:1:NAG:C8	1.79	1.10
1:A:232:LYS:CE	4:L:119:SER:OG	2.00	1.09
1:A:231:LYS:HD3	3:H:118:ALA:CB	1.82	1.09
1:G:229:LYS:HZ1	3:E:115:TYR:HA	1.09	1.08
1:G:231:LYS:HE2	3:E:119:TYR:H	1.18	1.08
1:A:268:GLU:O	4:L:71:TRP:NE1	1.87	1.07
1:G:232:LYS:CE	4:K:119:SER:OG	2.02	1.07
1:G:231:LYS:HD3	3:E:118:ALA:CB	1.85	1.07
1:A:231:LYS:HE2	3:H:119:TYR:H	1.16	1.06
1:G:268:GLU:O	4:K:71:TRP:NE1	1.88	1.06
1:F:85:HIS:NE2	3:C:114:SER:OG	1.90	1.04
1:F:230:ASP:OD2	3:C:119:TYR:OH	1.72	1.04
1:A:229:LYS:NZ	3:H:115:TYR:HA	1.72	1.04
1:F:231:LYS:HE2	3:C:119:TYR:H	1.17	1.04
1:A:130:GLN:CG	6:O:1:NAG:H81	1.88	1.03
1:A:130:GLN:HG2	6:O:1:NAG:H81	1.04	1.03
1:F:130:GLN:CG	6:a:1:NAG:H81	1.88	1.03
1:A:87:GLU:OE1	5:M:1:NAG:H81	1.59	1.03
1:G:130:GLN:CG	6:m:1:NAG:H81	1.88	1.03
1:A:229:LYS:O	3:H:116:SER:O	1.76	1.02
1:F:130:GLN:HG2	6:a:1:NAG:H81	1.04	1.02
1:F:231:LYS:HD3	3:C:118:ALA:CB	1.88	1.02
1:G:293:GLN:CD	6:q:1:NAG:HN2	1.67	1.02
1:F:293:GLN:CD	6:e:1:NAG:HN2	1.67	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLN:CD	6:S:1:NAG:HN2	1.67	1.01
1:F:229:LYS:NZ	3:C:115:TYR:HA	1.70	1.01
1:G:130:GLN:HG2	6:m:1:NAG:H81	1.04	1.01
1:F:87:GLU:OE1	5:Y:1:NAG:H81	1.59	1.01
1:F:229:LYS:O	3:C:116:SER:O	1.79	1.00
1:A:293:GLN:HE22	6:S:1:NAG:H3	1.26	1.00
1:G:230:ASP:OD2	3:E:119:TYR:OH	1.78	1.00
1:G:203:GLN:OE1	1:G:434:MET:HE3	1.61	1.00
1:A:85:HIS:NE2	3:H:114:SER:OG	1.95	1.00
1:F:203:GLN:OE1	1:F:434:MET:HE3	1.60	1.00
1:F:232:LYS:HE3	4:D:119:SER:CB	1.92	1.00
1:A:230:ASP:OD2	3:H:119:TYR:OH	1.78	1.00
1:G:229:LYS:NZ	3:E:115:TYR:HA	1.73	1.00
1:G:87:GLU:OE1	5:k:1:NAG:H81	1.59	0.99
1:G:229:LYS:O	3:E:116:SER:O	1.79	0.99
3:C:46:SER:O	5:Y:1:NAG:C2	2.11	0.99
1:G:293:GLN:HE22	6:q:1:NAG:H3	1.26	0.99
1:G:231:LYS:CE	4:K:52:TYR:OH	2.11	0.99
1:A:203:GLN:OE1	1:A:434:MET:HE3	1.60	0.98
1:F:241:SER:CA	3:C:112:TYR:OH	2.11	0.98
1:F:293:GLN:HE22	6:e:1:NAG:H3	1.26	0.98
1:F:231:LYS:CE	4:D:52:TYR:OH	2.10	0.98
1:A:231:LYS:CE	4:L:52:TYR:OH	2.10	0.98
1:G:241:SER:HA	3:E:112:TYR:HH	1.28	0.98
1:A:130:GLN:CG	6:O:1:NAG:C8	2.43	0.96
1:G:85:HIS:NE2	3:E:114:SER:OG	1.96	0.96
3:C:46:SER:O	5:Y:1:NAG:C1	2.14	0.95
1:F:241:SER:N	3:C:112:TYR:OH	1.99	0.95
1:G:130:GLN:CG	6:m:1:NAG:C8	2.43	0.95
1:F:231:LYS:NZ	4:D:52:TYR:CE2	2.34	0.94
1:A:232:LYS:HE3	4:L:119:SER:CB	1.97	0.94
1:F:230:ASP:HA	3:C:117:GLY:O	1.67	0.93
3:E:46:SER:O	5:k:1:NAG:C2	2.16	0.93
3:H:46:SER:O	5:M:1:NAG:C2	2.16	0.93
3:H:46:SER:O	5:M:1:NAG:C1	2.17	0.93
1:F:130:GLN:CG	6:a:1:NAG:C8	2.43	0.93
1:G:232:LYS:HE3	4:K:119:SER:CB	1.98	0.92
1:A:241:SER:CA	3:H:112:TYR:OH	2.17	0.92
1:G:241:SER:CA	3:E:112:TYR:OH	2.17	0.92
1:A:241:SER:N	3:H:112:TYR:OH	2.03	0.92
1:G:231:LYS:CE	4:K:52:TYR:HH	1.84	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:241:SER:N	3:E:112:TYR:OH	2.04	0.90
3:E:46:SER:O	5:k:1:NAG:C1	2.19	0.90
1:A:230:ASP:HA	3:H:117:GLY:O	1.72	0.90
1:A:231:LYS:HD3	3:H:118:ALA:HB1	1.53	0.89
1:F:231:LYS:HD3	3:C:118:ALA:HB1	1.54	0.88
1:A:230:ASP:HA	3:H:117:GLY:HA3	1.55	0.88
1:F:230:ASP:HA	3:C:117:GLY:C	1.98	0.88
1:F:231:LYS:NZ	4:D:52:TYR:OH	0.73	0.87
1:F:232:LYS:CE	4:D:119:SER:CB	2.51	0.87
1:G:231:LYS:NZ	4:K:52:TYR:OH	0.73	0.87
1:G:231:LYS:HD3	3:E:118:ALA:HB1	1.55	0.87
1:A:231:LYS:NZ	4:L:52:TYR:OH	0.72	0.87
1:A:230:ASP:HA	3:H:117:GLY:CA	2.05	0.87
1:A:230:ASP:HA	3:H:117:GLY:C	1.98	0.86
1:G:230:ASP:HA	3:E:117:GLY:O	1.73	0.86
1:F:231:LYS:NZ	4:D:52:TYR:HH	1.39	0.86
1:G:230:ASP:HA	3:E:117:GLY:C	2.01	0.86
1:F:241:SER:HA	3:C:112:TYR:HH	1.39	0.85
1:A:232:LYS:HE3	4:L:119:SER:HG	1.02	0.85
1:F:241:SER:HA	3:C:112:TYR:OH	1.73	0.85
1:G:232:LYS:HE3	4:K:119:SER:HG	1.42	0.84
1:F:85:HIS:HE2	3:C:114:SER:CB	1.91	0.84
1:G:230:ASP:HA	3:E:117:GLY:HA3	1.58	0.84
6:j:1:NAG:H61	6:j:2:NAG:HN2	1.43	0.84
1:F:85:HIS:NE2	3:C:114:SER:CB	2.40	0.84
1:G:230:ASP:HA	3:E:117:GLY:CA	2.07	0.84
1:G:85:HIS:HE2	3:E:114:SER:HG	1.26	0.83
1:A:232:LYS:CE	4:L:119:SER:CB	2.56	0.83
2:J:633:LYS:O	11:J:702:NAG:H82	1.79	0.83
2:B:633:LYS:O	11:B:702:NAG:H82	1.79	0.83
1:F:85:HIS:CE1	3:C:114:SER:C	2.56	0.83
1:G:231:LYS:HD3	3:E:118:ALA:HB2	1.61	0.83
1:G:232:LYS:CE	4:K:119:SER:CB	2.56	0.83
6:X:1:NAG:H61	6:X:2:NAG:HN2	1.43	0.82
6:v:1:NAG:H61	6:v:2:NAG:HN2	1.43	0.82
1:A:231:LYS:HD3	3:H:118:ALA:HB2	1.59	0.82
1:A:321(A):ASP:CG	6:N:1:NAG:H83	2.05	0.82
1:F:229:LYS:C	3:C:117:GLY:HA3	2.04	0.82
1:F:230:ASP:HA	3:C:117:GLY:CA	2.10	0.82
2:I:633:LYS:O	11:I:702:NAG:H82	1.79	0.82
1:G:321(A):ASP:CG	6:l:1:NAG:H83	2.05	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:ASP:OD1	3:C:119:TYR:HE2	1.62	0.82
1:F:321(A):ASP:CG	6:Z:1:NAG:H83	2.05	0.81
1:A:241:SER:HA	3:H:112:TYR:OH	1.80	0.81
1:G:241:SER:HA	3:E:112:TYR:OH	1.78	0.81
1:F:230:ASP:OD1	3:C:119:TYR:CE2	2.34	0.81
1:A:229:LYS:C	3:H:117:GLY:HA3	2.07	0.80
1:A:240:PRO:C	3:H:112:TYR:HH	1.89	0.79
1:G:130:GLN:HG3	6:m:1:NAG:H83	1.65	0.79
1:F:230:ASP:HA	3:C:117:GLY:HA3	1.63	0.79
1:F:130:GLN:HG3	6:a:1:NAG:H83	1.65	0.79
1:G:229:LYS:C	3:E:117:GLY:HA3	2.08	0.78
1:A:130:GLN:HG3	6:O:1:NAG:H83	1.65	0.78
1:A:230:ASP:CA	3:H:117:GLY:HA3	2.13	0.78
1:F:85:HIS:HE2	3:C:114:SER:HB2	1.49	0.78
1:G:85:HIS:NE2	3:E:114:SER:CB	2.46	0.78
1:G:85:HIS:HE2	3:E:114:SER:CB	1.97	0.77
1:G:85:HIS:CE1	3:E:114:SER:C	2.62	0.77
1:A:85:HIS:HE2	3:H:114:SER:CB	1.98	0.77
1:A:85:HIS:NE2	3:H:114:SER:CB	2.47	0.77
1:F:240:PRO:C	3:C:112:TYR:OH	2.27	0.76
1:A:85:HIS:CE1	3:H:114:SER:C	2.63	0.76
1:A:231:LYS:HE2	3:H:119:TYR:N	1.97	0.76
1:F:229:LYS:NZ	3:C:115:TYR:CA	2.43	0.76
1:A:229:LYS:NZ	3:H:115:TYR:CA	2.47	0.76
1:F:88:ASN:CG	3:C:47:GLN:HA	2.08	0.76
1:A:230:ASP:OD1	3:H:119:TYR:HE2	1.69	0.76
1:F:231:LYS:HD3	3:C:118:ALA:HB2	1.67	0.76
1:G:230:ASP:CA	3:E:117:GLY:HA3	2.16	0.75
1:F:241:SER:HB3	3:C:117:GLY:HA2	1.67	0.75
1:G:230:ASP:OD1	3:E:119:TYR:HE2	1.68	0.75
1:G:231:LYS:NZ	4:K:52:TYR:CE2	2.41	0.74
1:G:230:ASP:OD1	3:E:119:TYR:CE2	2.40	0.74
1:F:85:HIS:CE1	3:C:114:SER:CB	2.71	0.74
1:A:88:ASN:CG	3:H:47:GLN:HA	2.12	0.74
1:A:230:ASP:OD1	3:H:119:TYR:CE2	2.40	0.73
1:F:230:ASP:CA	3:C:117:GLY:HA3	2.18	0.73
1:G:85:HIS:HE2	3:E:114:SER:HB2	1.53	0.73
1:F:130:GLN:CG	6:a:1:NAG:H83	2.19	0.73
1:G:231:LYS:HE2	3:E:119:TYR:N	1.99	0.73
1:G:240:PRO:C	3:E:112:TYR:OH	2.32	0.73
1:G:130:GLN:CG	6:m:1:NAG:H83	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASP:N	3:H:117:GLY:HA3	2.05	0.72
1:A:231:LYS:HG2	3:H:118:ALA:HA	1.71	0.72
1:F:85:HIS:HE1	3:C:114:SER:C	1.96	0.72
1:A:241:SER:HB3	3:H:117:GLY:HA2	1.70	0.72
1:F:268:GLU:HG3	4:D:71:TRP:CZ2	2.23	0.72
1:G:88:ASN:CG	3:E:47:GLN:HA	2.13	0.72
1:A:241:SER:HA	3:H:112:TYR:HH	1.52	0.72
1:A:231:LYS:CD	3:H:118:ALA:HB1	2.19	0.72
1:F:293:GLN:NE2	6:e:1:NAG:H3	2.04	0.72
1:F:231:LYS:HE2	3:C:119:TYR:N	2.00	0.72
1:G:241:SER:HB3	3:E:117:GLY:HA2	1.71	0.72
1:A:240:PRO:C	3:H:112:TYR:OH	2.31	0.71
1:F:230:ASP:N	3:C:117:GLY:HA3	2.05	0.71
1:F:85:HIS:CE1	3:C:114:SER:OG	2.43	0.71
1:G:231:LYS:HG2	3:E:118:ALA:HA	1.73	0.70
1:A:130:GLN:CG	6:O:1:NAG:H83	2.19	0.70
1:A:231:LYS:CE	4:L:52:TYR:HH	1.94	0.70
1:A:231:LYS:NZ	4:L:52:TYR:CE2	2.41	0.70
1:F:231:LYS:HZ2	4:D:52:TYR:HH	1.02	0.70
1:A:85:HIS:HE2	3:H:114:SER:HB2	1.55	0.70
1:G:230:ASP:N	3:E:117:GLY:HA3	2.07	0.70
1:A:293:GLN:NE2	6:S:1:NAG:H3	2.03	0.69
1:G:85:HIS:CE1	3:E:114:SER:CB	2.75	0.69
1:A:231:LYS:CD	3:H:118:ALA:CB	2.67	0.69
1:F:268:GLU:HG3	4:D:71:TRP:CE2	2.26	0.69
1:F:85:HIS:NE2	3:C:114:SER:HB2	2.06	0.69
1:G:231:LYS:CD	3:E:118:ALA:HB1	2.21	0.69
1:A:85:HIS:CE1	3:H:114:SER:CB	2.76	0.69
1:G:85:HIS:CD2	3:E:114:SER:HG	2.09	0.69
1:A:293:GLN:NE2	6:S:1:NAG:HN2	1.91	0.69
1:F:231:LYS:CD	3:C:118:ALA:HB1	2.23	0.69
1:F:231:LYS:HG2	3:C:118:ALA:HA	1.75	0.68
3:H:212:ASN:O	3:H:234:ARG:NH1	2.27	0.68
1:A:85:HIS:CE1	3:H:114:SER:OG	2.46	0.68
1:F:240:PRO:C	3:C:112:TYR:HH	1.99	0.68
1:G:293:GLN:NE2	6:q:1:NAG:HN2	1.91	0.68
1:A:85:HIS:HE1	3:H:114:SER:C	2.02	0.68
1:A:268:GLU:HG3	4:L:71:TRP:CE2	2.28	0.68
3:E:212:ASN:O	3:E:234:ARG:NH1	2.27	0.68
1:G:268:GLU:HG3	4:K:71:TRP:CE2	2.29	0.67
1:A:363:ASN:OD1	1:A:364:SER:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:ASN:OD1	1:F:364:SER:O	2.12	0.67
1:G:229:LYS:NZ	3:E:115:TYR:CA	2.48	0.67
3:C:212:ASN:O	3:C:234:ARG:NH1	2.27	0.67
1:G:293:GLN:NE2	6:q:1:NAG:H3	2.04	0.67
3:C:46:SER:C	5:Y:1:NAG:HN2	2.00	0.67
1:F:293:GLN:NE2	6:e:1:NAG:HN2	1.91	0.67
1:G:268:GLU:HG3	4:K:71:TRP:CZ2	2.30	0.67
1:F:88:ASN:OD1	3:C:48:SER:N	2.28	0.66
1:G:363:ASN:OD1	1:G:364:SER:O	2.12	0.66
1:G:203:GLN:OE1	1:G:434:MET:CE	2.40	0.66
1:A:231:LYS:CE	3:H:118:ALA:HB1	2.26	0.66
1:F:85:HIS:HE1	3:C:114:SER:O	1.77	0.66
1:F:230:ASP:OD2	3:C:119:TYR:CZ	2.49	0.66
1:G:85:HIS:CE1	3:E:114:SER:OG	2.47	0.66
1:G:85:HIS:HE1	3:E:114:SER:C	2.02	0.65
1:G:85:HIS:NE2	3:E:114:SER:HB2	2.10	0.65
1:G:268:GLU:CG	4:K:71:TRP:CE2	2.79	0.65
1:A:268:GLU:HG3	4:L:71:TRP:CZ2	2.30	0.65
1:G:293:GLN:HE22	6:q:1:NAG:C3	2.06	0.65
1:G:241:SER:CA	3:E:112:TYR:HH	1.98	0.64
1:G:231:LYS:CD	3:E:118:ALA:CB	2.69	0.64
1:F:229:LYS:HB3	3:C:116:SER:C	2.23	0.64
1:G:231:LYS:CE	3:E:118:ALA:HB1	2.28	0.63
1:A:203:GLN:OE1	1:A:434:MET:CE	2.40	0.63
1:G:85:HIS:HE1	3:E:114:SER:O	1.82	0.63
3:E:46:SER:C	5:k:1:NAG:HN2	2.04	0.63
1:F:203:GLN:OE1	1:F:434:MET:CE	2.41	0.63
1:F:293:GLN:HE22	6:e:1:NAG:C3	2.06	0.63
1:A:72:HIS:N	1:A:72:HIS:CD2	2.67	0.62
1:A:293:GLN:NE2	6:S:1:NAG:N2	2.48	0.62
1:A:293:GLN:HE22	6:S:1:NAG:C3	2.06	0.62
1:G:293:GLN:NE2	6:q:1:NAG:N2	2.48	0.62
1:F:232:LYS:NZ	4:D:119:SER:CB	2.63	0.61
1:G:88:ASN:OD1	3:E:48:SER:N	2.32	0.61
1:F:293:GLN:CD	6:e:1:NAG:N2	2.51	0.61
1:F:321(A):ASP:OD1	6:Z:1:NAG:H82	2.00	0.61
1:F:293:GLN:NE2	6:e:1:NAG:N2	2.48	0.61
1:A:85:HIS:HE1	3:H:114:SER:O	1.83	0.61
1:A:85:HIS:NE2	3:H:114:SER:HB2	2.12	0.60
1:A:88:ASN:OD1	3:H:48:SER:N	2.34	0.60
1:A:268:GLU:O	4:L:71:TRP:CD1	2.53	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:321(A):ASP:OD1	6:l:1:NAG:C8	2.50	0.60
1:G:321(A):ASP:OD1	6:l:1:NAG:H82	2.01	0.60
3:H:46:SER:C	5:M:1:NAG:HN2	2.05	0.60
1:A:321(A):ASP:OD1	6:N:1:NAG:H82	2.01	0.60
1:G:293:GLN:CD	6:q:1:NAG:N2	2.51	0.60
1:A:229:LYS:HZ1	3:H:115:TYR:CA	1.98	0.60
1:F:321(A):ASP:OD1	6:Z:1:NAG:C8	2.50	0.60
1:F:241:SER:CB	3:C:117:GLY:HA2	2.30	0.60
1:A:321(A):ASP:OD1	6:N:1:NAG:C8	2.50	0.60
1:F:321(A):ASP:CG	6:Z:1:NAG:C8	2.75	0.60
1:G:321(A):ASP:CG	6:l:1:NAG:C8	2.75	0.60
1:A:232:LYS:NZ	4:L:119:SER:CB	2.64	0.59
1:F:231:LYS:CD	3:C:118:ALA:CB	2.73	0.59
1:G:230:ASP:OD2	3:E:119:TYR:CZ	2.55	0.59
1:A:230:ASP:OD2	3:H:119:TYR:CZ	2.55	0.59
1:F:268:GLU:O	4:D:71:TRP:CD1	2.54	0.59
1:G:72:HIS:CD2	1:G:72:HIS:N	2.67	0.59
1:A:230:ASP:OD1	3:H:117:GLY:O	2.20	0.59
1:F:87:GLU:CD	5:Y:1:NAG:H81	2.27	0.59
1:G:87:GLU:CD	5:k:1:NAG:H81	2.27	0.59
1:F:293:GLN:HB3	6:e:1:NAG:C8	2.33	0.59
1:G:293:GLN:NE2	6:q:1:NAG:C2	2.66	0.59
1:G:293:GLN:HB3	6:q:1:NAG:C8	2.33	0.59
1:F:231:LYS:CE	3:C:118:ALA:HB1	2.33	0.58
1:G:175:LEU:HD21	6:l:1:NAG:H82	1.85	0.58
1:A:175:LEU:HD21	6:N:1:NAG:H82	1.85	0.58
1:A:321(A):ASP:CG	6:N:1:NAG:C8	2.75	0.58
1:A:268:GLU:CG	4:L:71:TRP:CE2	2.79	0.58
1:A:293:GLN:NE2	6:S:1:NAG:C2	2.66	0.58
1:A:293:GLN:HB3	6:S:1:NAG:C8	2.33	0.58
1:G:229:LYS:HB3	3:E:116:SER:C	2.28	0.58
1:F:230:ASP:CG	3:C:119:TYR:CE2	2.82	0.58
1:F:293:GLN:NE2	6:e:1:NAG:C2	2.66	0.58
1:G:232:LYS:NZ	4:K:119:SER:CB	2.66	0.58
1:F:175:LEU:HD21	6:Z:1:NAG:H82	1.85	0.58
1:A:229:LYS:HB3	3:H:116:SER:C	2.28	0.58
1:F:85:HIS:CE1	3:C:114:SER:HB2	2.39	0.57
1:G:268:GLU:O	4:K:71:TRP:CD1	2.55	0.57
1:F:88:ASN:OD1	3:C:47:GLN:CB	2.51	0.57
1:F:72:HIS:CD2	1:F:72:HIS:N	2.67	0.57
2:J:634:GLU:O	11:J:702:NAG:H81	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLU:CD	5:M:1:NAG:H81	2.27	0.56
2:I:634:GLU:O	11:I:702:NAG:H81	2.05	0.56
1:G:230:ASP:OD1	3:E:117:GLY:O	2.23	0.56
1:F:88:ASN:OD1	3:C:47:GLN:C	2.47	0.56
2:I:634:GLU:HA	11:I:702:NAG:H81	1.87	0.56
2:B:633:LYS:O	11:B:702:NAG:C8	2.53	0.56
1:A:88:ASN:OD1	3:H:47:GLN:CB	2.54	0.56
1:A:241:SER:CB	3:H:117:GLY:HA2	2.36	0.56
1:A:293:GLN:NE2	6:S:1:NAG:C1	2.69	0.56
1:G:293:GLN:NE2	6:q:1:NAG:C1	2.69	0.56
2:J:634:GLU:HA	11:J:702:NAG:H81	1.87	0.56
2:B:634:GLU:O	11:B:702:NAG:H81	2.05	0.56
1:F:268:GLU:CG	4:D:71:TRP:CZ2	2.88	0.56
1:G:241:SER:CB	3:E:117:GLY:HA2	2.36	0.56
2:B:634:GLU:HA	11:B:702:NAG:H81	1.87	0.55
1:F:229:LYS:HB3	3:C:116:SER:O	2.05	0.55
1:F:241:SER:CA	3:C:112:TYR:HH	2.02	0.55
1:F:293:GLN:NE2	6:e:1:NAG:C1	2.69	0.55
2:J:633:LYS:O	11:J:702:NAG:C8	2.53	0.55
1:A:297:THR:CG2	6:U:1:NAG:H83	2.36	0.55
1:F:297:THR:CG2	6:g:1:NAG:H83	2.36	0.55
1:F:232:LYS:HE3	4:D:119:SER:HG	1.62	0.55
1:G:297:THR:CG2	6:s:1:NAG:H83	2.36	0.54
1:F:230:ASP:CA	3:C:117:GLY:O	2.49	0.54
1:G:88:ASN:OD1	3:E:47:GLN:CB	2.54	0.54
2:I:633:LYS:O	11:I:702:NAG:C8	2.53	0.54
1:F:230:ASP:OD1	3:C:117:GLY:O	2.25	0.54
1:G:85:HIS:CE1	3:E:114:SER:HB2	2.42	0.54
1:F:293:GLN:HB3	6:e:1:NAG:H82	1.90	0.54
1:F:268:GLU:CG	4:D:71:TRP:CE2	2.74	0.54
3:C:44:GLN:OE1	3:C:90:GLN:NE2	2.41	0.54
1:A:232:LYS:HG3	3:H:119:TYR:CD2	2.43	0.54
1:F:85:HIS:CE1	3:C:114:SER:O	2.58	0.53
1:A:85:HIS:CE1	3:H:114:SER:HB2	2.43	0.53
3:E:44:GLN:OE1	3:E:90:GLN:NE2	2.41	0.53
3:H:44:GLN:OE1	3:H:90:GLN:NE2	2.41	0.53
2:B:611:ASN:ND2	11:B:701:NAG:O7	2.42	0.53
2:I:611:ASN:ND2	11:I:701:NAG:O7	2.42	0.53
1:G:293:GLN:HB3	6:q:1:NAG:H82	1.90	0.52
1:F:297:THR:CG2	6:g:1:NAG:C8	2.88	0.52
2:J:611:ASN:ND2	11:J:701:NAG:O7	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:THR:CG2	6:U:1:NAG:C8	2.87	0.52
2:I:634:GLU:HA	11:I:702:NAG:C8	2.40	0.52
1:A:293:GLN:HB3	6:S:1:NAG:H82	1.90	0.52
1:G:88:ASN:OD1	3:E:47:GLN:C	2.52	0.52
2:J:634:GLU:HA	11:J:702:NAG:C8	2.40	0.52
1:G:297:THR:CG2	6:s:1:NAG:C8	2.87	0.51
1:A:88:ASN:OD1	3:H:47:GLN:C	2.53	0.51
2:B:634:GLU:HA	11:B:702:NAG:C8	2.40	0.51
1:G:246:GLN:OE1	1:G:246:GLN:N	2.36	0.51
5:Y:2:NAG:H3	5:Y:2:NAG:H83	1.93	0.51
1:G:232:LYS:HG3	3:E:119:TYR:CD2	2.46	0.51
1:A:246:GLN:OE1	1:A:246:GLN:N	2.36	0.51
1:A:230:ASP:CG	3:H:119:TYR:CE2	2.89	0.51
1:G:230:ASP:CG	3:E:119:TYR:CE2	2.89	0.50
5:k:2:NAG:H3	5:k:2:NAG:H83	1.92	0.50
1:F:229:LYS:HZ2	3:C:115:TYR:CA	2.21	0.50
5:M:2:NAG:H3	5:M:2:NAG:H83	1.92	0.50
4:K:193[A]:ARG:HD2	4:K:199:TYR:CZ	2.47	0.50
4:L:193[A]:ARG:HD2	4:L:199:TYR:OH	2.12	0.50
1:A:297:THR:HG22	6:U:1:NAG:H82	1.94	0.50
1:A:231:LYS:NZ	4:L:52:TYR:HH	1.09	0.50
1:A:293:GLN:CD	6:S:1:NAG:N2	2.51	0.50
1:F:267:GLU:OE2	4:D:76:ILE:HG21	2.12	0.49
4:D:193[A]:ARG:HD2	4:D:199:TYR:CZ	2.47	0.49
4:K:193[A]:ARG:HD2	4:K:199:TYR:OH	2.12	0.49
1:A:293:GLN:NE2	6:S:1:NAG:C3	2.71	0.49
1:G:293:GLN:NE2	6:q:1:NAG:C3	2.71	0.49
4:L:193[A]:ARG:HD2	4:L:199:TYR:CZ	2.47	0.49
1:F:363:ASN:OD1	1:F:363:ASN:C	2.56	0.49
1:A:232:LYS:HB2	3:H:119:TYR:CE2	2.47	0.49
1:G:268:GLU:CG	4:K:71:TRP:CZ2	2.95	0.49
4:D:193[A]:ARG:HD2	4:D:199:TYR:OH	2.12	0.49
1:A:229:LYS:HB3	3:H:116:SER:O	2.12	0.49
1:G:85:HIS:CE1	3:E:114:SER:O	2.63	0.49
1:G:229:LYS:HB3	3:E:116:SER:O	2.12	0.49
1:A:363:ASN:OD1	1:A:363:ASN:C	2.56	0.49
1:F:297:THR:HG22	6:g:1:NAG:H82	1.94	0.49
1:A:232:LYS:HB2	3:H:119:TYR:HE2	1.78	0.48
1:G:297:THR:HG22	6:s:1:NAG:H82	1.94	0.48
1:F:297:THR:HG22	6:g:1:NAG:C8	2.43	0.48
1:A:230:ASP:CA	3:H:117:GLY:O	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:THR:HG22	6:U:1:NAG:C8	2.43	0.48
1:G:363:ASN:OD1	1:G:363:ASN:C	2.56	0.48
1:F:232:LYS:HG3	3:C:119:TYR:CD2	2.48	0.48
1:G:297:THR:HG22	6:s:1:NAG:C8	2.43	0.48
1:A:231:LYS:HZ3	3:H:118:ALA:HB1	1.79	0.47
1:A:267:GLU:OE2	4:L:76:ILE:HG21	2.15	0.47
1:A:479:TRP:HA	1:A:479:TRP:CE3	2.49	0.47
1:A:232:LYS:NZ	4:L:119:SER:HB2	2.29	0.47
1:F:164:GLU:OE1	1:F:164:GLU:N	2.36	0.47
1:F:232:LYS:NZ	4:D:119:SER:HB2	2.28	0.47
1:F:232:LYS:HB2	3:C:119:TYR:CE2	2.49	0.47
1:G:230:ASP:CA	3:E:117:GLY:O	2.54	0.47
1:G:232:LYS:HB2	3:E:119:TYR:CE2	2.50	0.47
3:E:26:GLN:HG3	3:E:43[B]:CYS:SG	2.55	0.47
1:F:268:GLU:C	4:D:71:TRP:NE1	2.68	0.47
1:F:479:TRP:HA	1:F:479:TRP:CE3	2.50	0.47
1:G:479:TRP:HA	1:G:479:TRP:CE3	2.50	0.47
3:H:26:GLN:HG3	3:H:43[B]:CYS:SG	2.55	0.47
1:F:479:TRP:HA	1:F:479:TRP:HE3	1.80	0.47
1:G:479:TRP:HA	1:G:479:TRP:HE3	1.80	0.47
3:C:26:GLN:HG3	3:C:43[B]:CYS:SG	2.55	0.47
3:E:139:PRO:HB3	3:E:165:TYR:HB3	1.97	0.47
1:A:268:GLU:CG	4:L:71:TRP:CZ2	2.96	0.46
1:A:164:GLU:OE1	1:A:164:GLU:N	2.36	0.46
1:A:241:SER:CA	3:H:112:TYR:HH	2.10	0.46
1:A:479:TRP:HA	1:A:479:TRP:HE3	1.80	0.46
2:I:635:ILE:HG13	2:I:635:ILE:O	2.15	0.46
1:F:430:ILE:HD12	1:F:430:ILE:C	2.41	0.46
1:G:164:GLU:OE1	1:G:164:GLU:N	2.36	0.46
2:B:635:ILE:HG13	2:B:635:ILE:O	2.15	0.46
1:A:321(A):ASP:OD2	6:N:1:NAG:H83	2.16	0.46
3:H:139:PRO:HB3	3:H:165:TYR:HB3	1.97	0.46
6:v:1:NAG:H61	6:v:2:NAG:N2	2.22	0.46
1:F:230:ASP:OD2	3:C:119:TYR:CE2	2.68	0.46
1:F:241:SER:CB	3:C:117:GLY:CA	2.94	0.46
1:F:293:GLN:NE2	6:e:1:NAG:C3	2.71	0.46
1:G:267:GLU:OE2	4:K:76:ILE:HG21	2.15	0.46
1:G:232:LYS:NZ	4:K:119:SER:HB2	2.31	0.46
2:J:635:ILE:HG13	2:J:635:ILE:O	2.15	0.45
1:G:293:GLN:HB3	6:q:1:NAG:H83	1.98	0.45
1:G:430:ILE:C	1:G:430:ILE:HD12	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ILE:C	1:A:430:ILE:HD12	2.41	0.45
1:G:231:LYS:HZ3	3:E:118:ALA:HB1	1.81	0.45
1:G:297:THR:HG21	6:s:1:NAG:H83	1.97	0.45
3:E:142:LEU:HD13	4:K:160:THR:HB	1.99	0.45
1:A:241:SER:N	3:H:112:TYR:HH	1.96	0.45
1:F:229:LYS:HZ1	3:C:115:TYR:CA	2.00	0.45
1:F:321(A):ASP:OD2	6:Z:1:NAG:H83	2.16	0.45
3:C:142:LEU:HD13	4:D:160:THR:HB	1.99	0.45
6:f:1:NAG:H61	6:f:2:NAG:N2	2.32	0.45
1:F:293:GLN:HB3	6:e:1:NAG:H83	1.98	0.45
1:G:232:LYS:HZ1	4:K:119:SER:HB2	1.82	0.45
3:C:139:PRO:HB3	3:C:165:TYR:HB3	1.97	0.45
4:D:154:THR:HG22	4:D:155:PRO:HD2	1.99	0.45
9:h:1:NAG:H2	10:i:1:NAG:H5	1.99	0.45
1:A:231:LYS:CG	3:H:118:ALA:HA	2.44	0.45
1:A:268:GLU:OE2	4:L:71:TRP:CH2	2.55	0.45
1:A:293:GLN:HB3	6:S:1:NAG:H83	1.98	0.45
3:H:142:LEU:HD13	4:L:160:THR:HB	1.99	0.45
1:A:297:THR:HG21	6:U:1:NAG:H83	1.97	0.44
1:G:232:LYS:HB2	3:E:119:TYR:HE2	1.81	0.44
6:T:1:NAG:H61	6:T:2:NAG:N2	2.32	0.44
4:L:154:THR:HG22	4:L:155:PRO:HD2	1.99	0.44
9:V:1:NAG:H2	10:W:1:NAG:H5	1.99	0.44
1:G:321(A):ASP:OD2	6:l:1:NAG:H83	2.16	0.44
1:F:297:THR:HG21	6:g:1:NAG:H83	1.98	0.44
6:r:1:NAG:H61	6:r:2:NAG:N2	2.32	0.44
1:F:246:GLN:OE1	1:F:246:GLN:N	2.36	0.44
1:G:231:LYS:NZ	4:K:52:TYR:HH	0.98	0.44
4:K:154:THR:HG22	4:K:155:PRO:HD2	1.99	0.44
9:t:1:NAG:H2	10:u:1:NAG:H5	1.99	0.44
1:F:241:SER:CB	3:C:112:TYR:OH	2.64	0.43
6:X:1:NAG:H61	6:X:2:NAG:N2	2.22	0.43
3:C:133[A]:LYS:HA	3:C:166:PHE:CZ	2.53	0.43
3:E:133[A]:LYS:HA	3:E:166:PHE:CZ	2.53	0.43
1:A:232:LYS:HZ1	4:L:119:SER:HB2	1.84	0.43
3:E:212:ASN:HA	3:E:234:ARG:NE	2.34	0.43
3:H:133[A]:LYS:HA	3:H:166:PHE:CZ	2.53	0.43
1:A:232:LYS:CG	3:H:119:TYR:CD2	3.02	0.43
1:A:241:SER:CB	3:H:112:TYR:OH	2.66	0.43
3:H:212:ASN:HA	3:H:234:ARG:NE	2.34	0.43
1:F:232:LYS:HZ1	4:D:119:SER:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:290:THR:HB	1:G:291:PRO:HD2	2.01	0.42
1:G:240:PRO:C	3:E:112:TYR:HH	2.26	0.42
1:F:230:ASP:CG	3:C:119:TYR:HE2	2.22	0.42
1:F:231:LYS:CG	3:C:118:ALA:HA	2.48	0.42
1:F:232:LYS:HB2	3:C:119:TYR:HE2	1.83	0.42
1:G:479:TRP:CE3	1:G:479:TRP:CA	3.03	0.42
1:A:290:THR:HB	1:A:291:PRO:HD2	2.02	0.42
1:G:116:LEU:HD11	1:G:434:MET:SD	2.60	0.42
3:C:212:ASN:HA	3:C:234:ARG:NE	2.34	0.42
1:F:229:LYS:HE3	3:C:114:SER:O	2.20	0.42
1:F:290:THR:HB	1:F:291:PRO:HD2	2.02	0.42
1:F:479:TRP:CE3	1:F:479:TRP:CA	3.03	0.42
1:G:231:LYS:CG	3:E:118:ALA:HA	2.46	0.42
1:F:503:ARG:HB3	2:I:607:ASN:HB2	2.02	0.42
1:F:116:LEU:HD11	1:F:434:MET:SD	2.60	0.41
1:F:232:LYS:CE	4:D:119:SER:HB2	2.45	0.41
2:I:570:VAL:O	2:I:571:TRP:HB2	2.21	0.41
1:F:229:LYS:O	3:C:117:GLY:HA3	2.18	0.41
1:A:69:TRP:HA	1:A:69:TRP:CE3	2.56	0.41
1:A:479:TRP:CE3	1:A:479:TRP:CA	3.03	0.41
2:J:570:VAL:O	2:J:571:TRP:HB2	2.21	0.41
3:C:184:ILE:HA	3:C:203:THR:O	2.21	0.41
1:A:116:LEU:HD11	1:A:434:MET:SD	2.60	0.41
1:A:503:ARG:HB3	2:B:607:ASN:HB2	2.02	0.41
2:B:570:VAL:O	2:B:571:TRP:HB2	2.20	0.41
2:B:614:TRP:CD1	2:B:614:TRP:N	2.85	0.41
1:F:289:ASN:HD21	4:D:73:ALA:HB1	1.86	0.41
1:G:268:GLU:C	4:K:71:TRP:NE1	2.73	0.41
1:A:231:LYS:NZ	3:H:118:ALA:HB1	2.35	0.41
2:I:614:TRP:CD1	2:I:614:TRP:N	2.85	0.41
3:E:184:ILE:HA	3:E:203:THR:O	2.21	0.41
3:E:191:GLN:HG2	3:E:198:TYR:CE1	2.56	0.41
3:H:233:ASN:HB2	3:H:236:ASP:OD2	2.21	0.41
2:I:530:MET:HG2	2:I:628:TRP:HA	2.03	0.41
3:H:184:ILE:HA	3:H:203:THR:O	2.21	0.41
1:A:229:LYS:O	3:H:117:GLY:HA3	2.19	0.40
3:H:191:GLN:HG2	3:H:198:TYR:CE1	2.56	0.40
1:A:213:ILE:O	1:A:213:ILE:HG23	2.21	0.40
1:G:69:TRP:CE3	1:G:69:TRP:HA	2.55	0.40
1:G:232:LYS:CG	3:E:119:TYR:CD2	3.04	0.40
1:G:503:ARG:HB3	2:J:607:ASN:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:LYS:O	3:E:117:GLY:HA3	2.20	0.40
1:G:241:SER:CB	3:E:112:TYR:OH	2.67	0.40
1:G:241:SER:CB	3:E:117:GLY:CA	2.99	0.40
2:B:530:MET:HG2	2:B:628:TRP:HA	2.03	0.40
1:F:232:LYS:CG	3:C:119:TYR:CD2	3.05	0.40
2:J:530:MET:HG2	2:J:628:TRP:HA	2.04	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	436/481 (91%)	427 (98%)	9 (2%)	0	100	100
1	F	436/481 (91%)	427 (98%)	9 (2%)	0	100	100
1	G	436/481 (91%)	427 (98%)	9 (2%)	0	100	100
2	B	125/153 (82%)	122 (98%)	3 (2%)	0	100	100
2	I	125/153 (82%)	123 (98%)	2 (2%)	0	100	100
2	J	125/153 (82%)	122 (98%)	3 (2%)	0	100	100
3	C	222/217 (102%)	214 (96%)	8 (4%)	0	100	100
3	E	222/217 (102%)	214 (96%)	8 (4%)	0	100	100
3	H	222/217 (102%)	214 (96%)	8 (4%)	0	100	100
4	D	217/214 (101%)	213 (98%)	4 (2%)	0	100	100
4	K	217/214 (101%)	213 (98%)	4 (2%)	0	100	100
4	L	217/214 (101%)	213 (98%)	4 (2%)	0	100	100
All	All	3000/3195 (94%)	2929 (98%)	71 (2%)	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	397/428 (93%)	396 (100%)	1 (0%)	86	84
1	F	397/428 (93%)	396 (100%)	1 (0%)	86	84
1	G	397/428 (93%)	396 (100%)	1 (0%)	86	84
2	B	111/129 (86%)	111 (100%)	0	100	100
2	I	111/129 (86%)	111 (100%)	0	100	100
2	J	111/129 (86%)	111 (100%)	0	100	100
3	C	186/181 (103%)	175 (94%)	11 (6%)	18	40
3	E	186/181 (103%)	175 (94%)	11 (6%)	18	40
3	H	186/181 (103%)	175 (94%)	11 (6%)	18	40
4	D	182/177 (103%)	179 (98%)	3 (2%)	55	69
4	K	182/177 (103%)	179 (98%)	3 (2%)	55	69
4	L	182/177 (103%)	179 (98%)	3 (2%)	55	69
All	All	2628/2745 (96%)	2583 (98%)	45 (2%)	52	68

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	ASN
1	F	363	ASN
1	G	363	ASN
3	C	39	VAL
3	C	74	LEU
3	C	87	SER
3	C	89	THR
3	C	90	GLN
3	C	111	ASN
3	C	149	ASP
3	C	156	VAL
3	C	206	LEU
3	C	209	THR
3	C	216	GLU

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Mol	Chain	Res	Type
4	D	151	CYS
4	D	154	THR
4	D	201	LEU
3	E	39	VAL
3	E	74	LEU
3	E	87	SER
3	E	89	THR
3	E	90	GLN
3	E	111	ASN
3	E	149	ASP
3	E	156	VAL
3	E	206	LEU
3	E	209	THR
3	E	216	GLU
4	K	151	CYS
4	K	154	THR
4	K	201	LEU
3	H	39	VAL
3	H	74	LEU
3	H	87	SER
3	H	89	THR
3	H	90	GLN
3	H	111	ASN
3	H	149	ASP
3	H	156	VAL
3	H	206	LEU
3	H	209	THR
3	H	216	GLU
4	L	151	CYS
4	L	154	THR
4	L	201	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	293	GLN
2	B	640	GLN
1	F	66	HIS
1	F	293	GLN
2	I	640	GLN
1	G	66	HIS

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Mol	Chain	Res	Type
1	G	293	GLN
3	C	44	GLN
3	C	90	GLN
4	D	123	GLN
3	E	44	GLN
3	E	90	GLN
4	K	123	GLN
3	H	44	GLN
3	H	90	GLN
4	L	123	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

126 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	M	1	5,1	14,14,15	0.79	1 (7%)	17,19,21	0.92	1 (5%)
5	NAG	M	2	5	14,14,15	0.44	0	17,19,21	1.56	3 (17%)
5	BMA	M	3	5	11,11,12	1.15	1 (9%)	15,15,17	1.40	1 (6%)
6	NAG	N	1	1,6	14,14,15	0.26	0	17,19,21	0.55	0
6	NAG	N	2	6	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
6	NAG	O	1	1,6	14,14,15	0.43	0	17,19,21	0.46	0
6	NAG	O	2	6	14,14,15	0.29	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	P	1	1,6	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
6	NAG	P	2	6	14,14,15	0.53	0	17,19,21	1.32	3 (17%)
7	NAG	Q	1	1,7	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
7	NAG	Q	2	7	14,14,15	0.50	0	17,19,21	1.33	3 (17%)
7	BMA	Q	3	7	11,11,12	0.67	0	15,15,17	1.44	3 (20%)
7	MAN	Q	4	7	11,11,12	0.57	0	15,15,17	1.49	2 (13%)
7	MAN	Q	5	7	11,11,12	0.59	0	15,15,17	2.30	5 (33%)
7	MAN	Q	6	7	11,11,12	0.59	0	15,15,17	2.22	3 (20%)
7	MAN	Q	7	7	11,11,12	0.55	0	15,15,17	1.92	5 (33%)
8	NAG	R	1	8,1	14,14,15	0.77	1 (7%)	17,19,21	0.69	0
8	NAG	R	2	8	14,14,15	0.41	0	17,19,21	0.46	0
8	BMA	R	3	8	11,11,12	1.65	3 (27%)	15,15,17	1.80	2 (13%)
8	MAN	R	4	8	11,11,12	1.66	3 (27%)	15,15,17	1.28	2 (13%)
8	MAN	R	5	8	11,11,12	2.28	4 (36%)	15,15,17	1.68	3 (20%)
8	MAN	R	6	8	11,11,12	0.58	0	15,15,17	2.22	3 (20%)
8	MAN	R	7	8	11,11,12	0.58	0	15,15,17	1.92	5 (33%)
8	MAN	R	8	8	11,11,12	0.62	0	15,15,17	2.27	7 (46%)
6	NAG	S	1	1,6	14,14,15	0.31	0	17,19,21	0.73	0
6	NAG	S	2	6	14,14,15	0.66	0	17,19,21	0.54	0
6	NAG	T	1	1,6	14,14,15	0.44	0	17,19,21	0.43	0
6	NAG	T	2	6	14,14,15	0.63	0	17,19,21	0.57	0
6	NAG	U	1	1,6	14,14,15	0.40	0	17,19,21	0.76	1 (5%)
6	NAG	U	2	6	14,14,15	0.55	0	17,19,21	0.55	0
9	NAG	V	1	9,1	14,14,15	0.33	0	17,19,21	0.59	0
9	NAG	V	2	9	14,14,15	0.35	0	17,19,21	0.84	1 (5%)
9	BMA	V	3	9	11,11,12	0.66	0	15,15,17	1.44	3 (20%)
9	MAN	V	4	9	11,11,12	0.61	0	15,15,17	2.19	3 (20%)
9	MAN	V	5	9	11,11,12	0.54	0	15,15,17	1.93	5 (33%)
9	MAN	V	6	9	11,11,12	0.54	0	15,15,17	1.47	2 (13%)
10	NAG	W	1	1,10	14,14,15	0.97	1 (7%)	17,19,21	1.06	1 (5%)
10	NAG	W	2	10	14,14,15	0.49	0	17,19,21	0.56	0
10	BMA	W	3	10	11,11,12	0.64	0	15,15,17	1.42	3 (20%)
10	MAN	W	4	10	11,11,12	0.59	0	15,15,17	2.22	3 (20%)
6	NAG	X	1	1,6	14,14,15	0.51	0	17,19,21	0.57	0
6	NAG	X	2	6	14,14,15	0.39	0	17,19,21	0.45	0
5	NAG	Y	1	5,1	14,14,15	0.78	1 (7%)	17,19,21	0.92	1 (5%)
5	NAG	Y	2	5	14,14,15	0.43	0	17,19,21	1.56	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	Y	3	5	11,11,12	1.16	1 (9%)	15,15,17	1.40	1 (6%)
6	NAG	Z	1	1,6	14,14,15	0.27	0	17,19,21	0.55	0
6	NAG	Z	2	6	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
6	NAG	a	1	1,6	14,14,15	0.43	0	17,19,21	0.47	0
6	NAG	a	2	6	14,14,15	0.29	0	17,19,21	0.50	0
6	NAG	b	1	1,6	14,14,15	0.48	0	17,19,21	2.27	3 (17%)
6	NAG	b	2	6	14,14,15	0.51	0	17,19,21	1.34	3 (17%)
7	NAG	c	1	1,7	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
7	NAG	c	2	7	14,14,15	0.49	0	17,19,21	1.33	3 (17%)
7	BMA	c	3	7	11,11,12	0.66	0	15,15,17	1.44	3 (20%)
7	MAN	c	4	7	11,11,12	0.57	0	15,15,17	1.50	2 (13%)
7	MAN	c	5	7	11,11,12	0.58	0	15,15,17	2.30	5 (33%)
7	MAN	c	6	7	11,11,12	0.59	0	15,15,17	2.22	3 (20%)
7	MAN	c	7	7	11,11,12	0.57	0	15,15,17	1.93	5 (33%)
8	NAG	d	1	8,1	14,14,15	0.77	1 (7%)	17,19,21	0.68	0
8	NAG	d	2	8	14,14,15	0.40	0	17,19,21	0.47	0
8	BMA	d	3	8	11,11,12	1.66	4 (36%)	15,15,17	1.80	2 (13%)
8	MAN	d	4	8	11,11,12	1.65	3 (27%)	15,15,17	1.28	2 (13%)
8	MAN	d	5	8	11,11,12	2.28	4 (36%)	15,15,17	1.69	3 (20%)
8	MAN	d	6	8	11,11,12	0.60	0	15,15,17	2.22	3 (20%)
8	MAN	d	7	8	11,11,12	0.58	0	15,15,17	1.93	5 (33%)
8	MAN	d	8	8	11,11,12	0.61	0	15,15,17	2.26	7 (46%)
6	NAG	e	1	1,6	14,14,15	0.31	0	17,19,21	0.73	0
6	NAG	e	2	6	14,14,15	0.68	0	17,19,21	0.55	0
6	NAG	f	1	1,6	14,14,15	0.45	0	17,19,21	0.43	0
6	NAG	f	2	6	14,14,15	0.62	0	17,19,21	0.57	0
6	NAG	g	1	1,6	14,14,15	0.41	0	17,19,21	0.76	1 (5%)
6	NAG	g	2	6	14,14,15	0.58	0	17,19,21	0.55	0
9	NAG	h	1	9,1	14,14,15	0.33	0	17,19,21	0.59	0
9	NAG	h	2	9	14,14,15	0.35	0	17,19,21	0.83	1 (5%)
9	BMA	h	3	9	11,11,12	0.65	0	15,15,17	1.45	3 (20%)
9	MAN	h	4	9	11,11,12	0.62	0	15,15,17	2.19	3 (20%)
9	MAN	h	5	9	11,11,12	0.54	0	15,15,17	1.93	5 (33%)
9	MAN	h	6	9	11,11,12	0.54	0	15,15,17	1.47	2 (13%)
10	NAG	i	1	1,10	14,14,15	0.97	1 (7%)	17,19,21	1.05	1 (5%)
10	NAG	i	2	10	14,14,15	0.49	0	17,19,21	0.56	0
10	BMA	i	3	10	11,11,12	0.63	0	15,15,17	1.43	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	i	4	10	11,11,12	0.60	0	15,15,17	2.21	3 (20%)
6	NAG	j	1	1,6	14,14,15	0.48	0	17,19,21	0.58	0
6	NAG	j	2	6	14,14,15	0.40	0	17,19,21	0.46	0
5	NAG	k	1	5,1	14,14,15	0.80	1 (7%)	17,19,21	0.91	2 (11%)
5	NAG	k	2	5	14,14,15	0.45	0	17,19,21	1.55	3 (17%)
5	BMA	k	3	5	11,11,12	1.15	1 (9%)	15,15,17	1.40	1 (6%)
6	NAG	l	1	1,6	14,14,15	0.26	0	17,19,21	0.56	0
6	NAG	l	2	6	14,14,15	0.32	0	17,19,21	0.66	1 (5%)
6	NAG	m	1	1,6	14,14,15	0.44	0	17,19,21	0.47	0
6	NAG	m	2	6	14,14,15	0.28	0	17,19,21	0.51	0
6	NAG	n	1	1,6	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
6	NAG	n	2	6	14,14,15	0.52	0	17,19,21	1.32	3 (17%)
7	NAG	o	1	1,7	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
7	NAG	o	2	7	14,14,15	0.48	0	17,19,21	1.34	3 (17%)
7	BMA	o	3	7	11,11,12	0.65	0	15,15,17	1.43	3 (20%)
7	MAN	o	4	7	11,11,12	0.56	0	15,15,17	1.50	2 (13%)
7	MAN	o	5	7	11,11,12	0.59	0	15,15,17	2.30	5 (33%)
7	MAN	o	6	7	11,11,12	0.58	0	15,15,17	2.21	3 (20%)
7	MAN	o	7	7	11,11,12	0.55	0	15,15,17	1.92	5 (33%)
8	NAG	p	1	8,1	14,14,15	0.79	1 (7%)	17,19,21	0.69	0
8	NAG	p	2	8	14,14,15	0.41	0	17,19,21	0.47	0
8	BMA	p	3	8	11,11,12	1.65	4 (36%)	15,15,17	1.78	2 (13%)
8	MAN	p	4	8	11,11,12	1.66	3 (27%)	15,15,17	1.27	2 (13%)
8	MAN	p	5	8	11,11,12	2.27	4 (36%)	15,15,17	1.68	3 (20%)
8	MAN	p	6	8	11,11,12	0.61	0	15,15,17	2.22	3 (20%)
8	MAN	p	7	8	11,11,12	0.58	0	15,15,17	1.93	5 (33%)
8	MAN	p	8	8	11,11,12	0.61	0	15,15,17	2.26	7 (46%)
6	NAG	q	1	1,6	14,14,15	0.32	0	17,19,21	0.73	0
6	NAG	q	2	6	14,14,15	0.67	0	17,19,21	0.54	0
6	NAG	r	1	1,6	14,14,15	0.45	0	17,19,21	0.43	0
6	NAG	r	2	6	14,14,15	0.63	0	17,19,21	0.57	0
6	NAG	s	1	1,6	14,14,15	0.40	0	17,19,21	0.76	1 (5%)
6	NAG	s	2	6	14,14,15	0.55	0	17,19,21	0.55	0
9	NAG	t	1	9,1	14,14,15	0.34	0	17,19,21	0.59	0
9	NAG	t	2	9	14,14,15	0.36	0	17,19,21	0.84	1 (5%)
9	BMA	t	3	9	11,11,12	0.65	0	15,15,17	1.45	3 (20%)
9	MAN	t	4	9	11,11,12	0.61	0	15,15,17	2.20	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	t	5	9	11,11,12	0.56	0	15,15,17	1.93	6 (40%)
9	MAN	t	6	9	11,11,12	0.55	0	15,15,17	1.47	2 (13%)
10	NAG	u	1	1,10	14,14,15	0.95	1 (7%)	17,19,21	1.05	1 (5%)
10	NAG	u	2	10	14,14,15	0.50	0	17,19,21	0.56	0
10	BMA	u	3	10	11,11,12	0.65	0	15,15,17	1.42	3 (20%)
10	MAN	u	4	10	11,11,12	0.62	0	15,15,17	2.21	3 (20%)
6	NAG	v	1	1,6	14,14,15	0.50	0	17,19,21	0.57	0
6	NAG	v	2	6	14,14,15	0.41	0	17,19,21	0.45	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
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	6/6/23/26	0/1/1/1
5	BMA	M	3	5	-	2/2/19/22	0/1/1/1
6	NAG	N	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	NAG	O	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	NAG	P	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	P	2	6	-	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
7	BMA	Q	3	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	5	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	6	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	7	7	-	0/2/19/22	0/1/1/1
8	NAG	R	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	R	2	8	-	2/6/23/26	0/1/1/1
8	BMA	R	3	8	-	0/2/19/22	0/1/1/1
8	MAN	R	4	8	-	2/2/19/22	0/1/1/1
8	MAN	R	5	8	-	0/2/19/22	0/1/1/1
8	MAN	R	6	8	-	0/2/19/22	0/1/1/1
8	MAN	R	7	8	-	0/2/19/22	0/1/1/1
8	MAN	R	8	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	S	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	NAG	T	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	2/6/23/26	0/1/1/1
9	NAG	V	1	9,1	-	3/6/23/26	0/1/1/1
9	NAG	V	2	9	-	2/6/23/26	0/1/1/1
9	BMA	V	3	9	-	2/2/19/22	0/1/1/1
9	MAN	V	4	9	-	0/2/19/22	0/1/1/1
9	MAN	V	5	9	-	0/2/19/22	0/1/1/1
9	MAN	V	6	9	-	0/2/19/22	0/1/1/1
10	NAG	W	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	W	2	10	-	2/6/23/26	0/1/1/1
10	BMA	W	3	10	-	2/2/19/22	0/1/1/1
10	MAN	W	4	10	-	0/2/19/22	0/1/1/1
6	NAG	X	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
5	NAG	Y	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	6/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	2/2/19/22	0/1/1/1
6	NAG	Z	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	NAG	a	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	NAG	b	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	b	2	6	-	0/6/23/26	0/1/1/1
7	NAG	c	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
7	BMA	c	3	7	-	0/2/19/22	0/1/1/1
7	MAN	c	4	7	-	0/2/19/22	0/1/1/1
7	MAN	c	5	7	-	0/2/19/22	0/1/1/1
7	MAN	c	6	7	-	0/2/19/22	0/1/1/1
7	MAN	c	7	7	-	0/2/19/22	0/1/1/1
8	NAG	d	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	d	2	8	-	2/6/23/26	0/1/1/1
8	BMA	d	3	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	d	4	8	-	2/2/19/22	0/1/1/1
8	MAN	d	5	8	-	0/2/19/22	0/1/1/1
8	MAN	d	6	8	-	0/2/19/22	0/1/1/1
8	MAN	d	7	8	-	0/2/19/22	0/1/1/1
8	MAN	d	8	8	-	0/2/19/22	0/1/1/1
6	NAG	e	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1
6	NAG	f	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	NAG	g	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	g	2	6	-	2/6/23/26	0/1/1/1
9	NAG	h	1	9,1	-	3/6/23/26	0/1/1/1
9	NAG	h	2	9	-	2/6/23/26	0/1/1/1
9	BMA	h	3	9	-	2/2/19/22	0/1/1/1
9	MAN	h	4	9	-	0/2/19/22	0/1/1/1
9	MAN	h	5	9	-	0/2/19/22	0/1/1/1
9	MAN	h	6	9	-	0/2/19/22	0/1/1/1
10	NAG	i	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	i	2	10	-	2/6/23/26	0/1/1/1
10	BMA	i	3	10	-	2/2/19/22	0/1/1/1
10	MAN	i	4	10	-	0/2/19/22	0/1/1/1
6	NAG	j	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	j	2	6	-	2/6/23/26	0/1/1/1
5	NAG	k	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	k	2	5	-	6/6/23/26	0/1/1/1
5	BMA	k	3	5	-	2/2/19/22	0/1/1/1
6	NAG	l	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	l	2	6	-	2/6/23/26	0/1/1/1
6	NAG	m	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	m	2	6	-	2/6/23/26	0/1/1/1
6	NAG	n	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	n	2	6	-	0/6/23/26	0/1/1/1
7	NAG	o	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	o	2	7	-	0/6/23/26	0/1/1/1
7	BMA	o	3	7	-	0/2/19/22	0/1/1/1
7	MAN	o	4	7	-	0/2/19/22	0/1/1/1
7	MAN	o	5	7	-	0/2/19/22	0/1/1/1
7	MAN	o	6	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	o	7	7	-	0/2/19/22	0/1/1/1
8	NAG	p	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	p	2	8	-	2/6/23/26	0/1/1/1
8	BMA	p	3	8	-	0/2/19/22	0/1/1/1
8	MAN	p	4	8	-	2/2/19/22	0/1/1/1
8	MAN	p	5	8	-	0/2/19/22	0/1/1/1
8	MAN	p	6	8	-	0/2/19/22	0/1/1/1
8	MAN	p	7	8	-	0/2/19/22	0/1/1/1
8	MAN	p	8	8	-	0/2/19/22	0/1/1/1
6	NAG	q	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	q	2	6	-	0/6/23/26	0/1/1/1
6	NAG	r	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	r	2	6	-	2/6/23/26	0/1/1/1
6	NAG	s	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	s	2	6	-	2/6/23/26	0/1/1/1
9	NAG	t	1	9,1	-	3/6/23/26	0/1/1/1
9	NAG	t	2	9	-	2/6/23/26	0/1/1/1
9	BMA	t	3	9	-	2/2/19/22	0/1/1/1
9	MAN	t	4	9	-	0/2/19/22	0/1/1/1
9	MAN	t	5	9	-	0/2/19/22	0/1/1/1
9	MAN	t	6	9	-	0/2/19/22	0/1/1/1
10	NAG	u	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	u	2	10	-	2/6/23/26	0/1/1/1
10	BMA	u	3	10	-	2/2/19/22	0/1/1/1
10	MAN	u	4	10	-	0/2/19/22	0/1/1/1
6	NAG	v	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	v	2	6	-	2/6/23/26	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	5	MAN	C4-C5	4.38	1.62	1.53
8	d	5	MAN	C4-C5	4.35	1.62	1.53
8	p	5	MAN	C4-C5	4.31	1.62	1.53
8	d	5	MAN	C4-C3	3.69	1.61	1.52
8	p	5	MAN	C4-C3	3.68	1.61	1.52
8	R	5	MAN	C4-C3	3.67	1.61	1.52
10	i	1	NAG	O5-C1	3.42	1.49	1.43
10	W	1	NAG	O5-C1	3.41	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	u	1	NAG	O5-C1	3.34	1.49	1.43
8	p	4	MAN	O5-C5	3.17	1.49	1.43
8	R	4	MAN	O5-C5	3.16	1.49	1.43
8	d	4	MAN	O5-C5	3.13	1.49	1.43
8	d	5	MAN	C2-C3	2.92	1.57	1.52
8	R	5	MAN	C2-C3	2.87	1.56	1.52
8	p	5	MAN	C2-C3	2.86	1.56	1.52
8	d	4	MAN	C4-C3	2.46	1.58	1.52
8	R	4	MAN	C4-C5	2.46	1.58	1.53
8	p	4	MAN	C4-C5	2.45	1.58	1.53
8	d	4	MAN	C4-C5	2.45	1.58	1.53
8	d	3	BMA	O5-C5	2.43	1.48	1.43
8	p	3	BMA	O5-C5	2.43	1.48	1.43
8	d	3	BMA	C2-C3	2.42	1.56	1.52
8	p	4	MAN	C4-C3	2.42	1.58	1.52
8	R	3	BMA	O5-C5	2.42	1.48	1.43
8	R	4	MAN	C4-C3	2.41	1.58	1.52
8	R	3	BMA	C2-C3	2.37	1.56	1.52
8	p	3	BMA	C2-C3	2.37	1.56	1.52
8	p	5	MAN	O5-C5	2.36	1.48	1.43
8	p	1	NAG	O5-C1	-2.35	1.39	1.43
5	k	3	BMA	C1-C2	2.35	1.57	1.52
5	M	3	BMA	C1-C2	2.32	1.57	1.52
5	Y	3	BMA	C1-C2	2.32	1.57	1.52
8	d	1	NAG	O5-C1	-2.32	1.39	1.43
8	R	1	NAG	O5-C1	-2.27	1.39	1.43
8	R	5	MAN	O5-C5	2.26	1.47	1.43
8	d	5	MAN	O5-C5	2.25	1.47	1.43
5	k	1	NAG	O5-C1	-2.21	1.40	1.43
8	R	3	BMA	C4-C5	2.20	1.57	1.53
8	p	3	BMA	C4-C5	2.19	1.57	1.53
5	M	1	NAG	O5-C1	-2.19	1.40	1.43
5	Y	1	NAG	O5-C1	-2.19	1.40	1.43
8	d	3	BMA	C4-C5	2.16	1.57	1.53
8	d	3	BMA	O2-C2	2.03	1.47	1.43
8	p	3	BMA	O2-C2	2.03	1.47	1.43

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	c	1	NAG	O5-C1-C2	-7.52	99.66	111.29
7	o	1	NAG	O5-C1-C2	-7.51	99.66	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	1	NAG	O5-C1-C2	-7.51	99.67	111.29
6	P	1	NAG	O5-C1-C2	-7.50	99.68	111.29
6	b	1	NAG	O5-C1-C2	-7.48	99.71	111.29
6	n	1	NAG	O5-C1-C2	-7.46	99.76	111.29
8	R	6	MAN	C1-C2-C3	5.93	118.27	109.64
8	p	6	MAN	C1-C2-C3	5.93	118.27	109.64
10	W	4	MAN	C1-C2-C3	5.92	118.26	109.64
7	Q	6	MAN	C1-C2-C3	5.90	118.24	109.64
8	d	6	MAN	C1-C2-C3	5.89	118.23	109.64
10	u	4	MAN	C1-C2-C3	5.89	118.22	109.64
10	i	4	MAN	C1-C2-C3	5.89	118.21	109.64
7	c	6	MAN	C1-C2-C3	5.86	118.18	109.64
7	o	6	MAN	C1-C2-C3	5.86	118.18	109.64
9	t	4	MAN	C1-C2-C3	5.86	118.18	109.64
9	V	4	MAN	C1-C2-C3	5.84	118.14	109.64
9	h	4	MAN	C1-C2-C3	5.82	118.12	109.64
8	R	3	BMA	C1-O5-C5	5.76	119.90	112.19
8	d	3	BMA	C1-O5-C5	5.72	119.86	112.19
8	p	3	BMA	C1-O5-C5	5.67	119.78	112.19
7	c	5	MAN	C1-O5-C5	4.84	118.68	112.19
7	Q	5	MAN	C1-O5-C5	4.84	118.67	112.19
8	R	8	MAN	C6-C5-C4	-4.83	101.15	113.02
8	d	8	MAN	C6-C5-C4	-4.81	101.20	113.02
8	p	8	MAN	C6-C5-C4	-4.81	101.22	113.02
5	Y	2	NAG	C2-N2-C7	4.79	129.32	122.90
5	M	2	NAG	C2-N2-C7	4.79	129.31	122.90
7	o	5	MAN	C1-O5-C5	4.79	118.60	112.19
5	k	2	NAG	C2-N2-C7	4.74	129.25	122.90
7	o	5	MAN	O2-C2-C1	4.47	119.45	109.22
7	c	5	MAN	O2-C2-C1	4.45	119.41	109.22
7	Q	5	MAN	O2-C2-C1	4.44	119.39	109.22
7	o	6	MAN	C2-C3-C4	-4.06	103.72	110.86
7	Q	6	MAN	C2-C3-C4	-4.06	103.73	110.86
7	c	6	MAN	C2-C3-C4	-4.06	103.73	110.86
10	W	4	MAN	C2-C3-C4	-4.03	103.77	110.86
5	k	3	BMA	C1-O5-C5	4.03	117.59	112.19
5	M	3	BMA	C1-O5-C5	4.03	117.59	112.19
8	d	6	MAN	C2-C3-C4	-4.03	103.78	110.86
8	R	6	MAN	C2-C3-C4	-4.02	103.79	110.86
8	p	6	MAN	C2-C3-C4	-4.01	103.80	110.86
10	u	4	MAN	C2-C3-C4	-4.01	103.80	110.86
5	Y	3	BMA	C1-O5-C5	4.01	117.56	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	i	4	MAN	C2-C3-C4	-4.01	103.82	110.86
9	h	4	MAN	C2-C3-C4	-3.99	103.83	110.86
9	t	4	MAN	C2-C3-C4	-3.98	103.86	110.86
8	d	5	MAN	C1-O5-C5	3.96	117.49	112.19
7	o	5	MAN	O2-C2-C3	-3.95	101.97	110.15
9	V	4	MAN	C2-C3-C4	-3.95	103.91	110.86
7	Q	5	MAN	O2-C2-C3	-3.95	101.97	110.15
8	p	5	MAN	C1-O5-C5	3.94	117.47	112.19
8	R	5	MAN	C1-O5-C5	3.94	117.47	112.19
7	c	5	MAN	O2-C2-C3	-3.94	101.99	110.15
9	V	5	MAN	O4-C4-C3	-3.92	101.12	110.38
9	t	5	MAN	O4-C4-C3	-3.92	101.15	110.38
9	h	5	MAN	O4-C4-C3	-3.91	101.15	110.38
7	c	7	MAN	O4-C4-C3	-3.89	101.21	110.38
7	Q	7	MAN	O4-C4-C3	-3.89	101.22	110.38
8	d	7	MAN	O4-C4-C3	-3.86	101.27	110.38
7	o	7	MAN	O4-C4-C3	-3.86	101.28	110.38
8	R	7	MAN	O4-C4-C3	-3.84	101.32	110.38
8	p	7	MAN	O4-C4-C3	-3.84	101.33	110.38
8	d	4	MAN	C1-O5-C5	3.83	117.32	112.19
8	R	4	MAN	C1-O5-C5	3.80	117.28	112.19
8	p	4	MAN	C1-O5-C5	3.74	117.20	112.19
8	p	8	MAN	O4-C4-C3	-3.54	102.04	110.38
8	R	8	MAN	O4-C4-C3	-3.53	102.05	110.38
8	d	8	MAN	O4-C4-C3	-3.52	102.08	110.38
7	c	7	MAN	O4-C4-C5	3.27	117.39	109.32
9	t	5	MAN	O4-C4-C5	3.25	117.33	109.32
7	o	7	MAN	O4-C4-C5	3.24	117.31	109.32
8	p	7	MAN	O4-C4-C5	3.23	117.29	109.32
7	Q	7	MAN	O4-C4-C5	3.23	117.27	109.32
9	h	5	MAN	O4-C4-C5	3.23	117.27	109.32
9	V	5	MAN	O4-C4-C5	3.22	117.26	109.32
8	R	7	MAN	O4-C4-C5	3.22	117.25	109.32
8	d	7	MAN	O4-C4-C5	3.21	117.22	109.32
10	W	1	NAG	C1-O5-C5	3.16	116.42	112.19
10	i	1	NAG	C1-O5-C5	3.15	116.41	112.19
10	u	1	NAG	C1-O5-C5	3.15	116.40	112.19
7	o	2	NAG	O5-C5-C6	-3.14	101.55	107.66
7	c	2	NAG	O5-C5-C6	-3.13	101.58	107.66
7	Q	2	NAG	O5-C5-C6	-3.11	101.61	107.66
8	R	8	MAN	C3-C4-C5	-3.11	104.59	110.23
8	d	8	MAN	C3-C4-C5	-3.09	104.64	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	p	8	MAN	C3-C4-C5	-3.07	104.67	110.23
6	b	2	NAG	O5-C5-C6	-3.05	101.73	107.66
6	n	2	NAG	O5-C5-C6	-3.03	101.76	107.66
6	P	2	NAG	O5-C5-C6	-3.03	101.77	107.66
9	t	3	BMA	O2-C2-C3	2.98	116.33	110.15
7	c	3	BMA	O2-C2-C3	2.95	116.25	110.15
9	h	3	BMA	O2-C2-C3	2.94	116.23	110.15
7	o	3	BMA	O2-C2-C3	2.92	116.20	110.15
7	Q	3	BMA	O2-C2-C3	2.92	116.20	110.15
9	V	3	BMA	O2-C2-C3	2.92	116.19	110.15
7	Q	1	NAG	O7-C7-C8	-2.89	116.91	122.05
8	d	8	MAN	O2-C2-C3	-2.87	104.20	110.15
8	p	8	MAN	O2-C2-C3	-2.87	104.22	110.15
6	P	1	NAG	O7-C7-C8	-2.84	116.99	122.05
7	c	1	NAG	O7-C7-C8	-2.84	116.99	122.05
10	W	3	BMA	O2-C2-C3	2.84	116.04	110.15
10	u	3	BMA	O2-C2-C3	2.84	116.03	110.15
10	i	3	BMA	O2-C2-C3	2.84	116.03	110.15
8	R	8	MAN	O2-C2-C3	-2.84	104.28	110.15
6	b	1	NAG	O7-C7-C8	-2.83	117.01	122.05
7	o	1	NAG	O7-C7-C8	-2.82	117.03	122.05
6	n	1	NAG	O7-C7-C8	-2.82	117.03	122.05
8	d	5	MAN	C1-C2-C3	-2.81	105.56	109.64
8	R	5	MAN	C1-C2-C3	-2.74	105.65	109.64
8	p	5	MAN	C1-C2-C3	-2.74	105.66	109.64
6	P	1	NAG	C4-C3-C2	-2.71	107.05	111.02
6	n	1	NAG	C4-C3-C2	-2.70	107.06	111.02
7	Q	5	MAN	O4-C4-C3	-2.68	104.06	110.38
7	c	5	MAN	O4-C4-C3	-2.68	104.06	110.38
9	h	3	BMA	O4-C4-C5	-2.68	102.73	109.32
9	t	3	BMA	O4-C4-C5	-2.68	102.73	109.32
9	V	3	BMA	O4-C4-C5	-2.67	102.75	109.32
7	Q	1	NAG	C4-C3-C2	-2.67	107.11	111.02
6	b	1	NAG	C4-C3-C2	-2.66	107.12	111.02
7	o	5	MAN	O4-C4-C3	-2.66	104.11	110.38
10	i	3	BMA	O4-C4-C5	-2.66	102.78	109.32
7	c	3	BMA	O4-C4-C5	-2.65	102.80	109.32
7	c	1	NAG	C4-C3-C2	-2.64	107.14	111.02
7	Q	3	BMA	O4-C4-C5	-2.64	102.81	109.32
10	u	3	BMA	O4-C4-C5	-2.64	102.83	109.32
10	W	3	BMA	O4-C4-C5	-2.63	102.83	109.32
7	o	3	BMA	O4-C4-C5	-2.63	102.84	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	2	NAG	C1-C2-N2	2.62	114.56	110.43
7	o	1	NAG	C4-C3-C2	-2.61	107.19	111.02
5	k	2	NAG	C1-C2-N2	2.60	114.54	110.43
5	Y	2	NAG	C1-C2-N2	2.59	114.51	110.43
8	p	8	MAN	O5-C5-C6	2.54	112.62	107.66
9	h	5	MAN	O5-C5-C6	-2.54	102.71	107.66
7	o	7	MAN	O5-C5-C6	-2.54	102.72	107.66
7	Q	7	MAN	O5-C5-C6	-2.53	102.74	107.66
8	d	7	MAN	O5-C5-C6	-2.53	102.75	107.66
8	p	7	MAN	O5-C5-C6	-2.52	102.75	107.66
7	c	4	MAN	O5-C5-C6	2.52	112.57	107.66
8	R	7	MAN	O5-C5-C6	-2.52	102.75	107.66
9	V	5	MAN	O5-C5-C6	-2.51	102.78	107.66
7	c	7	MAN	O5-C5-C6	-2.51	102.78	107.66
7	o	4	MAN	O5-C5-C6	2.51	112.55	107.66
9	t	5	MAN	O5-C5-C6	-2.51	102.79	107.66
8	d	8	MAN	O5-C5-C6	2.50	112.52	107.66
8	R	8	MAN	O5-C5-C6	2.50	112.52	107.66
7	Q	4	MAN	O5-C5-C6	2.49	112.52	107.66
9	V	6	MAN	O5-C5-C6	2.42	112.38	107.66
9	h	6	MAN	O5-C5-C6	2.41	112.36	107.66
9	t	6	MAN	O5-C5-C6	2.41	112.35	107.66
6	b	2	NAG	O5-C1-C2	-2.40	107.58	111.29
7	Q	3	BMA	C6-C5-C4	-2.36	107.23	113.02
7	c	3	BMA	C6-C5-C4	-2.35	107.24	113.02
10	u	3	BMA	C6-C5-C4	-2.34	107.26	113.02
7	o	3	BMA	C6-C5-C4	-2.34	107.26	113.02
8	p	5	MAN	O3-C3-C4	2.34	115.89	110.38
7	o	2	NAG	O5-C1-C2	-2.34	107.67	111.29
6	n	2	NAG	O5-C1-C2	-2.33	107.69	111.29
6	P	2	NAG	O5-C1-C2	-2.33	107.69	111.29
8	R	5	MAN	O3-C3-C4	2.32	115.84	110.38
8	d	5	MAN	O3-C3-C4	2.32	115.84	110.38
9	V	5	MAN	C1-O5-C5	2.32	115.29	112.19
10	i	3	BMA	C6-C5-C4	-2.31	107.34	113.02
10	W	3	BMA	C6-C5-C4	-2.30	107.36	113.02
9	t	5	MAN	C1-O5-C5	2.30	115.27	112.19
9	t	3	BMA	C6-C5-C4	-2.30	107.38	113.02
8	d	7	MAN	C1-O5-C5	2.30	115.26	112.19
7	Q	2	NAG	O5-C1-C2	-2.30	107.74	111.29
9	h	3	BMA	C6-C5-C4	-2.30	107.38	113.02
7	c	2	NAG	O5-C1-C2	-2.30	107.74	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	t	2	NAG	C1-O5-C5	2.29	115.26	112.19
9	V	3	BMA	C6-C5-C4	-2.29	107.39	113.02
7	Q	5	MAN	O6-C6-C5	2.29	119.12	111.33
8	p	7	MAN	C1-O5-C5	2.28	115.25	112.19
5	k	1	NAG	C3-C4-C5	2.27	114.35	110.23
7	o	5	MAN	O6-C6-C5	2.27	119.06	111.33
5	M	1	NAG	C3-C4-C5	2.27	114.34	110.23
5	Y	1	NAG	C3-C4-C5	2.26	114.34	110.23
7	c	5	MAN	O6-C6-C5	2.26	119.04	111.33
9	V	2	NAG	C1-O5-C5	2.26	115.22	112.19
7	c	6	MAN	O5-C1-C2	-2.26	105.40	110.79
8	R	7	MAN	C1-O5-C5	2.25	115.21	112.19
9	h	2	NAG	C1-O5-C5	2.24	115.19	112.19
7	Q	6	MAN	O5-C1-C2	-2.24	105.45	110.79
7	o	6	MAN	O5-C1-C2	-2.24	105.45	110.79
10	W	4	MAN	O5-C1-C2	-2.24	105.46	110.79
7	c	7	MAN	C1-O5-C5	2.23	115.18	112.19
8	d	6	MAN	O5-C1-C2	-2.23	105.47	110.79
9	h	5	MAN	C1-O5-C5	2.23	115.17	112.19
8	p	6	MAN	O5-C1-C2	-2.23	105.48	110.79
8	R	6	MAN	O5-C1-C2	-2.22	105.50	110.79
10	u	4	MAN	O5-C1-C2	-2.21	105.51	110.79
7	Q	7	MAN	C1-O5-C5	2.21	115.14	112.19
8	d	3	BMA	O2-C2-C1	2.21	114.27	109.22
6	P	2	NAG	C4-C3-C2	-2.20	107.79	111.02
8	R	3	BMA	O2-C2-C1	2.20	114.27	109.22
5	Y	2	NAG	O4-C4-C5	-2.20	103.90	109.32
6	b	2	NAG	C4-C3-C2	-2.20	107.79	111.02
10	i	4	MAN	O5-C1-C2	-2.20	105.54	110.79
8	p	3	BMA	O2-C2-C1	2.19	114.25	109.22
7	c	7	MAN	O3-C3-C2	-2.19	105.58	110.05
9	t	4	MAN	O5-C1-C2	-2.19	105.57	110.79
5	M	2	NAG	O4-C4-C5	-2.19	103.94	109.32
5	k	2	NAG	O4-C4-C5	-2.19	103.94	109.32
7	Q	2	NAG	C4-C3-C2	-2.18	107.82	111.02
9	V	4	MAN	O5-C1-C2	-2.18	105.58	110.79
7	c	2	NAG	C4-C3-C2	-2.18	107.82	111.02
6	g	1	NAG	O4-C4-C5	-2.17	103.97	109.32
8	p	4	MAN	O2-C2-C3	-2.17	105.65	110.15
8	d	4	MAN	O2-C2-C3	-2.17	105.65	110.15
9	h	4	MAN	O5-C1-C2	-2.17	105.62	110.79
7	o	7	MAN	C1-O5-C5	2.17	115.09	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	s	1	NAG	O4-C4-C5	-2.16	103.99	109.32
8	R	4	MAN	O2-C2-C3	-2.16	105.67	110.15
7	o	2	NAG	C4-C3-C2	-2.16	107.85	111.02
8	d	8	MAN	O2-C2-C1	2.16	114.17	109.22
8	p	8	MAN	O2-C2-C1	2.16	114.17	109.22
6	U	1	NAG	O4-C4-C5	-2.16	104.01	109.32
7	o	7	MAN	O3-C3-C2	-2.15	105.67	110.05
7	Q	7	MAN	O3-C3-C2	-2.15	105.67	110.05
8	d	7	MAN	O3-C3-C2	-2.13	105.70	110.05
9	t	5	MAN	O3-C3-C2	-2.13	105.70	110.05
6	n	2	NAG	C4-C3-C2	-2.13	107.89	111.02
8	R	8	MAN	O2-C2-C1	2.13	114.11	109.22
8	p	7	MAN	O3-C3-C2	-2.13	105.71	110.05
9	V	5	MAN	O3-C3-C2	-2.12	105.72	110.05
8	R	7	MAN	O3-C3-C2	-2.12	105.72	110.05
9	h	5	MAN	O3-C3-C2	-2.12	105.72	110.05
7	o	4	MAN	O3-C3-C4	2.11	115.36	110.38
7	Q	4	MAN	O3-C3-C4	2.11	115.36	110.38
9	h	6	MAN	O3-C3-C4	2.10	115.33	110.38
9	V	6	MAN	O3-C3-C4	2.10	115.32	110.38
7	c	4	MAN	O3-C3-C4	2.10	115.32	110.38
9	t	6	MAN	O3-C3-C4	2.08	115.28	110.38
6	Z	2	NAG	C1-O5-C5	2.06	114.95	112.19
6	N	2	NAG	C1-O5-C5	2.06	114.95	112.19
6	l	2	NAG	C1-O5-C5	2.03	114.90	112.19
8	d	8	MAN	C2-C3-C4	2.02	114.41	110.86
8	R	8	MAN	C2-C3-C4	2.01	114.39	110.86
5	k	1	NAG	O4-C4-C5	-2.00	104.39	109.32
9	t	5	MAN	O3-C3-C4	2.00	115.09	110.38
8	p	8	MAN	C2-C3-C4	2.00	114.38	110.86

There are no chirality outliers.

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	3	BMA	C4-C5-C6-O6
5	Y	3	BMA	C4-C5-C6-O6
5	k	3	BMA	C4-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
6	e	1	NAG	O5-C5-C6-O6
6	q	1	NAG	O5-C5-C6-O6
6	r	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	T	1	NAG	O5-C5-C6-O6
6	f	1	NAG	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
6	m	2	NAG	O5-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
5	Y	3	BMA	O5-C5-C6-O6
5	k	3	BMA	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
5	k	1	NAG	O5-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
6	g	2	NAG	O5-C5-C6-O6
6	s	2	NAG	O5-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6
6	a	2	NAG	C4-C5-C6-O6
6	m	2	NAG	C4-C5-C6-O6
6	U	1	NAG	O5-C5-C6-O6
6	g	1	NAG	O5-C5-C6-O6
6	s	1	NAG	O5-C5-C6-O6
8	R	1	NAG	C4-C5-C6-O6
8	d	2	NAG	O5-C5-C6-O6
8	p	2	NAG	O5-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
6	e	1	NAG	C4-C5-C6-O6
6	f	1	NAG	C4-C5-C6-O6
6	q	1	NAG	C4-C5-C6-O6
6	r	1	NAG	C4-C5-C6-O6
8	d	1	NAG	C4-C5-C6-O6
8	p	1	NAG	C4-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	k	2	NAG	O5-C5-C6-O6
8	R	2	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
6	Z	1	NAG	O5-C5-C6-O6
6	l	1	NAG	O5-C5-C6-O6
9	V	1	NAG	O5-C5-C6-O6
9	h	1	NAG	O5-C5-C6-O6
9	t	1	NAG	O5-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	f	2	NAG	O5-C5-C6-O6
6	r	2	NAG	O5-C5-C6-O6
6	U	1	NAG	C4-C5-C6-O6
6	g	1	NAG	C4-C5-C6-O6
6	s	1	NAG	C4-C5-C6-O6
9	V	1	NAG	C4-C5-C6-O6
9	h	1	NAG	C4-C5-C6-O6
9	t	1	NAG	C4-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	Y	2	NAG	C4-C5-C6-O6
5	k	2	NAG	C4-C5-C6-O6
8	R	2	NAG	C4-C5-C6-O6
8	d	2	NAG	C4-C5-C6-O6
8	p	2	NAG	C4-C5-C6-O6
6	T	2	NAG	C4-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
6	f	2	NAG	C4-C5-C6-O6
6	g	2	NAG	C4-C5-C6-O6
6	r	2	NAG	C4-C5-C6-O6
6	s	2	NAG	C4-C5-C6-O6
8	R	4	MAN	O5-C5-C6-O6
8	d	4	MAN	O5-C5-C6-O6
8	p	4	MAN	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	l	2	NAG	O5-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
9	h	2	NAG	O5-C5-C6-O6
9	t	2	NAG	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6
5	k	1	NAG	C4-C5-C6-O6
9	V	2	NAG	C4-C5-C6-O6
9	h	2	NAG	C4-C5-C6-O6
9	t	2	NAG	C4-C5-C6-O6
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
5	Y	2	NAG	C8-C7-N2-C2
5	Y	2	NAG	O7-C7-N2-C2
5	k	2	NAG	C8-C7-N2-C2
5	k	2	NAG	O7-C7-N2-C2
6	X	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	j	2	NAG	O5-C5-C6-O6
6	v	2	NAG	O5-C5-C6-O6
9	V	3	BMA	O5-C5-C6-O6
9	h	3	BMA	O5-C5-C6-O6
9	t	3	BMA	O5-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
6	l	2	NAG	C4-C5-C6-O6
9	V	3	BMA	C4-C5-C6-O6
9	h	3	BMA	C4-C5-C6-O6
9	t	3	BMA	C4-C5-C6-O6
6	X	2	NAG	C4-C5-C6-O6
6	j	2	NAG	C4-C5-C6-O6
6	v	2	NAG	C4-C5-C6-O6
8	R	1	NAG	O5-C5-C6-O6
8	d	1	NAG	O5-C5-C6-O6
8	p	1	NAG	O5-C5-C6-O6
10	W	1	NAG	O5-C5-C6-O6
10	i	1	NAG	O5-C5-C6-O6
10	u	1	NAG	O5-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
6	l	1	NAG	C4-C5-C6-O6
8	R	4	MAN	C4-C5-C6-O6
8	p	4	MAN	C4-C5-C6-O6
8	d	4	MAN	C4-C5-C6-O6
6	a	1	NAG	O5-C5-C6-O6
6	m	1	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
10	W	2	NAG	C4-C5-C6-O6
10	i	2	NAG	C4-C5-C6-O6
10	u	2	NAG	C4-C5-C6-O6
10	W	3	BMA	C4-C5-C6-O6
10	u	3	BMA	C4-C5-C6-O6
10	i	3	BMA	C4-C5-C6-O6
10	u	3	BMA	O5-C5-C6-O6
10	W	3	BMA	O5-C5-C6-O6
10	i	3	BMA	O5-C5-C6-O6
10	W	1	NAG	C4-C5-C6-O6
10	i	1	NAG	C4-C5-C6-O6
10	u	1	NAG	C4-C5-C6-O6
10	i	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	W	2	NAG	O5-C5-C6-O6
10	u	2	NAG	O5-C5-C6-O6
5	M	2	NAG	C1-C2-N2-C7
5	Y	2	NAG	C1-C2-N2-C7
5	k	2	NAG	C1-C2-N2-C7
5	M	2	NAG	C3-C2-N2-C7
5	Y	2	NAG	C3-C2-N2-C7
5	k	2	NAG	C3-C2-N2-C7
9	V	1	NAG	C3-C2-N2-C7
9	h	1	NAG	C3-C2-N2-C7
9	t	1	NAG	C3-C2-N2-C7
7	c	1	NAG	O7-C7-N2-C2
6	P	1	NAG	O7-C7-N2-C2
6	b	1	NAG	O7-C7-N2-C2
7	Q	1	NAG	O7-C7-N2-C2
6	n	1	NAG	O7-C7-N2-C2
7	o	1	NAG	O7-C7-N2-C2

There are no ring outliers.

36 monomers are involved in 122 short contacts:

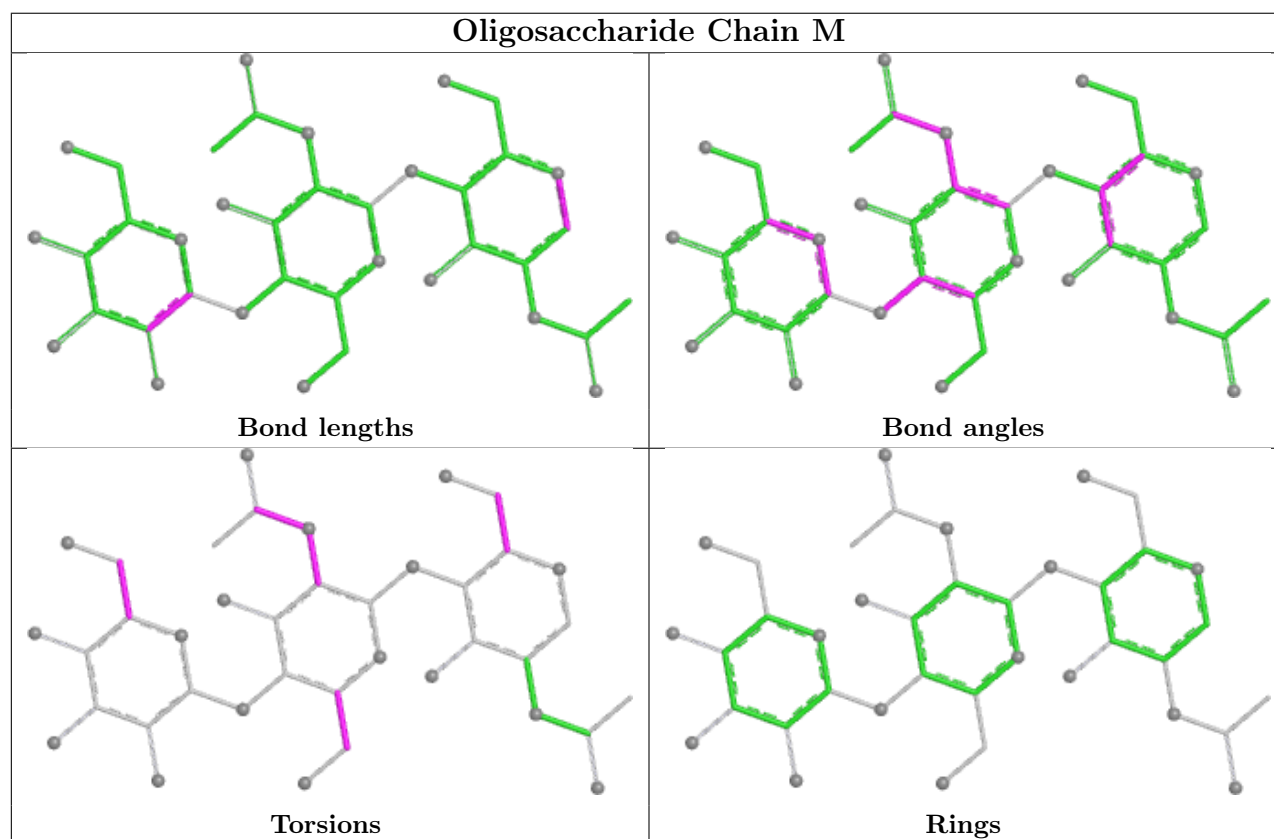
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	k	2	NAG	1	0
6	N	1	NAG	6	0
6	j	2	NAG	1	0
6	X	2	NAG	2	0
10	u	1	NAG	1	0
6	U	1	NAG	5	0
5	M	2	NAG	1	0
6	O	1	NAG	6	0
6	e	1	NAG	13	0
6	j	1	NAG	1	0
5	Y	2	NAG	1	0
6	v	2	NAG	2	0
9	V	1	NAG	1	0
6	l	1	NAG	6	0
5	k	1	NAG	6	0
6	q	1	NAG	13	0
6	a	1	NAG	6	0
9	t	1	NAG	1	0
6	r	1	NAG	1	0
6	r	2	NAG	1	0

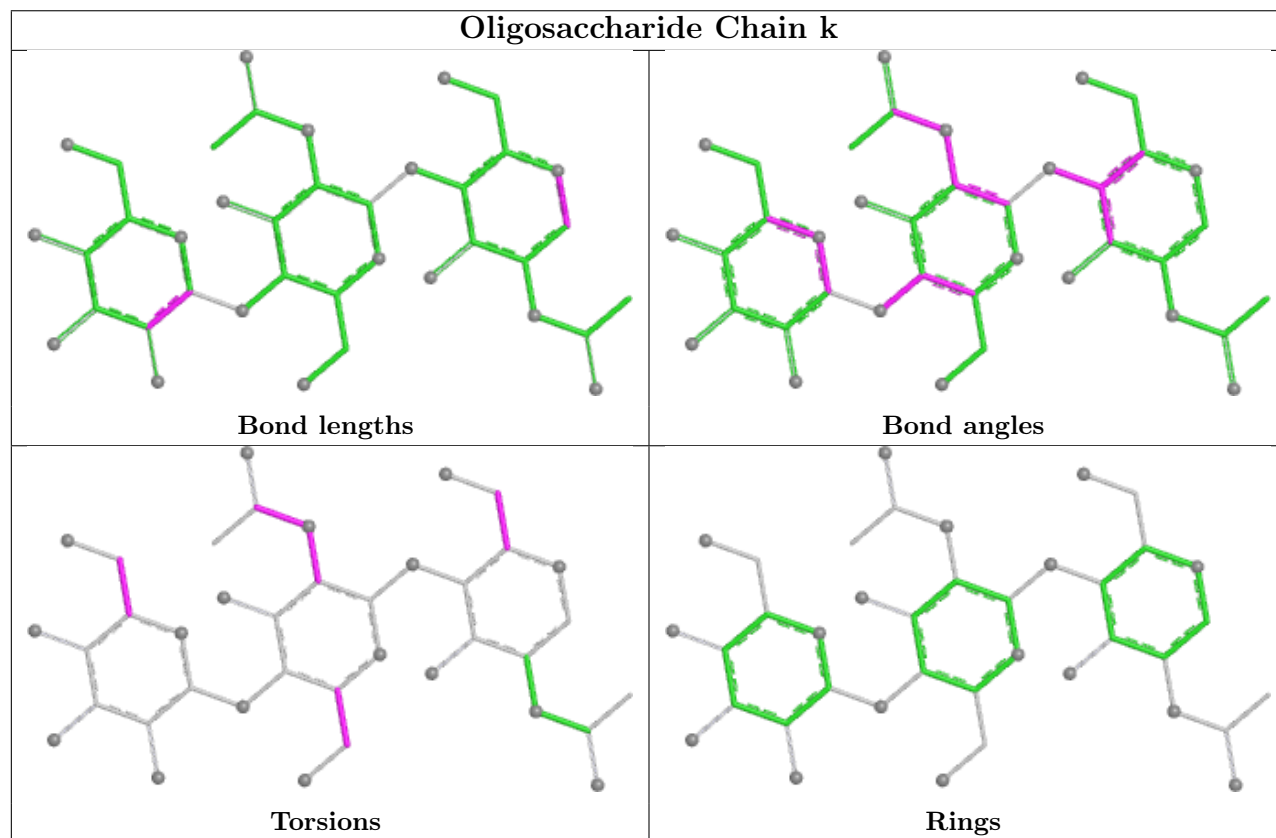
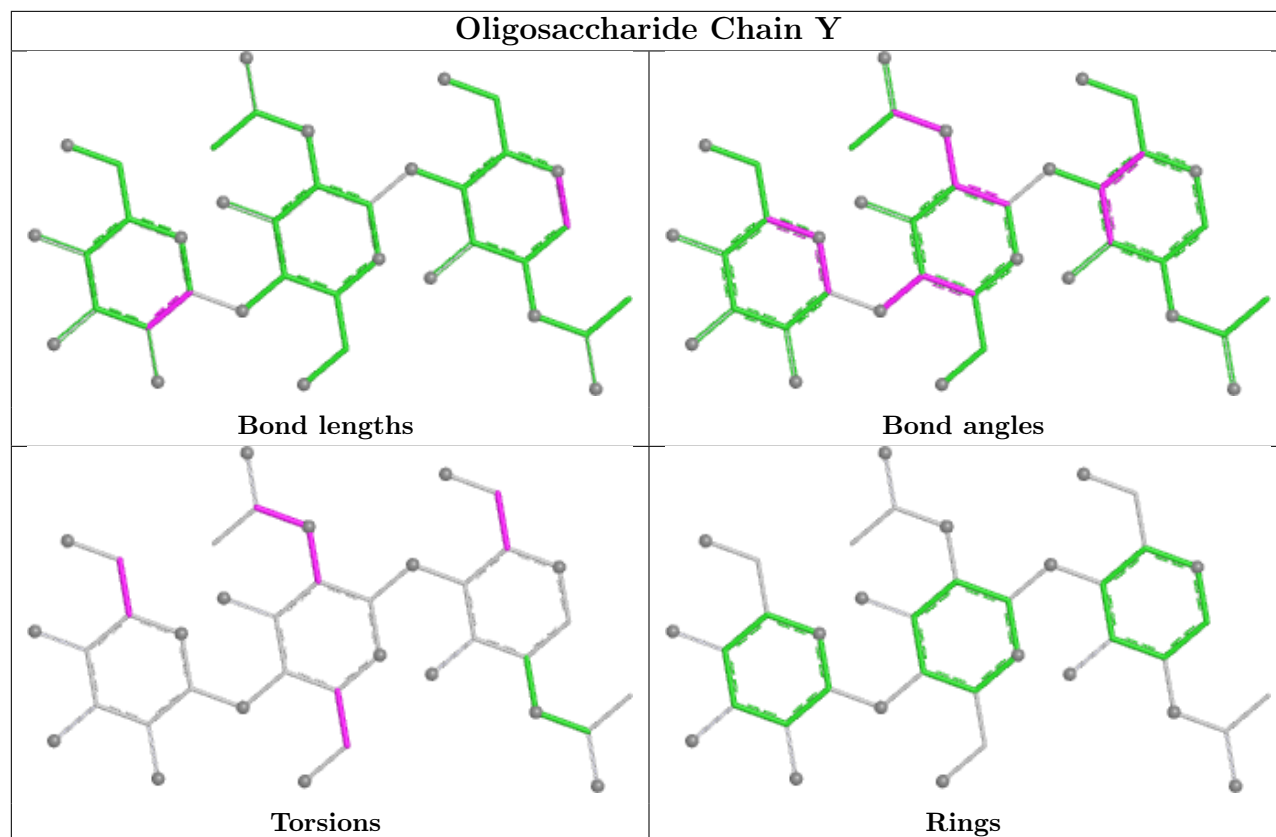
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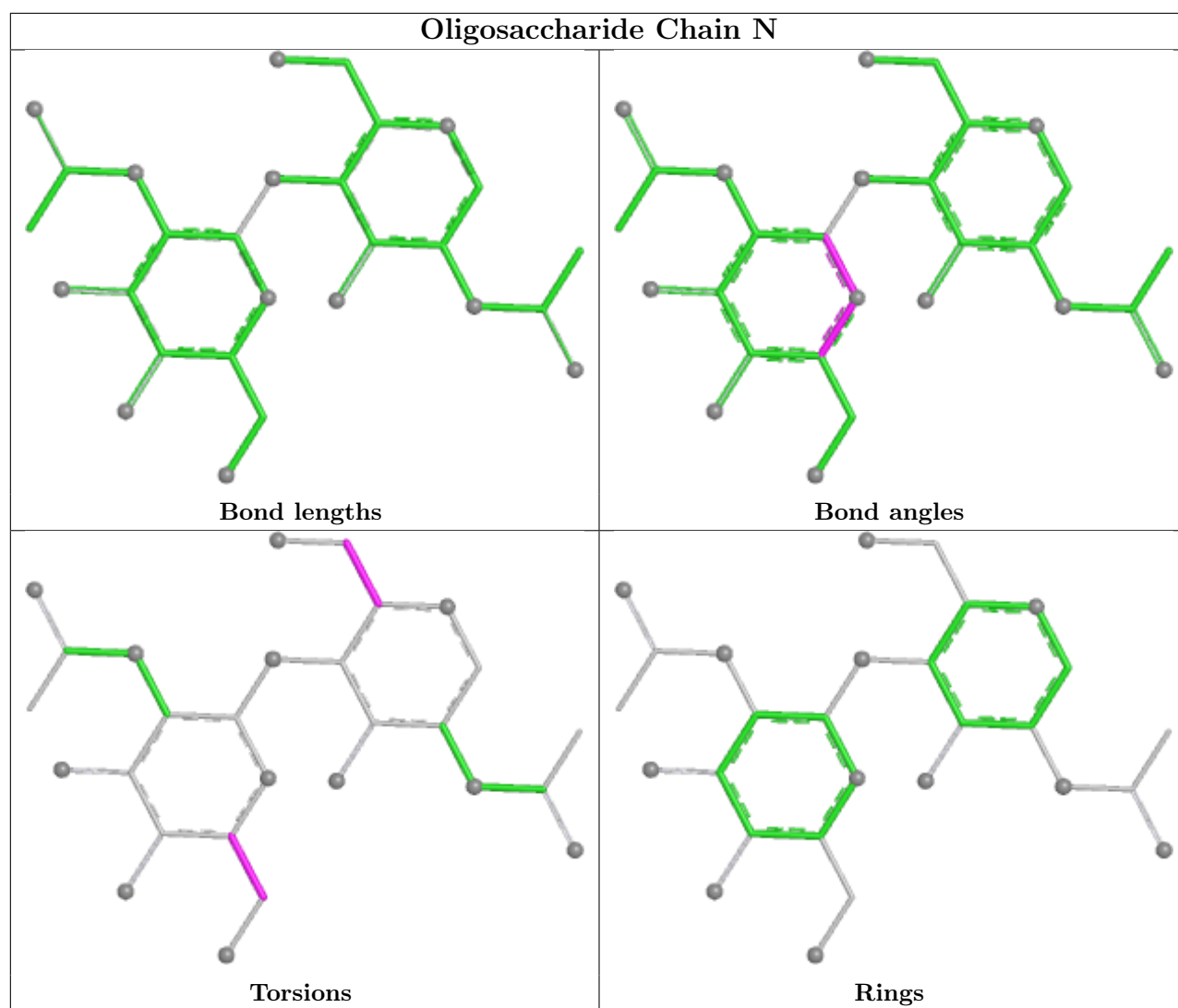
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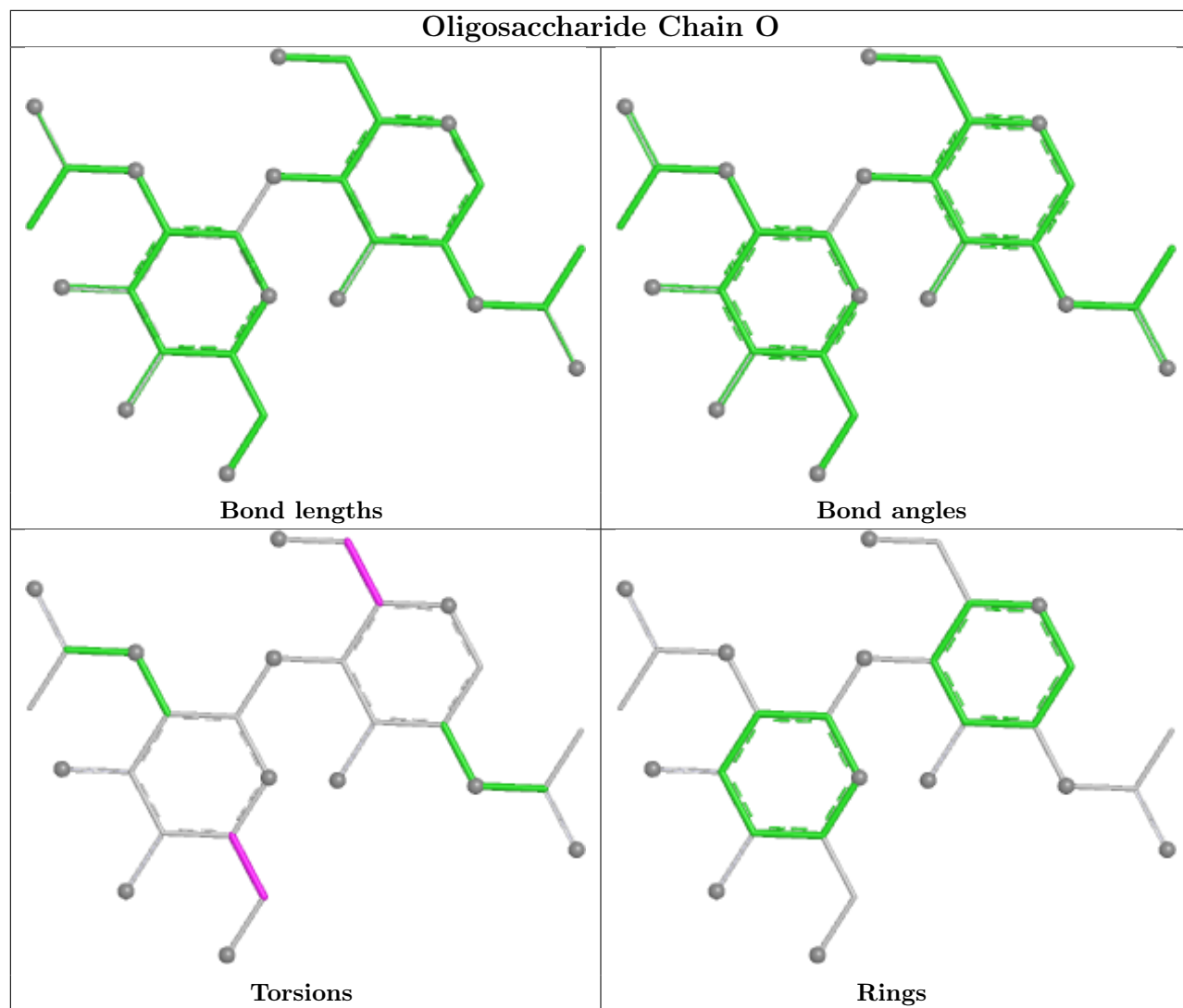
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	v	1	NAG	2	0
6	T	1	NAG	1	0
10	W	1	NAG	1	0
10	i	1	NAG	1	0
5	Y	1	NAG	6	0
6	T	2	NAG	1	0
6	f	2	NAG	1	0
6	f	1	NAG	1	0
5	M	1	NAG	6	0
6	S	1	NAG	13	0
9	h	1	NAG	1	0
6	g	1	NAG	5	0
6	s	1	NAG	5	0
6	m	1	NAG	6	0
6	Z	1	NAG	6	0
6	X	1	NAG	2	0

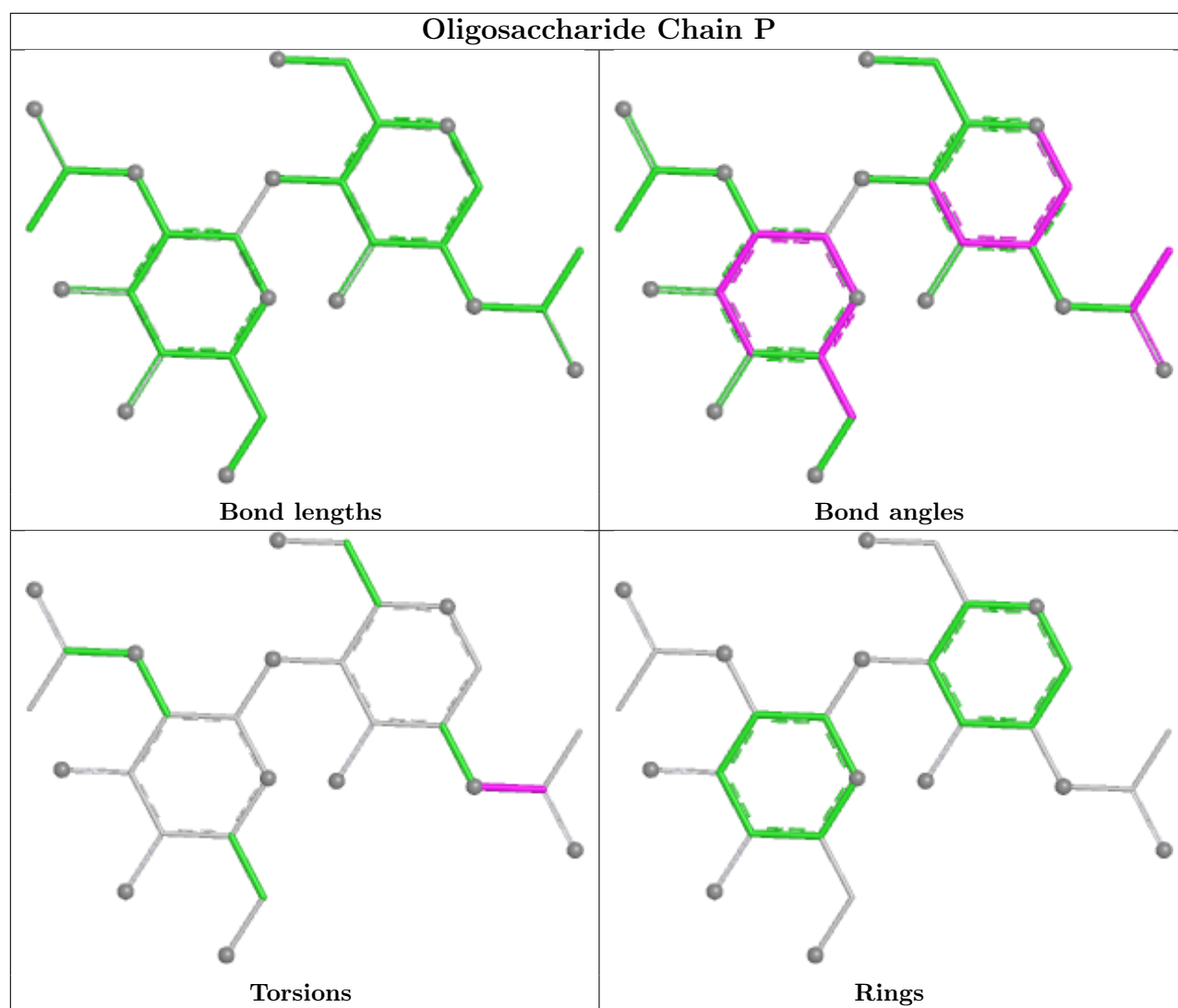
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

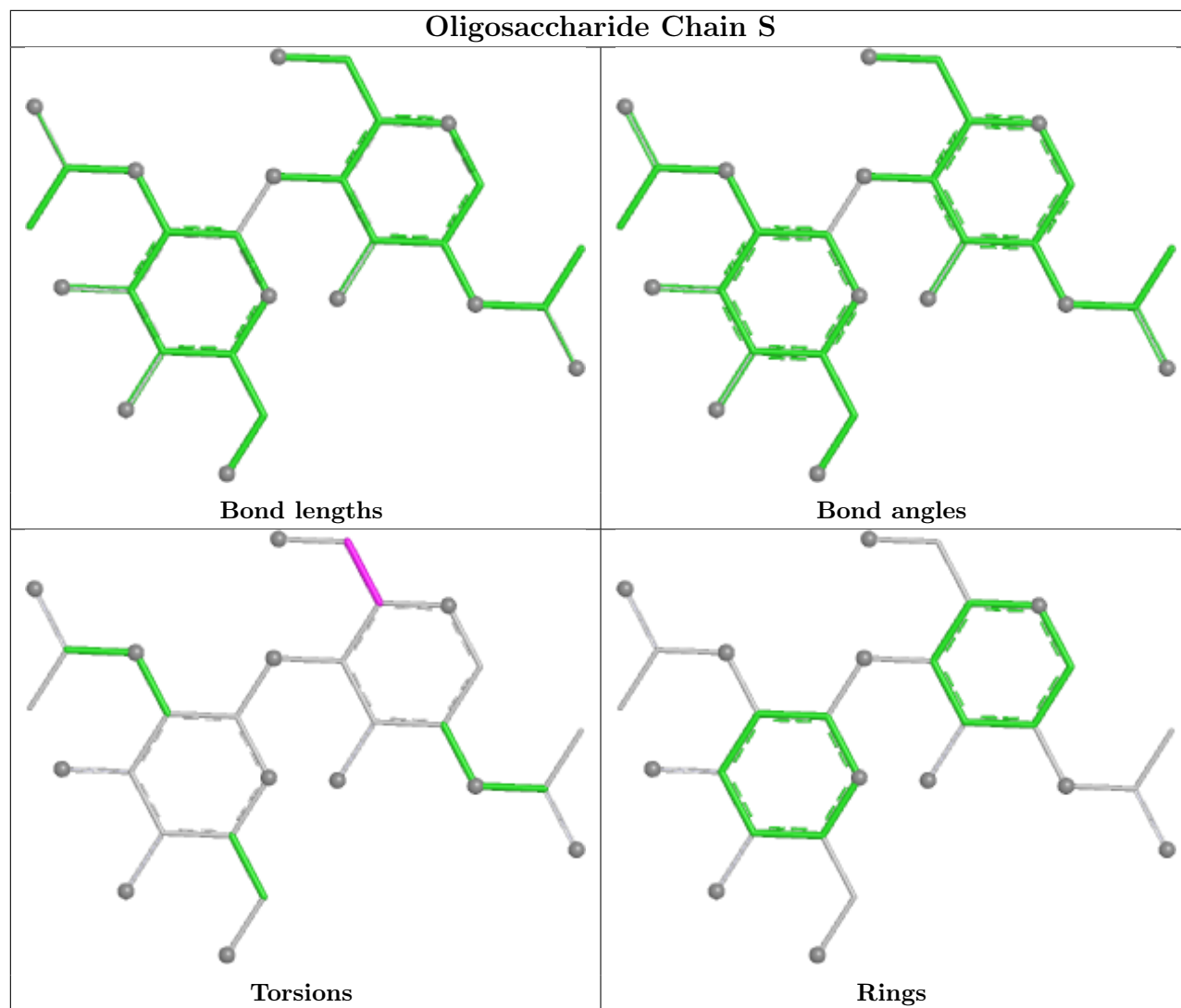


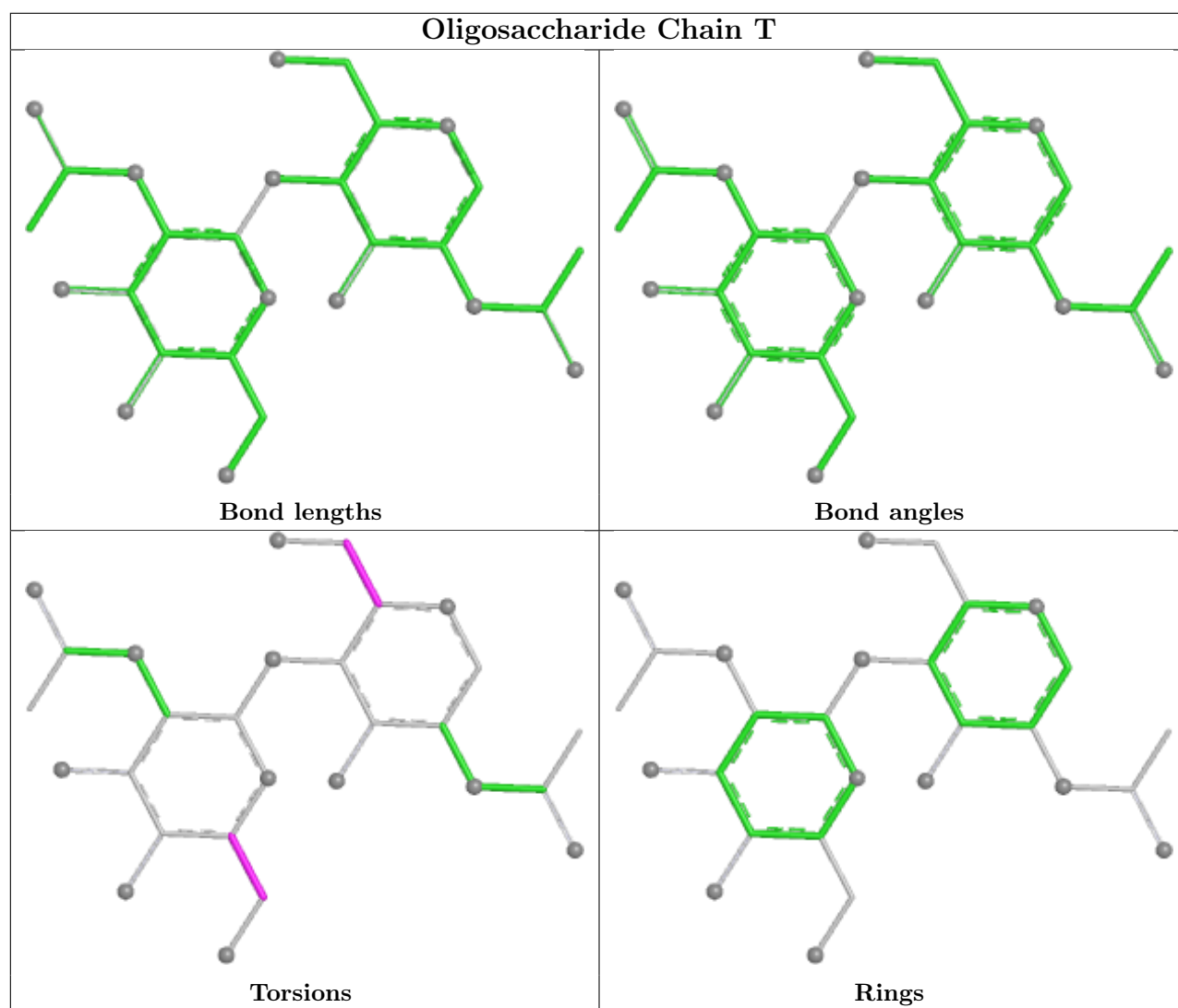


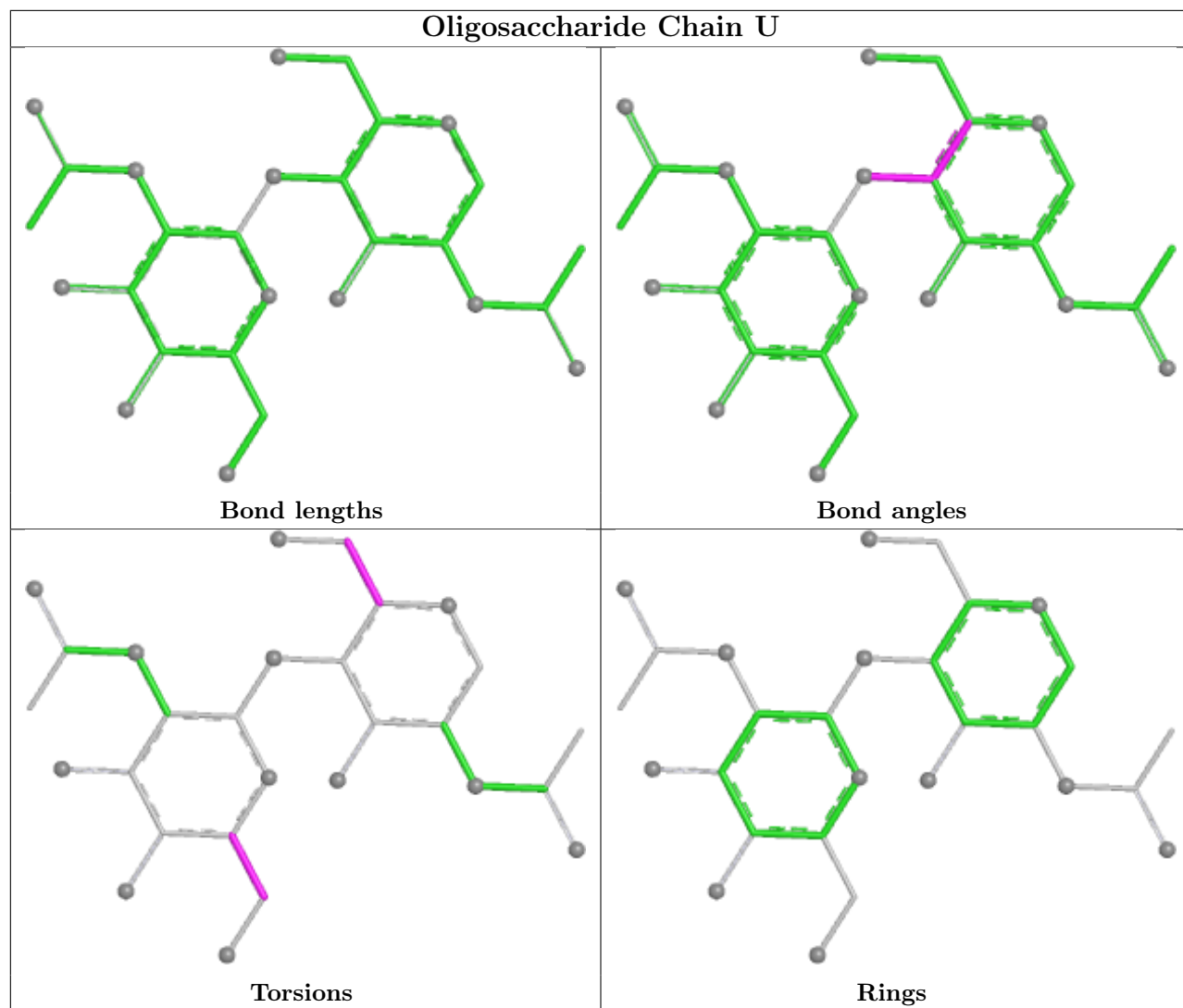


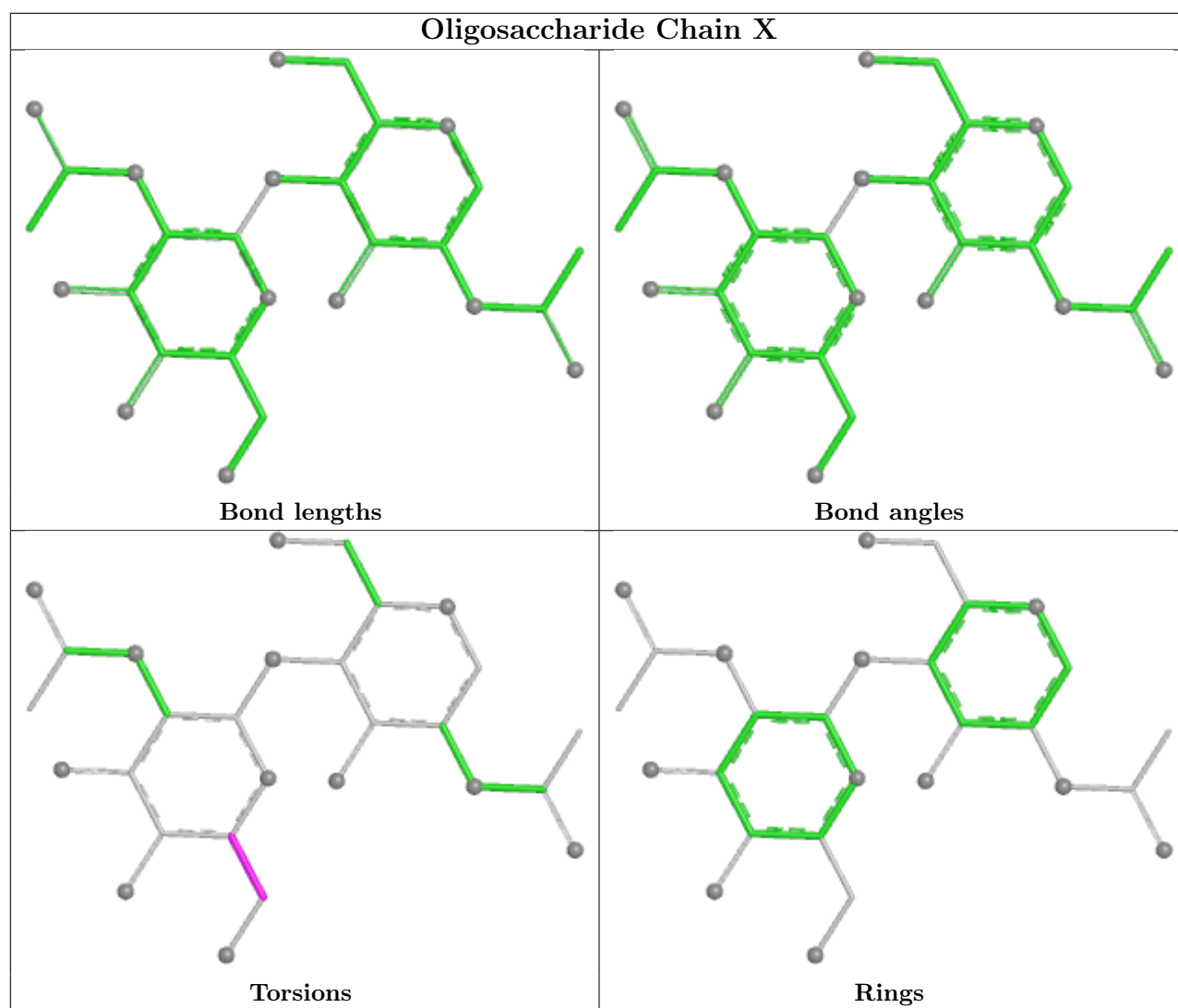


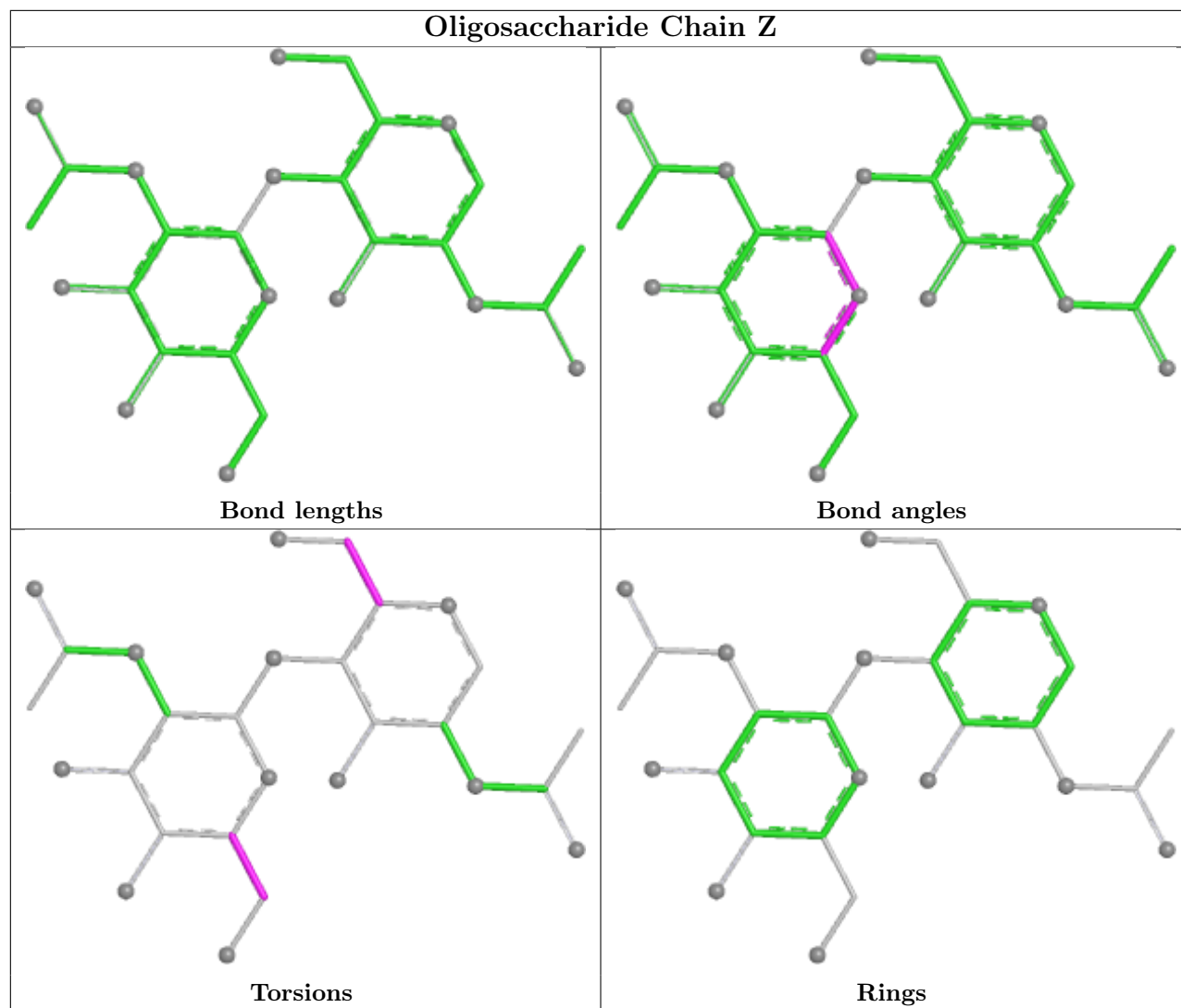


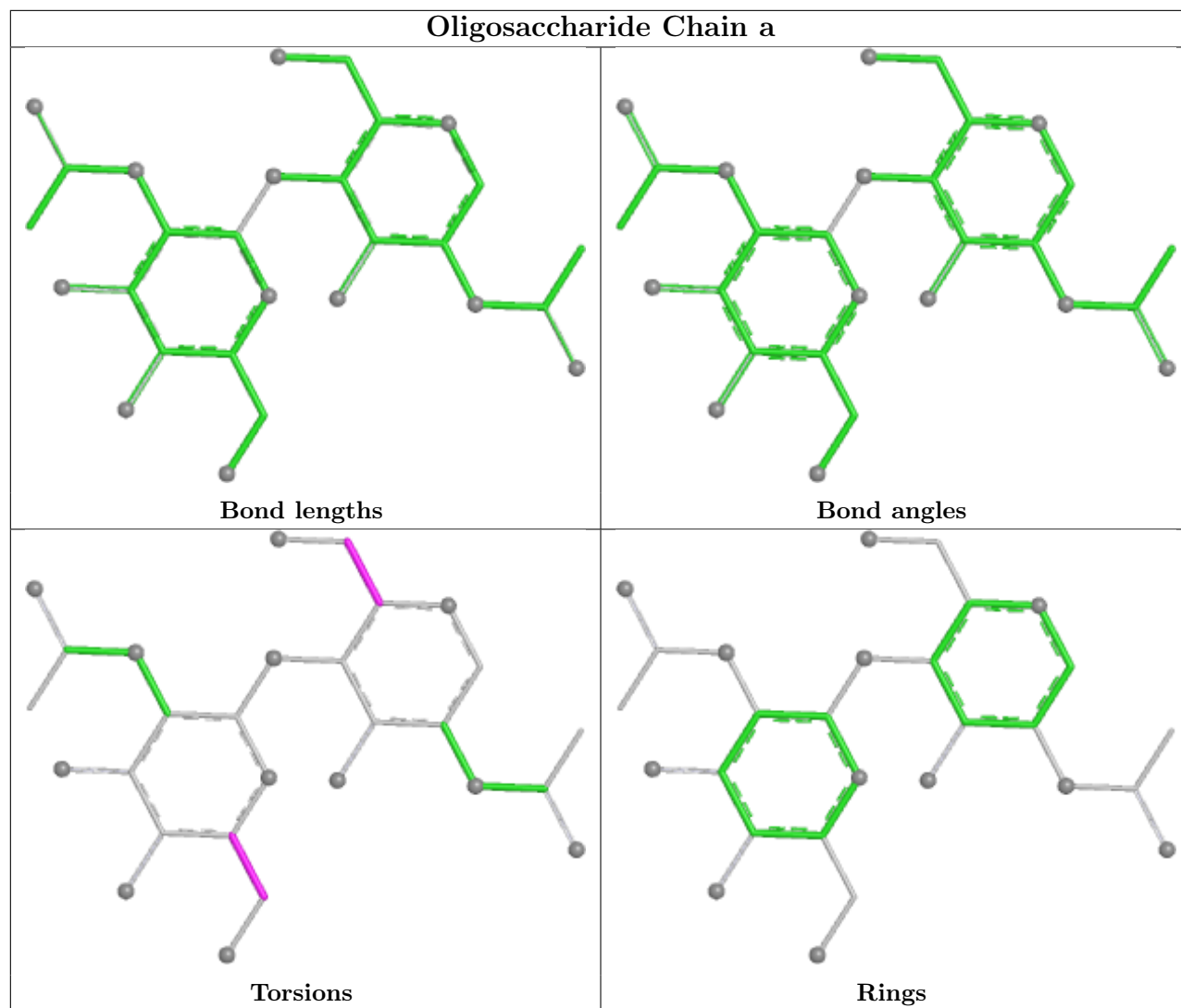


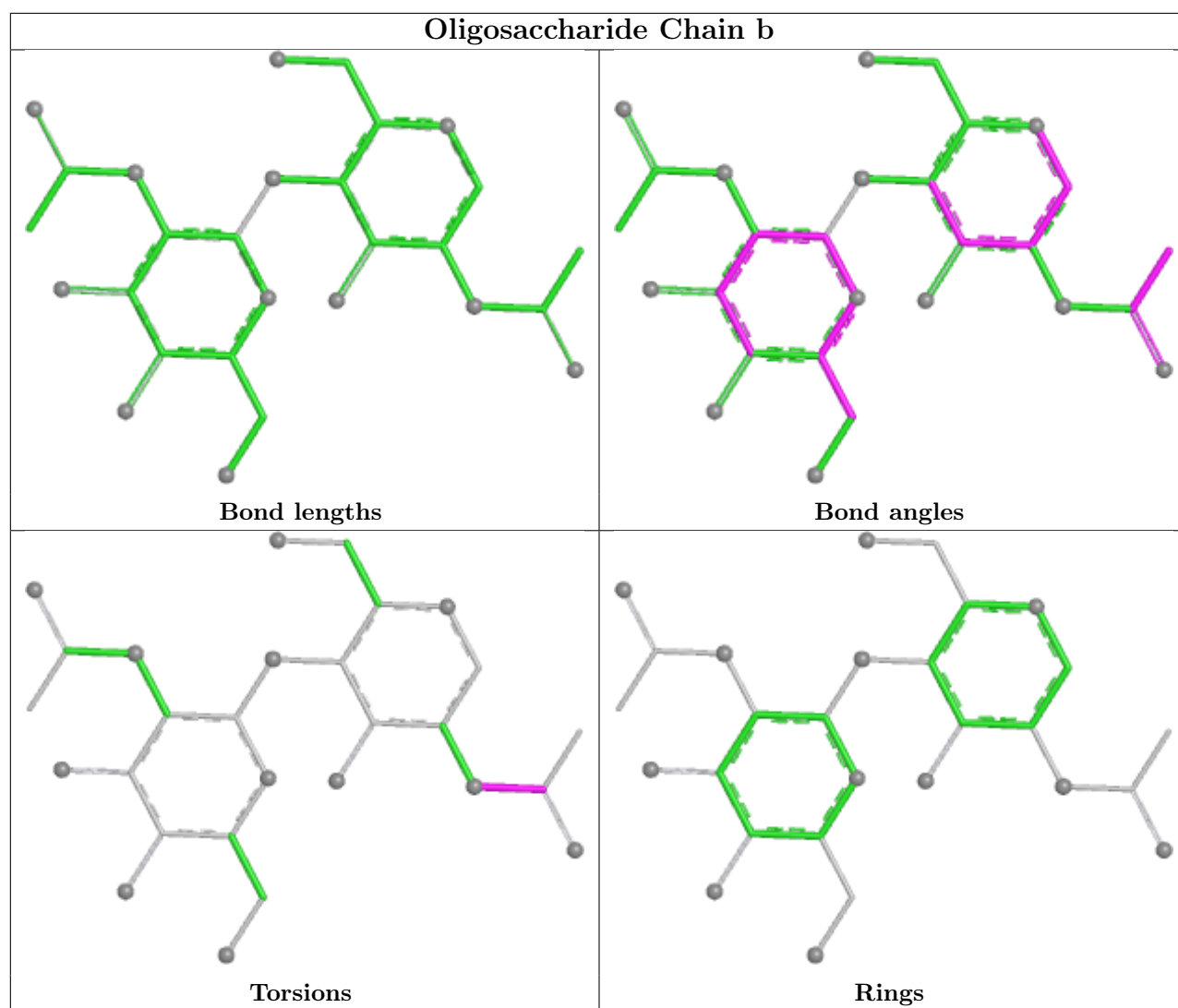


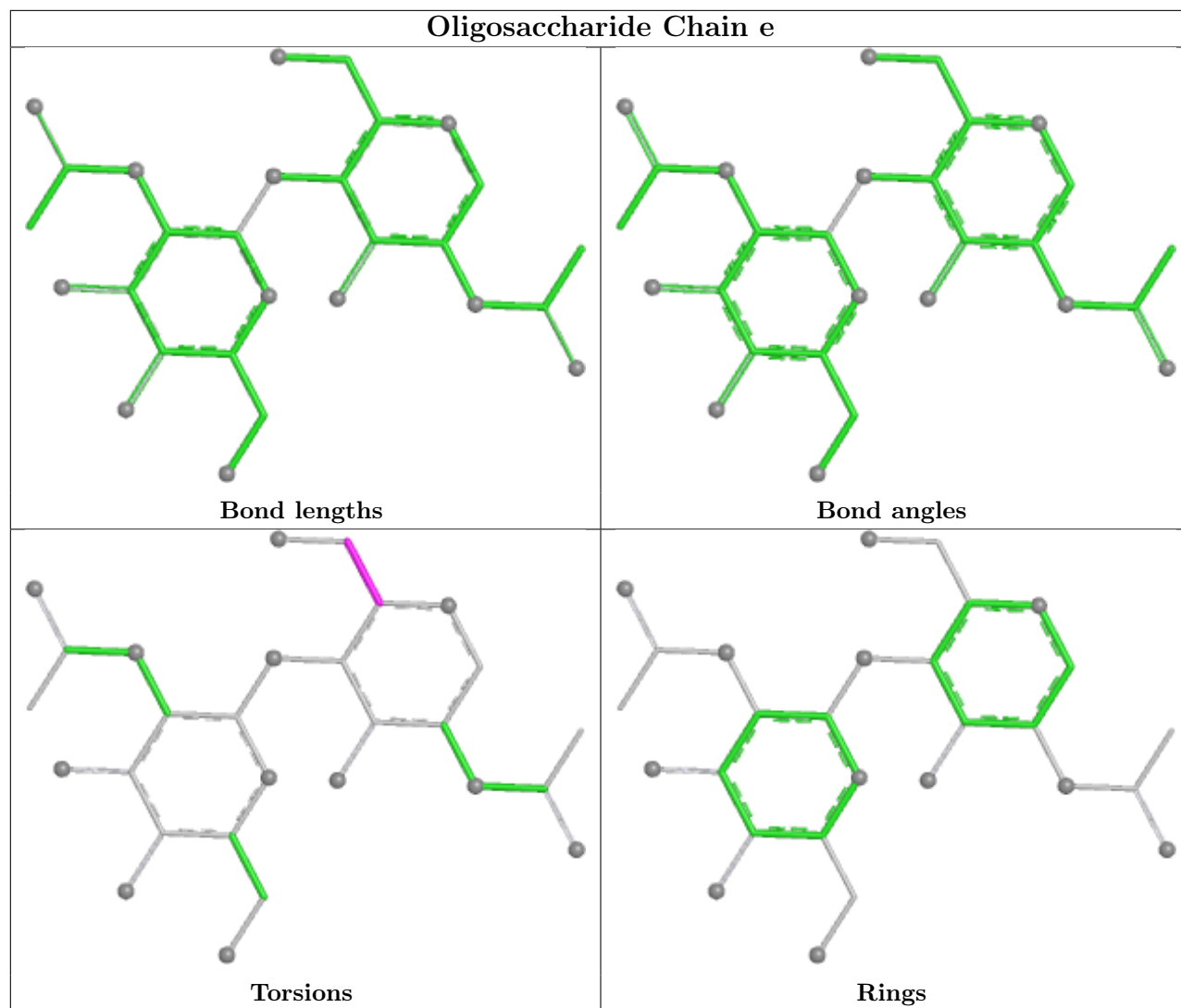


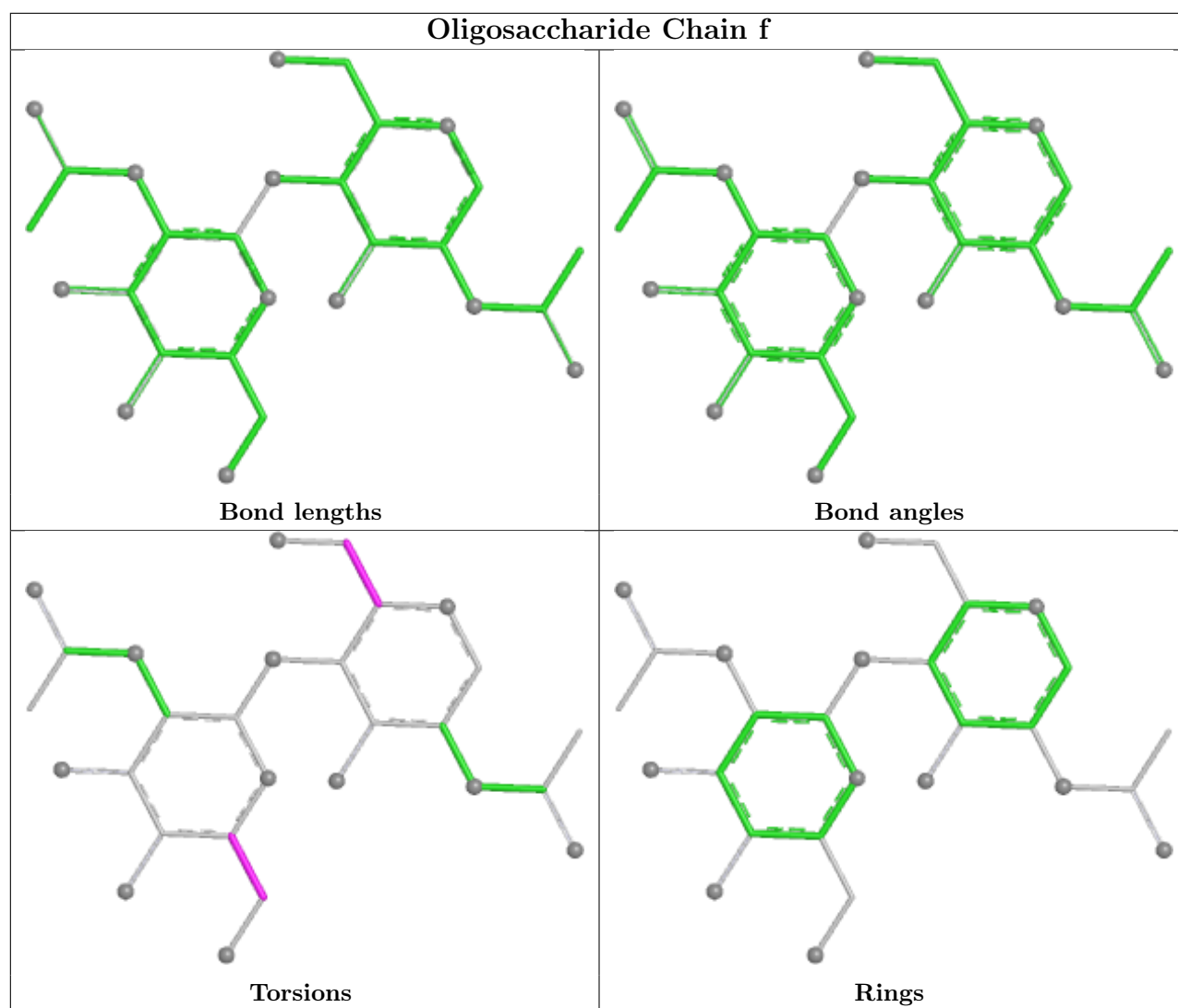


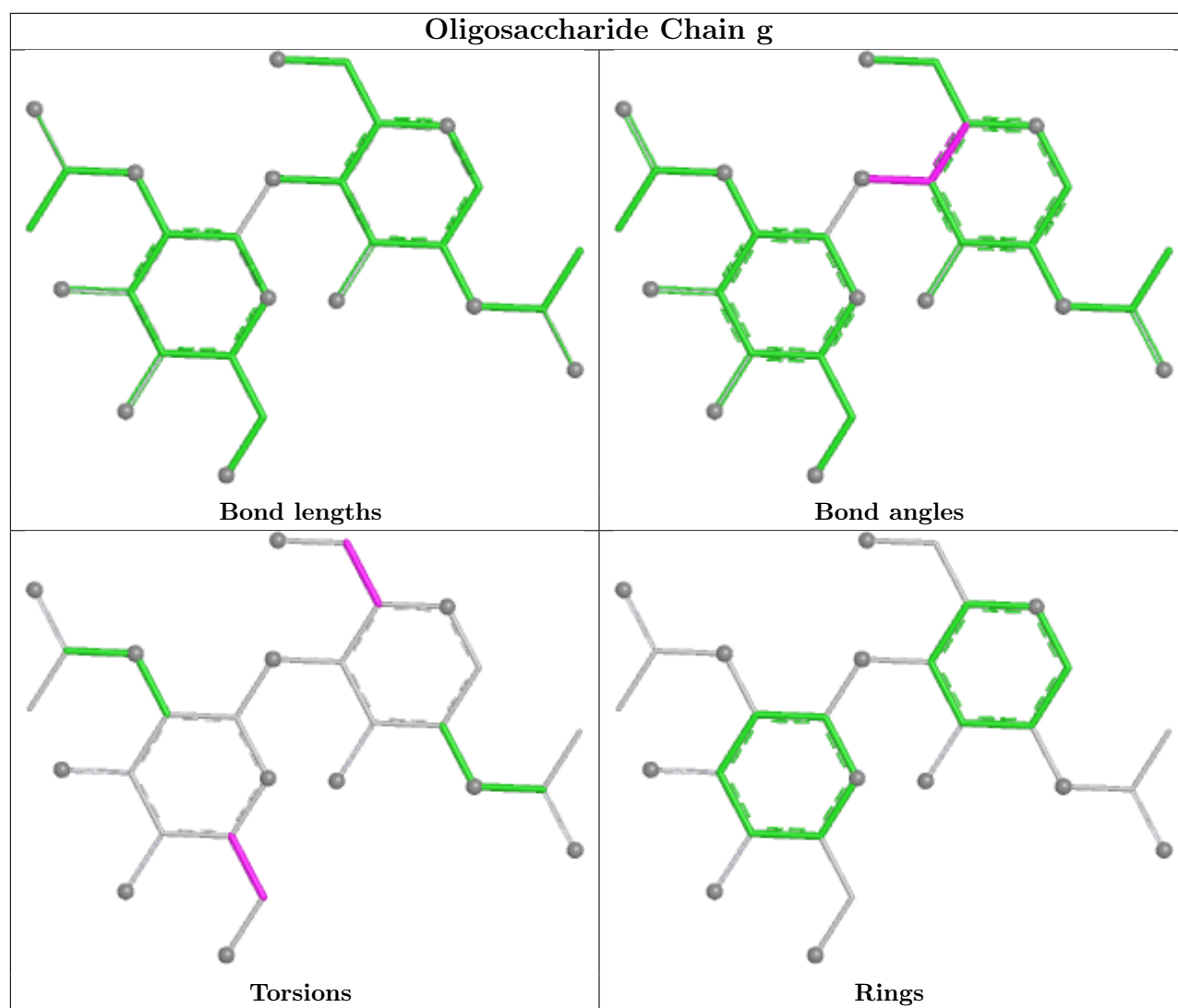


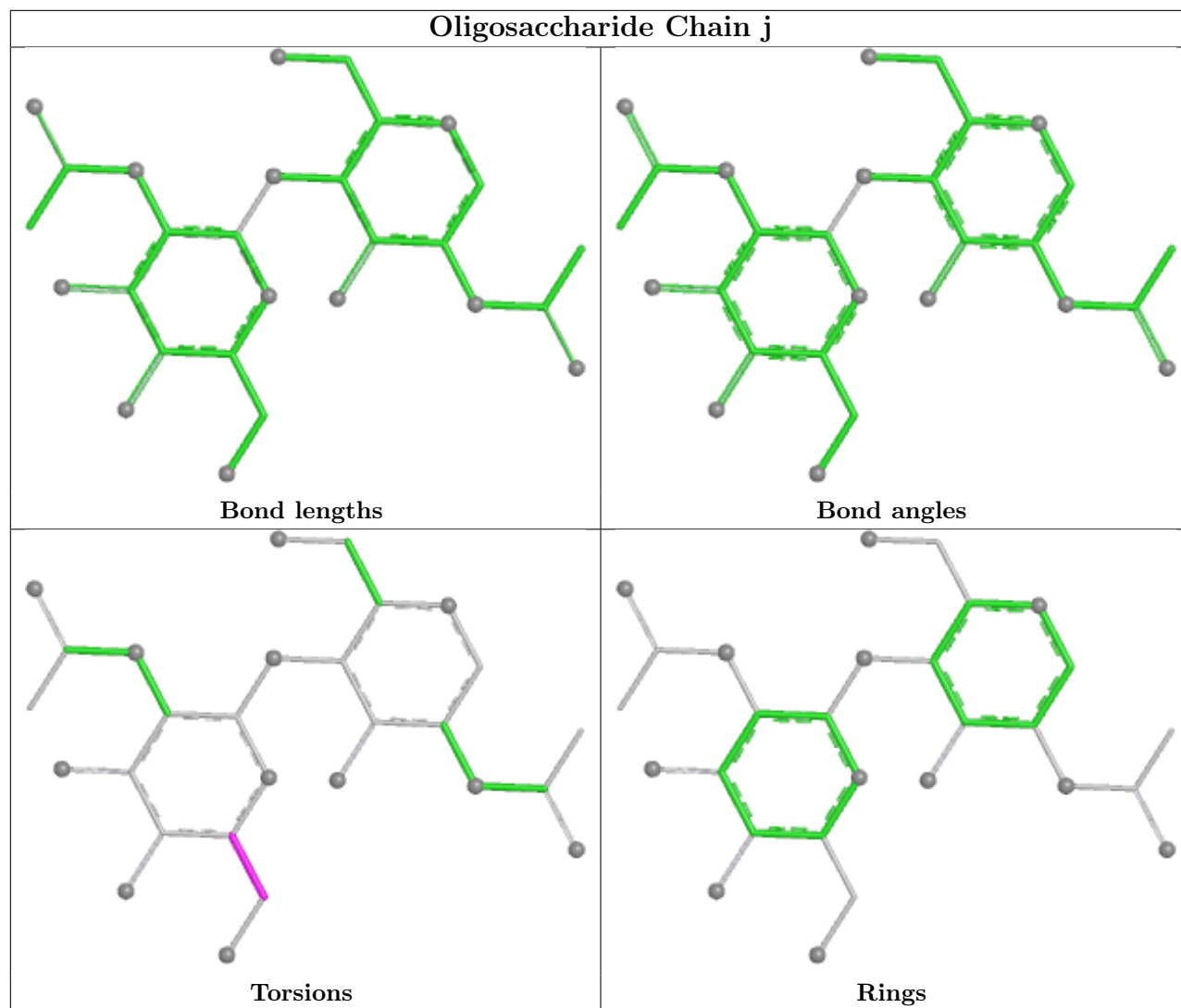


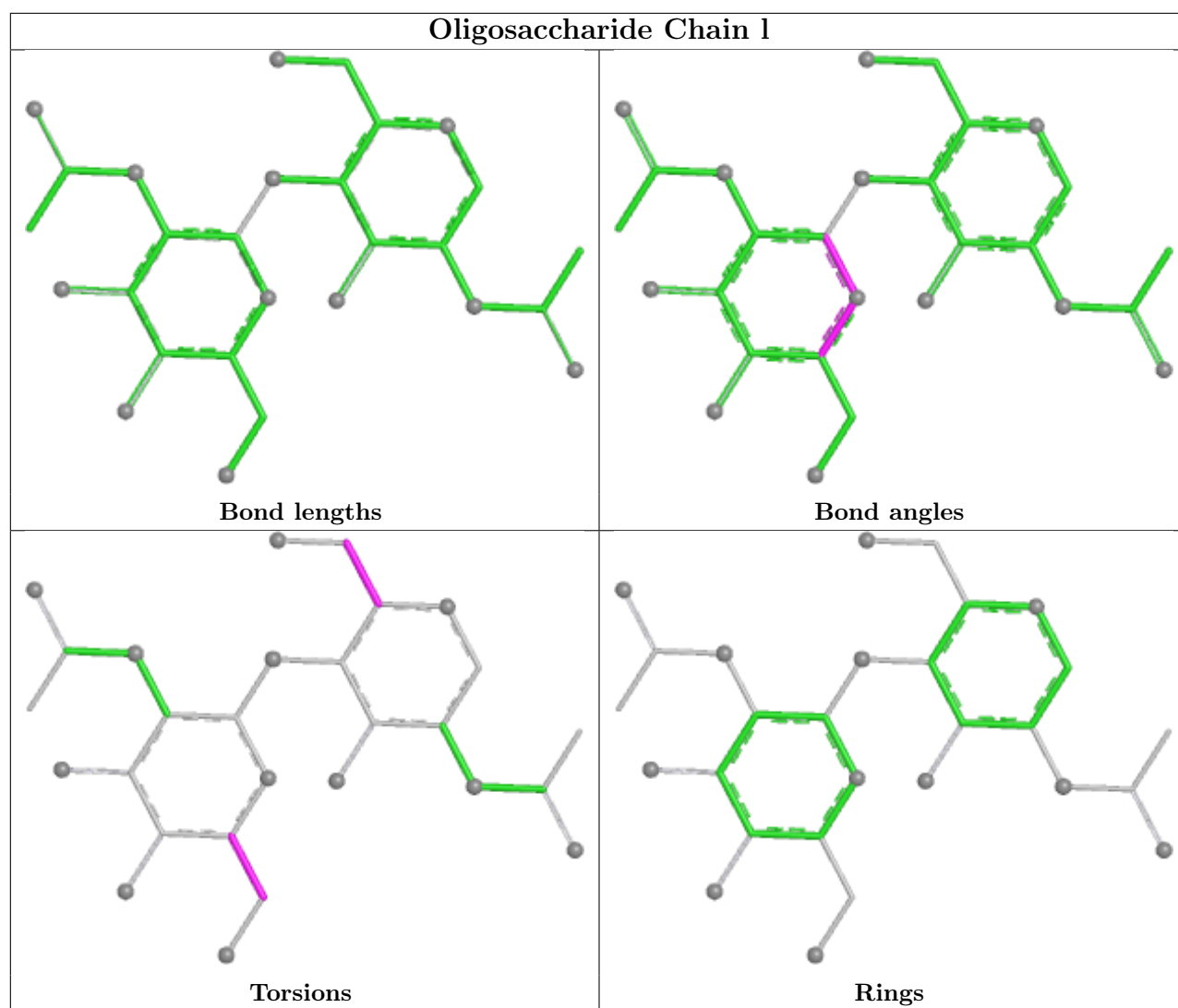


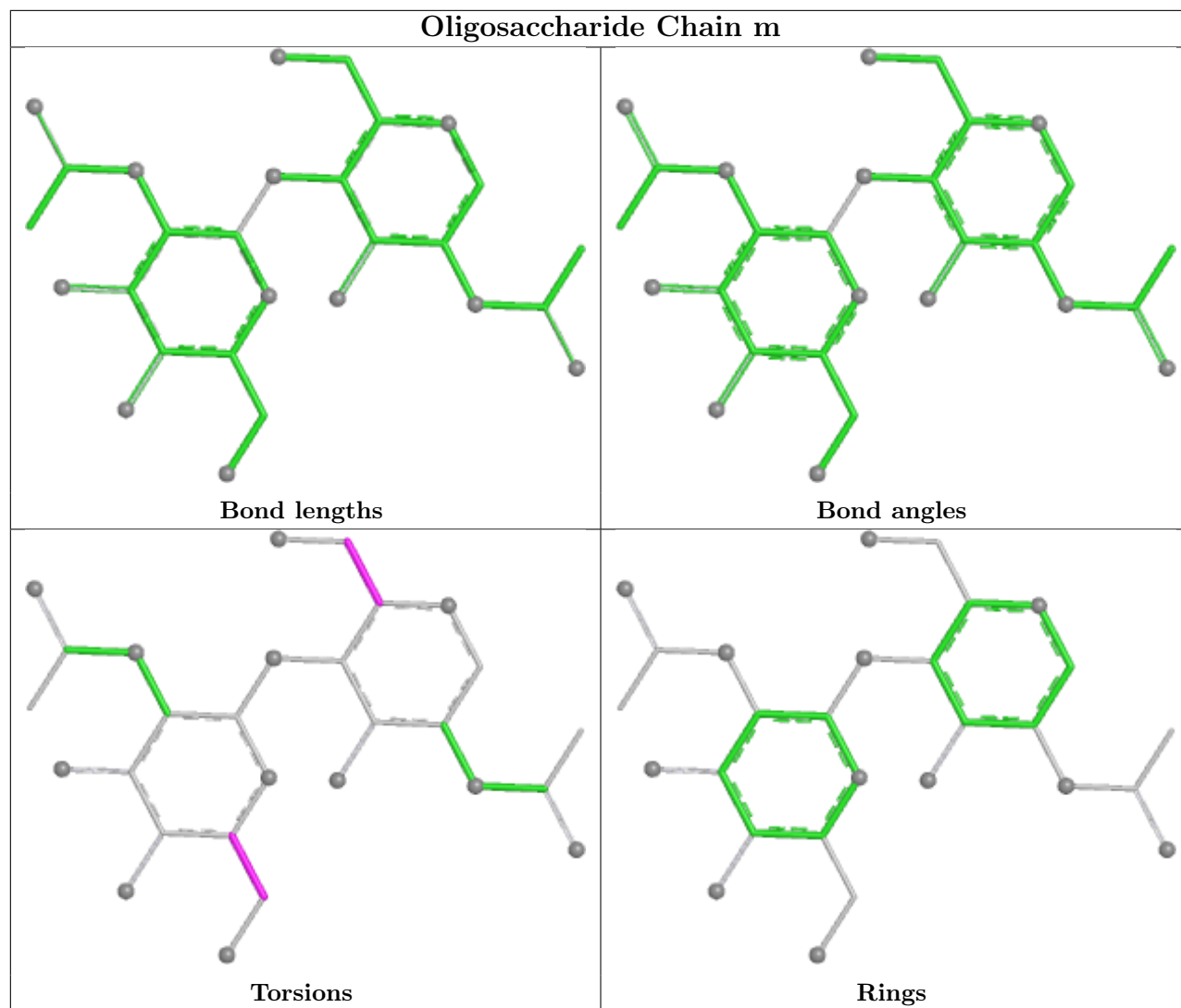


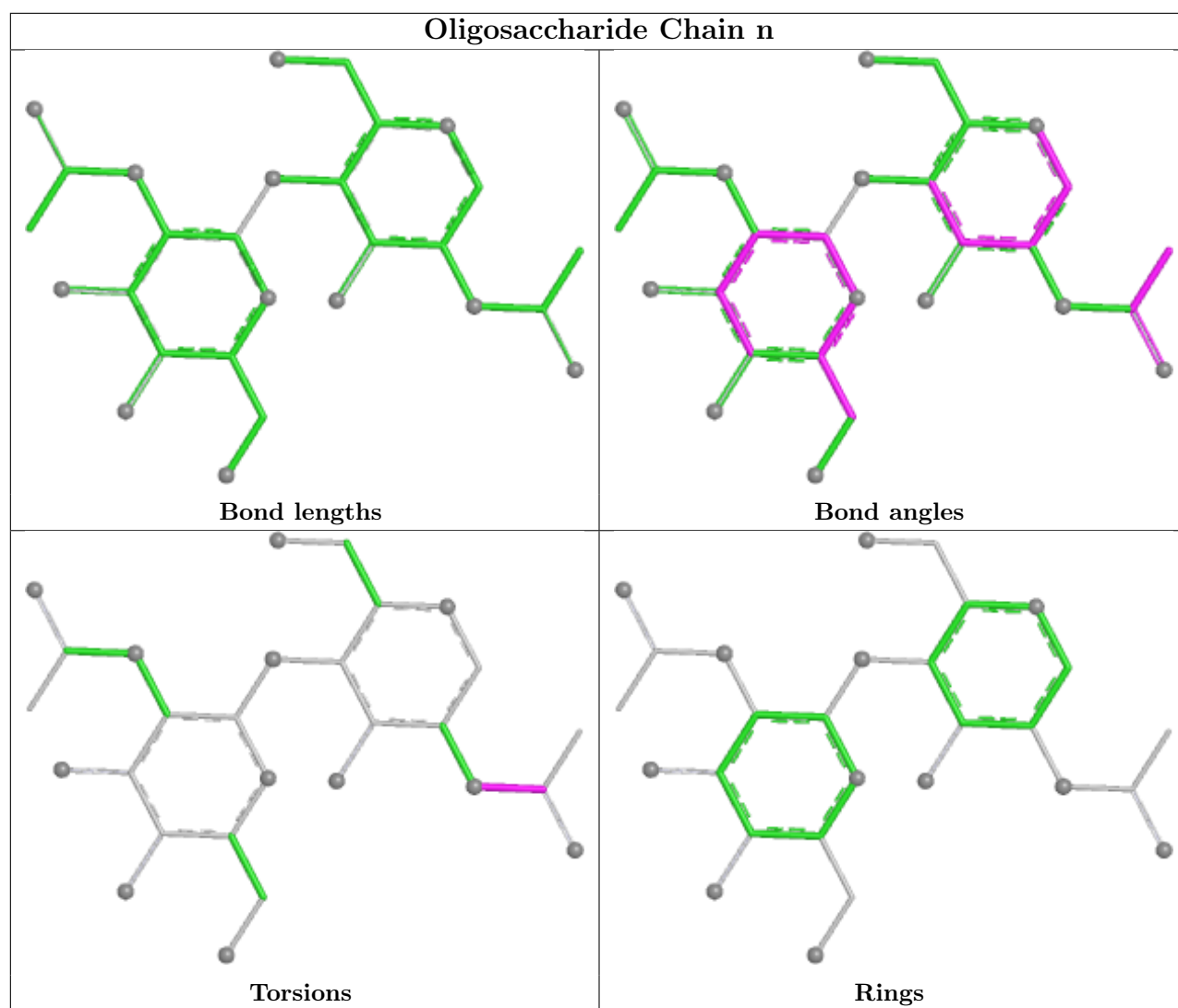


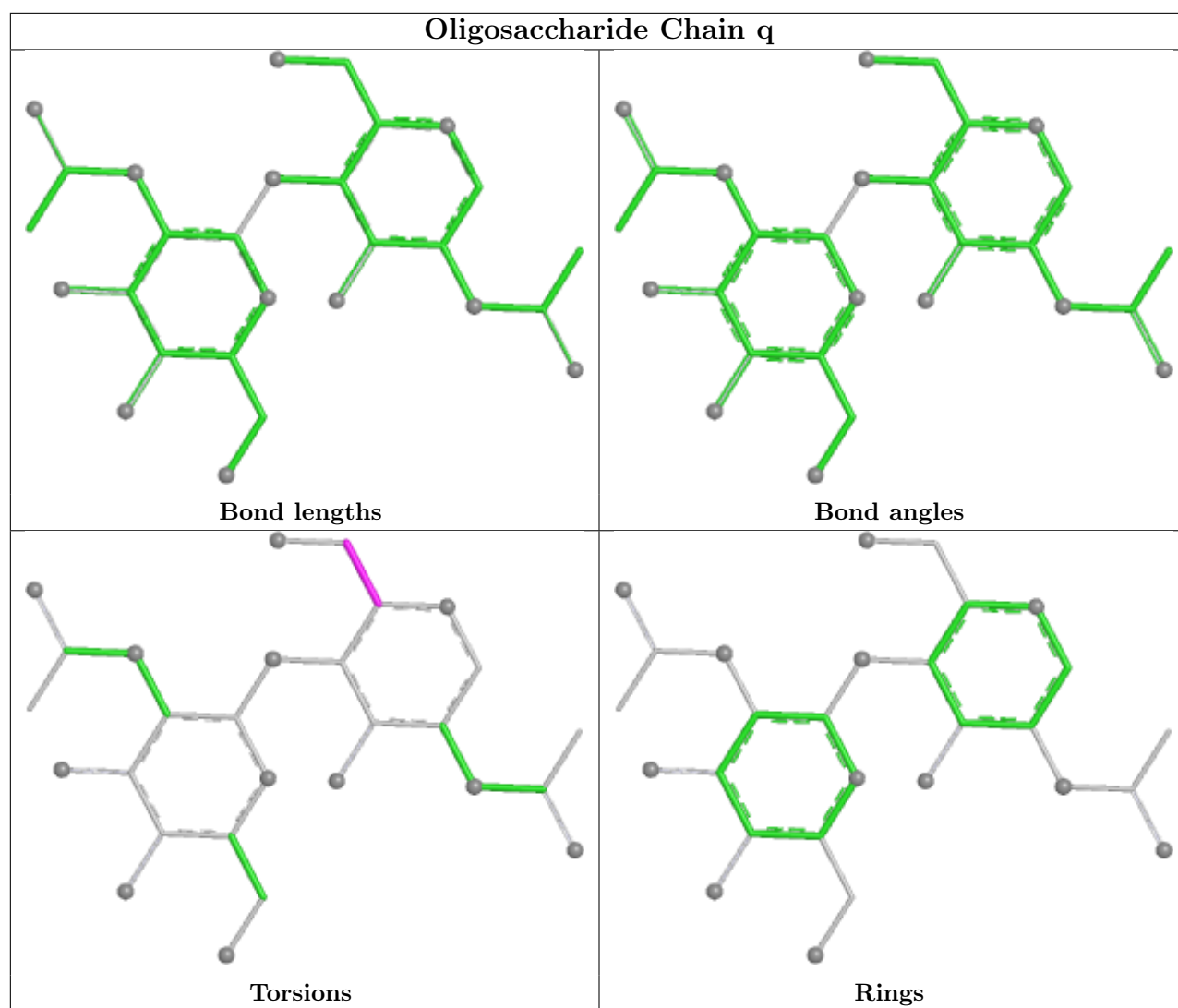


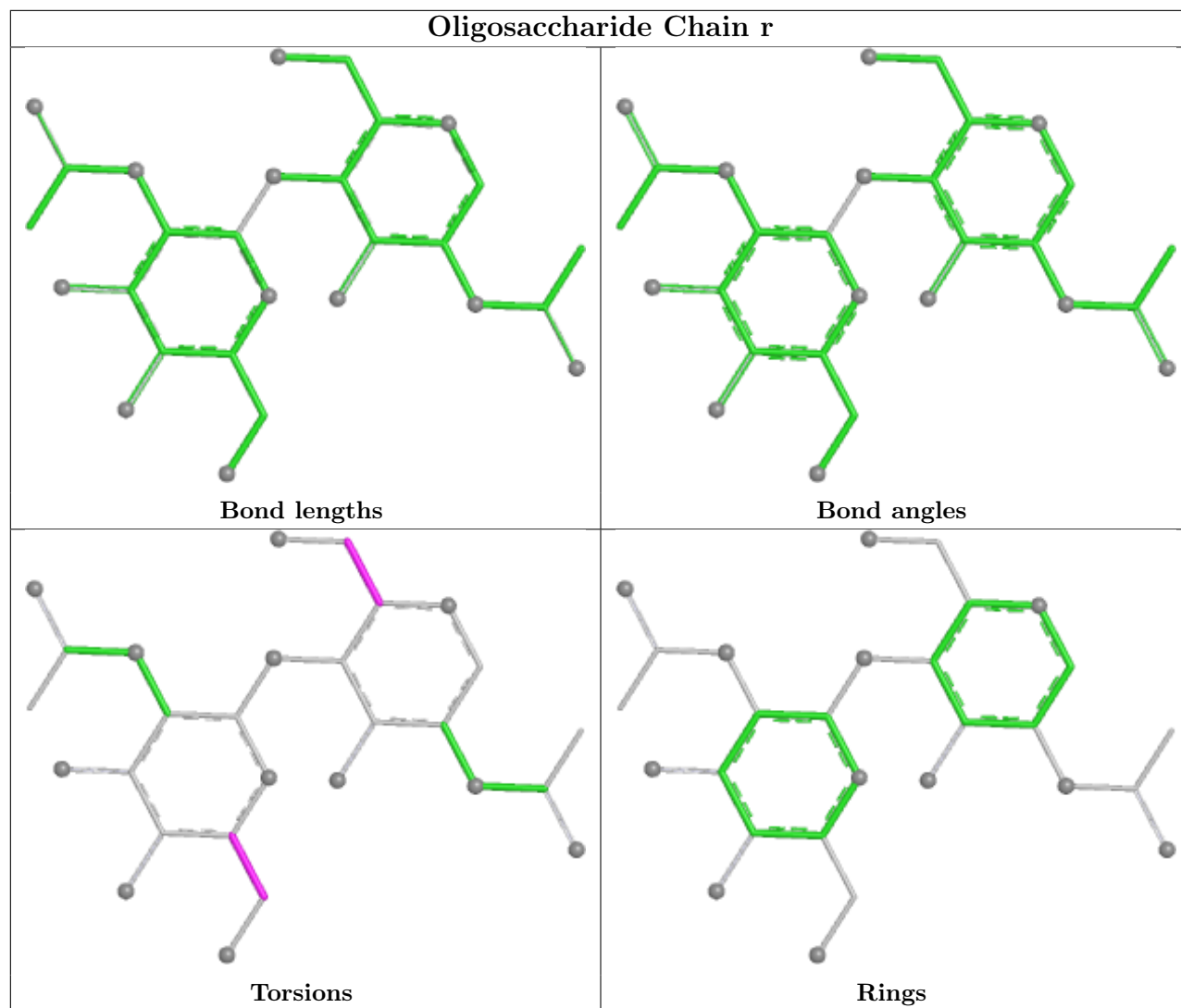


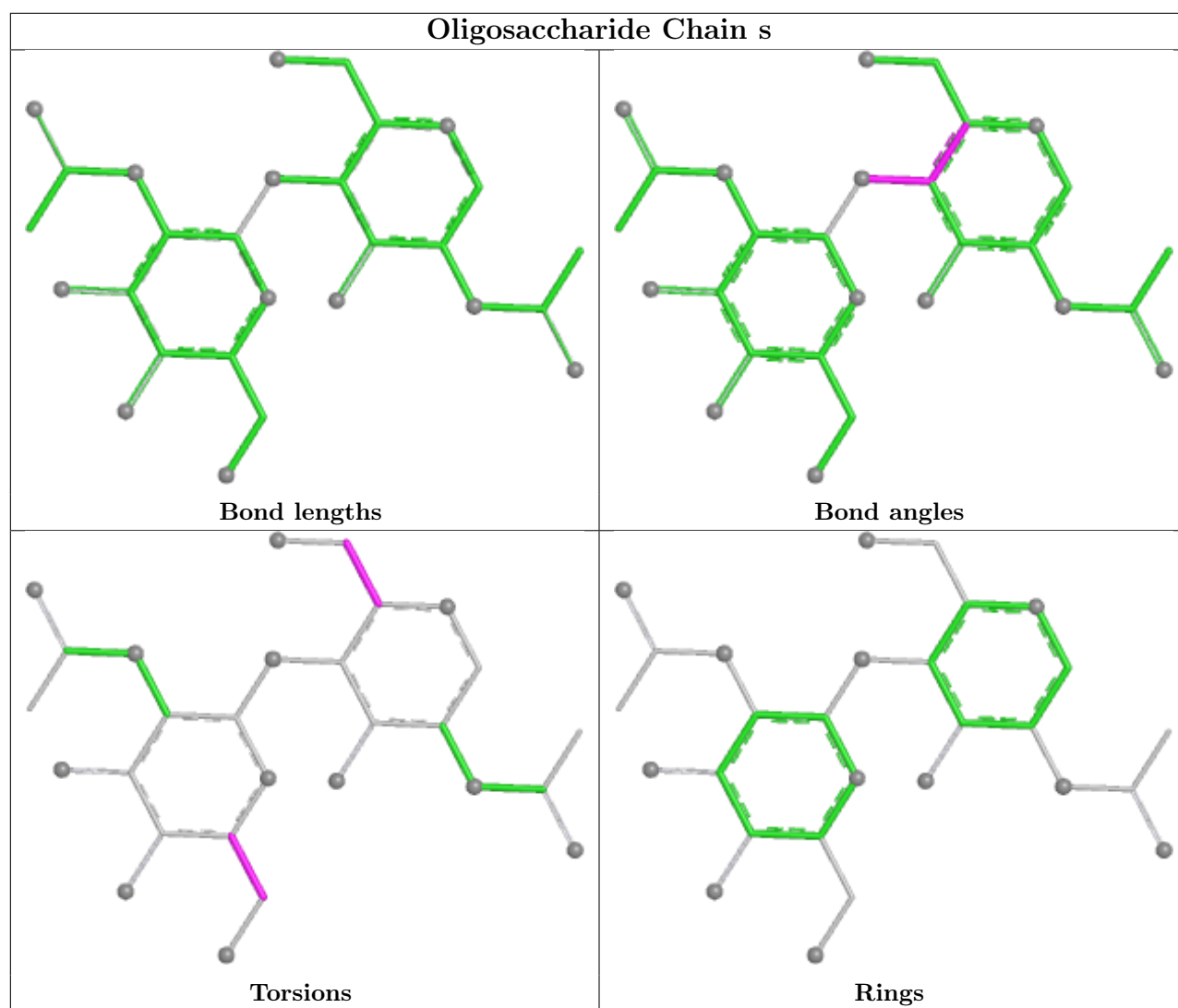


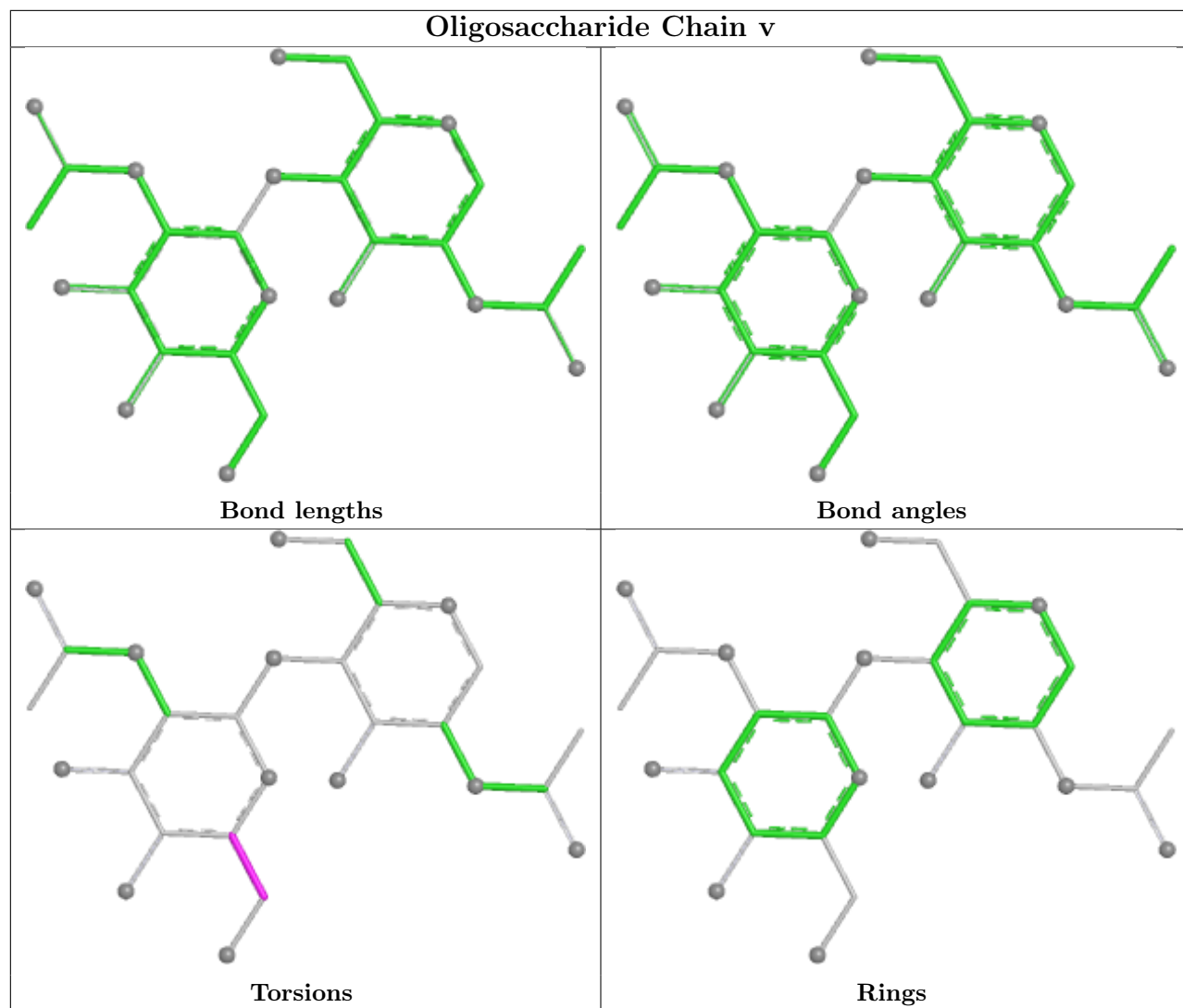


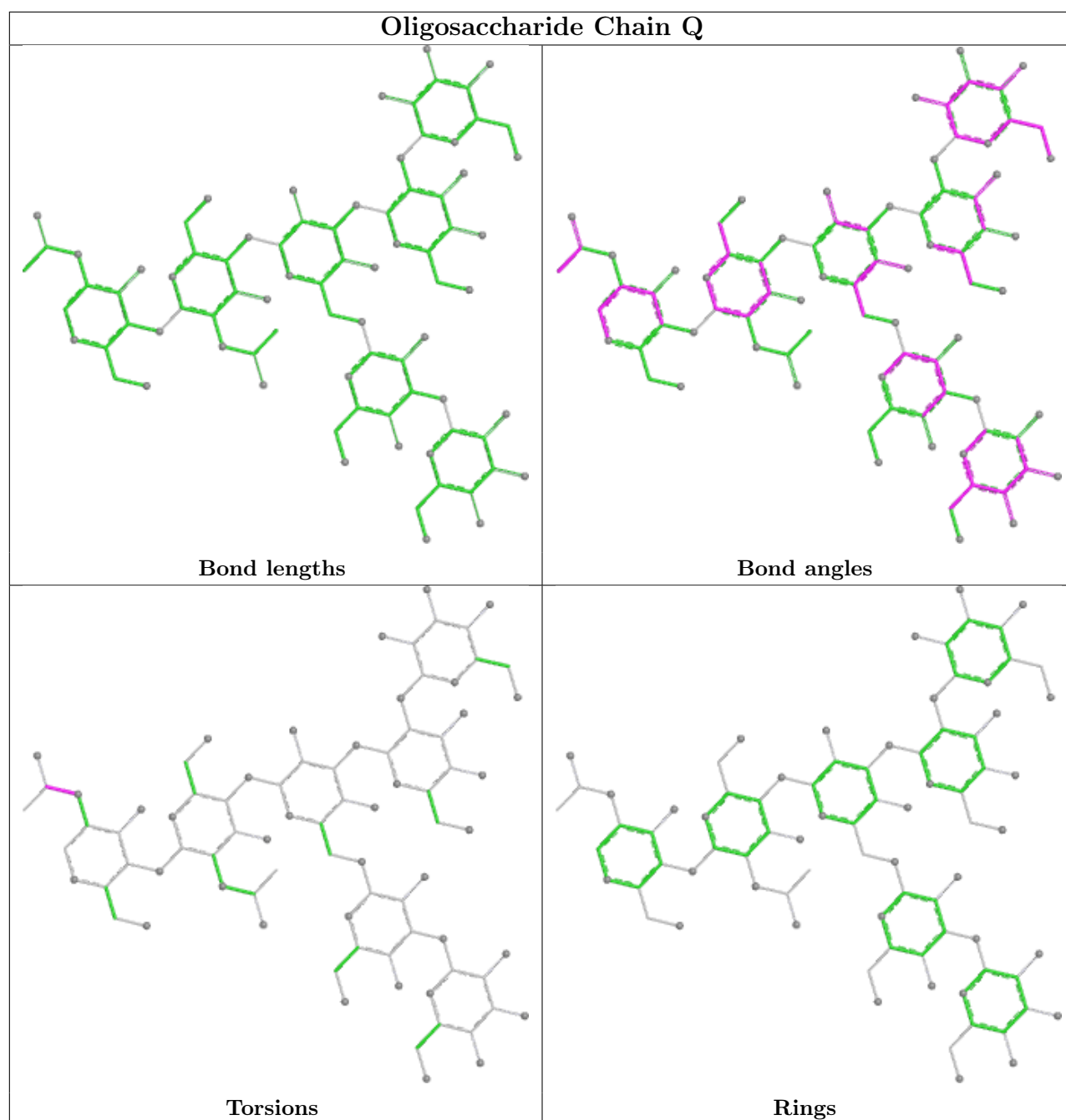


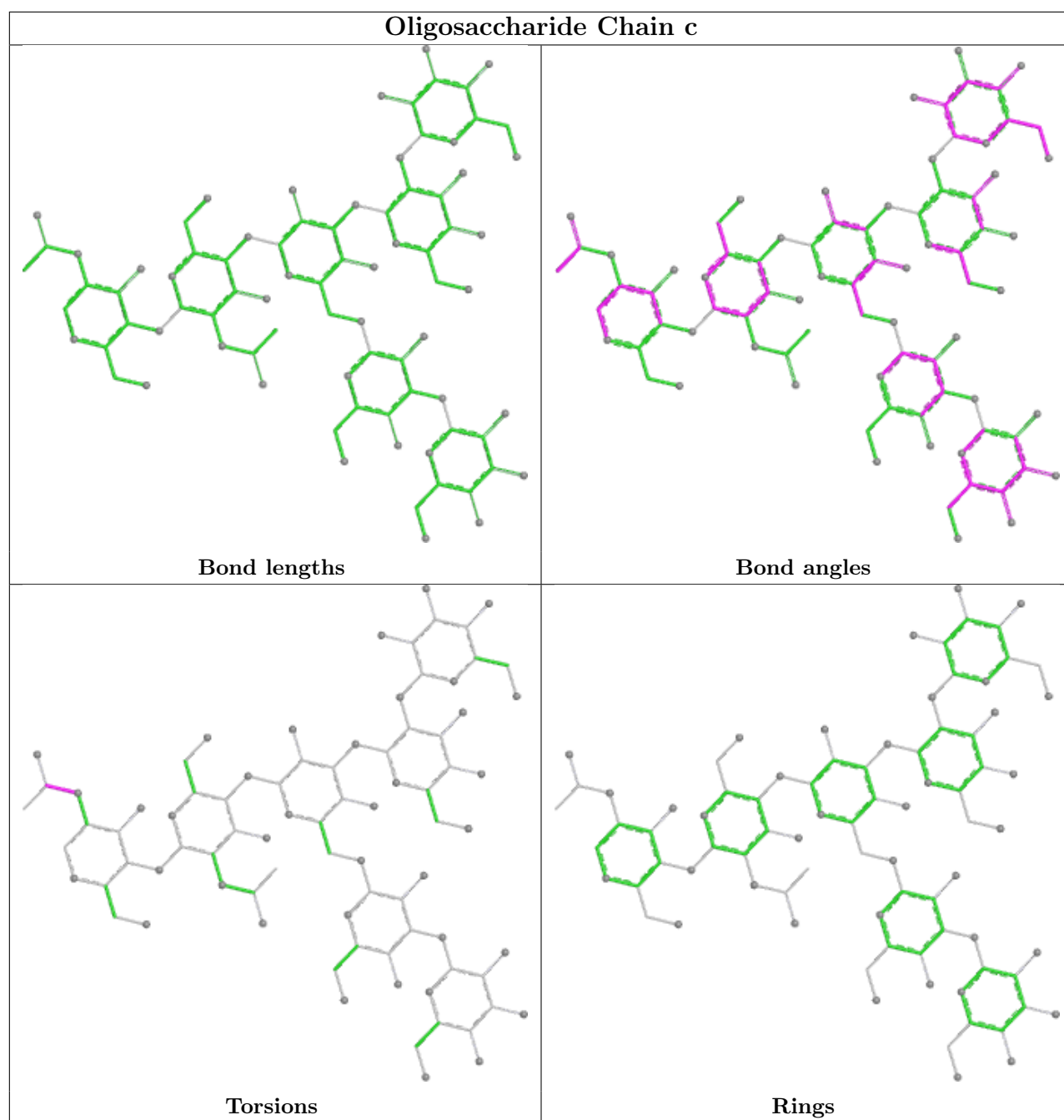


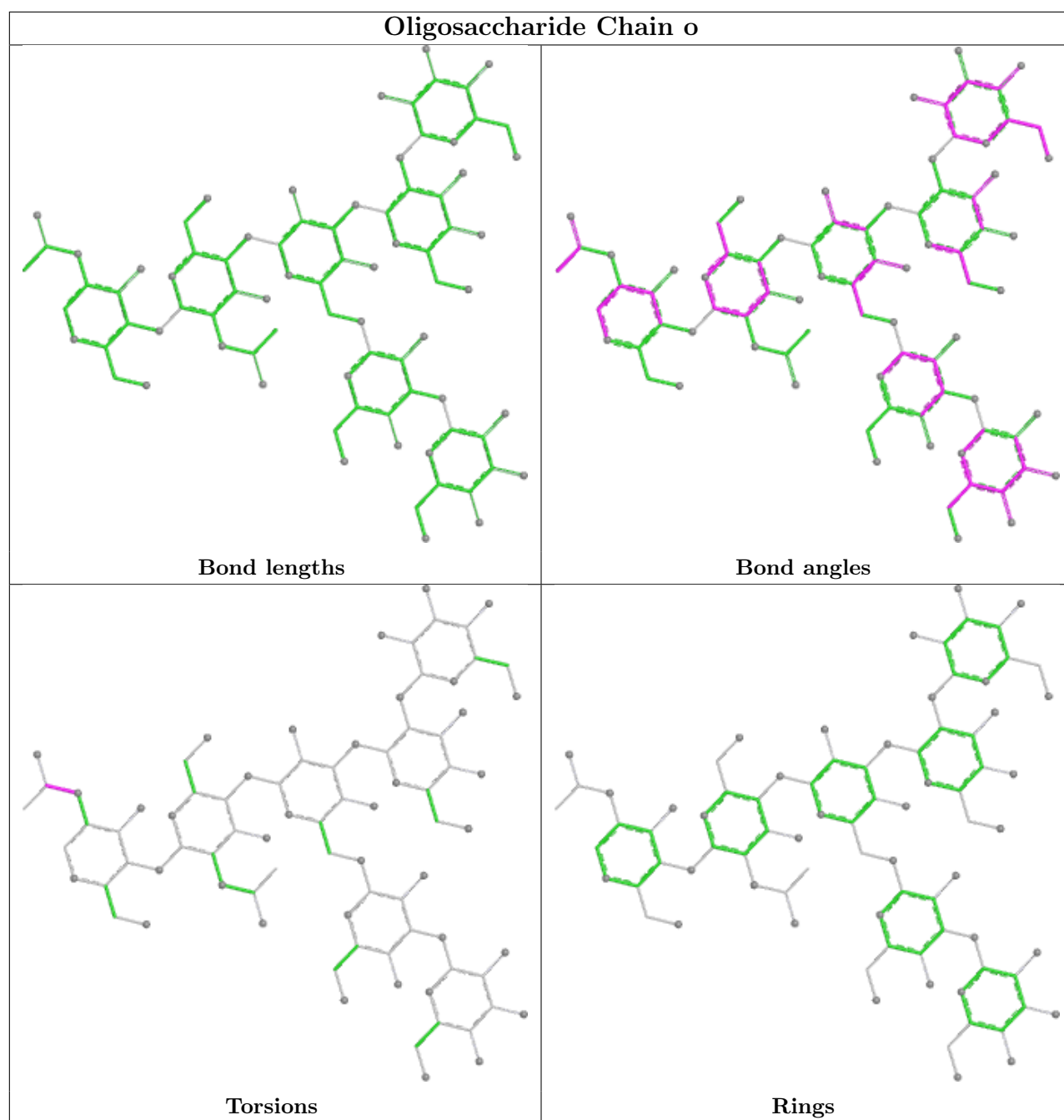


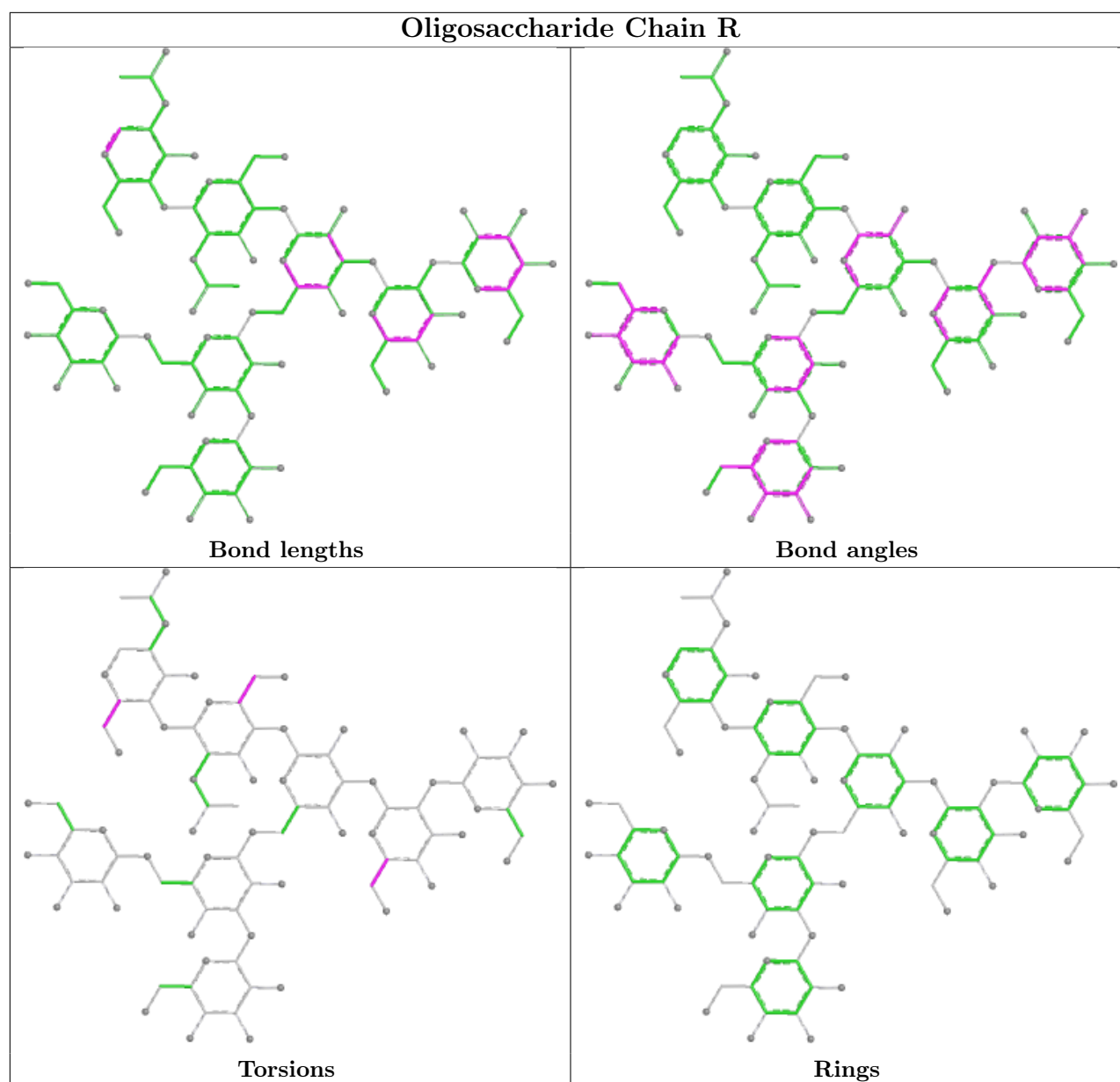


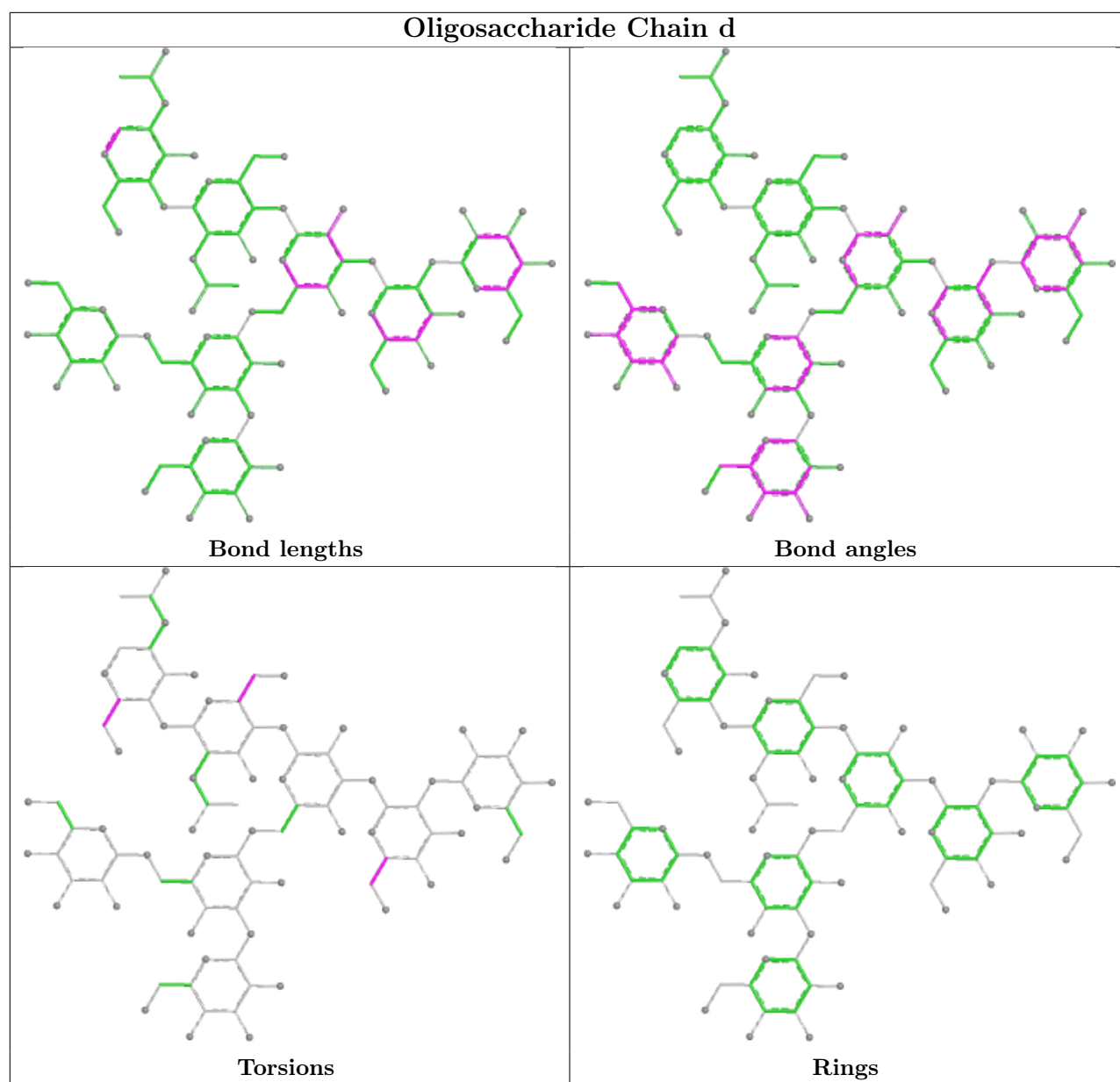


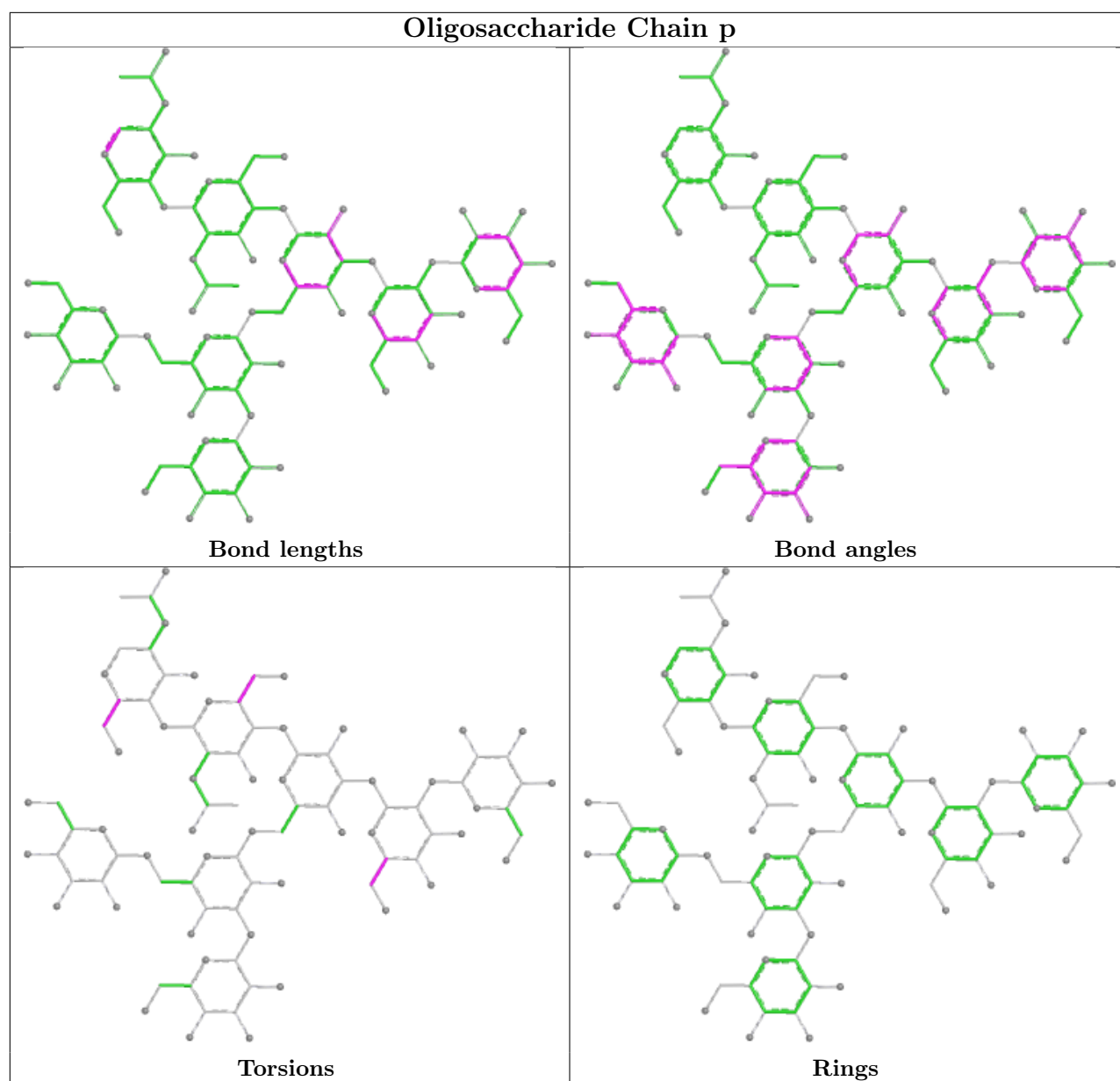


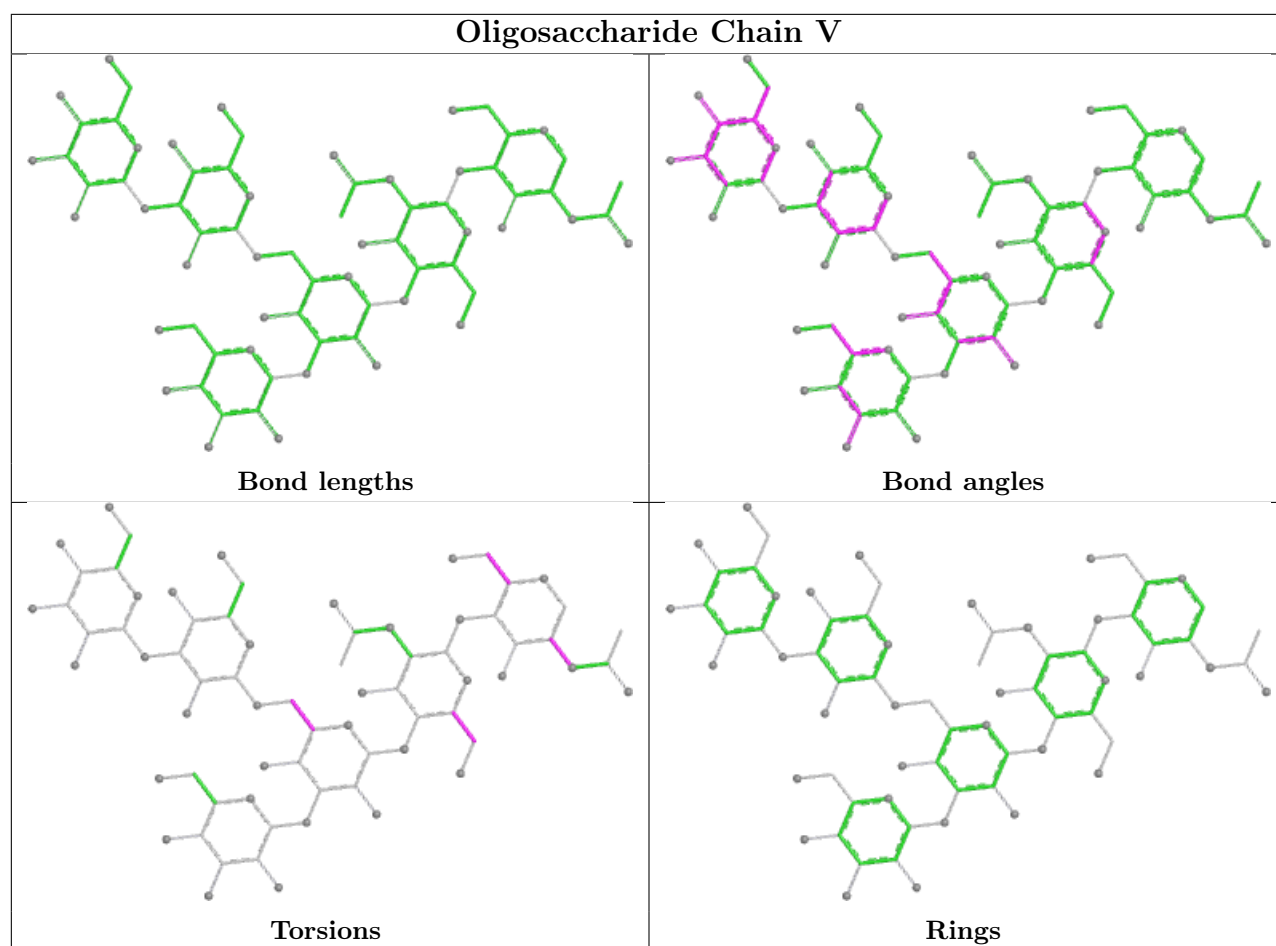


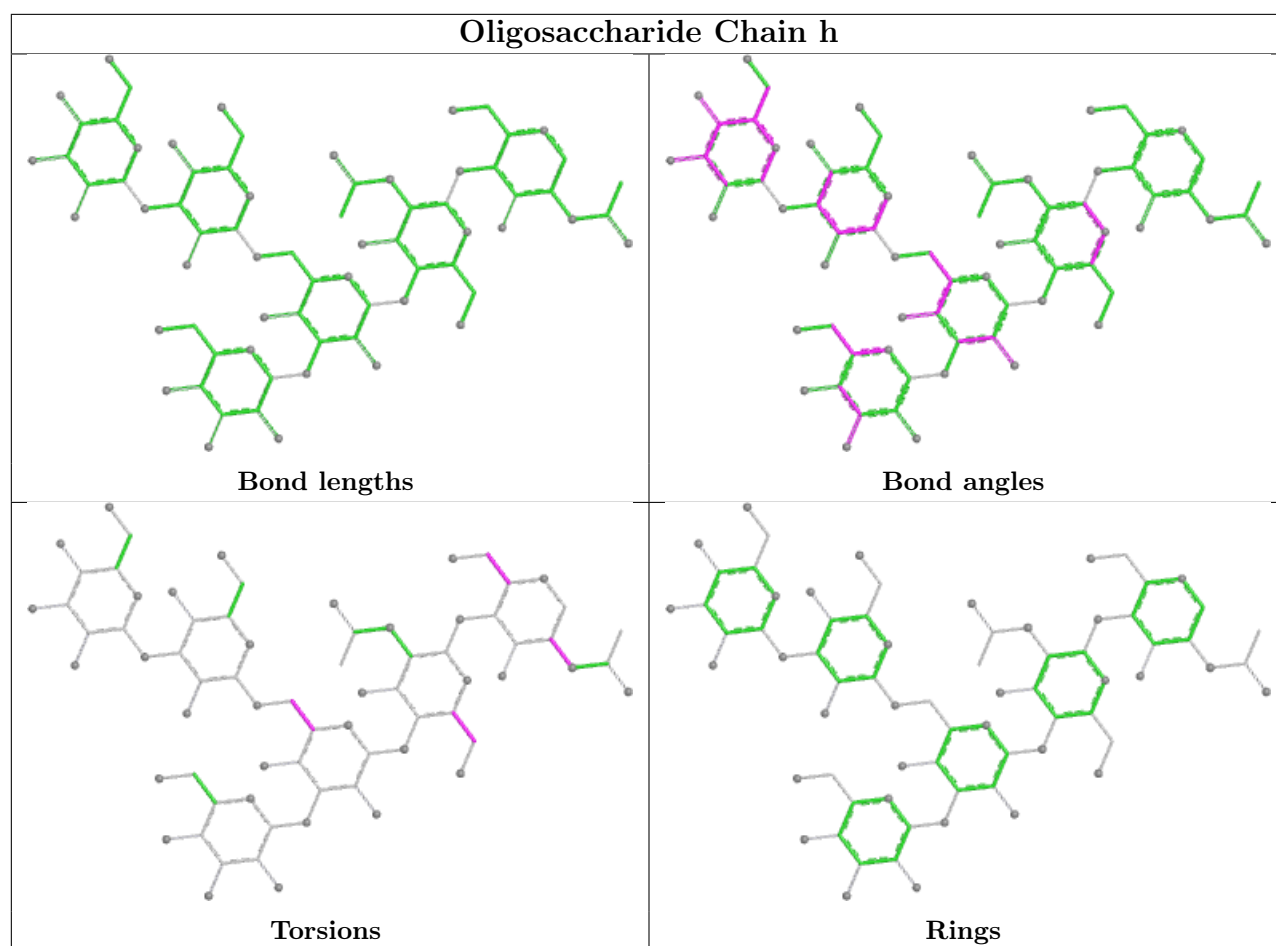


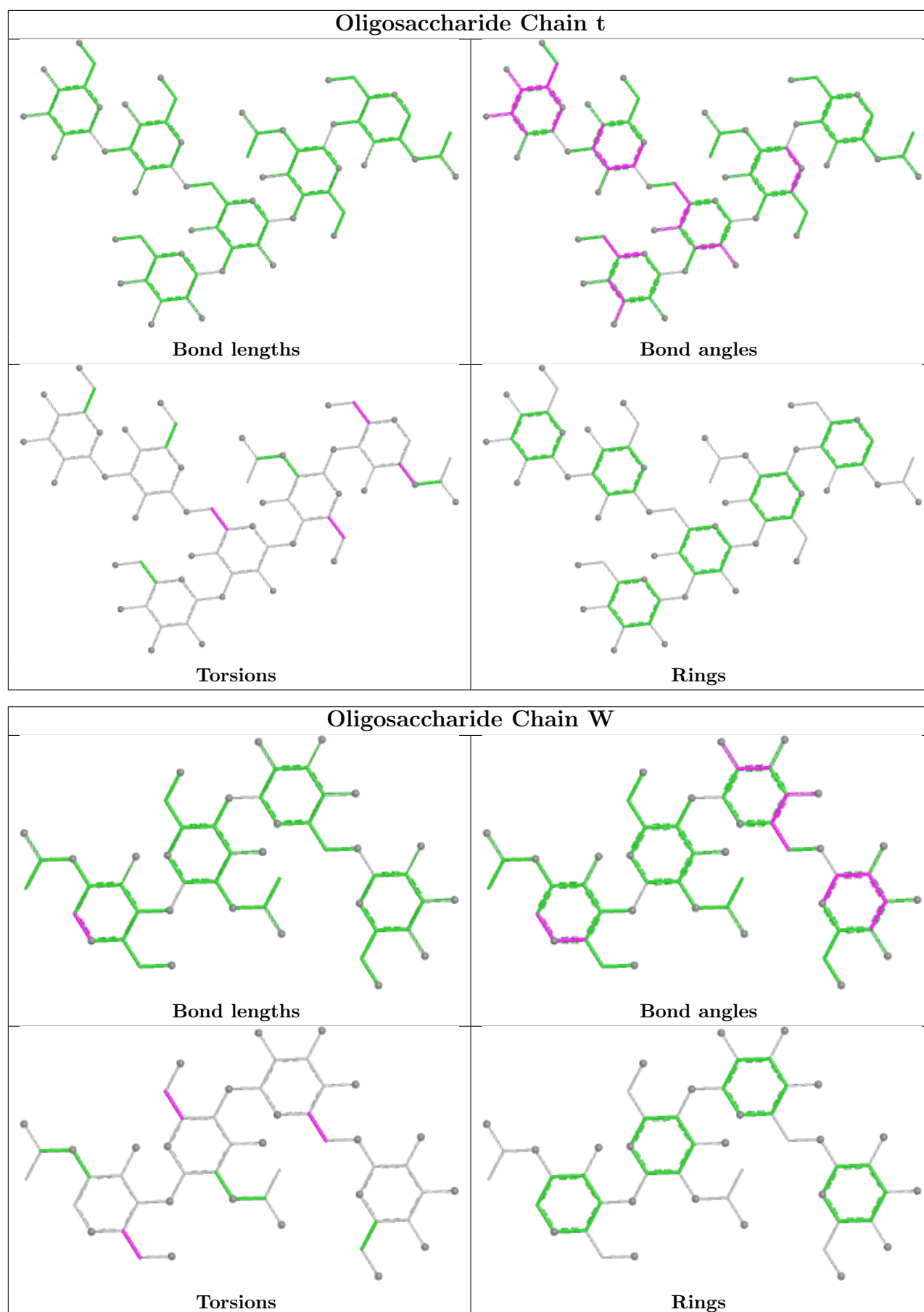


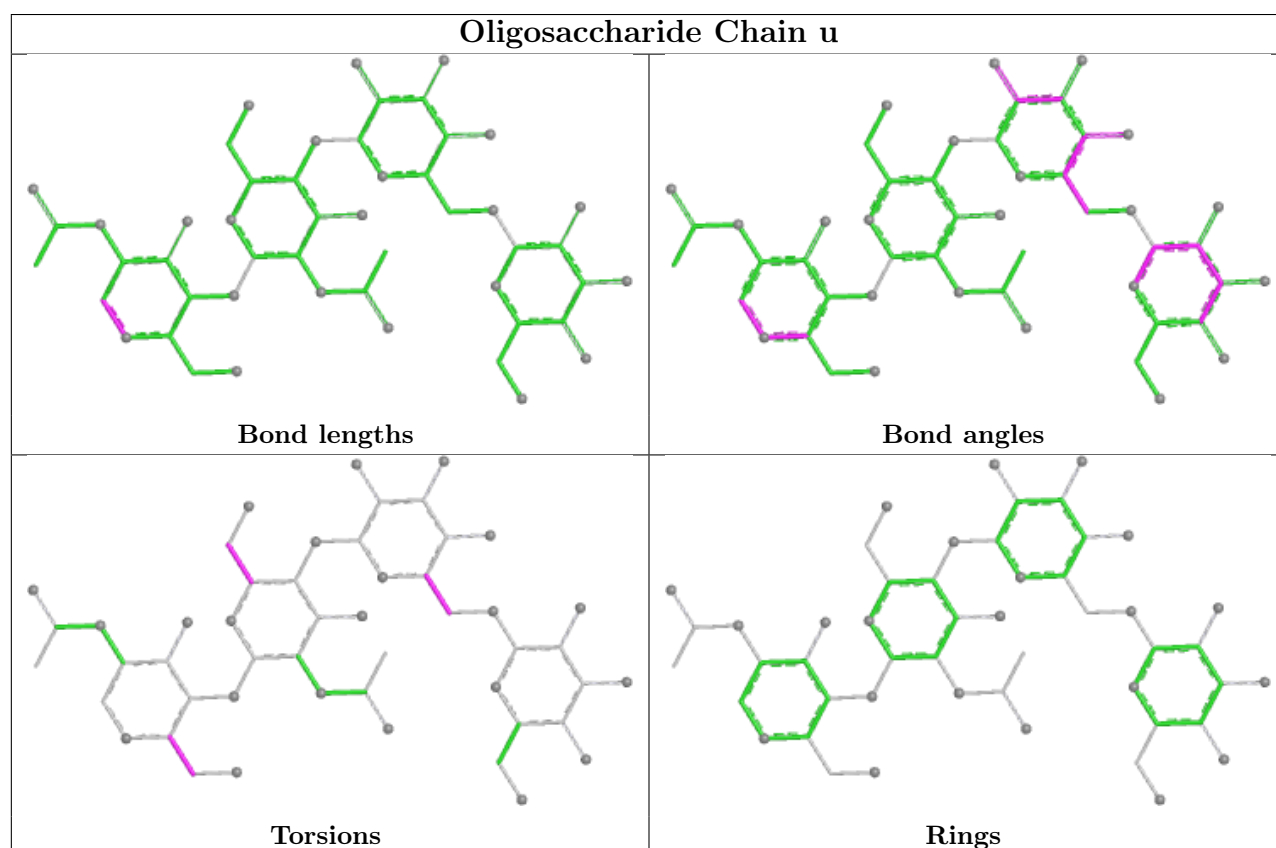
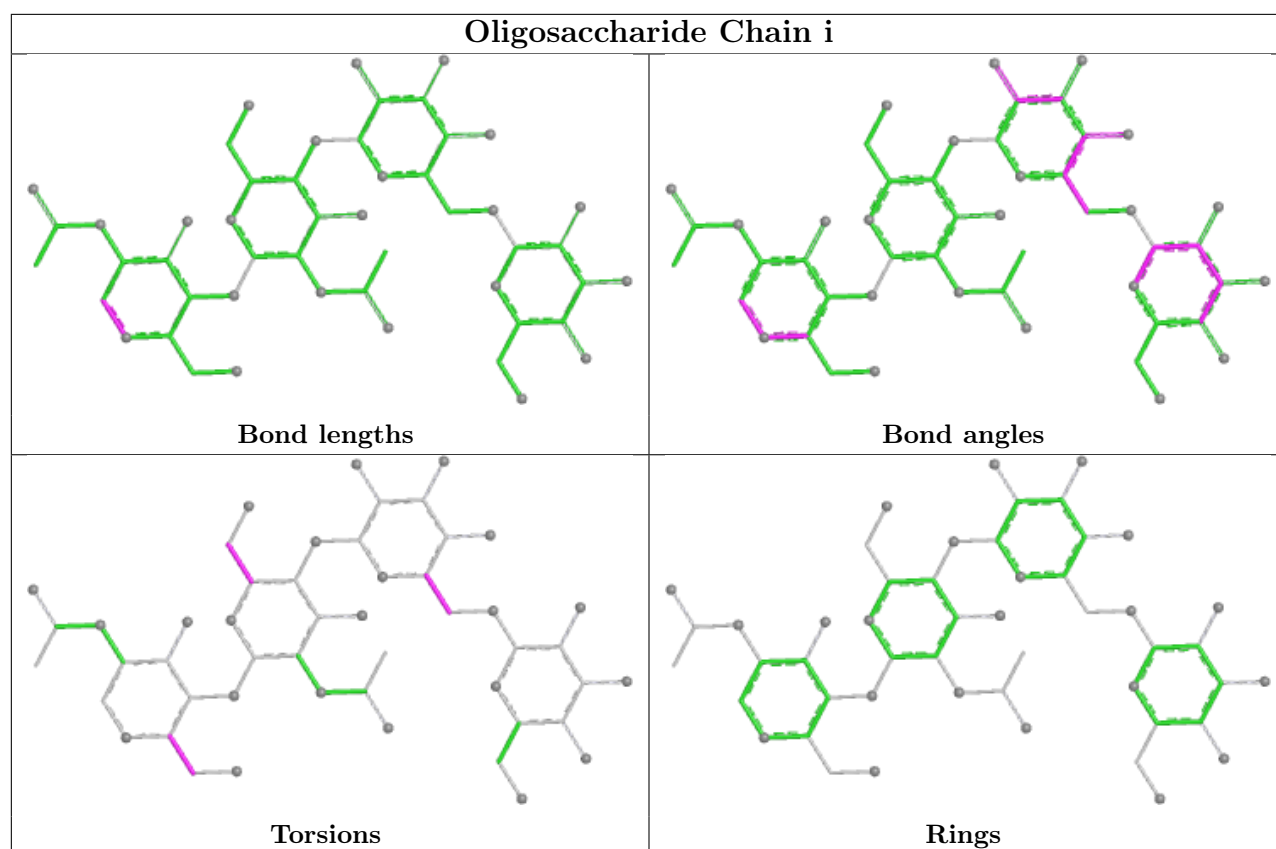












5.6 Ligand geometry

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	B	701	2	14,14,15	0.36	0	17,19,21	0.62	0
11	NAG	G	645	1	14,14,15	0.46	0	17,19,21	0.56	0
11	NAG	F	604	1	14,14,15	0.40	0	17,19,21	0.65	1 (5%)
11	NAG	A	645	1	14,14,15	0.47	0	17,19,21	0.55	0
11	NAG	F	634	1	14,14,15	0.32	0	17,19,21	0.41	0
11	NAG	G	633	1	14,14,15	0.34	0	17,19,21	0.41	0
11	NAG	F	645	1	14,14,15	0.47	0	17,19,21	0.56	0
11	NAG	G	604	1	14,14,15	0.42	0	17,19,21	0.65	1 (5%)
11	NAG	A	633	1	14,14,15	0.32	0	17,19,21	0.40	0
11	NAG	J	702	2	14,14,15	0.53	0	17,19,21	0.53	0
11	NAG	A	604	1	14,14,15	0.41	0	17,19,21	0.66	1 (5%)
11	NAG	G	611	1	14,14,15	0.54	0	17,19,21	0.52	0
11	NAG	I	702	2	14,14,15	0.53	0	17,19,21	0.54	0
11	NAG	F	631	1	14,14,15	0.50	0	17,19,21	0.41	0
11	NAG	J	701	2	14,14,15	0.36	0	17,19,21	0.61	0
11	NAG	A	634	1	14,14,15	0.51	0	17,19,21	0.41	0
11	NAG	B	702	2	14,14,15	0.52	0	17,19,21	0.53	0
11	NAG	A	611	1	14,14,15	0.53	0	17,19,21	0.52	0
11	NAG	G	634	1	14,14,15	0.50	0	17,19,21	0.42	0
11	NAG	I	701	2	14,14,15	0.35	0	17,19,21	0.62	0
11	NAG	F	611	1	14,14,15	0.53	0	17,19,21	0.51	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
11	NAG	B	701	2	-	3/6/23/26	0/1/1/1
11	NAG	G	645	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	F	604	1	-	2/6/23/26	0/1/1/1
11	NAG	A	645	1	-	0/6/23/26	0/1/1/1
11	NAG	F	634	1	-	2/6/23/26	0/1/1/1
11	NAG	G	633	1	-	2/6/23/26	0/1/1/1
11	NAG	F	645	1	-	0/6/23/26	0/1/1/1
11	NAG	G	604	1	-	2/6/23/26	0/1/1/1
11	NAG	A	633	1	-	2/6/23/26	0/1/1/1
11	NAG	J	702	2	-	2/6/23/26	0/1/1/1
11	NAG	A	604	1	-	2/6/23/26	0/1/1/1
11	NAG	G	611	1	-	2/6/23/26	0/1/1/1
11	NAG	I	702	2	-	2/6/23/26	0/1/1/1
11	NAG	F	631	1	-	2/6/23/26	0/1/1/1
11	NAG	J	701	2	-	3/6/23/26	0/1/1/1
11	NAG	A	634	1	-	2/6/23/26	0/1/1/1
11	NAG	B	702	2	-	2/6/23/26	0/1/1/1
11	NAG	A	611	1	-	2/6/23/26	0/1/1/1
11	NAG	G	634	1	-	2/6/23/26	0/1/1/1
11	NAG	I	701	2	-	3/6/23/26	0/1/1/1
11	NAG	F	611	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	604	NAG	C1-O5-C5	2.08	114.98	112.19
11	F	604	NAG	C1-O5-C5	2.06	114.95	112.19
11	G	604	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	633	NAG	O5-C5-C6-O6
11	A	634	NAG	O5-C5-C6-O6
11	F	631	NAG	O5-C5-C6-O6
11	F	634	NAG	O5-C5-C6-O6
11	G	633	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	G	634	NAG	O5-C5-C6-O6
11	B	701	NAG	O5-C5-C6-O6
11	B	702	NAG	O5-C5-C6-O6
11	I	702	NAG	O5-C5-C6-O6
11	J	702	NAG	O5-C5-C6-O6
11	I	701	NAG	O5-C5-C6-O6
11	J	701	NAG	O5-C5-C6-O6
11	A	634	NAG	C4-C5-C6-O6
11	F	631	NAG	C4-C5-C6-O6
11	G	634	NAG	C4-C5-C6-O6
11	B	701	NAG	C4-C5-C6-O6
11	I	701	NAG	C4-C5-C6-O6
11	J	701	NAG	C4-C5-C6-O6
11	A	604	NAG	O5-C5-C6-O6
11	F	604	NAG	O5-C5-C6-O6
11	G	604	NAG	O5-C5-C6-O6
11	A	611	NAG	O5-C5-C6-O6
11	F	611	NAG	O5-C5-C6-O6
11	G	611	NAG	O5-C5-C6-O6
11	A	633	NAG	C4-C5-C6-O6
11	F	634	NAG	C4-C5-C6-O6
11	G	633	NAG	C4-C5-C6-O6
11	B	702	NAG	C4-C5-C6-O6
11	I	702	NAG	C4-C5-C6-O6
11	J	702	NAG	C4-C5-C6-O6
11	G	611	NAG	C4-C5-C6-O6
11	A	611	NAG	C4-C5-C6-O6
11	F	611	NAG	C4-C5-C6-O6
11	A	604	NAG	C4-C5-C6-O6
11	F	604	NAG	C4-C5-C6-O6
11	G	604	NAG	C4-C5-C6-O6
11	B	701	NAG	C1-C2-N2-C7
11	I	701	NAG	C1-C2-N2-C7
11	J	701	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	701	NAG	1	0
11	J	702	NAG	5	0
11	I	702	NAG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	J	701	NAG	1	0
11	B	702	NAG	5	0
11	I	701	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

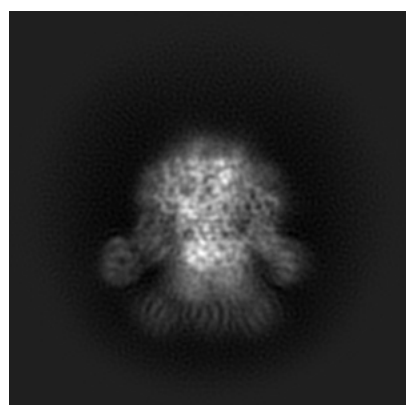
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7896. These allow visual inspection of the internal detail of the map and identification of artifacts.

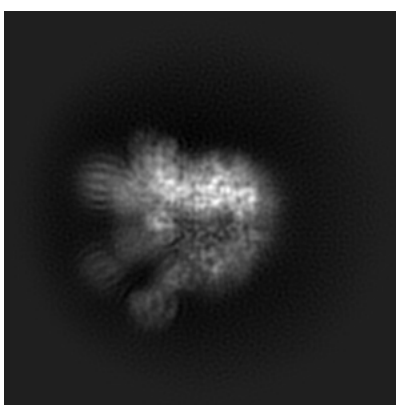
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

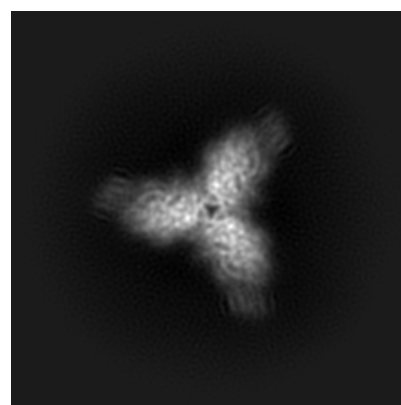
6.1.1 Primary map



X



Y

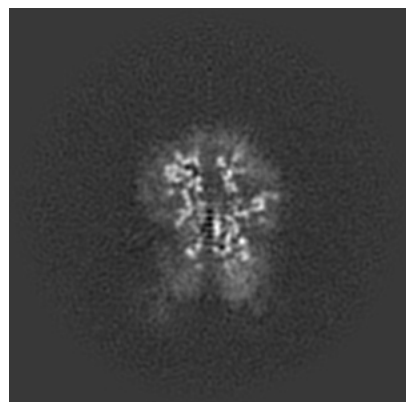


Z

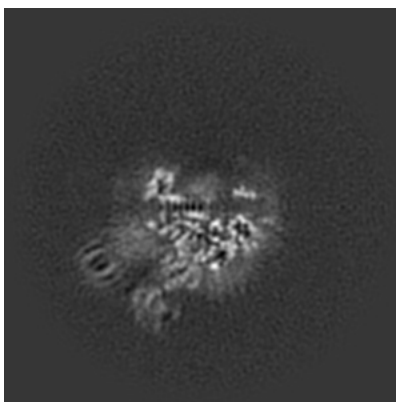
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

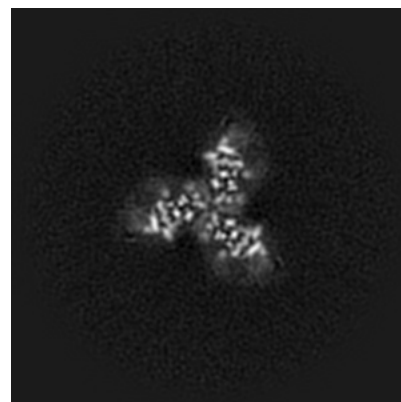
6.2.1 Primary map



X Index: 150



Y Index: 150

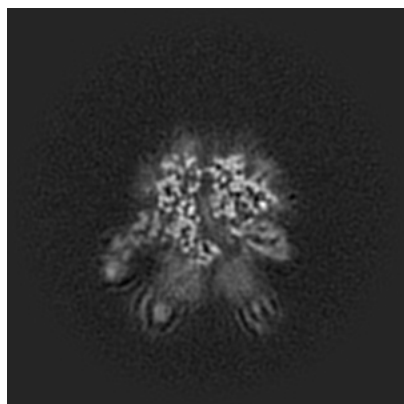


Z Index: 150

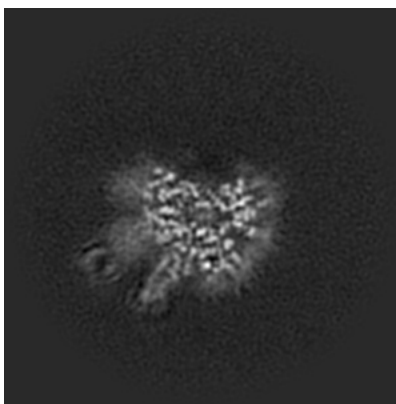
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

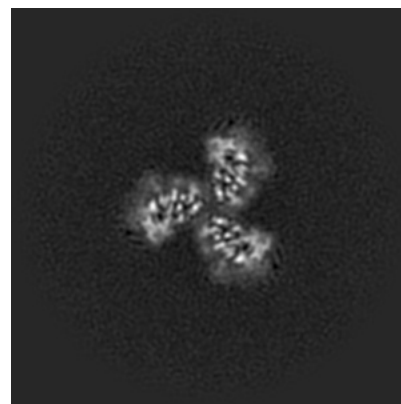
6.3.1 Primary map



X Index: 165



Y Index: 142

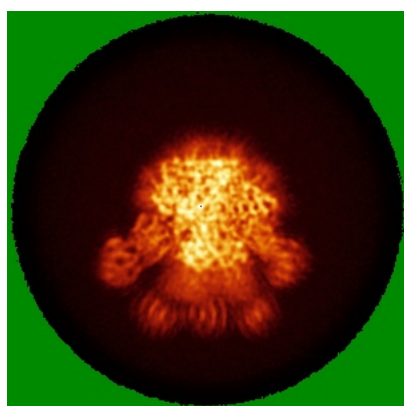


Z Index: 158

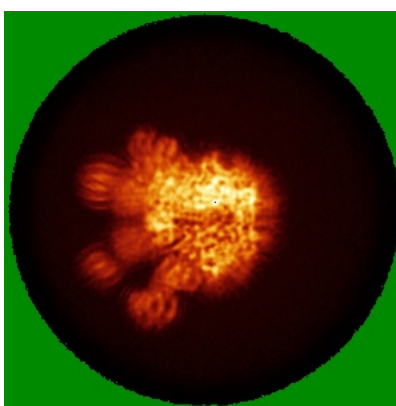
The images above show the largest variance slices of the map in three orthogonal directions.

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

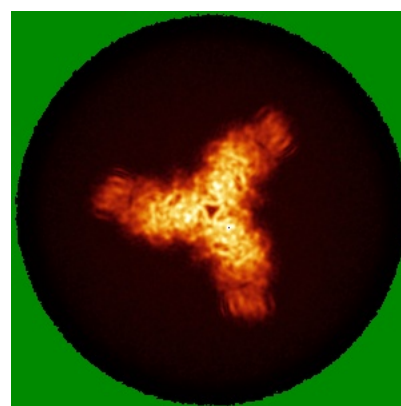
6.4.1 Primary map



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

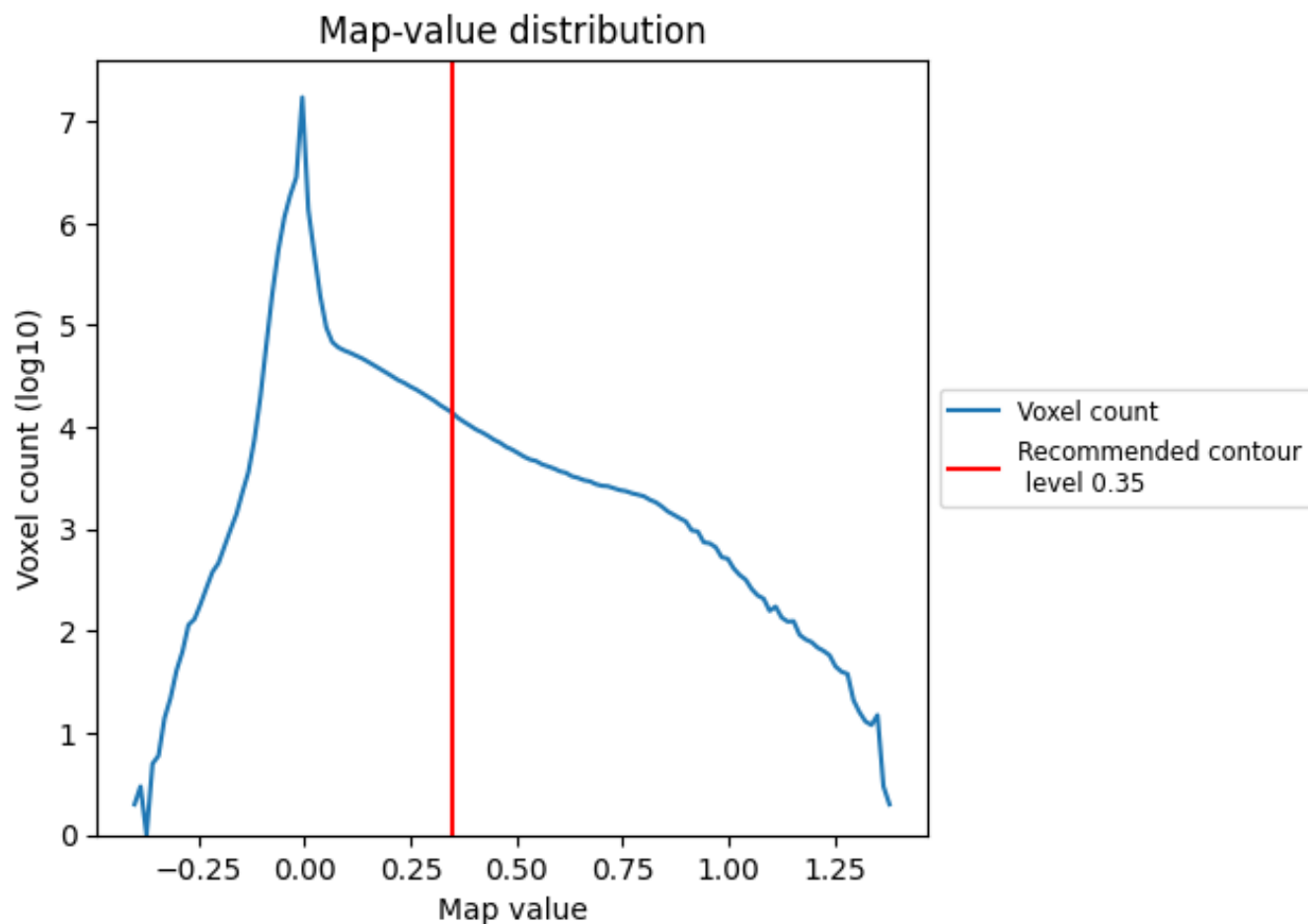
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

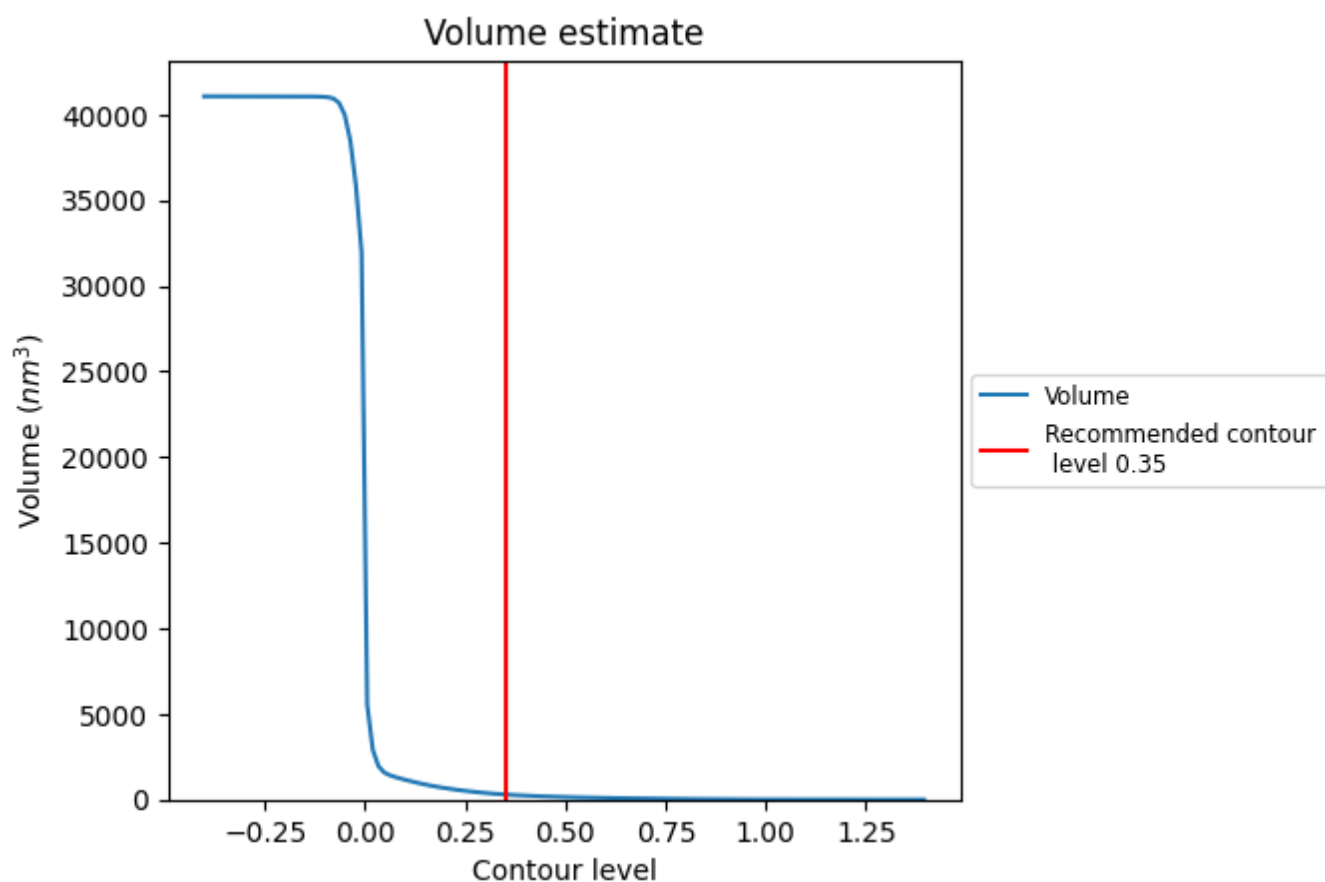
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

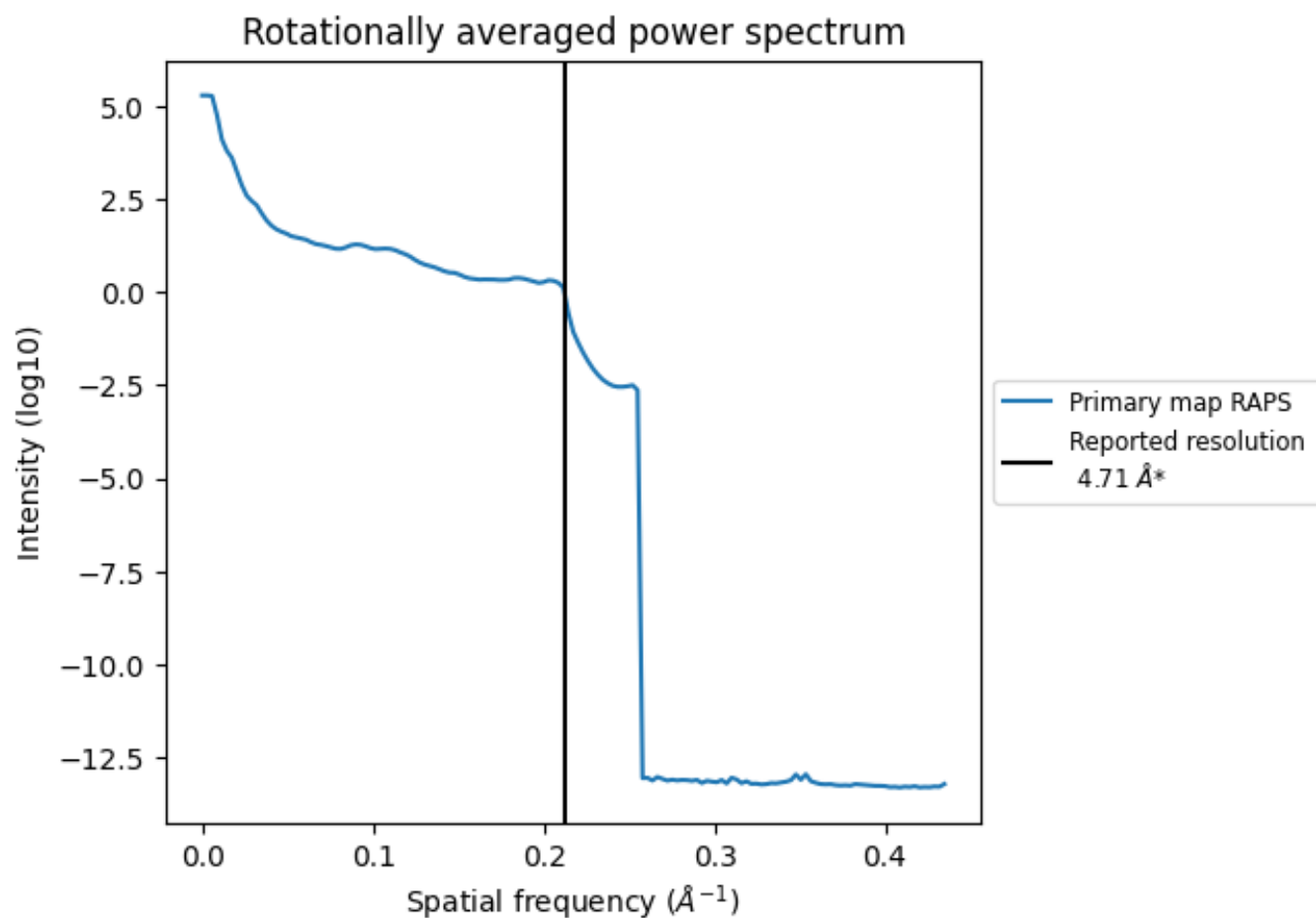
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 293 nm³; this corresponds to an approximate mass of 265 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 0.212 Å⁻¹

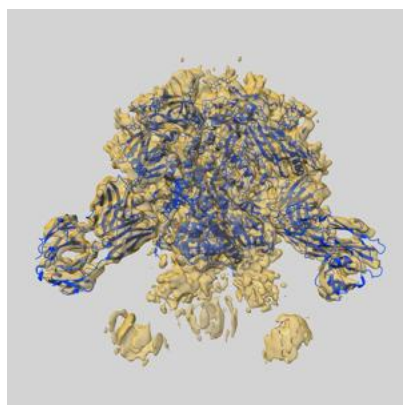
8 Fourier-Shell correlation ⓘ

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

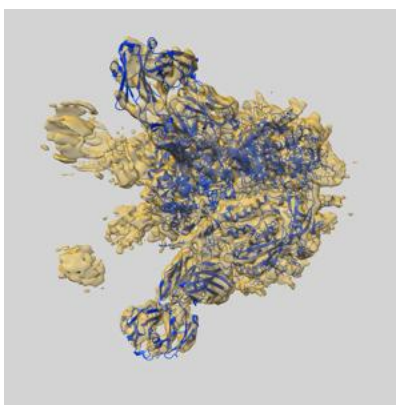
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7896 and PDB model 6DID. Per-residue inclusion information can be found in section [3](#) on page [12](#).

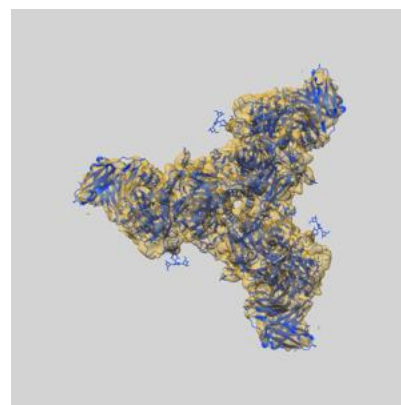
9.1 Map-model overlay [i](#)



X



Y



Z

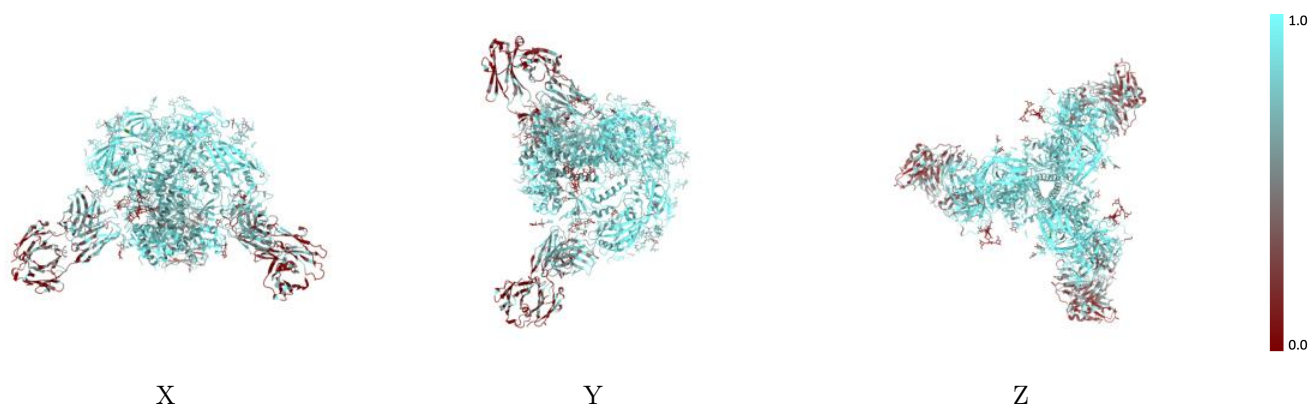
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



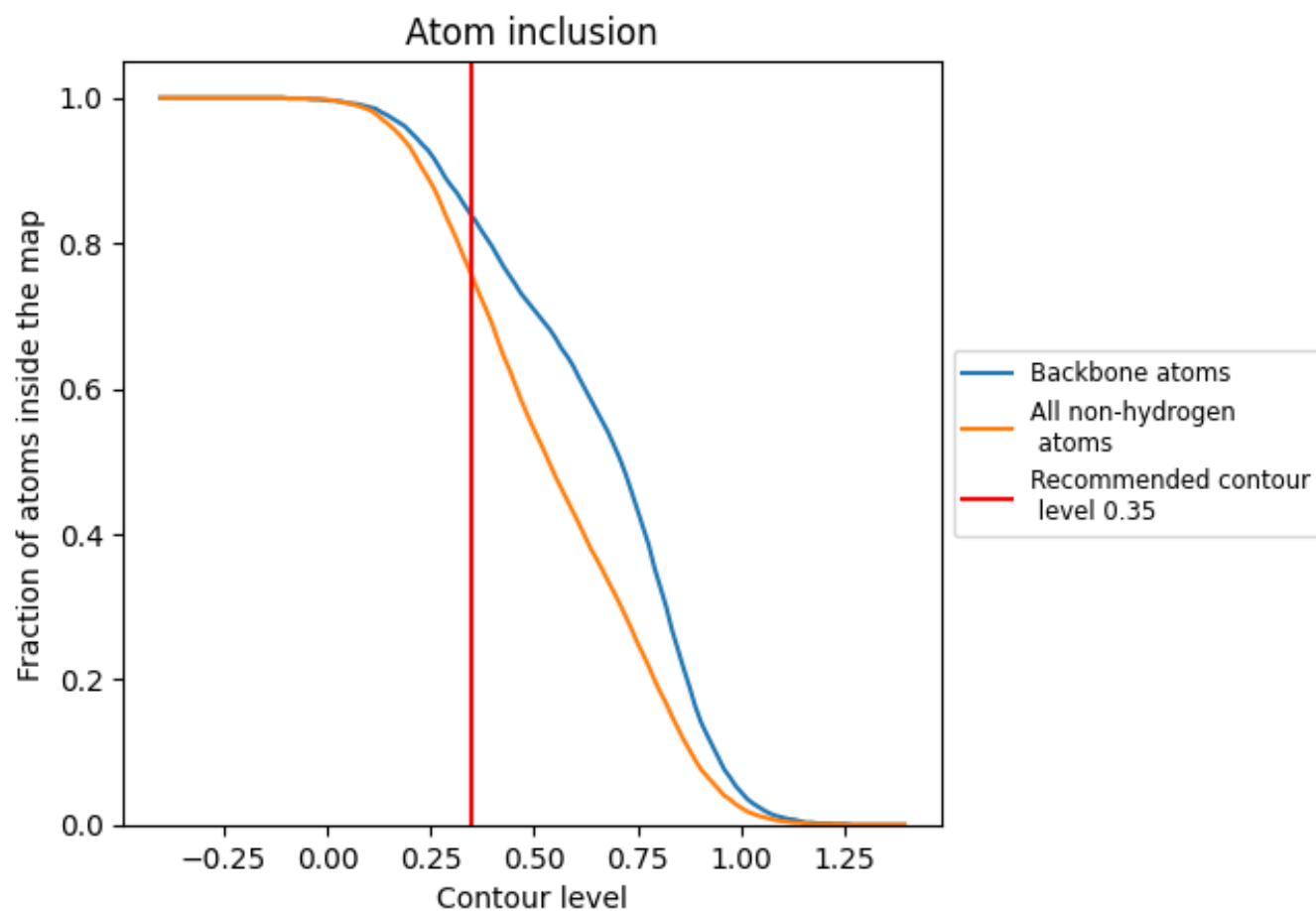
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7550	 0.2300
A	 0.8750	 0.3010
B	 0.8220	 0.2410
C	 0.4730	 0.1480
D	 0.4810	 0.1490
E	 0.4750	 0.1490
F	 0.8770	 0.3000
G	 0.8750	 0.3020
H	 0.4700	 0.1480
I	 0.8210	 0.2400
J	 0.8240	 0.2410
K	 0.4800	 0.1490
L	 0.4800	 0.1500
M	 0.3590	 0.1250
N	 0.8570	 0.3220
O	 0.7500	 0.3410
P	 0.8210	 0.3590
Q	 0.7590	 0.3320
R	 0.0000	 0.0070
S	 0.7860	 0.3000
T	 0.6070	 0.2720
U	 0.7860	 0.2600
V	 0.6810	 0.1890
W	 0.6600	 0.2010
X	 0.6790	 0.3210
Y	 0.3850	 0.1360
Z	 0.8570	 0.3210
a	 0.7860	 0.3220
b	 0.8210	 0.3660
c	 0.7590	 0.3340
d	 0.0000	 -0.0090
e	 0.7860	 0.2920
f	 0.6070	 0.2790
g	 0.7860	 0.2710
h	 0.6810	 0.1820



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Chain	Atom inclusion	Q-score
i	 0.6400	 0.1810
j	 0.7140	 0.2930
k	 0.3850	 0.1260
l	 0.8570	 0.3310
m	 0.7500	 0.3250
n	 0.8210	 0.3740
o	 0.7590	 0.3370
p	 0.0000	 -0.0000
q	 0.7860	 0.3090
r	 0.6070	 0.2750
s	 0.7860	 0.2840
t	 0.6810	 0.1810
u	 0.6400	 0.1880
v	 0.6790	 0.3220