



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 12:59 AM UTC

PDB ID : 6MPH / pdb_00006mph
EMDB ID : EMD-9189
Title : Cryo-EM structure at 3.8 Å resolution of HIV-1 fusion peptide-directed antibody, DF1W-a.01, elicited by vaccination of Rhesus macaques, in complex with stabilized HIV-1 Env BG505 DS-SOSIP, which was also bound to antibodies VRC03 and PGT122
Authors : Acharya, P.; Xu, K.; Kwong, P.D.
Deposited on : 2018-10-06
Resolution : 3.80 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:

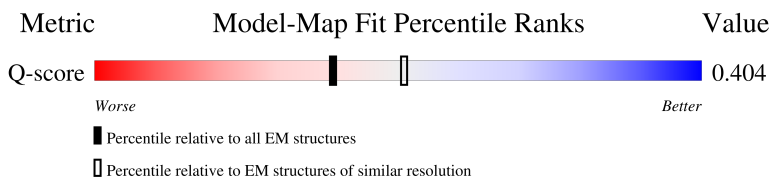
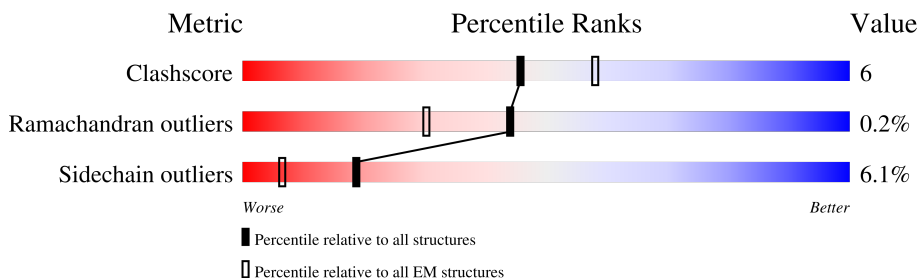
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	1	118	
1	3	118	
1	H	118	
2	2	112	

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Mol	Chain	Length	Quality of chain
2	4	112	27% 78% 20%
2	L	112	25% 79% 19%
3	6	153	71% 13% 14%
3	D	153	70% 15% 14%
3	E	153	69% 16% 14%
4	A	473	77% 16% .
4	B	473	77% 17% .
4	C	473	78% 15% .
5	M	132	8% 78% 21%
5	X	132	8% 80% 20%
5	Y	132	8% 80% 19%
6	N	107	7% 79% 18%
6	Z	107	7% 80% 16%
6	a	107	11% 79% 17%
7	Q	227	50% 6% 43%
7	f	227	49% 7% 43%
7	g	227	48% 8% 43%
8	R	102	86% 14%
8	h	102	85% 15%
8	i	102	84% 16%
9	9	5	20% 20% 80%
9	F	5	100%
9	J	5	40% 60% 40%
9	W	5	20% 20% 80%
9	j	5	40% 60% 40%



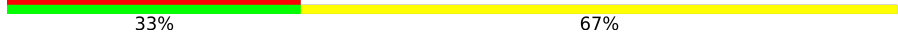
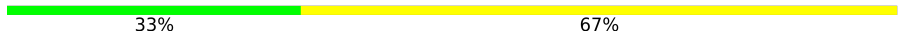


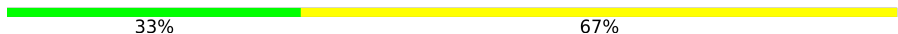
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Mol	Chain	Length	Quality of chain
9	r	5	20% 20% 80%
9	t	5	100%
9	w	5	40% 60% 40%
10	5	2	100%
10	7	2	50% 100%
10	G	2	50% 50%
10	O	2	100%
10	T	2	100%
10	U	2	50% 100%
10	d	2	50% 50%
10	l	2	100%
10	o	2	100%
10	p	2	50% 100%
10	u	2	50% 50%
10	y	2	100%
11	BA	4	50% 50%
11	CA	4	50% 50%
11	DA	4	50% 50%
11	I	4	25% 25% 75%
11	c	4	25% 75%
11	e	4	25% 25% 75%
11	v	4	25% 25% 75%
12	8	3	67% 33%
12	AA	3	67% 33% 67%
12	K	3	33% 33% 67%

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Mol	Chain	Length	Quality of chain
12	P	3	 33% 67%
12	V	3	 67% 33%
12	b	3	 33% 67%
12	k	3	 33% 67%
12	m	3	 33% 67%
12	q	3	 67% 33%
12	s	3	 33% 67%
12	x	3	 33% 67%
12	z	3	 33% 67%
13	0	6	 17% 33% 67%
13	S	6	 17% 33% 67%
13	n	6	 33% 67%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 32092 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DF1W-a.01 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	118	Total 915	C 588	N 154	O 171	S 2	0	0
1	3	118	Total 915	C 588	N 154	O 171	S 2	0	0
1	H	118	Total 915	C 588	N 154	O 171	S 2	0	0

- Molecule 2 is a protein called DF1W-a.01 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	112	Total 858	C 542	N 149	O 164	S 3	0	0
2	4	112	Total 858	C 542	N 149	O 164	S 3	0	0
2	L	112	Total 858	C 542	N 149	O 164	S 3	0	0

- Molecule 3 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	6	132	Total 1034	C 654	N 178	O 196	S 6	0	0
3	D	132	Total 1034	C 654	N 178	O 196	S 6	0	0
3	E	132	Total 1034	C 654	N 178	O 196	S 6	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	605	CYS	THR	conflict	UNP Q2N0S7
D	605	CYS	THR	conflict	UNP Q2N0S7
E	605	CYS	THR	conflict	UNP Q2N0S7

- Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	453	3564	2233	630	671	30	0	0
4	B	453	3564	2233	630	671	30	0	0
4	C	453	3564	2233	630	671	30	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	CYS	ILE	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	433	CYS	ALA	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
B	201	CYS	ILE	conflict	UNP Q2N0S6
B	332	ASN	THR	conflict	UNP Q2N0S6
B	433	CYS	ALA	conflict	UNP Q2N0S6
B	501	CYS	ALA	conflict	UNP Q2N0S6
C	201	CYS	ILE	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	433	CYS	ALA	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 5 is a protein called PGT122 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	132	1047	669	180	195	3	0	0
5	X	132	1047	669	180	195	3	0	0
5	Y	132	1047	669	180	195	3	0	0

- Molecule 6 is a protein called PGT122 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	103	787	491	137	157	2	0	0
6	Z	103	787	491	137	157	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	a	103	787	491	137	157	2	0	0

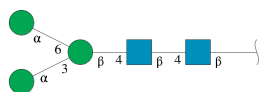
- Molecule 7 is a protein called VRC03 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Q	129	1029	660	176	187	6	0	0
7	f	129	1029	660	176	187	6	0	0
7	g	129	1029	660	176	187	6	0	0

- Molecule 8 is a protein called VRC03 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	R	102	802	510	137	152	3	0	0
8	h	102	802	510	137	152	3	0	0
8	i	102	802	510	137	152	3	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	F	5	61	34	2	25	0	0
9	J	5	61	34	2	25	0	0
9	W	5	61	34	2	25	0	0
9	j	5	61	34	2	25	0	0
9	r	5	61	34	2	25	0	0

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

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



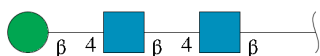
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	G	2	28	16	2	10	0	0
10	O	2	28	16	2	10	0	0
10	T	2	28	16	2	10	0	0
10	U	2	28	16	2	10	0	0
10	d	2	28	16	2	10	0	0
10	l	2	28	16	2	10	0	0
10	o	2	28	16	2	10	0	0
10	p	2	28	16	2	10	0	0
10	u	2	28	16	2	10	0	0
10	y	2	28	16	2	10	0	0
10	5	2	28	16	2	10	0	0
10	7	2	28	16	2	10	0	0

- Molecule 11 is an oligosaccharide called 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
11	I	4	Total	C	N	O	0	0
			50	28	2	20		
11	c	4	Total	C	N	O	0	0
			50	28	2	20		
11	e	4	Total	C	N	O	0	0
			50	28	2	20		
11	v	4	Total	C	N	O	0	0
			50	28	2	20		
11	BA	4	Total	C	N	O	0	0
			50	28	2	20		
11	CA	4	Total	C	N	O	0	0
			50	28	2	20		
11	DA	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 12 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.



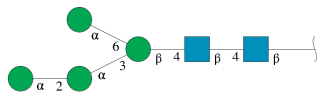
Mol	Chain	Residues	Atoms				AltConf	Trace
12	K	3	Total	C	N	O	0	0
			39	22	2	15		
12	P	3	Total	C	N	O	0	0
			39	22	2	15		
12	V	3	Total	C	N	O	0	0
			39	22	2	15		
12	b	3	Total	C	N	O	0	0
			39	22	2	15		
12	k	3	Total	C	N	O	0	0
			39	22	2	15		
12	m	3	Total	C	N	O	0	0
			39	22	2	15		
12	q	3	Total	C	N	O	0	0
			39	22	2	15		
12	s	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	x	3	Total 39	C 22	N 2	O 15	0	0
12	z	3	Total 39	C 22	N 2	O 15	0	0
12	8	3	Total 39	C 22	N 2	O 15	0	0
12	AA	3	Total 39	C 22	N 2	O 15	0	0

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
			Total	C	N	O		
13	S	6	Total 72	C 40	N 2	O 30	0	0
13	n	6	Total 72	C 40	N 2	O 30	0	0
13	0	6	Total 72	C 40	N 2	O 30	0	0

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

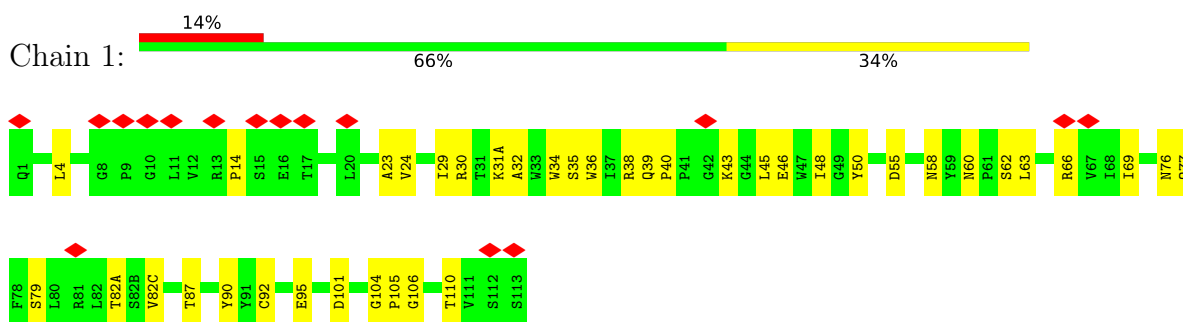


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
14	6	1	Total 14	8	1	5	0
14	A	1	Total 14	8	1	5	0
14	A	1	Total 14	8	1	5	0
14	B	1	Total 14	8	1	5	0
14	B	1	Total 14	8	1	5	0
14	C	1	Total 14	8	1	5	0
14	C	1	Total 14	8	1	5	0
14	D	1	Total 14	8	1	5	0
14	E	1	Total 14	8	1	5	0

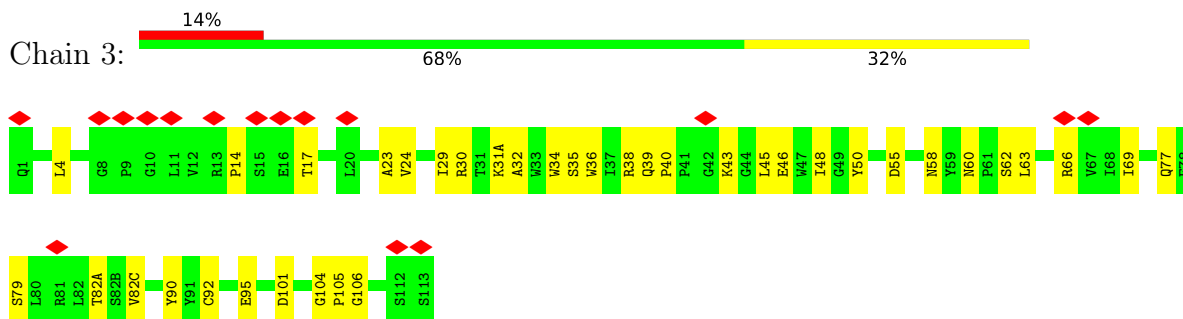
3 Residue-property plots [i](#)

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.

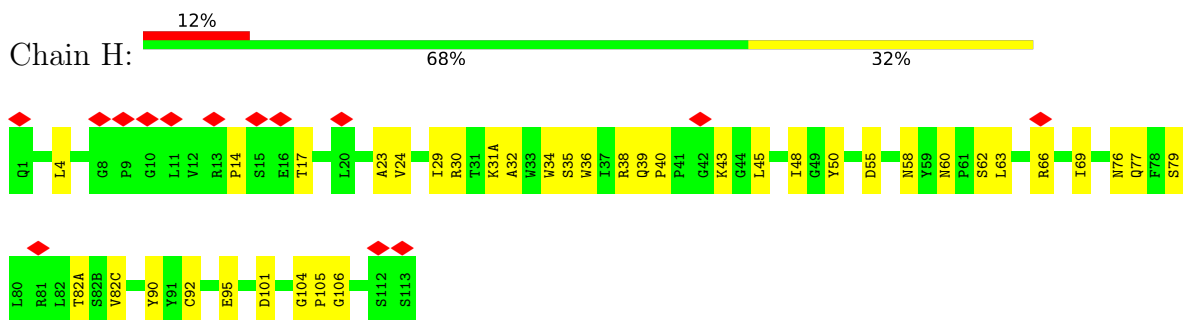
- Molecule 1: DF1W-a.01 heavy chain



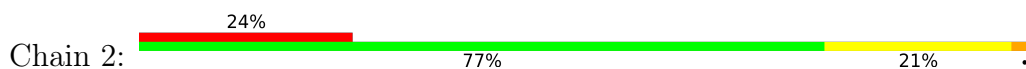
- Molecule 1: DF1W-a.01 heavy chain

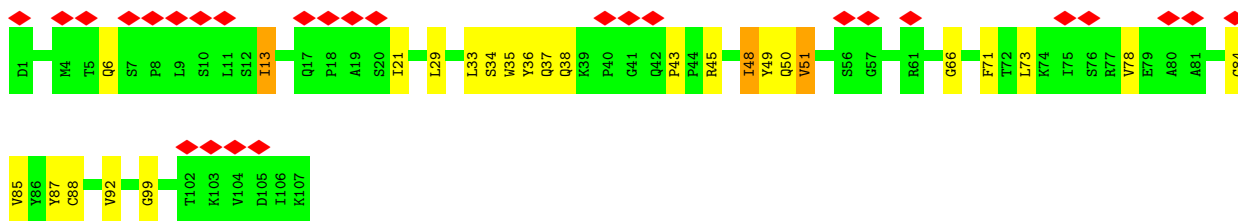


- Molecule 1: DF1W-a.01 heavy chain

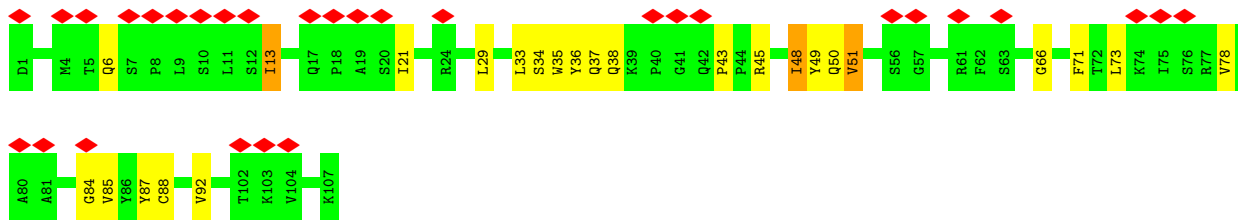
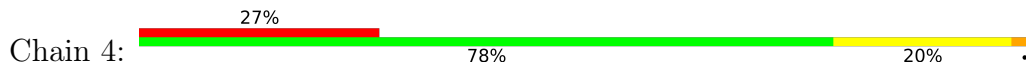


- Molecule 2: DF1W-a.01 Light chain

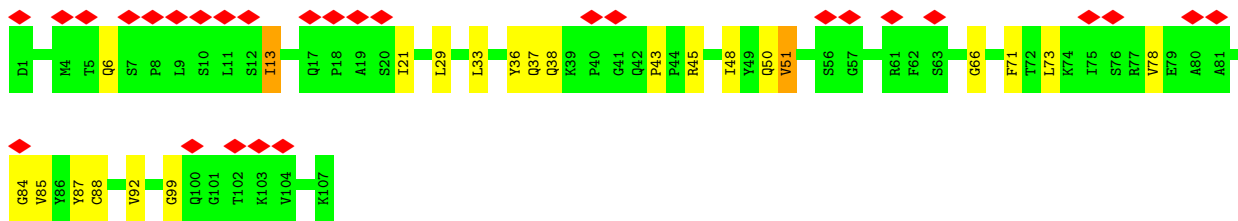
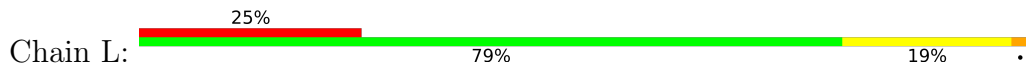




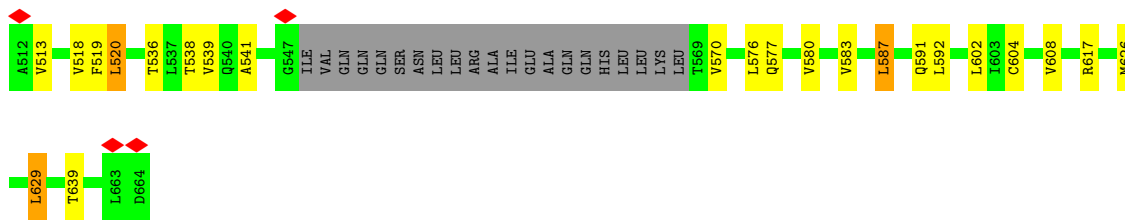
• Molecule 2: DF1W-a.01 Light chain



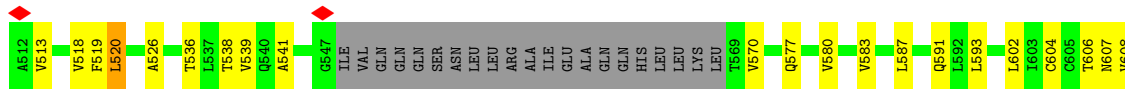
• Molecule 2: DF1W-a.01 Light chain

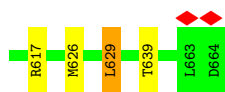


• Molecule 3: Envelope glycoprotein gp41

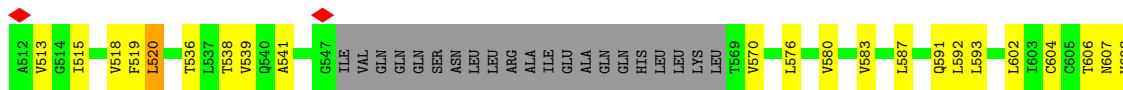


• Molecule 3: Envelope glycoprotein gp41

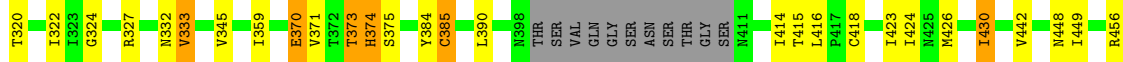
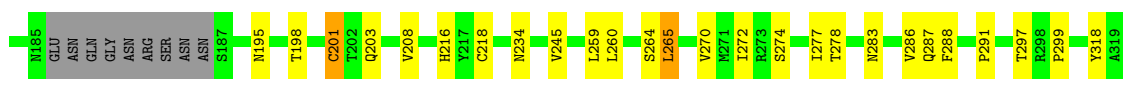
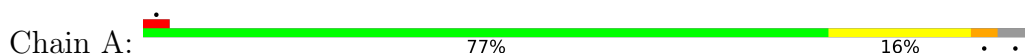




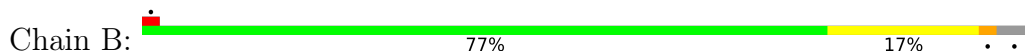
• Molecule 3: Envelope glycoprotein gp41



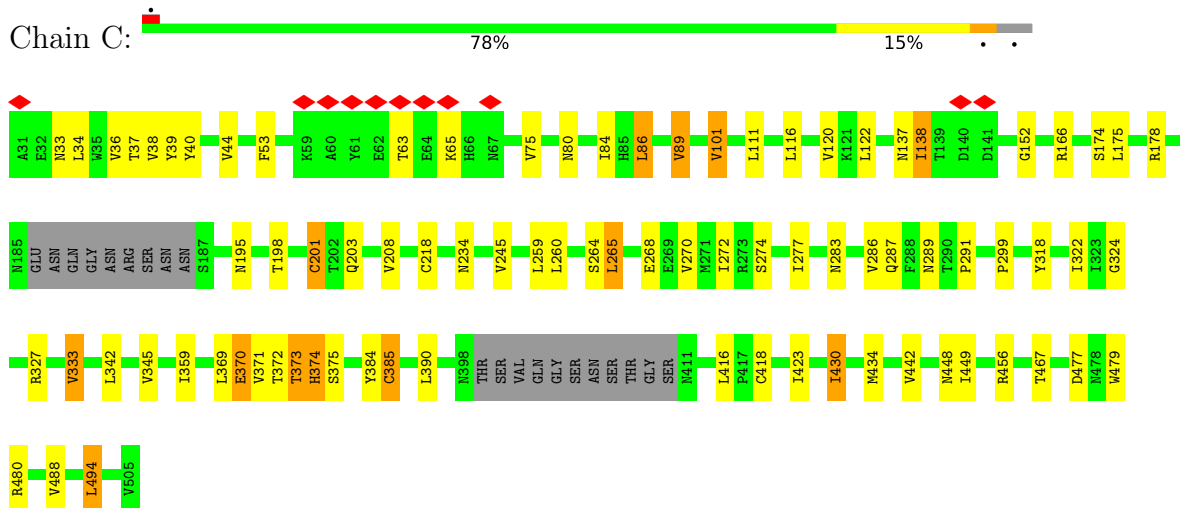
• Molecule 4: Envelope glycoprotein gp120



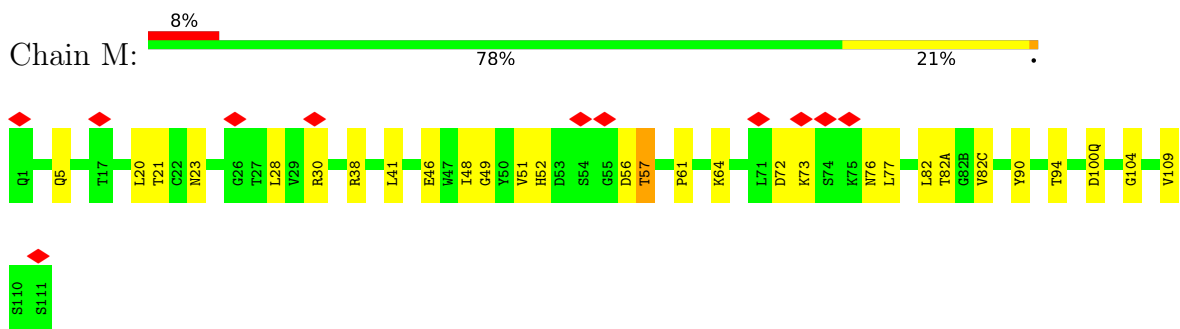
• Molecule 4: Envelope glycoprotein gp120



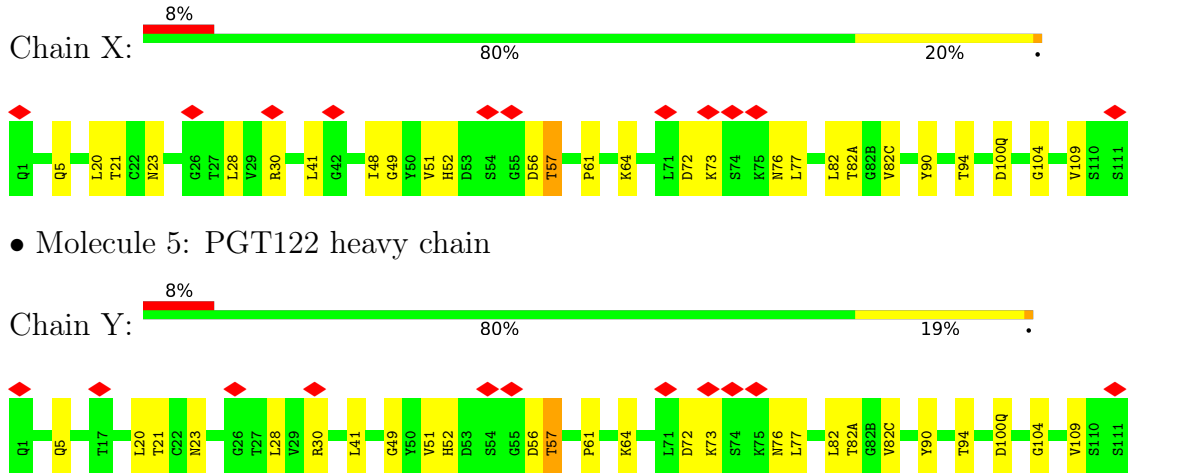
• Molecule 4: Envelope glycoprotein gp120



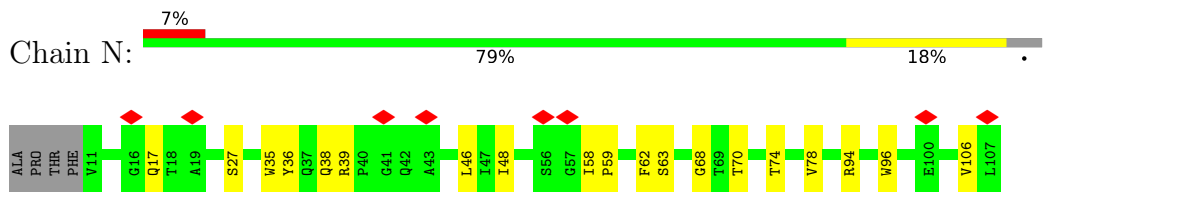
● Molecule 5: PGT122 heavy chain



● Molecule 5: PGT122 heavy chain

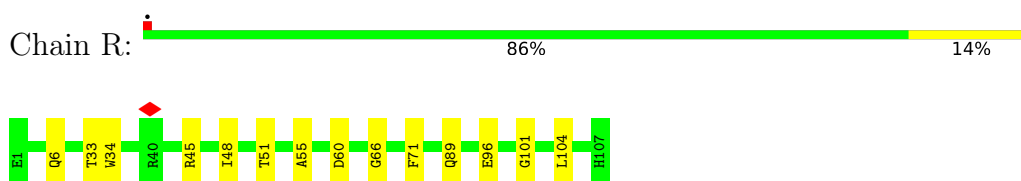


● Molecule 6: PGT122 Light Chain

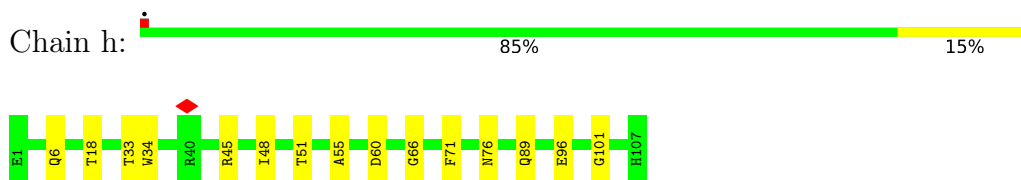


TYR
ILE
CYS
ASN
VAL
VAL
ASN
HIS
LYS
PHO
SER
SER
ASN
THR
THR
LYS
VAL
VAL
ASP
LYS
LYS
VAL
GLU
PRO
LYS

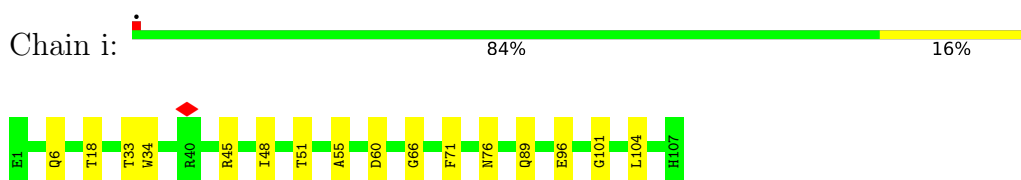
• Molecule 8: VRC03 Light Chain



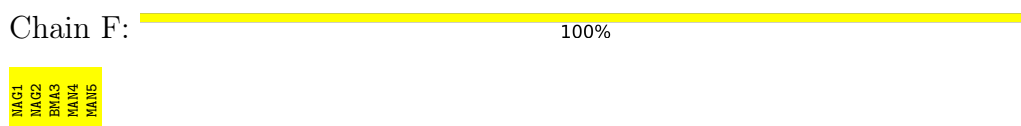
• Molecule 8: VRC03 Light Chain



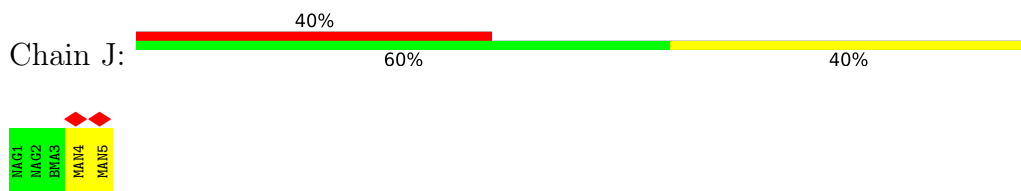
• Molecule 8: VRC03 Light Chain



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

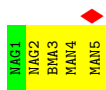


• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

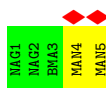
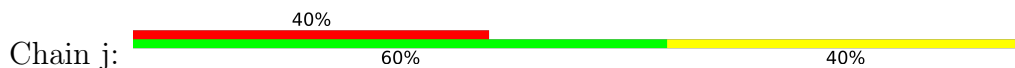


• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

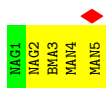




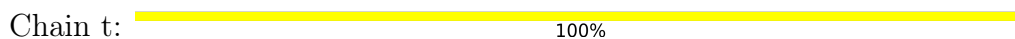
- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



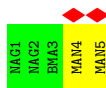
- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



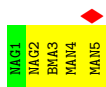
- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose

Chain G:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose

Chain O:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose

Chain T:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose

Chain U:  50% 100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose

Chain d:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose

Chain l:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose

Chain o:  100%


NAG1
NAG2

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

Chain p:  50% 100%


NAG1
NAG2

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

Chain u:  50% 50%


NAG1
NAG2

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

Chain y:  100%


NAG1
NAG2

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

Chain 5:  100%


NAG1
NAG2

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

Chain 7:  50% 100%


NAG1
NAG2

- Molecule 11: 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

Chain I:  25% 75%



- Molecule 11: 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

Chain c: 25% 75%



- Molecule 11: 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

Chain e: 25% 25% 75%



- Molecule 11: 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

Chain v: 25% 25% 75%



- Molecule 11: 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

Chain BA: 50% 50%



- Molecule 11: 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

Chain CA: 50% 50%



- Molecule 11: 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

Chain DA: 50% 50%



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

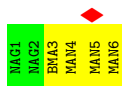


- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

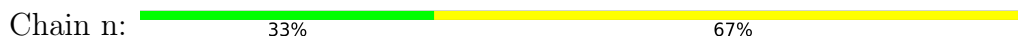




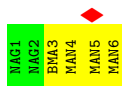
- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	120981	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.78	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.029	Depositor
Minimum map value	-1.585	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.126	Depositor
Recommended contour level	1	Depositor
Map size (Å)	407.03998, 407.03998, 407.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.19	0/941	0.43	0/1288
1	3	0.19	0/941	0.43	0/1288
1	H	0.19	0/941	0.44	0/1288
2	2	0.17	0/880	0.42	0/1197
2	4	0.17	0/880	0.42	0/1197
2	L	0.17	0/880	0.42	0/1197
3	6	0.24	0/1052	0.50	0/1427
3	D	0.24	0/1052	0.50	0/1427
3	E	0.24	0/1052	0.50	0/1427
4	A	0.31	0/3638	0.50	2/4939 (0.0%)
4	B	0.31	0/3638	0.49	0/4939
4	C	0.31	0/3638	0.49	0/4939
5	M	0.19	0/1076	0.44	0/1465
5	X	0.19	0/1076	0.43	0/1465
5	Y	0.19	0/1076	0.44	0/1465
6	N	0.22	0/807	0.42	0/1104
6	Z	0.21	0/807	0.42	0/1104
6	a	0.22	0/807	0.42	0/1104
7	Q	0.31	0/1062	0.46	0/1447
7	f	0.31	0/1062	0.46	0/1447
7	g	0.31	0/1062	0.46	0/1447
8	R	0.27	0/820	0.50	0/1107
8	h	0.27	0/820	0.51	0/1107
8	i	0.26	0/820	0.50	0/1107
All	All	0.26	0/30828	0.47	2/41922 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
2	4	0	1
2	L	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	332	ASN	CA-C-N	5.28	128.03	122.11
4	A	332	ASN	C-N-CA	5.28	128.03	122.11

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	50	GLN	Peptide
2	4	50	GLN	Peptide
2	L	50	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	915	0	902	22	0
1	3	915	0	902	23	0
1	H	915	0	902	22	0
2	2	858	0	845	18	0
2	4	858	0	845	16	0
2	L	858	0	845	15	0
3	6	1034	0	1013	11	0
3	D	1034	0	1013	11	0
3	E	1034	0	1013	11	0
4	A	3564	0	3497	45	0
4	B	3564	0	3497	41	0
4	C	3564	0	3497	41	0
5	M	1047	0	1026	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	X	1047	0	1026	17	0
5	Y	1047	0	1026	15	0
6	N	787	0	745	13	0
6	Z	787	0	745	11	0
6	a	787	0	745	10	0
7	Q	1029	0	976	10	0
7	f	1029	0	976	12	0
7	g	1029	0	976	14	0
8	R	802	0	780	7	0
8	h	802	0	780	7	0
8	i	802	0	780	8	0
9	9	61	0	52	0	0
9	F	61	0	52	0	0
9	J	61	0	52	0	0
9	W	61	0	52	0	0
9	j	61	0	52	0	0
9	r	61	0	52	0	0
9	t	61	0	52	0	0
9	w	61	0	52	0	0
10	5	28	0	25	0	0
10	7	28	0	25	0	0
10	G	28	0	25	1	0
10	O	28	0	25	0	0
10	T	28	0	25	0	0
10	U	28	0	25	0	0
10	d	28	0	25	1	0
10	l	28	0	25	0	0
10	o	28	0	25	0	0
10	p	28	0	25	0	0
10	u	28	0	25	1	0
10	y	28	0	25	0	0
11	BA	50	0	43	0	0
11	CA	50	0	43	0	0
11	DA	50	0	43	0	0
11	I	50	0	43	0	0
11	c	50	0	43	0	0
11	e	50	0	43	0	0
11	v	50	0	43	0	0
12	8	39	0	34	0	0
12	AA	39	0	34	0	0
12	K	39	0	34	0	0
12	P	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	V	39	0	34	0	0
12	b	39	0	34	0	0
12	k	39	0	34	0	0
12	m	39	0	34	1	0
12	q	39	0	34	0	0
12	s	39	0	34	0	0
12	x	39	0	34	0	0
12	z	39	0	34	1	0
13	0	72	0	61	0	0
13	S	72	0	61	0	0
13	n	72	0	61	0	0
14	6	14	0	13	0	0
14	A	28	0	26	0	0
14	B	28	0	26	0	0
14	C	28	0	26	0	0
14	D	14	0	13	0	0
14	E	14	0	13	0	0
All	All	32092	0	31077	390	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 6.

All (390) 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)
2:4:38:GLN:HB2	2:4:85:VAL:O	1.84	0.78
1:3:90:TYR:O	1:3:106:GLY:HA2	1.86	0.76
2:L:38:GLN:HB2	2:L:85:VAL:O	1.86	0.76
1:1:90:TYR:O	1:1:106:GLY:HA2	1.88	0.74
2:2:38:GLN:HB2	2:2:85:VAL:O	1.86	0.74
1:H:90:TYR:O	1:H:106:GLY:HA2	1.88	0.73
5:Y:52:HIS:HB3	5:Y:56:ASP:HB3	1.77	0.66
4:B:195:ASN:ND2	4:B:201:CYS:SG	2.69	0.66
4:C:373:THR:OG1	4:C:374:HIS:N	2.29	0.65
4:C:195:ASN:ND2	4:C:201:CYS:SG	2.70	0.65
5:X:52:HIS:HB3	5:X:56:ASP:HB3	1.78	0.65
4:A:195:ASN:ND2	4:A:201:CYS:SG	2.70	0.65
8:h:33:THR:HB	8:h:89:GLN:HB3	1.78	0.65
4:A:333:VAL:HG21	4:A:390:LEU:HD21	1.80	0.64
5:M:52:HIS:HB3	5:M:56:ASP:HB3	1.78	0.64
8:i:33:THR:HB	8:i:89:GLN:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:33:THR:HB	8:R:89:GLN:HB3	1.79	0.63
4:B:373:THR:OG1	4:B:374:HIS:N	2.29	0.62
2:L:36:TYR:HB2	2:L:87:TYR:HB2	1.81	0.62
2:2:36:TYR:HB2	2:2:87:TYR:HB2	1.81	0.61
2:4:36:TYR:HB2	2:4:87:TYR:HB2	1.81	0.61
4:A:373:THR:OG1	4:A:374:HIS:N	2.29	0.61
5:M:30:ARG:HH21	5:M:73:LYS:HD3	1.66	0.60
5:X:30:ARG:HH21	5:X:73:LYS:HD3	1.66	0.60
1:1:31(A):LYS:HG3	3:6:520:LEU:HD13	1.84	0.59
5:X:28:LEU:HA	5:X:76:ASN:HD21	1.67	0.59
5:Y:30:ARG:HH21	5:Y:73:LYS:HD3	1.67	0.59
5:Y:51:VAL:HG23	5:Y:57:THR:HG23	1.84	0.59
5:M:28:LEU:HA	5:M:76:ASN:HD21	1.67	0.59
5:Y:90:TYR:O	5:Y:104:GLY:HA2	2.03	0.59
5:X:51:VAL:HG23	5:X:57:THR:HG23	1.85	0.59
5:X:90:TYR:O	5:X:104:GLY:HA2	2.01	0.59
5:M:51:VAL:HG23	5:M:57:THR:HG23	1.84	0.58
5:M:90:TYR:O	5:M:104:GLY:HA2	2.02	0.58
5:Y:28:LEU:HA	5:Y:76:ASN:HD21	1.67	0.58
3:D:520:LEU:HD13	1:H:31(A):LYS:HG3	1.85	0.58
1:1:60:ASN:ND2	1:1:62:SER:OG	2.37	0.58
1:H:60:ASN:ND2	1:H:62:SER:OG	2.37	0.57
1:3:60:ASN:ND2	1:3:62:SER:OG	2.37	0.57
4:C:264:SER:O	4:C:287:GLN:NE2	2.38	0.56
1:H:50:TYR:OH	1:H:58:ASN:ND2	2.38	0.56
1:1:50:TYR:OH	1:1:58:ASN:ND2	2.38	0.56
1:3:50:TYR:OH	1:3:58:ASN:ND2	2.38	0.56
4:B:324:GLY:O	6:a:94:ARG:NH2	2.39	0.56
6:N:17:GLN:H	6:N:78:VAL:HG22	1.71	0.56
4:C:333:VAL:HG21	4:C:390:LEU:HD21	1.88	0.56
2:L:6:GLN:HE21	2:L:88:CYS:HB3	1.70	0.56
1:H:14:PRO:HA	1:H:82(C):VAL:HG23	1.88	0.55
5:X:5:GLN:HB3	5:X:23:ASN:HB2	1.88	0.55
1:3:31(A):LYS:HG3	3:E:520:LEU:HD13	1.87	0.55
5:M:5:GLN:HB3	5:M:23:ASN:HB2	1.87	0.55
5:Y:5:GLN:HB3	5:Y:23:ASN:HB2	1.88	0.55
2:L:38:GLN:O	2:L:84:GLY:HA3	2.06	0.55
2:4:6:GLN:HE21	2:4:88:CYS:HB3	1.72	0.55
4:A:264:SER:O	4:A:287:GLN:NE2	2.40	0.55
1:3:14:PRO:HA	1:3:82(C):VAL:HG23	1.88	0.55
4:C:40:TYR:HB3	3:D:602:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:14:PRO:HA	1:1:82(C):VAL:HG23	1.89	0.55
8:R:66:GLY:HA3	8:R:71:PHE:HA	1.89	0.54
4:A:203:GLN:HE22	4:A:318:TYR:H	1.55	0.54
8:h:6:GLN:HG3	8:h:101:GLY:H	1.72	0.54
4:B:203:GLN:HE22	4:B:318:TYR:H	1.55	0.54
2:4:38:GLN:O	2:4:84:GLY:HA3	2.07	0.54
3:6:617:ARG:NH1	3:6:626:MET:SD	2.81	0.54
4:C:277:ILE:O	4:C:456:ARG:NH1	2.40	0.54
8:i:60:ASP:OD1	8:i:60:ASP:N	2.41	0.54
2:2:38:GLN:O	2:2:84:GLY:HA3	2.07	0.54
4:C:324:GLY:O	6:N:94:ARG:NH2	2.41	0.54
8:i:66:GLY:HA3	8:i:71:PHE:HA	1.89	0.53
4:B:274:SER:HB3	4:B:277:ILE:HG13	1.89	0.53
4:A:274:SER:HB3	4:A:277:ILE:HG13	1.89	0.53
4:B:40:TYR:HB3	3:E:602:LEU:HD12	1.88	0.53
2:2:6:GLN:HE21	2:2:88:CYS:HB3	1.73	0.53
7:f:118:GLN:HE22	8:h:55:ALA:HB1	1.74	0.53
1:H:60:ASN:HB3	1:H:63:LEU:HD23	1.91	0.53
5:X:28:LEU:HG	5:X:30:ARG:H	1.73	0.53
6:a:17:GLN:H	6:a:78:VAL:HG22	1.72	0.53
1:H:36:TRP:HB3	1:H:48:ILE:HD12	1.90	0.53
5:M:28:LEU:HG	5:M:30:ARG:H	1.74	0.53
4:C:299:PRO:HA	4:C:442:VAL:HG13	1.91	0.53
4:A:324:GLY:O	6:Z:94:ARG:NH2	2.38	0.53
4:B:39:TYR:O	4:B:494:LEU:HA	2.09	0.53
4:B:264:SER:O	4:B:287:GLN:NE2	2.41	0.53
4:B:299:PRO:HA	4:B:442:VAL:HG13	1.90	0.53
3:6:602:LEU:HD12	4:A:40:TYR:HB3	1.91	0.52
4:A:39:TYR:O	4:A:494:LEU:HA	2.10	0.52
1:1:36:TRP:HB3	1:1:48:ILE:HD12	1.90	0.52
1:1:23:ALA:HA	1:1:77:GLN:HG2	1.92	0.52
1:3:36:TRP:HB3	1:3:48:ILE:HD12	1.90	0.52
8:h:66:GLY:HA3	8:h:71:PHE:HA	1.90	0.52
1:H:66:ARG:NH2	1:H:82(A):THR:O	2.40	0.52
4:C:274:SER:HB3	4:C:277:ILE:HG13	1.91	0.52
6:N:38:GLN:NE2	6:N:39:ARG:O	2.37	0.52
1:1:66:ARG:NH2	1:1:82(A):THR:O	2.39	0.52
3:D:617:ARG:NH1	3:D:626:MET:SD	2.83	0.52
2:2:38:GLN:O	2:2:84:GLY:CA	2.58	0.52
1:3:23:ALA:HA	1:3:77:GLN:HG2	1.92	0.52
1:3:40:PRO:HG2	1:3:43:LYS:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:60:ASN:HB3	1:3:63:LEU:HD23	1.90	0.52
4:C:86:LEU:HB3	4:C:89:VAL:HG11	1.92	0.52
1:1:4:LEU:HD11	1:1:34:TRP:HZ3	1.74	0.51
4:B:86:LEU:HB3	4:B:89:VAL:HG11	1.92	0.51
1:H:23:ALA:HA	1:H:77:GLN:HG2	1.92	0.51
1:H:40:PRO:HG2	1:H:43:LYS:HB2	1.92	0.51
8:R:60:ASP:N	8:R:60:ASP:OD1	2.43	0.51
2:L:38:GLN:O	2:L:84:GLY:CA	2.58	0.51
8:R:6:GLN:HG3	8:R:101:GLY:H	1.75	0.51
7:Q:118:GLN:HE22	8:R:55:ALA:HB1	1.74	0.51
6:Z:17:GLN:H	6:Z:78:VAL:HG22	1.73	0.51
1:H:4:LEU:HD11	1:H:34:TRP:HZ3	1.75	0.51
7:Q:40:ILE:HB	7:Q:43:LYS:HB2	1.93	0.51
1:1:40:PRO:HG2	1:1:43:LYS:HB2	1.91	0.51
1:1:92:CYS:O	1:1:104:GLY:N	2.43	0.51
4:B:53:PHE:HB3	4:B:218:CYS:O	2.11	0.51
4:C:203:GLN:HE22	4:C:318:TYR:H	1.56	0.51
5:X:20:LEU:HD11	5:X:90:TYR:HD2	1.76	0.51
1:3:66:ARG:NH2	1:3:82(A):THR:O	2.39	0.51
1:3:4:LEU:HD11	1:3:34:TRP:HZ3	1.76	0.51
2:4:38:GLN:O	2:4:84:GLY:CA	2.58	0.51
4:A:86:LEU:HB3	4:A:89:VAL:HG11	1.93	0.51
7:f:6:GLN:HE22	7:f:102:PHE:HA	1.76	0.51
1:1:69:ILE:HA	1:1:79:SER:O	2.11	0.51
4:C:39:TYR:O	4:C:494:LEU:HA	2.11	0.51
1:3:92:CYS:O	1:3:104:GLY:N	2.44	0.50
2:L:37:GLN:N	2:L:45:ARG:O	2.45	0.50
8:i:6:GLN:HG3	8:i:101:GLY:H	1.77	0.50
1:1:60:ASN:HB3	1:1:63:LEU:HD23	1.91	0.50
4:A:299:PRO:HA	4:A:442:VAL:HG13	1.91	0.50
7:g:118:GLN:HE22	8:i:55:ALA:HB1	1.76	0.50
2:2:37:GLN:N	2:2:45:ARG:O	2.45	0.50
4:C:101:VAL:HG23	4:C:479:TRP:HB2	1.93	0.50
8:h:60:ASP:N	8:h:60:ASP:OD1	2.44	0.50
4:B:152:GLY:O	4:B:178:ARG:NE	2.40	0.50
4:B:101:VAL:HG23	4:B:479:TRP:HB2	1.93	0.50
6:Z:38:GLN:NE2	6:Z:39:ARG:O	2.35	0.50
3:E:617:ARG:NH1	3:E:626:MET:SD	2.85	0.50
7:g:51:ILE:HD11	7:g:72:ARG:HB3	1.94	0.50
2:4:37:GLN:N	2:4:45:ARG:O	2.45	0.49
7:g:109:CYS:SG	7:g:112:CYS:N	2.84	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:CYS:O	1:H:104:GLY:N	2.43	0.49
7:g:51:ILE:HB	7:g:58:VAL:HG12	1.94	0.49
4:B:277:ILE:O	4:B:456:ARG:NH1	2.43	0.49
7:g:6:GLN:HE22	7:g:102:PHE:HA	1.77	0.49
1:1:4:LEU:HG	1:1:24:VAL:HG22	1.94	0.49
4:A:101:VAL:HG23	4:A:479:TRP:HB2	1.92	0.49
4:C:272:ILE:HG22	4:C:286:VAL:HG22	1.94	0.49
7:f:37:VAL:HG12	7:f:102:PHE:HB2	1.95	0.49
5:Y:20:LEU:HD11	5:Y:90:TYR:HD2	1.78	0.49
5:Y:28:LEU:HG	5:Y:30:ARG:H	1.77	0.49
6:a:59:PRO:HG2	6:a:62:PHE:HE2	1.78	0.49
7:f:109:CYS:SG	7:f:112:CYS:N	2.86	0.49
7:g:40:ILE:HB	7:g:43:LYS:HB2	1.95	0.49
1:H:69:ILE:HA	1:H:79:SER:O	2.12	0.49
7:Q:6:GLN:HE22	7:Q:102:PHE:HA	1.77	0.49
7:f:40:ILE:HB	7:f:43:LYS:HB2	1.94	0.49
7:Q:106:ARG:HA	7:Q:117:TRP:HA	1.95	0.48
4:A:174:SER:OG	4:A:175:LEU:N	2.47	0.48
6:a:35:TRP:HB2	6:a:48:ILE:HB	1.94	0.48
1:1:35:SER:HA	1:1:50:TYR:HA	1.95	0.48
1:1:105:PRO:HA	2:2:43:PRO:HD3	1.95	0.48
1:H:4:LEU:HG	1:H:24:VAL:HG22	1.94	0.48
1:3:4:LEU:HG	1:3:24:VAL:HG22	1.94	0.48
4:B:272:ILE:HG22	4:B:286:VAL:HG22	1.94	0.48
4:B:333:VAL:HG21	4:B:390:LEU:HD21	1.95	0.48
1:3:69:ILE:HA	1:3:79:SER:O	2.12	0.48
5:Y:72:ASP:O	5:Y:76:ASN:HA	2.14	0.48
4:C:430:ILE:H	4:C:430:ILE:HG13	1.55	0.48
6:Z:35:TRP:HB2	6:Z:48:ILE:HB	1.95	0.48
7:f:35:HIS:HB2	7:f:104:VAL:HG23	1.95	0.48
4:C:53:PHE:HB3	4:C:218:CYS:O	2.14	0.48
6:Z:59:PRO:HG2	6:Z:62:PHE:HE2	1.78	0.48
5:M:20:LEU:HD11	5:M:90:TYR:HD2	1.78	0.48
1:H:35:SER:HA	1:H:50:TYR:HA	1.95	0.48
7:g:35:HIS:HB2	7:g:104:VAL:HG23	1.95	0.48
1:H:32:ALA:HA	1:H:95:GLU:O	2.13	0.48
6:N:59:PRO:HG2	6:N:62:PHE:HE2	1.78	0.48
2:2:29:LEU:HA	2:2:92:VAL:HG11	1.96	0.47
3:D:519:PHE:HZ	3:D:539:VAL:HG21	1.79	0.47
6:N:35:TRP:HB2	6:N:48:ILE:HB	1.95	0.47
1:3:32:ALA:HA	1:3:95:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:541:ALA:O	3:E:591:GLN:NE2	2.47	0.47
1:3:105:PRO:HA	2:4:43:PRO:HD3	1.95	0.47
7:Q:35:HIS:HB2	7:Q:104:VAL:HG23	1.95	0.47
1:3:29:ILE:HG23	1:3:30:ARG:HG3	1.96	0.47
4:A:277:ILE:O	4:A:456:ARG:NH1	2.42	0.47
4:A:477:ASP:OD1	4:A:480:ARG:NH1	2.47	0.47
7:f:51:ILE:HB	7:f:58:VAL:HG12	1.96	0.47
6:a:63:SER:HB2	6:a:74:THR:HB	1.97	0.47
2:2:38:GLN:NE2	2:2:87:TYR:OH	2.48	0.47
3:6:519:PHE:HZ	3:6:539:VAL:HG21	1.79	0.47
3:6:591:GLN:NE2	3:D:541:ALA:O	2.48	0.47
6:a:38:GLN:NE2	6:a:39:ARG:O	2.38	0.47
7:f:51:ILE:HD11	7:f:72:ARG:HB3	1.96	0.47
7:Q:37:VAL:HG12	7:Q:102:PHE:HB2	1.96	0.47
6:Z:63:SER:HB2	6:Z:74:THR:HB	1.97	0.47
4:A:137:ASN:N	6:Z:94:ARG:O	2.48	0.47
6:N:63:SER:HB2	6:N:74:THR:HB	1.97	0.47
4:C:265:LEU:H	4:C:265:LEU:HG	1.49	0.46
4:C:477:ASP:OD1	4:C:480:ARG:NH1	2.48	0.46
1:H:105:PRO:HA	2:L:43:PRO:HD3	1.96	0.46
5:M:72:ASP:O	5:M:76:ASN:HA	2.14	0.46
4:A:265:LEU:H	4:A:265:LEU:HG	1.50	0.46
3:E:606:THR:OG1	3:E:607:ASN:N	2.48	0.46
8:R:34:TRP:HB2	8:R:48:ILE:HB	1.97	0.46
2:2:66:GLY:HA3	2:2:71:PHE:HA	1.97	0.46
3:E:519:PHE:HZ	3:E:539:VAL:HG21	1.80	0.46
5:M:21:THR:HB	5:M:77:LEU:HD23	1.97	0.46
5:Y:21:THR:HB	5:Y:77:LEU:HD23	1.98	0.46
1:3:35:SER:HA	1:3:50:TYR:HA	1.96	0.46
4:A:55:ALA:HB3	4:A:216:HIS:HB2	1.97	0.46
4:B:174:SER:OG	4:B:175:LEU:N	2.48	0.46
5:X:72:ASP:O	5:X:76:ASN:HA	2.15	0.46
4:C:152:GLY:O	4:C:178:ARG:NE	2.42	0.46
2:L:29:LEU:HA	2:L:92:VAL:HG11	1.96	0.46
2:L:66:GLY:HA3	2:L:71:PHE:HA	1.98	0.46
1:1:39:GLN:HB2	1:1:45:LEU:HD23	1.98	0.46
7:g:82:ASP:OD1	7:g:82:ASP:N	2.41	0.46
2:4:38:GLN:NE2	2:4:87:TYR:OH	2.49	0.46
5:X:21:THR:HB	5:X:77:LEU:HD23	1.97	0.46
7:g:12:LYS:NZ	7:g:17:SER:O	2.40	0.46
7:g:37:VAL:HG12	7:g:102:PHE:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:39:GLN:HB2	1:3:45:LEU:HD23	1.98	0.46
4:A:430:ILE:H	4:A:430:ILE:HG13	1.56	0.46
4:B:299:PRO:HG2	4:B:327:ARG:HB2	1.96	0.46
1:1:32:ALA:HA	1:1:95:GLU:O	2.16	0.45
7:Q:109:CYS:SG	7:Q:112:CYS:N	2.87	0.45
1:1:29:ILE:HG23	1:1:30:ARG:HG3	1.98	0.45
4:B:137:ASN:N	6:a:94:ARG:O	2.49	0.45
2:L:38:GLN:NE2	2:L:87:TYR:OH	2.49	0.45
4:C:137:ASN:N	6:N:94:ARG:O	2.50	0.45
4:C:174:SER:OG	4:C:175:LEU:N	2.49	0.45
3:D:580:VAL:HA	3:D:583:VAL:HG22	1.97	0.45
3:D:591:GLN:NE2	3:E:541:ALA:O	2.50	0.45
2:4:66:GLY:HA3	2:4:71:PHE:HA	1.97	0.45
4:A:53:PHE:HB3	4:A:218:CYS:HB2	1.99	0.45
4:A:299:PRO:HG2	4:A:327:ARG:HB2	1.99	0.45
4:A:385:CYS:HA	4:A:418:CYS:HA	1.99	0.45
4:B:116:LEU:HD21	4:B:434:MET:HE2	1.99	0.45
4:C:283:ASN:ND2	4:C:477:ASP:OD2	2.48	0.45
3:E:580:VAL:HA	3:E:583:VAL:HG22	1.98	0.45
3:6:580:VAL:HA	3:6:583:VAL:HG22	1.98	0.45
4:C:299:PRO:HG2	4:C:327:ARG:HB2	1.98	0.45
4:B:44:VAL:HG23	3:E:629:LEU:HD23	1.99	0.45
4:A:259:LEU:HD23	4:A:449:ILE:HD13	1.99	0.45
2:4:29:LEU:HA	2:4:92:VAL:HG11	1.98	0.45
4:C:86:LEU:HD21	3:D:526:ALA:HB3	1.98	0.45
4:B:457:ASP:OD2	7:g:65:GLN:NE2	2.50	0.44
7:Q:51:ILE:HB	7:Q:58:VAL:HG12	1.99	0.44
8:i:34:TRP:HB2	8:i:48:ILE:HB	1.99	0.44
6:Z:36:TYR:HD1	6:Z:46:LEU:HA	1.83	0.44
4:A:152:GLY:O	4:A:178:ARG:NE	2.41	0.44
7:f:82:ASP:OD1	7:f:82:ASP:N	2.39	0.44
4:A:138:ILE:H	4:A:138:ILE:HG13	1.49	0.44
1:3:38:ARG:O	1:3:46:GLU:N	2.44	0.44
4:A:333:VAL:HG23	4:A:414:ILE:HB	2.00	0.44
7:g:104:VAL:HB	7:g:117:TRP:HB3	1.99	0.44
10:G:1:NAG:O4	10:G:1:NAG:O7	2.36	0.44
4:B:53:PHE:CB	4:B:218:CYS:O	2.66	0.44
4:B:477:ASP:OD1	4:B:480:ARG:NH1	2.51	0.44
10:d:1:NAG:O4	10:d:1:NAG:O7	2.36	0.44
4:B:373:THR:HG21	4:B:384:TYR:HB3	1.99	0.44
6:N:27:SER:OG	6:N:68:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:104:VAL:HB	7:Q:117:TRP:HB3	2.00	0.44
5:Y:72:ASP:O	5:Y:76:ASN:N	2.51	0.44
4:A:166:ARG:HD3	4:A:166:ARG:HA	1.81	0.44
2:4:13:ILE:H	2:4:13:ILE:HG13	1.66	0.43
5:X:49:GLY:HA2	6:Z:96:TRP:HZ3	1.83	0.43
8:i:104:LEU:HD12	8:i:104:LEU:HA	1.87	0.43
4:B:55:ALA:HB3	4:B:216:HIS:HB2	2.01	0.43
4:B:257:THR:OG1	4:B:258:GLN:N	2.51	0.43
1:H:29:ILE:HG23	1:H:30:ARG:HG3	1.99	0.43
6:N:58:ILE:HD12	6:N:58:ILE:HA	1.95	0.43
8:h:34:TRP:HB2	8:h:48:ILE:HB	1.99	0.43
5:M:94:THR:OG1	5:M:100(Q):ASP:OD1	2.36	0.43
4:A:52:LEU:HD23	4:A:52:LEU:HA	1.87	0.43
4:B:385:CYS:HA	4:B:418:CYS:HA	1.99	0.43
4:A:234:ASN:ND2	12:P:1:NAG:O5	2.52	0.43
4:A:288:PHE:HZ	4:A:449:ILE:HG22	1.83	0.43
4:A:322:ILE:O	6:Z:94:ARG:NH2	2.36	0.43
4:C:234:ASN:ND2	12:z:1:NAG:O5	2.52	0.43
4:B:234:ASN:ND2	12:m:1:NAG:O5	2.51	0.43
3:E:592:LEU:HD23	3:E:592:LEU:HA	1.89	0.43
7:f:104:VAL:HB	7:f:117:TRP:HB3	2.01	0.43
10:u:1:NAG:O4	10:u:1:NAG:O7	2.36	0.43
1:1:38:ARG:O	1:1:46:GLU:N	2.45	0.43
4:B:283:ASN:ND2	4:B:477:ASP:OD2	2.48	0.43
4:C:166:ARG:HA	4:C:166:ARG:HD3	1.82	0.43
4:C:369:LEU:O	4:C:372:THR:OG1	2.37	0.43
5:Y:49:GLY:HA2	6:a:96:TRP:HZ3	1.83	0.43
4:C:53:PHE:CB	4:C:218:CYS:O	2.67	0.43
5:Y:94:THR:OG1	5:Y:100(Q):ASP:OD1	2.36	0.43
6:a:36:TYR:HD1	6:a:46:LEU:HA	1.83	0.43
2:4:34:SER:HA	2:4:49:TYR:HA	2.01	0.43
4:A:270:VAL:HG11	4:A:345:VAL:HG12	2.01	0.43
5:X:94:THR:OG1	5:X:100(Q):ASP:OD1	2.37	0.43
1:3:40:PRO:HB2	1:3:43:LYS:HD3	2.01	0.42
4:B:65:LYS:HE2	4:B:65:LYS:HB3	1.87	0.42
4:B:268:GLU:O	4:B:289:ASN:ND2	2.52	0.42
3:D:606:THR:OG1	3:D:607:ASN:N	2.46	0.42
6:N:36:TYR:HD1	6:N:46:LEU:HA	1.83	0.42
7:f:12:LYS:NZ	7:f:17:SER:O	2.40	0.42
4:A:272:ILE:HG22	4:A:286:VAL:HG22	1.99	0.42
4:B:291:PRO:HB2	4:B:448:ASN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:49:GLY:HA2	6:N:96:TRP:HZ3	1.85	0.42
8:R:104:LEU:HD12	8:R:104:LEU:HA	1.88	0.42
2:2:34:SER:HA	2:2:49:TYR:HA	2.02	0.42
4:A:291:PRO:HB2	4:A:448:ASN:HB3	2.01	0.42
4:B:265:LEU:H	4:B:265:LEU:HG	1.48	0.42
4:C:138:ILE:H	4:C:138:ILE:HG13	1.50	0.42
5:M:72:ASP:O	5:M:76:ASN:CA	2.67	0.42
2:4:13:ILE:HB	2:4:78:VAL:HG21	2.01	0.42
4:A:84:ILE:H	4:A:84:ILE:HG12	1.59	0.42
4:C:44:VAL:HG23	3:D:629:LEU:HD23	2.00	0.42
5:M:38:ARG:NE	5:M:46:GLU:OE1	2.47	0.42
3:6:592:LEU:HD23	3:6:592:LEU:HA	1.89	0.42
1:H:40:PRO:HB2	1:H:43:LYS:HD3	2.01	0.42
7:Q:82:ASP:OD1	7:Q:82:ASP:N	2.42	0.42
5:X:61:PRO:HA	5:X:64:LYS:HB2	2.01	0.42
5:Y:72:ASP:O	5:Y:76:ASN:CA	2.66	0.42
1:1:40:PRO:HB2	1:1:43:LYS:HD3	2.02	0.42
2:2:21:ILE:HD12	2:2:73:LEU:HD23	2.02	0.42
2:L:6:GLN:HE22	2:L:99:GLY:HA3	1.84	0.42
8:h:18:THR:HG22	8:h:76:ASN:HA	2.02	0.42
2:2:6:GLN:HE22	2:2:99:GLY:HA3	1.85	0.42
4:C:342:LEU:HD23	4:C:342:LEU:HA	1.89	0.42
2:L:21:ILE:HD12	2:L:73:LEU:HD23	2.02	0.42
2:2:29:LEU:HD12	2:2:71:PHE:HE2	1.85	0.42
4:C:116:LEU:HD21	4:C:434:MET:HE2	2.02	0.42
2:4:35:TRP:N	2:4:48:ILE:O	2.53	0.41
4:A:65:LYS:HB3	4:A:65:LYS:HE2	1.88	0.41
4:B:259:LEU:HD23	4:B:449:ILE:HD13	2.02	0.41
4:C:385:CYS:HA	4:C:418:CYS:HA	2.00	0.41
3:D:577:GLN:HA	3:D:580:VAL:HG22	2.02	0.41
1:H:17:THR:HG23	1:H:82(A):THR:HG22	2.02	0.41
2:2:13:ILE:HB	2:2:78:VAL:HG21	2.02	0.41
2:4:21:ILE:HD12	2:4:73:LEU:HD23	2.03	0.41
4:A:283:ASN:ND2	4:A:477:ASP:OD2	2.53	0.41
4:B:258:GLN:NE2	4:B:470:PRO:O	2.54	0.41
4:C:259:LEU:HD23	4:C:449:ILE:HD13	2.01	0.41
7:g:106:ARG:HA	7:g:117:TRP:HA	2.01	0.41
6:Z:58:ILE:HD12	6:Z:58:ILE:HA	1.94	0.41
4:A:33:ASN:OD1	4:A:33:ASN:N	2.49	0.41
4:C:268:GLU:O	4:C:289:ASN:ND2	2.54	0.41
4:C:370:GLU:H	4:C:370:GLU:HG2	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:370:GLU:HB3	4:C:384:TYR:HE1	1.85	0.41
1:H:38:ARG:HB3	1:H:48:ILE:HD11	2.02	0.41
1:H:39:GLN:HB2	1:H:45:LEU:HD23	2.01	0.41
5:M:72:ASP:O	5:M:76:ASN:N	2.53	0.41
3:6:629:LEU:HD23	4:A:44:VAL:HG23	2.01	0.41
4:C:291:PRO:HB2	4:C:448:ASN:HB3	2.01	0.41
5:M:61:PRO:HA	5:M:64:LYS:HB2	2.01	0.41
4:B:52:LEU:H	4:B:103:GLN:HE22	1.68	0.41
5:X:72:ASP:O	5:X:76:ASN:CA	2.69	0.41
5:X:72:ASP:O	5:X:76:ASN:N	2.54	0.41
4:A:370:GLU:HB3	4:A:384:TYR:HE1	1.85	0.41
5:M:72:ASP:HB3	5:M:77:LEU:H	1.86	0.41
4:A:53:PHE:HB3	4:A:218:CYS:O	2.20	0.41
5:M:48:ILE:H	5:M:48:ILE:HG13	1.72	0.41
3:6:587:LEU:HD12	3:6:587:LEU:HA	1.92	0.41
4:B:212:PRO:HB2	4:B:252:LYS:HB2	2.02	0.41
4:C:322:ILE:O	6:N:94:ARG:NH2	2.37	0.41
1:3:17:THR:HG23	1:3:82(A):THR:HG22	2.03	0.41
2:4:66:GLY:HA3	2:4:71:PHE:HD1	1.86	0.41
3:6:577:GLN:HA	3:6:580:VAL:HG22	2.02	0.41
4:A:175:LEU:HB2	4:A:320:THR:HB	2.02	0.41
4:C:65:LYS:HE2	4:C:65:LYS:HB3	1.87	0.41
2:L:29:LEU:HD12	2:L:71:PHE:HE2	1.86	0.41
6:N:36:TYR:HE1	6:N:46:LEU:HD12	1.86	0.41
5:X:48:ILE:H	5:X:48:ILE:HG13	1.72	0.41
5:X:100(Q):ASP:OD1	5:X:100(Q):ASP:N	2.46	0.41
1:1:87:THR:HG23	1:1:110:THR:HA	2.03	0.40
2:2:35:TRP:N	2:2:48:ILE:O	2.54	0.40
3:E:515:ILE:HD12	3:E:515:ILE:HA	1.97	0.40
2:L:66:GLY:HA3	2:L:71:PHE:HD1	1.86	0.40
7:g:6:GLN:HE21	7:g:121:GLY:HA3	1.87	0.40
1:3:63:LEU:HD13	1:3:63:LEU:HA	1.97	0.40
4:B:426:MET:HE3	4:B:426:MET:HB2	1.85	0.40
2:2:66:GLY:HA3	2:2:71:PHE:HD1	1.86	0.40
4:B:270:VAL:HG11	4:B:345:VAL:HG12	2.02	0.40
2:L:13:ILE:HB	2:L:78:VAL:HG21	2.03	0.40
2:2:13:ILE:H	2:2:13:ILE:HG13	1.66	0.40
4:A:278:THR:O	4:A:456:ARG:NH2	2.53	0.40
4:C:270:VAL:HG11	4:C:345:VAL:HG12	2.03	0.40
8:i:18:THR:HG22	8:i:76:ASN:HA	2.03	0.40
4:A:53:PHE:CB	4:A:218:CYS:O	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:424:ILE:HD12	4:A:426:MET:HG2	2.04	0.40
4:B:67:ASN:OD1	4:B:67:ASN:N	2.55	0.40
5:Y:61:PRO:HA	5:Y:64:LYS:HB2	2.03	0.40
6:a:27:SER:OG	6:a:68:GLY:N	2.50	0.40
7:f:6:GLN:HE21	7:f:121:GLY:HA3	1.87	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	1	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
1	3	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
1	H	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
2	2	110/112 (98%)	106 (96%)	3 (3%)	1 (1%)	14	45
2	4	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	14	45
2	L	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	14	45
3	6	128/153 (84%)	121 (94%)	7 (6%)	0	100	100
3	D	128/153 (84%)	121 (94%)	7 (6%)	0	100	100
3	E	128/153 (84%)	121 (94%)	7 (6%)	0	100	100
4	A	447/473 (94%)	414 (93%)	33 (7%)	0	100	100
4	B	447/473 (94%)	415 (93%)	32 (7%)	0	100	100
4	C	447/473 (94%)	416 (93%)	31 (7%)	0	100	100
5	M	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
5	X	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
5	Y	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
6	N	101/107 (94%)	96 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Z	101/107 (94%)	96 (95%)	5 (5%)	0	100	100
6	a	101/107 (94%)	97 (96%)	4 (4%)	0	100	100
7	Q	127/227 (56%)	123 (97%)	4 (3%)	0	100	100
7	f	127/227 (56%)	123 (97%)	4 (3%)	0	100	100
7	g	127/227 (56%)	122 (96%)	5 (4%)	0	100	100
8	R	100/102 (98%)	95 (95%)	4 (4%)	1 (1%)	12	43
8	h	100/102 (98%)	95 (95%)	4 (4%)	1 (1%)	12	43
8	i	100/102 (98%)	94 (94%)	5 (5%)	1 (1%)	12	43
All	All	3777/4272 (88%)	3572 (95%)	199 (5%)	6 (0%)	44	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	h	96	GLU
8	i	96	GLU
8	R	96	GLU
2	2	51	VAL
2	4	51	VAL
2	L	51	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	100/100 (100%)	97 (97%)	3 (3%)	36	57
1	3	100/100 (100%)	98 (98%)	2 (2%)	48	65
1	H	100/100 (100%)	97 (97%)	3 (3%)	36	57
2	2	97/97 (100%)	93 (96%)	4 (4%)	27	51
2	4	97/97 (100%)	93 (96%)	4 (4%)	27	51
2	L	97/97 (100%)	93 (96%)	4 (4%)	27	51
3	6	110/129 (85%)	98 (89%)	12 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	110/129 (85%)	98 (89%)	12 (11%)	6	25
3	E	110/129 (85%)	97 (88%)	13 (12%)	5	22
4	A	405/422 (96%)	367 (91%)	38 (9%)	8	30
4	B	405/422 (96%)	369 (91%)	36 (9%)	9	32
4	C	405/422 (96%)	369 (91%)	36 (9%)	9	32
5	M	116/116 (100%)	110 (95%)	6 (5%)	21	46
5	X	116/116 (100%)	110 (95%)	6 (5%)	21	46
5	Y	116/116 (100%)	110 (95%)	6 (5%)	21	46
6	N	86/89 (97%)	84 (98%)	2 (2%)	44	63
6	Z	86/89 (97%)	84 (98%)	2 (2%)	44	63
6	a	86/89 (97%)	84 (98%)	2 (2%)	44	63
7	Q	109/193 (56%)	107 (98%)	2 (2%)	51	67
7	f	109/193 (56%)	107 (98%)	2 (2%)	51	67
7	g	109/193 (56%)	107 (98%)	2 (2%)	51	67
8	R	86/86 (100%)	84 (98%)	2 (2%)	44	63
8	h	86/86 (100%)	84 (98%)	2 (2%)	44	63
8	i	86/86 (100%)	84 (98%)	2 (2%)	44	63
All	All	3327/3696 (90%)	3124 (94%)	203 (6%)	19	43

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	55	ASP
1	1	76	ASN
1	1	101	ASP
2	2	13	ILE
2	2	33	LEU
2	2	48	ILE
2	2	51	VAL
1	3	55	ASP
1	3	101	ASP
2	4	13	ILE
2	4	33	LEU
2	4	48	ILE
2	4	51	VAL
3	6	513	VAL

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Mol	Chain	Res	Type
3	6	518	VAL
3	6	520	LEU
3	6	536	THR
3	6	538	THR
3	6	570	VAL
3	6	576	LEU
3	6	587	LEU
3	6	604	CYS
3	6	608	VAL
3	6	629	LEU
3	6	639	THR
4	A	33	ASN
4	A	34	LEU
4	A	36	VAL
4	A	37	THR
4	A	38	VAL
4	A	63	THR
4	A	75	VAL
4	A	80	ASN
4	A	84	ILE
4	A	86	LEU
4	A	89	VAL
4	A	101	VAL
4	A	111	LEU
4	A	120	VAL
4	A	122	LEU
4	A	138	ILE
4	A	198	THR
4	A	201	CYS
4	A	208	VAL
4	A	245	VAL
4	A	260	LEU
4	A	265	LEU
4	A	297	THR
4	A	333	VAL
4	A	359	ILE
4	A	370	GLU
4	A	371	VAL
4	A	373	THR
4	A	374	HIS
4	A	375	SER
4	A	385	CYS

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Mol	Chain	Res	Type
4	A	415	THR
4	A	416	LEU
4	A	423	ILE
4	A	430	ILE
4	A	467	THR
4	A	488	VAL
4	A	494	LEU
4	B	33	ASN
4	B	34	LEU
4	B	36	VAL
4	B	37	THR
4	B	38	VAL
4	B	63	THR
4	B	75	VAL
4	B	80	ASN
4	B	84	ILE
4	B	86	LEU
4	B	89	VAL
4	B	101	VAL
4	B	111	LEU
4	B	120	VAL
4	B	122	LEU
4	B	138	ILE
4	B	198	THR
4	B	201	CYS
4	B	208	VAL
4	B	245	VAL
4	B	260	LEU
4	B	265	LEU
4	B	333	VAL
4	B	359	ILE
4	B	370	GLU
4	B	371	VAL
4	B	373	THR
4	B	374	HIS
4	B	375	SER
4	B	385	CYS
4	B	415	THR
4	B	416	LEU
4	B	423	ILE
4	B	430	ILE
4	B	488	VAL

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Mol	Chain	Res	Type
4	B	494	LEU
4	C	33	ASN
4	C	34	LEU
4	C	36	VAL
4	C	37	THR
4	C	38	VAL
4	C	63	THR
4	C	75	VAL
4	C	80	ASN
4	C	84	ILE
4	C	86	LEU
4	C	89	VAL
4	C	101	VAL
4	C	111	LEU
4	C	120	VAL
4	C	122	LEU
4	C	138	ILE
4	C	198	THR
4	C	201	CYS
4	C	208	VAL
4	C	245	VAL
4	C	260	LEU
4	C	265	LEU
4	C	333	VAL
4	C	359	ILE
4	C	370	GLU
4	C	371	VAL
4	C	373	THR
4	C	374	HIS
4	C	375	SER
4	C	385	CYS
4	C	416	LEU
4	C	423	ILE
4	C	430	ILE
4	C	467	THR
4	C	488	VAL
4	C	494	LEU
3	D	513	VAL
3	D	518	VAL
3	D	520	LEU
3	D	536	THR
3	D	538	THR

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Mol	Chain	Res	Type
3	D	570	VAL
3	D	587	LEU
3	D	593	LEU
3	D	604	CYS
3	D	608	VAL
3	D	629	LEU
3	D	639	THR
3	E	513	VAL
3	E	518	VAL
3	E	520	LEU
3	E	536	THR
3	E	538	THR
3	E	570	VAL
3	E	576	LEU
3	E	587	LEU
3	E	593	LEU
3	E	604	CYS
3	E	608	VAL
3	E	629	LEU
3	E	639	THR
1	H	55	ASP
1	H	76	ASN
1	H	101	ASP
2	L	13	ILE
2	L	33	LEU
2	L	48	ILE
2	L	51	VAL
5	M	41	LEU
5	M	57	THR
5	M	82	LEU
5	M	82(A)	THR
5	M	82(C)	VAL
5	M	109	VAL
6	N	70	THR
6	N	106	VAL
7	Q	37	VAL
7	Q	51	ILE
8	R	45	ARG
8	R	51	THR
5	X	41	LEU
5	X	57	THR
5	X	82	LEU

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Mol	Chain	Res	Type
5	X	82(A)	THR
5	X	82(C)	VAL
5	X	109	VAL
5	Y	41	LEU
5	Y	57	THR
5	Y	82	LEU
5	Y	82(A)	THR
5	Y	82(C)	VAL
5	Y	109	VAL
6	Z	70	THR
6	Z	106	VAL
6	a	70	THR
6	a	106	VAL
7	f	37	VAL
7	f	51	ILE
7	g	37	VAL
7	g	51	ILE
8	h	45	ARG
8	h	51	THR
8	i	45	ARG
8	i	51	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	58	ASN
1	1	60	ASN
1	1	76	ASN
2	2	38	GLN
1	3	58	ASN
1	3	60	ASN
1	3	76	ASN
2	4	38	GLN
3	6	611	ASN
4	A	72	HIS
4	A	103	GLN
4	A	114	GLN
4	A	203	GLN
4	A	234	ASN
4	A	258	GLN
4	A	289	ASN
4	A	330	HIS

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Mol	Chain	Res	Type
4	B	72	HIS
4	B	103	GLN
4	B	114	GLN
4	B	156	ASN
4	B	203	GLN
4	B	234	ASN
4	B	258	GLN
4	B	287	GLN
4	B	289	ASN
4	C	72	HIS
4	C	103	GLN
4	C	114	GLN
4	C	203	GLN
4	C	258	GLN
4	C	289	ASN
3	D	611	ASN
3	E	577	GLN
3	E	611	ASN
1	H	58	ASN
1	H	60	ASN
1	H	76	ASN
2	L	38	GLN
5	M	23	ASN
6	N	17	GLN
7	Q	6	GLN
7	Q	118	GLN
8	R	6	GLN
8	R	90	GLN
5	X	23	ASN
5	Y	23	ASN
6	Z	17	GLN
6	a	17	GLN
7	f	6	GLN
7	f	118	GLN
7	g	6	GLN
7	g	118	GLN
8	h	6	GLN
8	i	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

146 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
13	NAG	0	1	13	14,14,15	0.39	0	17,19,21	0.41	0
13	NAG	0	2	13	14,14,15	0.19	0	17,19,21	0.40	0
13	BMA	0	3	13	11,11,12	0.60	0	15,15,17	0.91	1 (6%)
13	MAN	0	4	13	11,11,12	0.65	0	15,15,17	1.31	2 (13%)
13	MAN	0	5	13	11,11,12	0.70	0	15,15,17	1.21	2 (13%)
13	MAN	0	6	13	11,11,12	0.88	0	15,15,17	0.99	2 (13%)
10	NAG	5	1	4,10	14,14,15	0.19	0	17,19,21	0.50	0
10	NAG	5	2	10	14,14,15	0.28	0	17,19,21	0.56	0
10	NAG	7	1	10	14,14,15	0.30	0	17,19,21	0.60	0
10	NAG	7	2	10	14,14,15	0.35	0	17,19,21	0.44	0
12	NAG	8	1	4,12	14,14,15	0.24	0	17,19,21	0.58	0
12	NAG	8	2	12	14,14,15	0.35	0	17,19,21	0.60	0
12	BMA	8	3	12	11,11,12	0.61	0	15,15,17	1.14	2 (13%)
9	NAG	9	1	9,4	14,14,15	0.29	0	17,19,21	0.58	0
9	NAG	9	2	9	14,14,15	0.48	0	17,19,21	1.04	2 (11%)
9	BMA	9	3	9	11,11,12	0.86	0	15,15,17	0.82	1 (6%)
9	MAN	9	4	9	11,11,12	0.80	0	15,15,17	0.99	2 (13%)
9	MAN	9	5	9	11,11,12	0.74	0	15,15,17	1.04	2 (13%)
12	NAG	AA	1	4,12	14,14,15	0.61	0	17,19,21	1.33	3 (17%)
12	NAG	AA	2	12	14,14,15	0.40	0	17,19,21	0.55	0
12	BMA	AA	3	12	11,11,12	0.73	0	15,15,17	1.00	1 (6%)
11	NAG	BA	1	11	14,14,15	0.19	0	17,19,21	0.56	0
11	NAG	BA	2	11	14,14,15	0.37	0	17,19,21	0.74	1 (5%)
11	BMA	BA	3	11	11,11,12	0.91	0	15,15,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	BA	4	11	11,11,12	0.78	0	15,15,17	1.15	2 (13%)
11	NAG	CA	1	11	14,14,15	0.19	0	17,19,21	0.57	0
11	NAG	CA	2	11	14,14,15	0.36	0	17,19,21	0.74	1 (5%)
11	BMA	CA	3	11	11,11,12	0.92	0	15,15,17	0.75	0
11	MAN	CA	4	11	11,11,12	0.76	0	15,15,17	1.15	2 (13%)
11	NAG	DA	1	11	14,14,15	0.25	0	17,19,21	0.62	0
11	NAG	DA	2	11	14,14,15	0.36	0	17,19,21	0.73	1 (5%)
11	BMA	DA	3	11	11,11,12	0.93	0	15,15,17	0.76	0
11	MAN	DA	4	11	11,11,12	0.79	0	15,15,17	1.13	2 (13%)
9	NAG	F	1	9,4	14,14,15	0.24	0	17,19,21	0.86	1 (5%)
9	NAG	F	2	9	14,14,15	0.28	0	17,19,21	0.83	1 (5%)
9	BMA	F	3	9	11,11,12	0.80	0	15,15,17	1.23	2 (13%)
9	MAN	F	4	9	11,11,12	0.69	0	15,15,17	1.20	2 (13%)
9	MAN	F	5	9	11,11,12	0.71	0	15,15,17	1.08	2 (13%)
10	NAG	G	1	10	14,14,15	0.79	1 (7%)	17,19,21	1.24	1 (5%)
10	NAG	G	2	10	14,14,15	0.41	0	17,19,21	0.46	0
11	NAG	I	1	11	14,14,15	0.21	0	17,19,21	0.54	0
11	NAG	I	2	11	14,14,15	0.33	0	17,19,21	0.94	1 (5%)
11	BMA	I	3	11	11,11,12	0.82	0	15,15,17	1.18	1 (6%)
11	MAN	I	4	11	11,11,12	0.91	0	15,15,17	1.51	2 (13%)
9	NAG	J	1	9	14,14,15	0.23	0	17,19,21	0.50	0
9	NAG	J	2	9	14,14,15	0.20	0	17,19,21	0.57	0
9	BMA	J	3	9	11,11,12	0.74	0	15,15,17	0.80	0
9	MAN	J	4	9	11,11,12	0.83	0	15,15,17	1.06	2 (13%)
9	MAN	J	5	9	11,11,12	0.69	0	15,15,17	1.07	2 (13%)
12	NAG	K	1	4,12	14,14,15	0.57	0	17,19,21	1.12	1 (5%)
12	NAG	K	2	12	14,14,15	0.24	0	17,19,21	0.57	0
12	BMA	K	3	12	11,11,12	0.59	0	15,15,17	0.85	1 (6%)
10	NAG	O	1	10	14,14,15	0.42	0	17,19,21	0.57	0
10	NAG	O	2	10	14,14,15	0.30	0	17,19,21	0.52	0
12	NAG	P	1	12	14,14,15	0.19	0	17,19,21	0.54	0
12	NAG	P	2	12	14,14,15	0.22	0	17,19,21	0.58	0
12	BMA	P	3	12	11,11,12	0.72	0	15,15,17	1.01	1 (6%)
13	NAG	S	1	13	14,14,15	0.33	0	17,19,21	0.43	0
13	NAG	S	2	13	14,14,15	0.19	0	17,19,21	0.40	0
13	BMA	S	3	13	11,11,12	0.64	0	15,15,17	0.92	1 (6%)
13	MAN	S	4	13	11,11,12	0.64	0	15,15,17	1.29	2 (13%)
13	MAN	S	5	13	11,11,12	0.70	0	15,15,17	1.20	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	MAN	S	6	13	11,11,12	0.87	0	15,15,17	0.99	2 (13%)
10	NAG	T	1	4,10	14,14,15	0.26	0	17,19,21	0.48	0
10	NAG	T	2	10	14,14,15	0.27	0	17,19,21	0.54	0
10	NAG	U	1	10	14,14,15	0.33	0	17,19,21	0.59	0
10	NAG	U	2	10	14,14,15	0.38	0	17,19,21	0.43	0
12	NAG	V	1	4,12	14,14,15	0.29	0	17,19,21	0.64	0
12	NAG	V	2	12	14,14,15	0.31	0	17,19,21	0.57	0
12	BMA	V	3	12	11,11,12	0.60	0	15,15,17	1.15	2 (13%)
9	NAG	W	1	9,4	14,14,15	0.27	0	17,19,21	0.60	0
9	NAG	W	2	9	14,14,15	0.50	0	17,19,21	1.02	2 (11%)
9	BMA	W	3	9	11,11,12	0.87	0	15,15,17	0.84	1 (6%)
9	MAN	W	4	9	11,11,12	0.81	0	15,15,17	1.00	2 (13%)
9	MAN	W	5	9	11,11,12	0.73	0	15,15,17	1.03	2 (13%)
12	NAG	b	1	4,12	14,14,15	0.66	0	17,19,21	1.32	3 (17%)
12	NAG	b	2	12	14,14,15	0.41	0	17,19,21	0.56	0
12	BMA	b	3	12	11,11,12	0.71	0	15,15,17	0.99	1 (6%)
11	NAG	c	1	4,11	14,14,15	0.24	0	17,19,21	1.00	2 (11%)
11	NAG	c	2	11	14,14,15	0.39	0	17,19,21	1.09	1 (5%)
11	BMA	c	3	11	11,11,12	1.05	0	15,15,17	1.01	0
11	MAN	c	4	11	11,11,12	1.17	2 (18%)	15,15,17	1.10	1 (6%)
10	NAG	d	1	10	14,14,15	0.78	1 (7%)	17,19,21	1.24	1 (5%)
10	NAG	d	2	10	14,14,15	0.44	0	17,19,21	0.46	0
11	NAG	e	1	11	14,14,15	0.20	0	17,19,21	0.55	0
11	NAG	e	2	11	14,14,15	0.31	0	17,19,21	0.94	1 (5%)
11	BMA	e	3	11	11,11,12	0.82	0	15,15,17	1.18	1 (6%)
11	MAN	e	4	11	11,11,12	0.92	0	15,15,17	1.49	2 (13%)
9	NAG	j	1	9	14,14,15	0.23	0	17,19,21	0.51	0
9	NAG	j	2	9	14,14,15	0.21	0	17,19,21	0.56	0
9	BMA	j	3	9	11,11,12	0.74	0	15,15,17	0.83	0
9	MAN	j	4	9	11,11,12	0.82	0	15,15,17	1.03	2 (13%)
9	MAN	j	5	9	11,11,12	0.67	0	15,15,17	1.11	2 (13%)
12	NAG	k	1	4,12	14,14,15	0.60	1 (7%)	17,19,21	1.11	1 (5%)
12	NAG	k	2	12	14,14,15	0.24	0	17,19,21	0.57	0
12	BMA	k	3	12	11,11,12	0.60	0	15,15,17	0.85	1 (6%)
10	NAG	l	1	10	14,14,15	0.44	0	17,19,21	0.58	0
10	NAG	l	2	10	14,14,15	0.27	0	17,19,21	0.54	0
12	NAG	m	1	12	14,14,15	0.21	0	17,19,21	0.53	0
12	NAG	m	2	12	14,14,15	0.23	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	BMA	m	3	12	11,11,12	0.71	0	15,15,17	1.01	1 (6%)
13	NAG	n	1	13	14,14,15	0.36	0	17,19,21	0.41	0
13	NAG	n	2	13	14,14,15	0.19	0	17,19,21	0.41	0
13	BMA	n	3	13	11,11,12	0.59	0	15,15,17	0.90	1 (6%)
13	MAN	n	4	13	11,11,12	0.66	0	15,15,17	1.32	2 (13%)
13	MAN	n	5	13	11,11,12	0.69	0	15,15,17	1.22	2 (13%)
13	MAN	n	6	13	11,11,12	0.90	0	15,15,17	0.97	2 (13%)
10	NAG	o	1	4,10	14,14,15	0.23	0	17,19,21	0.47	0
10	NAG	o	2	10	14,14,15	0.30	0	17,19,21	0.55	0
10	NAG	p	1	10	14,14,15	0.34	0	17,19,21	0.62	0
10	NAG	p	2	10	14,14,15	0.36	0	17,19,21	0.45	0
12	NAG	q	1	4,12	14,14,15	0.28	0	17,19,21	0.66	0
12	NAG	q	2	12	14,14,15	0.33	0	17,19,21	0.59	0
12	BMA	q	3	12	11,11,12	0.60	0	15,15,17	1.14	2 (13%)
9	NAG	r	1	9,4	14,14,15	0.27	0	17,19,21	0.59	0
9	NAG	r	2	9	14,14,15	0.47	0	17,19,21	1.01	2 (11%)
9	BMA	r	3	9	11,11,12	0.87	0	15,15,17	0.81	1 (6%)
9	MAN	r	4	9	11,11,12	0.80	0	15,15,17	0.99	2 (13%)
9	MAN	r	5	9	11,11,12	0.73	0	15,15,17	1.04	2 (13%)
12	NAG	s	1	4,12	14,14,15	0.66	0	17,19,21	1.33	2 (11%)
12	NAG	s	2	12	14,14,15	0.31	0	17,19,21	0.57	0
12	BMA	s	3	12	11,11,12	0.73	0	15,15,17	1.03	1 (6%)
9	NAG	t	1	9,4	14,14,15	0.48	0	17,19,21	0.73	1 (5%)
9	NAG	t	2	9	14,14,15	0.40	0	17,19,21	0.75	1 (5%)
9	BMA	t	3	9	11,11,12	1.23	1 (9%)	15,15,17	1.17	2 (13%)
9	MAN	t	4	9	11,11,12	1.08	1 (9%)	15,15,17	1.18	1 (6%)
9	MAN	t	5	9	11,11,12	0.67	0	15,15,17	1.12	2 (13%)
10	NAG	u	1	10	14,14,15	0.79	1 (7%)	17,19,21	1.23	1 (5%)
10	NAG	u	2	10	14,14,15	0.31	0	17,19,21	0.47	0
11	NAG	v	1	11	14,14,15	0.23	0	17,19,21	0.54	0
11	NAG	v	2	11	14,14,15	0.32	0	17,19,21	0.92	1 (5%)
11	BMA	v	3	11	11,11,12	0.80	0	15,15,17	1.18	1 (6%)
11	MAN	v	4	11	11,11,12	0.89	0	15,15,17	1.51	2 (13%)
9	NAG	w	1	9	14,14,15	0.21	0	17,19,21	0.53	0
9	NAG	w	2	9	14,14,15	0.21	0	17,19,21	0.57	0
9	BMA	w	3	9	11,11,12	0.72	0	15,15,17	0.81	0
9	MAN	w	4	9	11,11,12	0.77	0	15,15,17	1.05	2 (13%)
9	MAN	w	5	9	11,11,12	0.68	0	15,15,17	1.09	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	x	1	4,12	14,14,15	0.54	0	17,19,21	1.13	1 (5%)
12	NAG	x	2	12	14,14,15	0.25	0	17,19,21	0.57	0
12	BMA	x	3	12	11,11,12	0.58	0	15,15,17	0.84	1 (6%)
10	NAG	y	1	10	14,14,15	0.39	0	17,19,21	0.55	0
10	NAG	y	2	10	14,14,15	0.31	0	17,19,21	0.55	0
12	NAG	z	1	12	14,14,15	0.20	0	17,19,21	0.53	0
12	NAG	z	2	12	14,14,15	0.23	0	17,19,21	0.57	0
12	BMA	z	3	12	11,11,12	0.73	0	15,15,17	1.01	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	0	1	13	-	0/6/23/26	0/1/1/1
13	NAG	0	2	13	-	2/6/23/26	0/1/1/1
13	BMA	0	3	13	-	0/2/19/22	0/1/1/1
13	MAN	0	4	13	-	2/2/19/22	0/1/1/1
13	MAN	0	5	13	-	2/2/19/22	0/1/1/1
13	MAN	0	6	13	-	2/2/19/22	0/1/1/1
10	NAG	5	1	4,10	-	2/6/23/26	0/1/1/1
10	NAG	5	2	10	-	0/6/23/26	0/1/1/1
10	NAG	7	1	10	-	1/6/23/26	0/1/1/1
10	NAG	7	2	10	-	2/6/23/26	0/1/1/1
12	NAG	8	1	4,12	-	0/6/23/26	0/1/1/1
12	NAG	8	2	12	-	2/6/23/26	0/1/1/1
12	BMA	8	3	12	-	2/2/19/22	0/1/1/1
9	NAG	9	1	9,4	-	2/6/23/26	0/1/1/1
9	NAG	9	2	9	-	2/6/23/26	0/1/1/1
9	BMA	9	3	9	-	0/2/19/22	0/1/1/1
9	MAN	9	4	9	-	1/2/19/22	0/1/1/1
9	MAN	9	5	9	-	0/2/19/22	0/1/1/1
12	NAG	AA	1	4,12	-	2/6/23/26	0/1/1/1
12	NAG	AA	2	12	-	1/6/23/26	0/1/1/1
12	BMA	AA	3	12	-	0/2/19/22	0/1/1/1
11	NAG	BA	1	11	-	2/6/23/26	0/1/1/1
11	NAG	BA	2	11	-	1/6/23/26	0/1/1/1
11	BMA	BA	3	11	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	BA	4	11	-	0/2/19/22	0/1/1/1
11	NAG	CA	1	11	-	2/6/23/26	0/1/1/1
11	NAG	CA	2	11	-	1/6/23/26	0/1/1/1
11	BMA	CA	3	11	-	2/2/19/22	0/1/1/1
11	MAN	CA	4	11	-	0/2/19/22	0/1/1/1
11	NAG	DA	1	11	-	2/6/23/26	0/1/1/1
11	NAG	DA	2	11	-	1/6/23/26	0/1/1/1
11	BMA	DA	3	11	-	2/2/19/22	0/1/1/1
11	MAN	DA	4	11	-	0/2/19/22	0/1/1/1
9	NAG	F	1	9,4	-	2/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
9	BMA	F	3	9	-	0/2/19/22	0/1/1/1
9	MAN	F	4	9	-	2/2/19/22	0/1/1/1
9	MAN	F	5	9	-	2/2/19/22	0/1/1/1
10	NAG	G	1	10	-	2/6/23/26	0/1/1/1
10	NAG	G	2	10	-	2/6/23/26	0/1/1/1
11	NAG	I	1	11	-	1/6/23/26	0/1/1/1
11	NAG	I	2	11	-	0/6/23/26	0/1/1/1
11	BMA	I	3	11	-	0/2/19/22	0/1/1/1
11	MAN	I	4	11	-	0/2/19/22	0/1/1/1
9	NAG	J	1	9	-	2/6/23/26	0/1/1/1
9	NAG	J	2	9	-	0/6/23/26	0/1/1/1
9	BMA	J	3	9	-	2/2/19/22	0/1/1/1
9	MAN	J	4	9	-	1/2/19/22	0/1/1/1
9	MAN	J	5	9	-	0/2/19/22	0/1/1/1
12	NAG	K	1	4,12	-	3/6/23/26	0/1/1/1
12	NAG	K	2	12	-	0/6/23/26	0/1/1/1
12	BMA	K	3	12	-	0/2/19/22	0/1/1/1
10	NAG	O	1	10	-	0/6/23/26	0/1/1/1
10	NAG	O	2	10	-	2/6/23/26	0/1/1/1
12	NAG	P	1	12	-	2/6/23/26	0/1/1/1
12	NAG	P	2	12	-	0/6/23/26	0/1/1/1
12	BMA	P	3	12	-	2/2/19/22	0/1/1/1
13	NAG	S	1	13	-	0/6/23/26	0/1/1/1
13	NAG	S	2	13	-	2/6/23/26	0/1/1/1
13	BMA	S	3	13	-	0/2/19/22	0/1/1/1
13	MAN	S	4	13	-	2/2/19/22	0/1/1/1
13	MAN	S	5	13	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MAN	S	6	13	-	2/2/19/22	0/1/1/1
10	NAG	T	1	4,10	-	2/6/23/26	0/1/1/1
10	NAG	T	2	10	-	1/6/23/26	0/1/1/1
10	NAG	U	1	10	-	1/6/23/26	0/1/1/1
10	NAG	U	2	10	-	2/6/23/26	0/1/1/1
12	NAG	V	1	4,12	-	0/6/23/26	0/1/1/1
12	NAG	V	2	12	-	2/6/23/26	0/1/1/1
12	BMA	V	3	12	-	2/2/19/22	0/1/1/1
9	NAG	W	1	9,4	-	2/6/23/26	0/1/1/1
9	NAG	W	2	9	-	2/6/23/26	0/1/1/1
9	BMA	W	3	9	-	0/2/19/22	0/1/1/1
9	MAN	W	4	9	-	1/2/19/22	0/1/1/1
9	MAN	W	5	9	-	0/2/19/22	0/1/1/1
12	NAG	b	1	4,12	-	2/6/23/26	0/1/1/1
12	NAG	b	2	12	-	1/6/23/26	0/1/1/1
12	BMA	b	3	12	-	0/2/19/22	0/1/1/1
11	NAG	c	1	4,11	-	2/6/23/26	0/1/1/1
11	NAG	c	2	11	-	2/6/23/26	0/1/1/1
11	BMA	c	3	11	-	1/2/19/22	0/1/1/1
11	MAN	c	4	11	-	2/2/19/22	0/1/1/1
10	NAG	d	1	10	-	2/6/23/26	0/1/1/1
10	NAG	d	2	10	-	2/6/23/26	0/1/1/1
11	NAG	e	1	11	-	1/6/23/26	0/1/1/1
11	NAG	e	2	11	-	1/6/23/26	0/1/1/1
11	BMA	e	3	11	-	0/2/19/22	0/1/1/1
11	MAN	e	4	11	-	0/2/19/22	0/1/1/1
9	NAG	j	1	9	-	2/6/23/26	0/1/1/1
9	NAG	j	2	9	-	0/6/23/26	0/1/1/1
9	BMA	j	3	9	-	2/2/19/22	0/1/1/1
9	MAN	j	4	9	-	1/2/19/22	0/1/1/1
9	MAN	j	5	9	-	0/2/19/22	0/1/1/1
12	NAG	k	1	4,12	-	2/6/23/26	0/1/1/1
12	NAG	k	2	12	-	0/6/23/26	0/1/1/1
12	BMA	k	3	12	-	0/2/19/22	0/1/1/1
10	NAG	l	1	10	-	0/6/23/26	0/1/1/1
10	NAG	l	2	10	-	2/6/23/26	0/1/1/1
12	NAG	m	1	12	-	2/6/23/26	0/1/1/1
12	NAG	m	2	12	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BMA	m	3	12	-	2/2/19/22	0/1/1/1
13	NAG	n	1	13	-	0/6/23/26	0/1/1/1
13	NAG	n	2	13	-	2/6/23/26	0/1/1/1
13	BMA	n	3	13	-	0/2/19/22	0/1/1/1
13	MAN	n	4	13	-	2/2/19/22	0/1/1/1
13	MAN	n	5	13	-	2/2/19/22	0/1/1/1
13	MAN	n	6	13	-	2/2/19/22	0/1/1/1
10	NAG	o	1	4,10	-	1/6/23/26	0/1/1/1
10	NAG	o	2	10	-	0/6/23/26	0/1/1/1
10	NAG	p	1	10	-	1/6/23/26	0/1/1/1
10	NAG	p	2	10	-	2/6/23/26	0/1/1/1
12	NAG	q	1	4,12	-	0/6/23/26	0/1/1/1
12	NAG	q	2	12	-	2/6/23/26	0/1/1/1
12	BMA	q	3	12	-	2/2/19/22	0/1/1/1
9	NAG	r	1	9,4	-	2/6/23/26	0/1/1/1
9	NAG	r	2	9	-	2/6/23/26	0/1/1/1
9	BMA	r	3	9	-	0/2/19/22	0/1/1/1
9	MAN	r	4	9	-	1/2/19/22	0/1/1/1
9	MAN	r	5	9	-	0/2/19/22	0/1/1/1
12	NAG	s	1	4,12	-	2/6/23/26	0/1/1/1
12	NAG	s	2	12	-	1/6/23/26	0/1/1/1
12	BMA	s	3	12	-	0/2/19/22	0/1/1/1
9	NAG	t	1	9,4	-	0/6/23/26	0/1/1/1
9	NAG	t	2	9	-	2/6/23/26	0/1/1/1
9	BMA	t	3	9	-	0/2/19/22	0/1/1/1
9	MAN	t	4	9	-	2/2/19/22	0/1/1/1
9	MAN	t	5	9	-	2/2/19/22	0/1/1/1
10	NAG	u	1	10	-	2/6/23/26	0/1/1/1
10	NAG	u	2	10	-	2/6/23/26	0/1/1/1
11	NAG	v	1	11	-	1/6/23/26	0/1/1/1
11	NAG	v	2	11	-	0/6/23/26	0/1/1/1
11	BMA	v	3	11	-	0/2/19/22	0/1/1/1
11	MAN	v	4	11	-	0/2/19/22	0/1/1/1
9	NAG	w	1	9	-	2/6/23/26	0/1/1/1
9	NAG	w	2	9	-	0/6/23/26	0/1/1/1
9	BMA	w	3	9	-	2/2/19/22	0/1/1/1
9	MAN	w	4	9	-	1/2/19/22	0/1/1/1
9	MAN	w	5	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	x	1	4,12	-	2/6/23/26	0/1/1/1
12	NAG	x	2	12	-	0/6/23/26	0/1/1/1
12	BMA	x	3	12	-	0/2/19/22	0/1/1/1
10	NAG	y	1	10	-	0/6/23/26	0/1/1/1
10	NAG	y	2	10	-	2/6/23/26	0/1/1/1
12	NAG	z	1	12	-	2/6/23/26	0/1/1/1
12	NAG	z	2	12	-	0/6/23/26	0/1/1/1
12	BMA	z	3	12	-	2/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	t	3	BMA	O5-C1	-3.02	1.38	1.43
9	t	4	MAN	C1-C2	2.66	1.58	1.52
10	u	1	NAG	O5-C1	-2.51	1.39	1.43
10	G	1	NAG	O5-C1	-2.48	1.39	1.43
10	d	1	NAG	O5-C1	-2.47	1.39	1.43
11	c	4	MAN	O5-C1	-2.27	1.39	1.43
11	c	4	MAN	C1-C2	2.11	1.57	1.52
12	k	1	NAG	C1-C2	2.04	1.55	1.52

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	v	4	MAN	C1-O5-C5	5.11	119.03	112.19
11	I	4	MAN	C1-O5-C5	5.08	119.00	112.19
11	e	4	MAN	C1-O5-C5	5.00	118.89	112.19
13	n	4	MAN	C1-O5-C5	3.96	117.49	112.19
13	0	4	MAN	C1-O5-C5	3.91	117.43	112.19
13	S	4	MAN	C1-O5-C5	3.87	117.37	112.19
11	e	3	BMA	C1-O5-C5	3.85	117.34	112.19
11	I	3	BMA	C1-O5-C5	3.83	117.31	112.19
11	v	3	BMA	C1-O5-C5	3.79	117.26	112.19
13	n	5	MAN	C1-O5-C5	3.70	117.14	112.19
13	S	5	MAN	C1-O5-C5	3.66	117.09	112.19
13	0	5	MAN	C1-O5-C5	3.65	117.08	112.19
9	F	4	MAN	C1-O5-C5	3.61	117.03	112.19
11	c	2	NAG	C1-O5-C5	3.44	116.80	112.19
10	G	1	NAG	C2-N2-C7	3.39	127.44	122.90
12	V	3	BMA	C1-O5-C5	3.38	116.71	112.19
10	u	1	NAG	C2-N2-C7	3.35	127.39	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	d	1	NAG	C2-N2-C7	3.34	127.38	122.90
12	q	3	BMA	C1-O5-C5	3.33	116.65	112.19
12	8	3	BMA	C1-O5-C5	3.30	116.61	112.19
12	AA	1	NAG	C1-O5-C5	3.25	116.55	112.19
12	b	1	NAG	C3-C4-C5	3.24	116.11	110.23
11	CA	4	MAN	C1-O5-C5	3.24	116.52	112.19
12	s	1	NAG	C3-C4-C5	3.23	116.09	110.23
9	F	3	BMA	C1-O5-C5	3.22	116.50	112.19
9	j	5	MAN	C1-O5-C5	3.19	116.46	112.19
11	BA	4	MAN	C1-O5-C5	3.17	116.43	112.19
12	AA	1	NAG	C3-C4-C5	3.13	115.91	110.23
12	s	1	NAG	C1-O5-C5	3.12	116.36	112.19
12	b	1	NAG	C1-O5-C5	3.07	116.31	112.19
9	w	5	MAN	C1-O5-C5	3.06	116.29	112.19
12	x	1	NAG	C2-N2-C7	3.06	127.00	122.90
12	K	1	NAG	C2-N2-C7	3.06	127.00	122.90
11	DA	4	MAN	C1-O5-C5	3.05	116.27	112.19
12	k	1	NAG	C2-N2-C7	3.03	126.97	122.90
9	J	5	MAN	C1-O5-C5	3.02	116.24	112.19
9	F	5	MAN	C1-O5-C5	2.89	116.05	112.19
9	t	4	MAN	O2-C2-C3	-2.85	104.25	110.15
11	e	2	NAG	C1-O5-C5	2.82	115.96	112.19
11	I	2	NAG	C1-O5-C5	2.79	115.93	112.19
12	m	3	BMA	C1-O5-C5	2.79	115.93	112.19
12	P	3	BMA	C1-O5-C5	2.76	115.89	112.19
12	z	3	BMA	C1-O5-C5	2.75	115.87	112.19
11	v	2	NAG	C1-O5-C5	2.75	115.87	112.19
9	t	5	MAN	O2-C2-C3	-2.73	104.49	110.15
9	r	5	MAN	C1-O5-C5	2.70	115.81	112.19
9	9	5	MAN	C1-O5-C5	2.69	115.79	112.19
9	t	5	MAN	C1-O5-C5	2.65	115.74	112.19
9	W	5	MAN	C1-O5-C5	2.65	115.74	112.19
9	9	2	NAG	C1-O5-C5	2.62	115.69	112.19
9	W	2	NAG	C1-O5-C5	2.58	115.64	112.19
9	t	3	BMA	C1-O5-C5	2.56	115.62	112.19
9	W	4	MAN	C1-O5-C5	2.56	115.61	112.19
9	r	2	NAG	C1-O5-C5	2.54	115.59	112.19
11	c	1	NAG	O4-C4-C5	-2.51	103.14	109.32
9	r	4	MAN	C1-O5-C5	2.48	115.50	112.19
9	9	4	MAN	C1-O5-C5	2.45	115.47	112.19
9	F	5	MAN	O2-C2-C3	-2.45	105.08	110.15
11	c	4	MAN	O2-C2-C3	-2.40	105.17	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	1	NAG	O4-C4-C5	-2.39	103.43	109.32
12	V	3	BMA	O2-C2-C3	-2.38	105.22	110.15
12	8	3	BMA	O2-C2-C3	-2.38	105.22	110.15
12	q	3	BMA	O2-C2-C3	-2.37	105.24	110.15
13	n	6	MAN	O2-C2-C3	-2.37	105.24	110.15
13	0	6	MAN	O2-C2-C3	-2.37	105.25	110.15
9	9	2	NAG	O4-C4-C3	2.36	115.94	110.38
13	S	6	MAN	O2-C2-C3	-2.36	105.27	110.15
9	W	3	BMA	C1-O5-C5	2.36	115.34	112.19
12	s	3	BMA	C1-O5-C5	2.35	115.34	112.19
13	0	4	MAN	O2-C2-C3	-2.34	105.31	110.15
9	W	5	MAN	O2-C2-C3	-2.33	105.32	110.15
9	w	4	MAN	C1-O5-C5	2.33	115.31	112.19
9	F	2	NAG	C1-O5-C5	2.33	115.30	112.19
9	W	2	NAG	O4-C4-C3	2.32	115.86	110.38
13	S	6	MAN	C1-O5-C5	2.32	115.30	112.19
13	n	4	MAN	O2-C2-C3	-2.32	105.35	110.15
9	9	5	MAN	O2-C2-C3	-2.31	105.36	110.15
13	S	4	MAN	O2-C2-C3	-2.30	105.38	110.15
9	w	5	MAN	O2-C2-C3	-2.30	105.39	110.15
11	c	1	NAG	C1-O5-C5	2.30	115.26	112.19
9	r	5	MAN	O2-C2-C3	-2.29	105.40	110.15
9	r	2	NAG	O4-C4-C3	2.29	115.78	110.38
12	AA	3	BMA	C1-O5-C5	2.27	115.23	112.19
9	J	5	MAN	O2-C2-C3	-2.26	105.47	110.15
9	j	5	MAN	O2-C2-C3	-2.26	105.47	110.15
12	b	3	BMA	C1-O5-C5	2.26	115.22	112.19
9	J	4	MAN	C1-O5-C5	2.24	115.18	112.19
9	9	3	BMA	C1-O5-C5	2.24	115.18	112.19
9	r	3	BMA	C1-O5-C5	2.23	115.17	112.19
13	0	6	MAN	C1-O5-C5	2.23	115.17	112.19
9	t	3	BMA	O2-C2-C3	-2.22	105.56	110.15
11	I	4	MAN	O2-C2-C3	-2.21	105.57	110.15
9	t	1	NAG	C1-O5-C5	2.20	115.14	112.19
9	w	4	MAN	O2-C2-C3	-2.20	105.60	110.15
11	CA	2	NAG	C1-O5-C5	2.20	115.13	112.19
11	e	4	MAN	O2-C2-C3	-2.19	105.61	110.15
9	J	4	MAN	O2-C2-C3	-2.19	105.61	110.15
9	j	4	MAN	O2-C2-C3	-2.18	105.63	110.15
13	n	6	MAN	C1-O5-C5	2.18	115.10	112.19
11	v	4	MAN	O2-C2-C3	-2.17	105.66	110.15
11	BA	4	MAN	O2-C2-C3	-2.16	105.68	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	DA	4	MAN	O2-C2-C3	-2.16	105.68	110.15
11	BA	2	NAG	C1-O5-C5	2.16	115.08	112.19
9	j	4	MAN	C1-O5-C5	2.15	115.07	112.19
11	CA	4	MAN	O2-C2-C3	-2.15	105.69	110.15
13	0	5	MAN	O2-C2-C3	-2.12	105.76	110.15
13	n	5	MAN	O2-C2-C3	-2.12	105.77	110.15
11	DA	2	NAG	C1-O5-C5	2.11	115.02	112.19
12	K	3	BMA	C1-O5-C5	2.10	115.00	112.19
9	r	4	MAN	O2-C2-C3	-2.08	105.84	110.15
9	t	2	NAG	C1-O5-C5	2.08	114.97	112.19
13	n	3	BMA	C1-O5-C5	2.08	114.97	112.19
13	S	5	MAN	O2-C2-C3	-2.07	105.86	110.15
9	F	4	MAN	O2-C2-C3	-2.06	105.88	110.15
9	W	4	MAN	O2-C2-C3	-2.06	105.89	110.15
9	F	3	BMA	O2-C2-C3	-2.06	105.89	110.15
13	0	3	BMA	C1-O5-C5	2.05	114.94	112.19
13	S	3	BMA	C1-O5-C5	2.05	114.94	112.19
12	k	3	BMA	C1-O5-C5	2.05	114.93	112.19
12	AA	1	NAG	C4-C3-C2	2.04	114.01	111.02
12	b	1	NAG	C4-C3-C2	2.04	114.00	111.02
12	x	3	BMA	C1-O5-C5	2.03	114.91	112.19
9	9	4	MAN	O2-C2-C3	-2.03	105.94	110.15

There are no chirality outliers.

All (167) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	V	3	BMA	C4-C5-C6-O6
9	r	2	NAG	O5-C5-C6-O6
11	BA	1	NAG	O5-C5-C6-O6
11	DA	1	NAG	O5-C5-C6-O6
12	8	3	BMA	C4-C5-C6-O6
9	W	2	NAG	O5-C5-C6-O6
10	d	2	NAG	O5-C5-C6-O6
9	9	2	NAG	O5-C5-C6-O6
13	S	5	MAN	O5-C5-C6-O6
12	q	3	BMA	C4-C5-C6-O6
9	J	1	NAG	O5-C5-C6-O6
9	t	4	MAN	O5-C5-C6-O6
10	G	2	NAG	O5-C5-C6-O6
10	u	2	NAG	O5-C5-C6-O6
11	c	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	CA	1	NAG	O5-C5-C6-O6
12	P	1	NAG	O5-C5-C6-O6
12	V	2	NAG	O5-C5-C6-O6
12	m	1	NAG	O5-C5-C6-O6
12	z	1	NAG	O5-C5-C6-O6
9	W	2	NAG	C4-C5-C6-O6
9	9	2	NAG	C4-C5-C6-O6
9	w	1	NAG	O5-C5-C6-O6
12	q	2	NAG	O5-C5-C6-O6
12	8	2	NAG	O5-C5-C6-O6
9	r	2	NAG	C4-C5-C6-O6
10	G	2	NAG	C4-C5-C6-O6
10	u	2	NAG	C4-C5-C6-O6
12	s	1	NAG	C4-C5-C6-O6
12	AA	1	NAG	C4-C5-C6-O6
10	U	2	NAG	O5-C5-C6-O6
11	BA	1	NAG	C4-C5-C6-O6
11	CA	1	NAG	C4-C5-C6-O6
11	DA	1	NAG	C4-C5-C6-O6
9	j	1	NAG	O5-C5-C6-O6
10	7	2	NAG	O5-C5-C6-O6
13	0	5	MAN	O5-C5-C6-O6
12	V	2	NAG	C4-C5-C6-O6
10	p	2	NAG	O5-C5-C6-O6
13	n	5	MAN	O5-C5-C6-O6
10	d	2	NAG	C4-C5-C6-O6
12	b	1	NAG	C4-C5-C6-O6
13	0	4	MAN	O5-C5-C6-O6
12	q	3	BMA	O5-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
10	O	2	NAG	O5-C5-C6-O6
12	V	3	BMA	O5-C5-C6-O6
12	q	2	NAG	C4-C5-C6-O6
12	8	2	NAG	C4-C5-C6-O6
12	8	3	BMA	O5-C5-C6-O6
11	BA	3	BMA	C4-C5-C6-O6
11	DA	3	BMA	C4-C5-C6-O6
13	n	4	MAN	O5-C5-C6-O6
13	n	5	MAN	C4-C5-C6-O6
13	S	4	MAN	O5-C5-C6-O6
11	c	4	MAN	C4-C5-C6-O6
12	m	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	0	5	MAN	C4-C5-C6-O6
10	l	2	NAG	O5-C5-C6-O6
13	S	5	MAN	C4-C5-C6-O6
10	y	2	NAG	O5-C5-C6-O6
11	CA	3	BMA	C4-C5-C6-O6
12	P	1	NAG	C4-C5-C6-O6
12	z	1	NAG	C4-C5-C6-O6
12	b	1	NAG	O5-C5-C6-O6
12	s	1	NAG	O5-C5-C6-O6
9	t	4	MAN	C4-C5-C6-O6
12	AA	1	NAG	O5-C5-C6-O6
9	J	3	BMA	O5-C5-C6-O6
12	z	3	BMA	O5-C5-C6-O6
10	O	2	NAG	C4-C5-C6-O6
9	j	3	BMA	O5-C5-C6-O6
13	0	2	NAG	C4-C5-C6-O6
9	J	1	NAG	C4-C5-C6-O6
10	T	1	NAG	O5-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6
9	w	3	BMA	O5-C5-C6-O6
12	P	3	BMA	O5-C5-C6-O6
13	n	6	MAN	O5-C5-C6-O6
9	J	3	BMA	C4-C5-C6-O6
9	w	1	NAG	C4-C5-C6-O6
13	0	6	MAN	O5-C5-C6-O6
9	j	3	BMA	C4-C5-C6-O6
13	S	2	NAG	C4-C5-C6-O6
12	m	3	BMA	O5-C5-C6-O6
11	BA	3	BMA	O5-C5-C6-O6
11	DA	3	BMA	O5-C5-C6-O6
13	S	6	MAN	O5-C5-C6-O6
9	w	3	BMA	C4-C5-C6-O6
10	l	2	NAG	C4-C5-C6-O6
9	F	5	MAN	O5-C5-C6-O6
10	U	1	NAG	O5-C5-C6-O6
10	p	1	NAG	O5-C5-C6-O6
10	y	2	NAG	C4-C5-C6-O6
9	t	2	NAG	O5-C5-C6-O6
9	F	5	MAN	C4-C5-C6-O6
10	5	1	NAG	O5-C5-C6-O6
11	CA	3	BMA	O5-C5-C6-O6
9	t	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	7	2	NAG	C4-C5-C6-O6
13	n	2	NAG	C4-C5-C6-O6
9	j	1	NAG	C4-C5-C6-O6
9	w	4	MAN	O5-C5-C6-O6
9	J	4	MAN	O5-C5-C6-O6
10	7	1	NAG	O5-C5-C6-O6
11	c	2	NAG	O5-C5-C6-O6
10	U	2	NAG	C4-C5-C6-O6
9	j	4	MAN	O5-C5-C6-O6
13	0	2	NAG	O5-C5-C6-O6
10	p	2	NAG	C4-C5-C6-O6
9	9	1	NAG	C4-C5-C6-O6
9	r	1	NAG	C4-C5-C6-O6
13	S	2	NAG	O5-C5-C6-O6
9	t	5	MAN	O5-C5-C6-O6
10	o	1	NAG	O5-C5-C6-O6
9	r	4	MAN	O5-C5-C6-O6
9	W	4	MAN	O5-C5-C6-O6
9	9	4	MAN	O5-C5-C6-O6
11	CA	2	NAG	O5-C5-C6-O6
9	W	1	NAG	C4-C5-C6-O6
9	t	5	MAN	C4-C5-C6-O6
12	z	3	BMA	C4-C5-C6-O6
11	DA	2	NAG	O5-C5-C6-O6
11	I	1	NAG	O5-C5-C6-O6
11	v	1	NAG	O5-C5-C6-O6
9	F	4	MAN	C4-C5-C6-O6
12	b	2	NAG	O5-C5-C6-O6
12	AA	2	NAG	O5-C5-C6-O6
11	BA	2	NAG	O5-C5-C6-O6
12	s	2	NAG	O5-C5-C6-O6
11	e	1	NAG	O5-C5-C6-O6
12	P	3	BMA	C4-C5-C6-O6
13	n	2	NAG	O5-C5-C6-O6
9	F	4	MAN	O5-C5-C6-O6
12	m	3	BMA	C4-C5-C6-O6
13	0	4	MAN	C4-C5-C6-O6
13	n	6	MAN	C4-C5-C6-O6
9	r	1	NAG	O5-C5-C6-O6
11	c	1	NAG	C4-C5-C6-O6
9	9	1	NAG	O5-C5-C6-O6
13	0	6	MAN	C4-C5-C6-O6

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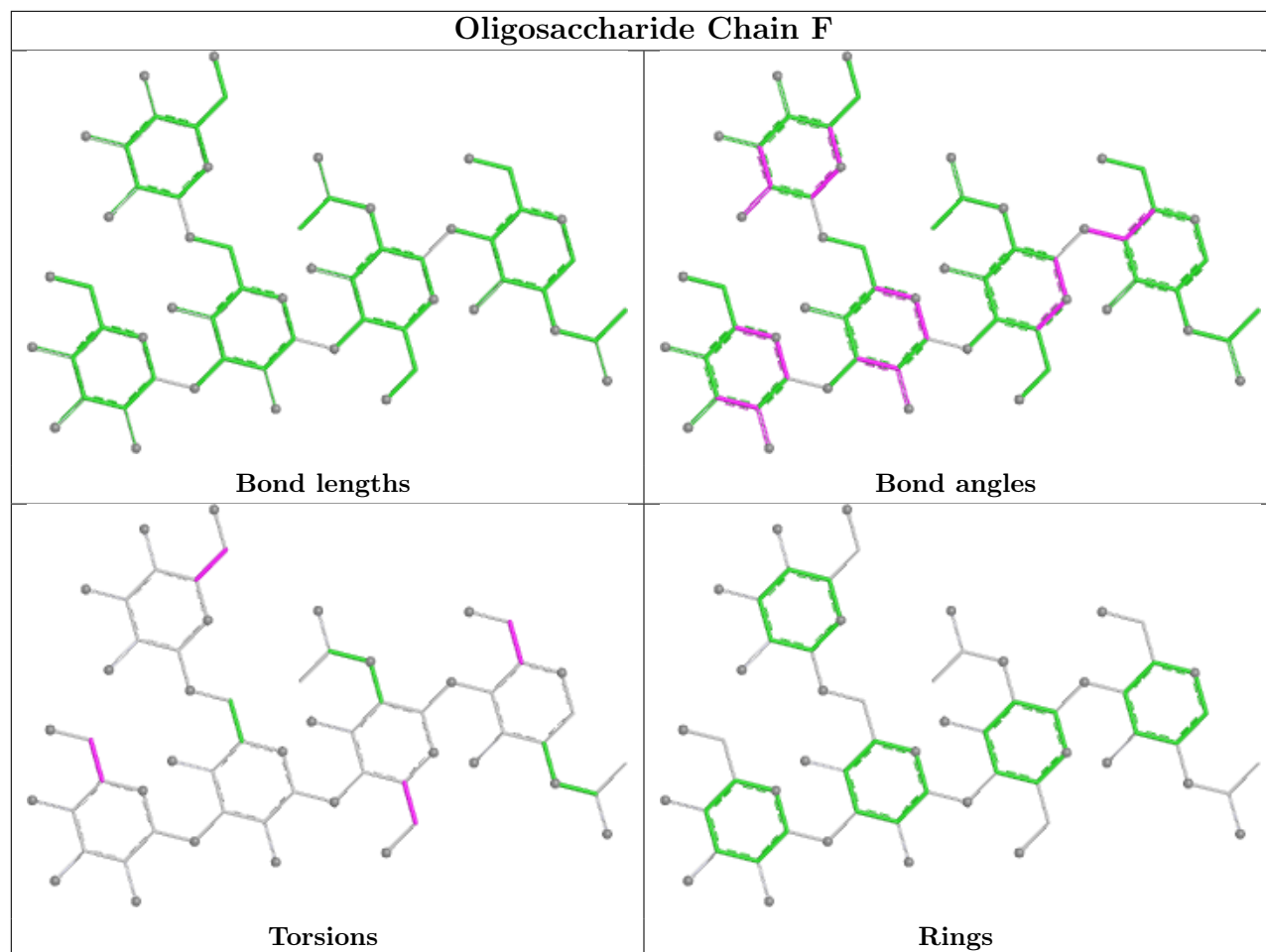
Mol	Chain	Res	Type	Atoms
10	G	1	NAG	C1-C2-N2-C7
10	d	1	NAG	C1-C2-N2-C7
10	u	1	NAG	C1-C2-N2-C7
13	n	4	MAN	C4-C5-C6-O6
13	S	6	MAN	C4-C5-C6-O6
13	S	4	MAN	C4-C5-C6-O6
9	W	1	NAG	O5-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6
10	G	1	NAG	C3-C2-N2-C7
10	d	1	NAG	C3-C2-N2-C7
10	u	1	NAG	C3-C2-N2-C7
12	K	1	NAG	C3-C2-N2-C7
11	c	1	NAG	O5-C5-C6-O6
10	T	1	NAG	C4-C5-C6-O6
10	T	2	NAG	C1-C2-N2-C7
10	5	1	NAG	C1-C2-N2-C7
11	e	2	NAG	C1-C2-N2-C7
12	K	1	NAG	C1-C2-N2-C7
12	k	1	NAG	C1-C2-N2-C7
12	x	1	NAG	C1-C2-N2-C7
12	k	1	NAG	C3-C2-N2-C7
12	x	1	NAG	C3-C2-N2-C7
11	c	2	NAG	C4-C5-C6-O6
9	F	1	NAG	O5-C5-C6-O6
12	K	1	NAG	C4-C5-C6-O6
11	c	3	BMA	O5-C5-C6-O6

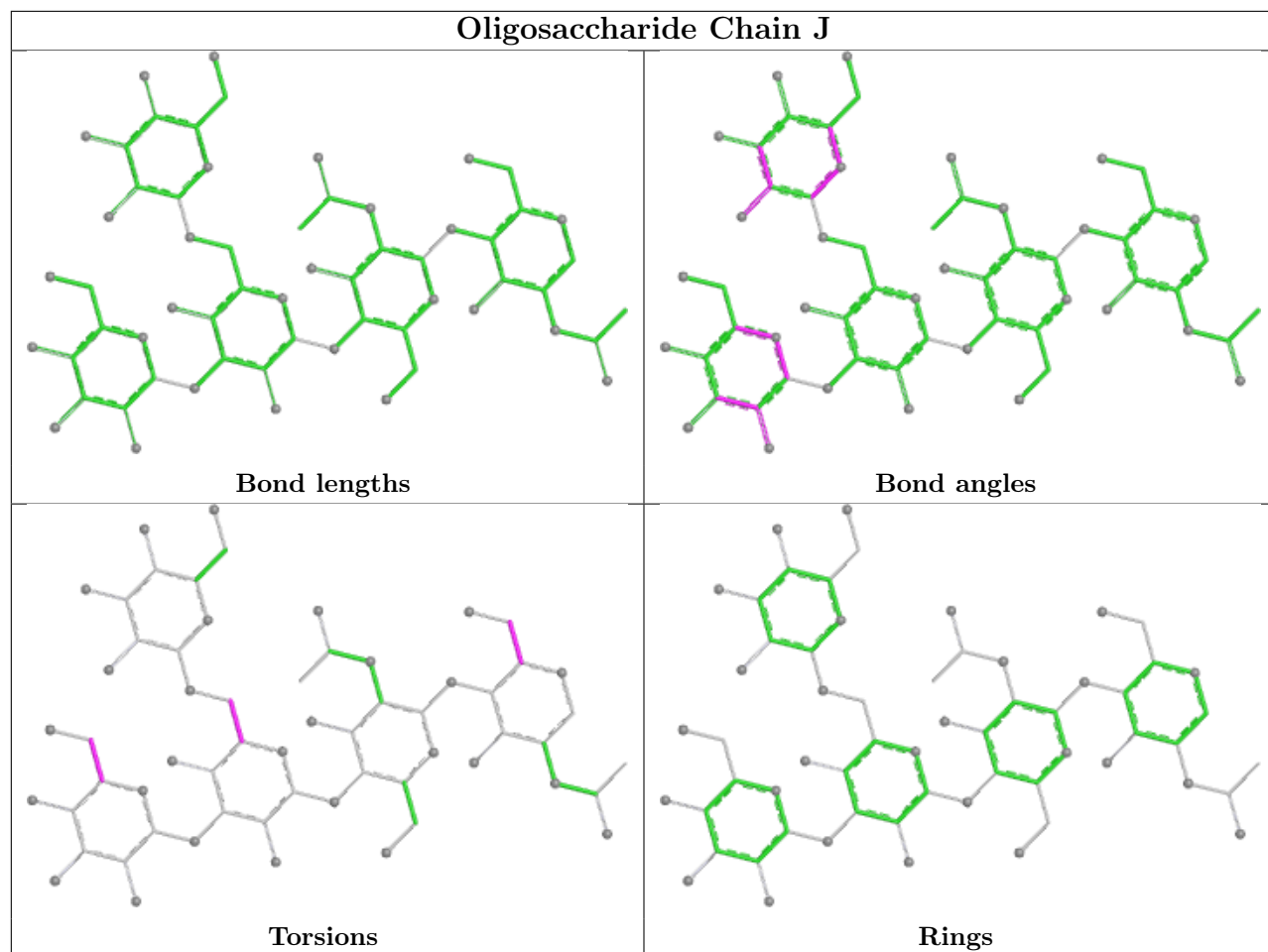
There are no ring outliers.

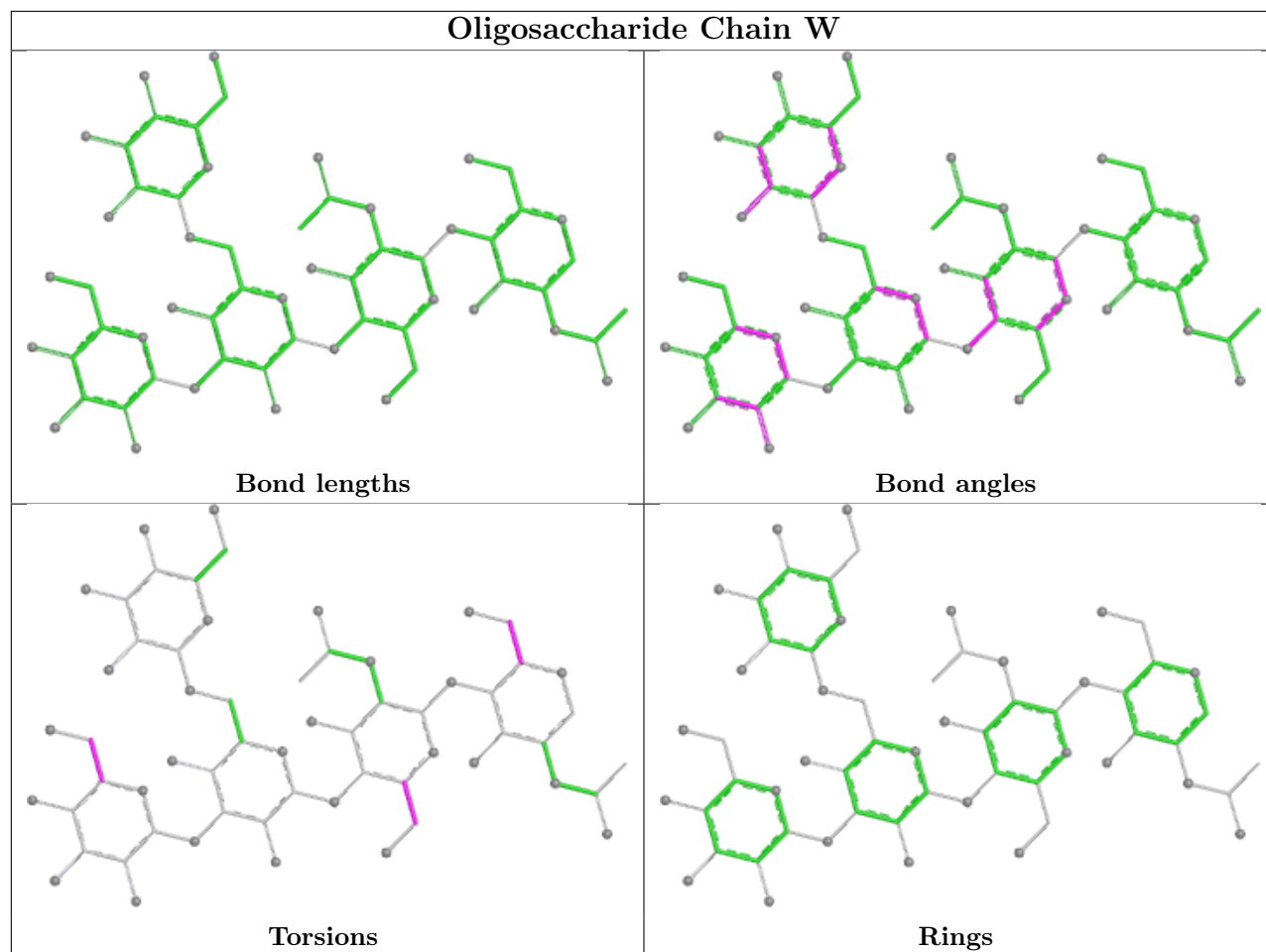
6 monomers are involved in 6 short contacts:

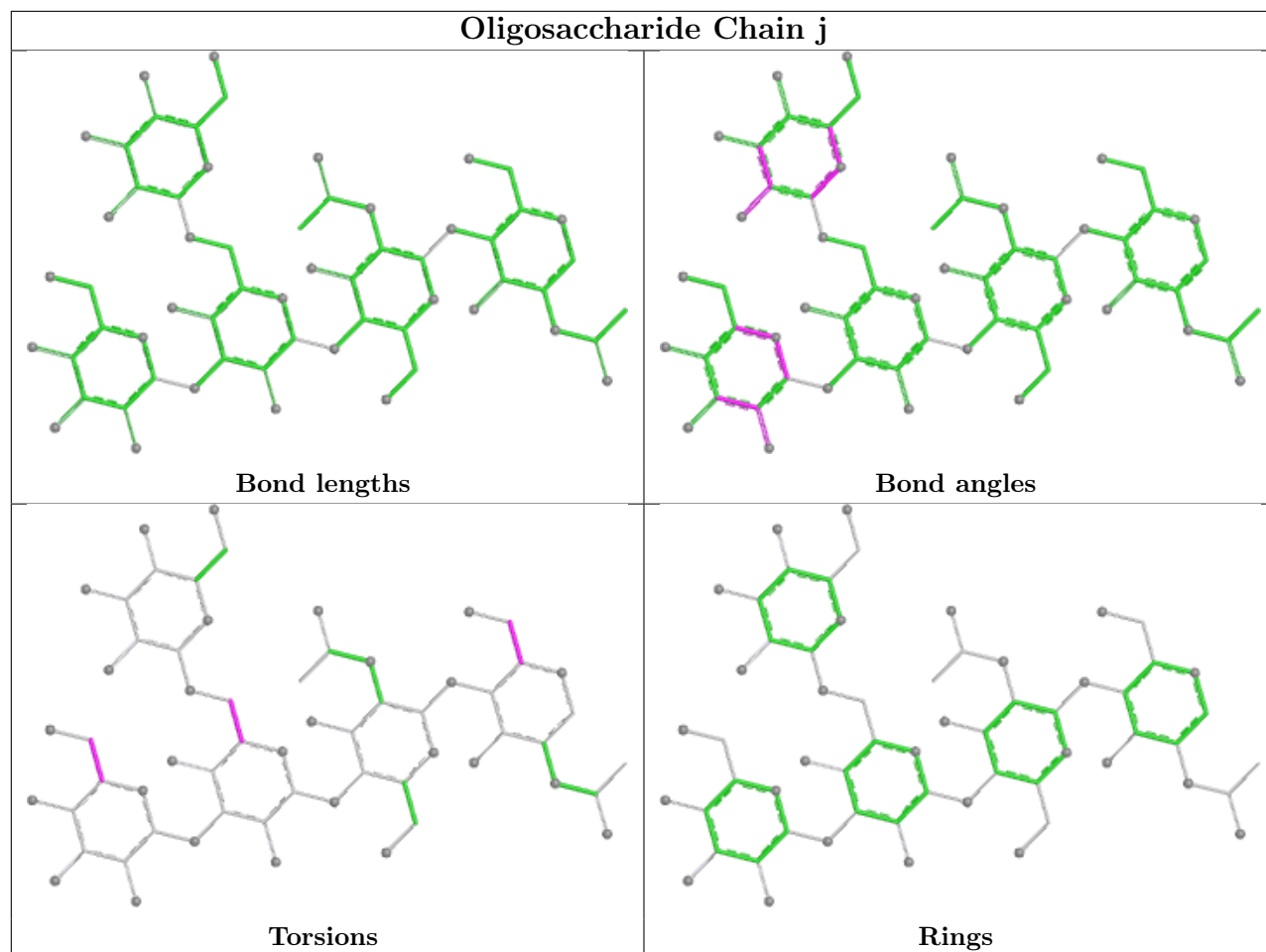
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	G	1	NAG	1	0
12	z	1	NAG	1	0
12	P	1	NAG	1	0
10	u	1	NAG	1	0
12	m	1	NAG	1	0
10	d	1	NAG	1	0

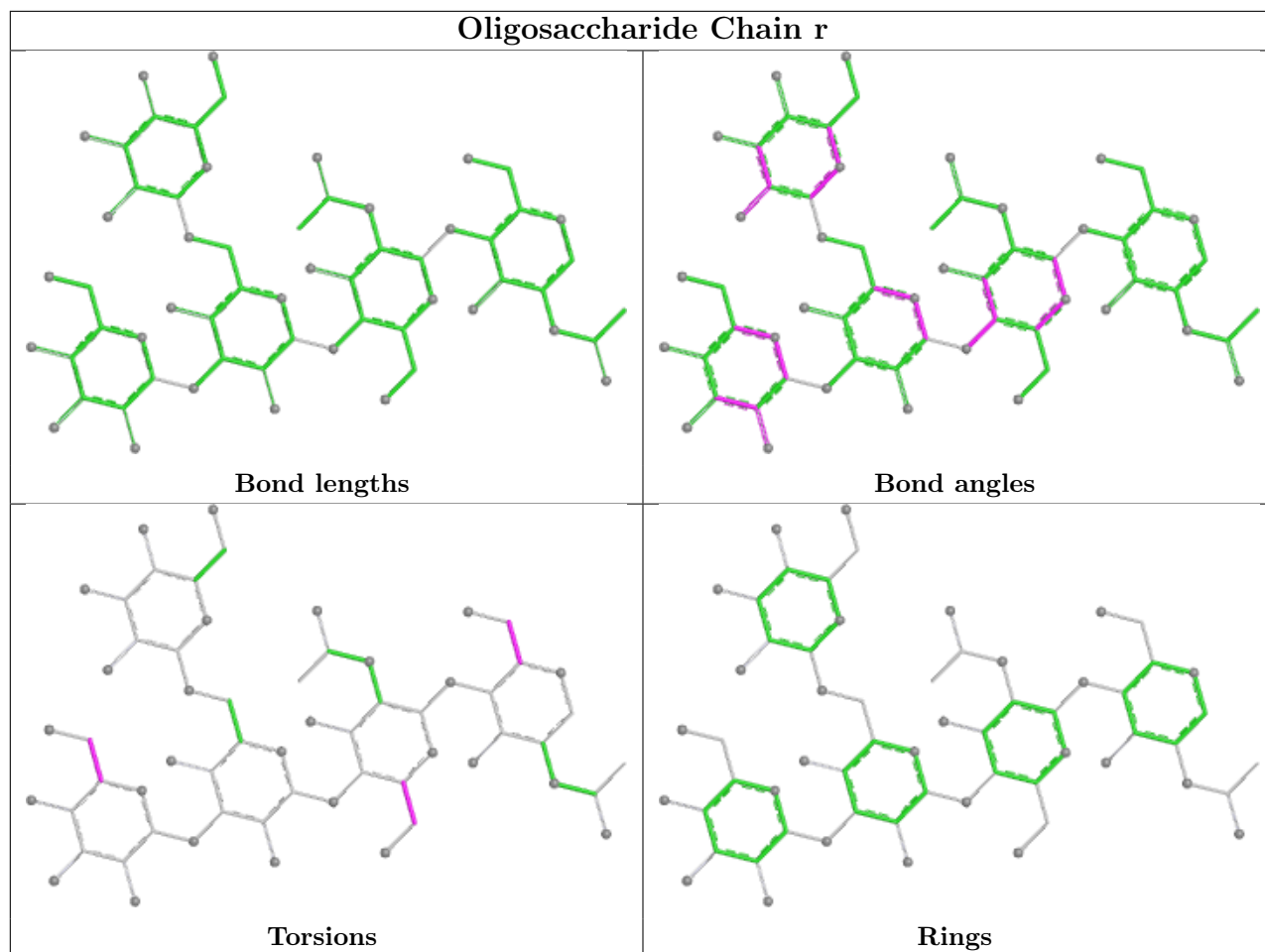
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

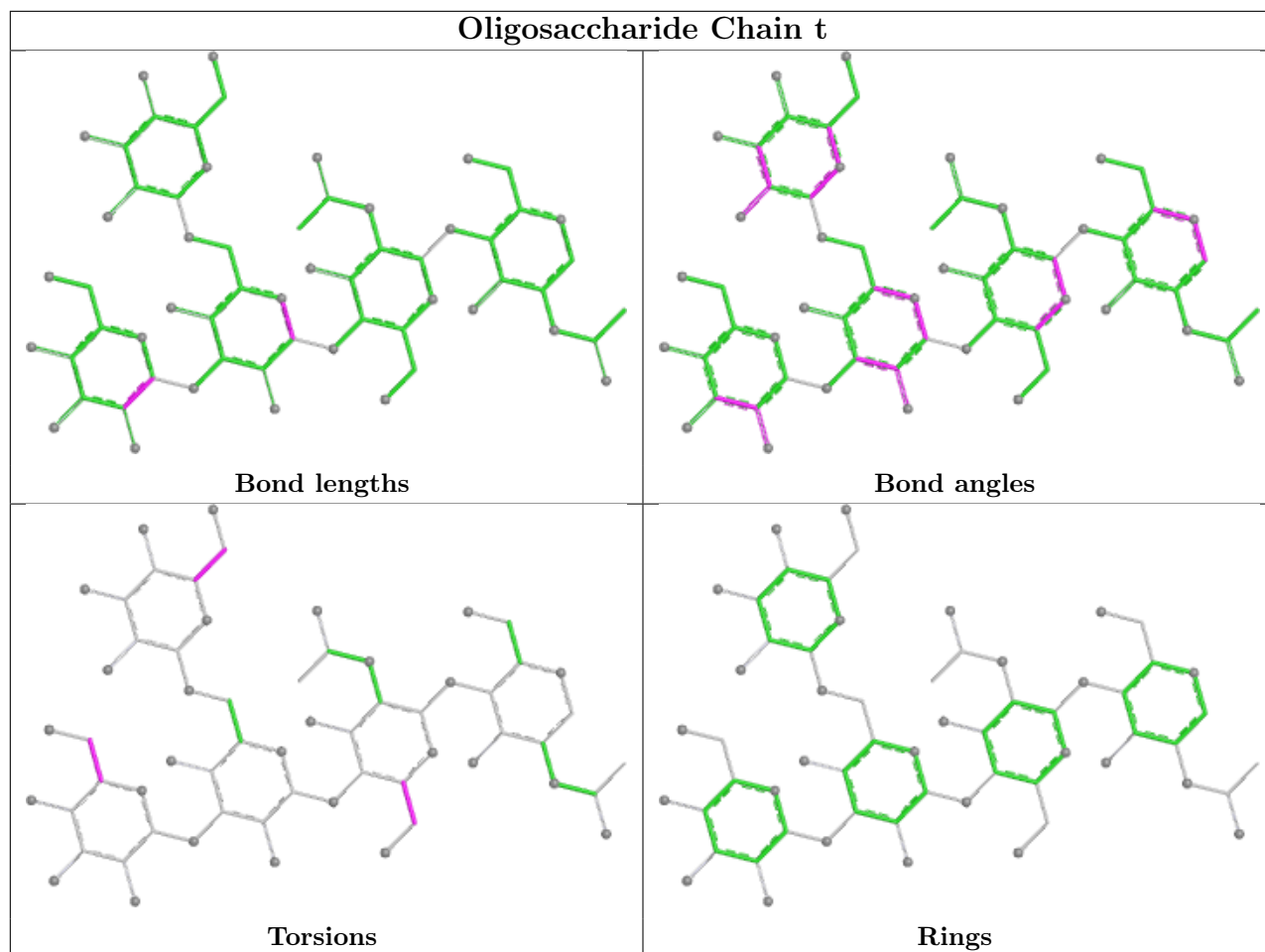


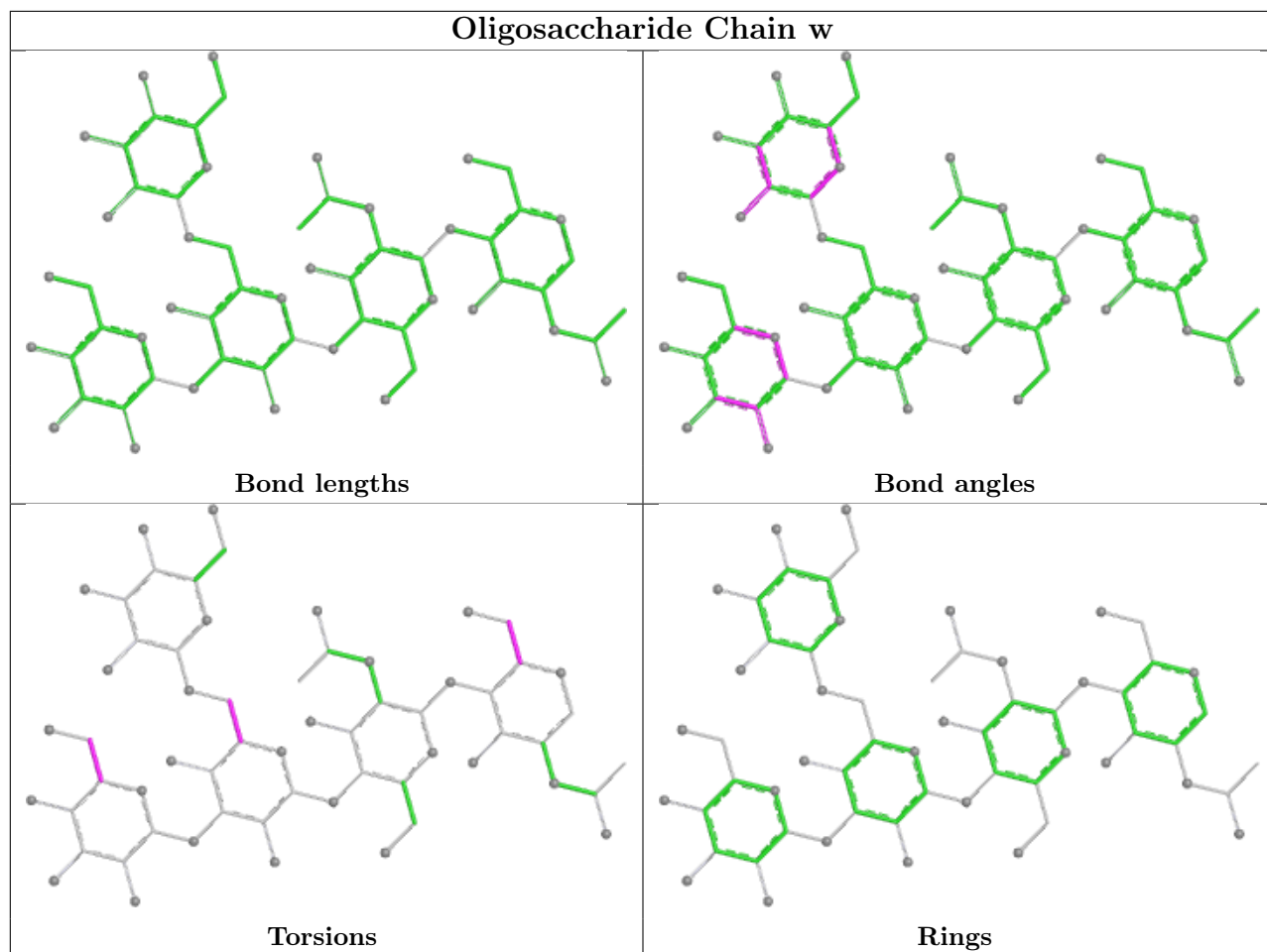


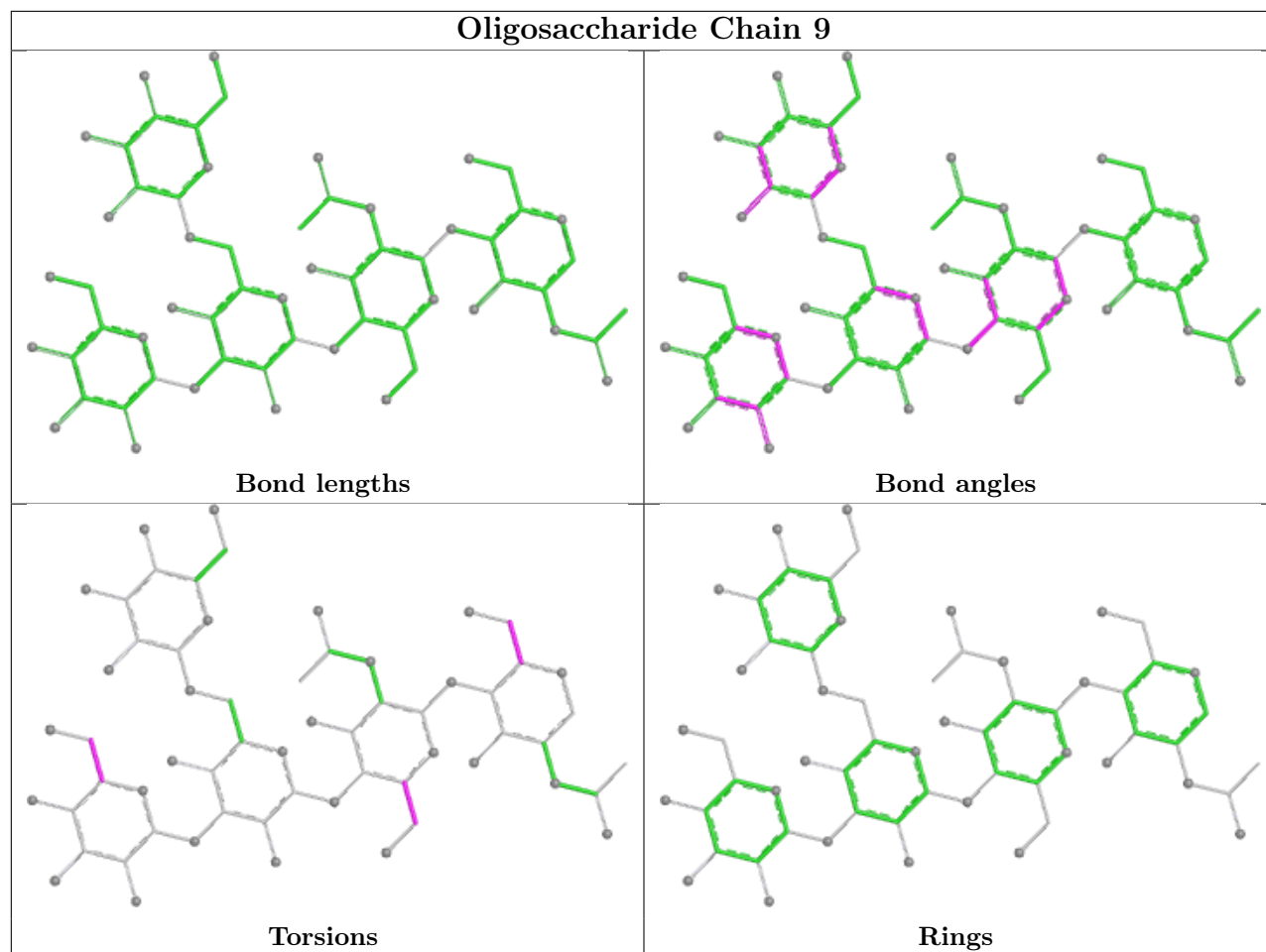


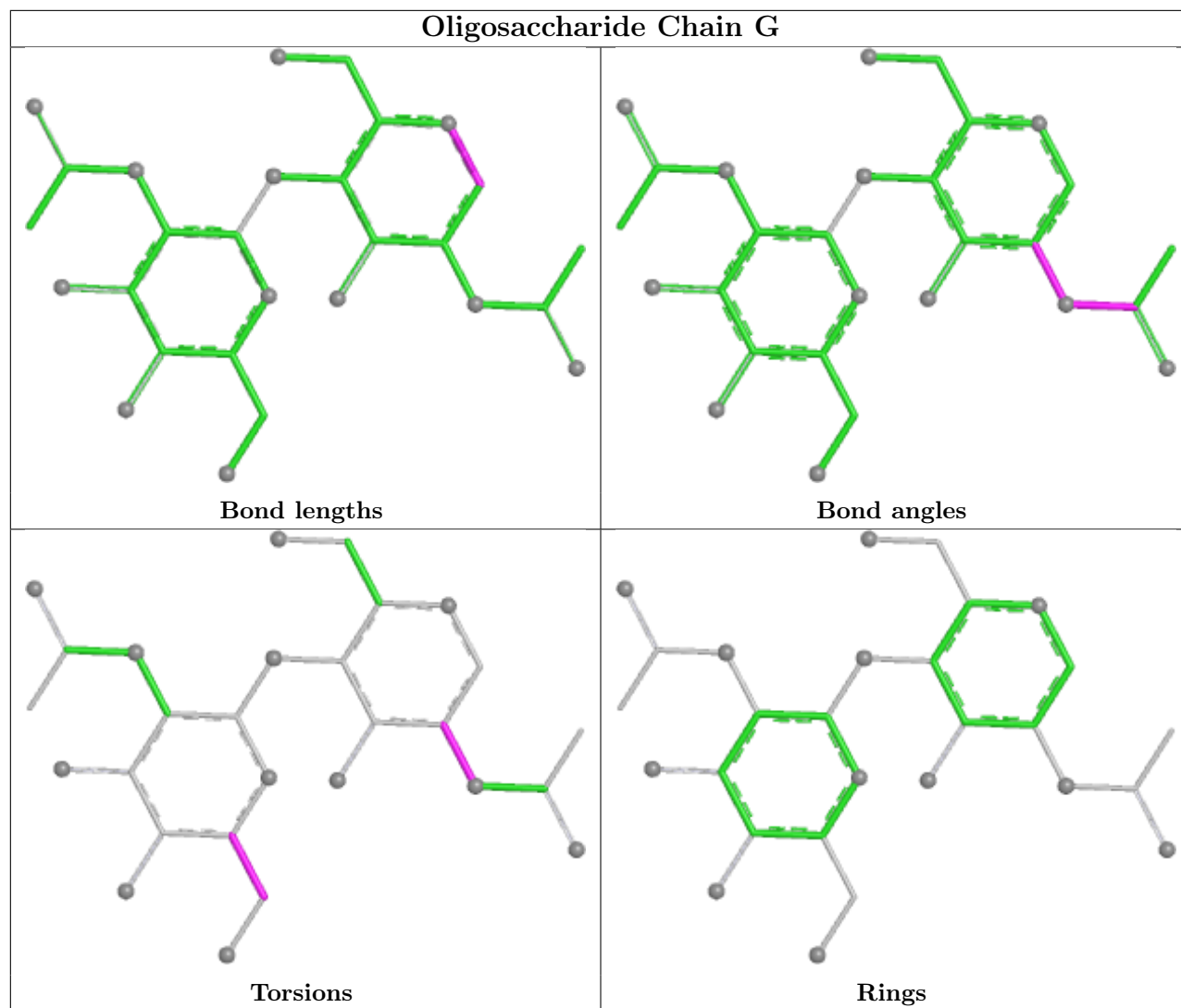


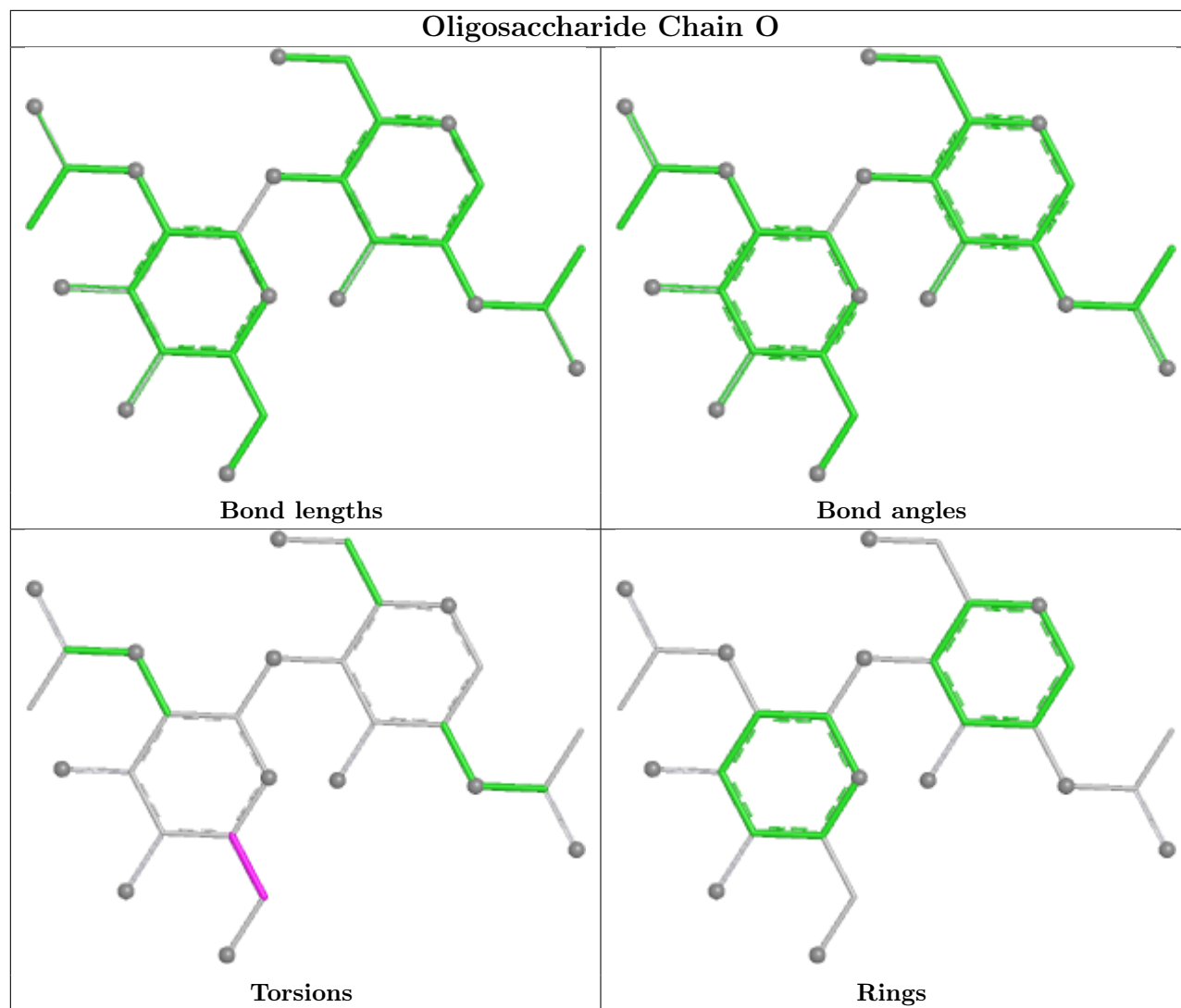


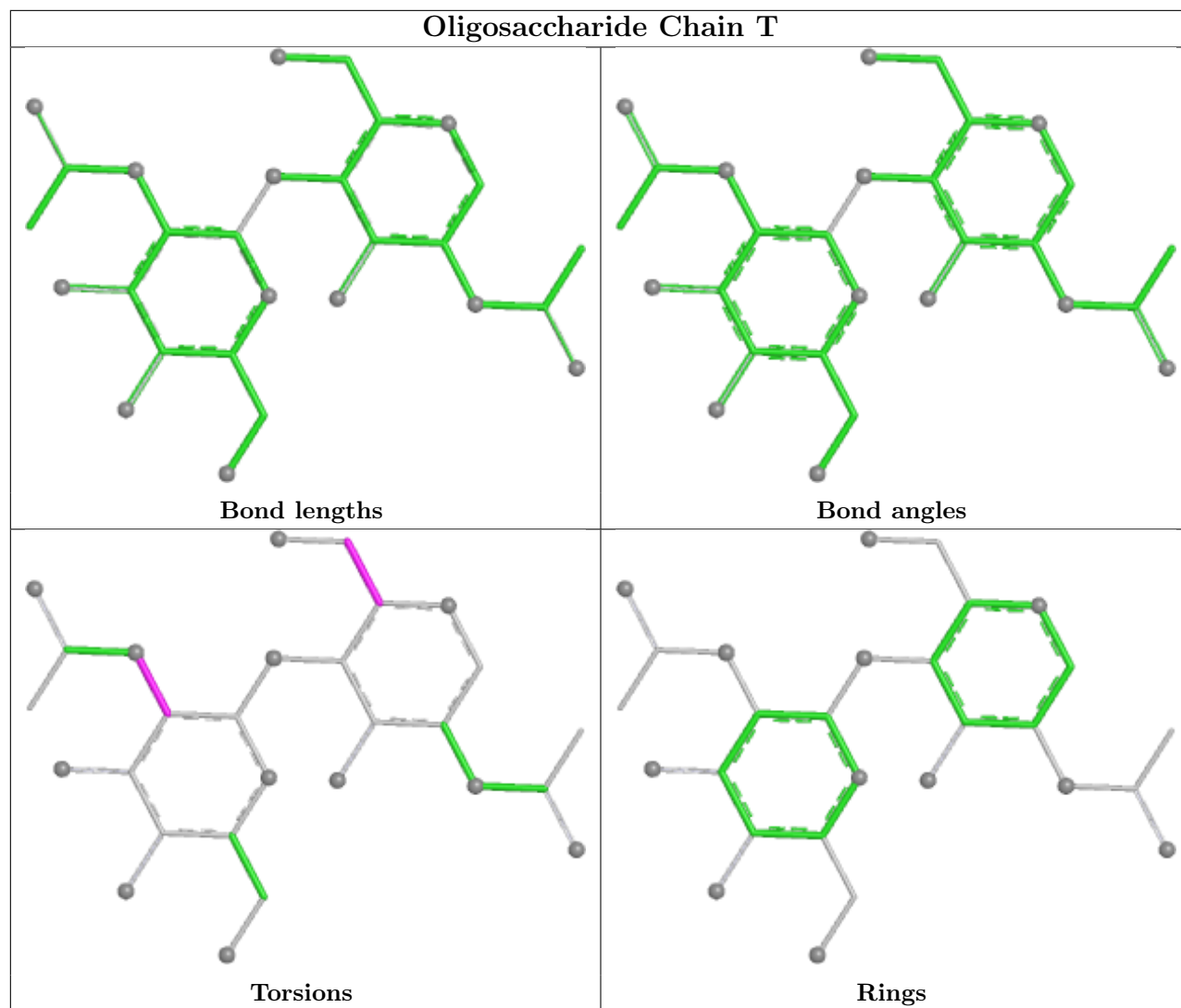


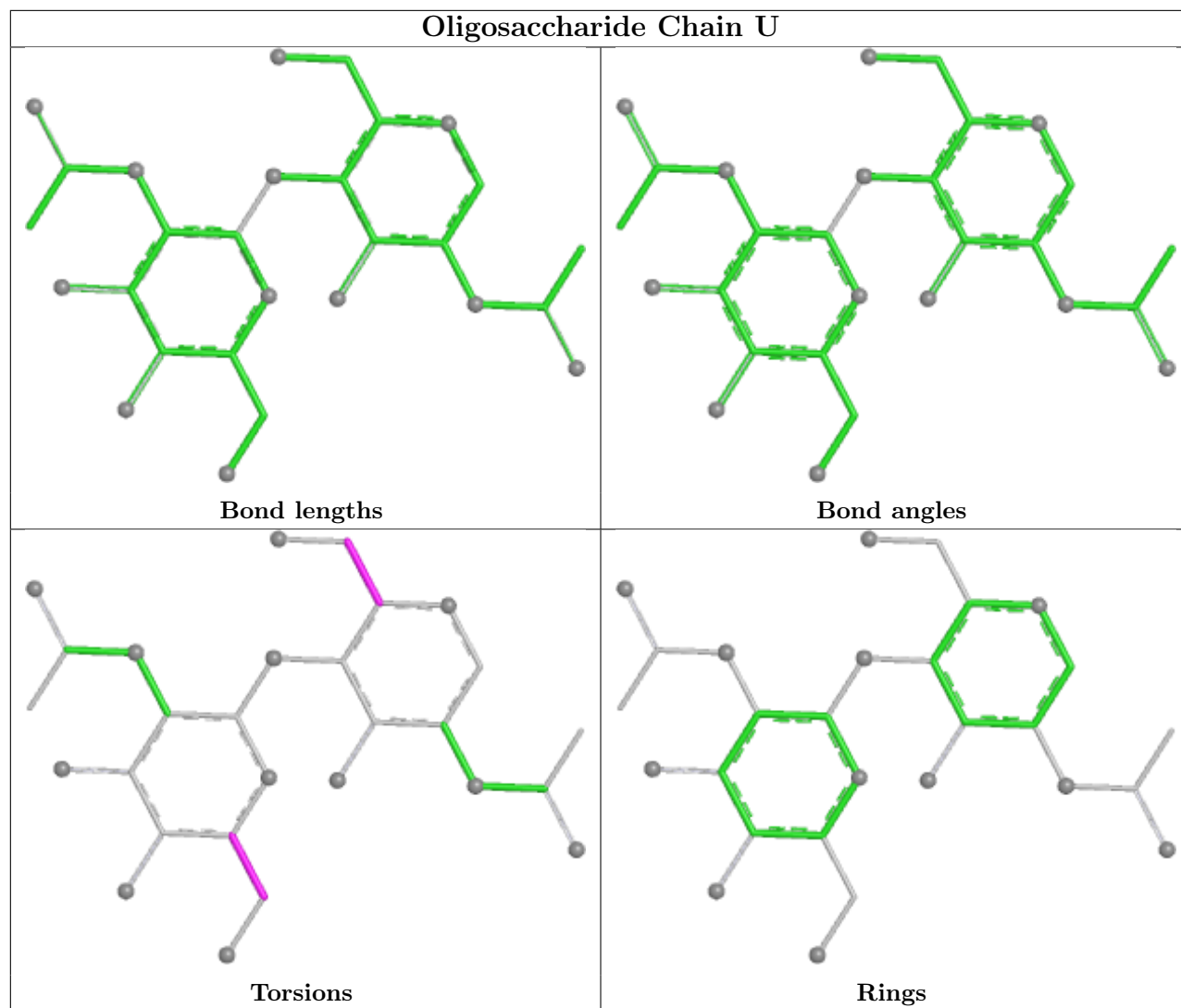


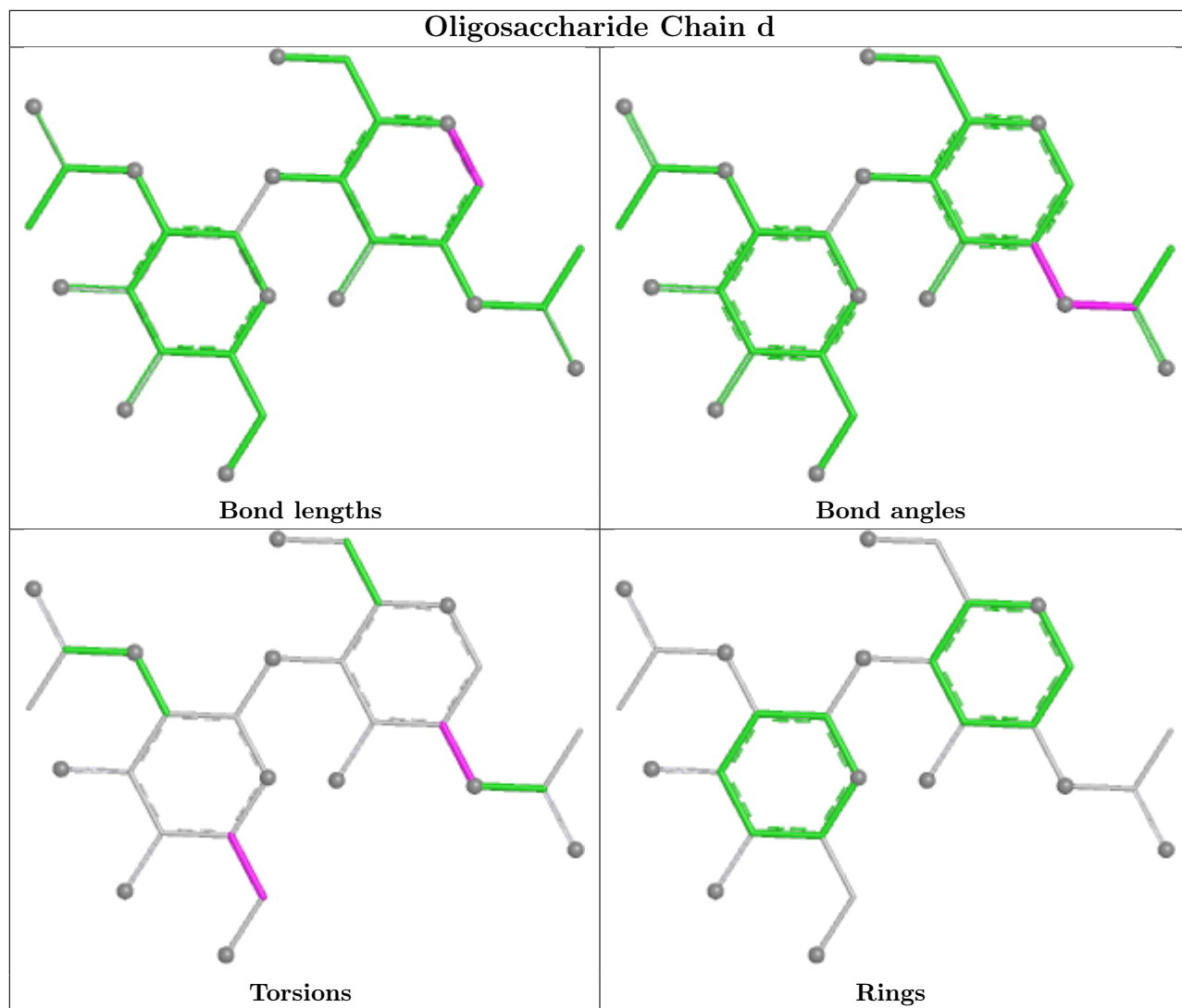


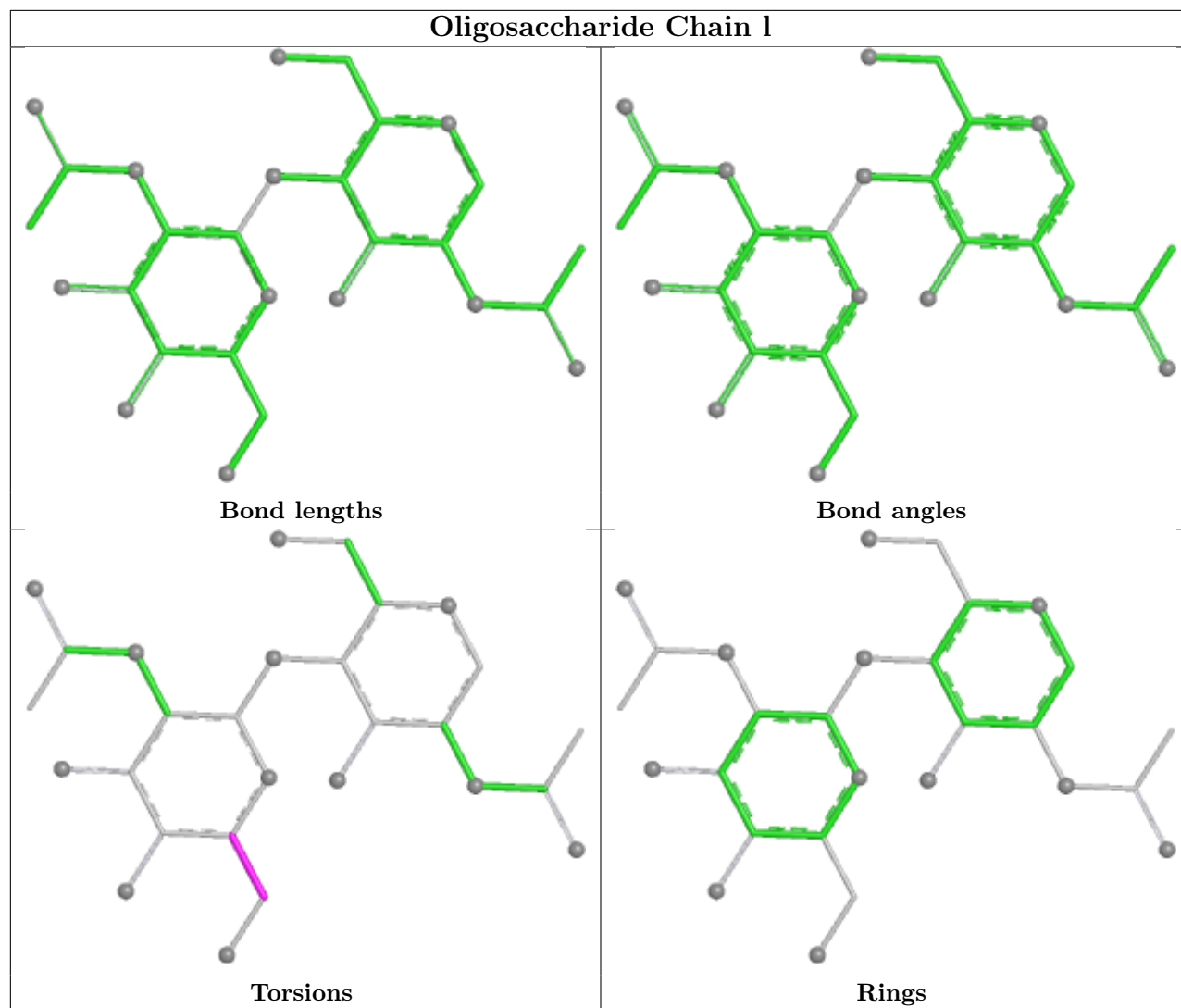


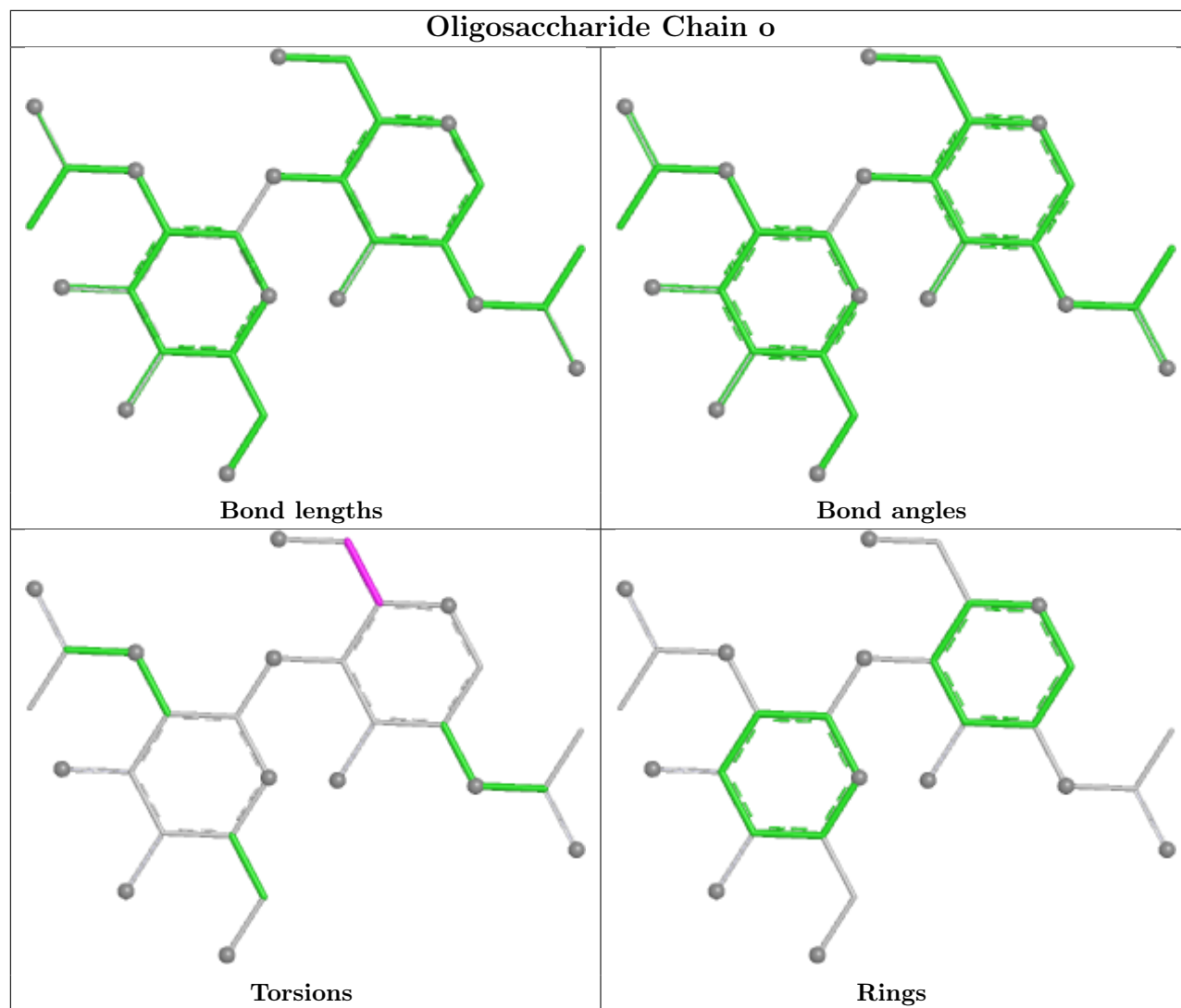


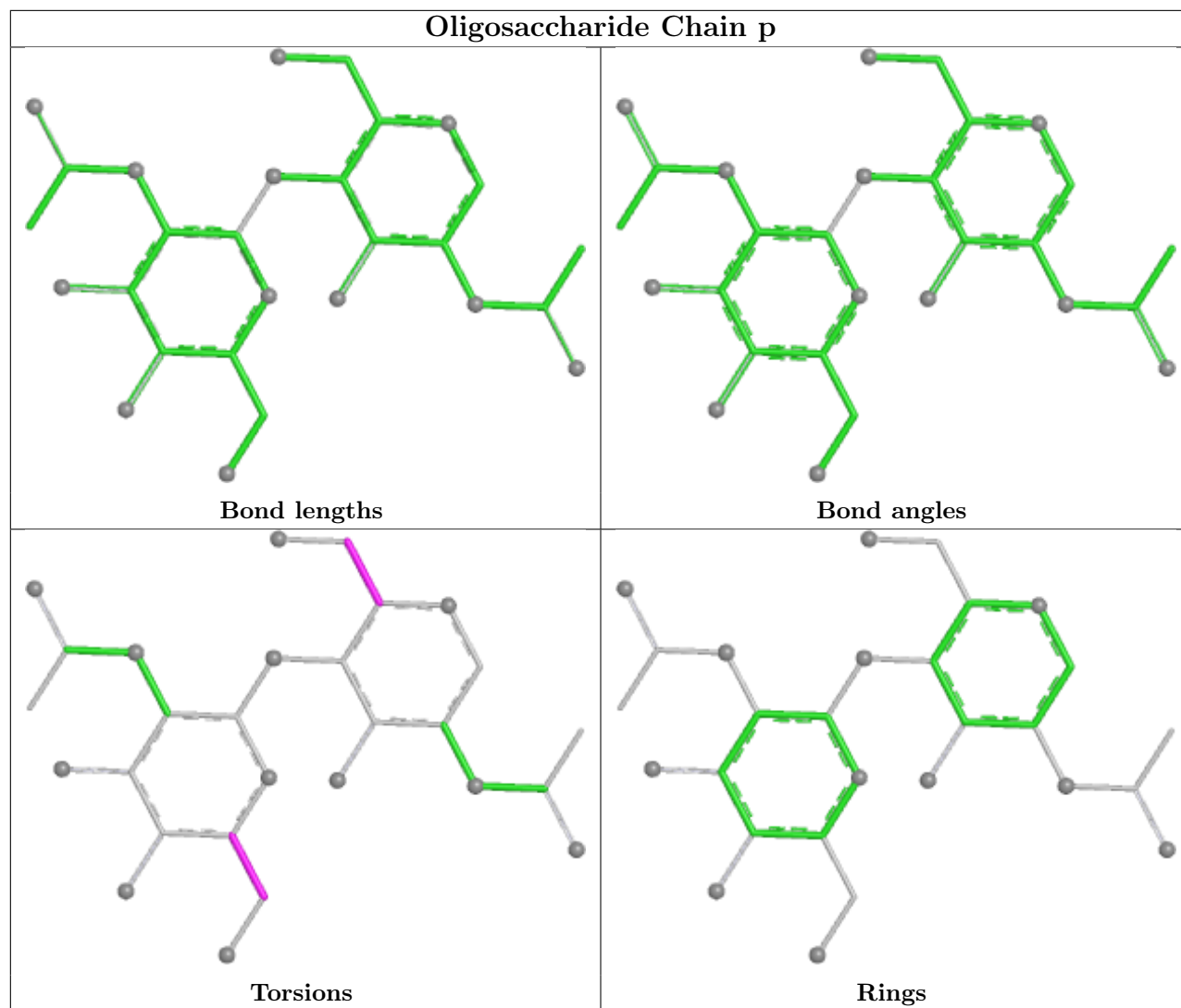


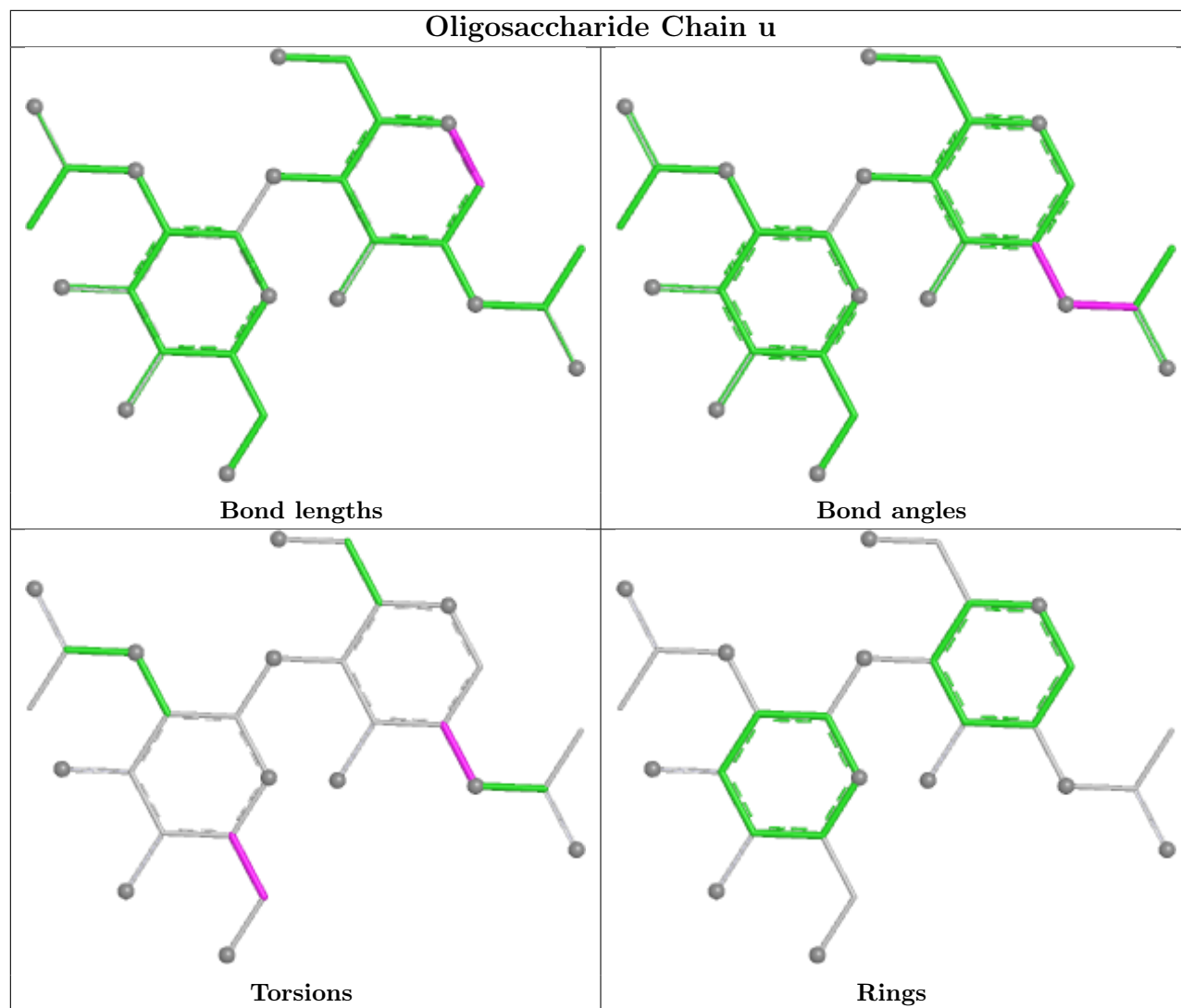


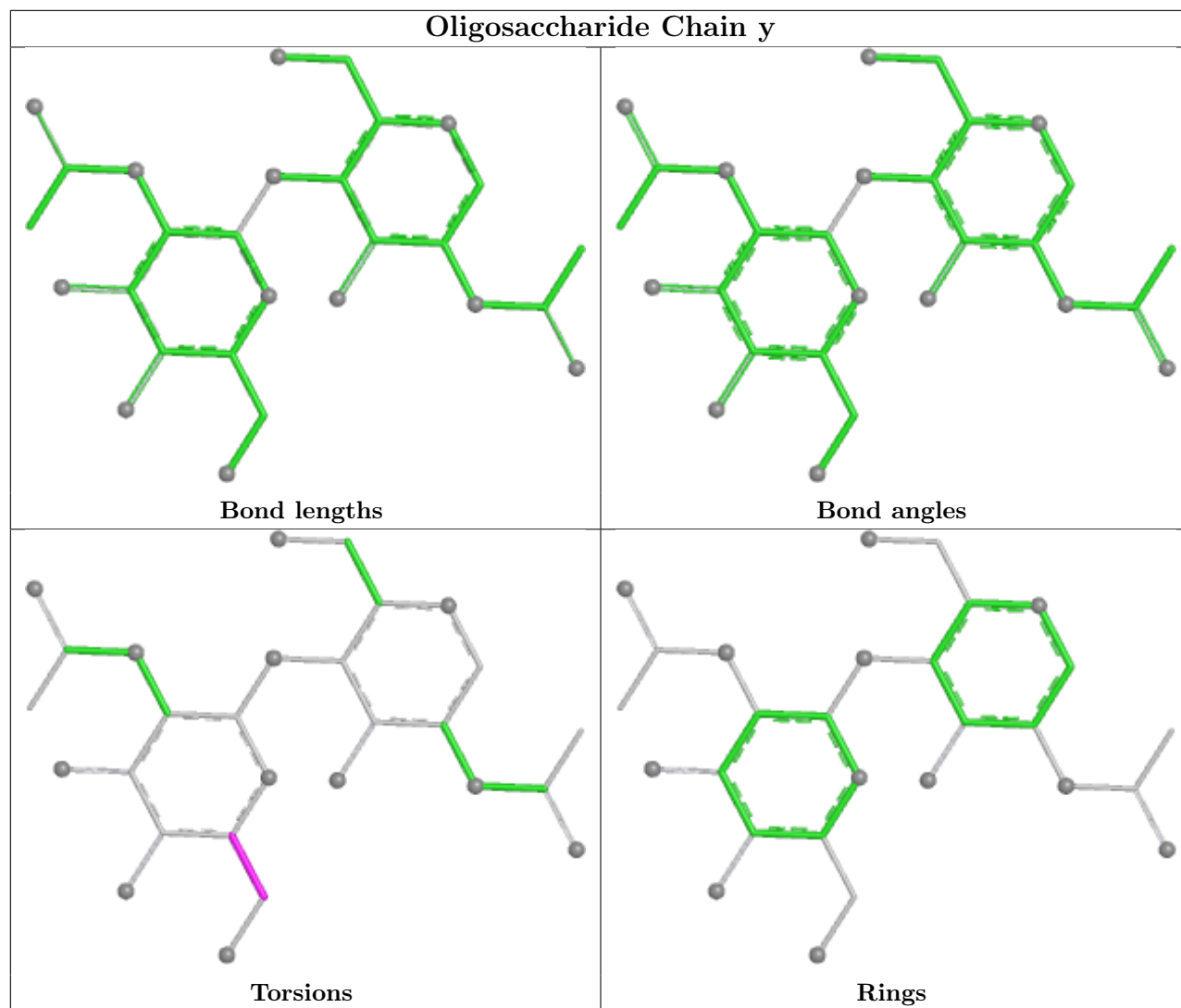


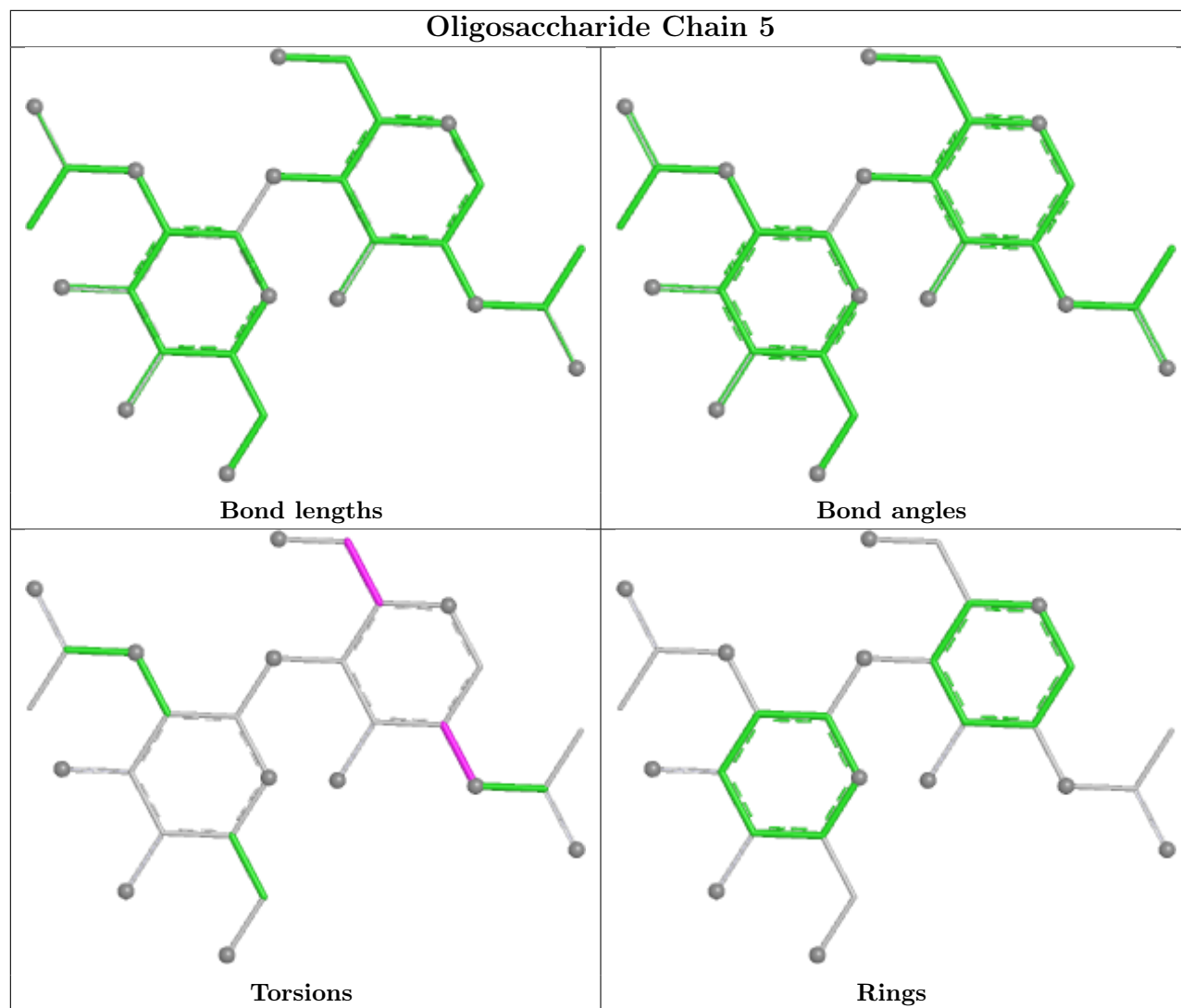


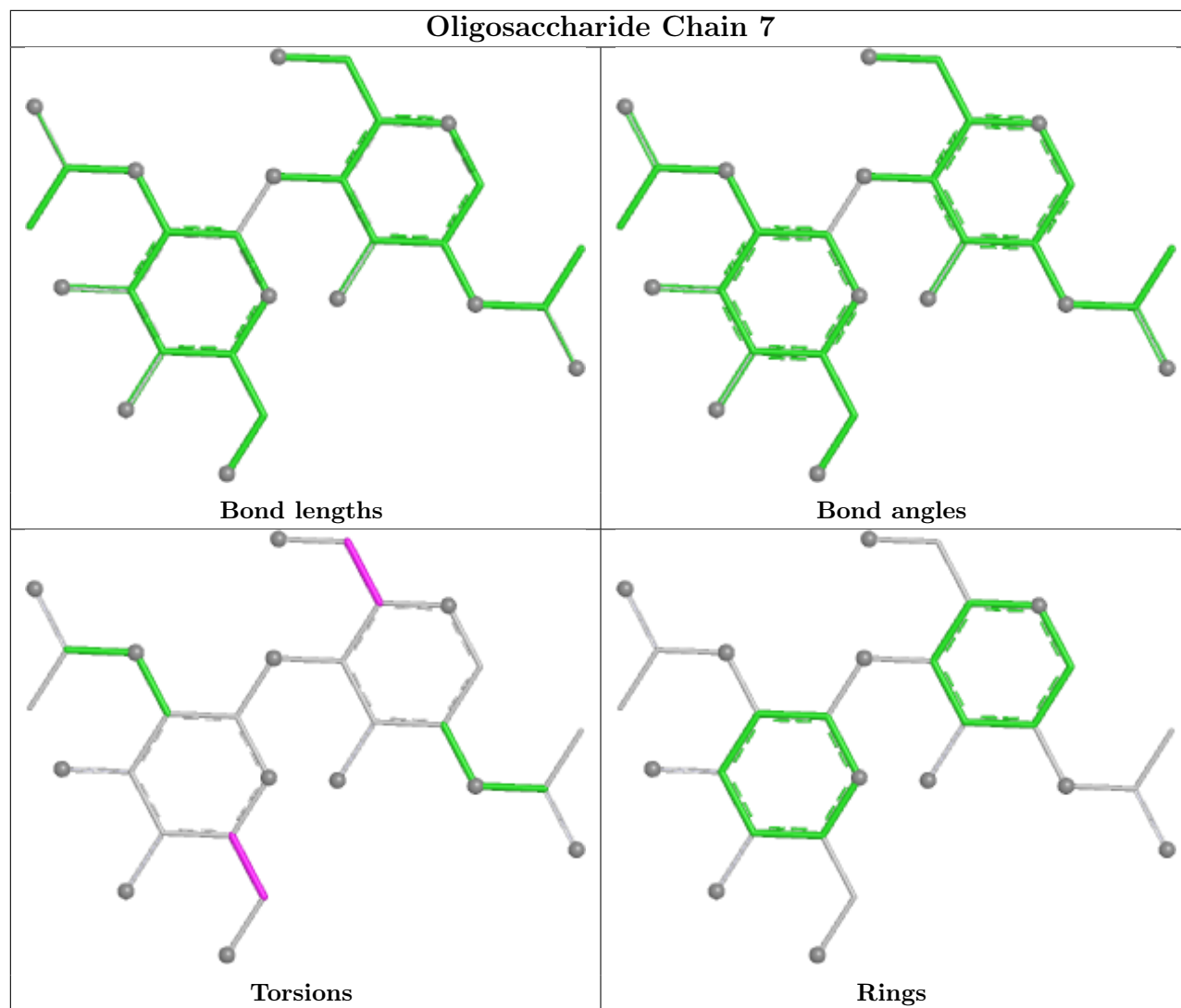


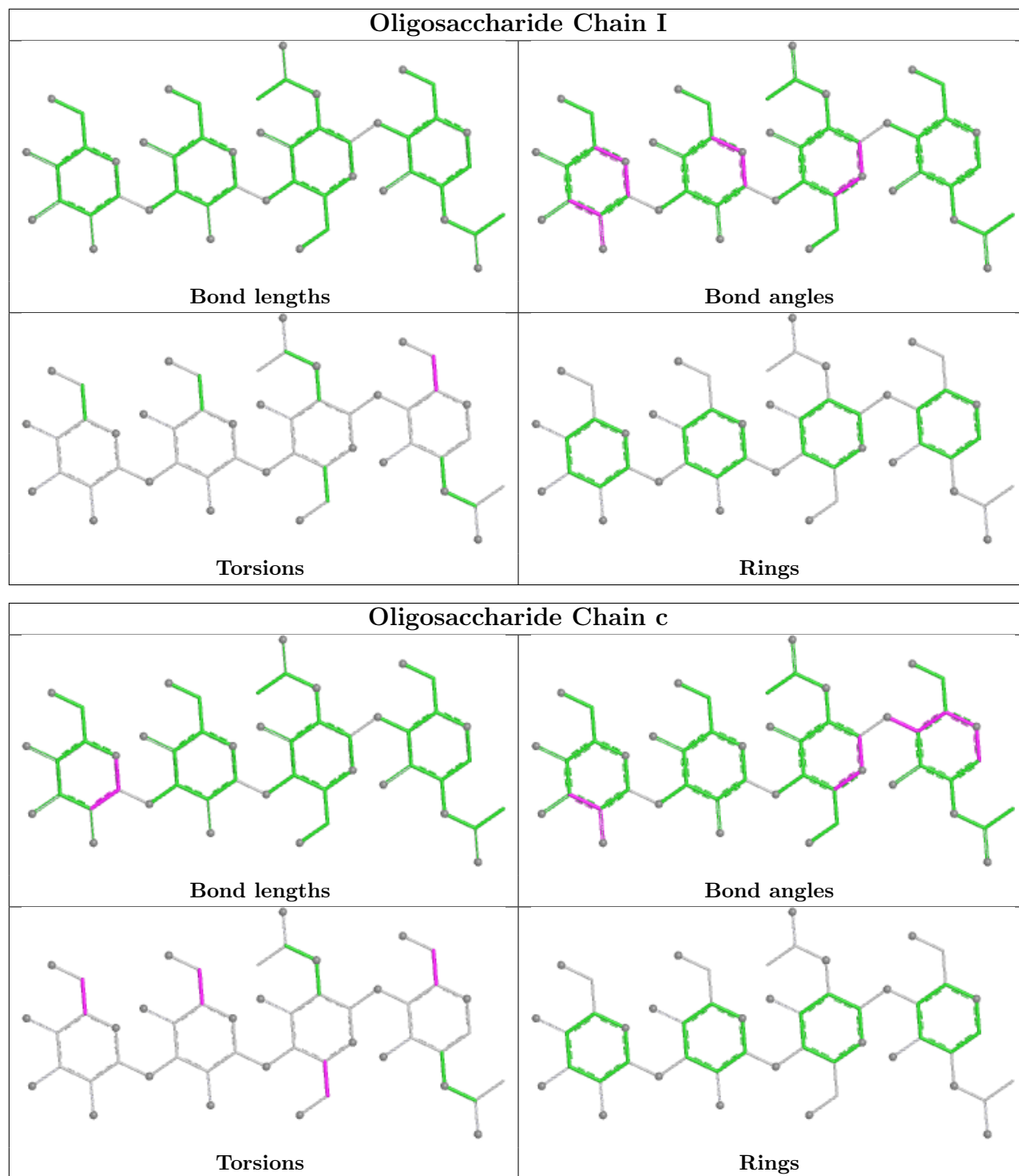


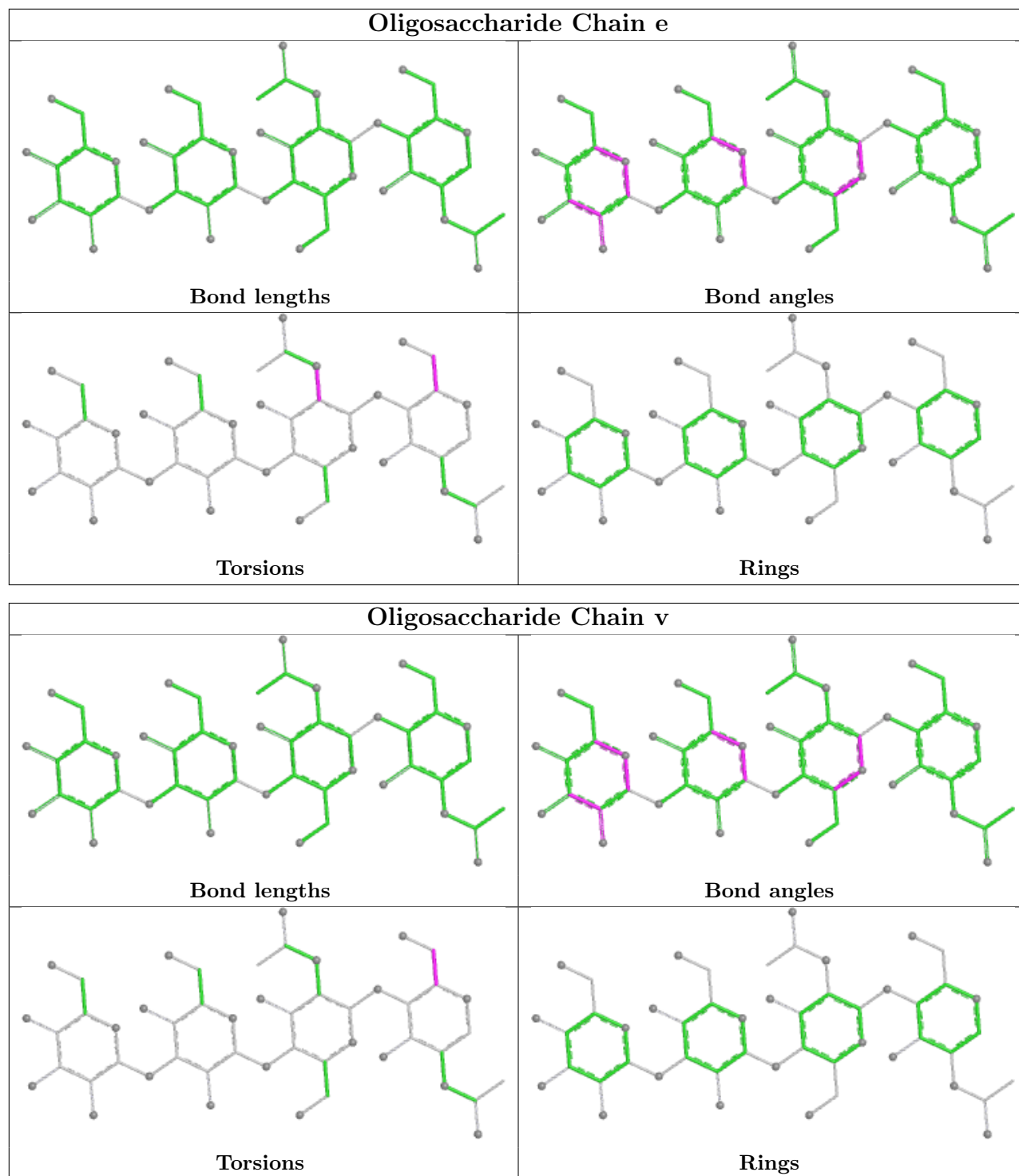


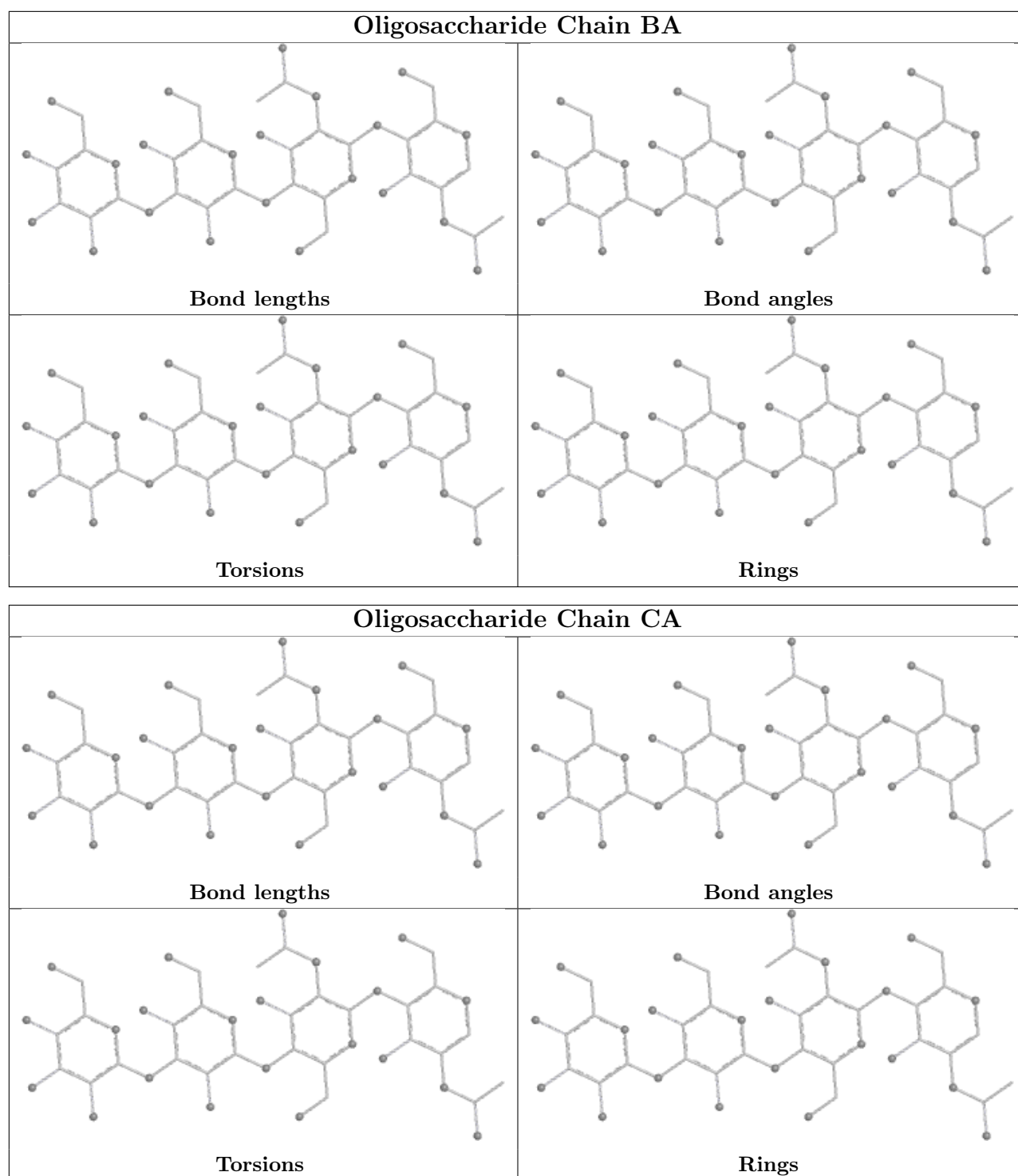


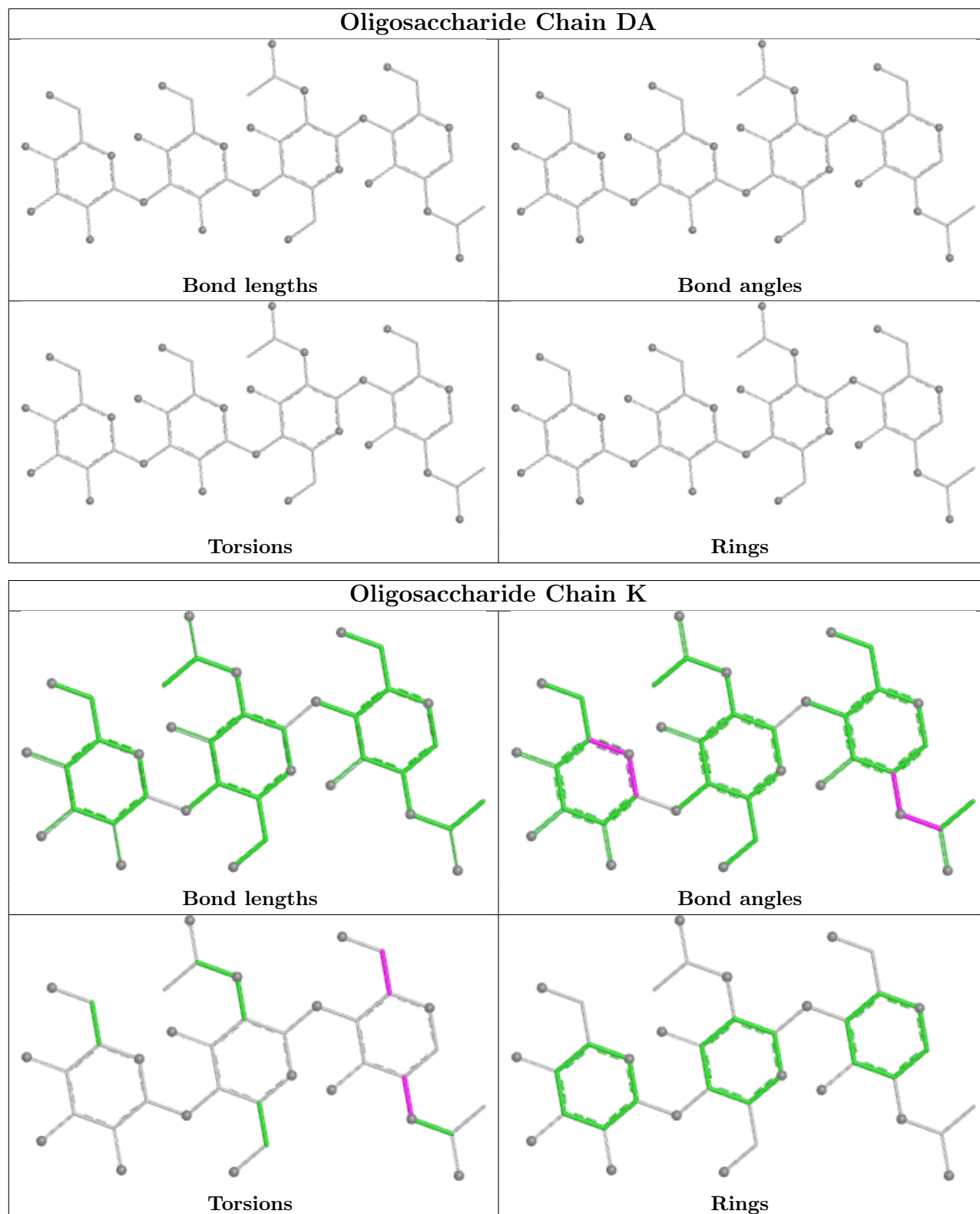


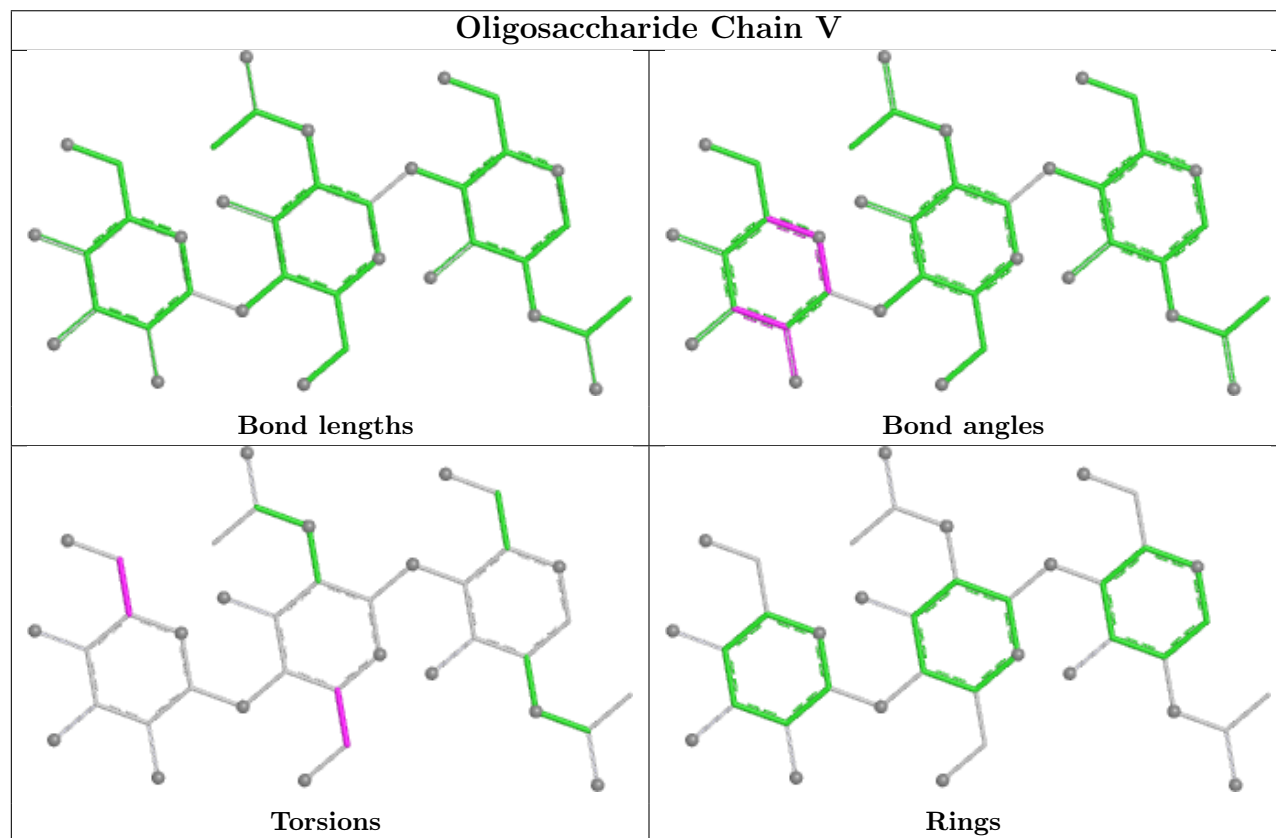
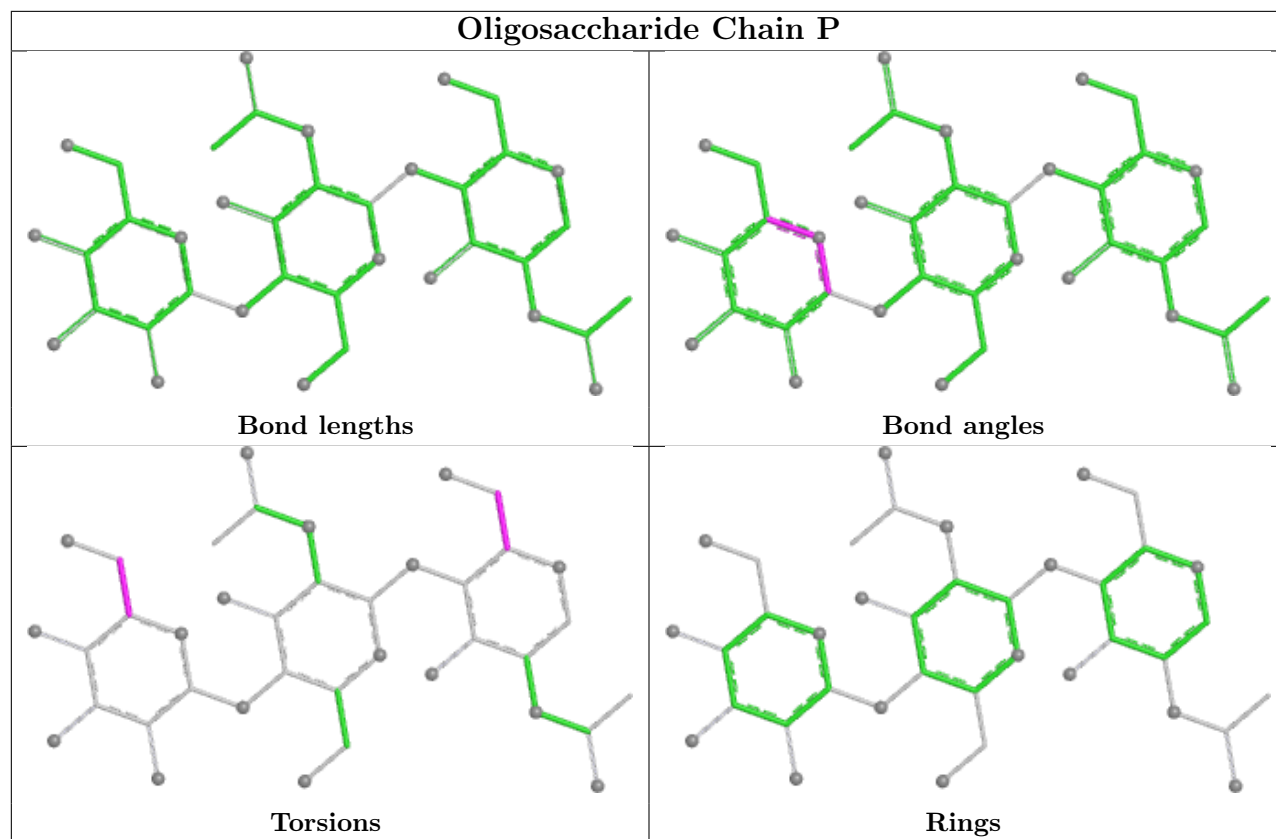


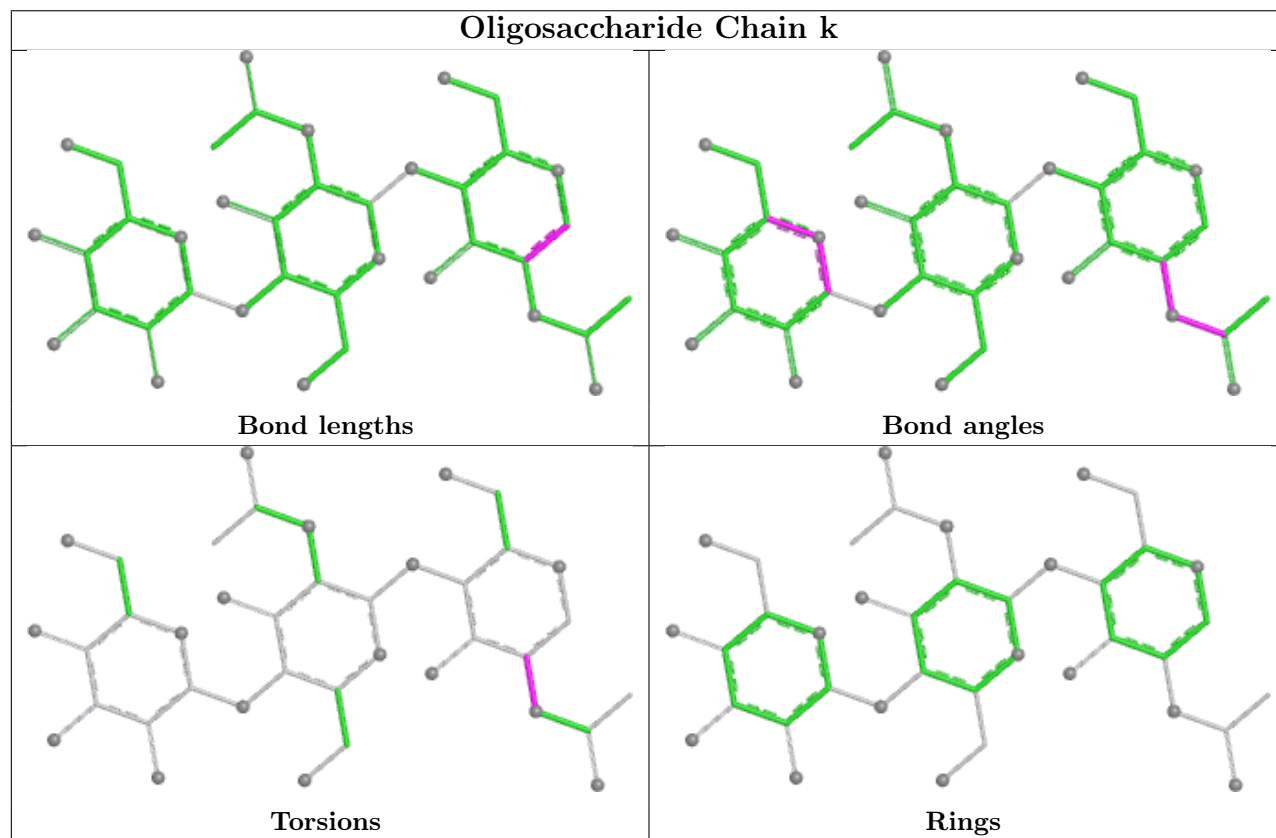
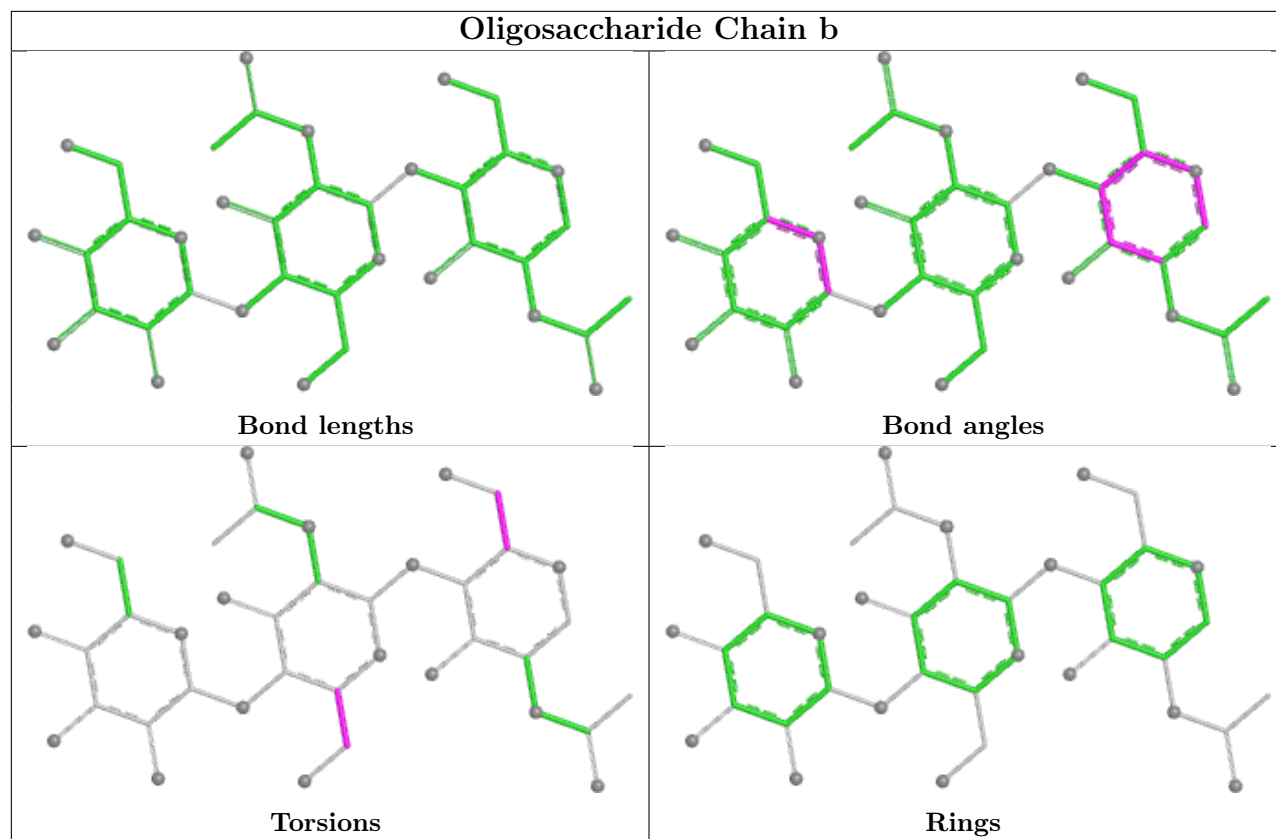


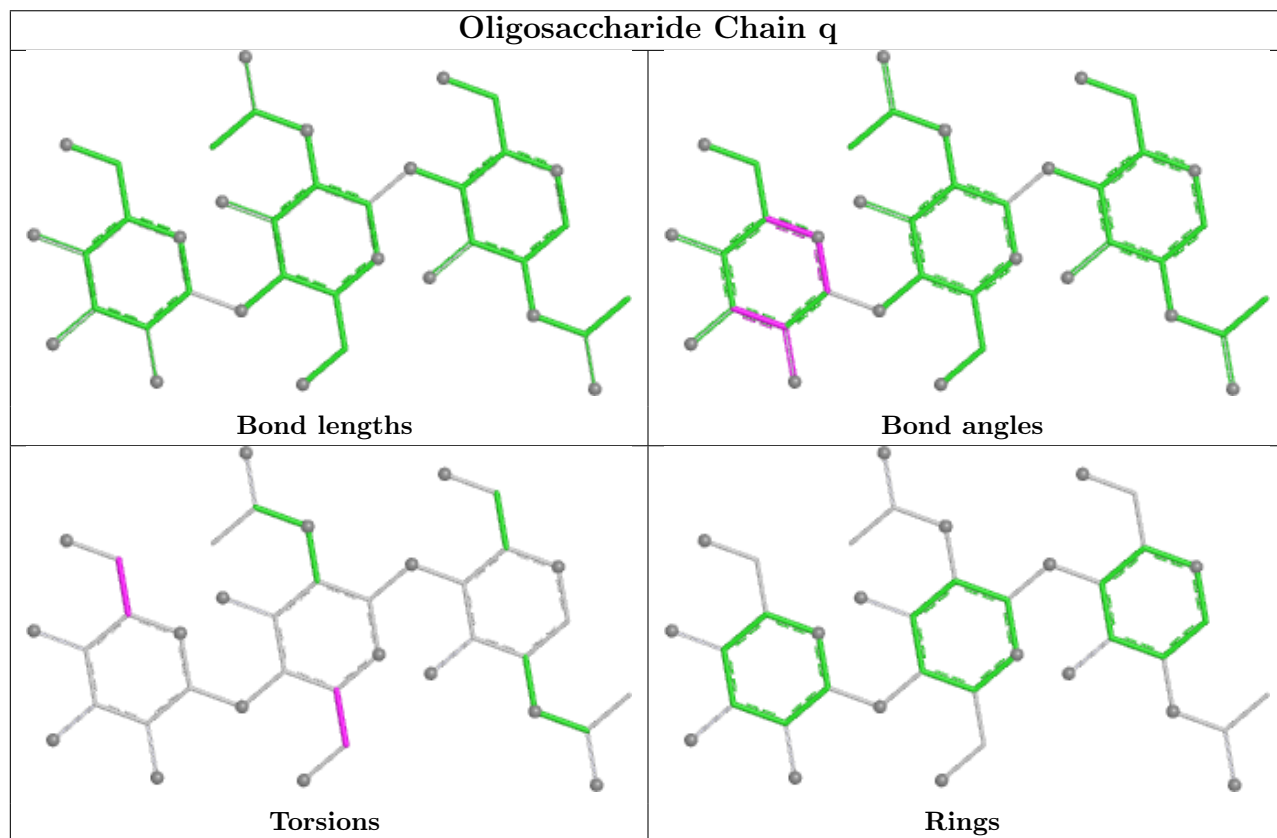
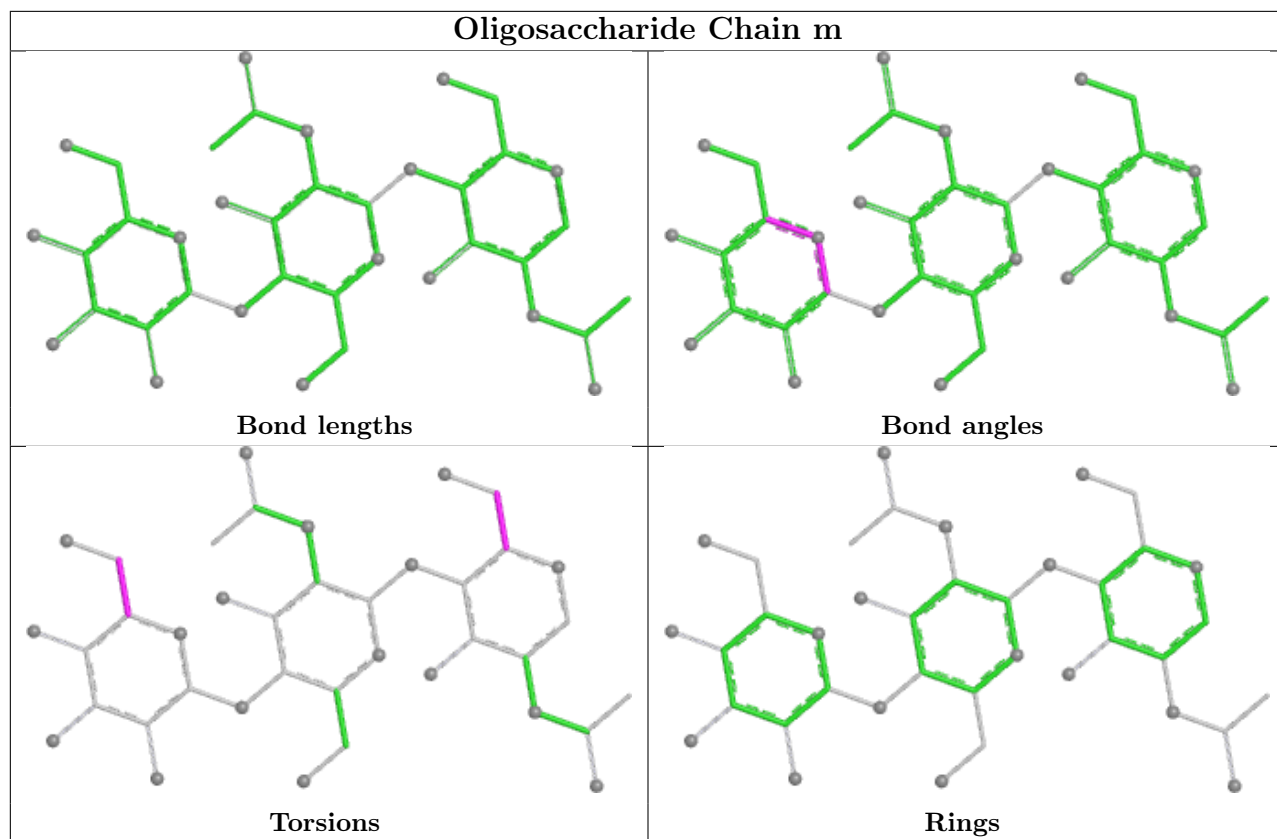


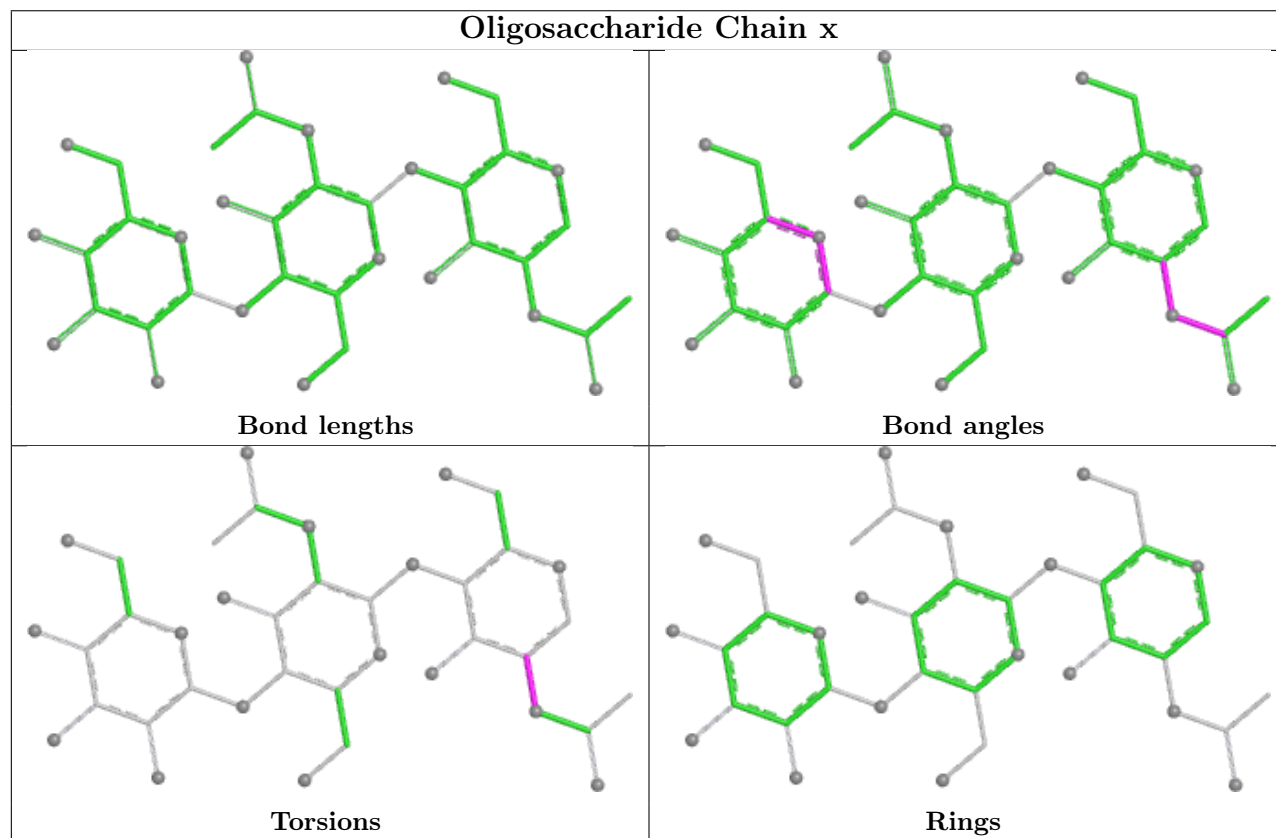
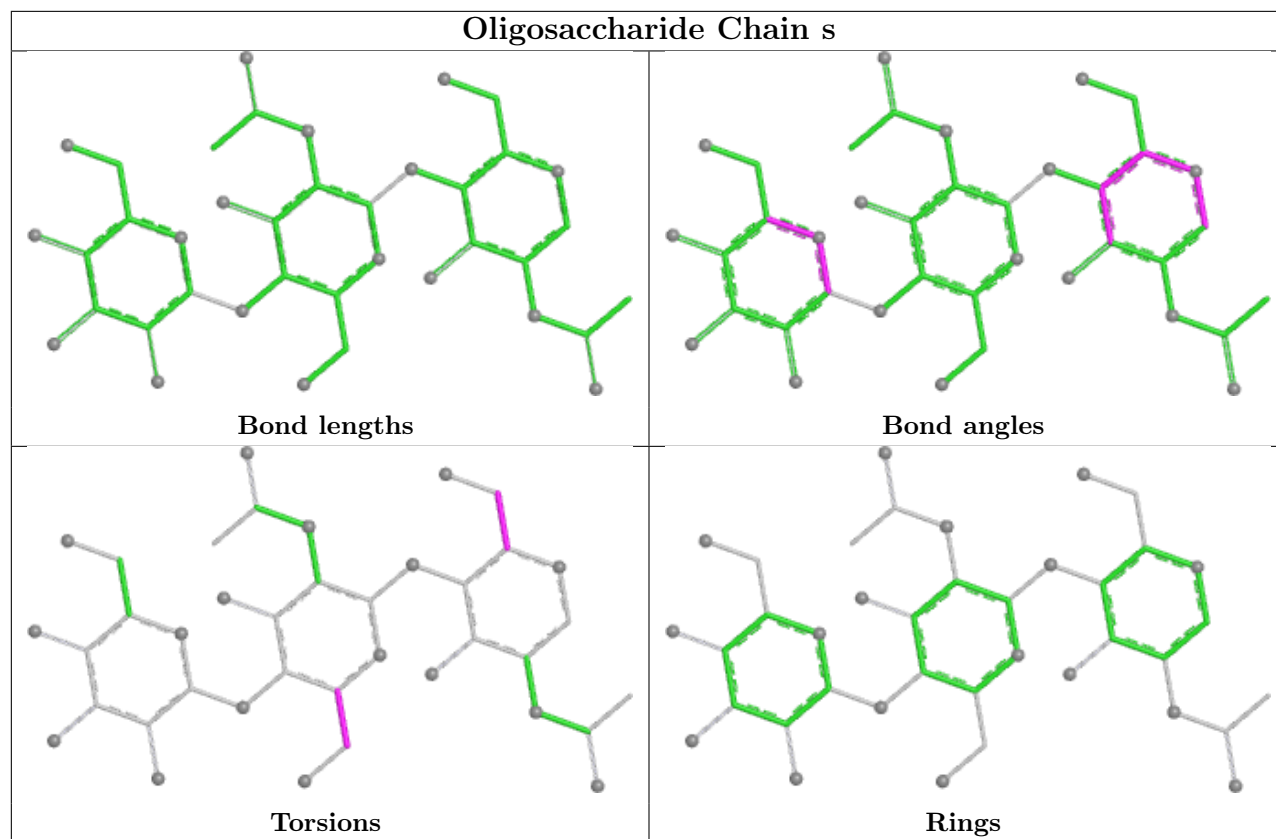


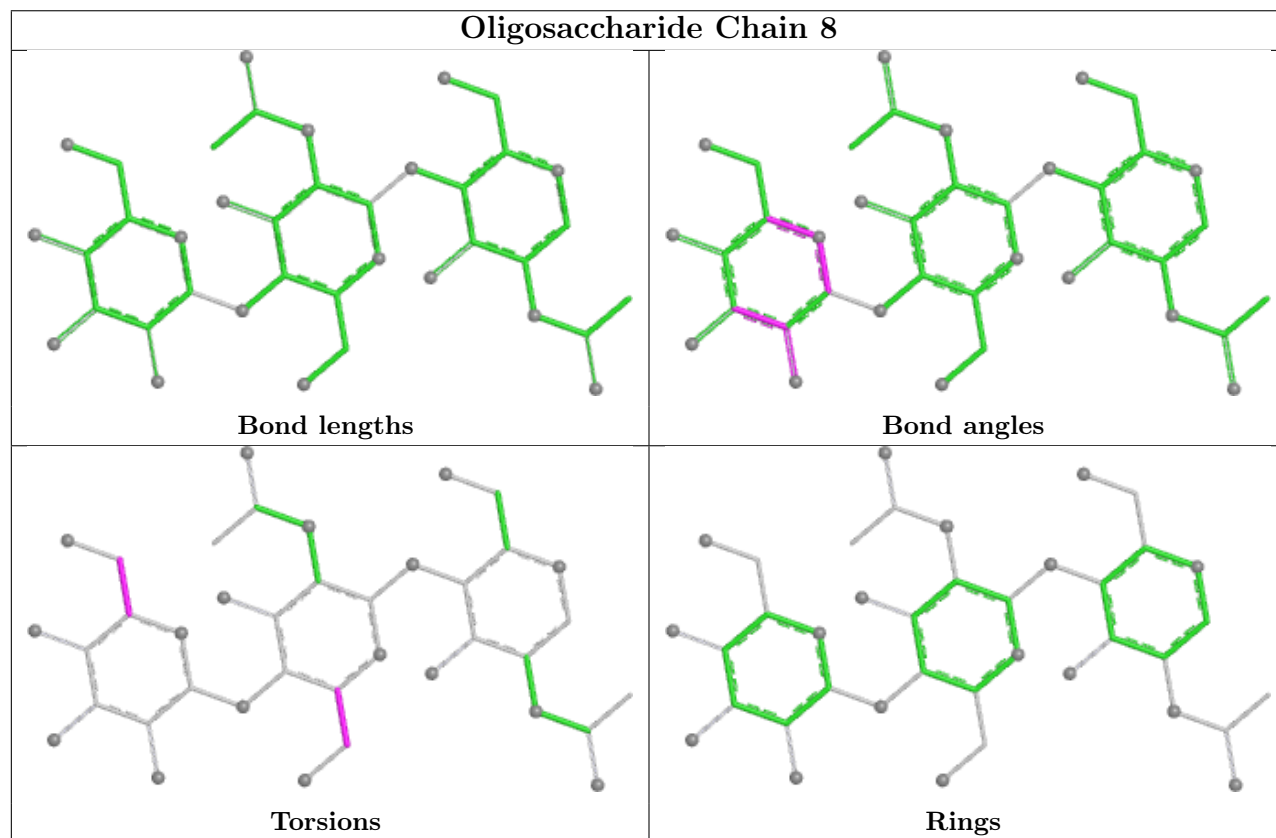
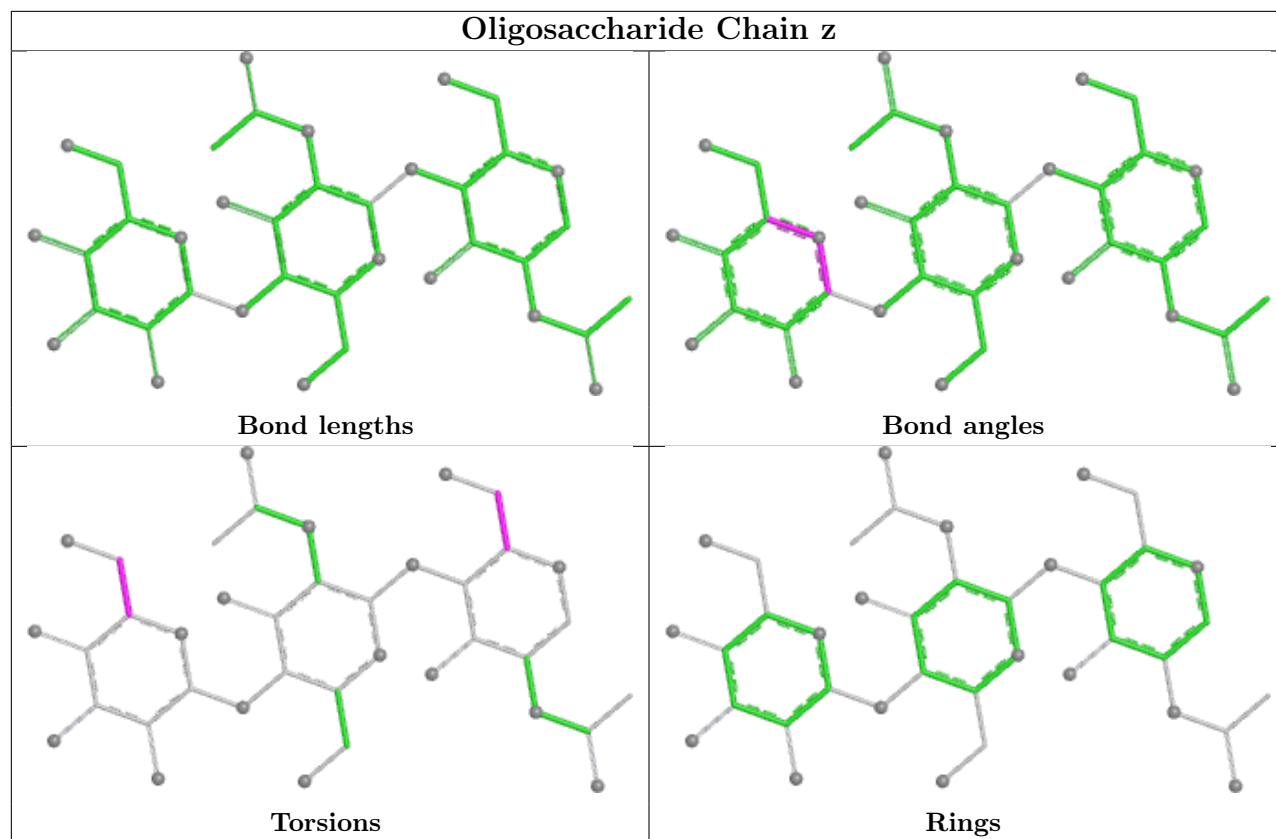


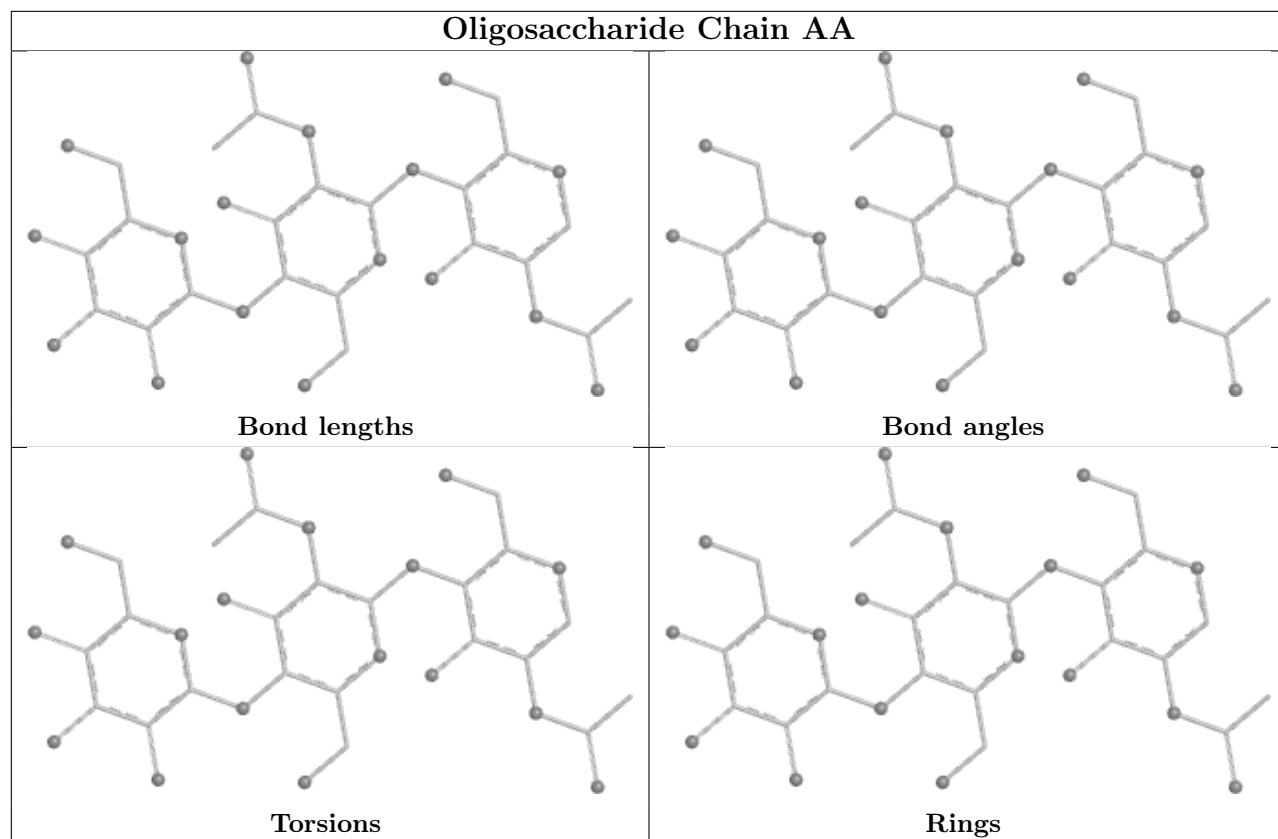


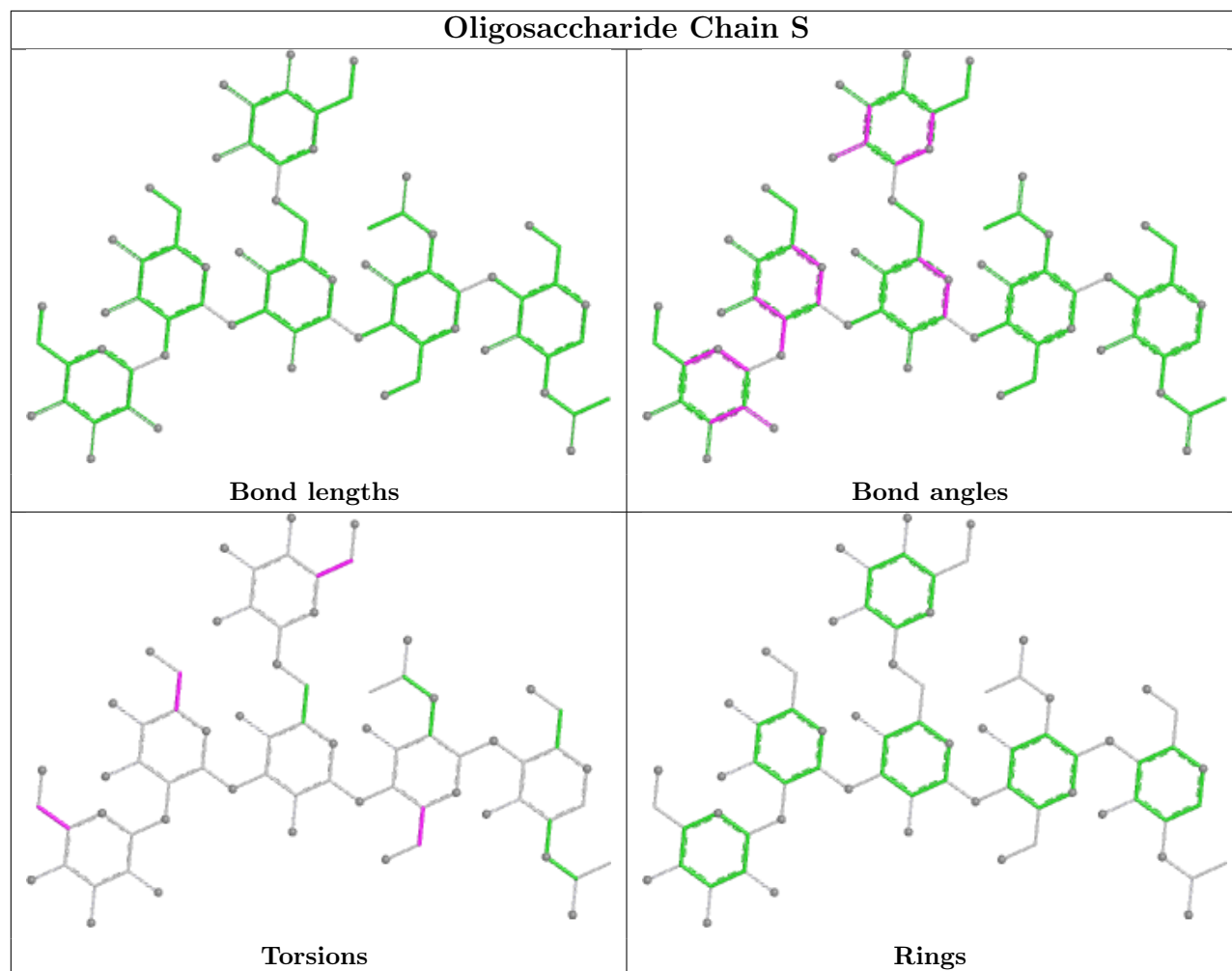


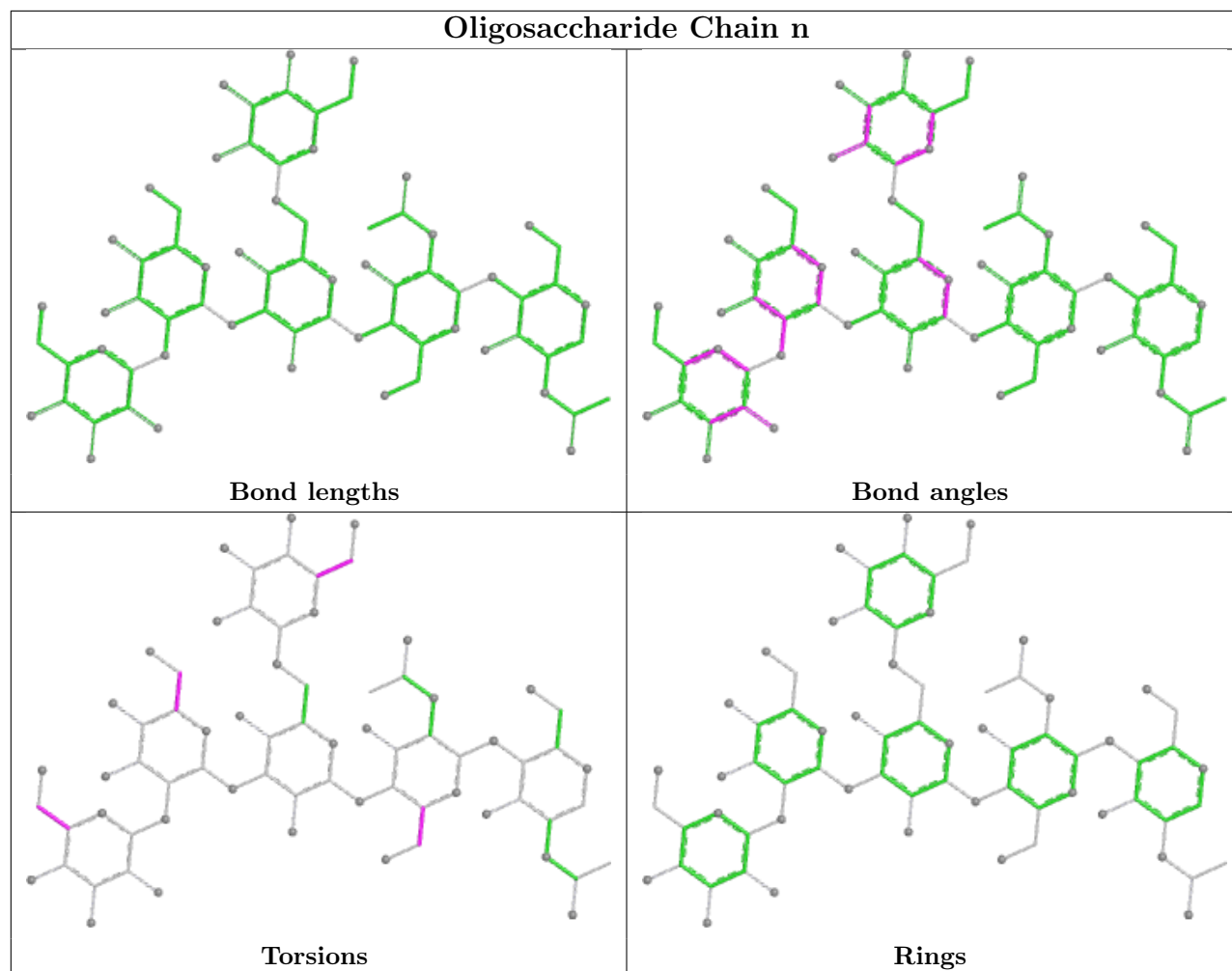


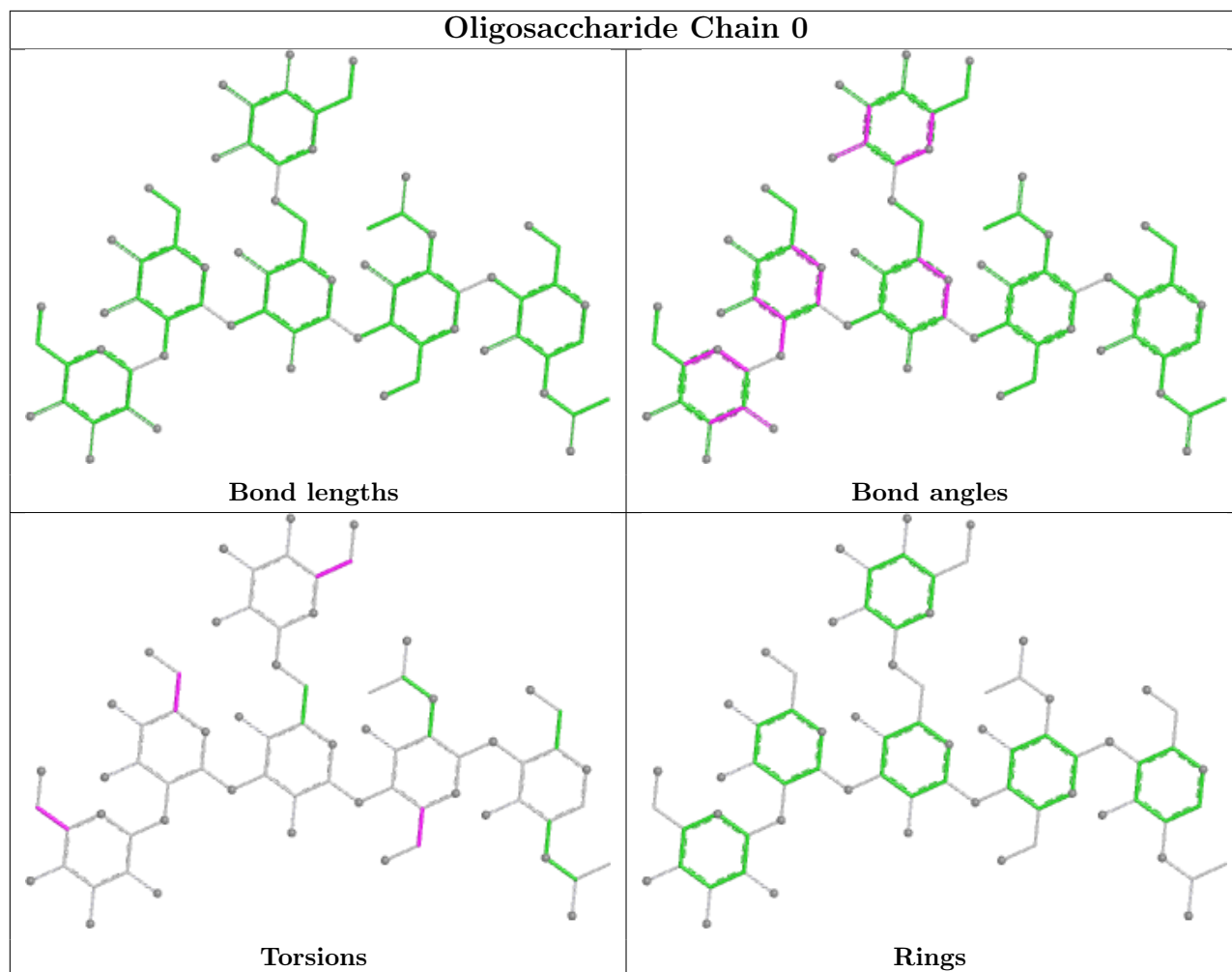












5.6 Ligand geometry [i](#)

9 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
14	NAG	A	635	4	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
14	NAG	C	635	4	14,14,15	0.33	0	17,19,21	0.65	1 (5%)
14	NAG	B	646	4	14,14,15	0.69	1 (7%)	17,19,21	0.60	0
14	NAG	A	647	4	14,14,15	0.33	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	B	634	4	14,14,15	0.35	0	17,19,21	0.67	1 (5%)
14	NAG	6	701	3	14,14,15	0.34	0	17,19,21	0.46	0
14	NAG	C	647	4	14,14,15	0.56	0	17,19,21	0.65	0
14	NAG	D	701	3	14,14,15	0.38	0	17,19,21	0.47	0
14	NAG	E	701	3	14,14,15	0.36	0	17,19,21	0.46	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
14	NAG	A	635	4	-	0/6/23/26	0/1/1/1
14	NAG	C	635	4	-	0/6/23/26	0/1/1/1
14	NAG	B	646	4	-	1/6/23/26	0/1/1/1
14	NAG	A	647	4	-	1/6/23/26	0/1/1/1
14	NAG	B	634	4	-	0/6/23/26	0/1/1/1
14	NAG	6	701	3	-	0/6/23/26	0/1/1/1
14	NAG	C	647	4	-	0/6/23/26	0/1/1/1
14	NAG	D	701	3	-	0/6/23/26	0/1/1/1
14	NAG	E	701	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	646	NAG	O5-C1	2.39	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	634	NAG	C1-O5-C5	2.32	115.30	112.19
14	A	635	NAG	C1-O5-C5	2.29	115.25	112.19
14	C	635	NAG	C1-O5-C5	2.23	115.18	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	647	NAG	C1-C2-N2-C7
14	B	646	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

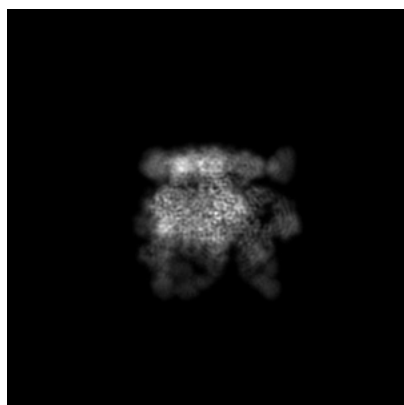
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9189. These allow visual inspection of the internal detail of the map and identification of artifacts.

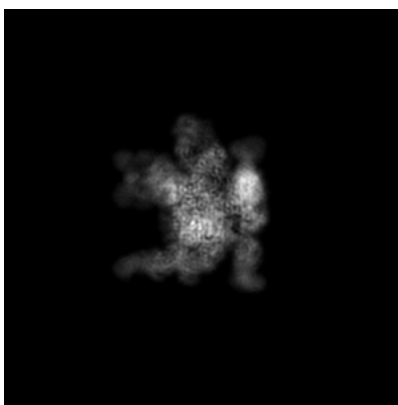
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

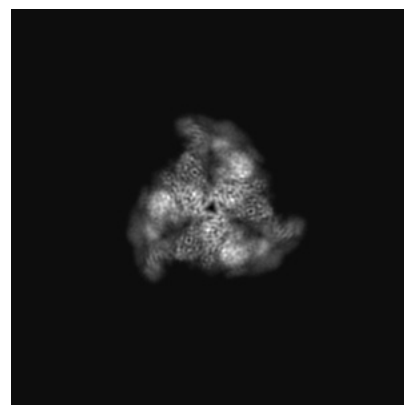
6.1.1 Primary map



X



Y

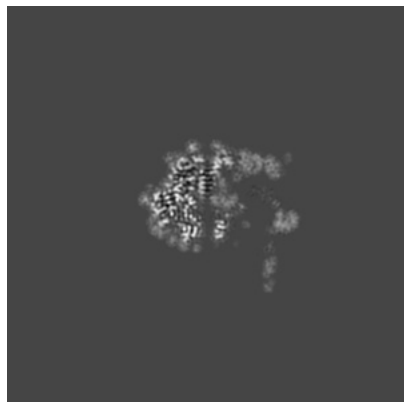


Z

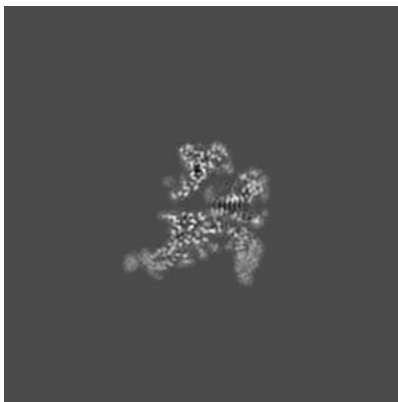
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

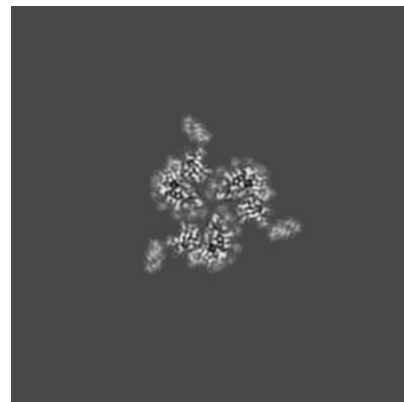
6.2.1 Primary map



X Index: 192



Y Index: 192

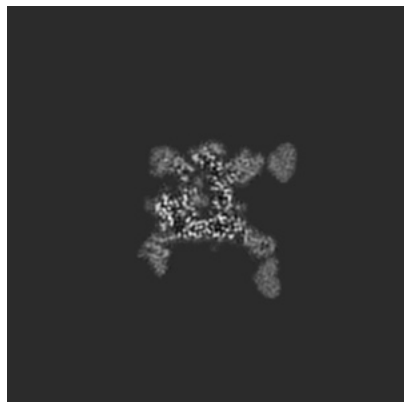


Z Index: 192

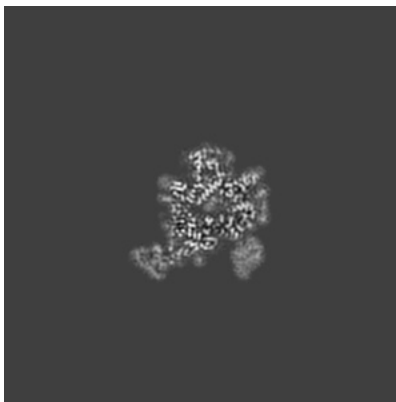
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

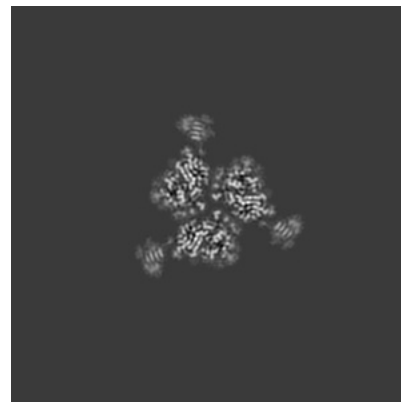
6.3.1 Primary map



X Index: 204



Y Index: 200

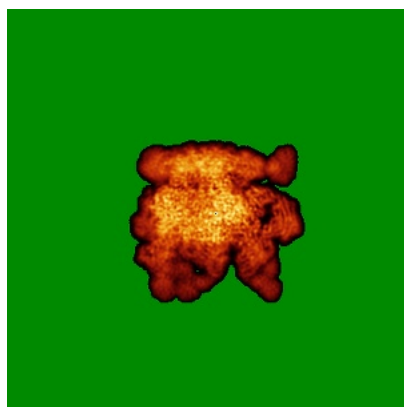


Z Index: 187

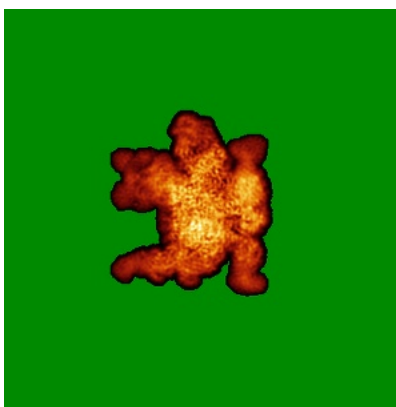
The images above show the largest variance slices of the map in three orthogonal directions.

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

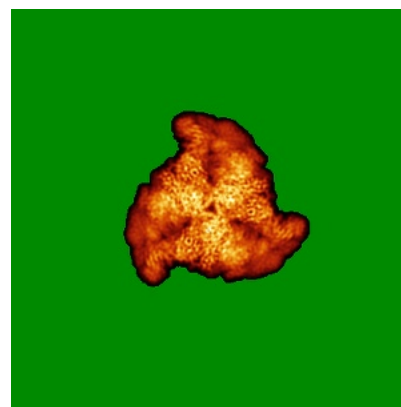
6.4.1 Primary map



X



Y

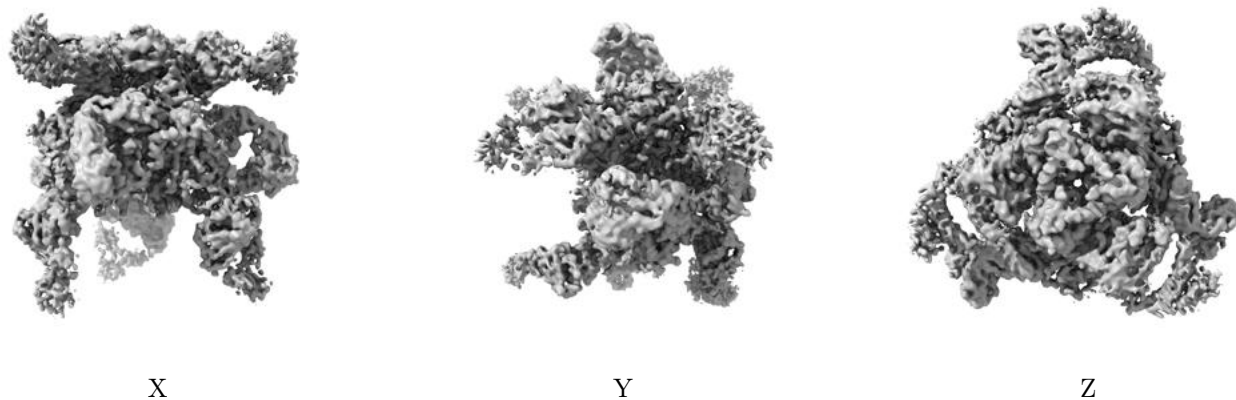


Z

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

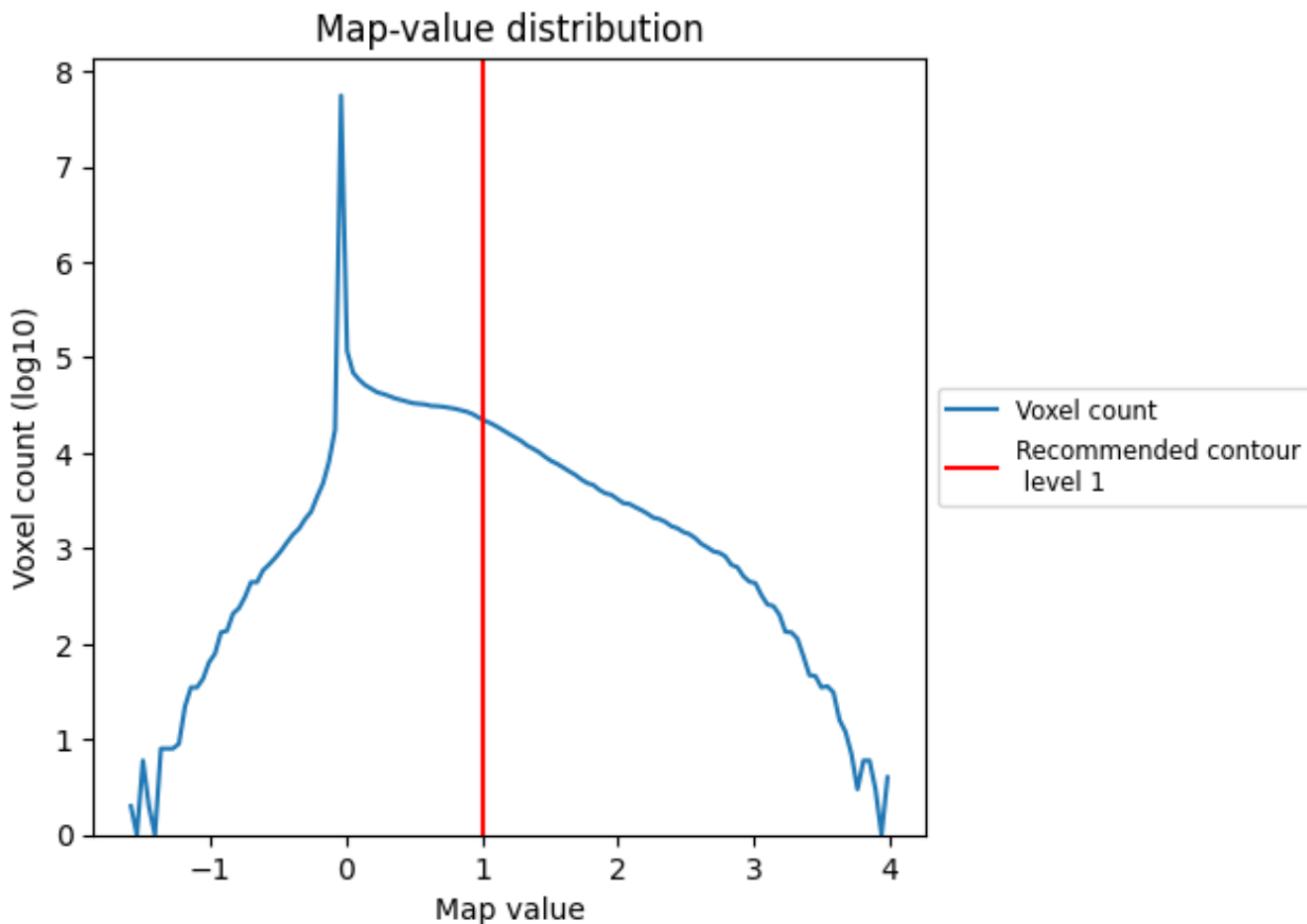
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

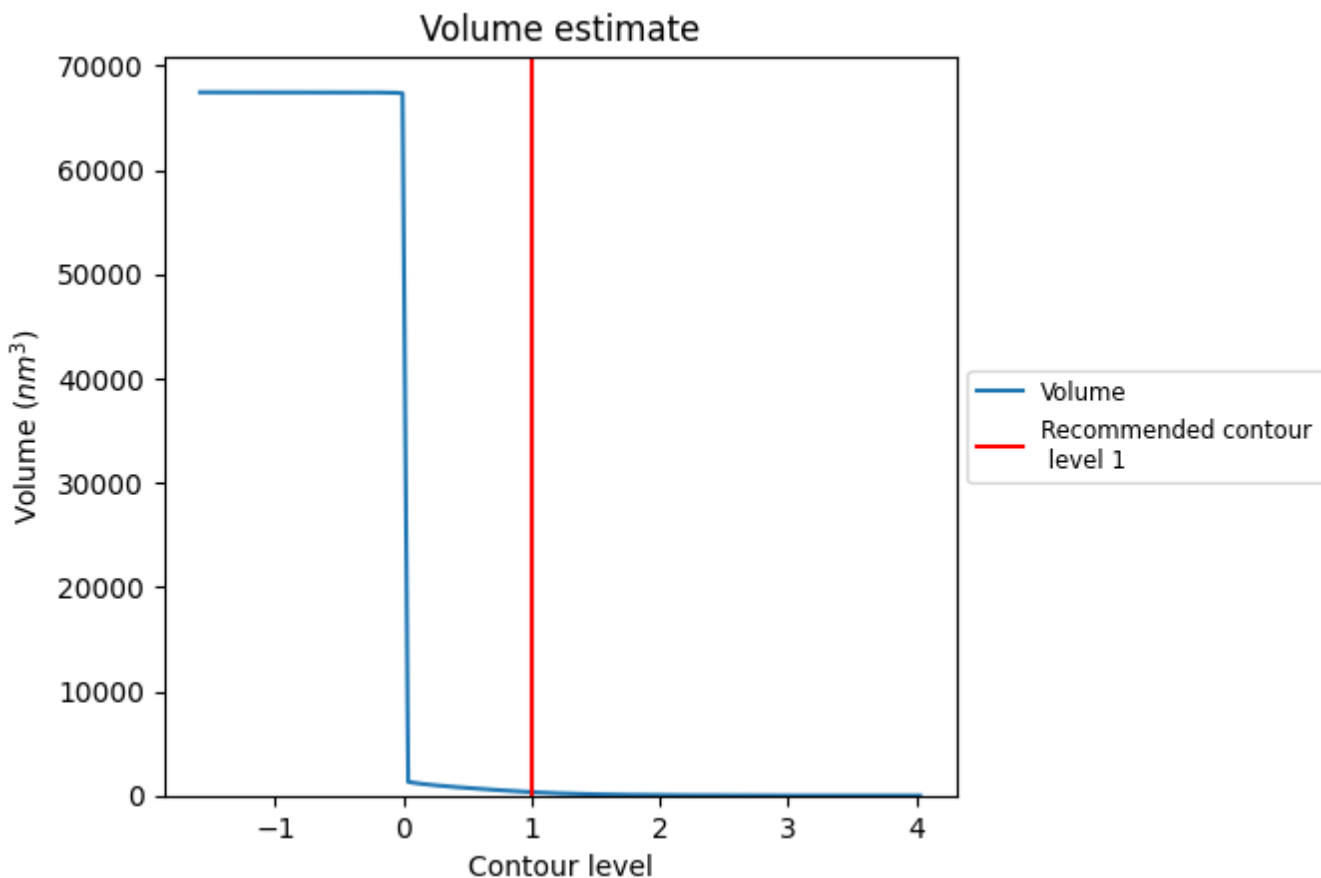
This section contains the results of statistical analysis of the map.

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.

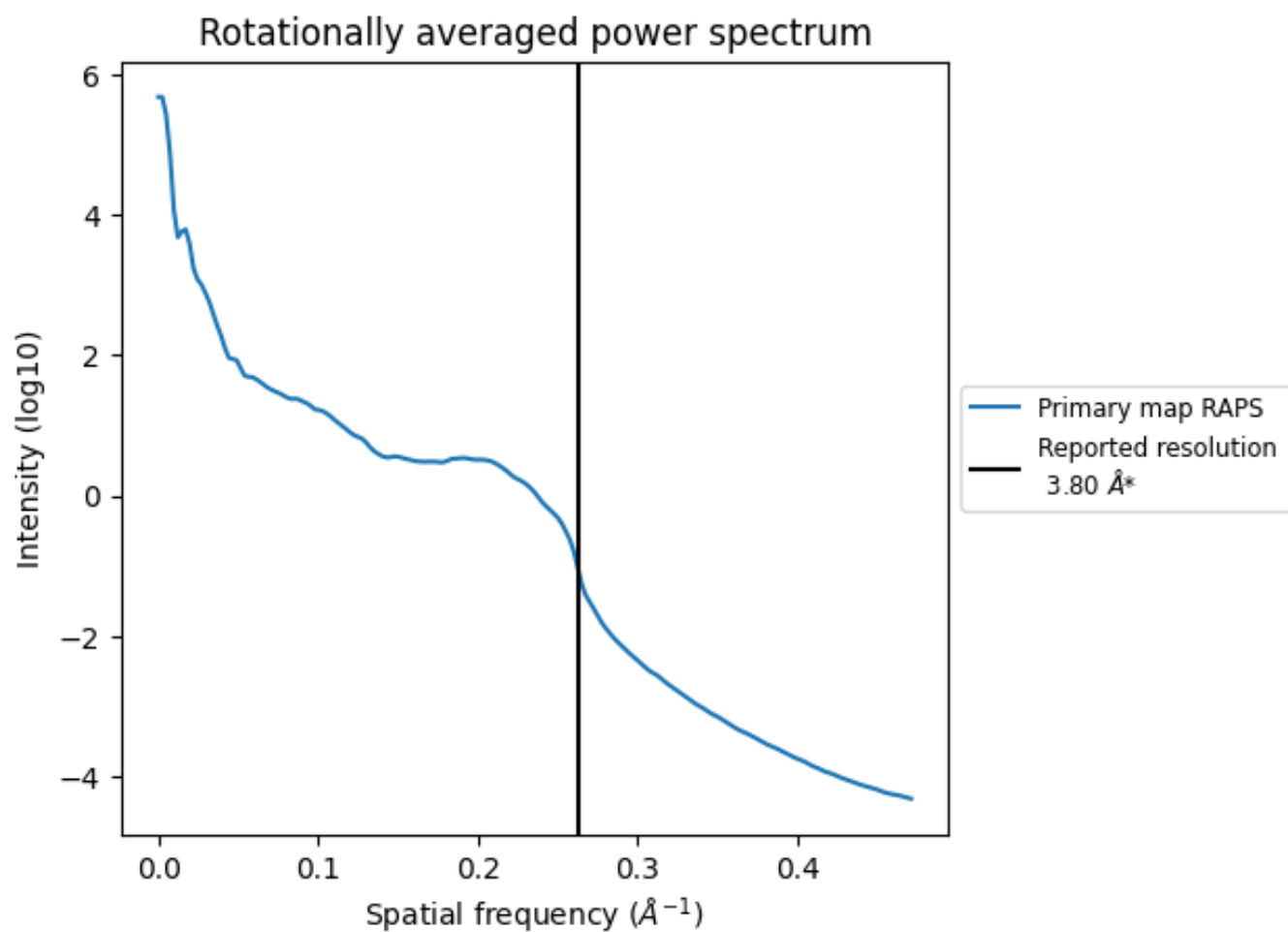
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 330 nm³; this corresponds to an approximate mass of 298 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

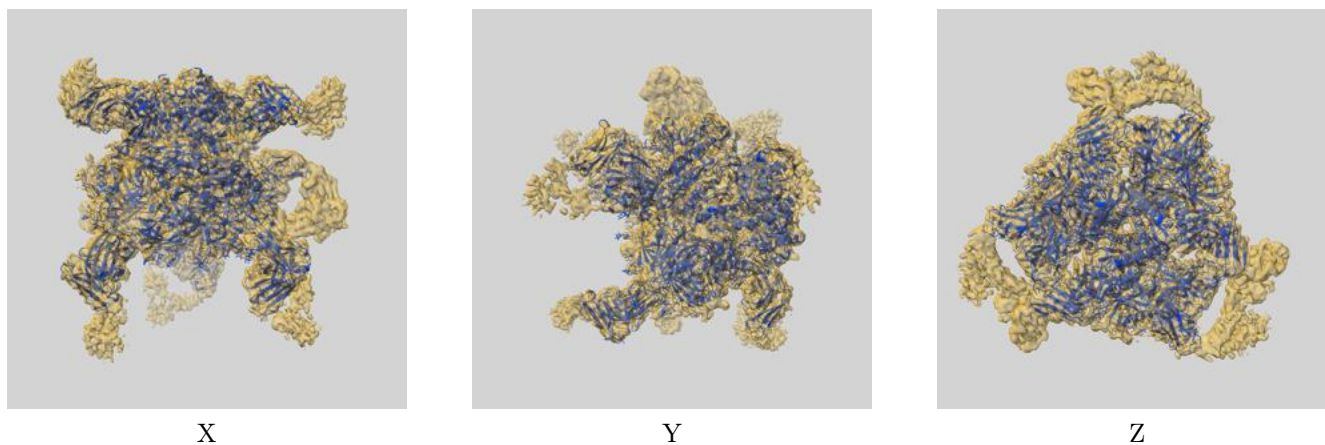
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

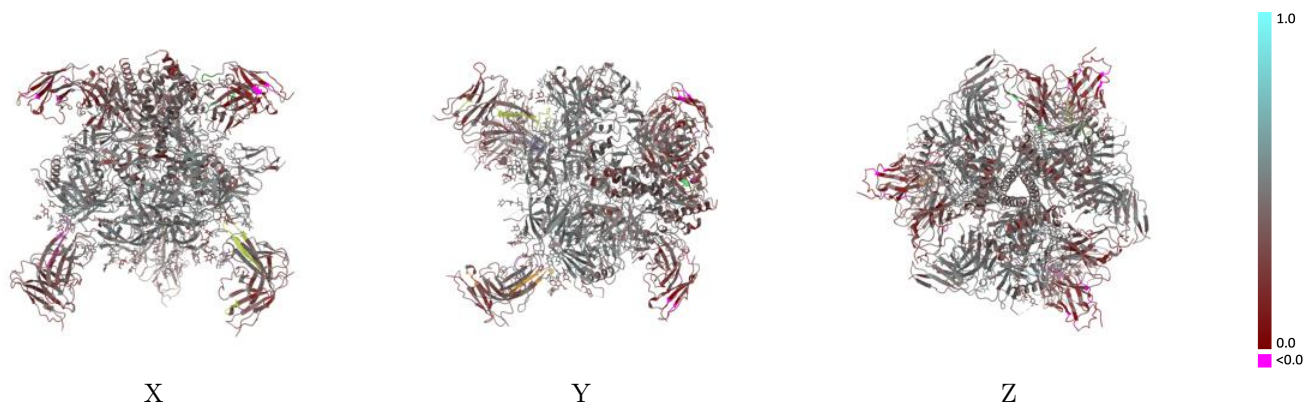
This section contains information regarding the fit between EMDB map EMD-9189 and PDB model 6MPH. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



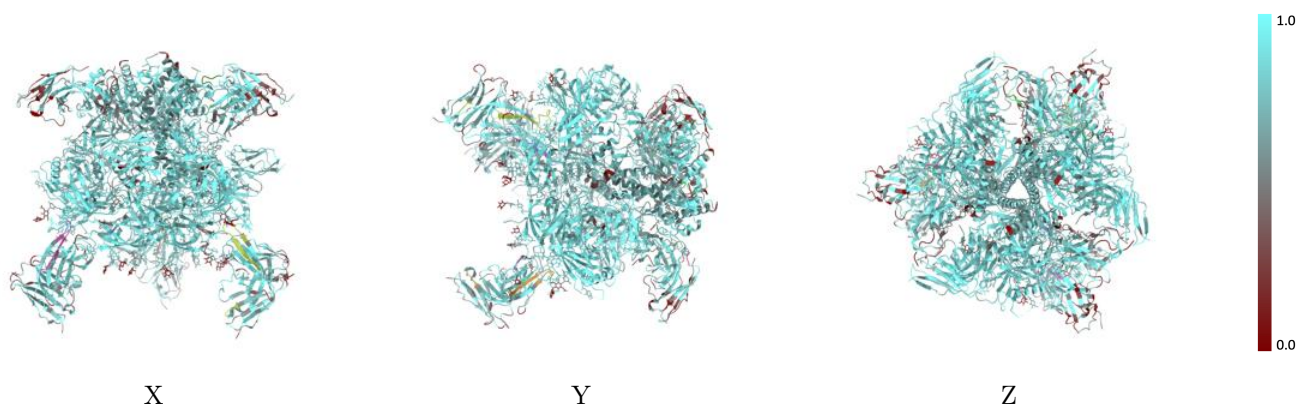
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



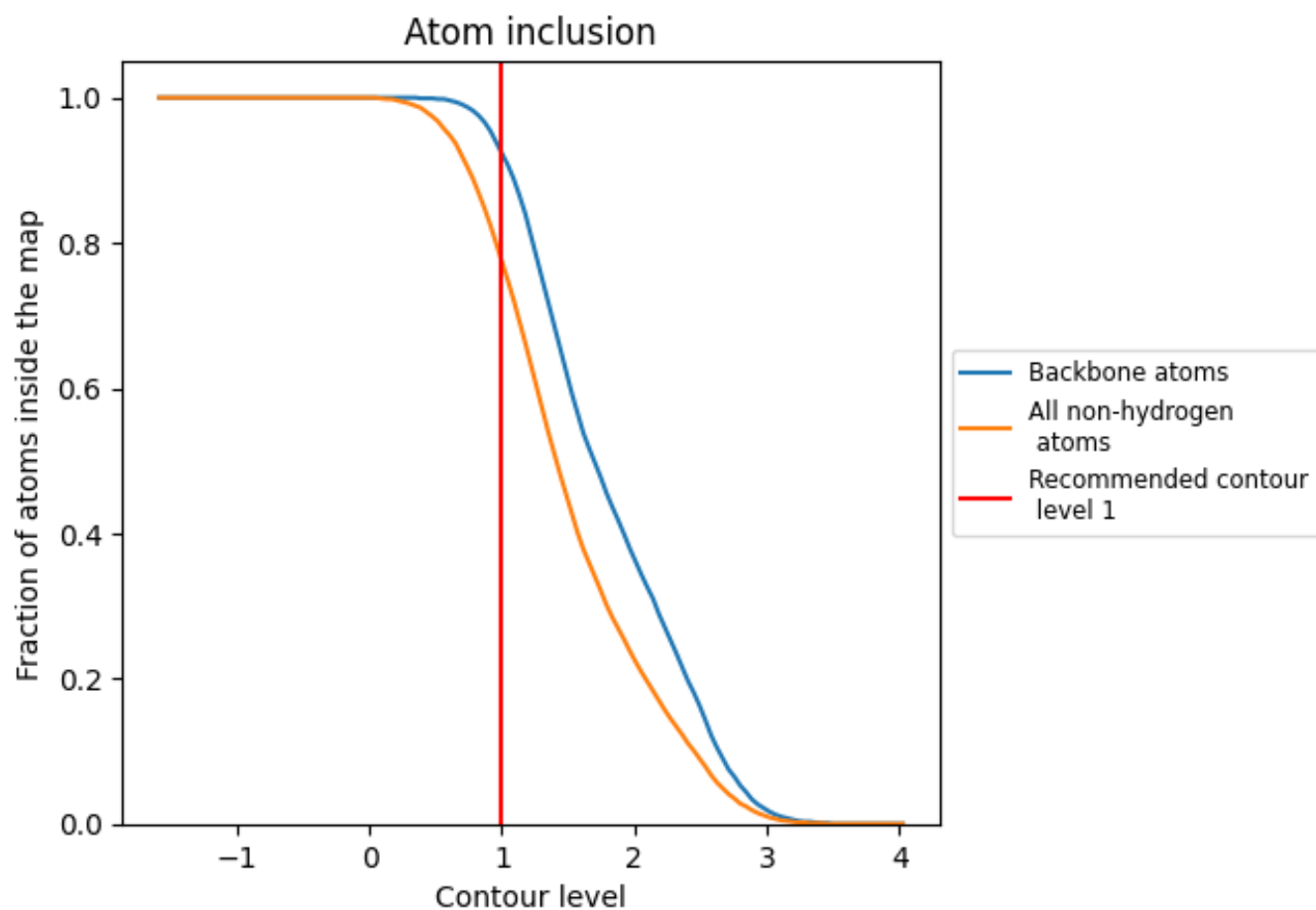
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 78% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7750	 0.4040
0	 0.7080	 0.4700
1	 0.6850	 0.3150
2	 0.6560	 0.2650
3	 0.6840	 0.3100
4	 0.6550	 0.2600
5	 0.6430	 0.4640
6	 0.7640	 0.3790
7	 0.5360	 0.3520
8	 0.7690	 0.4670
9	 0.7540	 0.4210
A	 0.8310	 0.4550
AA	 0.3080	 0.2980
B	 0.8280	 0.4530
BA	 0.7200	 0.4430
C	 0.8330	 0.4550
CA	 0.7600	 0.4500
D	 0.7620	 0.3810
DA	 0.7000	 0.4530
E	 0.7660	 0.3790
F	 0.9180	 0.4950
G	 0.6430	 0.3980
H	 0.6950	 0.3180
I	 0.6000	 0.4160
J	 0.5570	 0.3980
K	 0.4870	 0.4100
L	 0.6670	 0.2620
M	 0.7260	 0.3600
N	 0.7440	 0.3750
O	 0.6070	 0.4690
P	 0.7180	 0.4600
Q	 0.8670	 0.4810
R	 0.8370	 0.4400
S	 0.6670	 0.4600
T	 0.6070	 0.4290



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Chain	Atom inclusion	Q-score
U	0.4640	0.3470
V	0.7950	0.4600
W	0.7540	0.4230
X	0.7310	0.3580
Y	0.7320	0.3600
Z	0.7450	0.3740
a	0.7430	0.3780
b	0.3330	0.3010
c	0.9000	0.4960
d	0.6430	0.3790
e	0.5800	0.3980
f	0.8670	0.4820
g	0.8650	0.4800
h	0.8340	0.4390
i	0.8290	0.4380
j	0.5410	0.4060
k	0.5130	0.4200
l	0.6070	0.4640
m	0.7180	0.4360
n	0.6940	0.4610
o	0.6430	0.4490
p	0.5000	0.3510
q	0.8210	0.4650
r	0.7540	0.4070
s	0.3330	0.3130
t	0.9340	0.4930
u	0.6070	0.3750
v	0.5800	0.4160
w	0.5410	0.4120
x	0.4870	0.4310
y	0.5710	0.4780
z	0.7440	0.4530