



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 09:24 PM UTC

PDB ID : 7SGD / pdb_00007sgd
EMDB ID : EMD-25107
Title : Lassa virus glycoprotein construct(Josiah GPCysR4) recovered from GPC-I53-50 nanoparticle by localized reconstruction
Authors : Antanasijevic, A.; Brouwer, P.J.M.; Ward, A.B.
Deposited on : 2021-10-05
Resolution : 3.97 Å(reported)
Based on initial model : 5VK2

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

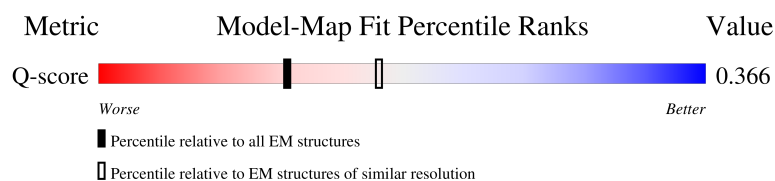
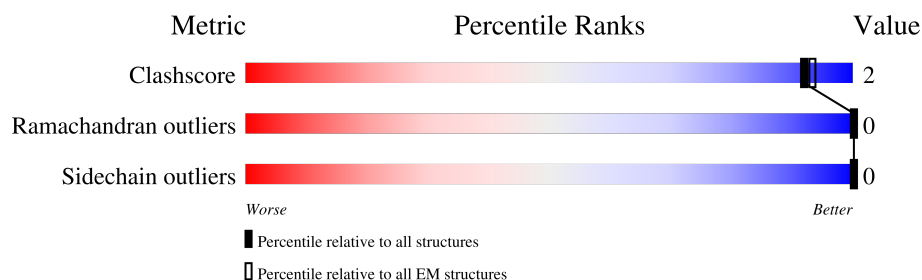
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.97 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.



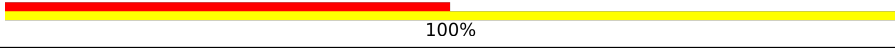
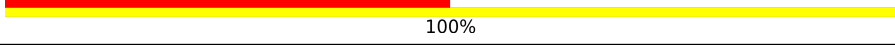
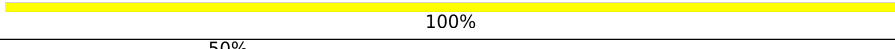
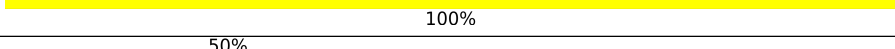
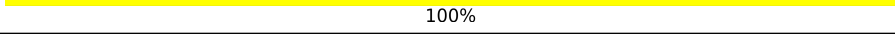
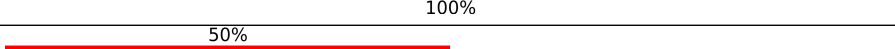
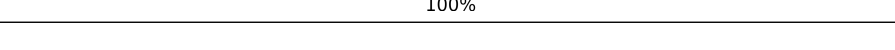
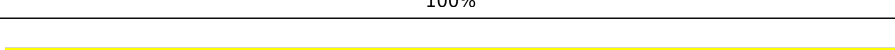
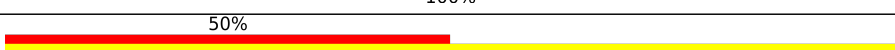
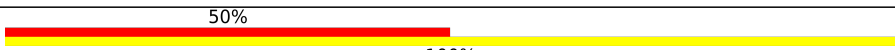
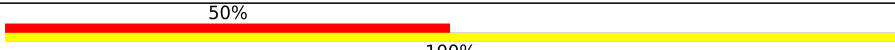
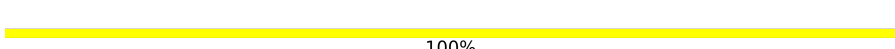
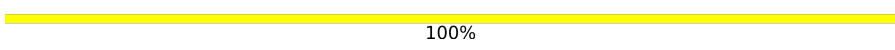
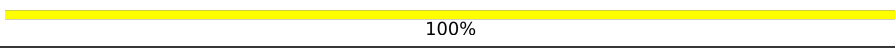
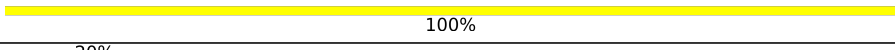
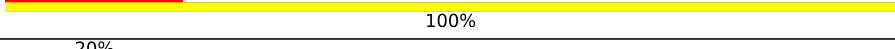
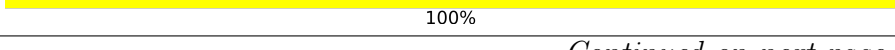
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7578 (3.47 - 4.47)

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

Mol	Chain	Length	Quality of chain
1	A	665	 25% 74%
1	B	665	 25% 74%
1	C	665	 25% 74%
1	a	665	 23% 75%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	b	665	
1	c	665	
2	D	2	
2	E	2	
2	G	2	
2	H	2	
2	I	2	
2	K	2	
2	M	2	
2	N	2	
2	P	2	
2	Q	2	
2	R	2	
2	T	2	
2	V	2	
2	W	2	
2	Y	2	
2	Z	2	
2	d	2	
2	f	2	
3	F	3	
3	O	3	
3	X	3	
4	J	5	
4	S	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	e	5	20% 100%
5	L	3	67% 100%
5	U	3	67% 100%
5	g	3	67% 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9120 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 Josiah GPCysR4 I53-50A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	174	Total	C	N	O	S	0	0
			1371	863	230	262	16		
1	a	164	Total	C	N	O	S	0	0
			1335	840	226	254	15		
1	B	174	Total	C	N	O	S	0	0
			1371	863	230	262	16		
1	b	164	Total	C	N	O	S	0	0
			1335	840	226	254	15		
1	C	174	Total	C	N	O	S	0	0
			1371	863	230	262	16		
1	c	164	Total	C	N	O	S	0	0
			1335	840	226	254	15		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	CYS	ARG	conflict	UNP Q6GWS0
A	258	ARG	LEU	conflict	UNP Q6GWS0
A	259	ARG	LEU	conflict	UNP Q6GWS0
A	329	PRO	GLU	conflict	UNP Q6GWS0
A	360	CYS	GLY	conflict	UNP Q6GWS0
a	207	CYS	ARG	conflict	UNP Q6GWS0
a	258	ARG	LEU	conflict	UNP Q6GWS0
a	259	ARG	LEU	conflict	UNP Q6GWS0
a	329	PRO	GLU	conflict	UNP Q6GWS0
a	360	CYS	GLY	conflict	UNP Q6GWS0
B	207	CYS	ARG	conflict	UNP Q6GWS0
B	258	ARG	LEU	conflict	UNP Q6GWS0
B	259	ARG	LEU	conflict	UNP Q6GWS0
B	329	PRO	GLU	conflict	UNP Q6GWS0
B	360	CYS	GLY	conflict	UNP Q6GWS0
b	207	CYS	ARG	conflict	UNP Q6GWS0
b	258	ARG	LEU	conflict	UNP Q6GWS0
b	259	ARG	LEU	conflict	UNP Q6GWS0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
b	329	PRO	GLU	conflict	UNP Q6GWS0
b	360	CYS	GLY	conflict	UNP Q6GWS0
C	207	CYS	ARG	conflict	UNP Q6GWS0
C	258	ARG	LEU	conflict	UNP Q6GWS0
C	259	ARG	LEU	conflict	UNP Q6GWS0
C	329	PRO	GLU	conflict	UNP Q6GWS0
C	360	CYS	GLY	conflict	UNP Q6GWS0
c	207	CYS	ARG	conflict	UNP Q6GWS0
c	258	ARG	LEU	conflict	UNP Q6GWS0
c	259	ARG	LEU	conflict	UNP Q6GWS0
c	329	PRO	GLU	conflict	UNP Q6GWS0
c	360	CYS	GLY	conflict	UNP Q6GWS0

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



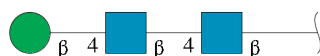
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

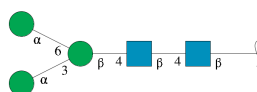
Mol	Chain	Residues	Atoms				AltConf	Trace
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	f	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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.



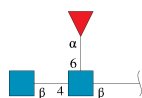
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		
3	X	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 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.



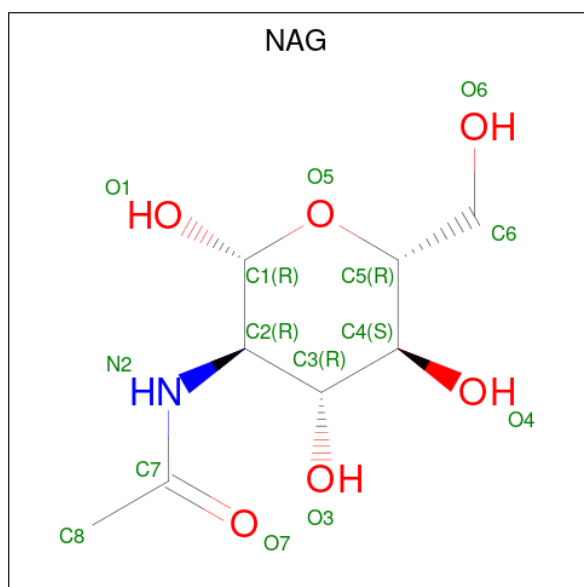
Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	5	Total	C	N	O	0	0
			61	34	2	25		
4	S	5	Total	C	N	O	0	0
			61	34	2	25		
4	e	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	3	Total	C	N	O	0	0
			38	22	2	14		
5	U	3	Total	C	N	O	0	0
			38	22	2	14		
5	g	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

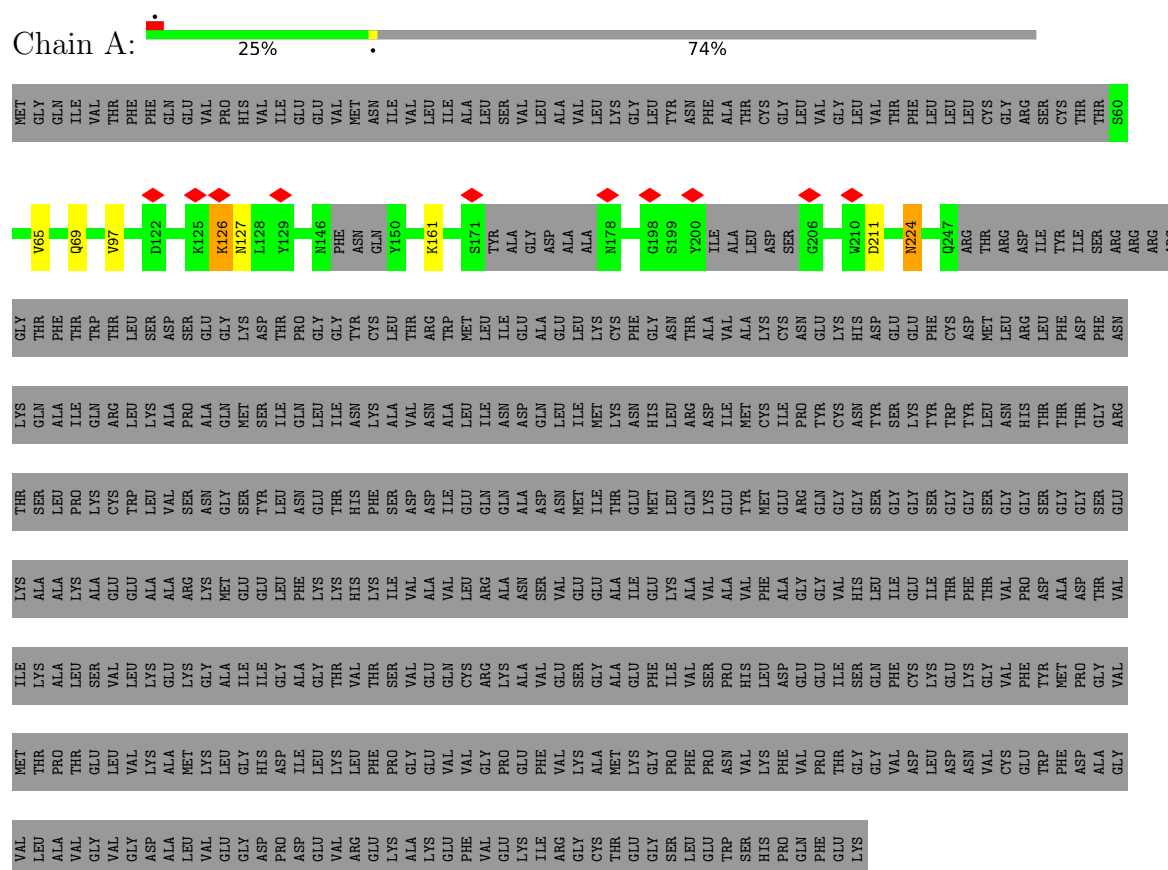


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	a	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	b	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	c	1	Total	C	N	O	0
			14	8	1	5	

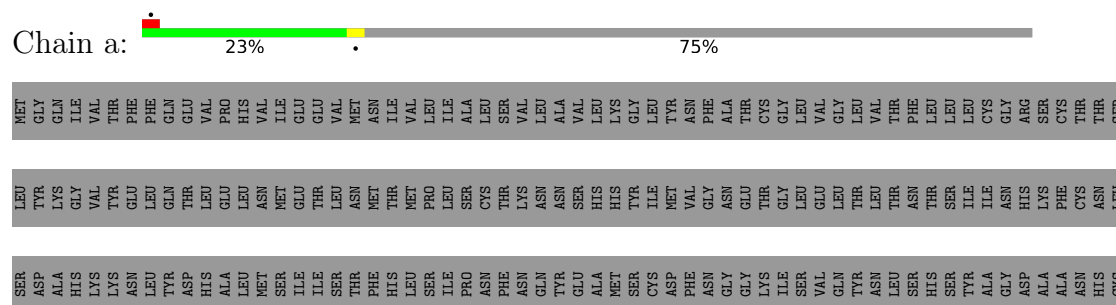
3 Residue-property plots

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

• Molecule 1: Josiah GPCysR4 I53-50A



• Molecule 1: Josiah GPCysR4 I53-50A







ASP	LEU	ASP	VAL	CYS	GLU	GLY	THR	TRP	GLY	THR	GLY	ASP	LEU	MET
ASP	ASP	GLY	THR	GLY	THR	GLY	GLY	LEU	THR	VAL	GLY	ALA	TYR	GLY
ASN	ASN	GLY	THR	GLY	THR	GLY	LEU	LEU	ASN	ALA	ALA	HIS	GLN	LYS
VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	SER	GLY	VAL	GLY	LYS	VAL	THR
CYS	CYS	VAL	VAL	VAL	VAL	VAL	GLY	GLN	GLY	VAL	VAL	ASN	GLU	THR
GLU	GLU	PHE	PRO	PHE	ASP	GLY	GLY	GLN	THR	THR	THR	ASN	LEU	PHE
TRP	TRP	ASP	ASP	ASP	ASP	GLY	ARG	ARG	THR	GLN	GLN	THR	LEU	GLY
PHE	PHE	PRO	ALA	GLY	THR	GLY	THR	ASP	PHE	THR	THR	HIS	LEU	PHE
ALA	ALA	VAL	VAL	VAL	VAL	GLY	GLY	ILE	GLY	THR	THR	ALA	LEU	VAL
GLY	GLY	VAL	VAL	VAL	VAL	GLY	GLY	ILE	THR	THR	THR	ARG	LEU	HIS
VAL	VAL	MET	ILE	MET	ILE	LYS	THR	TRP	ARG	ARG	ARG	MET	ASN	VAL
LEU	LEU	PRO	ALA	ALA	ALA	ALA	ILE	ILE	SER	SER	SER	ILE	ASN	VAL
VAL	VAL	PRO	ALA	ALA	ALA	ALA	SER	THR	THR	THR	THR	ILE	GLY	GLY
VAL	VAL	THR	THR	THR	THR	THR	LYS	ARG	ARG	ARG	ARG	ILE	GLU	GLY
VAL	VAL	GLU	SER	ALA	GLY	GLY	ALA	ARG	ARG	GLY	GLY	ILE	THR	VAL
VAL	VAL	LEU	VAL	LEU	LEU	GLY	GLY	ARG	ARG	GLY	SER	ASN	LEU	MET
GLY	GLY	VAL	VAL	VAL	VAL	GLY	VAL	ARG	GLY	THR	THR	THR	LEU	VAL
ASP	ASP	LYS	LYS	LYS	LYS	ALA	ALA	G260	GLY	THR	THR	PHE	MET	ASN
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	D268	ALA	ALA	ALA	HIS	THR	THR
VAL	VAL	MET	LYS	LYS	GLY	ARG	LYS	S269	THR	LEU	LEU	MET	PRO	LEU
VAL	VAL	LYS	GLY	MET	ALA	GLY	ALA	E270	ASP	ASP	ILE	SER	LEU	ILE
GLY	GLY	LEU	ILE	GLY	ILE	GLY	GLY	G271	SER	GLY	GLY	CYS	THR	SER
ASP	ASP	HIS	ILE	ASP	ILE	GLY	GLY	K272	THR	CYS	GLY	PHE	LEU	VAL
ASP	ASP	ILE	ALA	PHE	PHE	PHE	LYS	D273	GLY	ASN	GLN	ASN	LYS	VAL
GLY	GLY	LEU	THR	LYS	THR	LYS	LYS	T274	THR	THR	THR	ASN	ASN	ALA
VAL	VAL	LYS	VAL	HIS	VAL	HIS	LYS		ASP	ASP	GLY	SER	ASN	VAL
ARG	ARG	LEU	THR	PHE	THR	THR	LYS	E303	CYS	CYS	ALA	HIS	LEU	VAL
GLY	GLY	PRO	SER	ILE	VAL	ILE	ILE	K304	ILE	ILE	MET	HIS	GLY	LYS
LYS	LYS	PRO	VAL	VAL	VAL	VAL	VAL	B305	MET	MET	SER	TYR	GLY	LYS
LYS	LYS	GLY	GLY	ALA	ALA	ALA	ALA	D306	THR	THR	CYS	ILE	LEU	LEU
GLU	GLU	VAL	GLN	VAL	GLN	VAL	VAL		SER	SER	ASP	MET	TYR	THR
PHE	PHE	VAL	VAL	VAL	VAL	VAL	VAL	K327	THR	THR	PHE	VAL	ASN	ASN
VAL	VAL	GLY	ARG	ARG	ARG	ARG	ARG	A328	GLN	GLN	ASN	GLY	ASN	PHE
GLU	GLU	PRO	LYS	ALA	ALA	ALA	ALA	P329	THR	THR	GLY	ASN	GLY	THR
LYS	LYS	PHE	ALA	ASN	ASN	ASN	ASN	A330	LEU	LEU	GLY	THR	THR	CYS
ILE	ILE	GLU	VAL	VAL	VAL	VAL	VAL	Q331	ILE	ILE	LYS	THR	THR	GLY
ARG	ARG	VAL	GLY	VAL	GLY	VAL	VAL		ILE	ILE	ILE	GLY	GLY	GLY
CYS	CYS	LYS	SER	GLY	SER	GLY	GLY	Q335	GLN	GLN	SER	LEU	LEU	VAL
GLY	GLY	ALA	GLY	GLY	GLY	GLY	GLY		ASN	ASN	VAL	GLU	GLU	VAL
THR	THR	MET	GLY	ILE	GLY	ILE	ILE		THR	THR	GLN	THR	LEU	GLY
GLY	GLY	LYS	PHE	GLY	PHE	GLY	GLY	I345	THR	THR	THR	THR	LEU	THR
PRO	PRO													

NAG1
NAG2

NAG1
NAG2

NAG1
NAG2

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



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



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



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



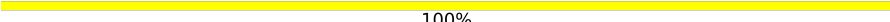
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain Q:  100%

MAG1
MAG2

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

Chain R:  50%
100%

MAG1
MAG2

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

Chain T:  50%
50%

MAG1
MAG2

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

Chain V:  50%
100%

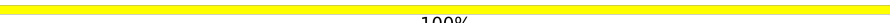
MAG1
MAG2

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

Chain W:  50%
100%

MAG1
MAG2

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

Chain Y:  100%

MAG1
MAG2

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



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



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



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



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



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



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

nose



● Molecule 4: 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 4: 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 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]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	124891	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 ($e^-/\text{\AA}^2$)	50.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.032	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	226.59999, 226.59999, 226.59999	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.18	0/1401	1.31	5/1895 (0.3%)
1	B	1.18	0/1401	1.31	5/1895 (0.3%)
1	C	1.18	0/1401	1.31	5/1895 (0.3%)
1	a	1.19	0/1363	1.21	5/1840 (0.3%)
1	b	1.19	0/1363	1.21	4/1840 (0.2%)
1	c	1.18	0/1363	1.21	5/1840 (0.3%)
All	All	1.18	0/8292	1.26	29/11205 (0.3%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ASN	N-CA-CB	7.37	120.80	110.26
1	C	224	ASN	N-CA-CB	7.36	120.78	110.26
1	B	224	ASN	N-CA-CB	7.35	120.77	110.26
1	C	65	VAL	N-CA-C	7.07	121.13	113.43
1	B	65	VAL	N-CA-C	7.04	121.11	113.43
1	A	65	VAL	N-CA-C	7.03	121.09	113.43
1	a	331	GLN	CA-C-N	-6.57	111.75	120.95
1	a	331	GLN	C-N-CA	-6.57	111.75	120.95
1	c	331	GLN	CA-C-N	-6.55	111.77	120.95
1	c	331	GLN	C-N-CA	-6.55	111.77	120.95
1	b	331	GLN	CA-C-N	-6.55	111.78	120.95
1	b	331	GLN	C-N-CA	-6.55	111.78	120.95
1	B	126	LYS	N-CA-C	-5.62	102.58	110.50
1	A	126	LYS	N-CA-C	-5.62	102.58	110.50
1	C	126	LYS	N-CA-C	-5.62	102.58	110.50
1	c	345	ILE	N-CA-C	5.60	116.01	108.17
1	a	382	LEU	N-CA-C	-5.59	102.72	109.83
1	b	382	LEU	N-CA-C	-5.59	102.73	109.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	345	ILE	N-CA-C	5.59	115.99	108.17
1	a	345	ILE	N-CA-C	5.58	115.99	108.17
1	c	382	LEU	N-CA-C	-5.58	102.75	109.83
1	B	97	VAL	N-CA-C	5.30	115.49	107.75
1	A	97	VAL	N-CA-C	5.29	115.48	107.75
1	C	97	VAL	N-CA-C	5.26	115.44	107.75
1	c	331	GLN	N-CA-C	-5.23	102.31	110.42
1	a	331	GLN	N-CA-C	-5.23	102.31	110.42
1	A	211	ASP	N-CA-C	5.07	117.47	111.33
1	C	211	ASP	N-CA-C	5.07	117.46	111.33
1	B	211	ASP	N-CA-C	5.06	117.45	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1371	0	1294	3	0
1	B	1371	0	1294	3	0
1	C	1371	0	1294	4	0
1	a	1335	0	1282	6	0
1	b	1335	0	1282	7	0
1	c	1335	0	1282	7	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	K	28	0	25	1	0
2	M	28	0	25	0	0
2	N	28	0	25	1	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
2	T	28	0	25	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	28	0	25	0	0
2	W	28	0	25	1	0
2	Y	28	0	25	0	0
2	Z	28	0	25	0	0
2	d	28	0	25	0	0
2	f	28	0	25	1	0
3	F	39	0	34	0	0
3	O	39	0	34	0	0
3	X	39	0	34	0	0
4	J	61	0	52	0	0
4	S	61	0	52	0	0
4	e	61	0	52	0	0
5	L	38	0	34	0	0
5	U	38	0	34	0	0
5	g	38	0	34	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
6	a	14	0	13	0	0
6	b	14	0	13	0	0
6	c	14	0	13	0	0
All	All	9120	0	8616	27	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 2.

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LYS:HA	1:B:224:ASN:OD1	2.04	0.58
1:C:161:LYS:HA	1:C:224:ASN:OD1	2.04	0.57
1:A:161:LYS:HA	1:A:224:ASN:OD1	2.04	0.56
1:a:380:THR:HG21	2:K:1:NAG:H82	1.90	0.54
1:c:380:THR:HG21	2:f:1:NAG:H82	1.90	0.53
1:b:380:THR:HG21	2:T:1:NAG:H82	1.90	0.52
1:C:126:LYS:O	1:C:127:ASN:C	2.54	0.49
1:A:126:LYS:O	1:A:127:ASN:C	2.54	0.48
1:b:303:GLU:OE2	1:c:304:LYS:NZ	2.48	0.47
1:B:69:GLN:NE2	1:b:373:ASN:HD22	2.13	0.47
1:C:69:GLN:NE2	1:c:373:ASN:HD22	2.13	0.47
1:a:304:LYS:NZ	1:c:303:GLU:OE2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:NAG:H62	2:E:2:NAG:C7	2.45	0.46
1:b:367:SER:OG	1:b:368:LYS:N	2.49	0.46
1:a:367:SER:OG	1:a:368:LYS:N	2.49	0.46
1:A:69:GLN:NE2	1:a:373:ASN:HD22	2.13	0.46
1:B:126:LYS:O	1:B:127:ASN:C	2.54	0.46
2:N:1:NAG:H62	2:N:2:NAG:C7	2.45	0.46
1:a:303:GLU:OE2	1:b:304:LYS:NZ	2.48	0.45
2:W:1:NAG:H62	2:W:2:NAG:C7	2.45	0.45
1:c:367:SER:OG	1:c:368:LYS:N	2.49	0.44
1:a:306:ASP:OD1	1:a:306:ASP:N	2.49	0.44
1:c:306:ASP:OD1	1:c:306:ASP:N	2.49	0.43
1:b:306:ASP:OD1	1:b:306:ASP:N	2.49	0.43
1:b:347:ASP:OD1	1:b:347:ASP:N	2.52	0.42
1:C:130:ASP:C	1:C:130:ASP:OD1	2.65	0.40
1:c:347:ASP:OD1	1:c:347:ASP:N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/665 (25%)	163 (98%)	3 (2%)	0	100	100
1	B	166/665 (25%)	163 (98%)	3 (2%)	0	100	100
1	C	166/665 (25%)	163 (98%)	3 (2%)	0	100	100
1	a	162/665 (24%)	159 (98%)	3 (2%)	0	100	100
1	b	162/665 (24%)	159 (98%)	3 (2%)	0	100	100
1	c	162/665 (24%)	159 (98%)	3 (2%)	0	100	100
All	All	984/3990 (25%)	966 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	156/565 (28%)	156 (100%)	0	100	100
1	B	156/565 (28%)	156 (100%)	0	100	100
1	C	156/565 (28%)	156 (100%)	0	100	100
1	a	148/565 (26%)	148 (100%)	0	100	100
1	b	148/565 (26%)	148 (100%)	0	100	100
1	c	148/565 (26%)	148 (100%)	0	100	100
All	All	912/3390 (27%)	912 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	69	GLN
1	A	92	HIS
1	A	158	ASN
1	A	209	ASN
1	a	321	GLN
1	a	405	GLN
1	B	69	GLN
1	B	92	HIS
1	B	209	ASN
1	b	321	GLN
1	b	405	GLN
1	C	69	GLN
1	C	92	HIS
1	C	158	ASN
1	C	209	ASN
1	c	321	GLN
1	c	405	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

69 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	1,2	14,14,15	2.06	6 (42%)	17,19,21	1.00	1 (5%)
2	NAG	D	2	2	14,14,15	2.06	5 (35%)	17,19,21	0.88	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.40	0	17,19,21	0.73	0
2	NAG	E	2	2	14,14,15	0.39	0	17,19,21	0.46	0
3	NAG	F	1	3,1	14,14,15	1.88	4 (28%)	17,19,21	1.51	6 (35%)
3	NAG	F	2	3	14,14,15	2.00	5 (35%)	17,19,21	0.93	0
3	BMA	F	3	3	11,11,12	1.86	5 (45%)	15,15,17	0.87	1 (6%)
2	NAG	G	1	1,2	14,14,15	2.21	6 (42%)	17,19,21	1.19	2 (11%)
2	NAG	G	2	2	14,14,15	2.01	5 (35%)	17,19,21	0.85	1 (5%)
2	NAG	H	1	1,2	14,14,15	2.14	5 (35%)	17,19,21	1.13	1 (5%)
2	NAG	H	2	2	14,14,15	2.01	5 (35%)	17,19,21	0.90	1 (5%)
2	NAG	I	1	1,2	14,14,15	2.25	6 (42%)	17,19,21	1.03	1 (5%)
2	NAG	I	2	2	14,14,15	2.16	5 (35%)	17,19,21	0.92	1 (5%)
4	NAG	J	1	1,4	14,14,15	1.80	3 (21%)	17,19,21	1.42	2 (11%)
4	NAG	J	2	4	14,14,15	1.75	5 (35%)	17,19,21	1.43	4 (23%)
4	BMA	J	3	4	11,11,12	1.46	3 (27%)	15,15,17	0.64	0
4	MAN	J	4	4	11,11,12	1.88	4 (36%)	15,15,17	0.66	0
4	MAN	J	5	4	11,11,12	1.79	5 (45%)	15,15,17	0.75	0
2	NAG	K	1	1,2	14,14,15	0.37	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	K	2	2	14,14,15	0.38	0	17,19,21	0.44	0
5	NAG	L	1	1,5	14,14,15	1.63	3 (21%)	17,19,21	1.07	1 (5%)
5	NAG	L	2	5	14,14,15	2.39	5 (35%)	17,19,21	1.22	3 (17%)
5	FUC	L	3	5	10,10,11	1.88	5 (50%)	14,14,16	0.67	0
2	NAG	M	1	1,2	14,14,15	2.07	6 (42%)	17,19,21	1.01	1 (5%)
2	NAG	M	2	2	14,14,15	2.06	5 (35%)	17,19,21	0.87	1 (5%)
2	NAG	N	1	1,2	14,14,15	0.41	0	17,19,21	0.74	0
2	NAG	N	2	2	14,14,15	0.39	0	17,19,21	0.46	0
3	NAG	O	1	3,1	14,14,15	1.88	4 (28%)	17,19,21	1.51	6 (35%)
3	NAG	O	2	3	14,14,15	2.00	5 (35%)	17,19,21	0.92	0
3	BMA	O	3	3	11,11,12	1.85	5 (45%)	15,15,17	0.87	1 (6%)
2	NAG	P	1	1,2	14,14,15	2.21	6 (42%)	17,19,21	1.18	2 (11%)
2	NAG	P	2	2	14,14,15	2.01	5 (35%)	17,19,21	0.85	1 (5%)
2	NAG	Q	1	1,2	14,14,15	2.14	5 (35%)	17,19,21	1.13	1 (5%)
2	NAG	Q	2	2	14,14,15	2.01	5 (35%)	17,19,21	0.90	1 (5%)
2	NAG	R	1	1,2	14,14,15	2.25	6 (42%)	17,19,21	1.04	1 (5%)
2	NAG	R	2	2	14,14,15	2.15	5 (35%)	17,19,21	0.92	1 (5%)
4	NAG	S	1	1,4	14,14,15	1.80	3 (21%)	17,19,21	1.42	2 (11%)
4	NAG	S	2	4	14,14,15	1.75	5 (35%)	17,19,21	1.43	4 (23%)
4	BMA	S	3	4	11,11,12	1.47	3 (27%)	15,15,17	0.64	0
4	MAN	S	4	4	11,11,12	1.88	4 (36%)	15,15,17	0.66	0
4	MAN	S	5	4	11,11,12	1.78	5 (45%)	15,15,17	0.75	0
2	NAG	T	1	1,2	14,14,15	0.37	0	17,19,21	0.49	0
2	NAG	T	2	2	14,14,15	0.38	0	17,19,21	0.44	0
5	NAG	U	1	1,5	14,14,15	1.63	3 (21%)	17,19,21	1.06	1 (5%)
5	NAG	U	2	5	14,14,15	2.39	5 (35%)	17,19,21	1.21	2 (11%)
5	FUC	U	3	5	10,10,11	1.87	5 (50%)	14,14,16	0.67	0
2	NAG	V	1	1,2	14,14,15	2.07	6 (42%)	17,19,21	1.00	1 (5%)
2	NAG	V	2	2	14,14,15	2.06	5 (35%)	17,19,21	0.88	1 (5%)
2	NAG	W	1	1,2	14,14,15	0.40	0	17,19,21	0.73	0
2	NAG	W	2	2	14,14,15	0.38	0	17,19,21	0.46	0
3	NAG	X	1	3,1	14,14,15	1.89	4 (28%)	17,19,21	1.51	6 (35%)
3	NAG	X	2	3	14,14,15	2.00	5 (35%)	17,19,21	0.93	0
3	BMA	X	3	3	11,11,12	1.84	5 (45%)	15,15,17	0.87	1 (6%)
2	NAG	Y	1	1,2	14,14,15	2.20	6 (42%)	17,19,21	1.19	2 (11%)
2	NAG	Y	2	2	14,14,15	2.00	5 (35%)	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Z	1	1,2	14,14,15	2.14	5 (35%)	17,19,21	1.13	1 (5%)
2	NAG	Z	2	2	14,14,15	2.01	5 (35%)	17,19,21	0.90	1 (5%)
2	NAG	d	1	1,2	14,14,15	2.24	6 (42%)	17,19,21	1.04	1 (5%)
2	NAG	d	2	2	14,14,15	2.17	5 (35%)	17,19,21	0.92	1 (5%)
4	NAG	e	1	1,4	14,14,15	1.80	3 (21%)	17,19,21	1.42	2 (11%)
4	NAG	e	2	4	14,14,15	1.76	5 (35%)	17,19,21	1.43	4 (23%)
4	BMA	e	3	4	11,11,12	1.46	3 (27%)	15,15,17	0.64	0
4	MAN	e	4	4	11,11,12	1.88	5 (45%)	15,15,17	0.66	0
4	MAN	e	5	4	11,11,12	1.79	5 (45%)	15,15,17	0.75	0
2	NAG	f	1	1,2	14,14,15	0.37	0	17,19,21	0.49	0
2	NAG	f	2	2	14,14,15	0.38	0	17,19,21	0.43	0
5	NAG	g	1	1,5	14,14,15	1.63	3 (21%)	17,19,21	1.07	1 (5%)
5	NAG	g	2	5	14,14,15	2.39	5 (35%)	17,19,21	1.21	3 (17%)
5	FUC	g	3	5	10,10,11	1.89	5 (50%)	14,14,16	0.67	0

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	d	2	2	-	0/6/23/26	0/1/1/1
4	NAG	e	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
4	BMA	e	3	4	-	2/2/19/22	0/1/1/1
4	MAN	e	4	4	-	2/2/19/22	0/1/1/1
4	MAN	e	5	4	-	0/2/19/22	0/1/1/1
2	NAG	f	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	f	2	2	-	4/6/23/26	0/1/1/1
5	NAG	g	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	g	2	5	-	3/6/23/26	0/1/1/1
5	FUC	g	3	5	-	-	0/1/1/1

All (271) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	2	NAG	C1-C2	6.41	1.61	1.52
5	g	2	NAG	C1-C2	6.40	1.61	1.52
5	U	2	NAG	C1-C2	6.40	1.61	1.52
2	d	1	NAG	C1-C2	6.10	1.60	1.52
2	R	1	NAG	C1-C2	6.10	1.60	1.52
2	I	1	NAG	C1-C2	6.09	1.60	1.52
2	G	1	NAG	C1-C2	5.94	1.60	1.52
2	Y	1	NAG	C1-C2	5.93	1.60	1.52
2	P	1	NAG	C1-C2	5.91	1.60	1.52
2	d	2	NAG	C1-C2	5.65	1.60	1.52
2	I	2	NAG	C1-C2	5.61	1.60	1.52
2	R	2	NAG	C1-C2	5.56	1.59	1.52
2	H	1	NAG	C1-C2	5.50	1.59	1.52
2	Q	1	NAG	C1-C2	5.48	1.59	1.52
2	Z	1	NAG	C1-C2	5.46	1.59	1.52
3	X	1	NAG	C1-C2	4.97	1.59	1.52
2	D	2	NAG	C1-C2	4.96	1.59	1.52
3	F	1	NAG	C1-C2	4.95	1.59	1.52
2	M	2	NAG	C1-C2	4.95	1.59	1.52
2	V	2	NAG	C1-C2	4.93	1.59	1.52
3	O	1	NAG	C1-C2	4.92	1.59	1.52
2	P	2	NAG	C1-C2	4.86	1.59	1.52
2	G	2	NAG	C1-C2	4.83	1.58	1.52
2	Y	2	NAG	C1-C2	4.81	1.58	1.52
3	X	2	NAG	C1-C2	4.79	1.58	1.52
3	O	2	NAG	C1-C2	4.78	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	C1-C2	4.76	1.58	1.52
2	M	1	NAG	C1-C2	4.70	1.58	1.52
2	Q	2	NAG	C1-C2	4.69	1.58	1.52
2	V	1	NAG	C1-C2	4.67	1.58	1.52
2	H	2	NAG	C1-C2	4.66	1.58	1.52
2	Z	2	NAG	C1-C2	4.66	1.58	1.52
2	D	1	NAG	C1-C2	4.65	1.58	1.52
4	e	1	NAG	C1-C2	4.25	1.58	1.52
4	S	1	NAG	C1-C2	4.23	1.58	1.52
4	J	1	NAG	C1-C2	4.23	1.58	1.52
5	U	1	NAG	C1-C2	4.19	1.58	1.52
5	L	1	NAG	C1-C2	4.19	1.58	1.52
5	g	1	NAG	C1-C2	4.18	1.58	1.52
4	S	2	NAG	C1-C2	3.75	1.57	1.52
4	e	2	NAG	C1-C2	3.74	1.57	1.52
4	J	2	NAG	C1-C2	3.74	1.57	1.52
2	Z	1	NAG	O5-C5	3.42	1.50	1.43
2	Q	1	NAG	O5-C5	3.39	1.50	1.43
2	H	1	NAG	O5-C5	3.39	1.50	1.43
5	g	2	NAG	O5-C5	3.35	1.50	1.43
5	U	2	NAG	O5-C5	3.33	1.49	1.43
5	L	2	NAG	O5-C5	3.31	1.49	1.43
2	M	2	NAG	O5-C5	3.29	1.49	1.43
2	D	2	NAG	O5-C5	3.27	1.49	1.43
2	V	2	NAG	O5-C5	3.27	1.49	1.43
2	Y	2	NAG	O5-C5	3.25	1.49	1.43
2	G	2	NAG	O5-C5	3.24	1.49	1.43
4	e	4	MAN	O5-C5	3.22	1.49	1.43
4	J	4	MAN	O5-C5	3.21	1.49	1.43
4	S	4	MAN	O5-C5	3.21	1.49	1.43
3	F	3	BMA	C2-C3	3.21	1.57	1.52
2	P	2	NAG	O5-C5	3.20	1.49	1.43
2	V	1	NAG	O5-C5	3.20	1.49	1.43
3	O	3	BMA	C2-C3	3.18	1.57	1.52
2	M	1	NAG	O5-C5	3.16	1.49	1.43
2	Z	2	NAG	O5-C5	3.16	1.49	1.43
2	D	1	NAG	O5-C5	3.14	1.49	1.43
2	H	2	NAG	O5-C5	3.11	1.49	1.43
2	Q	2	NAG	O5-C5	3.11	1.49	1.43
3	X	3	BMA	C2-C3	3.10	1.57	1.52
2	d	2	NAG	O5-C5	3.10	1.49	1.43
2	I	2	NAG	O5-C5	3.09	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	2	NAG	O5-C5	3.07	1.49	1.43
3	O	2	NAG	O5-C5	3.02	1.49	1.43
3	X	2	NAG	O5-C5	3.02	1.49	1.43
3	F	2	NAG	O5-C5	3.01	1.49	1.43
4	J	4	MAN	C2-C3	3.00	1.57	1.52
4	S	4	MAN	C2-C3	3.00	1.57	1.52
4	e	4	MAN	C2-C3	2.99	1.57	1.52
2	R	1	NAG	O5-C5	2.92	1.49	1.43
2	I	1	NAG	O5-C5	2.91	1.49	1.43
2	d	1	NAG	O5-C5	2.90	1.49	1.43
4	S	5	MAN	C2-C3	2.88	1.56	1.52
4	J	5	MAN	C2-C3	2.88	1.56	1.52
4	e	5	MAN	O5-C5	2.86	1.49	1.43
4	e	5	MAN	C2-C3	2.86	1.56	1.52
5	U	2	NAG	C3-C2	2.85	1.58	1.52
5	L	2	NAG	C3-C2	2.85	1.58	1.52
5	g	2	NAG	C3-C2	2.82	1.58	1.52
4	J	5	MAN	O5-C5	2.82	1.48	1.43
4	S	5	MAN	O5-C5	2.79	1.48	1.43
5	U	1	NAG	O5-C5	2.76	1.48	1.43
5	g	1	NAG	O5-C5	2.76	1.48	1.43
5	L	1	NAG	O5-C5	2.75	1.48	1.43
3	O	3	BMA	O5-C5	2.74	1.48	1.43
2	Y	1	NAG	O5-C5	2.74	1.48	1.43
2	G	1	NAG	O5-C5	2.73	1.48	1.43
2	P	1	NAG	O5-C5	2.72	1.48	1.43
3	F	3	BMA	O5-C5	2.72	1.48	1.43
5	g	3	FUC	C1-C2	2.71	1.58	1.52
3	X	3	BMA	O5-C5	2.71	1.48	1.43
2	R	2	NAG	C3-C2	2.70	1.58	1.52
5	L	3	FUC	C1-C2	2.69	1.58	1.52
2	I	2	NAG	C3-C2	2.69	1.58	1.52
2	d	2	NAG	C3-C2	2.69	1.58	1.52
5	L	3	FUC	C2-C3	2.69	1.56	1.52
5	U	3	FUC	C2-C3	2.67	1.56	1.52
5	g	3	FUC	C2-C3	2.67	1.56	1.52
5	U	3	FUC	C1-C2	2.66	1.58	1.52
5	g	3	FUC	O5-C5	2.66	1.48	1.43
2	P	1	NAG	C4-C5	2.65	1.58	1.53
5	L	3	FUC	O5-C5	2.64	1.48	1.43
3	O	3	BMA	C1-C2	2.64	1.58	1.52
3	F	3	BMA	C1-C2	2.63	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	NAG	C4-C5	2.63	1.58	1.53
2	Y	1	NAG	C4-C5	2.63	1.58	1.53
5	U	3	FUC	O5-C5	2.63	1.48	1.43
3	X	3	BMA	C1-C2	2.63	1.58	1.52
2	Q	2	NAG	C3-C2	2.62	1.58	1.52
2	H	2	NAG	C3-C2	2.61	1.58	1.52
4	S	3	BMA	O5-C5	2.60	1.48	1.43
4	e	2	NAG	O5-C5	2.58	1.48	1.43
2	Z	2	NAG	C3-C2	2.58	1.57	1.52
5	g	3	FUC	C4-C5	2.58	1.58	1.52
5	L	3	FUC	C4-C5	2.56	1.58	1.52
4	J	2	NAG	O5-C5	2.56	1.48	1.43
5	U	3	FUC	C4-C5	2.56	1.58	1.52
4	J	3	BMA	O5-C5	2.55	1.48	1.43
4	S	2	NAG	O5-C5	2.55	1.48	1.43
5	U	2	NAG	C2-N2	2.54	1.50	1.46
2	M	1	NAG	C4-C5	2.53	1.58	1.53
5	L	2	NAG	C2-N2	2.53	1.50	1.46
5	g	2	NAG	C2-N2	2.53	1.50	1.46
2	Q	1	NAG	O5-C1	2.52	1.47	1.43
4	S	1	NAG	O5-C5	2.52	1.48	1.43
4	e	3	BMA	O5-C5	2.52	1.48	1.43
4	e	1	NAG	O5-C5	2.52	1.48	1.43
2	H	1	NAG	O5-C1	2.51	1.47	1.43
2	D	1	NAG	C4-C5	2.50	1.58	1.53
2	V	1	NAG	C4-C5	2.50	1.58	1.53
4	J	1	NAG	O5-C5	2.50	1.48	1.43
2	Z	1	NAG	O5-C1	2.49	1.47	1.43
2	M	2	NAG	C3-C2	2.49	1.57	1.52
4	S	5	MAN	C4-C5	2.49	1.58	1.53
4	e	5	MAN	C4-C5	2.49	1.58	1.53
4	e	4	MAN	C1-C2	2.48	1.58	1.52
2	V	2	NAG	C3-C2	2.47	1.57	1.52
4	J	5	MAN	C4-C5	2.47	1.58	1.53
2	D	2	NAG	C3-C2	2.46	1.57	1.52
4	J	4	MAN	C1-C2	2.46	1.58	1.52
3	O	2	NAG	C4-C5	2.44	1.58	1.53
2	D	1	NAG	O5-C1	2.43	1.47	1.43
4	S	4	MAN	C1-C2	2.43	1.58	1.52
4	S	1	NAG	C3-C2	2.43	1.57	1.52
5	L	2	NAG	C4-C5	2.42	1.58	1.53
3	F	2	NAG	C4-C5	2.42	1.58	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	2	NAG	C4-C5	2.42	1.58	1.53
3	O	1	NAG	O5-C5	2.41	1.48	1.43
2	V	1	NAG	O5-C1	2.40	1.47	1.43
4	J	1	NAG	C3-C2	2.40	1.57	1.52
2	Z	1	NAG	C4-C5	2.40	1.58	1.53
2	Q	1	NAG	C4-C5	2.40	1.58	1.53
3	F	1	NAG	O5-C5	2.40	1.48	1.43
2	M	1	NAG	O5-C1	2.40	1.47	1.43
2	H	1	NAG	C4-C5	2.39	1.58	1.53
3	X	1	NAG	O5-C5	2.39	1.48	1.43
5	U	2	NAG	C4-C5	2.39	1.58	1.53
2	Y	2	NAG	C3-C2	2.39	1.57	1.52
4	e	1	NAG	C3-C2	2.39	1.57	1.52
5	g	2	NAG	C4-C5	2.38	1.58	1.53
2	P	2	NAG	C3-C2	2.38	1.57	1.52
2	G	2	NAG	C3-C2	2.38	1.57	1.52
3	X	2	NAG	C4-C3	2.37	1.58	1.52
4	e	5	MAN	C1-C2	2.37	1.57	1.52
4	S	5	MAN	C1-C2	2.37	1.57	1.52
4	J	5	MAN	C1-C2	2.37	1.57	1.52
3	F	2	NAG	C4-C3	2.36	1.58	1.52
3	O	2	NAG	C4-C3	2.35	1.58	1.52
2	Z	2	NAG	C4-C5	2.34	1.58	1.53
4	J	4	MAN	C4-C5	2.34	1.58	1.53
4	S	4	MAN	C4-C5	2.34	1.58	1.53
2	V	2	NAG	C4-C5	2.33	1.58	1.53
2	Q	2	NAG	C4-C5	2.33	1.58	1.53
4	S	2	NAG	C4-C3	2.32	1.58	1.52
4	J	2	NAG	C4-C3	2.32	1.58	1.52
2	d	1	NAG	C4-C5	2.32	1.58	1.53
2	M	2	NAG	C4-C5	2.32	1.58	1.53
2	H	2	NAG	C4-C5	2.32	1.58	1.53
4	e	2	NAG	C4-C3	2.31	1.58	1.52
2	I	1	NAG	C4-C5	2.31	1.57	1.53
2	R	1	NAG	C4-C5	2.31	1.57	1.53
4	e	4	MAN	C4-C5	2.31	1.57	1.53
2	D	2	NAG	C4-C5	2.31	1.57	1.53
2	G	2	NAG	C4-C5	2.29	1.57	1.53
2	P	2	NAG	C4-C5	2.29	1.57	1.53
2	Y	2	NAG	C4-C5	2.28	1.57	1.53
3	O	3	BMA	C4-C5	2.27	1.57	1.53
3	F	3	BMA	C4-C5	2.27	1.57	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	3	BMA	C4-C5	2.26	1.57	1.53
2	I	1	NAG	C3-C2	2.26	1.57	1.52
3	X	1	NAG	C4-C5	2.26	1.57	1.53
2	R	1	NAG	C3-C2	2.25	1.57	1.52
2	d	1	NAG	C3-C2	2.25	1.57	1.52
3	F	2	NAG	C3-C2	2.25	1.57	1.52
3	X	2	NAG	C3-C2	2.24	1.57	1.52
3	O	2	NAG	C3-C2	2.23	1.57	1.52
4	e	2	NAG	C3-C2	2.23	1.57	1.52
4	J	3	BMA	C1-C2	2.23	1.57	1.52
4	S	3	BMA	C1-C2	2.22	1.57	1.52
3	O	1	NAG	C4-C5	2.22	1.57	1.53
3	F	1	NAG	C4-C5	2.22	1.57	1.53
4	e	3	BMA	C1-C2	2.20	1.57	1.52
4	J	2	NAG	C3-C2	2.20	1.57	1.52
2	I	1	NAG	O5-C1	2.19	1.47	1.43
4	S	2	NAG	C3-C2	2.19	1.57	1.52
4	S	3	BMA	C2-C3	2.18	1.55	1.52
4	e	3	BMA	C2-C3	2.18	1.55	1.52
2	D	1	NAG	C3-C2	2.18	1.57	1.52
2	V	1	NAG	C3-C2	2.17	1.57	1.52
2	M	1	NAG	C3-C2	2.17	1.57	1.52
2	R	1	NAG	O5-C1	2.17	1.47	1.43
2	d	1	NAG	O5-C1	2.16	1.47	1.43
2	Y	1	NAG	C3-C2	2.15	1.57	1.52
2	V	2	NAG	C2-N2	2.15	1.49	1.46
2	P	1	NAG	C3-C2	2.15	1.57	1.52
4	J	3	BMA	C2-C3	2.15	1.55	1.52
2	G	1	NAG	C3-C2	2.15	1.57	1.52
2	V	1	NAG	C4-C3	2.14	1.57	1.52
2	D	1	NAG	C4-C3	2.14	1.57	1.52
2	d	2	NAG	C4-C5	2.14	1.57	1.53
2	R	2	NAG	C4-C5	2.13	1.57	1.53
2	D	2	NAG	C2-N2	2.12	1.49	1.46
2	I	2	NAG	C4-C5	2.12	1.57	1.53
2	M	1	NAG	C4-C3	2.11	1.57	1.52
2	M	2	NAG	C2-N2	2.10	1.49	1.46
4	S	2	NAG	C4-C5	2.10	1.57	1.53
2	P	1	NAG	C2-N2	2.10	1.49	1.46
2	d	2	NAG	C2-N2	2.09	1.49	1.46
2	R	2	NAG	C2-N2	2.08	1.49	1.46
3	X	1	NAG	C3-C2	2.08	1.56	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	NAG	C2-N2	2.08	1.49	1.46
3	F	1	NAG	C3-C2	2.08	1.56	1.52
2	Q	1	NAG	C3-C2	2.08	1.56	1.52
3	O	1	NAG	C3-C2	2.07	1.56	1.52
2	Z	2	NAG	C2-N2	2.07	1.49	1.46
4	J	2	NAG	C4-C5	2.07	1.57	1.53
2	G	1	NAG	C2-N2	2.06	1.49	1.46
2	G	1	NAG	C4-C3	2.06	1.57	1.52
4	e	2	NAG	C4-C5	2.05	1.57	1.53
4	J	5	MAN	C4-C3	2.05	1.57	1.52
2	H	1	NAG	C3-C2	2.05	1.56	1.52
2	H	2	NAG	C2-N2	2.05	1.49	1.46
5	L	3	FUC	C4-C3	2.04	1.57	1.52
3	X	3	BMA	C4-C3	2.04	1.57	1.52
2	G	2	NAG	C4-C3	2.04	1.57	1.52
3	F	3	BMA	C4-C3	2.04	1.57	1.52
2	Y	2	NAG	C4-C3	2.04	1.57	1.52
2	Y	1	NAG	C4-C3	2.03	1.57	1.52
2	P	2	NAG	C4-C3	2.03	1.57	1.52
2	Q	2	NAG	C2-N2	2.03	1.49	1.46
5	g	3	FUC	C4-C3	2.03	1.57	1.52
3	O	3	BMA	C4-C3	2.03	1.57	1.52
5	U	3	FUC	C4-C3	2.03	1.57	1.52
2	Y	1	NAG	C2-N2	2.03	1.49	1.46
2	I	1	NAG	C4-C3	2.03	1.57	1.52
2	R	1	NAG	C4-C3	2.03	1.57	1.52
2	d	1	NAG	C4-C3	2.03	1.57	1.52
4	e	5	MAN	C4-C3	2.03	1.57	1.52
2	P	1	NAG	C4-C3	2.03	1.57	1.52
5	L	1	NAG	C4-C5	2.02	1.57	1.53
2	Z	1	NAG	C3-C2	2.02	1.56	1.52
5	g	1	NAG	C4-C5	2.01	1.57	1.53
4	e	4	MAN	C4-C3	2.01	1.57	1.52
4	S	5	MAN	C4-C3	2.01	1.57	1.52
5	U	1	NAG	C4-C5	2.00	1.57	1.53

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	1	NAG	C2-N2-C7	3.41	127.47	122.90
4	J	1	NAG	C2-N2-C7	3.41	127.47	122.90
4	e	1	NAG	C2-N2-C7	3.41	127.47	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1	NAG	O5-C5-C6	-3.20	101.44	107.66
3	F	1	NAG	O5-C5-C6	-3.18	101.47	107.66
3	X	1	NAG	O5-C5-C6	-3.18	101.47	107.66
4	S	2	NAG	C8-C7-N2	2.97	121.05	116.12
4	e	2	NAG	C8-C7-N2	2.96	121.03	116.12
4	J	2	NAG	C8-C7-N2	2.96	121.03	116.12
5	L	2	NAG	C1-C2-N2	2.66	114.62	110.43
5	U	2	NAG	C1-C2-N2	2.65	114.61	110.43
5	g	2	NAG	C1-C2-N2	2.65	114.60	110.43
4	J	2	NAG	O4-C4-C5	-2.64	102.83	109.32
4	e	2	NAG	O4-C4-C5	-2.64	102.83	109.32
4	S	2	NAG	O4-C4-C5	-2.63	102.84	109.32
4	J	2	NAG	O7-C7-C8	-2.58	117.46	122.05
4	S	2	NAG	O7-C7-C8	-2.58	117.47	122.05
4	e	2	NAG	O7-C7-C8	-2.57	117.48	122.05
2	D	1	NAG	C1-C2-N2	-2.47	106.54	110.43
4	J	1	NAG	O7-C7-C8	-2.47	117.66	122.05
2	M	1	NAG	C1-C2-N2	-2.47	106.55	110.43
2	V	1	NAG	C1-C2-N2	-2.47	106.55	110.43
4	S	1	NAG	O7-C7-C8	-2.46	117.67	122.05
4	e	1	NAG	O7-C7-C8	-2.45	117.69	122.05
3	O	3	BMA	C1-O5-C5	2.45	115.46	112.19
2	G	1	NAG	O4-C4-C3	-2.44	104.63	110.38
3	F	3	BMA	C1-O5-C5	2.44	115.45	112.19
3	X	3	BMA	C1-O5-C5	2.44	115.45	112.19
2	P	1	NAG	O4-C4-C3	-2.43	104.66	110.38
2	Y	1	NAG	O4-C4-C3	-2.43	104.66	110.38
3	O	1	NAG	C8-C7-N2	2.37	120.05	116.12
3	X	1	NAG	C8-C7-N2	2.36	120.03	116.12
3	F	1	NAG	C8-C7-N2	2.36	120.03	116.12
5	L	2	NAG	C2-N2-C7	2.34	126.04	122.90
5	g	2	NAG	C2-N2-C7	2.34	126.03	122.90
5	U	2	NAG	C2-N2-C7	2.31	126.00	122.90
2	H	2	NAG	C8-C7-N2	2.26	119.86	116.12
2	Q	2	NAG	C8-C7-N2	2.25	119.86	116.12
2	Z	2	NAG	C8-C7-N2	2.25	119.85	116.12
3	X	1	NAG	C1-C2-N2	-2.24	106.91	110.43
3	O	1	NAG	C1-C2-N2	-2.24	106.91	110.43
3	F	1	NAG	C1-C2-N2	-2.24	106.91	110.43
2	H	1	NAG	C1-C2-N2	-2.20	106.97	110.43
2	Q	1	NAG	C1-C2-N2	-2.19	106.98	110.43
2	Z	1	NAG	C1-C2-N2	-2.19	106.98	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	NAG	O4-C4-C3	-2.19	105.21	110.38
4	S	2	NAG	O4-C4-C3	-2.19	105.21	110.38
4	e	2	NAG	O4-C4-C3	-2.19	105.22	110.38
5	g	1	NAG	C8-C7-N2	2.18	119.73	116.12
5	L	1	NAG	C8-C7-N2	2.17	119.72	116.12
5	U	1	NAG	C8-C7-N2	2.17	119.72	116.12
3	X	1	NAG	O7-C7-C8	-2.15	118.22	122.05
3	F	1	NAG	O7-C7-C8	-2.15	118.23	122.05
3	O	1	NAG	O7-C7-C8	-2.14	118.24	122.05
2	Y	1	NAG	C8-C7-N2	2.12	119.64	116.12
3	X	1	NAG	C1-O5-C5	2.12	115.02	112.19
2	I	2	NAG	C8-C7-N2	2.11	119.62	116.12
2	R	2	NAG	C8-C7-N2	2.11	119.62	116.12
2	d	2	NAG	C8-C7-N2	2.10	119.61	116.12
2	G	1	NAG	C8-C7-N2	2.10	119.60	116.12
2	D	2	NAG	C8-C7-N2	2.09	119.58	116.12
3	F	1	NAG	C1-O5-C5	2.08	114.98	112.19
2	M	2	NAG	C8-C7-N2	2.08	119.57	116.12
2	P	1	NAG	C8-C7-N2	2.08	119.56	116.12
2	V	2	NAG	C8-C7-N2	2.08	119.56	116.12
2	R	1	NAG	C8-C7-N2	2.07	119.56	116.12
2	Y	2	NAG	C8-C7-N2	2.07	119.55	116.12
2	d	1	NAG	C8-C7-N2	2.07	119.55	116.12
3	O	1	NAG	C1-O5-C5	2.06	114.95	112.19
2	P	2	NAG	C8-C7-N2	2.05	119.51	116.12
2	I	1	NAG	C8-C7-N2	2.04	119.50	116.12
2	G	2	NAG	C8-C7-N2	2.04	119.50	116.12
3	X	1	NAG	O4-C4-C3	-2.02	105.61	110.38
3	F	1	NAG	O4-C4-C3	-2.02	105.61	110.38
5	L	2	NAG	C8-C7-N2	2.02	119.46	116.12
5	g	2	NAG	C8-C7-N2	2.02	119.46	116.12
3	O	1	NAG	O4-C4-C3	-2.01	105.64	110.38

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	NAG	C1-C2-N2-C7
2	T	2	NAG	C1-C2-N2-C7
2	f	2	NAG	C1-C2-N2-C7
4	J	1	NAG	C3-C2-N2-C7
4	S	1	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	e	1	NAG	C3-C2-N2-C7
4	J	3	BMA	C4-C5-C6-O6
4	S	3	BMA	C4-C5-C6-O6
4	e	3	BMA	C4-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
4	S	3	BMA	O5-C5-C6-O6
4	e	3	BMA	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	N	2	NAG	C8-C7-N2-C2
2	W	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	N	2	NAG	O7-C7-N2-C2
2	W	2	NAG	O7-C7-N2-C2
4	J	4	MAN	C4-C5-C6-O6
4	S	4	MAN	C4-C5-C6-O6
4	e	4	MAN	C4-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
5	g	1	NAG	C4-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
5	g	1	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	f	2	NAG	O5-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6
4	S	4	MAN	O5-C5-C6-O6
4	e	4	MAN	O5-C5-C6-O6
5	L	2	NAG	C1-C2-N2-C7
5	U	2	NAG	C1-C2-N2-C7
5	g	2	NAG	C1-C2-N2-C7
2	K	2	NAG	C8-C7-N2-C2
2	T	2	NAG	C8-C7-N2-C2
2	f	2	NAG	C8-C7-N2-C2
2	E	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	K	2	NAG	O7-C7-N2-C2
2	T	2	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

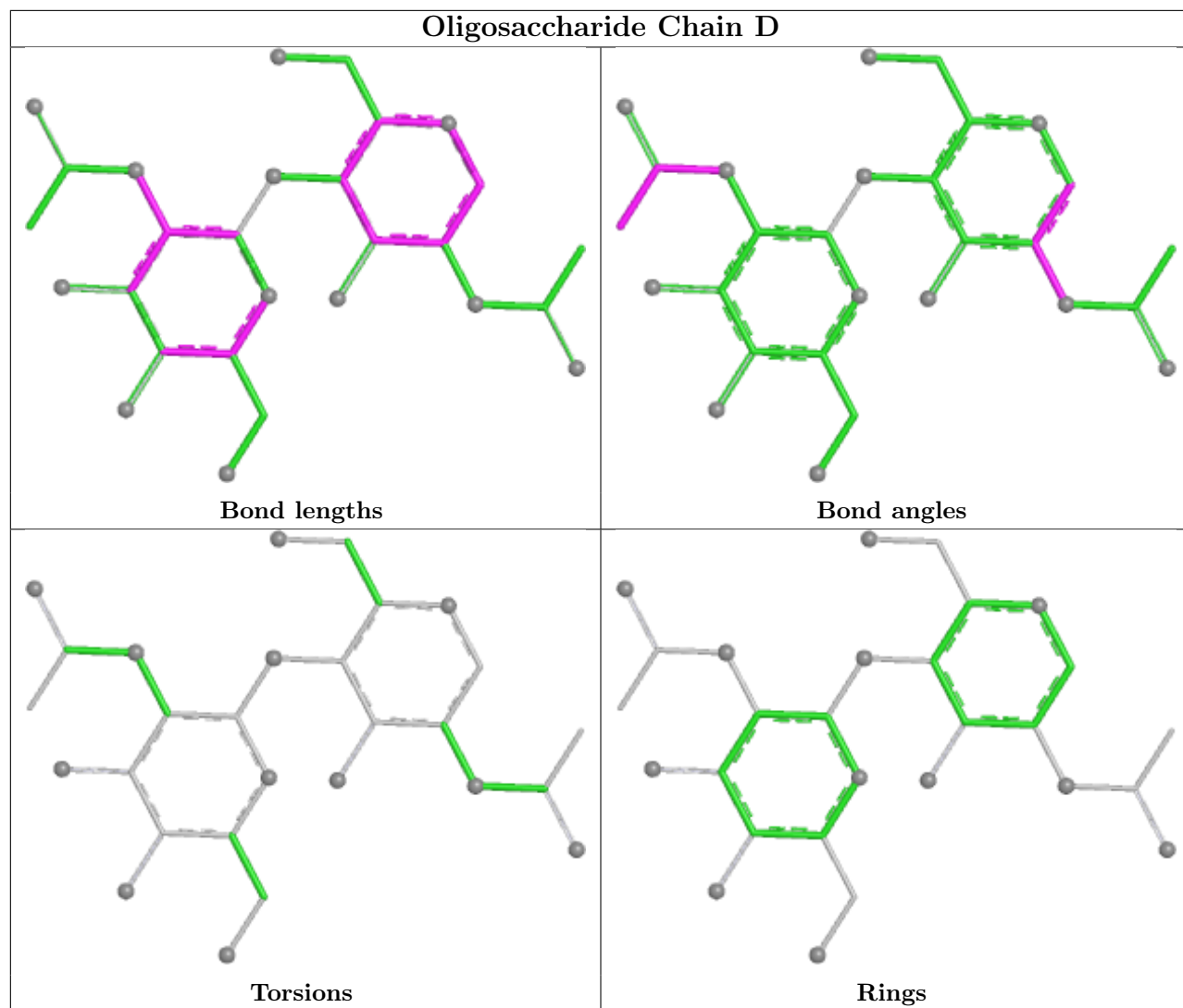
Mol	Chain	Res	Type	Atoms
2	f	2	NAG	O7-C7-N2-C2
5	L	2	NAG	C3-C2-N2-C7
5	U	2	NAG	C3-C2-N2-C7
5	g	2	NAG	C3-C2-N2-C7

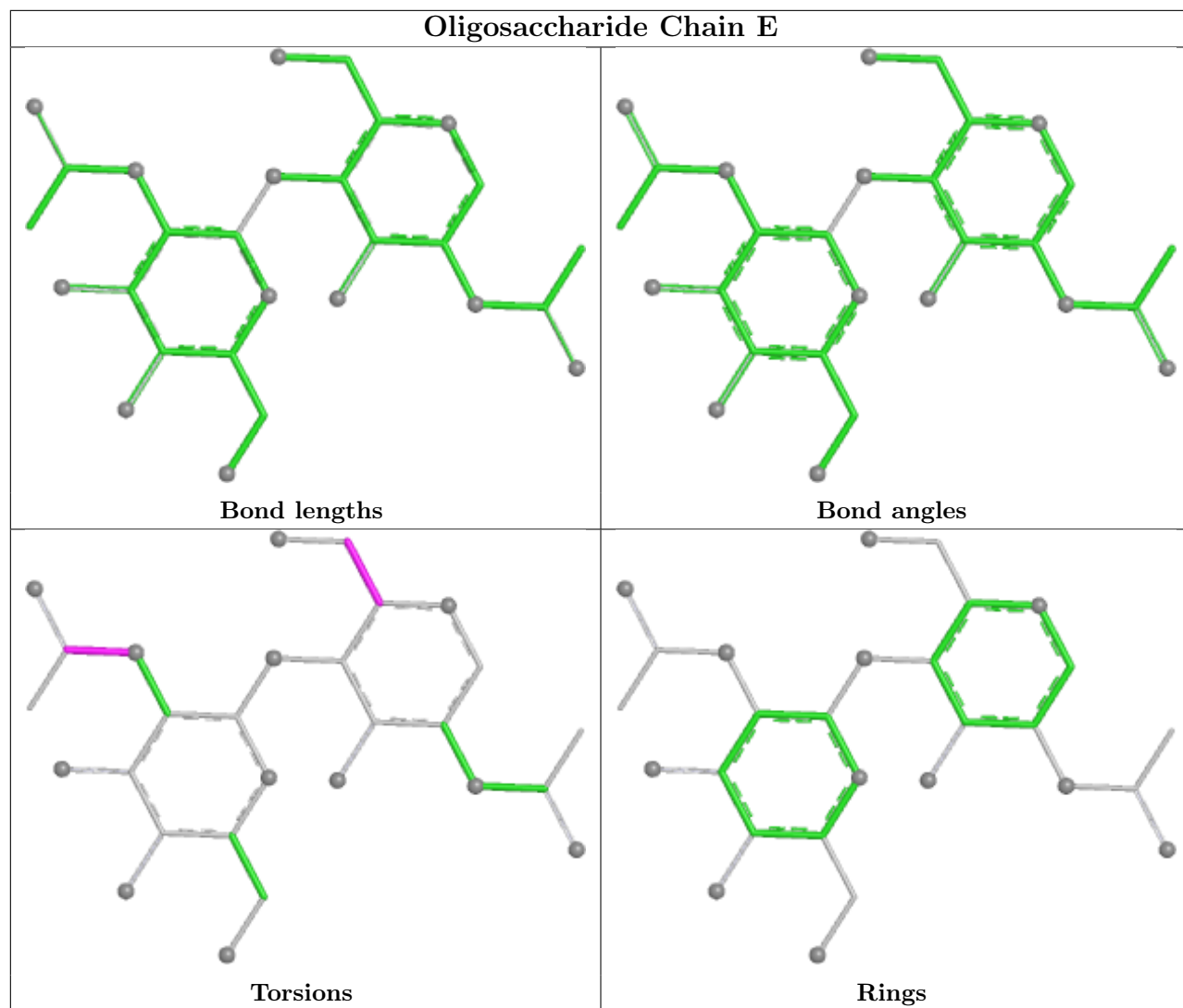
There are no ring outliers.

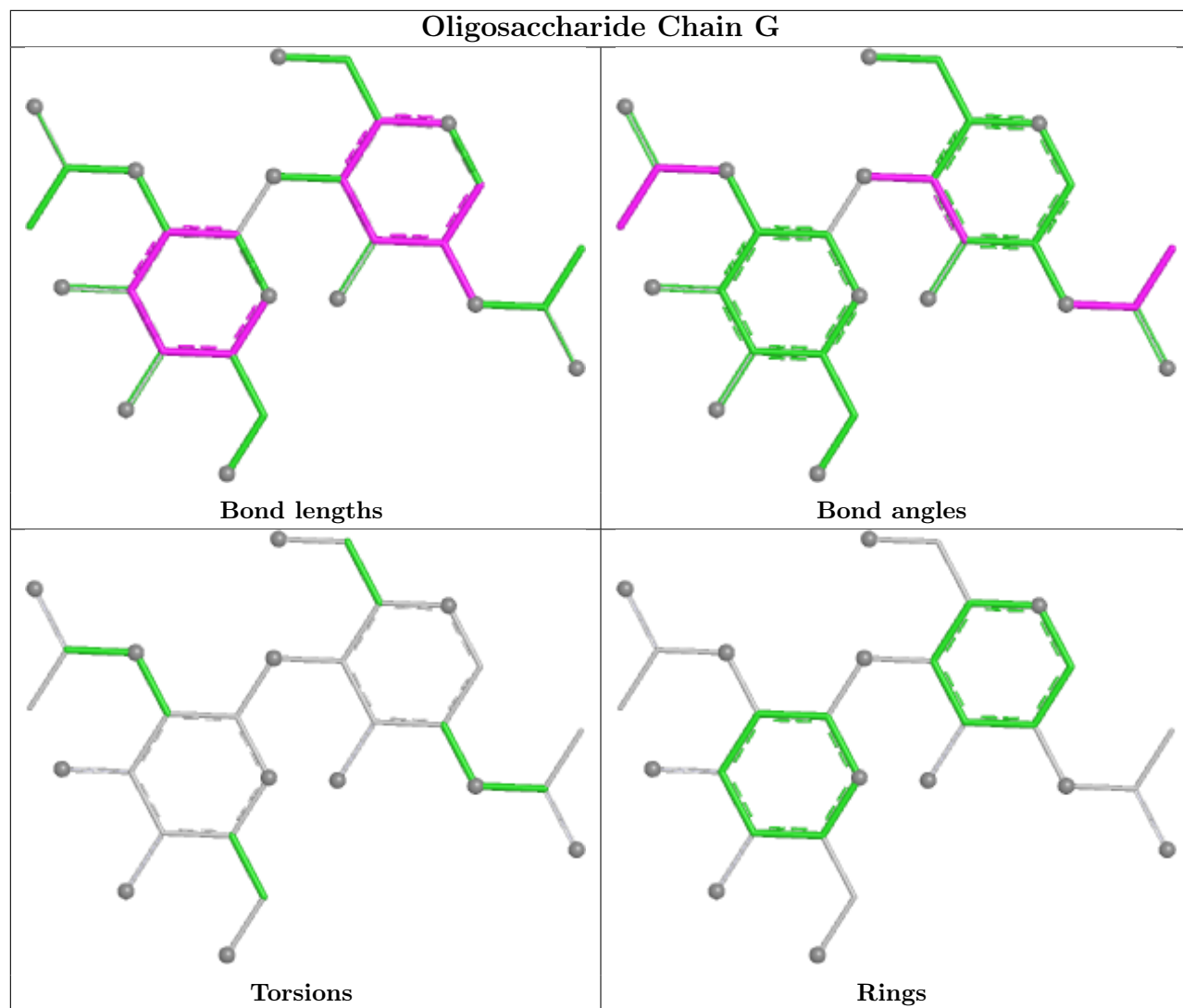
9 monomers are involved in 6 short contacts:

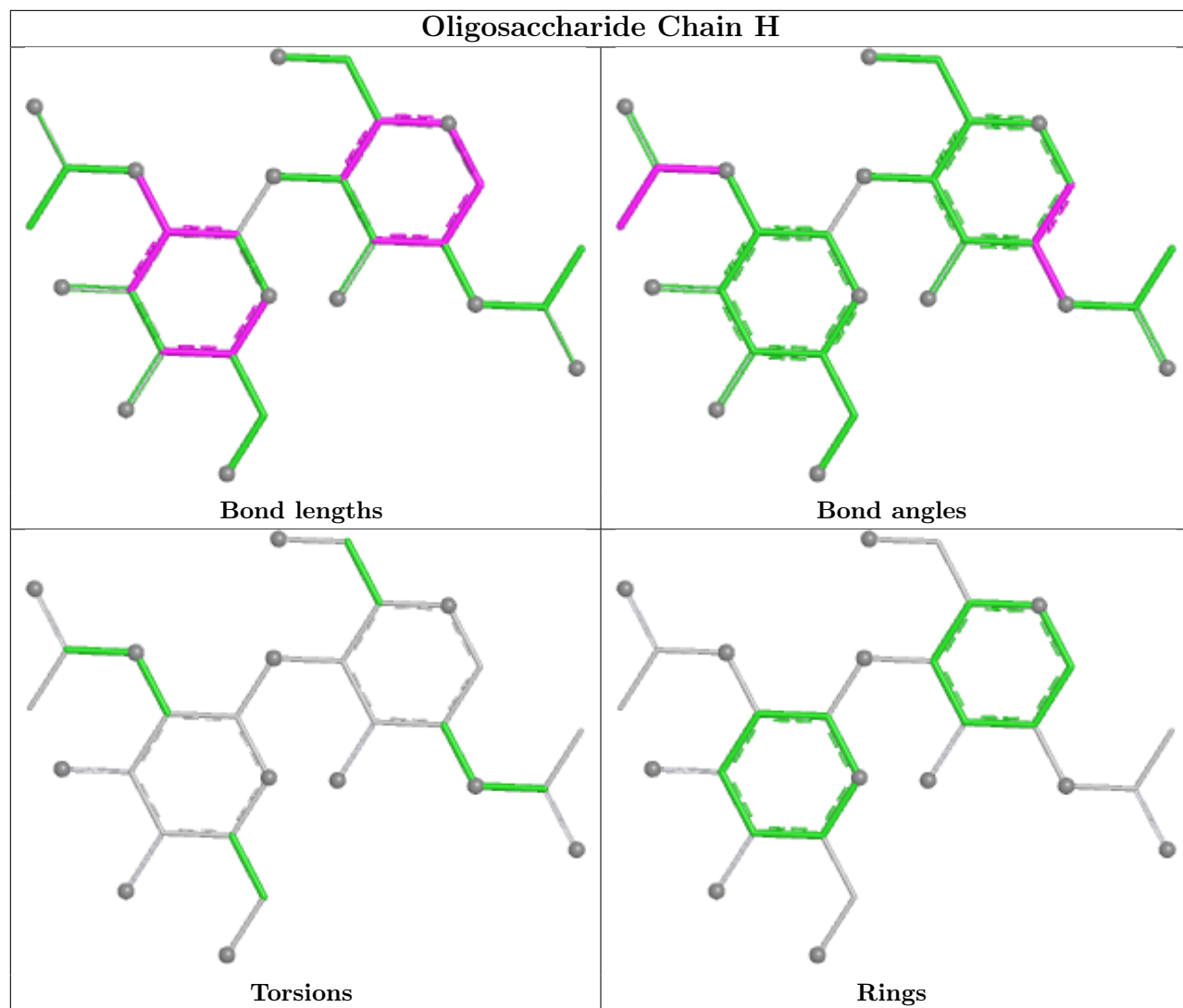
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	1	NAG	1	0
2	K	1	NAG	1	0
2	N	2	NAG	1	0
2	T	1	NAG	1	0
2	W	2	NAG	1	0
2	N	1	NAG	1	0
2	E	1	NAG	1	0
2	f	1	NAG	1	0
2	E	2	NAG	1	0

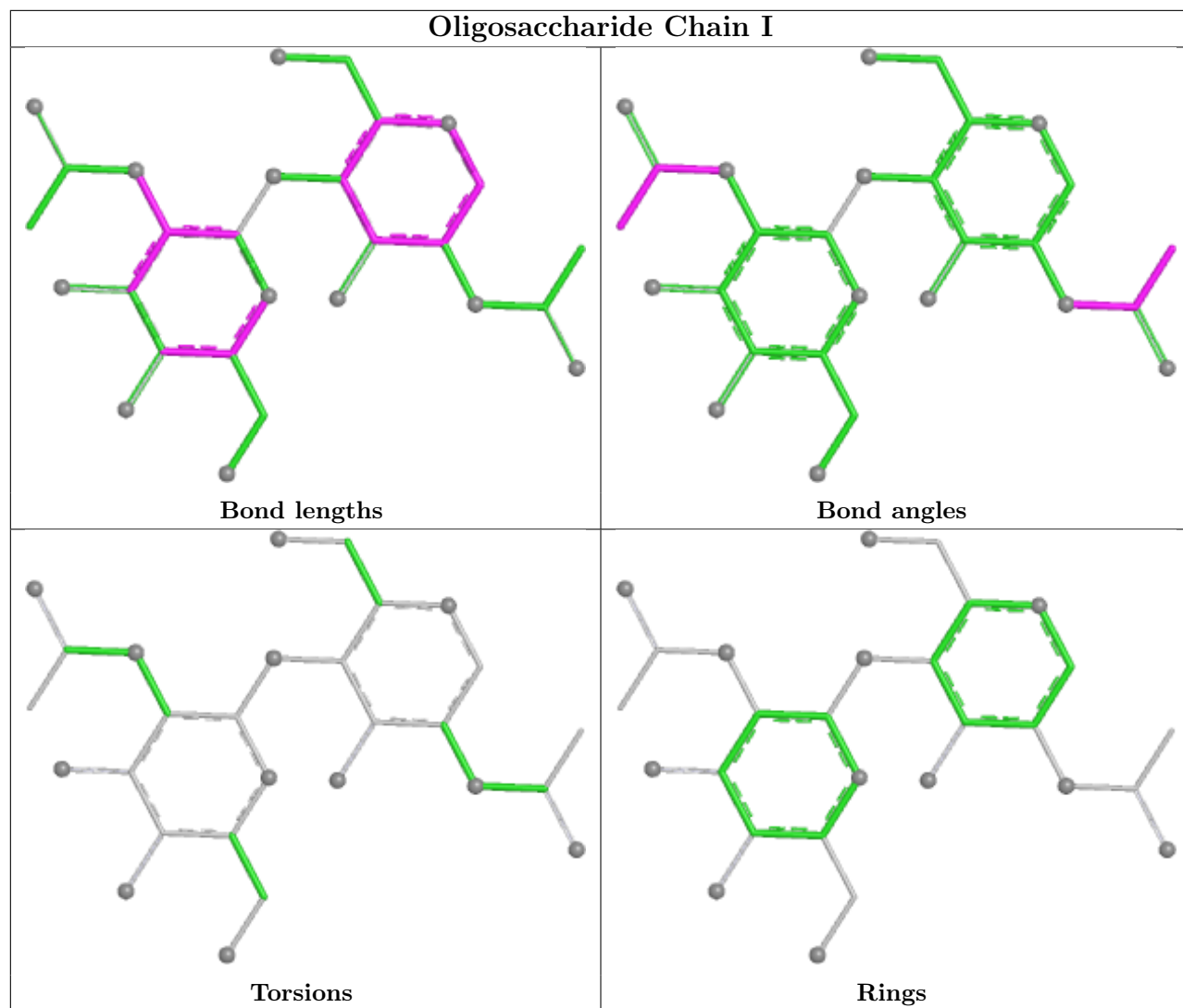
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

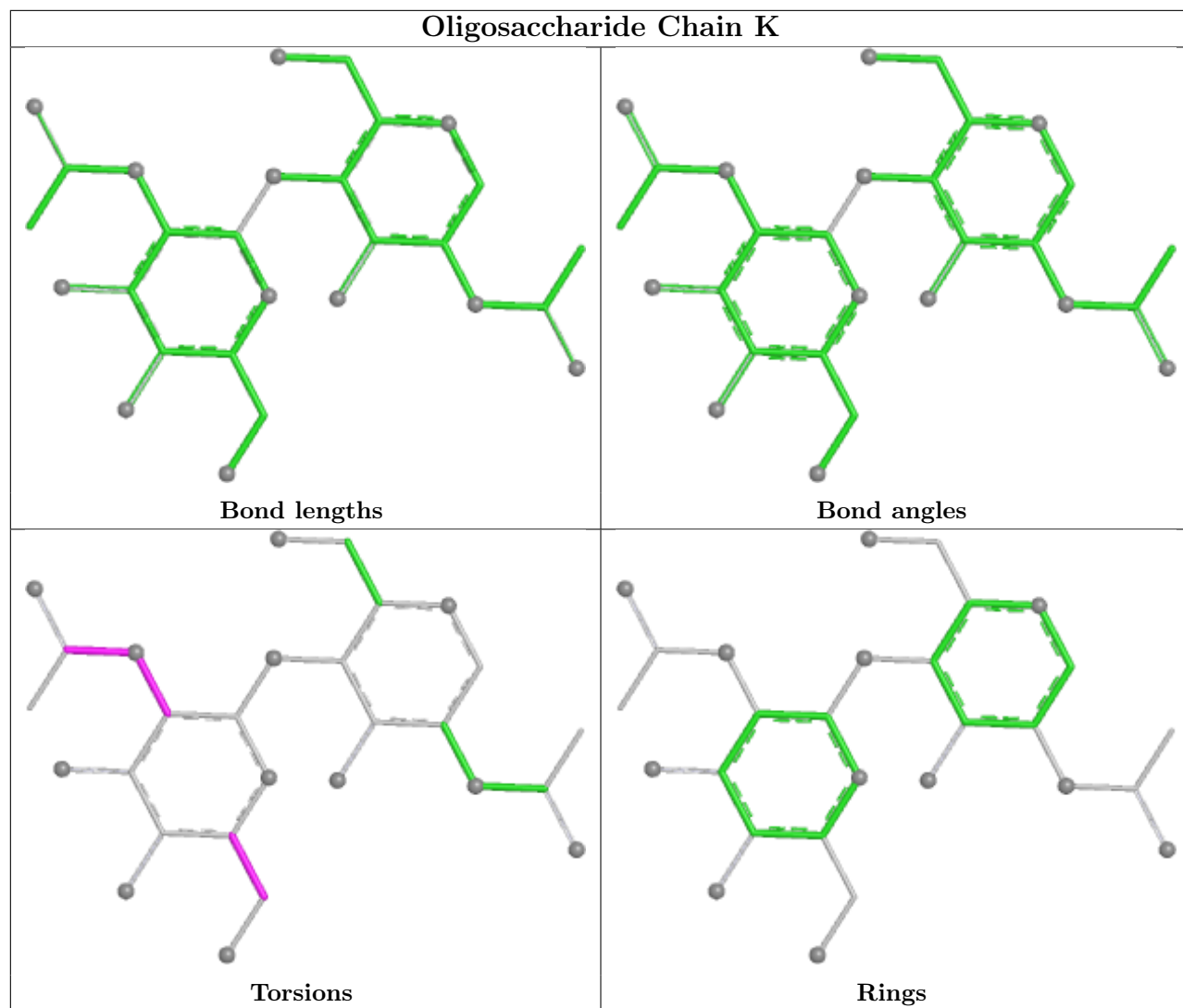


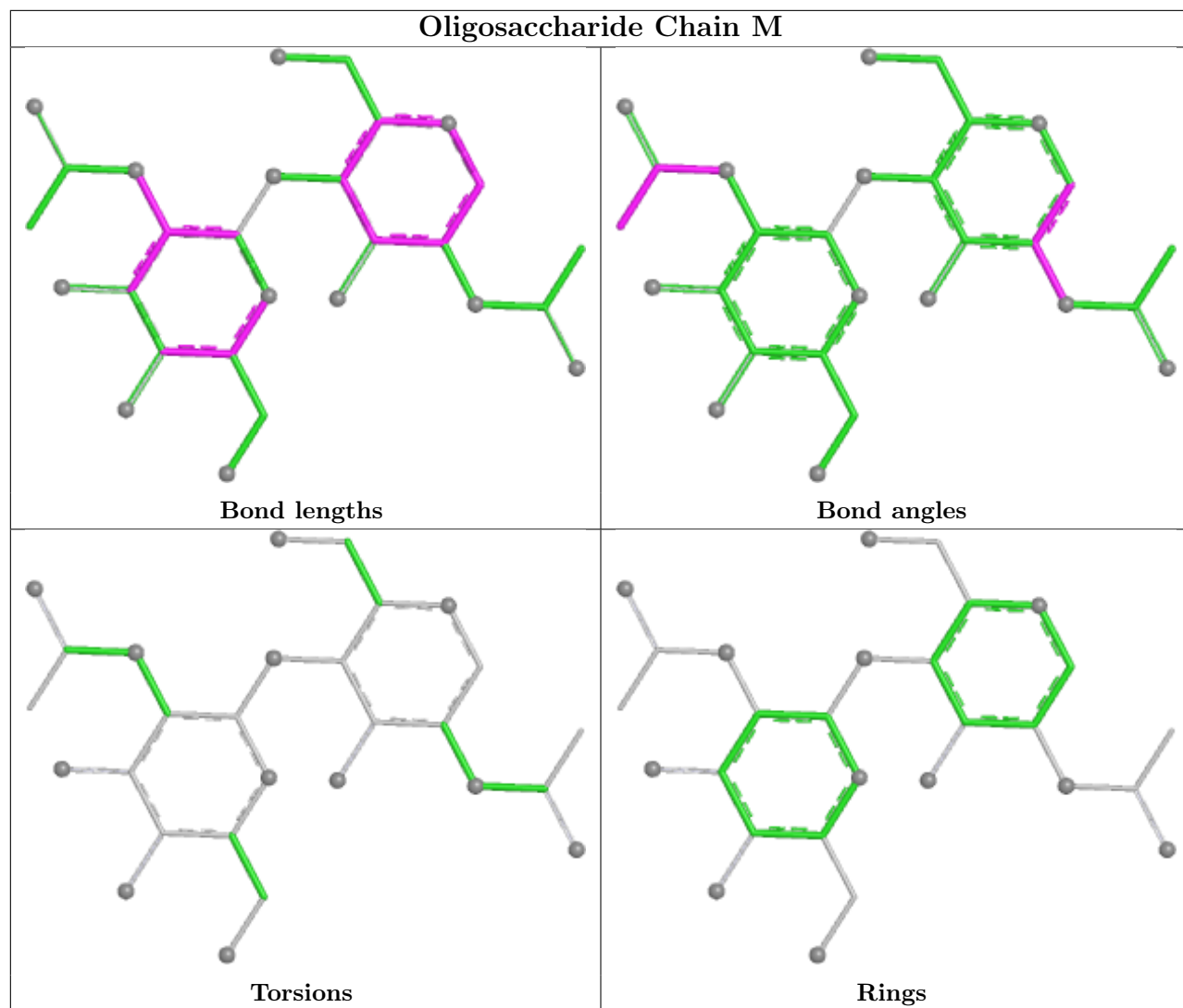


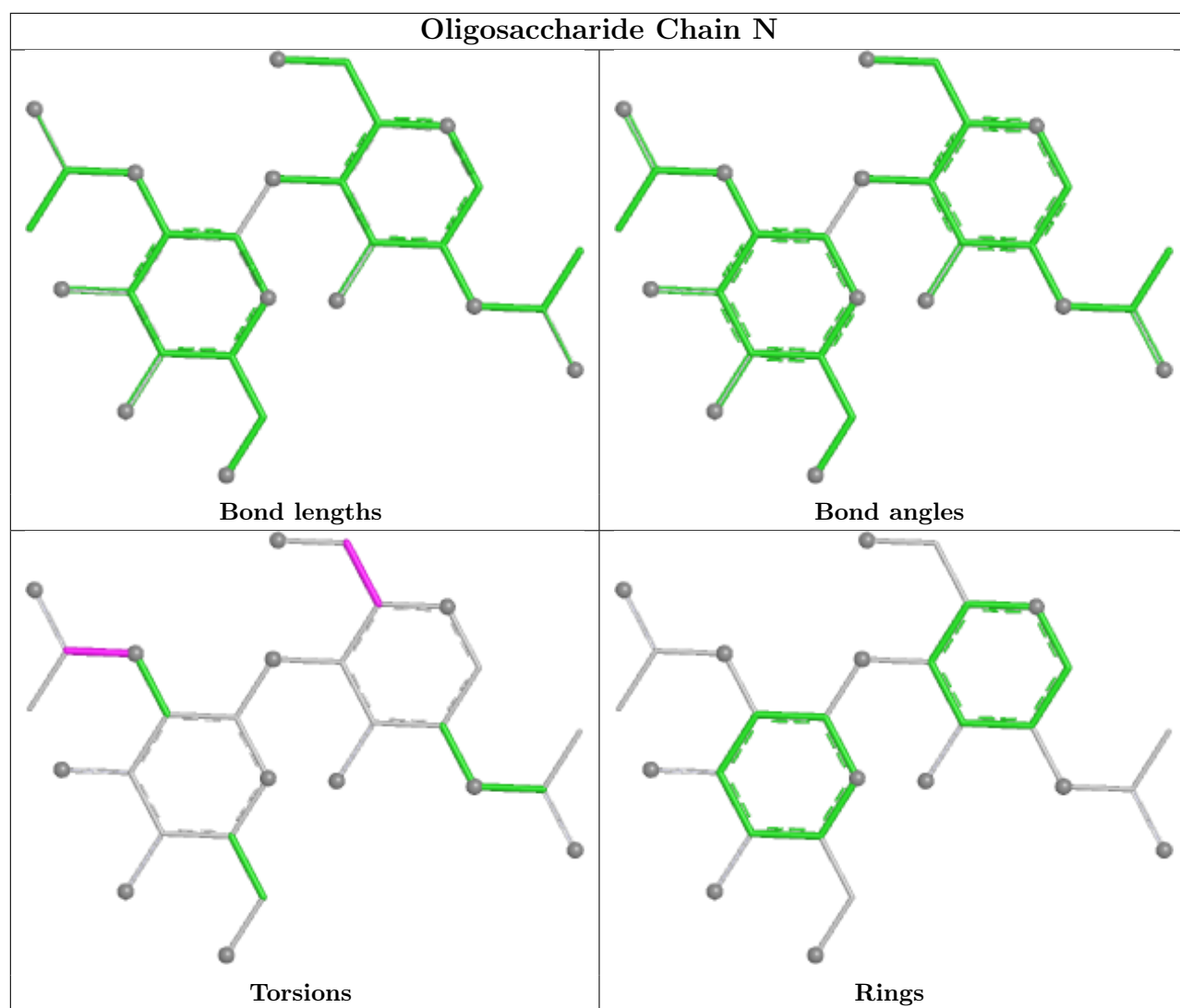


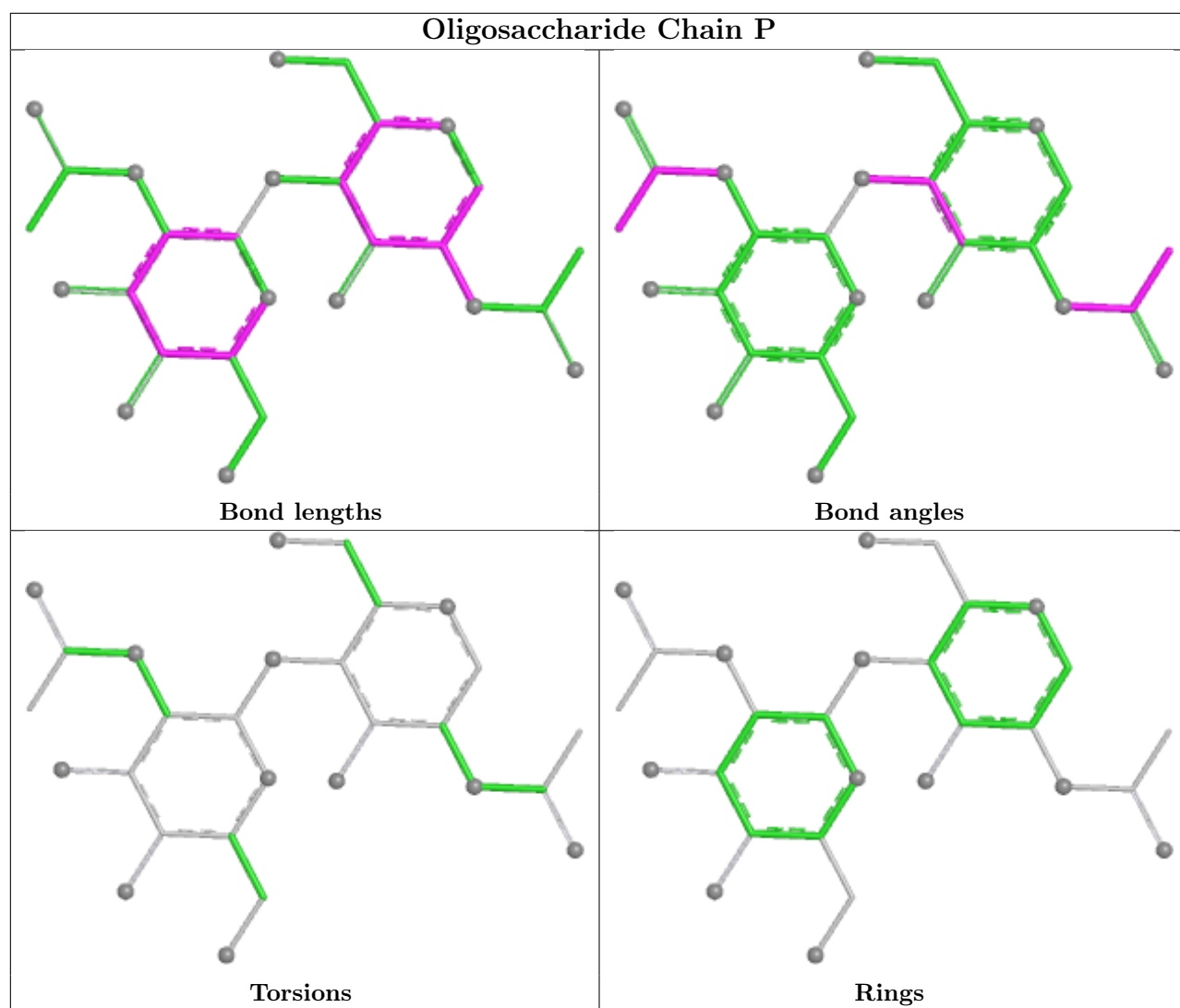


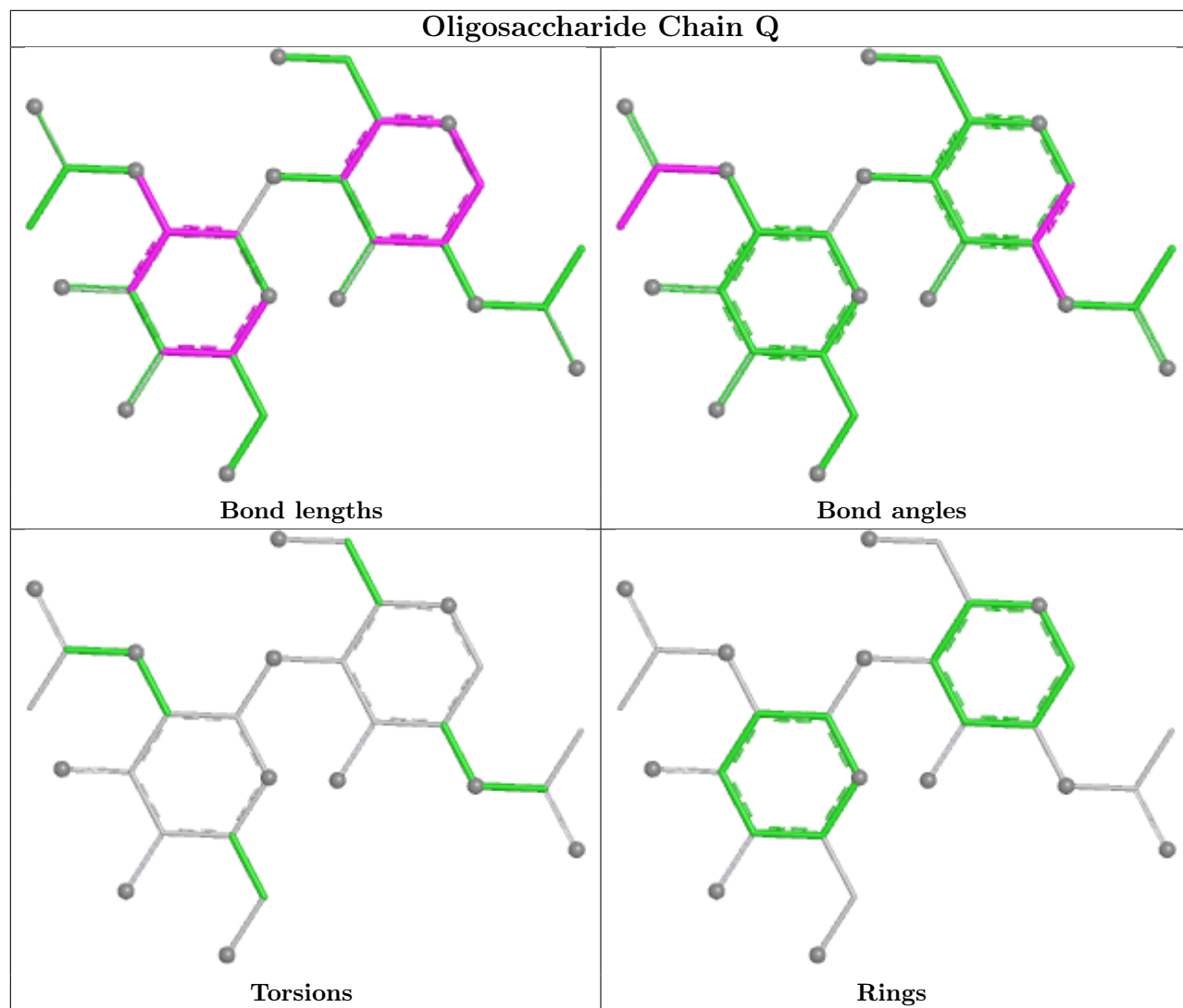


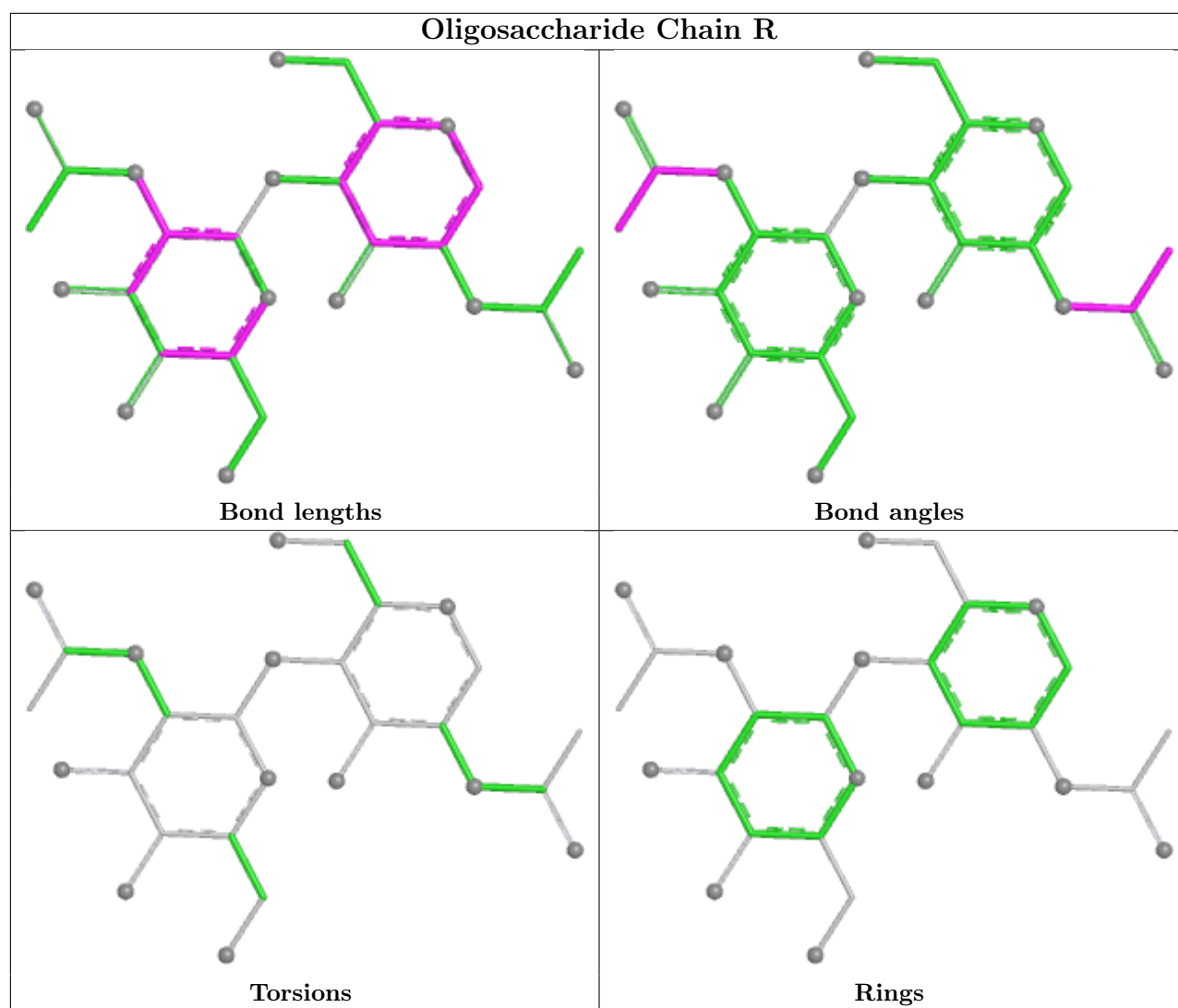


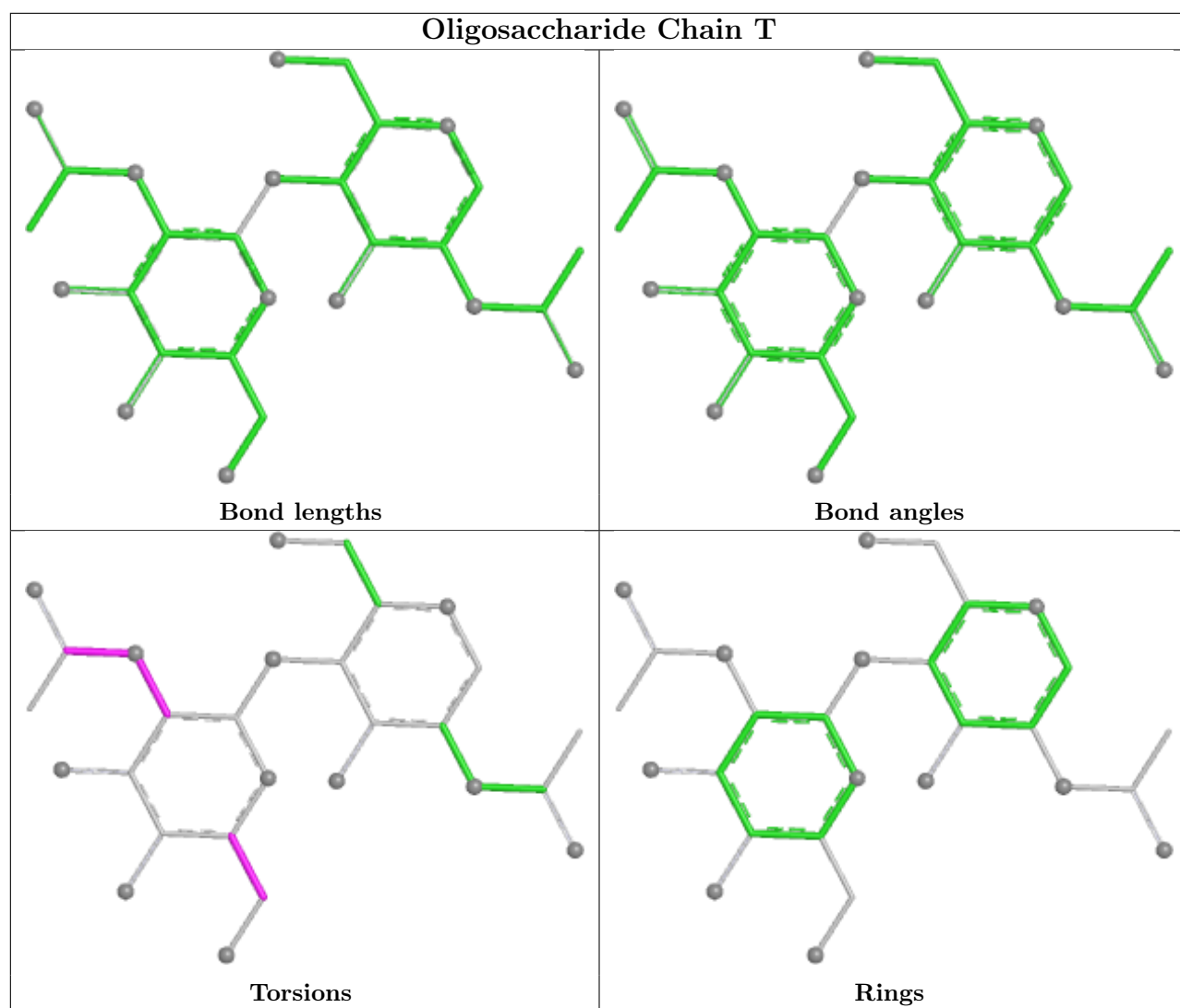


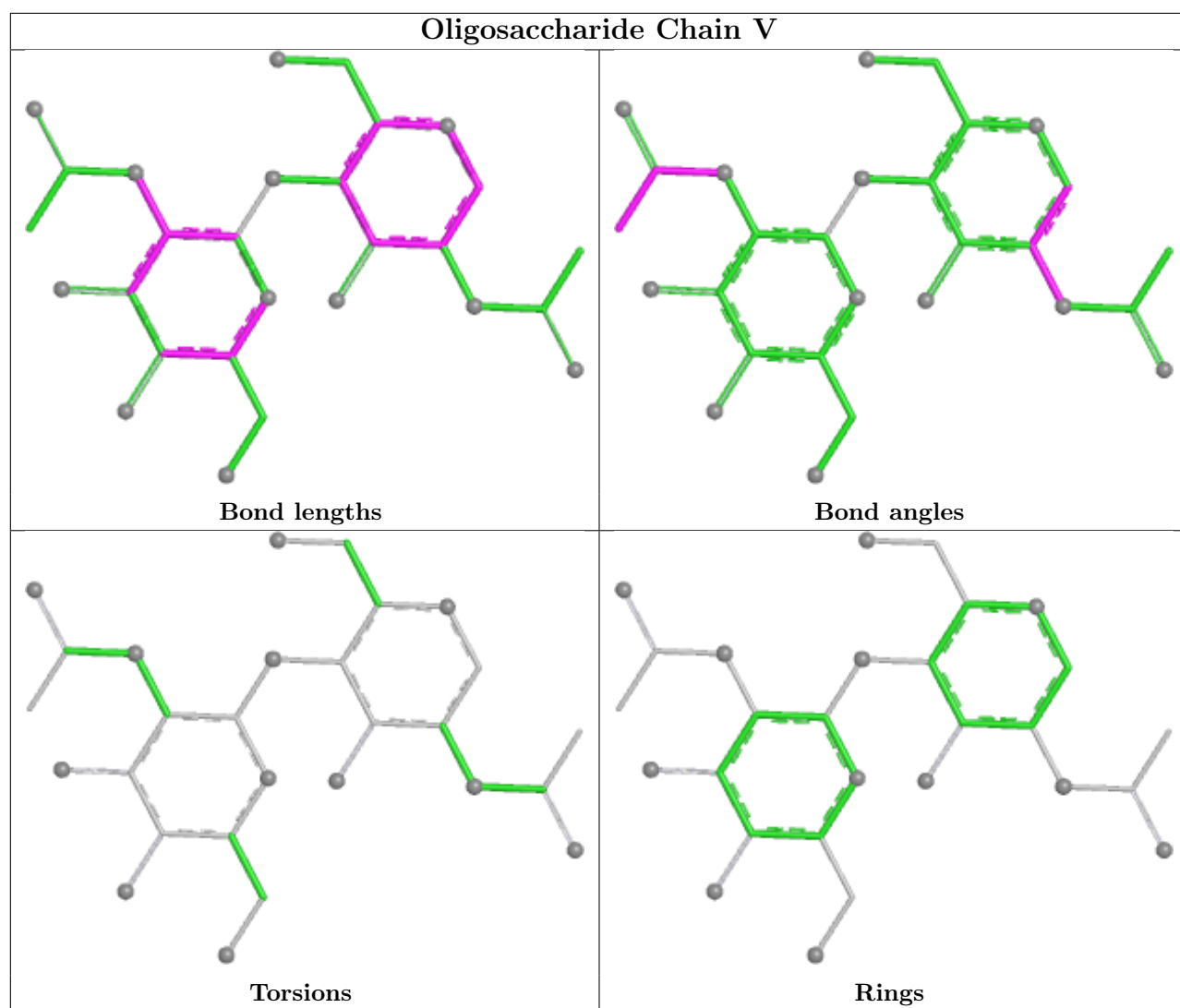


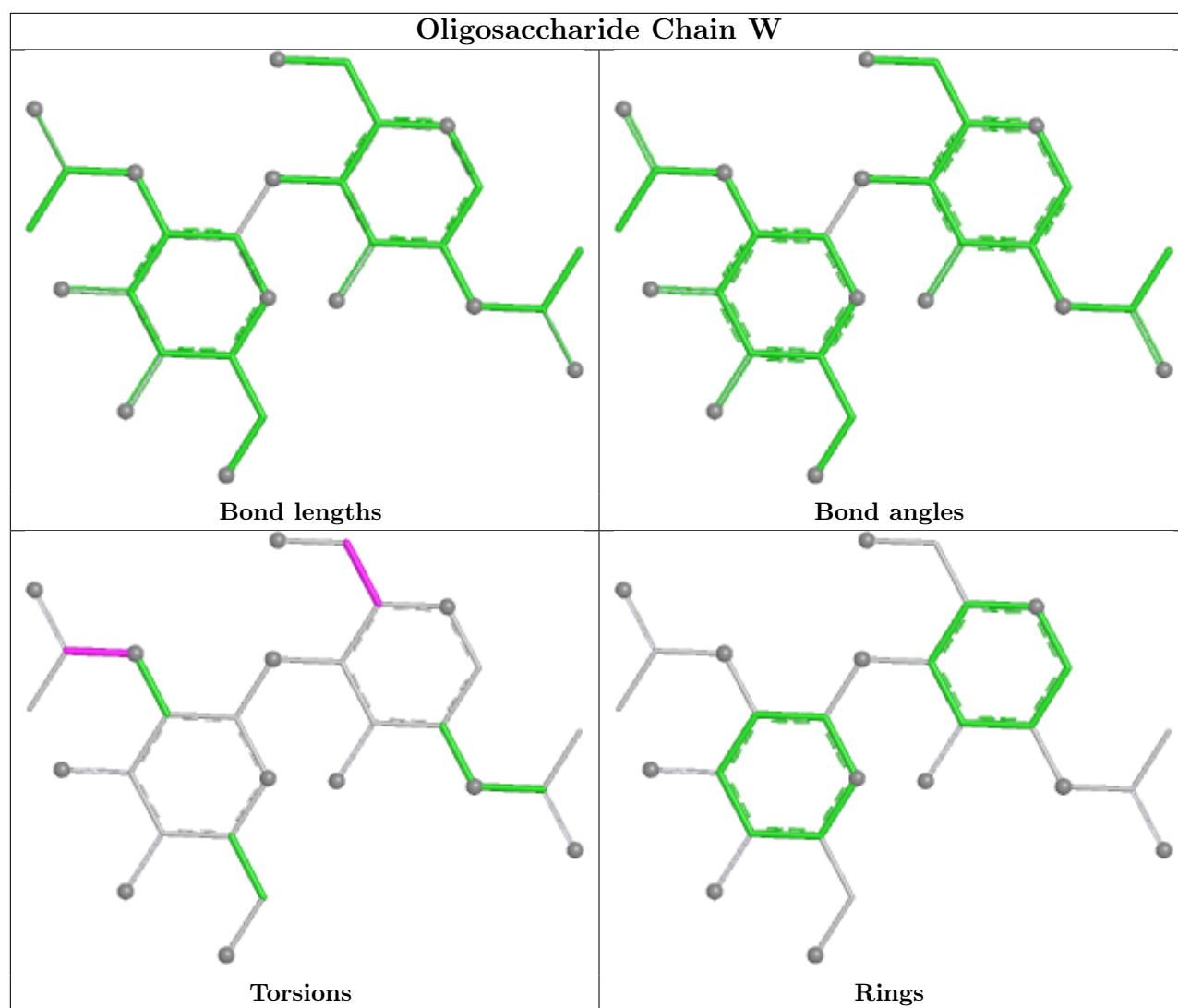


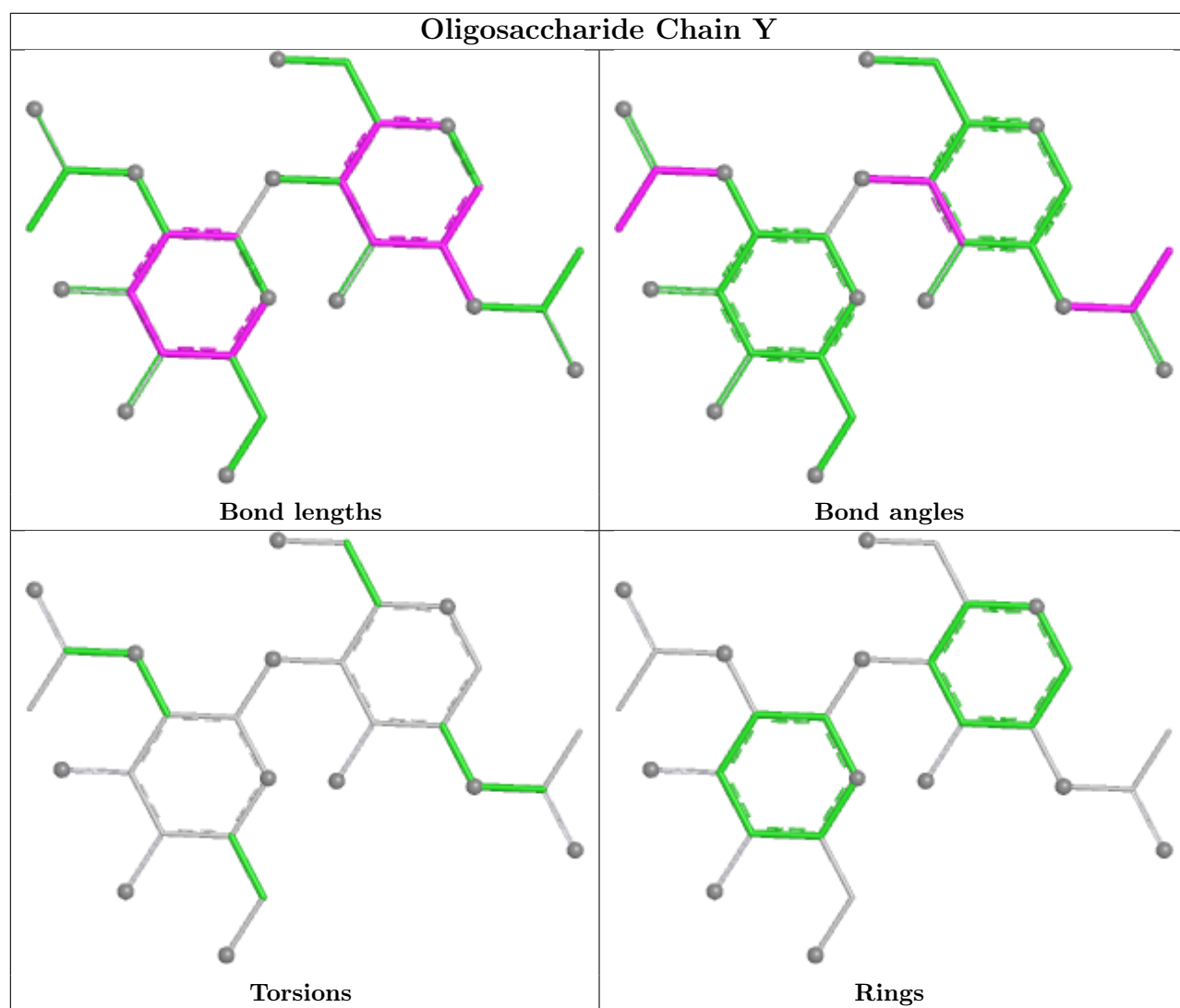


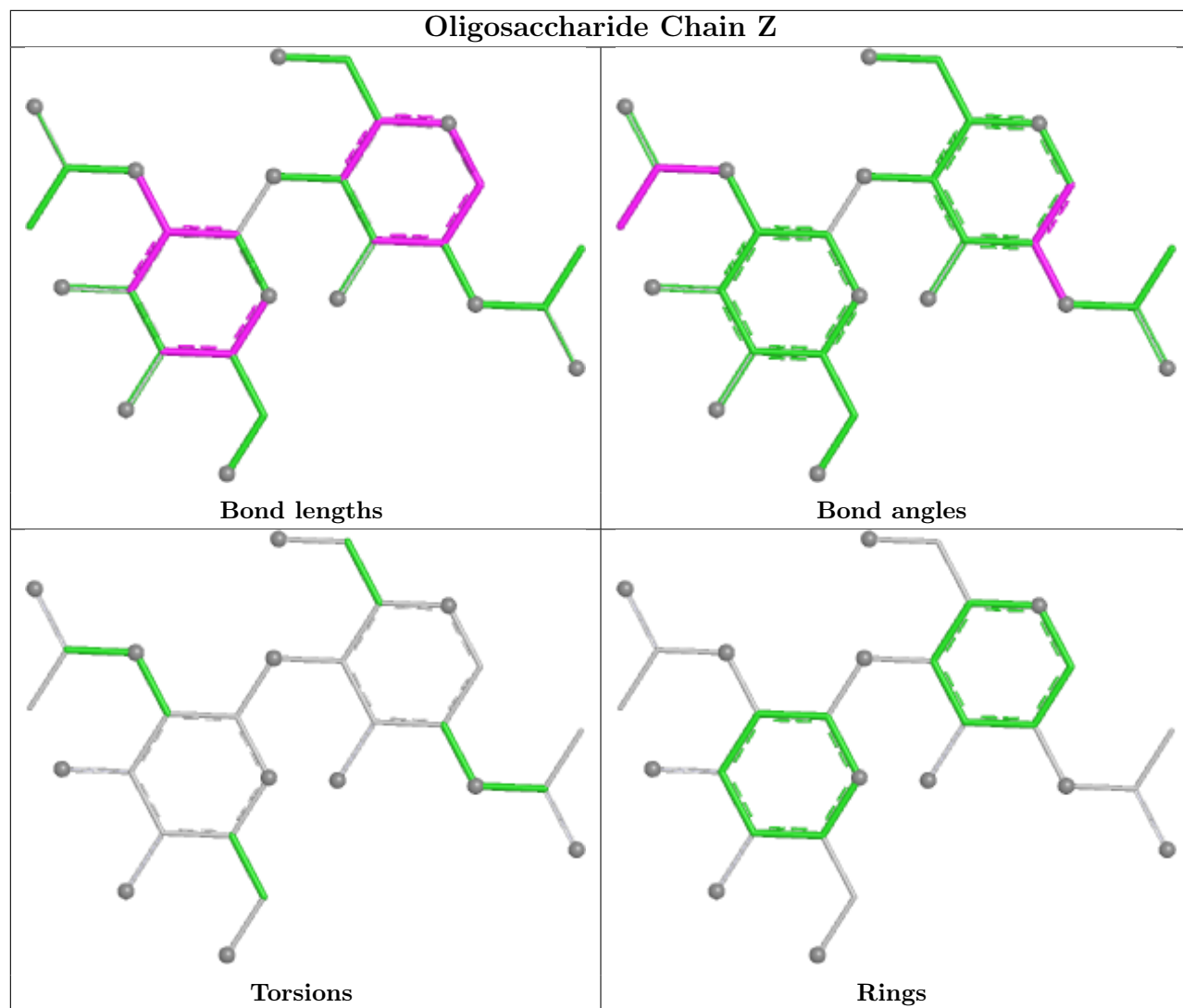


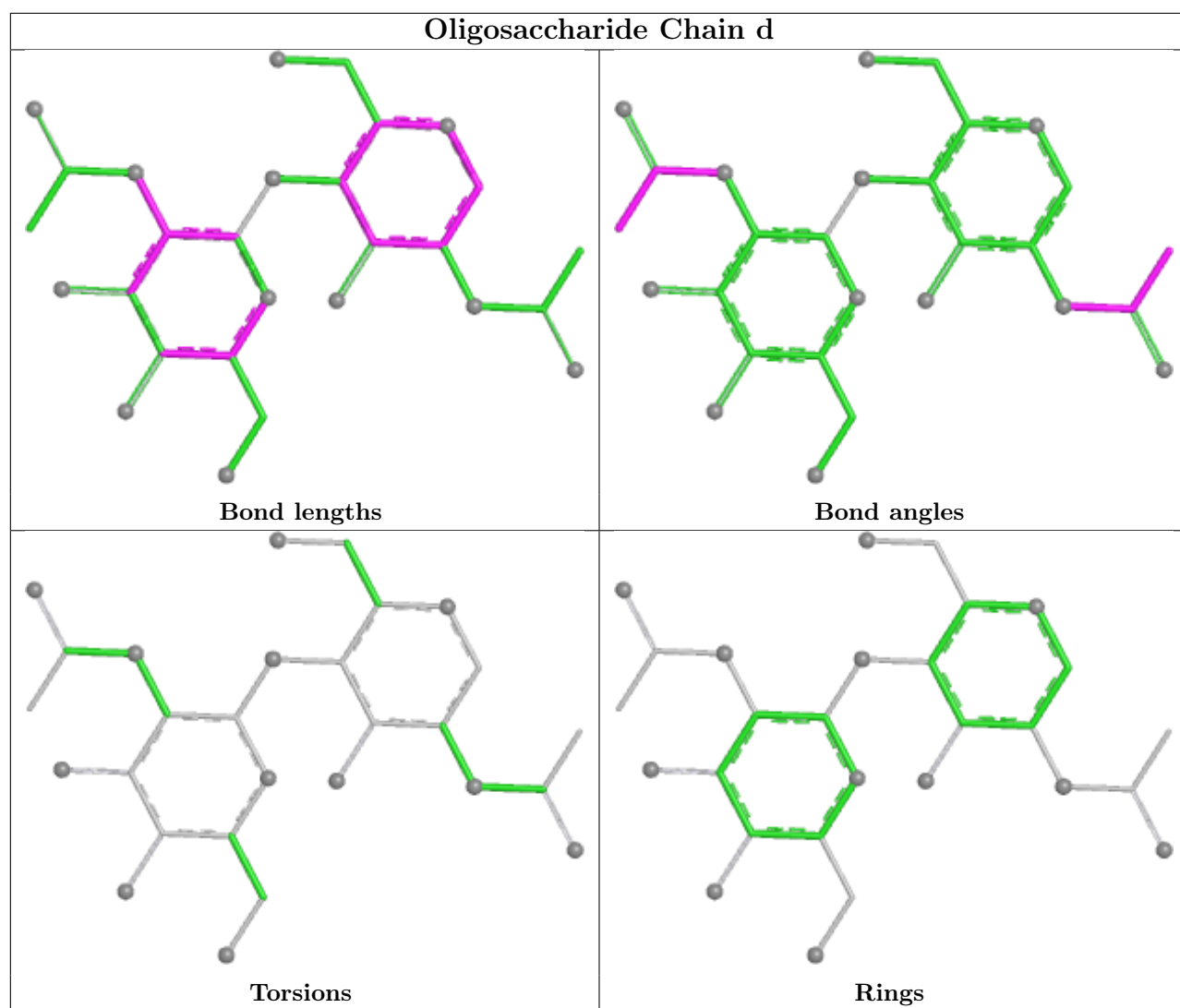


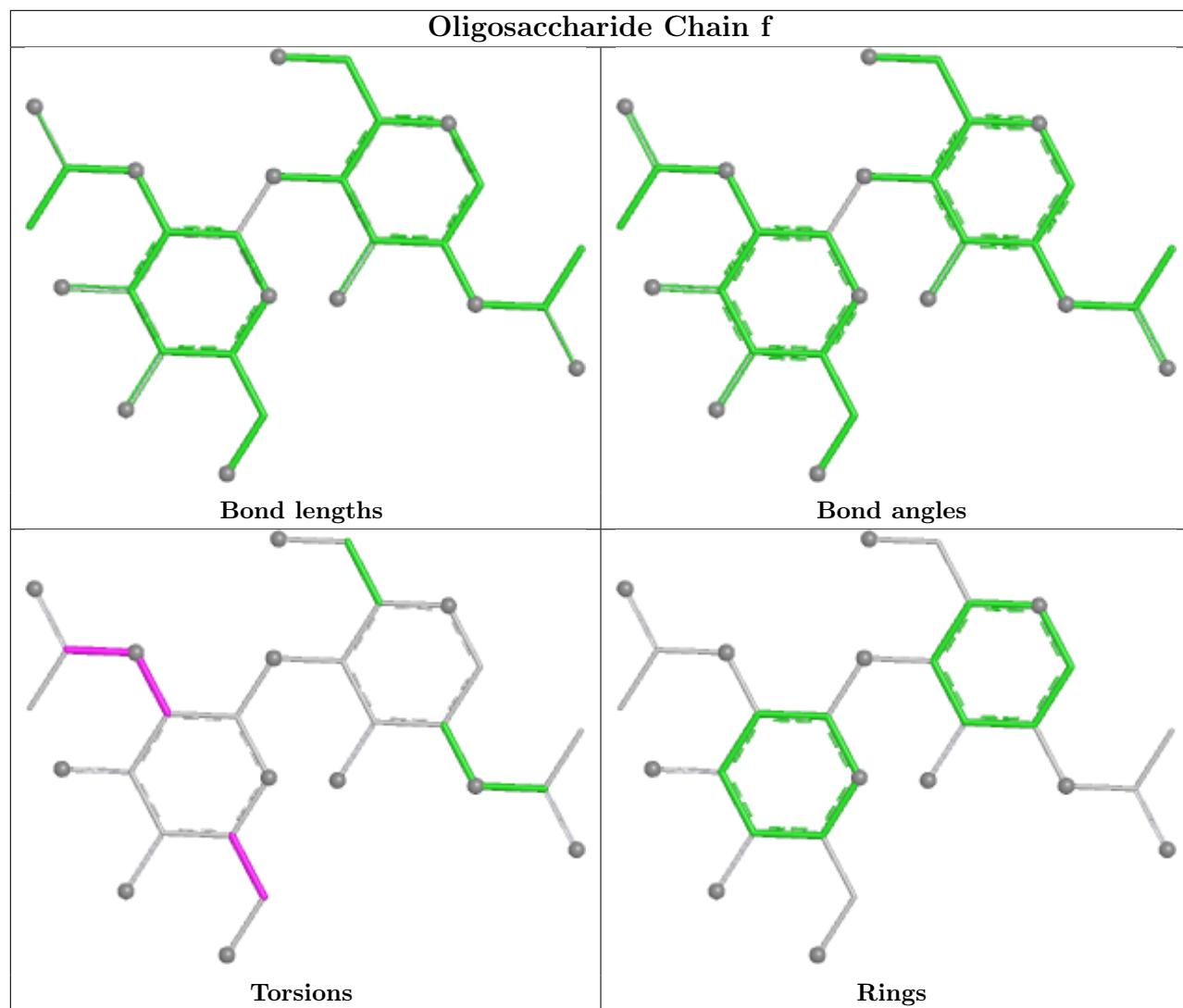


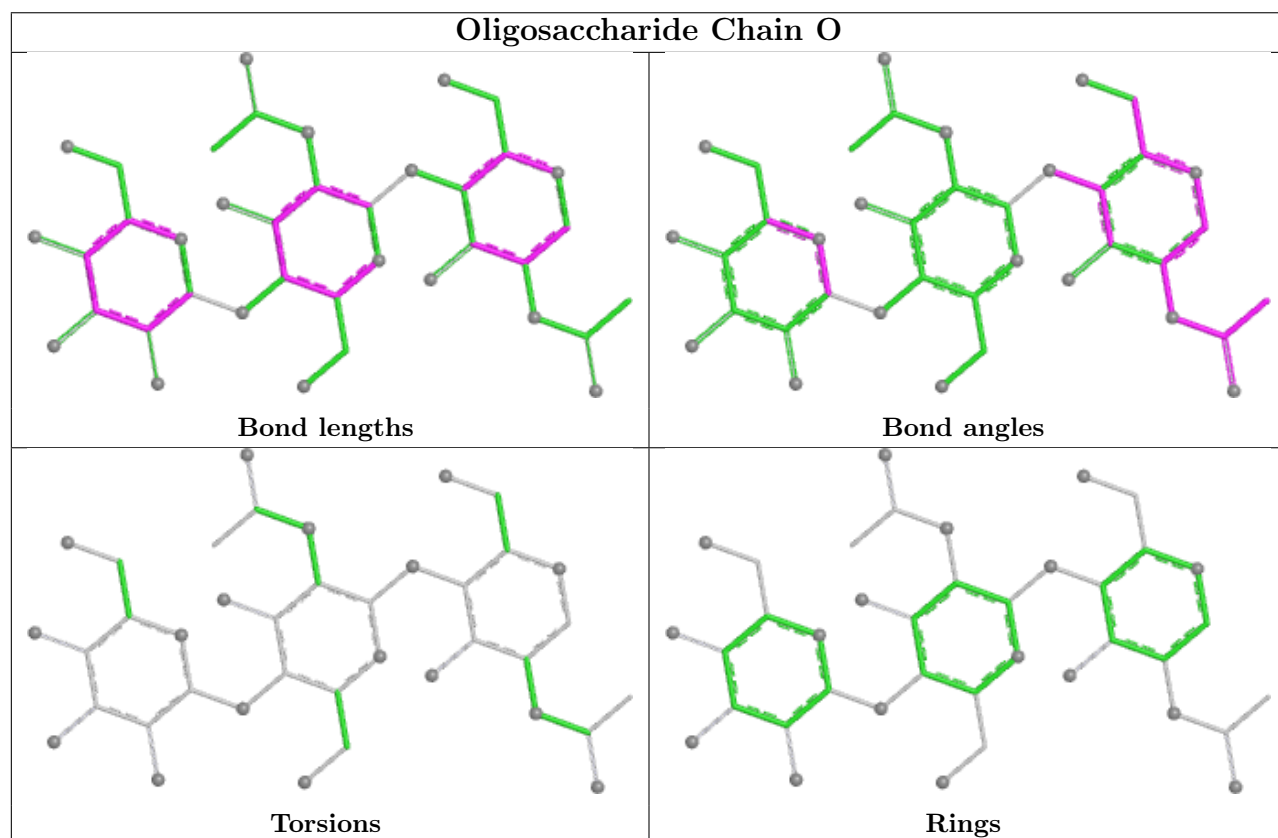
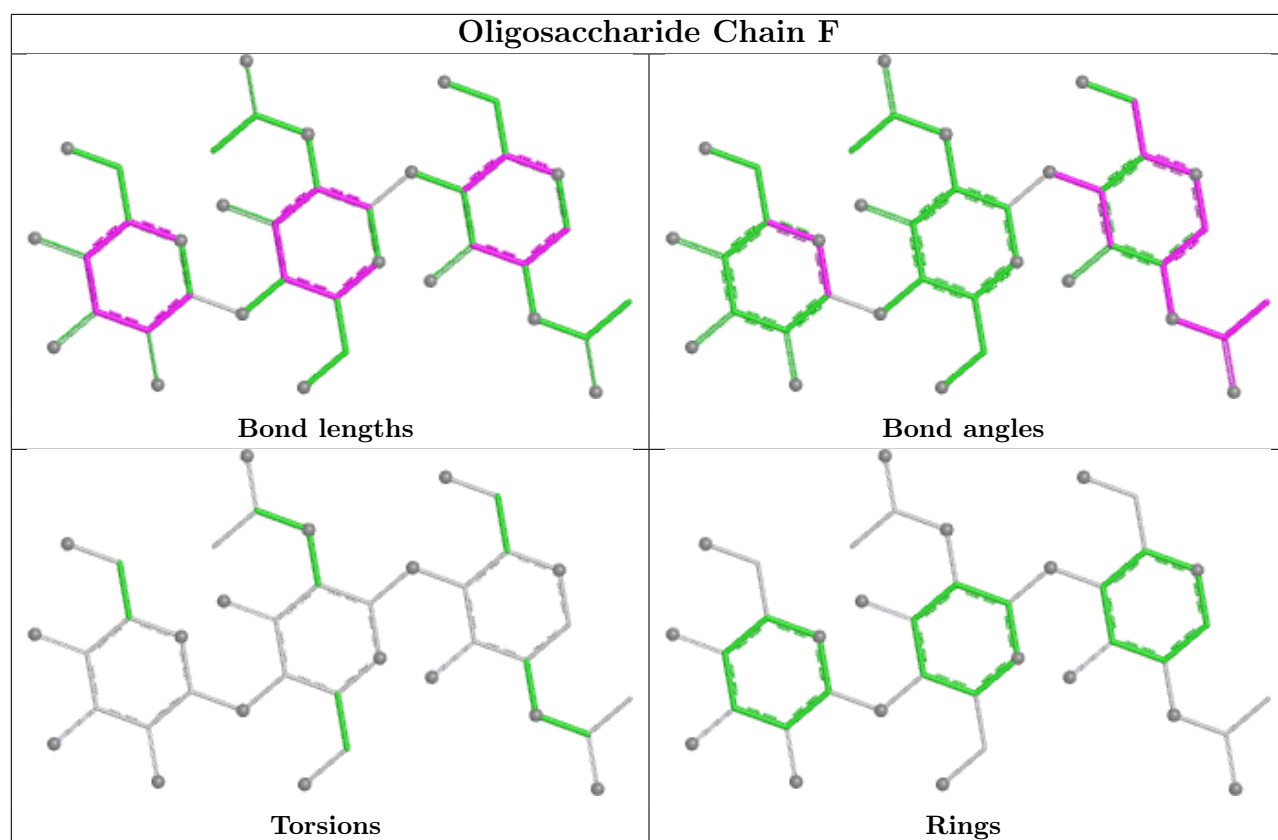


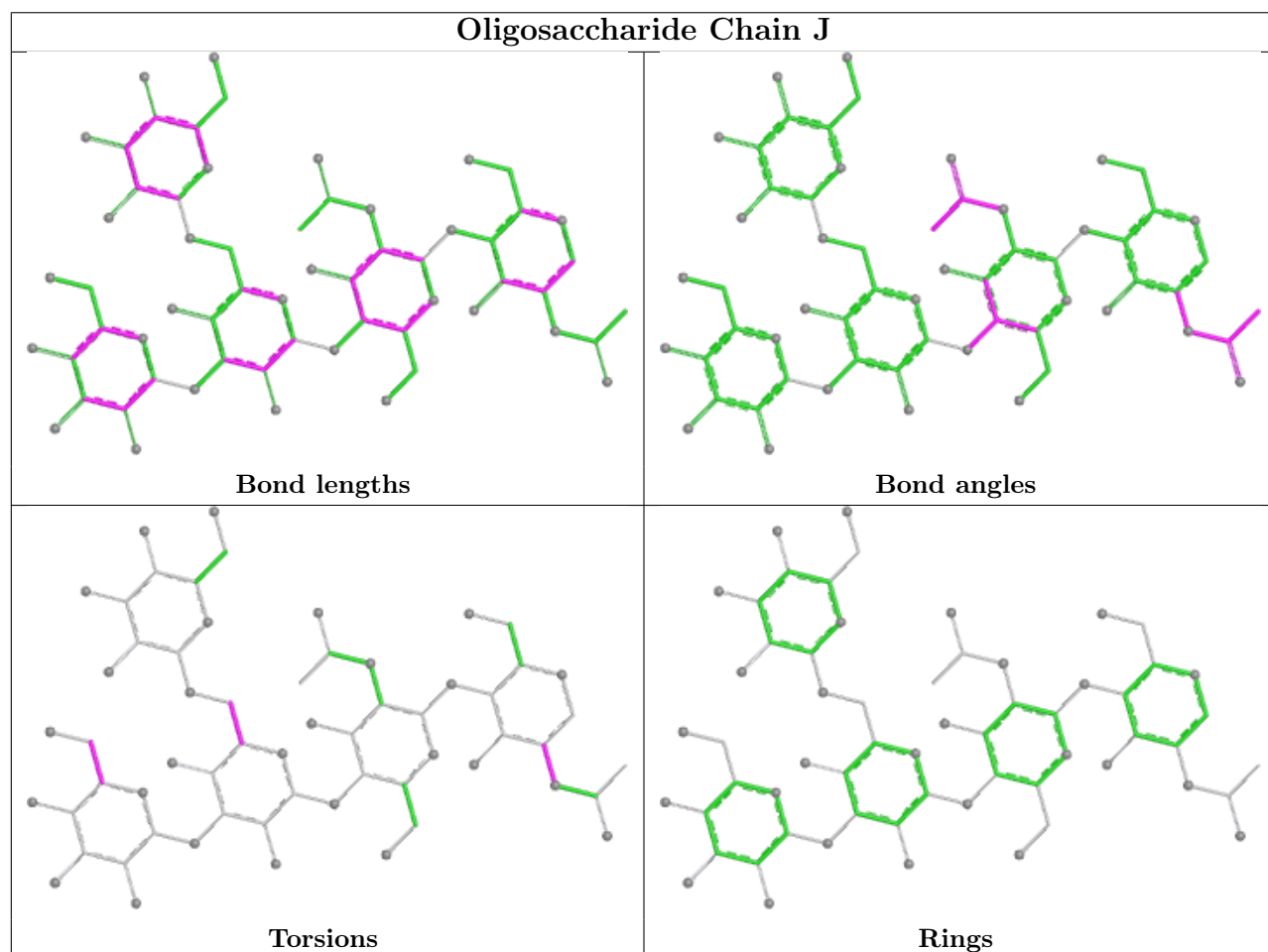
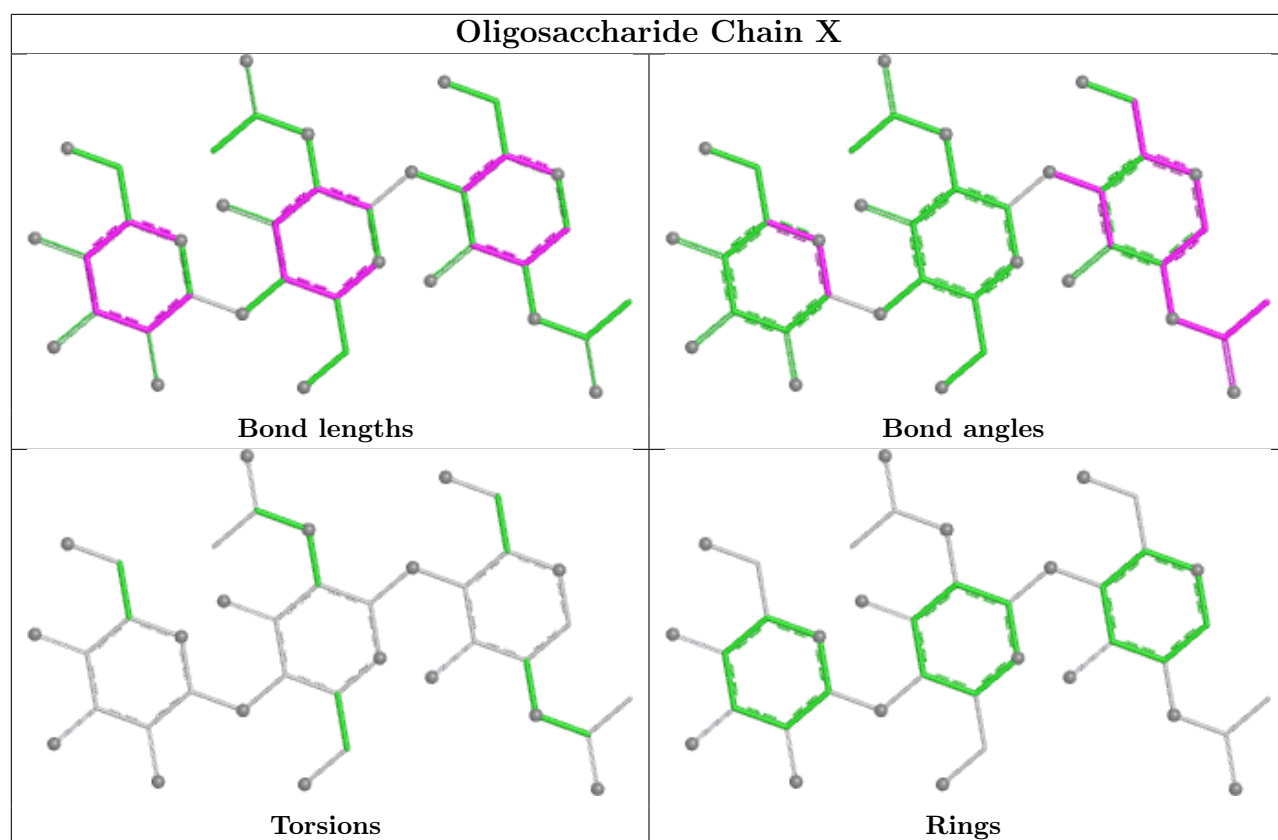


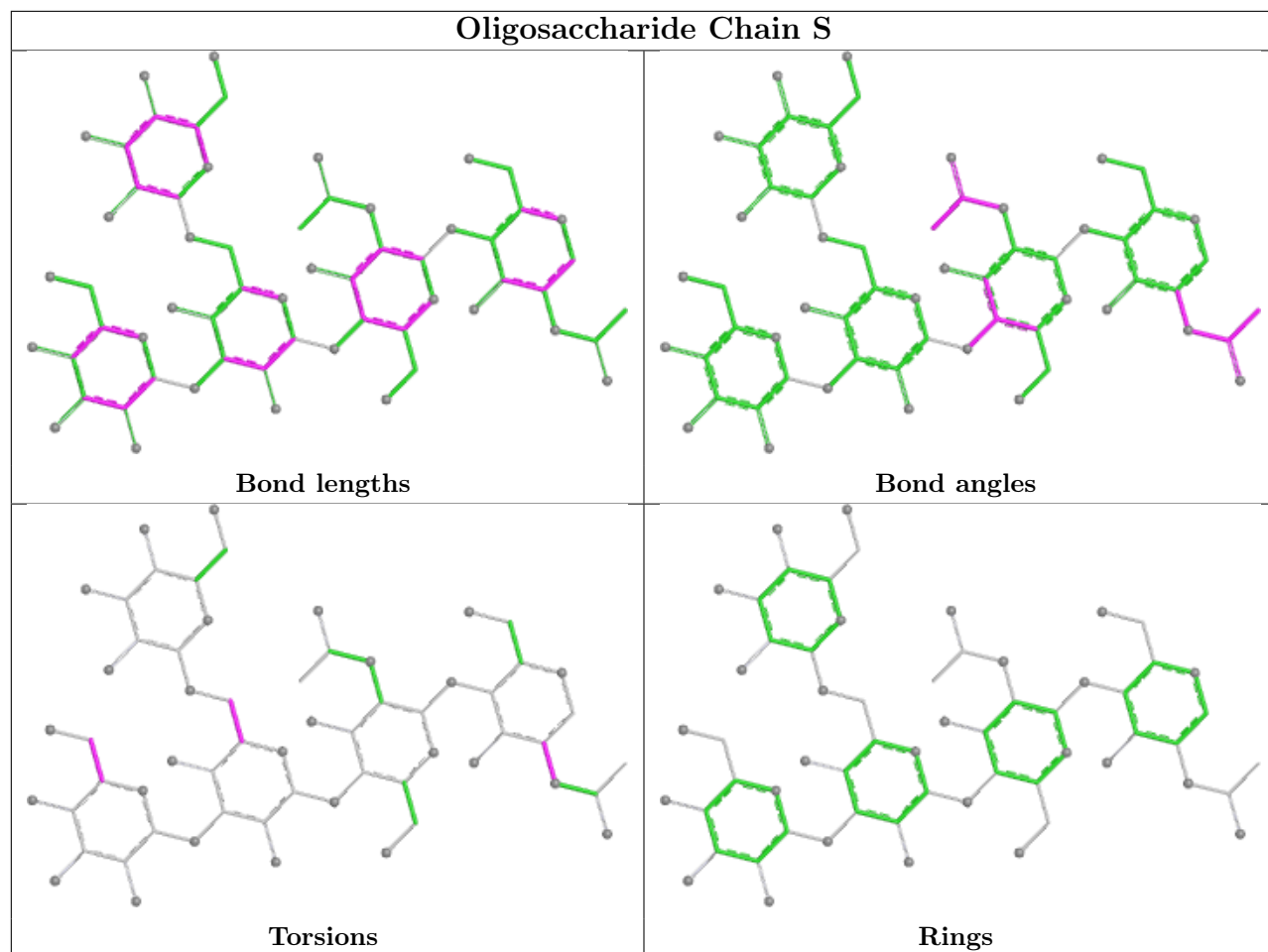


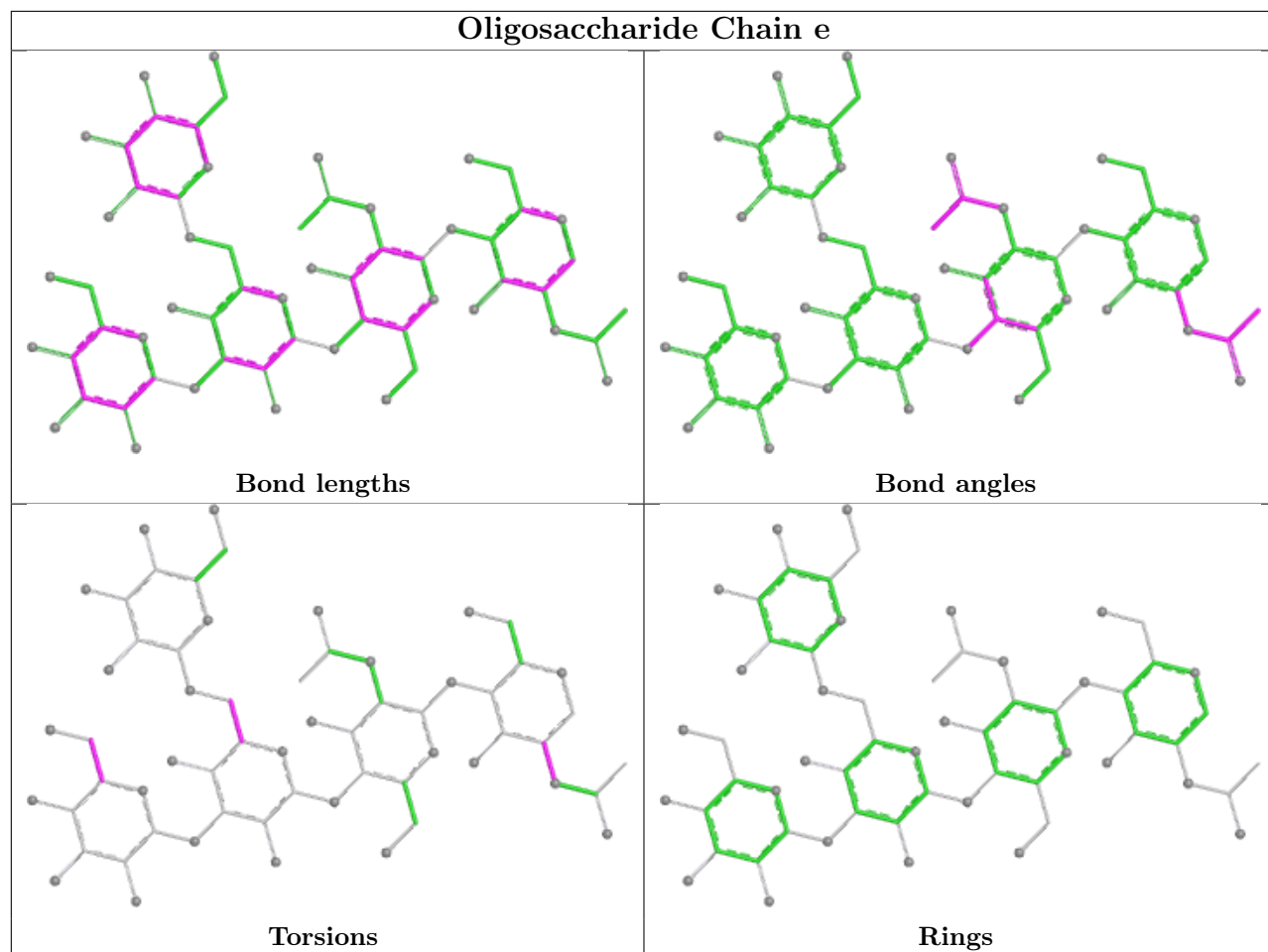


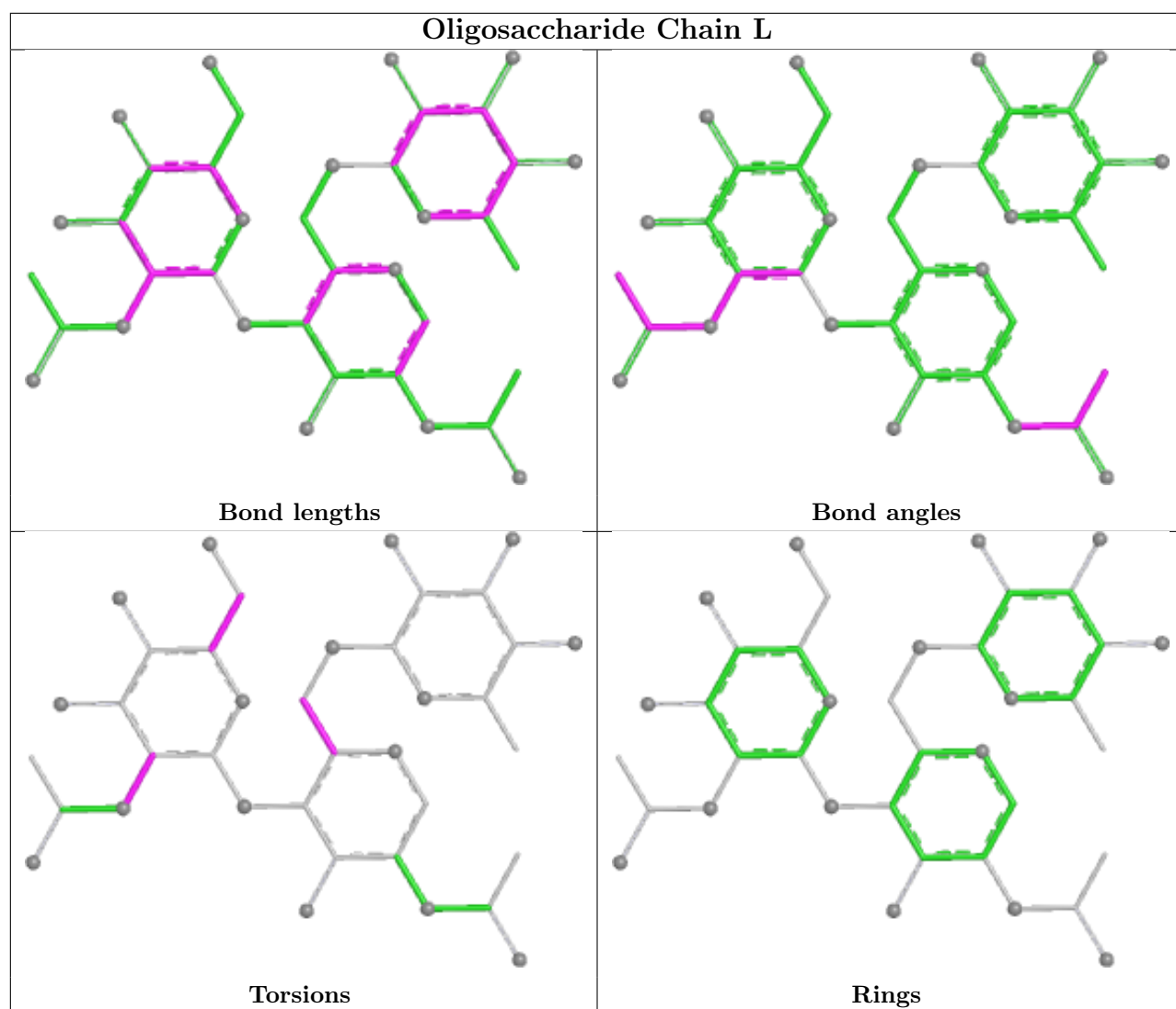


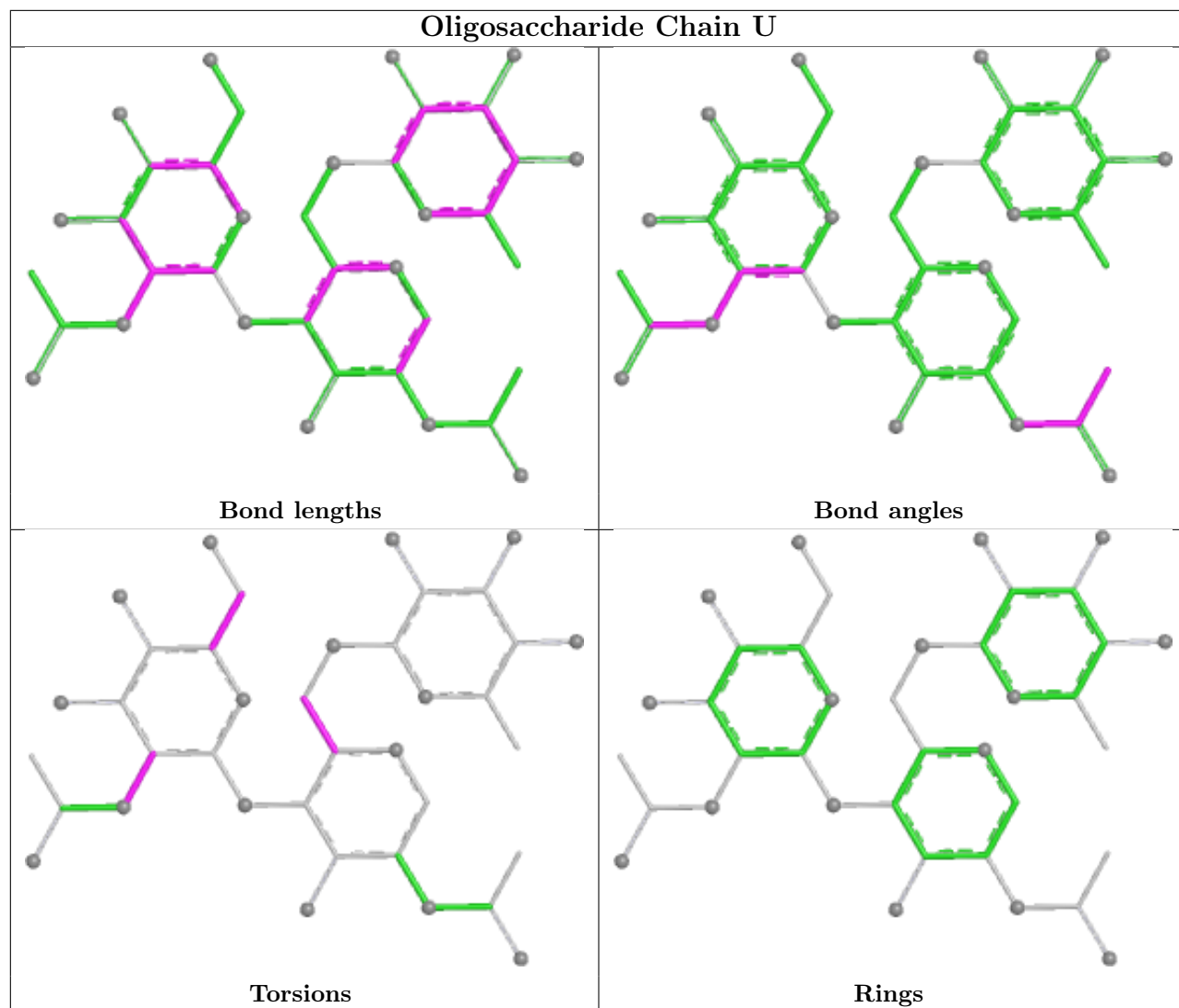


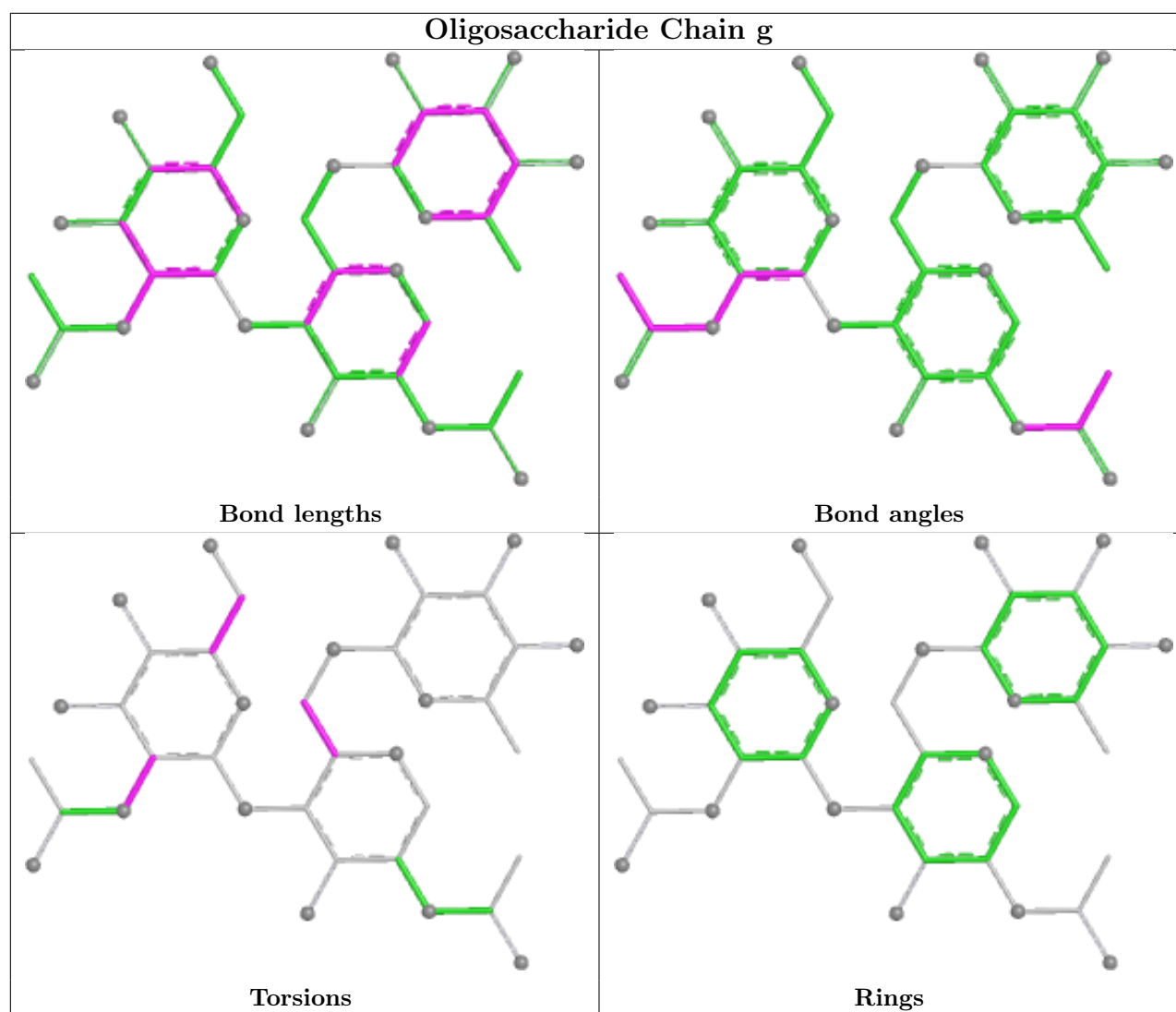












5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
6	NAG	C	701	1	14,14,15	2.13	6 (42%)	17,19,21	1.21	2 (11%)
6	NAG	a	701	1	14,14,15	2.26	7 (50%)	17,19,21	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	701	1	14,14,15	2.13	6 (42%)	17,19,21	1.21	2 (11%)
6	NAG	b	701	1	14,14,15	2.26	7 (50%)	17,19,21	1.05	0
6	NAG	B	701	1	14,14,15	2.13	6 (42%)	17,19,21	1.21	2 (11%)
6	NAG	c	701	1	14,14,15	2.26	6 (42%)	17,19,21	1.05	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
6	NAG	C	701	1	-	0/6/23/26	0/1/1/1
6	NAG	a	701	1	-	2/6/23/26	0/1/1/1
6	NAG	A	701	1	-	0/6/23/26	0/1/1/1
6	NAG	b	701	1	-	2/6/23/26	0/1/1/1
6	NAG	B	701	1	-	0/6/23/26	0/1/1/1
6	NAG	c	701	1	-	2/6/23/26	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	701	NAG	C1-C2	5.61	1.60	1.52
6	b	701	NAG	C1-C2	5.60	1.60	1.52
6	c	701	NAG	C1-C2	5.59	1.60	1.52
6	B	701	NAG	C1-C2	5.02	1.59	1.52
6	A	701	NAG	C1-C2	5.01	1.59	1.52
6	C	701	NAG	C1-C2	4.96	1.59	1.52
6	C	701	NAG	O5-C5	3.51	1.50	1.43
6	c	701	NAG	O5-C5	3.51	1.50	1.43
6	B	701	NAG	O5-C5	3.50	1.50	1.43
6	A	701	NAG	O5-C5	3.49	1.50	1.43
6	b	701	NAG	O5-C5	3.47	1.50	1.43
6	a	701	NAG	O5-C5	3.46	1.50	1.43
6	C	701	NAG	O5-C1	2.74	1.48	1.43
6	B	701	NAG	O5-C1	2.71	1.48	1.43
6	A	701	NAG	O5-C1	2.70	1.48	1.43
6	b	701	NAG	O5-C1	2.69	1.48	1.43
6	a	701	NAG	O5-C1	2.68	1.48	1.43
6	c	701	NAG	O5-C1	2.66	1.48	1.43
6	c	701	NAG	C3-C2	2.53	1.57	1.52
6	b	701	NAG	C3-C2	2.53	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	701	NAG	C3-C2	2.51	1.57	1.52
6	c	701	NAG	C2-N2	2.28	1.50	1.46
6	a	701	NAG	C2-N2	2.27	1.50	1.46
6	b	701	NAG	C2-N2	2.27	1.50	1.46
6	B	701	NAG	C4-C5	2.20	1.57	1.53
6	C	701	NAG	C4-C5	2.19	1.57	1.53
6	A	701	NAG	C4-C5	2.18	1.57	1.53
6	C	701	NAG	C2-N2	2.18	1.49	1.46
6	b	701	NAG	C4-C5	2.15	1.57	1.53
6	a	701	NAG	C4-C5	2.15	1.57	1.53
6	A	701	NAG	C2-N2	2.15	1.49	1.46
6	c	701	NAG	C4-C5	2.14	1.57	1.53
6	B	701	NAG	C2-N2	2.13	1.49	1.46
6	B	701	NAG	C3-C2	2.09	1.56	1.52
6	C	701	NAG	C3-C2	2.09	1.56	1.52
6	A	701	NAG	C3-C2	2.08	1.56	1.52
6	a	701	NAG	C4-C3	2.02	1.57	1.52
6	b	701	NAG	C4-C3	2.01	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	701	NAG	C8-C7-N2	3.44	121.82	116.12
6	B	701	NAG	C8-C7-N2	3.44	121.82	116.12
6	C	701	NAG	C8-C7-N2	3.43	121.81	116.12
6	A	701	NAG	O7-C7-C8	-2.19	118.15	122.05
6	B	701	NAG	O7-C7-C8	-2.19	118.16	122.05
6	C	701	NAG	O7-C7-C8	-2.18	118.17	122.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	a	701	NAG	C3-C2-N2-C7
6	b	701	NAG	C3-C2-N2-C7
6	c	701	NAG	C3-C2-N2-C7
6	a	701	NAG	C1-C2-N2-C7
6	b	701	NAG	C1-C2-N2-C7
6	c	701	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

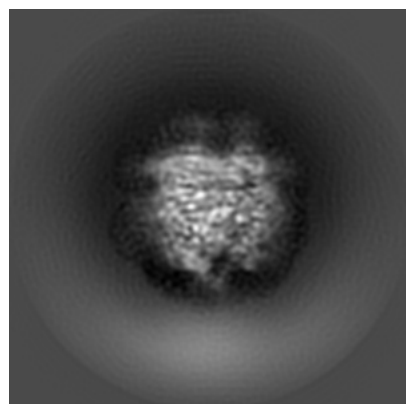
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25107. These allow visual inspection of the internal detail of the map and identification of artifacts.

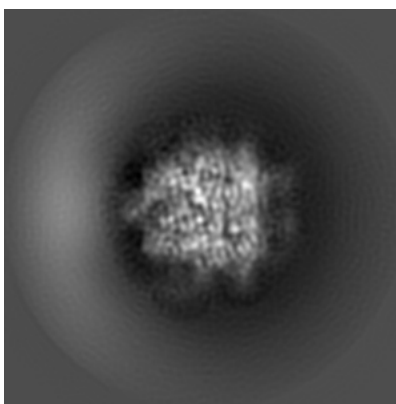
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

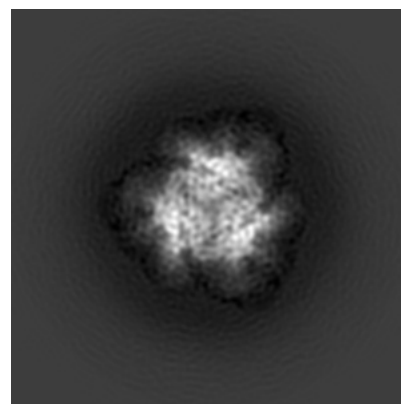
6.1.1 Primary map



X

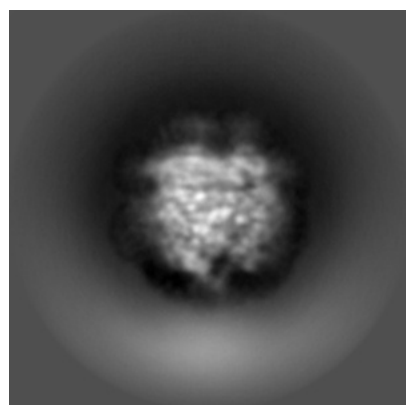


Y

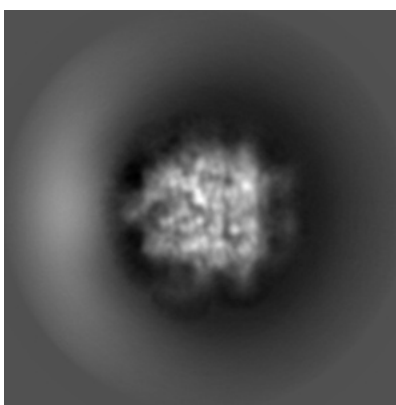


Z

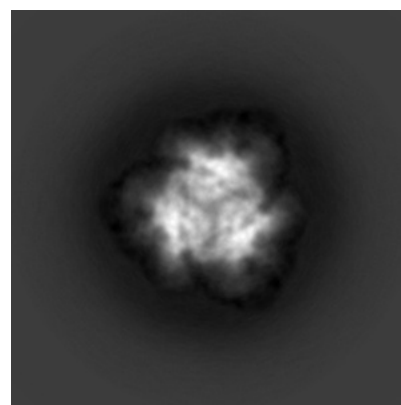
6.1.2 Raw map



X



Y

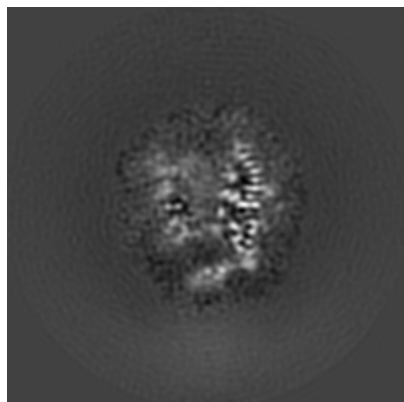


Z

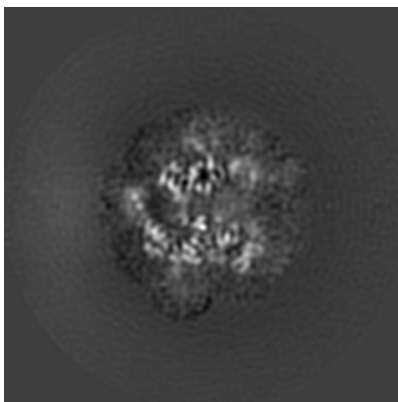
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

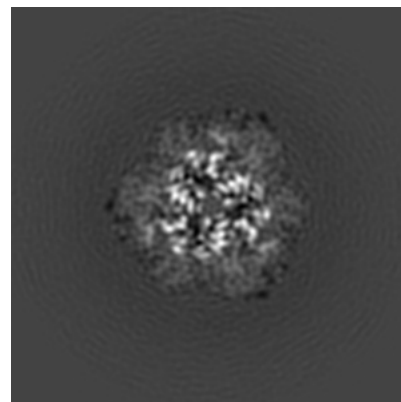
6.2.1 Primary map



X Index: 110

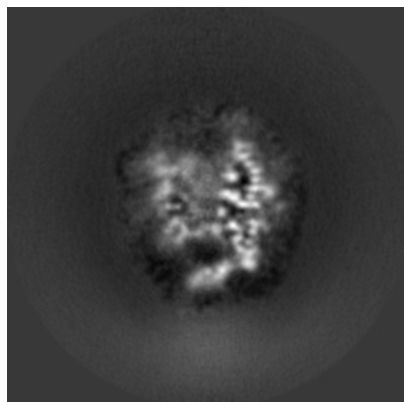


Y Index: 110

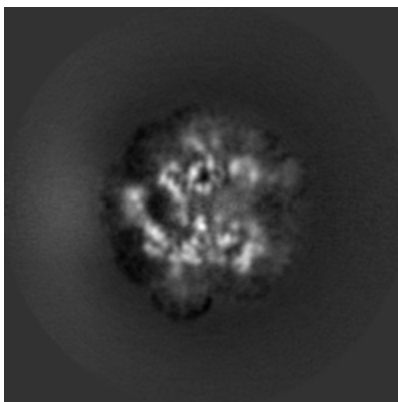


Z Index: 110

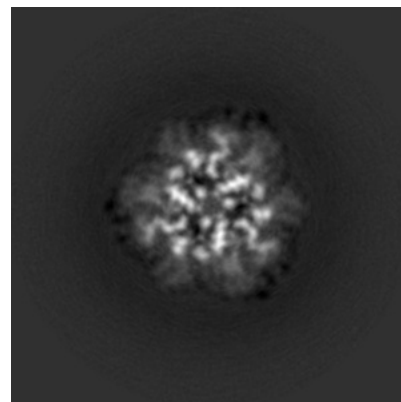
6.2.2 Raw map



X Index: 110



Y Index: 110

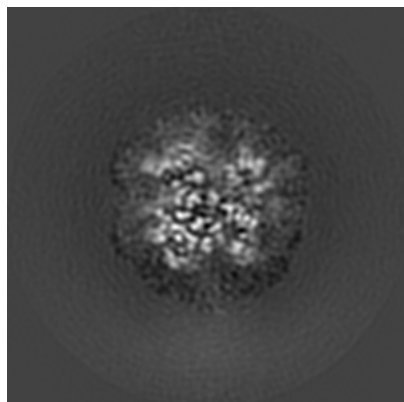


Z Index: 110

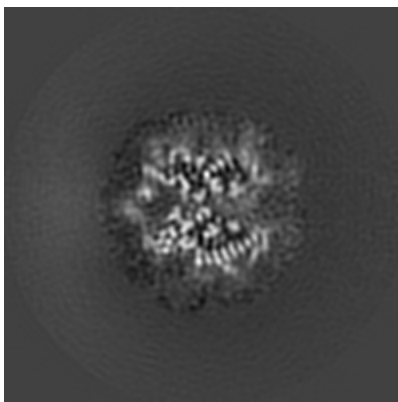
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

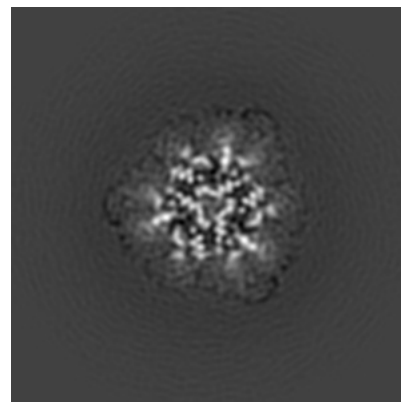
6.3.1 Primary map



X Index: 123

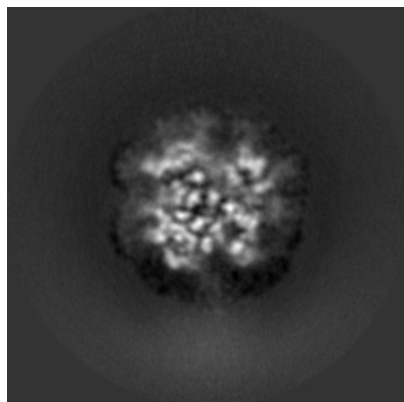


Y Index: 102

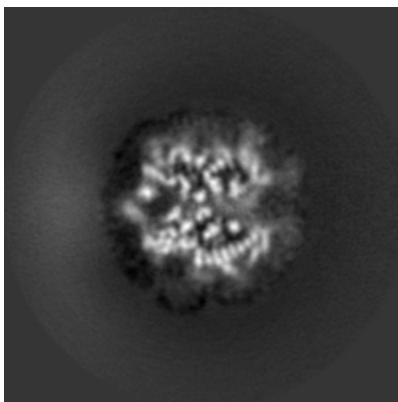


Z Index: 107

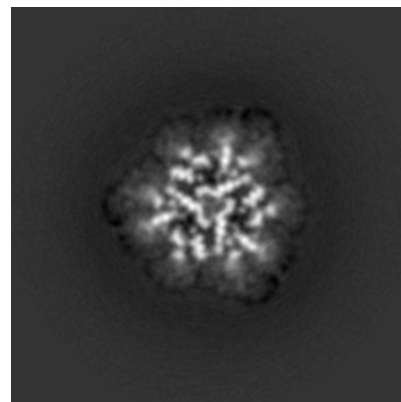
6.3.2 Raw map



X Index: 123



Y Index: 102

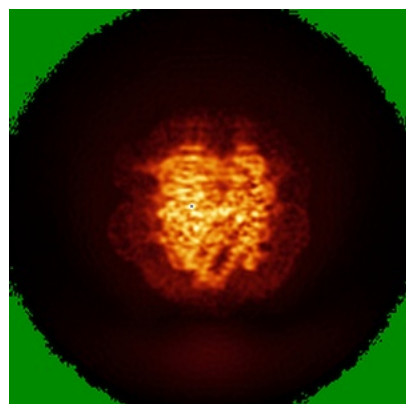


Z Index: 107

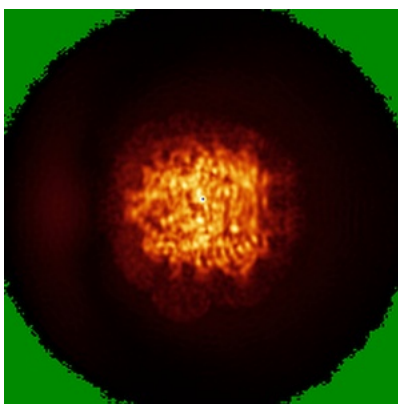
The images above show the largest variance slices of the map in three orthogonal directions.

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

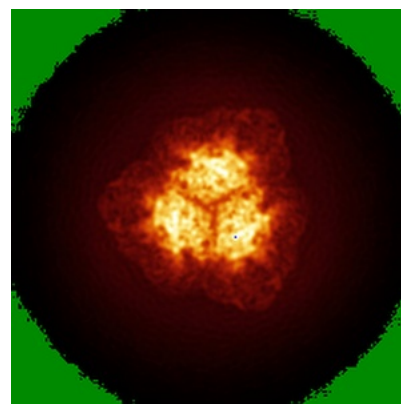
6.4.1 Primary map



X

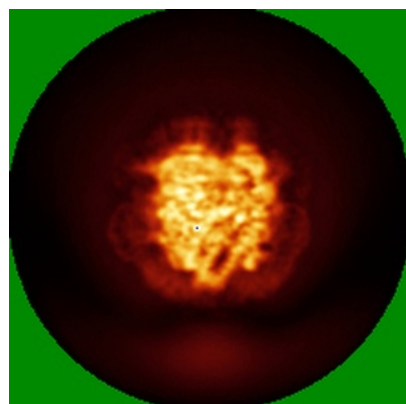


Y

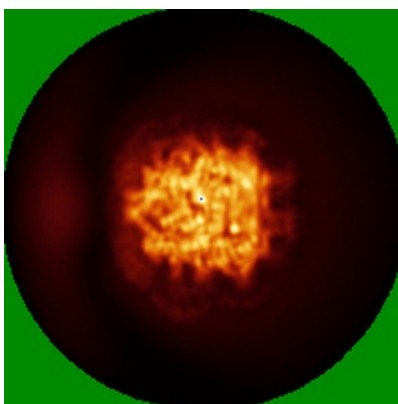


Z

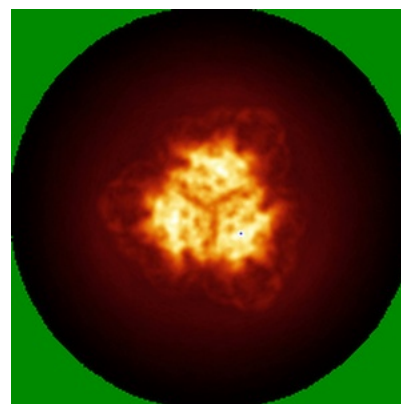
6.4.2 Raw map



X



Y

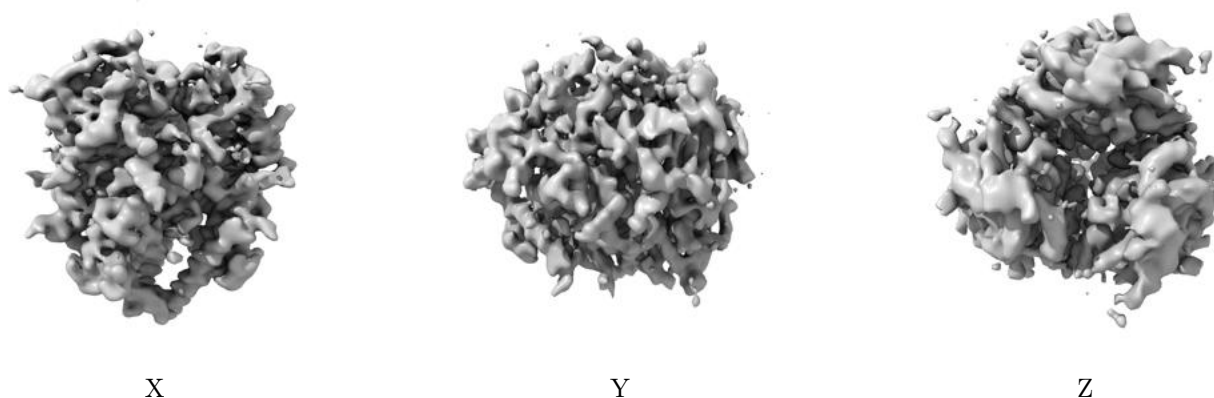


Z

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

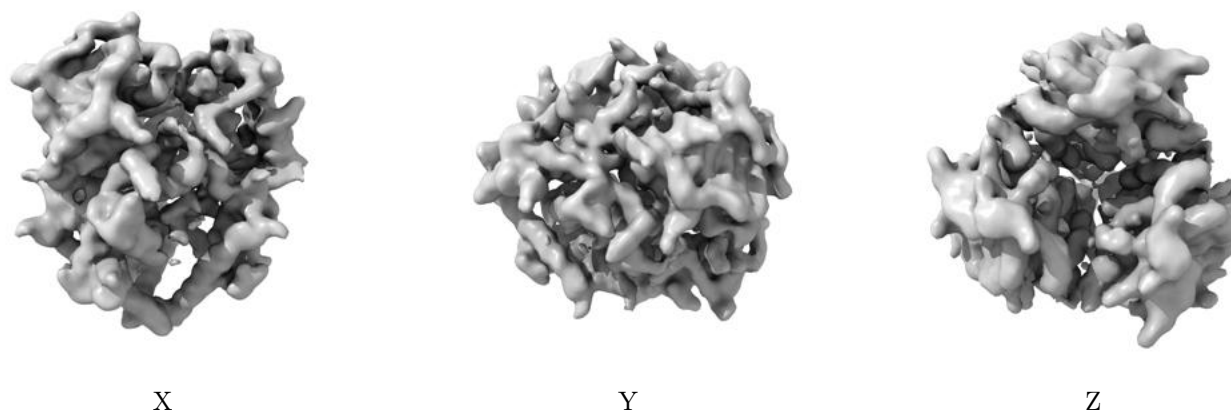
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

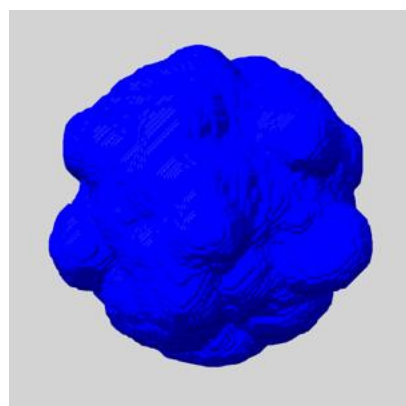
6.6 Mask visualisation [i](#)

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

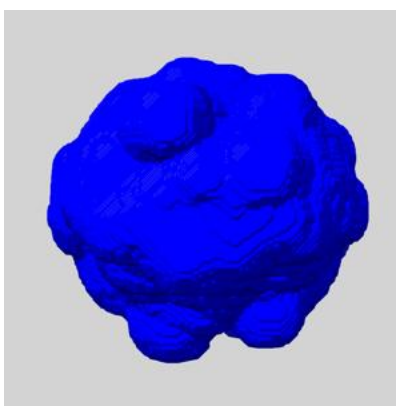
A mask typically either:

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

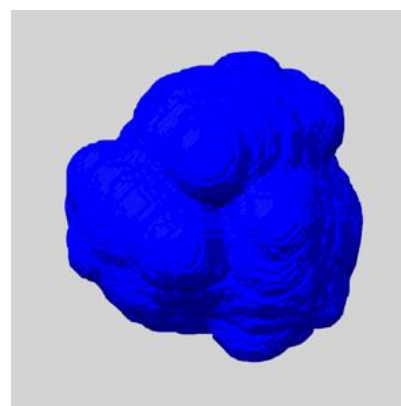
6.6.1 emd_25107_msk_1.map [i](#)



X



Y

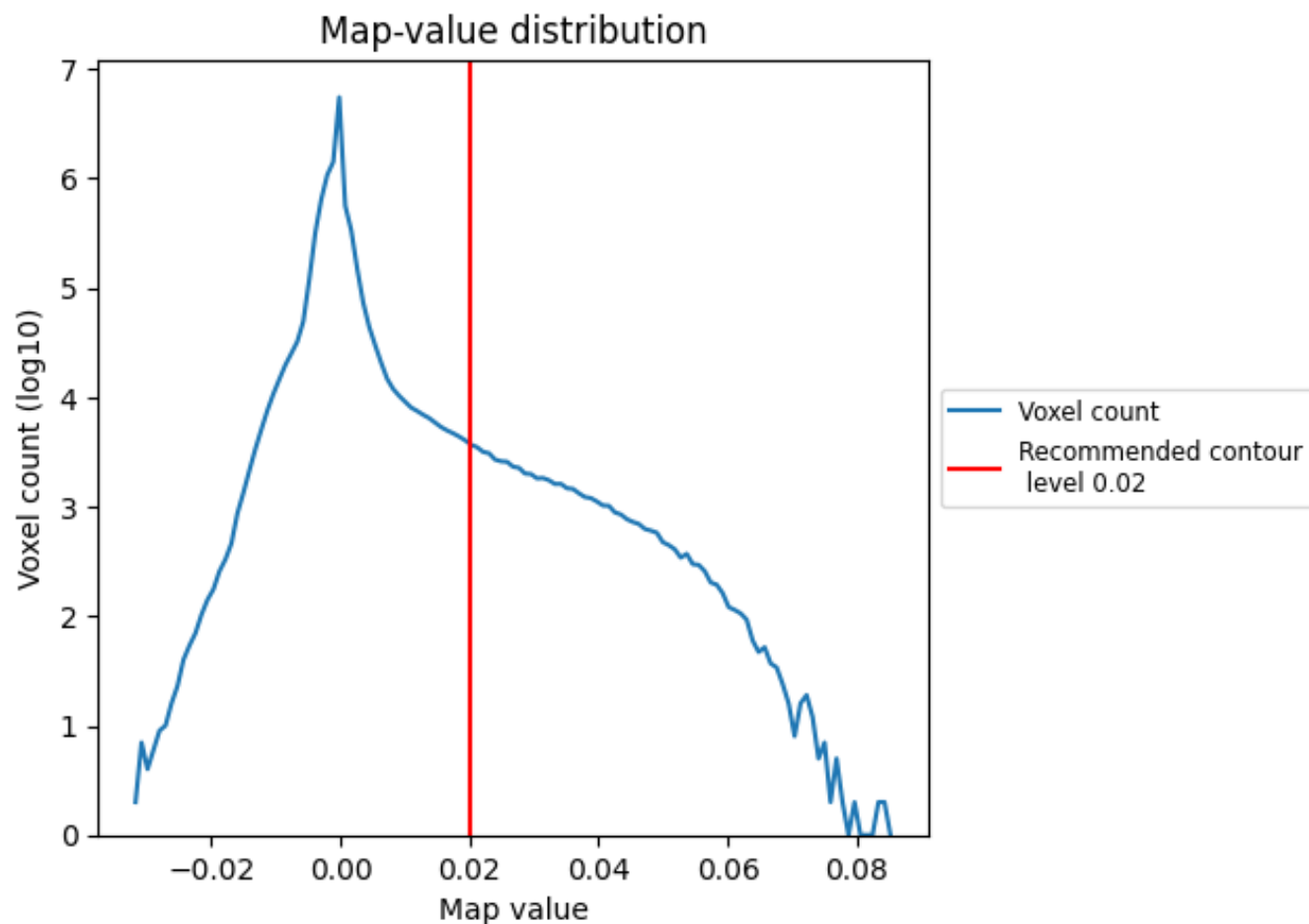


Z

7 Map analysis [i](#)

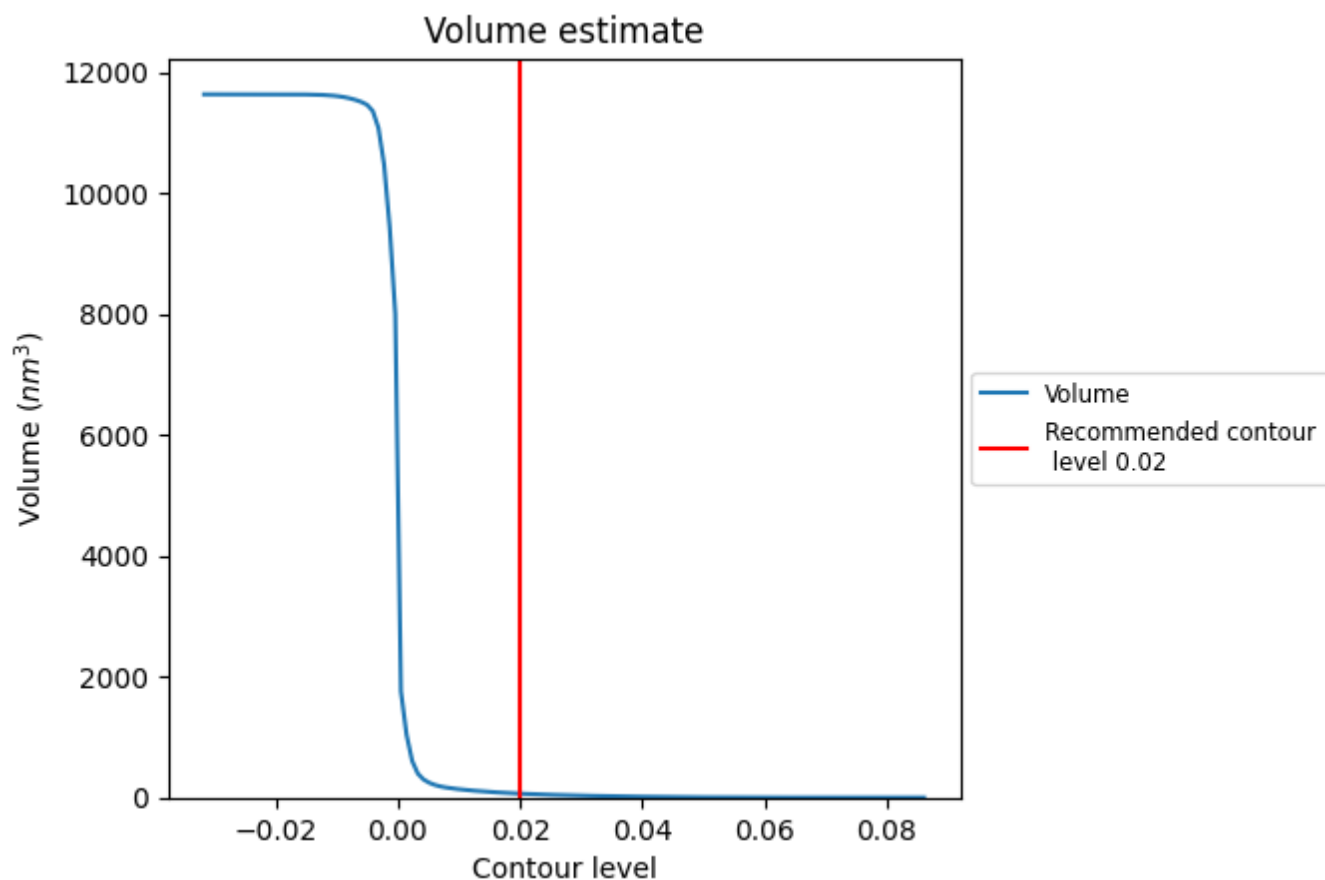
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

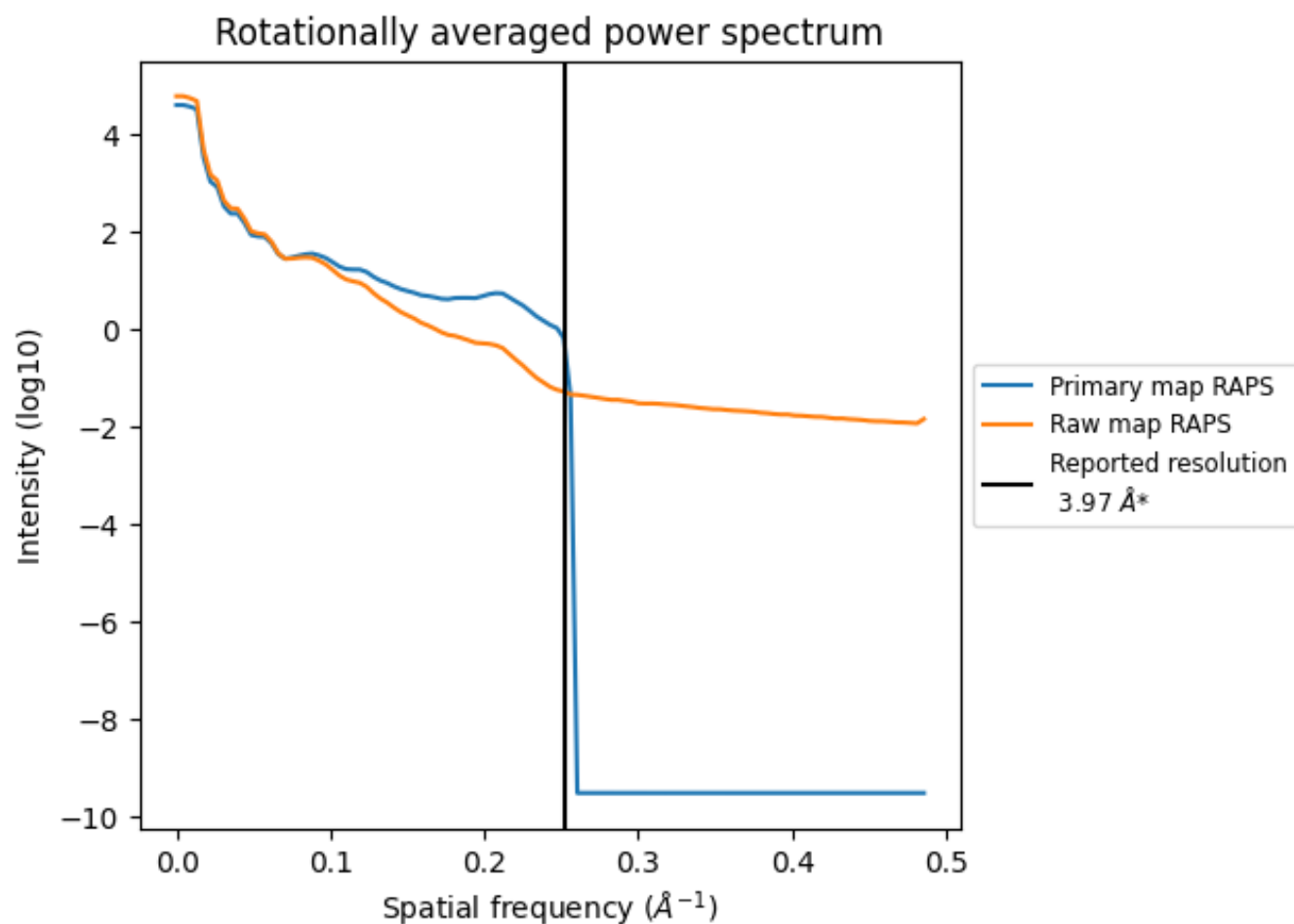
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65 nm³; this corresponds to an approximate mass of 59 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

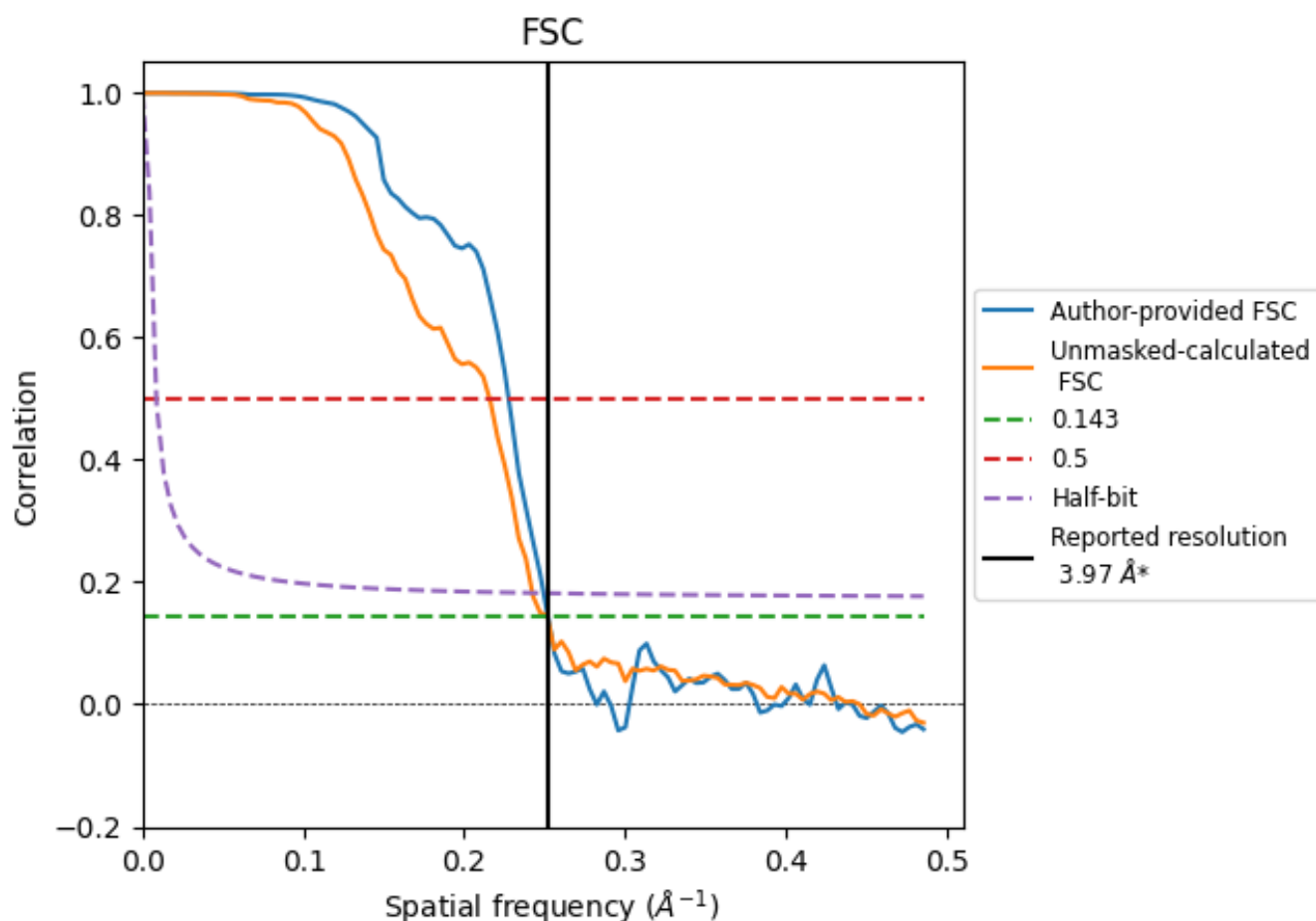


*Reported resolution corresponds to spatial frequency of 0.252 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.252 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

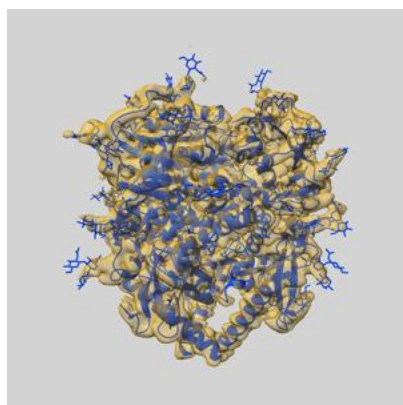
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.97	-	-
Author-provided FSC curve	3.97	4.40	4.01
Unmasked-calculated*	3.97	4.63	4.13

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

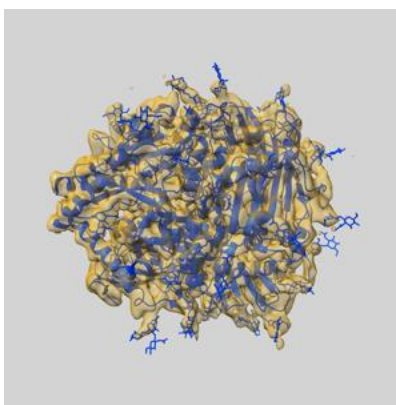
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25107 and PDB model 7SGD. Per-residue inclusion information can be found in section 3 on page 10.

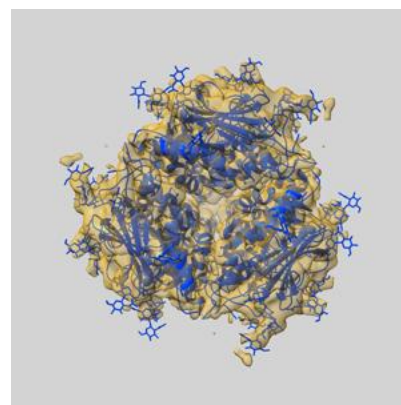
9.1 Map-model overlay [i](#)



X



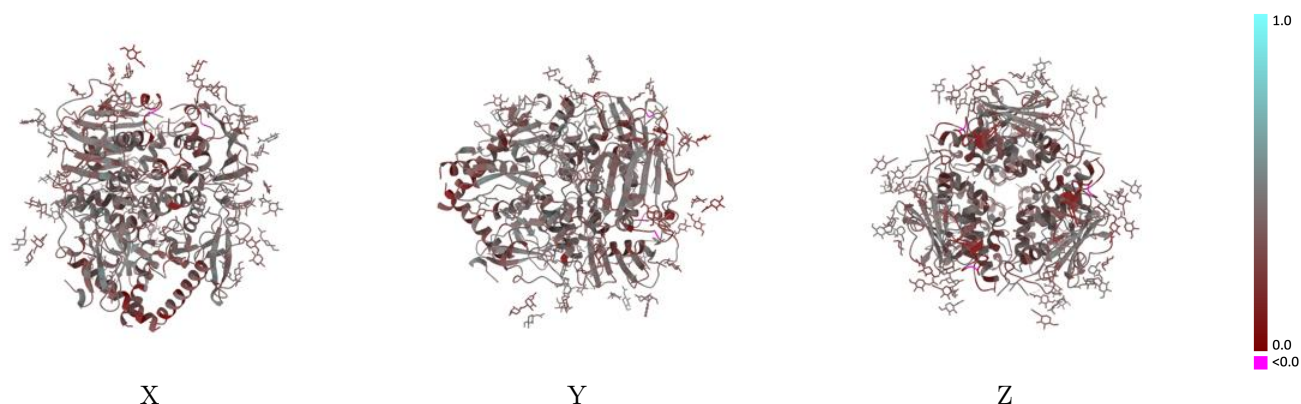
Y



Z

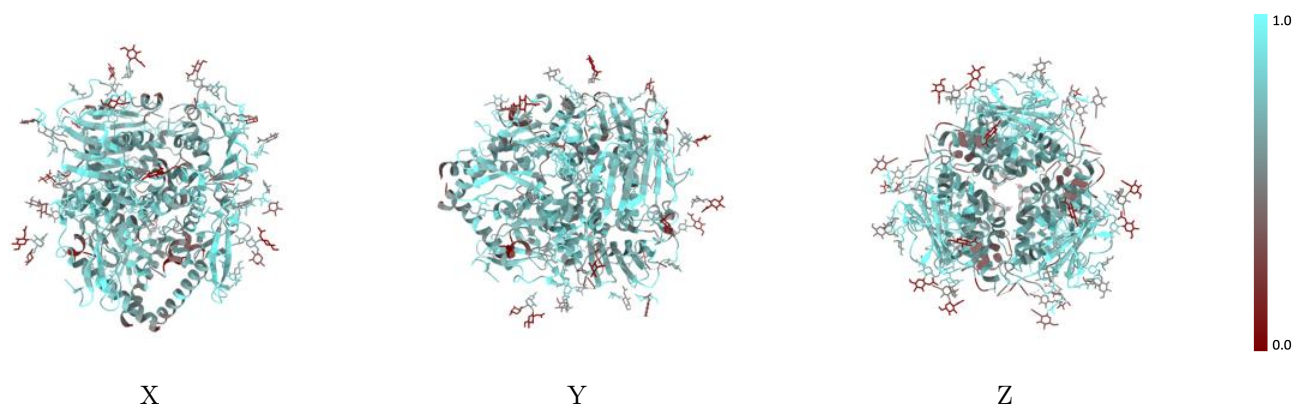
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



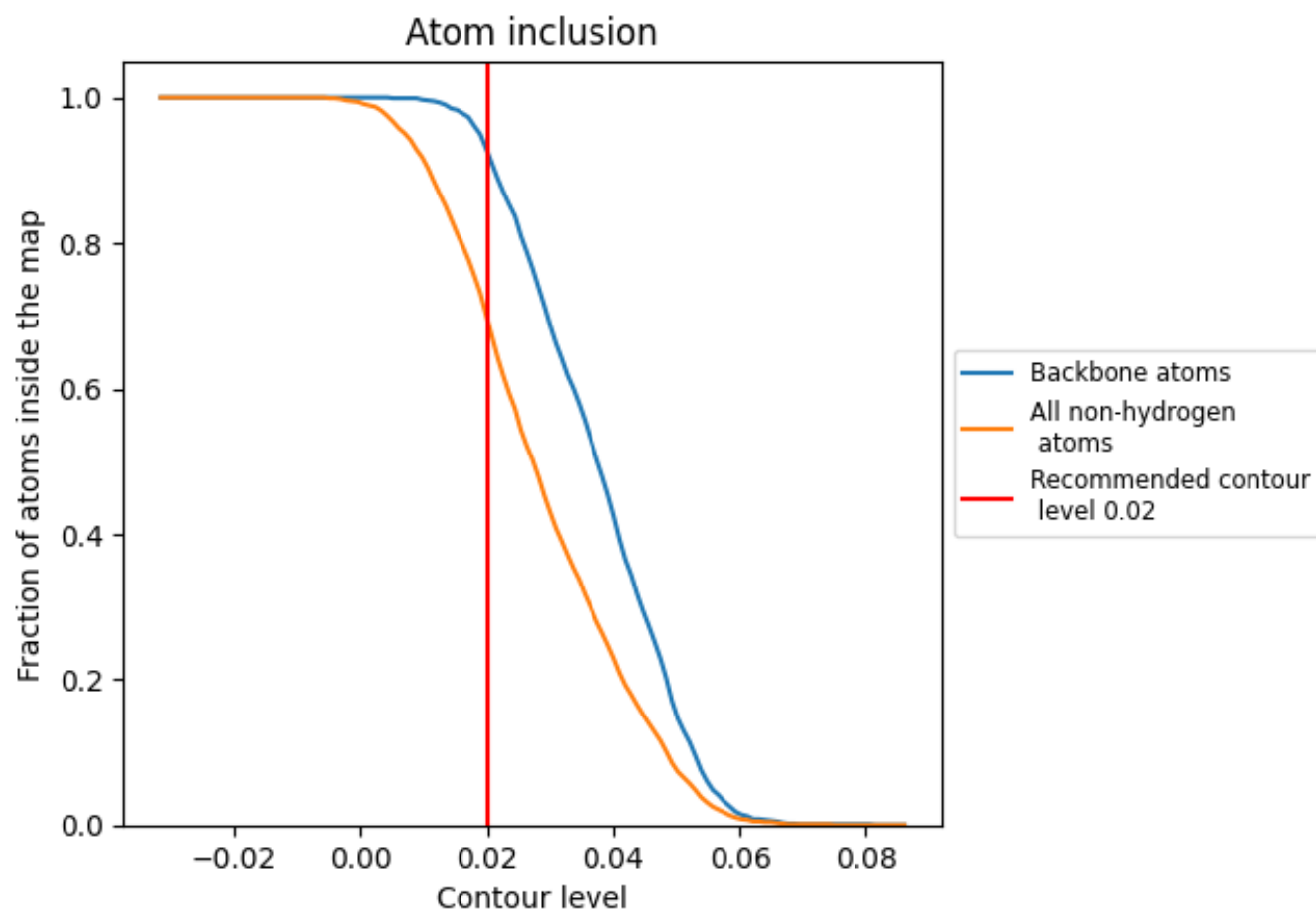
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6980	 0.3660
A	 0.7300	 0.3590
B	 0.7270	 0.3610
C	 0.7270	 0.3600
D	 0.2140	 0.3620
E	 0.3930	 0.2680
F	 0.7180	 0.3710
G	 0.6070	 0.4120
H	 0.6070	 0.3850
I	 0.3210	 0.2210
J	 0.6890	 0.3990
K	 0.7500	 0.3830
L	 0.2630	 0.3610
M	 0.2140	 0.3560
N	 0.3930	 0.2720
O	 0.7440	 0.3640
P	 0.6070	 0.4320
Q	 0.6790	 0.3830
R	 0.2860	 0.2160
S	 0.6890	 0.4020
T	 0.7500	 0.3960
U	 0.2890	 0.3680
V	 0.2140	 0.3630
W	 0.3930	 0.2820
X	 0.7180	 0.3640
Y	 0.6070	 0.4330
Z	 0.6070	 0.3900
a	 0.7060	 0.3720
b	 0.7050	 0.3720
c	 0.7070	 0.3740
d	 0.3210	 0.2170
e	 0.6890	 0.4070
f	 0.7140	 0.3700
g	 0.2630	 0.3460

