



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 04:05 PM EST

PDB ID : 1ZPU  
Title : Crystal Structure of Fet3p, a Multicopper Oxidase that Functions in Iron Import  
Authors : Taylor, A.B.; Stoj, C.S.; Ziegler, L.; Kosman, D.J.; Hart, P.J.  
Deposited on : 2005-05-17  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

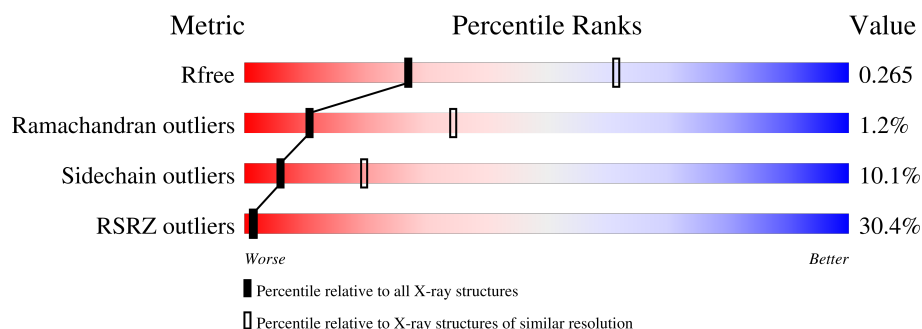
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.



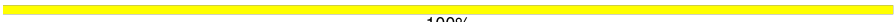
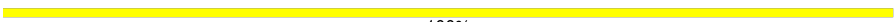
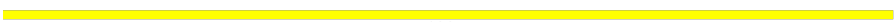











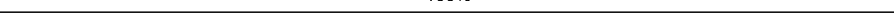
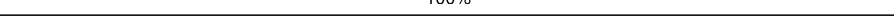
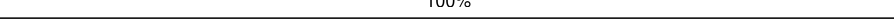

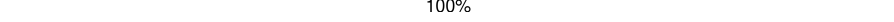
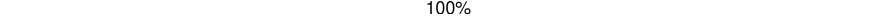

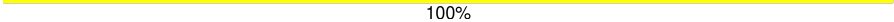

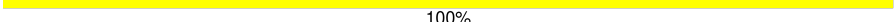
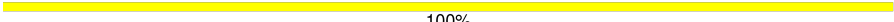
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3657 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	534	<div> <div>26%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
1	B	534	<div> <div>10%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	C	534	<div> <div>36%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	D	534	<div> <div>21%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	E	534	<div> <div>23%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	F	534	<div> <div>64%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
2	G	5	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	5	 100%
2	M	5	 100%
2	O	5	 100%
2	S	5	 100%
2	U	5	 100%
2	Y	5	 100%
2	a	5	 100%
2	d	5	 40% 60%
2	f	5	 20% 80%
2	i	5	 20% 80%
2	k	5	 100%
3	H	6	 17% 83%
3	N	6	 100%
3	Z	6	 100%
3	j	6	 100%
4	I	2	 100%
4	P	2	 50% 50%
4	Q	2	 100%
4	V	2	 100%
4	b	2	 50% 50%
4	g	2	 100%
5	K	3	 33% 67%
5	L	3	 100%
5	W	3	 100%
5	X	3	 33% 67%

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Mol	Chain	Length	Quality of chain
5	c	3	<div><div style="width: 33%;"></div>33%<div style="width: 67%;"></div>67%</div>
5	h	3	<div><div style="width: 100%;"></div>100%</div>
5	l	3	<div><div style="width: 100%;"></div>100%</div>
6	R	4	<div><div style="width: 100%;"></div>100%</div>
7	T	7	<div><div style="width: 29%;"></div>29%<div style="width: 71%;"></div>71%</div>
7	e	7	<div><div style="width: 100%;"></div>100%</div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	a	1	X	-	-	-
2	NAG	f	1	X	-	-	-
3	NAG	H	1	X	-	-	-
3	NAG	N	1	X	-	-	-
3	NAG	Z	1	X	-	-	-
3	NAG	j	1	X	-	-	-
4	NAG	b	1	X	-	-	-
5	NAG	L	1	X	-	-	-
5	NAG	X	1	X	-	-	-
5	NAG	c	1	X	-	-	-
5	NAG	h	1	X	-	-	-
5	NAG	l	1	X	-	-	-
6	NAG	R	1	X	-	-	-
7	NAG	T	1	X	-	-	-
7	NAG	e	1	X	-	-	-
8	NAG	A	2006	X	-	-	-
8	NAG	A	2012	X	-	-	-
8	NAG	A	2018	X	-	-	-
8	NAG	B	2006	X	-	-	-
8	NAG	B	2012	X	-	-	-
8	NAG	B	2018	X	-	-	-
8	NAG	C	2012	X	-	-	-
8	NAG	C	2018	X	-	-	-
8	NAG	D	2006	X	-	-	-
8	NAG	E	2012	X	-	-	-
8	NAG	F	2005	X	-	-	-
8	NAG	F	2006	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	F	2009	X	-	-	-
8	NAG	F	2012	X	-	-	-

## 2 Entry composition [i](#)

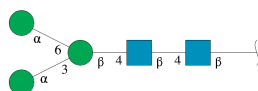
There are 9 unique types of molecules in this entry. The entry contains 27659 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Iron transport multicopper oxidase FET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	B	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	C	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	D	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	E	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	F	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			

- Molecule 2 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.



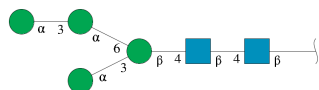
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	O	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	U	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	Y	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	a	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	d	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	f	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	i	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	k	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



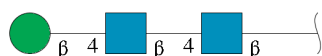
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	N	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	Z	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	j	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	g	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	c	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	h	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	l	3	Total	C	N	O	0	0	0
			39	22	2	15			

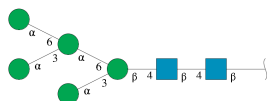
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





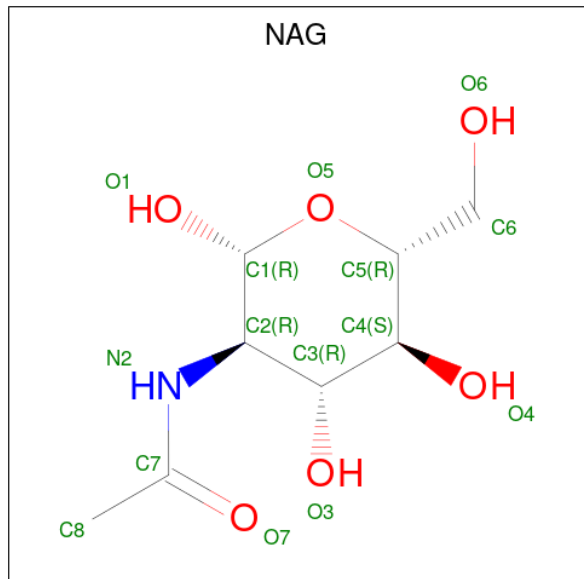
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	T	7	Total	C	N	O	0	0	0
			83	46	2	35			
7	e	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		

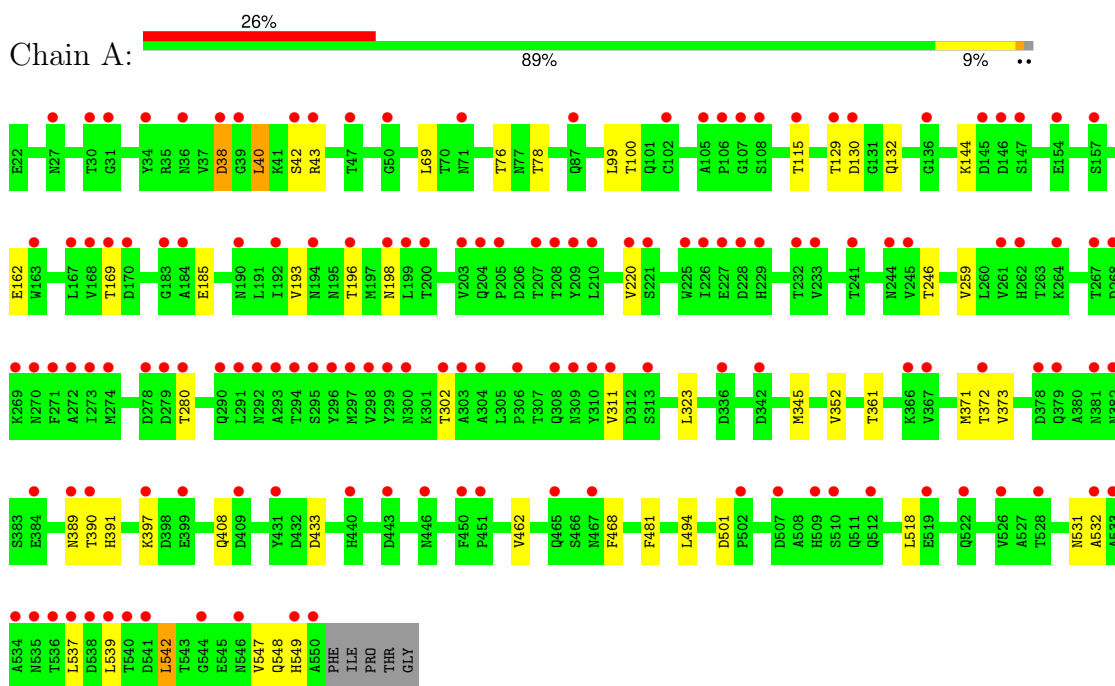
- Molecule 9 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Cu	0	0
			4	4		
9	B	4	Total	Cu	0	0
			4	4		
9	C	4	Total	Cu	0	0
			4	4		
9	D	4	Total	Cu	0	0
			4	4		
9	E	4	Total	Cu	0	0
			4	4		
9	F	4	Total	Cu	0	0
			4	4		

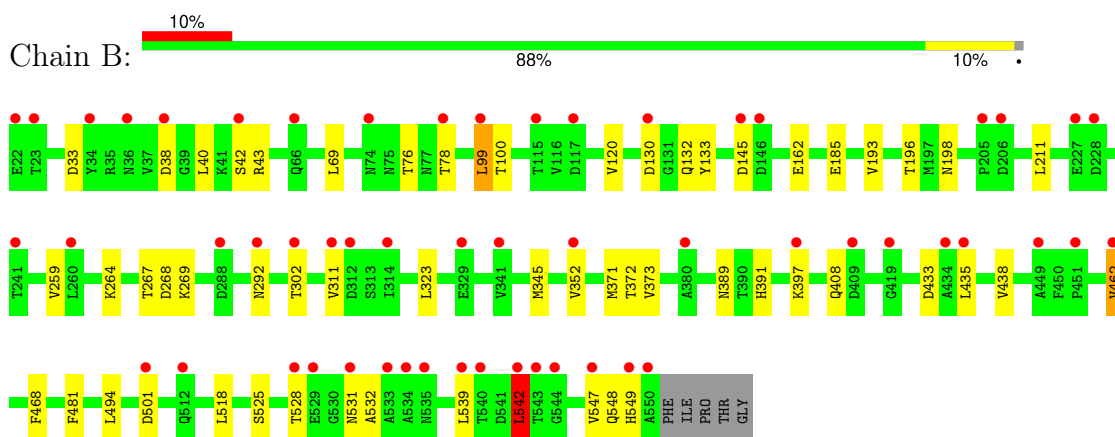
### 3 Residue-property plots

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. 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. 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.

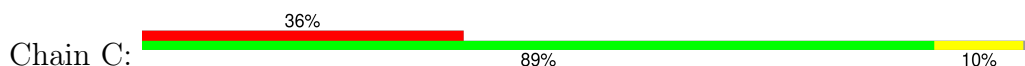
#### • Molecule 1: Iron transport multicopper oxidase FET3

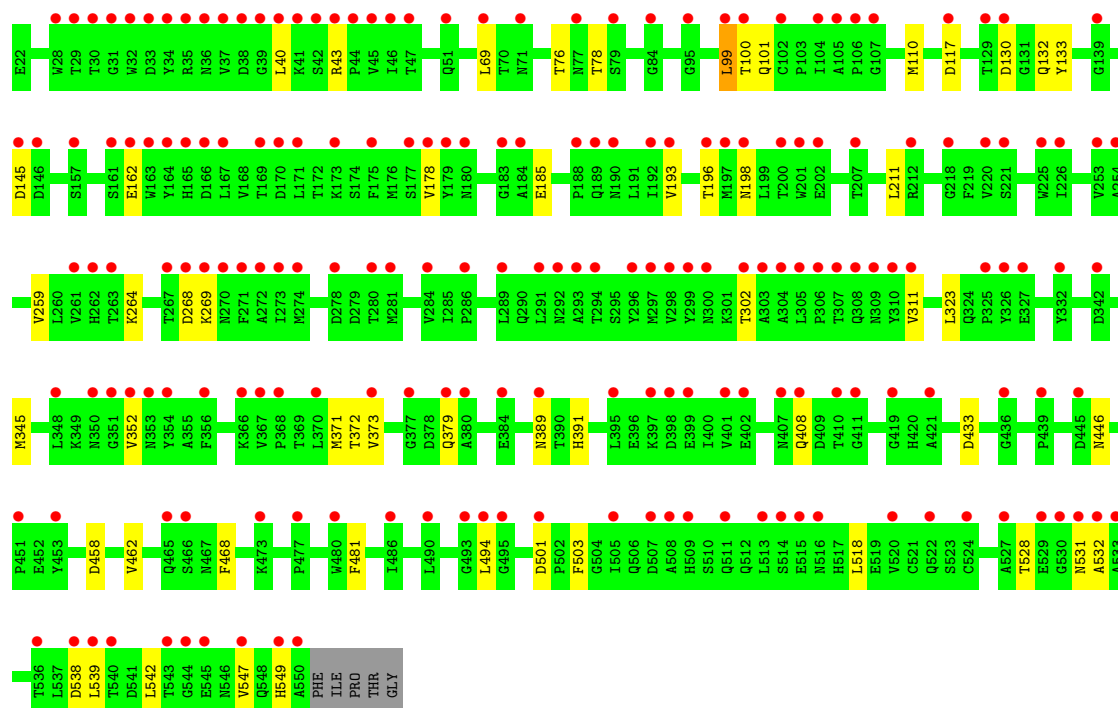


#### • Molecule 1: Iron transport multicopper oxidase FET3

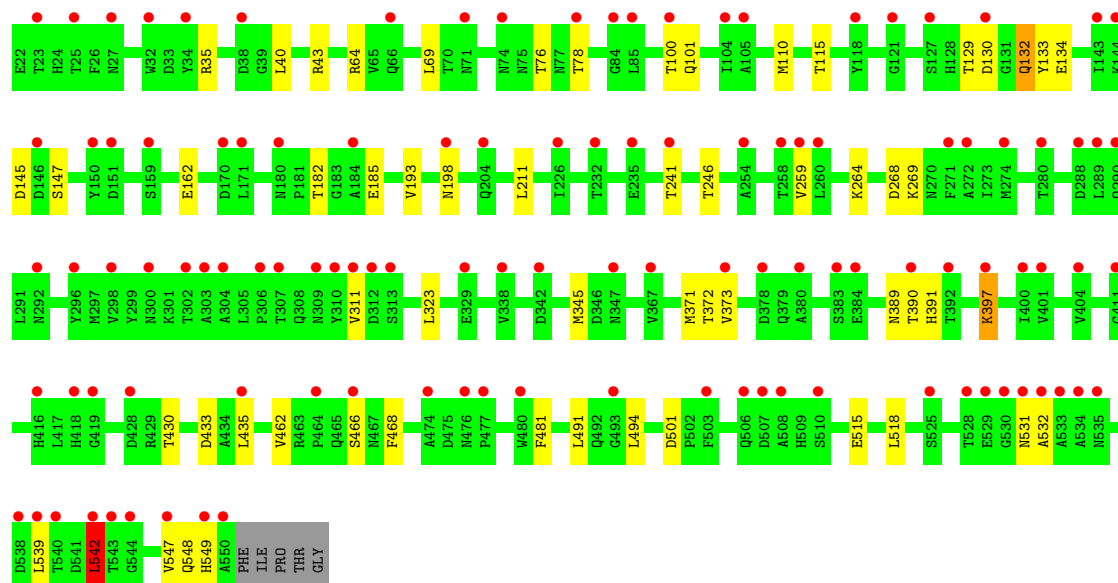
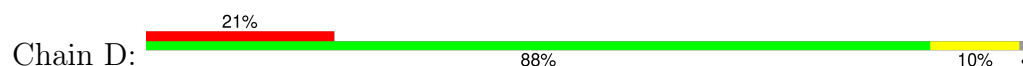


#### • Molecule 1: Iron transport multicopper oxidase FET3

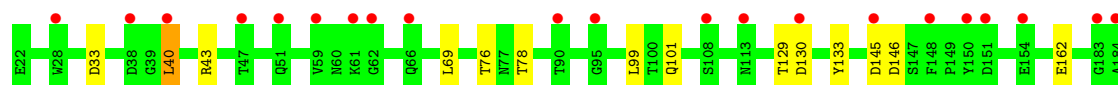


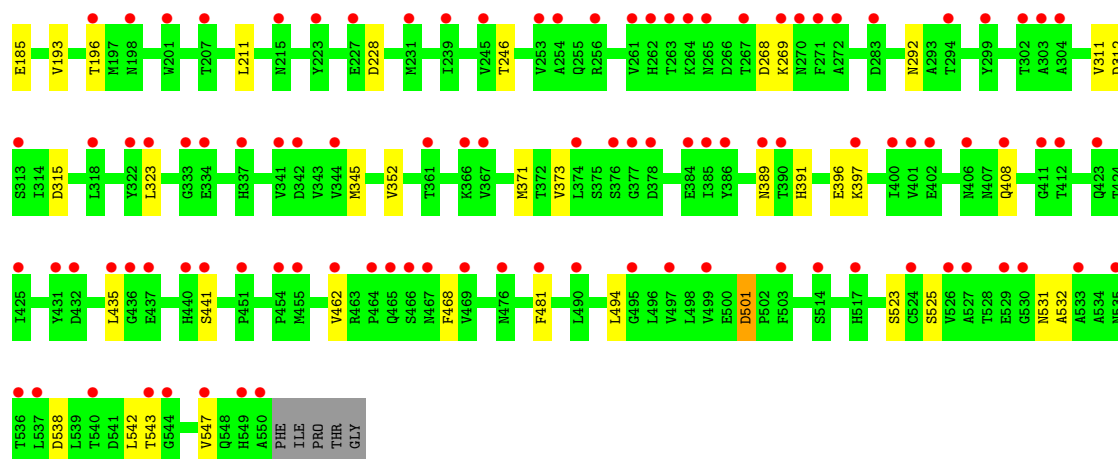


• Molecule 1: Iron transport multicopper oxidase FET3

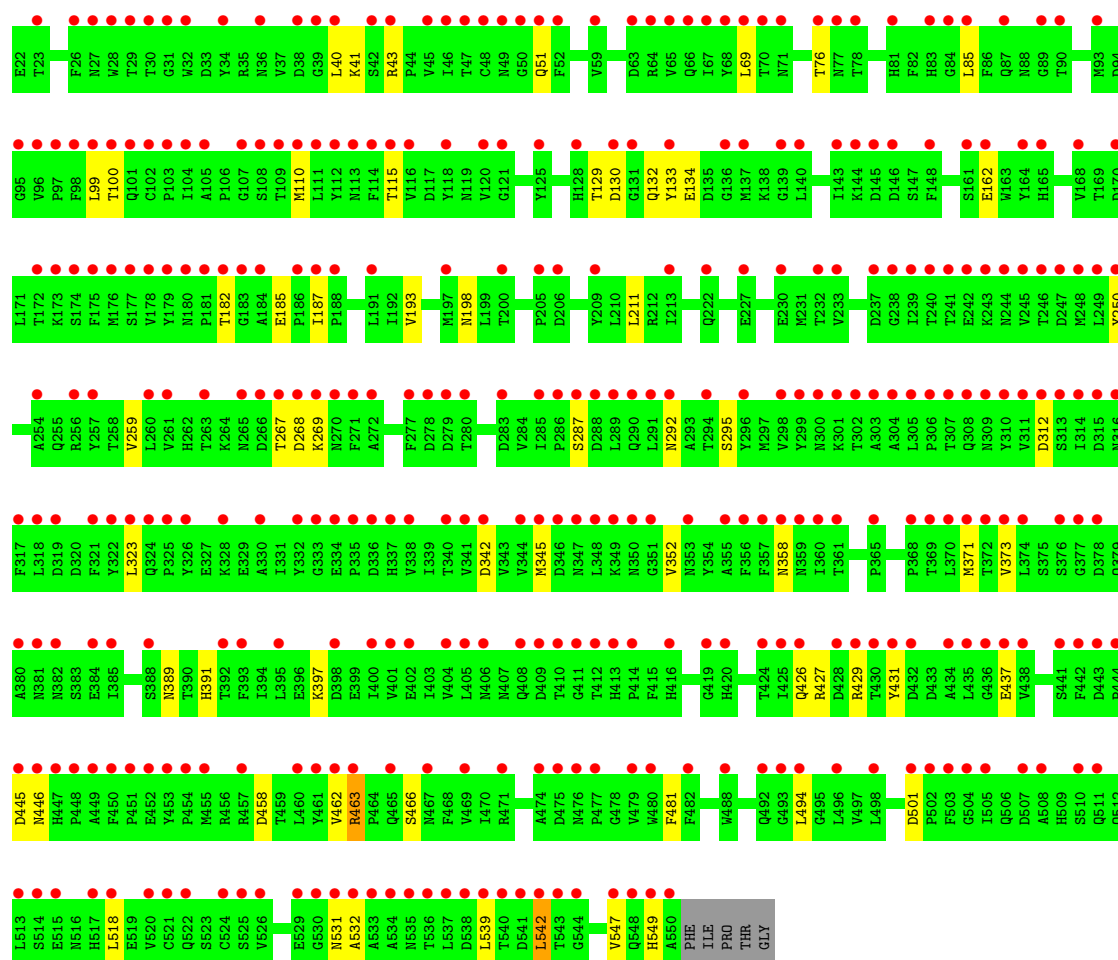
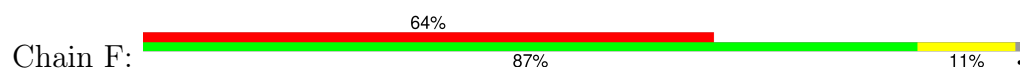


• Molecule 1: Iron transport multicopper oxidase FET3






• Molecule 1: Iron transport multicopper oxidase FET3



• Molecule 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

Chain G:  100%


MAG1  
MAG2  
BMA3  
MAN4  
MAN5

● Molecule 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

Chain J:  100%


MAG1  
MAG2  
BMA3  
MAN4  
MAN5

● Molecule 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

Chain M:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

● Molecule 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

Chain O:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

● Molecule 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

Chain S:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

● Molecule 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

Chain U:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5


● Molecule 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

nose

Chain Y:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

• Molecule 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

Chain a:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

• Molecule 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

Chain d:  40% 60%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

• Molecule 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

Chain f:  20% 80%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

• Molecule 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

Chain i:  20% 80%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

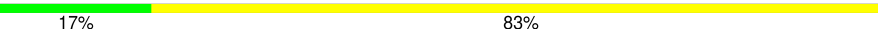
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5



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

Chain H:  17% 83%

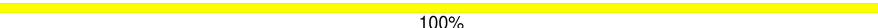
NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain N:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain Z:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain j:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain I:  100%

NAG1  
NAG2

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

Chain P:  50% 50%

NAG1  
NAG2

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

Chain Q:  100%

MAG1  
MAG2

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

Chain V:  100%

MAG1  
MAG2

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

Chain b:  50% 50%

MAG1  
MAG2

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

Chain g:  100%

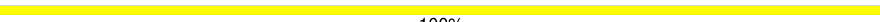
MAG1  
MAG2

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

Chain K:  33% 67%

MAG1  
MAG2  
BMA3

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

Chain L:  100%


MAG1  
MAG2  
BMA3

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

Chain W:  100%


MAG1  
MAG2  
BMA3

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

Chain X:  33% 67%

MAG1  
MAG2  
BMA3

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

Chain c:  33% 67%

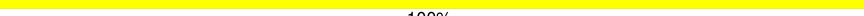
MAG1  
MAG2  
BMA3

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

Chain h:  100%

MAG1  
MAG2  
BMA3

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

Chain l:  100%

MAG1  
MAG2  
BMA3

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

Chain R:  100%

MAG1  
MAG2  
BMA3  
MAN4

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

Chain T:  29% 71%

MAG1	MAG2	BMA3	MAN4	MAN5	MAN6	MAN7
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- Molecule 7:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\alpha$ -D-mannopyranose-(1-6)-[ $\alpha$ -D-mannopyranose-(1-3)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain e:

100%

MAG1	MAG2	BMA3	MAN4	MAN5	MAN6	MAN7
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.53Å 168.53Å 174.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.80) 98.2 (50.00-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.226 , 0.257 0.235 , 0.265	Depositor DCC
$R_{free}$ test set	6726 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 70.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.010 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	27659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3641e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, CU1, NAG, 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	A	0.50	0/4373	0.66	2/5981 (0.0%)
1	B	0.50	0/4373	0.66	3/5981 (0.1%)
1	C	0.55	5/4373 (0.1%)	0.64	2/5981 (0.0%)
1	D	0.51	3/4373 (0.1%)	0.60	2/5981 (0.0%)
1	E	0.44	1/4373 (0.0%)	0.58	1/5981 (0.0%)
1	F	0.99	20/4373 (0.5%)	0.77	11/5981 (0.2%)
All	All	0.61	29/26238 (0.1%)	0.65	21/35886 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	463	ARG	CZ-NH1	40.06	1.85	1.33
1	F	250	TYR	CE2-CZ	15.67	1.58	1.38
1	F	250	TYR	CG-CD2	15.35	1.59	1.39
1	D	515	GLU	CD-OE1	13.48	1.40	1.25
1	F	250	TYR	CE1-CZ	13.27	1.55	1.38
1	F	250	TYR	CG-CD1	11.36	1.53	1.39
1	F	358	ASN	CG-OD1	10.61	1.47	1.24
1	F	445	ASP	CG-OD2	9.77	1.47	1.25
1	F	431	TYR	CE1-CZ	9.44	1.50	1.38
1	C	538	ASP	CG-OD2	9.41	1.47	1.25
1	D	515	GLU	CD-OE2	8.80	1.35	1.25
1	D	35	ARG	CZ-NH1	8.75	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	431	TYR	CG-CD2	7.97	1.49	1.39
1	F	312	ASP	CG-OD2	7.86	1.43	1.25
1	F	431	TYR	CG-CD1	7.78	1.49	1.39
1	F	426	GLN	CD-OE1	7.58	1.40	1.24
1	F	446	ASN	CG-OD1	7.40	1.40	1.24
1	C	379	GLN	CG-CD	7.34	1.68	1.51
1	C	538	ASP	CB-CG	7.01	1.66	1.51
1	F	429	ARG	NE-CZ	6.76	1.41	1.33
1	C	503	PHE	CD2-CE2	6.44	1.52	1.39
1	F	463	ARG	CD-NE	6.35	1.57	1.46
1	F	312	ASP	CG-OD1	6.22	1.39	1.25
1	F	463	ARG	NE-CZ	5.97	1.40	1.33
1	F	445	ASP	CG-OD1	5.95	1.39	1.25
1	F	437	GLU	CD-OE1	5.86	1.32	1.25
1	F	437	GLU	CD-OE2	5.60	1.31	1.25
1	C	379	GLN	CD-NE2	5.29	1.46	1.32
1	E	396	GLU	CD-OE1	5.10	1.31	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	463	ARG	NE-CZ-NH2	-25.91	107.34	120.30
1	F	463	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	F	445	ASP	CB-CG-OD2	-9.31	109.92	118.30
1	F	429	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	F	463	ARG	NH1-CZ-NH2	-8.13	110.46	119.40
1	F	250	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	C	458	ASP	CB-CA-C	-7.02	96.35	110.40
1	F	250	TYR	CD1-CG-CD2	6.90	125.49	117.90
1	D	542	LEU	CA-CB-CG	6.81	130.96	115.30
1	B	542	LEU	CA-CB-CG	6.34	129.88	115.30
1	F	312	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	F	431	TYR	CG-CD2-CE2	-5.88	116.60	121.30
1	F	250	TYR	CG-CD1-CE1	-5.71	116.73	121.30
1	B	462	VAL	CB-CA-C	-5.59	100.79	111.40
1	E	40	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	38	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	D	35	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	99	LEU	CA-CB-CG	5.43	127.79	115.30
1	F	250	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	A	40	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	99	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	463	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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	527/534 (99%)	497 (94%)	23 (4%)	7 (1%)	10	32
1	B	527/534 (99%)	498 (94%)	23 (4%)	6 (1%)	12	37
1	C	527/534 (99%)	495 (94%)	27 (5%)	5 (1%)	14	42
1	D	527/534 (99%)	497 (94%)	22 (4%)	8 (2%)	8	29
1	E	527/534 (99%)	497 (94%)	24 (5%)	6 (1%)	12	37
1	F	527/534 (99%)	498 (94%)	23 (4%)	6 (1%)	12	37
All	All	3162/3204 (99%)	2982 (94%)	142 (4%)	38 (1%)	11	34

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ASP
1	B	531	ASN
1	C	130	ASP
1	D	130	ASP
1	E	130	ASP
1	E	531	ASN
1	F	130	ASP
1	A	531	ASN

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Mol	Chain	Res	Type
1	B	130	ASP
1	B	542	LEU
1	C	531	ASN
1	D	531	ASN
1	D	542	LEU
1	F	531	ASN
1	A	542	LEU
1	C	542	LEU
1	E	542	LEU
1	F	542	LEU
1	A	132	GLN
1	A	501	ASP
1	B	501	ASP
1	B	532	ALA
1	C	501	ASP
1	D	501	ASP
1	E	501	ASP
1	E	532	ALA
1	F	501	ASP
1	B	132	GLN
1	C	532	ALA
1	D	129	THR
1	D	132	GLN
1	D	397	LYS
1	D	532	ALA
1	E	129	THR
1	F	532	ALA
1	A	129	THR
1	A	532	ALA
1	F	129	THR

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	477/481 (99%)	430 (90%)	47 (10%)	6 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	477/481 (99%)	425 (89%)	52 (11%)	5	17
1	C	477/481 (99%)	431 (90%)	46 (10%)	7	22
1	D	477/481 (99%)	425 (89%)	52 (11%)	5	17
1	E	477/481 (99%)	432 (91%)	45 (9%)	7	23
1	F	477/481 (99%)	429 (90%)	48 (10%)	6	20
All	All	2862/2886 (99%)	2572 (90%)	290 (10%)	6	20

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	40	LEU
1	A	42	SER
1	A	43	ARG
1	A	69	LEU
1	A	76	THR
1	A	78	THR
1	A	99	LEU
1	A	100	THR
1	A	115	THR
1	A	144	LYS
1	A	162	GLU
1	A	169	THR
1	A	185	GLU
1	A	193	VAL
1	A	196	THR
1	A	198	ASN
1	A	220	VAL
1	A	246	THR
1	A	259	VAL
1	A	280	THR
1	A	302	THR
1	A	311	VAL
1	A	323	LEU
1	A	345	MET
1	A	352	VAL
1	A	361	THR
1	A	371	MET
1	A	372	THR
1	A	373	VAL

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Mol	Chain	Res	Type
1	A	389	ASN
1	A	390	THR
1	A	391	HIS
1	A	397	LYS
1	A	408	GLN
1	A	433	ASP
1	A	462	VAL
1	A	468	PHE
1	A	481	PHE
1	A	494	LEU
1	A	518	LEU
1	A	537	LEU
1	A	539	LEU
1	A	542	LEU
1	A	547	VAL
1	A	548	GLN
1	A	549	HIS
1	B	33	ASP
1	B	38	ASP
1	B	40	LEU
1	B	42	SER
1	B	43	ARG
1	B	69	LEU
1	B	76	THR
1	B	78	THR
1	B	99	LEU
1	B	100	THR
1	B	120	VAL
1	B	133	TYR
1	B	145	ASP
1	B	162	GLU
1	B	185	GLU
1	B	193	VAL
1	B	196	THR
1	B	198	ASN
1	B	211	LEU
1	B	259	VAL
1	B	264	LYS
1	B	267	THR
1	B	268	ASP
1	B	269	LYS
1	B	292	ASN

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Mol	Chain	Res	Type
1	B	302	THR
1	B	311	VAL
1	B	323	LEU
1	B	345	MET
1	B	352	VAL
1	B	371	MET
1	B	372	THR
1	B	373	VAL
1	B	389	ASN
1	B	391	HIS
1	B	397	LYS
1	B	408	GLN
1	B	433	ASP
1	B	435	LEU
1	B	438	VAL
1	B	462	VAL
1	B	468	PHE
1	B	481	PHE
1	B	494	LEU
1	B	518	LEU
1	B	525	SER
1	B	528	THR
1	B	539	LEU
1	B	542	LEU
1	B	547	VAL
1	B	548	GLN
1	B	549	HIS
1	C	40	LEU
1	C	43	ARG
1	C	69	LEU
1	C	76	THR
1	C	78	THR
1	C	99	LEU
1	C	100	THR
1	C	101	GLN
1	C	110	MET
1	C	117	ASP
1	C	132	GLN
1	C	133	TYR
1	C	145	ASP
1	C	162	GLU
1	C	178	VAL

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Mol	Chain	Res	Type
1	C	185	GLU
1	C	193	VAL
1	C	196	THR
1	C	198	ASN
1	C	211	LEU
1	C	259	VAL
1	C	264	LYS
1	C	268	ASP
1	C	269	LYS
1	C	302	THR
1	C	311	VAL
1	C	323	LEU
1	C	345	MET
1	C	352	VAL
1	C	371	MET
1	C	372	THR
1	C	373	VAL
1	C	389	ASN
1	C	391	HIS
1	C	408	GLN
1	C	433	ASP
1	C	446	ASN
1	C	462	VAL
1	C	468	PHE
1	C	481	PHE
1	C	494	LEU
1	C	518	LEU
1	C	528	THR
1	C	539	LEU
1	C	547	VAL
1	C	549	HIS
1	D	40	LEU
1	D	43	ARG
1	D	64	ARG
1	D	69	LEU
1	D	76	THR
1	D	78	THR
1	D	100	THR
1	D	101	GLN
1	D	110	MET
1	D	115	THR
1	D	132	GLN

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Mol	Chain	Res	Type
1	D	133	TYR
1	D	134	GLU
1	D	145	ASP
1	D	147	SER
1	D	162	GLU
1	D	182	THR
1	D	185	GLU
1	D	193	VAL
1	D	198	ASN
1	D	211	LEU
1	D	241	THR
1	D	246	THR
1	D	259	VAL
1	D	264	LYS
1	D	268	ASP
1	D	269	LYS
1	D	311	VAL
1	D	323	LEU
1	D	345	MET
1	D	371	MET
1	D	372	THR
1	D	373	VAL
1	D	389	ASN
1	D	390	THR
1	D	391	HIS
1	D	397	LYS
1	D	430	THR
1	D	433	ASP
1	D	435	LEU
1	D	462	VAL
1	D	466	SER
1	D	468	PHE
1	D	481	PHE
1	D	491	LEU
1	D	494	LEU
1	D	518	LEU
1	D	539	LEU
1	D	542	LEU
1	D	547	VAL
1	D	548	GLN
1	D	549	HIS
1	E	33	ASP

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Mol	Chain	Res	Type
1	E	40	LEU
1	E	43	ARG
1	E	69	LEU
1	E	76	THR
1	E	78	THR
1	E	99	LEU
1	E	101	GLN
1	E	133	TYR
1	E	145	ASP
1	E	146	ASP
1	E	162	GLU
1	E	185	GLU
1	E	193	VAL
1	E	196	THR
1	E	211	LEU
1	E	228	ASP
1	E	246	THR
1	E	268	ASP
1	E	269	LYS
1	E	292	ASN
1	E	311	VAL
1	E	312	ASP
1	E	315	ASP
1	E	323	LEU
1	E	345	MET
1	E	352	VAL
1	E	371	MET
1	E	373	VAL
1	E	389	ASN
1	E	391	HIS
1	E	397	LYS
1	E	408	GLN
1	E	435	LEU
1	E	441	SER
1	E	462	VAL
1	E	468	PHE
1	E	481	PHE
1	E	494	LEU
1	E	501	ASP
1	E	523	SER
1	E	525	SER
1	E	538	ASP

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Mol	Chain	Res	Type
1	E	543	THR
1	E	547	VAL
1	F	40	LEU
1	F	41	LYS
1	F	43	ARG
1	F	51	GLN
1	F	69	LEU
1	F	76	THR
1	F	85	LEU
1	F	99	LEU
1	F	100	THR
1	F	110	MET
1	F	115	THR
1	F	132	GLN
1	F	133	TYR
1	F	134	GLU
1	F	162	GLU
1	F	182	THR
1	F	185	GLU
1	F	187	ILE
1	F	193	VAL
1	F	198	ASN
1	F	211	LEU
1	F	259	VAL
1	F	267	THR
1	F	268	ASP
1	F	269	LYS
1	F	287	SER
1	F	292	ASN
1	F	295	SER
1	F	323	LEU
1	F	342	ASP
1	F	345	MET
1	F	352	VAL
1	F	371	MET
1	F	373	VAL
1	F	389	ASN
1	F	391	HIS
1	F	397	LYS
1	F	427	ARG
1	F	458	ASP
1	F	462	VAL

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Mol	Chain	Res	Type
1	F	466	SER
1	F	481	PHE
1	F	494	LEU
1	F	518	LEU
1	F	539	LEU
1	F	542	LEU
1	F	547	VAL
1	F	549	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	255	GLN
1	B	222	GLN
1	B	255	GLN
1	B	275	GLN
1	B	324	GLN
1	B	517	HIS
1	C	51	GLN
1	C	66	GLN
1	C	517	HIS
1	D	324	GLN
1	E	195	ASN
1	E	382	ASN
1	E	549	HIS
1	F	309	ASN

### 5.3.3 RNA [i](#)

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](#)

135 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	G	1	2,1	14,14,15	0.71	0	17,19,21	1.37	3 (17%)
2	NAG	G	2	2	14,14,15	0.53	0	17,19,21	1.07	2 (11%)
2	BMA	G	3	2	11,11,12	0.81	0	15,15,17	1.71	2 (13%)
2	MAN	G	4	2	11,11,12	0.58	0	15,15,17	1.33	1 (6%)
2	MAN	G	5	2	11,11,12	0.73	0	15,15,17	2.09	2 (13%)
3	NAG	H	1	3,1	14,14,15	0.78	0	17,19,21	2.11	4 (23%)
3	NAG	H	2	3	14,14,15	0.63	0	17,19,21	0.85	0
3	BMA	H	3	3	11,11,12	0.73	0	15,15,17	1.82	3 (20%)
3	MAN	H	4	3	11,11,12	0.60	0	15,15,17	1.03	1 (6%)
3	MAN	H	5	3	11,11,12	0.71	0	15,15,17	1.09	1 (6%)
3	MAN	H	6	3	11,11,12	0.67	0	15,15,17	1.54	3 (20%)
4	NAG	I	1	4,1	14,14,15	0.63	0	17,19,21	2.17	5 (29%)
4	NAG	I	2	4	14,14,15	1.09	1 (7%)	17,19,21	1.32	2 (11%)
2	NAG	J	1	2,1	14,14,15	0.72	0	17,19,21	1.73	4 (23%)
2	NAG	J	2	2	14,14,15	0.62	0	17,19,21	2.05	3 (17%)
2	BMA	J	3	2	11,11,12	0.71	0	15,15,17	1.30	2 (13%)
2	MAN	J	4	2	11,11,12	0.72	0	15,15,17	1.59	2 (13%)
2	MAN	J	5	2	11,11,12	0.69	0	15,15,17	1.74	1 (6%)
5	NAG	K	1	1,5	14,14,15	0.51	0	17,19,21	2.04	3 (17%)
5	NAG	K	2	5	14,14,15	0.47	0	17,19,21	0.94	0
5	BMA	K	3	5	11,11,12	0.92	0	15,15,17	1.07	1 (6%)
5	NAG	L	1	1,5	14,14,15	0.49	0	17,19,21	1.88	5 (29%)
5	NAG	L	2	5	14,14,15	0.54	0	17,19,21	1.14	2 (11%)
5	BMA	L	3	5	11,11,12	0.63	0	15,15,17	1.92	2 (13%)
2	NAG	M	1	2,1	14,14,15	0.70	0	17,19,21	0.99	1 (5%)
2	NAG	M	2	2	14,14,15	0.60	0	17,19,21	1.10	1 (5%)
2	BMA	M	3	2	11,11,12	0.75	0	15,15,17	0.92	1 (6%)
2	MAN	M	4	2	11,11,12	0.70	0	15,15,17	2.65	5 (33%)
2	MAN	M	5	2	11,11,12	0.45	0	15,15,17	1.34	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	N	1	3,1	14,14,15	0.69	0	17,19,21	1.53	4 (23%)
3	NAG	N	2	3	14,14,15	0.57	0	17,19,21	1.04	1 (5%)
3	BMA	N	3	3	11,11,12	0.75	0	15,15,17	1.37	2 (13%)
3	MAN	N	4	3	11,11,12	0.61	0	15,15,17	2.08	2 (13%)
3	MAN	N	5	3	11,11,12	0.54	0	15,15,17	1.22	1 (6%)
3	MAN	N	6	3	11,11,12	0.55	0	15,15,17	1.06	1 (6%)
2	NAG	O	1	2,1	14,14,15	0.56	0	17,19,21	1.68	3 (17%)
2	NAG	O	2	2	14,14,15	0.74	0	17,19,21	1.28	3 (17%)
2	BMA	O	3	2	11,11,12	0.75	0	15,15,17	1.51	4 (26%)
2	MAN	O	4	2	11,11,12	0.61	0	15,15,17	1.93	5 (33%)
2	MAN	O	5	2	11,11,12	1.67	2 (18%)	15,15,17	2.23	4 (26%)
4	NAG	P	1	4,1	14,14,15	0.56	0	17,19,21	0.96	0
4	NAG	P	2	4	14,14,15	0.50	0	17,19,21	0.98	1 (5%)
4	NAG	Q	1	4,1	14,14,15	0.47	0	17,19,21	1.87	4 (23%)
4	NAG	Q	2	4	14,14,15	0.48	0	17,19,21	1.18	1 (5%)
6	NAG	R	1	1,6	14,14,15	0.73	0	17,19,21	1.61	2 (11%)
6	NAG	R	2	6	14,14,15	0.62	0	17,19,21	1.21	2 (11%)
6	BMA	R	3	6	11,11,12	0.54	0	15,15,17	0.90	1 (6%)
6	MAN	R	4	6	11,11,12	0.53	0	15,15,17	2.04	4 (26%)
2	NAG	S	1	2,1	14,14,15	0.74	0	17,19,21	1.37	5 (29%)
2	NAG	S	2	2	14,14,15	0.61	0	17,19,21	1.36	3 (17%)
2	BMA	S	3	2	11,11,12	0.56	0	15,15,17	1.77	3 (20%)
2	MAN	S	4	2	11,11,12	0.56	0	15,15,17	1.36	2 (13%)
2	MAN	S	5	2	11,11,12	0.62	0	15,15,17	1.18	1 (6%)
7	NAG	T	1	1,7	14,14,15	0.91	1 (7%)	17,19,21	2.10	7 (41%)
7	NAG	T	2	7	14,14,15	0.44	0	17,19,21	0.94	0
7	BMA	T	3	7	11,11,12	0.58	0	15,15,17	1.80	3 (20%)
7	MAN	T	4	7	11,11,12	0.60	0	15,15,17	1.28	1 (6%)
7	MAN	T	5	7	11,11,12	0.70	0	15,15,17	0.75	0
7	MAN	T	6	7	11,11,12	0.55	0	15,15,17	2.10	1 (6%)
7	MAN	T	7	7	11,11,12	0.75	0	15,15,17	1.72	3 (20%)
2	NAG	U	1	2,1	14,14,15	0.48	0	17,19,21	1.98	2 (11%)
2	NAG	U	2	2	14,14,15	0.74	1 (7%)	17,19,21	1.30	4 (23%)
2	BMA	U	3	2	11,11,12	0.68	0	15,15,17	1.16	2 (13%)
2	MAN	U	4	2	11,11,12	0.77	0	15,15,17	1.43	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	U	5	2	11,11,12	0.59	0	15,15,17	1.61	2 (13%)
4	NAG	V	1	4,1	14,14,15	0.51	0	17,19,21	1.16	1 (5%)
4	NAG	V	2	4	14,14,15	1.20	2 (14%)	17,19,21	1.46	2 (11%)
5	NAG	W	1	1,5	14,14,15	1.99	3 (21%)	17,19,21	0.92	0
5	NAG	W	2	5	14,14,15	1.77	3 (21%)	17,19,21	2.25	4 (23%)
5	BMA	W	3	5	11,11,12	2.48	1 (9%)	15,15,17	1.70	4 (26%)
5	NAG	X	1	1,5	14,14,15	0.49	0	17,19,21	1.80	5 (29%)
5	NAG	X	2	5	14,14,15	0.42	0	17,19,21	1.21	2 (11%)
5	BMA	X	3	5	11,11,12	0.66	0	15,15,17	0.88	0
2	NAG	Y	1	2,1	14,14,15	0.54	0	17,19,21	0.95	1 (5%)
2	NAG	Y	2	2	14,14,15	0.58	0	17,19,21	1.23	3 (17%)
2	BMA	Y	3	2	11,11,12	0.57	0	15,15,17	1.29	2 (13%)
2	MAN	Y	4	2	11,11,12	0.57	0	15,15,17	1.25	1 (6%)
2	MAN	Y	5	2	11,11,12	0.62	0	15,15,17	1.08	1 (6%)
3	NAG	Z	1	3,1	14,14,15	0.62	0	17,19,21	1.77	3 (17%)
3	NAG	Z	2	3	14,14,15	0.69	0	17,19,21	0.96	1 (5%)
3	BMA	Z	3	3	11,11,12	0.70	0	15,15,17	1.75	4 (26%)
3	MAN	Z	4	3	11,11,12	0.59	0	15,15,17	1.09	1 (6%)
3	MAN	Z	5	3	11,11,12	0.62	0	15,15,17	0.91	1 (6%)
3	MAN	Z	6	3	11,11,12	1.07	1 (9%)	15,15,17	1.83	3 (20%)
2	NAG	a	1	2,1	14,14,15	0.40	0	17,19,21	1.23	1 (5%)
2	NAG	a	2	2	14,14,15	0.57	0	17,19,21	1.01	2 (11%)
2	BMA	a	3	2	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
2	MAN	a	4	2	11,11,12	0.54	0	15,15,17	1.46	1 (6%)
2	MAN	a	5	2	11,11,12	0.60	0	15,15,17	1.53	2 (13%)
4	NAG	b	1	4,1	14,14,15	1.38	2 (14%)	17,19,21	1.66	3 (17%)
4	NAG	b	2	4	14,14,15	0.50	0	17,19,21	0.69	0
5	NAG	c	1	1,5	14,14,15	0.53	0	17,19,21	1.38	2 (11%)
5	NAG	c	2	5	14,14,15	0.54	0	17,19,21	0.82	0
5	BMA	c	3	5	11,11,12	0.54	0	15,15,17	0.88	1 (6%)
2	NAG	d	1	2,1	14,14,15	0.60	0	17,19,21	1.11	1 (5%)
2	NAG	d	2	2	14,14,15	0.54	0	17,19,21	0.82	0
2	BMA	d	3	2	11,11,12	0.76	0	15,15,17	1.91	4 (26%)
2	MAN	d	4	2	11,11,12	0.59	0	15,15,17	0.61	0
2	MAN	d	5	2	11,11,12	0.54	0	15,15,17	1.38	1 (6%)
7	NAG	e	1	1,7	14,14,15	0.56	0	17,19,21	1.08	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	e	2	7	14,14,15	0.49	0	17,19,21	1.26	2 (11%)
7	BMA	e	3	7	11,11,12	0.61	0	15,15,17	1.41	4 (26%)
7	MAN	e	4	7	11,11,12	0.62	0	15,15,17	1.42	3 (20%)
7	MAN	e	5	7	11,11,12	0.55	0	15,15,17	0.98	1 (6%)
7	MAN	e	6	7	11,11,12	0.70	0	15,15,17	1.54	2 (13%)
7	MAN	e	7	7	11,11,12	0.52	0	15,15,17	1.52	1 (6%)
2	NAG	f	1	2,1	14,14,15	0.53	0	17,19,21	1.45	3 (17%)
2	NAG	f	2	2	14,14,15	0.50	0	17,19,21	0.95	0
2	BMA	f	3	2	11,11,12	0.62	0	15,15,17	0.97	1 (6%)
2	MAN	f	4	2	11,11,12	0.56	0	15,15,17	1.34	1 (6%)
2	MAN	f	5	2	11,11,12	0.56	0	15,15,17	1.37	1 (6%)
4	NAG	g	1	4,1	14,14,15	0.55	0	17,19,21	1.22	2 (11%)
4	NAG	g	2	4	14,14,15	0.59	0	17,19,21	1.05	1 (5%)
5	NAG	h	1	1,5	14,14,15	0.60	0	17,19,21	1.68	4 (23%)
5	NAG	h	2	5	14,14,15	0.61	0	17,19,21	1.11	1 (5%)
5	BMA	h	3	5	11,11,12	0.86	0	15,15,17	1.78	3 (20%)
2	NAG	i	1	2,1	14,14,15	0.60	0	17,19,21	0.96	0
2	NAG	i	2	2	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
2	BMA	i	3	2	11,11,12	0.64	0	15,15,17	1.31	3 (20%)
2	MAN	i	4	2	11,11,12	0.64	0	15,15,17	1.79	3 (20%)
2	MAN	i	5	2	11,11,12	0.49	0	15,15,17	1.57	1 (6%)
3	NAG	j	1	3,1	14,14,15	0.63	0	17,19,21	1.49	3 (17%)
3	NAG	j	2	3	14,14,15	0.75	0	17,19,21	1.50	2 (11%)
3	BMA	j	3	3	11,11,12	0.78	0	15,15,17	0.90	2 (13%)
3	MAN	j	4	3	11,11,12	1.19	1 (9%)	15,15,17	1.42	2 (13%)
3	MAN	j	5	3	11,11,12	0.94	1 (9%)	15,15,17	0.92	1 (6%)
3	MAN	j	6	3	11,11,12	0.58	0	15,15,17	1.55	2 (13%)
2	NAG	k	1	2,1	14,14,15	0.52	0	17,19,21	1.24	1 (5%)
2	NAG	k	2	2	14,14,15	0.55	0	17,19,21	1.07	2 (11%)
2	BMA	k	3	2	11,11,12	0.69	0	15,15,17	1.22	1 (6%)
2	MAN	k	4	2	11,11,12	0.66	0	15,15,17	0.87	1 (6%)
2	MAN	k	5	2	11,11,12	1.57	1 (9%)	15,15,17	1.70	2 (13%)
5	NAG	l	1	1,5	14,14,15	0.51	0	17,19,21	1.11	1 (5%)
5	NAG	l	2	5	14,14,15	0.57	0	17,19,21	1.52	4 (23%)
5	BMA	l	3	5	11,11,12	1.84	2 (18%)	15,15,17	0.98	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	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
2	MAN	G	5	2	-	2/2/19/22	1/1/1/1
3	NAG	H	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	MAN	H	4	3	-	2/2/19/22	0/1/1/1
3	MAN	H	5	3	-	0/2/19/22	0/1/1/1
3	MAN	H	6	3	-	2/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	5/6/23/26	0/1/1/1
2	BMA	J	3	2	-	2/2/19/22	0/1/1/1
2	MAN	J	4	2	-	2/2/19/22	0/1/1/1
2	MAN	J	5	2	-	1/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	5/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	NAG	L	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/6/23/26	0/1/1/1
2	BMA	M	3	2	-	0/2/19/22	0/1/1/1
2	MAN	M	4	2	-	1/2/19/22	0/1/1/1
2	MAN	M	5	2	-	1/2/19/22	1/1/1/1
3	NAG	N	1	3,1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	MAN	N	4	3	-	1/2/19/22	0/1/1/1
3	MAN	N	5	3	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	X	2	5	-	0/6/23/26	0/1/1/1
5	BMA	X	3	5	-	2/2/19/22	0/1/1/1
2	NAG	Y	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	2/6/23/26	0/1/1/1
2	BMA	Y	3	2	-	2/2/19/22	0/1/1/1
2	MAN	Y	4	2	-	2/2/19/22	0/1/1/1
2	MAN	Y	5	2	-	1/2/19/22	0/1/1/1
3	NAG	Z	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Z	3	3	-	0/2/19/22	0/1/1/1
3	MAN	Z	4	3	-	0/2/19/22	0/1/1/1
3	MAN	Z	5	3	-	2/2/19/22	0/1/1/1
3	MAN	Z	6	3	-	2/2/19/22	0/1/1/1
2	NAG	a	1	2,1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	a	2	2	-	2/6/23/26	0/1/1/1
2	BMA	a	3	2	-	2/2/19/22	0/1/1/1
2	MAN	a	4	2	-	1/2/19/22	0/1/1/1
2	MAN	a	5	2	-	2/2/19/22	0/1/1/1
4	NAG	b	1	4,1	1/1/5/7	6/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
5	NAG	c	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	BMA	c	3	5	-	0/2/19/22	0/1/1/1
2	NAG	d	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	4/6/23/26	0/1/1/1
2	BMA	d	3	2	-	2/2/19/22	0/1/1/1
2	MAN	d	4	2	-	2/2/19/22	0/1/1/1
2	MAN	d	5	2	-	2/2/19/22	0/1/1/1
7	NAG	e	1	1,7	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	e	2	7	-	4/6/23/26	0/1/1/1
7	BMA	e	3	7	-	2/2/19/22	0/1/1/1
7	MAN	e	4	7	-	2/2/19/22	0/1/1/1
7	MAN	e	5	7	-	0/2/19/22	0/1/1/1
7	MAN	e	6	7	-	2/2/19/22	0/1/1/1
7	MAN	e	7	7	-	2/2/19/22	0/1/1/1
2	NAG	f	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1

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

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	3	BMA	O6-C6	7.78	1.75	1.42
2	k	5	MAN	O6-C6	4.89	1.63	1.42
5	l	3	BMA	O6-C6	4.81	1.62	1.42
5	W	1	NAG	C8-C7	4.59	1.60	1.50
5	W	2	NAG	C8-C7	4.54	1.60	1.50
5	W	1	NAG	O7-C7	4.47	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	1	NAG	C8-C7	4.04	1.58	1.50
2	O	5	MAN	O6-C6	3.83	1.58	1.42
3	j	4	MAN	O6-C6	3.54	1.57	1.42
5	W	2	NAG	O7-C7	3.40	1.30	1.23
2	O	5	MAN	C2-C3	3.17	1.57	1.52
5	W	1	NAG	O6-C6	3.11	1.55	1.42
5	W	2	NAG	C7-N2	2.91	1.43	1.34
3	Z	6	MAN	O6-C6	2.83	1.54	1.42
4	V	2	NAG	O7-C7	2.61	1.29	1.23
3	j	5	MAN	O6-C6	2.61	1.53	1.42
4	V	2	NAG	C8-C7	2.60	1.55	1.50
4	b	1	NAG	O7-C7	2.54	1.28	1.23
4	I	2	NAG	C1-C2	2.52	1.55	1.52
5	l	3	BMA	C4-C3	2.52	1.58	1.52
7	T	1	NAG	O5-C1	-2.13	1.40	1.43
2	U	2	NAG	O7-C7	2.02	1.27	1.23

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	5	MAN	C1-O5-C5	7.27	121.93	112.19
2	M	4	MAN	C1-O5-C5	7.15	121.77	112.19
2	O	5	MAN	C1-O5-C5	6.84	121.35	112.19
2	U	1	NAG	C1-O5-C5	6.74	121.22	112.19
7	T	6	MAN	C1-O5-C5	6.61	121.04	112.19
2	J	2	NAG	C2-N2-C7	6.51	131.63	122.90
3	N	4	MAN	C1-O5-C5	6.43	120.80	112.19
5	W	2	NAG	C2-N2-C7	-6.34	114.40	122.90
2	J	5	MAN	C1-O5-C5	6.17	120.46	112.19
7	e	7	MAN	C1-O5-C5	5.58	119.67	112.19
2	k	5	MAN	C1-O5-C5	5.50	119.56	112.19
6	R	4	MAN	C1-O5-C5	5.45	119.48	112.19
5	L	3	BMA	C1-O5-C5	5.30	119.29	112.19
2	i	5	MAN	C1-O5-C5	5.30	119.29	112.19
3	H	1	NAG	C2-N2-C7	5.22	129.90	122.90
4	Q	1	NAG	C2-N2-C7	5.13	129.77	122.90
7	T	1	NAG	O5-C1-C2	-5.10	103.40	111.29
5	L	1	NAG	C1-O5-C5	4.95	118.81	112.19
3	Z	1	NAG	C2-N2-C7	4.91	129.48	122.90
2	M	4	MAN	C3-C4-C5	4.85	119.03	110.23
2	O	1	NAG	C1-O5-C5	4.84	118.67	112.19
5	K	1	NAG	C2-N2-C7	4.84	129.38	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	5	MAN	C1-O5-C5	4.81	118.63	112.19
3	Z	6	MAN	C1-C2-C3	4.81	116.64	109.64
2	d	3	BMA	C1-C2-C3	4.76	116.58	109.64
4	b	1	NAG	C2-N2-C7	4.75	129.27	122.90
4	I	1	NAG	O5-C1-C2	-4.69	104.04	111.29
2	i	4	MAN	C1-O5-C5	4.65	118.42	112.19
6	R	1	NAG	O5-C1-C2	-4.63	104.13	111.29
3	j	6	MAN	C1-O5-C5	4.54	118.27	112.19
5	W	2	NAG	O7-C7-N2	-4.54	113.95	121.98
4	I	1	NAG	C4-C3-C2	4.54	117.67	111.02
7	T	4	MAN	C1-O5-C5	4.52	118.25	112.19
5	X	1	NAG	O5-C1-C2	-4.47	104.38	111.29
2	S	3	BMA	C1-C2-C3	4.44	116.11	109.64
3	j	4	MAN	C1-O5-C5	4.42	118.11	112.19
2	J	1	NAG	C1-O5-C5	4.36	118.03	112.19
5	K	1	NAG	C1-C2-N2	4.34	117.28	110.43
5	L	3	BMA	C1-C2-C3	4.34	115.96	109.64
3	Z	3	BMA	O3-C3-C2	4.28	118.79	110.05
2	G	3	BMA	C3-C4-C5	4.28	117.99	110.23
3	H	1	NAG	O5-C1-C2	-4.25	104.72	111.29
2	a	4	MAN	C1-C2-C3	-4.22	103.50	109.64
2	U	5	MAN	C1-O5-C5	4.17	117.78	112.19
2	f	5	MAN	C1-O5-C5	4.16	117.76	112.19
3	j	1	NAG	O5-C1-C2	-4.16	104.86	111.29
5	h	1	NAG	C1-O5-C5	4.15	117.75	112.19
2	a	1	NAG	C1-O5-C5	4.15	117.75	112.19
4	V	2	NAG	C4-C3-C2	4.14	117.09	111.02
7	T	3	BMA	O3-C3-C2	4.09	118.40	110.05
2	a	5	MAN	C1-O5-C5	4.06	117.63	112.19
3	H	3	BMA	O3-C3-C2	4.05	118.32	110.05
2	G	4	MAN	C1-O5-C5	4.03	117.59	112.19
2	f	4	MAN	C1-O5-C5	4.02	117.57	112.19
2	O	4	MAN	C1-C2-C3	-4.01	103.81	109.64
7	T	7	MAN	C3-C4-C5	3.98	117.45	110.23
3	N	1	NAG	O5-C1-C2	-3.93	105.21	111.29
2	k	1	NAG	C1-O5-C5	3.93	117.45	112.19
4	I	2	NAG	C2-N2-C7	3.83	128.03	122.90
7	e	6	MAN	C3-C4-C5	3.79	117.10	110.23
2	i	4	MAN	C3-C4-C5	3.79	117.10	110.23
3	j	2	NAG	C4-C3-C2	3.78	116.56	111.02
5	c	1	NAG	O5-C1-C2	-3.75	105.50	111.29
2	J	4	MAN	C1-C2-C3	-3.74	104.20	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	h	3	BMA	C3-C4-C5	3.69	116.93	110.23
2	i	2	NAG	C1-O5-C5	3.67	117.11	112.19
3	N	4	MAN	C3-C4-C5	3.63	116.81	110.23
3	N	5	MAN	C1-O5-C5	3.60	117.01	112.19
2	O	3	BMA	O3-C3-C2	-3.60	102.71	110.05
4	Q	1	NAG	O5-C1-C2	-3.59	105.73	111.29
5	W	3	BMA	O6-C6-C5	-3.58	99.13	111.33
2	S	3	BMA	O5-C5-C6	3.57	114.61	107.66
2	U	4	MAN	C1-C2-C3	-3.53	104.50	109.64
7	T	3	BMA	C1-O5-C5	3.51	116.89	112.19
5	X	2	NAG	C1-O5-C5	3.48	116.85	112.19
3	H	3	BMA	O3-C3-C4	3.47	118.56	110.38
5	K	1	NAG	O5-C1-C2	-3.46	105.94	111.29
3	N	3	BMA	O3-C3-C2	3.45	117.10	110.05
2	J	3	BMA	C1-C2-C3	3.44	114.66	109.64
2	O	1	NAG	C2-N2-C7	-3.42	118.31	122.90
6	R	4	MAN	C1-C2-C3	3.42	114.62	109.64
2	Y	4	MAN	C3-C4-C5	3.41	116.42	110.23
5	h	3	BMA	C1-C2-C3	3.39	114.58	109.64
3	H	6	MAN	C3-C4-C5	3.37	116.34	110.23
2	M	5	MAN	C1-O5-C5	3.36	116.69	112.19
7	e	4	MAN	C1-O5-C5	3.35	116.68	112.19
5	h	3	BMA	C2-C3-C4	3.35	116.75	110.86
5	W	3	BMA	C1-C2-C3	3.32	114.48	109.64
2	G	3	BMA	C1-C2-C3	3.30	114.45	109.64
2	S	2	NAG	O4-C4-C3	-3.28	102.65	110.38
4	I	1	NAG	C2-N2-C7	3.27	127.29	122.90
2	d	3	BMA	C2-C3-C4	3.27	116.61	110.86
3	j	6	MAN	C1-C2-C3	3.26	114.40	109.64
4	b	1	NAG	C1-C2-N2	3.24	115.55	110.43
4	V	1	NAG	C1-O5-C5	3.24	116.53	112.19
2	f	1	NAG	C4-C3-C2	3.22	115.74	111.02
2	O	4	MAN	C1-O5-C5	3.21	116.49	112.19
3	j	2	NAG	C2-N2-C7	3.21	127.20	122.90
3	Z	4	MAN	C1-O5-C5	3.21	116.49	112.19
3	Z	1	NAG	C1-O5-C5	3.20	116.47	112.19
2	S	4	MAN	C3-C4-C5	3.18	115.99	110.23
5	l	2	NAG	C1-O5-C5	3.17	116.44	112.19
5	X	1	NAG	C8-C7-N2	3.17	121.38	116.12
2	J	2	NAG	C8-C7-N2	3.17	121.38	116.12
2	k	3	BMA	C3-C4-C5	3.17	115.97	110.23
3	H	3	BMA	C3-C4-C5	-3.14	104.53	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	1	NAG	C2-N2-C7	3.13	127.09	122.90
2	U	5	MAN	C3-C4-C5	3.11	115.87	110.23
2	a	5	MAN	C3-C4-C5	3.09	115.84	110.23
2	M	2	NAG	C1-O5-C5	3.09	116.33	112.19
2	S	2	NAG	C2-N2-C7	-3.09	118.76	122.90
3	H	5	MAN	C1-O5-C5	3.06	116.29	112.19
2	Y	2	NAG	C1-O5-C5	3.04	116.26	112.19
2	O	5	MAN	C3-C4-C5	3.02	115.72	110.23
5	W	2	NAG	O7-C7-C8	3.01	127.42	122.05
2	O	4	MAN	C3-C4-C5	3.00	115.68	110.23
2	G	1	NAG	C1-O5-C5	2.98	116.18	112.19
2	d	3	BMA	C3-C4-C5	2.98	115.63	110.23
3	Z	6	MAN	C2-C3-C4	2.97	116.08	110.86
2	U	1	NAG	C2-N2-C7	-2.97	118.92	122.90
2	J	2	NAG	O5-C1-C2	-2.94	106.75	111.29
4	Q	2	NAG	C1-O5-C5	2.93	116.12	112.19
5	h	1	NAG	C2-N2-C7	2.92	126.82	122.90
7	T	7	MAN	O5-C1-C2	-2.92	103.82	110.79
2	U	2	NAG	C1-C2-N2	2.92	115.03	110.43
5	L	1	NAG	C3-C4-C5	-2.91	104.95	110.23
3	H	6	MAN	C1-O5-C5	2.90	116.08	112.19
4	g	2	NAG	C4-C3-C2	2.90	115.27	111.02
7	e	6	MAN	C1-O5-C5	2.88	116.04	112.19
7	e	2	NAG	C1-O5-C5	2.86	116.02	112.19
2	J	1	NAG	O5-C5-C6	2.85	113.20	107.66
2	M	4	MAN	O5-C5-C4	2.84	117.74	110.83
5	l	2	NAG	O5-C1-C2	-2.84	106.90	111.29
7	e	5	MAN	C1-O5-C5	2.83	115.98	112.19
7	e	3	BMA	O3-C3-C2	2.81	115.79	110.05
5	K	3	BMA	C1-C2-C3	2.80	113.72	109.64
3	Z	3	BMA	C3-C4-C5	-2.80	105.15	110.23
3	H	4	MAN	C1-O5-C5	2.80	115.94	112.19
5	X	1	NAG	C3-C4-C5	-2.77	105.22	110.23
7	T	1	NAG	C4-C3-C2	2.76	115.06	111.02
5	l	2	NAG	C2-N2-C7	-2.75	119.21	122.90
3	j	5	MAN	C1-O5-C5	2.74	115.86	112.19
7	T	3	BMA	O3-C3-C4	2.73	116.82	110.38
2	i	3	BMA	C1-O5-C5	2.72	115.83	112.19
2	S	5	MAN	C1-C2-C3	-2.70	105.71	109.64
2	k	2	NAG	C4-C3-C2	2.70	114.97	111.02
5	h	2	NAG	C4-C3-C2	2.70	114.97	111.02
2	J	4	MAN	O2-C2-C1	2.69	115.39	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	4	MAN	O5-C1-C2	2.69	117.20	110.79
2	a	3	BMA	O3-C3-C2	-2.68	104.58	110.05
4	I	1	NAG	C8-C7-N2	2.68	120.56	116.12
4	b	1	NAG	O5-C1-C2	-2.66	107.18	111.29
5	L	1	NAG	O5-C1-C2	-2.66	107.18	111.29
7	T	1	NAG	C3-C4-C5	-2.64	105.45	110.23
5	l	1	NAG	C1-O5-C5	2.64	115.72	112.19
2	d	1	NAG	O5-C1-C2	-2.64	107.21	111.29
5	L	2	NAG	C1-O5-C5	2.63	115.72	112.19
2	a	3	BMA	O3-C3-C4	2.63	116.57	110.38
3	Z	6	MAN	C1-O5-C5	2.62	115.70	112.19
3	Z	3	BMA	O3-C3-C4	2.62	116.55	110.38
3	Z	5	MAN	C1-O5-C5	2.61	115.69	112.19
7	e	3	BMA	C1-C2-C3	-2.61	105.85	109.64
2	O	2	NAG	O7-C7-N2	2.60	126.58	121.98
6	R	4	MAN	C3-C4-C5	2.60	114.95	110.23
7	e	4	MAN	C1-C2-C3	2.58	113.40	109.64
2	i	3	BMA	C1-C2-C3	2.58	113.40	109.64
4	Q	1	NAG	C1-O5-C5	2.58	115.64	112.19
2	M	4	MAN	C2-C3-C4	2.58	115.39	110.86
2	G	2	NAG	C1-O5-C5	2.58	115.64	112.19
5	h	1	NAG	C8-C7-N2	2.57	120.38	116.12
2	O	2	NAG	C4-C3-C2	2.57	114.78	111.02
2	i	3	BMA	C3-C4-C5	2.57	114.89	110.23
3	j	1	NAG	C2-N2-C7	2.56	126.33	122.90
5	X	1	NAG	O7-C7-C8	-2.56	117.50	122.05
3	H	6	MAN	O5-C1-C2	-2.55	104.71	110.79
2	O	5	MAN	C1-C2-C3	2.55	113.35	109.64
2	J	3	BMA	O3-C3-C2	-2.54	104.86	110.05
3	Z	3	BMA	C1-O5-C5	2.54	115.59	112.19
2	Y	3	BMA	C1-C2-C3	2.52	113.32	109.64
2	S	1	NAG	O7-C7-C8	-2.52	117.57	122.05
2	U	3	BMA	O3-C3-C2	-2.51	104.92	110.05
7	T	1	NAG	C6-C5-C4	2.50	119.15	113.02
2	O	4	MAN	O2-C2-C1	2.49	114.93	109.22
2	J	1	NAG	C1-C2-N2	2.49	114.36	110.43
6	R	4	MAN	O5-C5-C6	2.49	112.50	107.66
2	k	5	MAN	C1-C2-C3	2.48	113.25	109.64
3	j	1	NAG	C8-C7-N2	2.47	120.22	116.12
2	Y	3	BMA	O5-C5-C6	2.46	112.45	107.66
6	R	2	NAG	O4-C4-C3	-2.46	104.58	110.38
5	W	3	BMA	C2-C3-C4	2.45	115.16	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	5	MAN	C2-C3-C4	-2.44	106.57	110.86
2	a	2	NAG	O5-C1-C2	-2.44	107.52	111.29
2	U	3	BMA	C1-C2-C3	2.44	113.19	109.64
2	S	1	NAG	O5-C1-C2	-2.43	107.53	111.29
2	O	3	BMA	O3-C3-C4	2.43	116.11	110.38
2	O	1	NAG	O5-C5-C6	2.42	112.37	107.66
3	H	1	NAG	C8-C7-N2	2.41	120.12	116.12
2	Y	1	NAG	O5-C1-C2	-2.41	107.56	111.29
7	T	1	NAG	C8-C7-N2	2.39	120.08	116.12
2	f	1	NAG	C3-C4-C5	2.38	114.56	110.23
7	e	1	NAG	O5-C1-C2	-2.36	107.64	111.29
2	f	1	NAG	C1-C2-N2	-2.35	106.72	110.43
7	e	3	BMA	O3-C3-C4	2.35	115.92	110.38
4	g	1	NAG	C2-N2-C7	2.34	126.04	122.90
2	U	2	NAG	O5-C1-C2	-2.34	107.67	111.29
2	G	1	NAG	C6-C5-C4	-2.34	107.28	113.02
5	l	2	NAG	C4-C3-C2	-2.34	107.59	111.02
2	U	2	NAG	C1-O5-C5	2.32	115.30	112.19
3	N	1	NAG	C2-N2-C7	2.32	126.01	122.90
2	G	5	MAN	O5-C5-C6	2.31	112.16	107.66
7	e	4	MAN	C3-C4-C5	2.31	114.42	110.23
5	c	1	NAG	C8-C7-N2	2.30	119.93	116.12
5	X	1	NAG	C1-O5-C5	2.30	115.26	112.19
4	V	2	NAG	C3-C4-C5	2.30	114.39	110.23
2	k	2	NAG	C2-N2-C7	2.29	125.97	122.90
2	G	2	NAG	O5-C1-C2	-2.29	107.75	111.29
2	S	1	NAG	C4-C3-C2	2.28	114.36	111.02
2	S	2	NAG	C1-O5-C5	2.28	115.25	112.19
7	T	1	NAG	O5-C5-C4	-2.28	105.28	110.83
4	g	1	NAG	C1-C2-N2	2.28	114.02	110.43
5	W	3	BMA	C1-O5-C5	2.27	115.23	112.19
2	M	5	MAN	O5-C5-C6	2.26	112.07	107.66
6	R	2	NAG	C1-O5-C5	-2.26	109.16	112.19
2	Y	5	MAN	C3-C4-C5	2.26	114.33	110.23
3	N	6	MAN	C1-O5-C5	2.26	115.21	112.19
3	Z	2	NAG	C1-O5-C5	2.25	115.21	112.19
4	P	2	NAG	C3-C4-C5	2.22	114.27	110.23
5	L	1	NAG	O7-C7-C8	-2.22	118.09	122.05
3	Z	1	NAG	O5-C1-C2	-2.22	107.86	111.29
5	h	1	NAG	O7-C7-C8	-2.22	118.11	122.05
5	X	2	NAG	O5-C1-C2	-2.22	107.86	111.29
2	O	5	MAN	O5-C5-C4	2.21	116.21	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	3	BMA	C1-O5-C5	2.21	115.15	112.19
4	Q	1	NAG	C1-C2-N2	2.20	113.89	110.43
2	J	1	NAG	C2-N2-C7	-2.20	119.96	122.90
2	U	2	NAG	C2-N2-C7	2.20	125.84	122.90
2	i	4	MAN	O5-C5-C4	2.19	116.14	110.83
2	Y	2	NAG	O4-C4-C3	-2.18	105.25	110.38
5	L	2	NAG	O5-C1-C2	-2.16	107.96	111.29
7	T	7	MAN	C2-C3-C4	2.15	114.65	110.86
3	N	3	BMA	O3-C3-C4	2.15	115.45	110.38
3	j	3	BMA	C1-O5-C5	2.14	115.06	112.19
6	R	3	BMA	C1-C2-C3	2.14	112.76	109.64
2	O	3	BMA	O5-C5-C6	2.13	111.81	107.66
2	d	3	BMA	O5-C5-C6	2.13	111.81	107.66
2	k	4	MAN	O5-C5-C6	2.12	111.79	107.66
4	I	1	NAG	O4-C4-C3	-2.12	105.38	110.38
2	O	3	BMA	C3-C4-C5	2.09	114.03	110.23
2	U	4	MAN	O2-C2-C1	2.09	114.01	109.22
2	a	2	NAG	C3-C4-C5	2.09	114.02	110.23
3	j	4	MAN	C3-C4-C5	2.08	114.00	110.23
3	N	1	NAG	C8-C7-N2	2.07	119.56	116.12
2	G	1	NAG	O5-C1-C2	-2.07	108.08	111.29
5	c	3	BMA	C1-O5-C5	2.06	114.95	112.19
7	e	2	NAG	C3-C4-C5	2.06	113.97	110.23
3	H	1	NAG	C3-C4-C5	-2.06	106.50	110.23
6	R	1	NAG	C2-N2-C7	-2.06	120.15	122.90
2	O	2	NAG	C8-C7-N2	-2.05	112.72	116.12
3	N	1	NAG	C1-O5-C5	2.05	114.93	112.19
2	f	3	BMA	O3-C3-C2	-2.05	105.87	110.05
4	I	2	NAG	C4-C3-C2	2.05	114.02	111.02
3	j	3	BMA	C1-C2-C3	2.04	112.61	109.64
5	W	2	NAG	C1-O5-C5	2.04	114.92	112.19
2	O	4	MAN	O3-C3-C2	-2.04	105.90	110.05
3	N	2	NAG	C2-N2-C7	2.03	125.62	122.90
2	U	4	MAN	O5-C5-C6	2.03	111.61	107.66
2	S	1	NAG	C1-C2-N2	2.03	113.63	110.43
2	S	4	MAN	C1-C2-C3	-2.03	106.69	109.64
2	S	3	BMA	O3-C3-C2	-2.03	105.92	110.05
7	e	3	BMA	C1-O5-C5	2.03	114.90	112.19
2	S	1	NAG	O4-C4-C3	-2.01	105.63	110.38
2	M	1	NAG	O7-C7-C8	-2.01	118.47	122.05
2	Y	2	NAG	C4-C3-C2	2.01	113.96	111.02
5	L	1	NAG	O4-C4-C5	2.00	114.25	109.32



All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	a	1	NAG	C1
2	f	1	NAG	C1
3	H	1	NAG	C1
3	N	1	NAG	C1
3	Z	1	NAG	C1
3	j	1	NAG	C1
4	b	1	NAG	C1
5	L	1	NAG	C1
5	X	1	NAG	C1
5	c	1	NAG	C1
5	h	1	NAG	C1
5	l	1	NAG	C1
6	R	1	NAG	C1
7	T	1	NAG	C1
7	e	1	NAG	C1

All (250) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	U	1	NAG	C8-C7-N2-C2
2	U	1	NAG	O7-C7-N2-C2
2	U	2	NAG	C1-C2-N2-C7
2	U	2	NAG	C8-C7-N2-C2
2	U	2	NAG	O7-C7-N2-C2
2	a	1	NAG	C8-C7-N2-C2
2	a	1	NAG	O7-C7-N2-C2
2	d	2	NAG	C8-C7-N2-C2
2	d	2	NAG	O7-C7-N2-C2
2	f	2	NAG	C8-C7-N2-C2
2	f	2	NAG	O7-C7-N2-C2
2	k	1	NAG	C8-C7-N2-C2
2	k	1	NAG	O7-C7-N2-C2
2	k	2	NAG	C3-C2-N2-C7
2	k	2	NAG	C8-C7-N2-C2
2	k	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	N	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	N	1	NAG	O7-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
3	Z	1	NAG	C8-C7-N2-C2
3	Z	1	NAG	O7-C7-N2-C2
3	j	2	NAG	C8-C7-N2-C2
3	j	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	Q	1	NAG	C3-C2-N2-C7
4	Q	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
4	b	1	NAG	C8-C7-N2-C2
4	b	1	NAG	O7-C7-N2-C2
4	g	1	NAG	C1-C2-N2-C7
4	g	1	NAG	C8-C7-N2-C2
4	g	1	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	L	1	NAG	C8-C7-N2-C2
5	L	1	NAG	O7-C7-N2-C2
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
5	c	1	NAG	C8-C7-N2-C2
5	c	1	NAG	O7-C7-N2-C2
5	l	2	NAG	C8-C7-N2-C2
5	l	2	NAG	O7-C7-N2-C2
6	R	1	NAG	C8-C7-N2-C2
6	R	1	NAG	O7-C7-N2-C2
7	e	1	NAG	C8-C7-N2-C2
7	e	1	NAG	O7-C7-N2-C2
7	e	2	NAG	C8-C7-N2-C2
7	e	2	NAG	O7-C7-N2-C2
2	Y	2	NAG	C8-C7-N2-C2
2	Y	2	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	j	1	NAG	C8-C7-N2-C2
2	J	4	MAN	C4-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	U	1	NAG	O5-C5-C6-O6
2	U	4	MAN	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
7	e	3	BMA	O5-C5-C6-O6
2	U	4	MAN	C4-C5-C6-O6
5	X	3	BMA	C4-C5-C6-O6
2	J	4	MAN	O5-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
2	i	2	NAG	O5-C5-C6-O6
3	Z	6	MAN	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	X	3	BMA	O5-C5-C6-O6
3	Z	2	NAG	C8-C7-N2-C2
3	Z	2	NAG	O7-C7-N2-C2
2	G	4	MAN	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	d	4	MAN	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
7	e	4	MAN	O5-C5-C6-O6
2	S	3	BMA	O5-C5-C6-O6
2	a	5	MAN	O5-C5-C6-O6
2	k	1	NAG	O5-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
2	O	3	BMA	O5-C5-C6-O6
2	d	5	MAN	O5-C5-C6-O6
2	f	1	NAG	O5-C5-C6-O6
3	j	3	BMA	O5-C5-C6-O6
5	h	3	BMA	O5-C5-C6-O6
2	a	2	NAG	C4-C5-C6-O6
2	O	5	MAN	O5-C5-C6-O6
2	Y	3	BMA	O5-C5-C6-O6
7	T	7	MAN	O5-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	i	2	NAG	C4-C5-C6-O6
3	j	1	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
7	e	3	BMA	C4-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
2	Y	4	MAN	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
3	H	6	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	U	1	NAG	C4-C5-C6-O6
2	f	5	MAN	C4-C5-C6-O6
3	Z	6	MAN	C4-C5-C6-O6
3	N	6	MAN	O5-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
2	d	3	BMA	O5-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6
2	k	4	MAN	O5-C5-C6-O6
7	T	6	MAN	O5-C5-C6-O6
2	J	3	BMA	C4-C5-C6-O6
2	d	5	MAN	C4-C5-C6-O6
5	h	2	NAG	C4-C5-C6-O6
7	e	6	MAN	O5-C5-C6-O6
2	d	3	BMA	C4-C5-C6-O6
3	N	6	MAN	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
3	j	3	BMA	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
3	j	1	NAG	O7-C7-N2-C2
7	T	1	NAG	C8-C7-N2-C2
2	S	3	BMA	C4-C5-C6-O6
2	Y	3	BMA	C4-C5-C6-O6
2	Y	4	MAN	C4-C5-C6-O6
2	d	4	MAN	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
2	O	5	MAN	C4-C5-C6-O6
2	i	4	MAN	O5-C5-C6-O6
3	j	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
3	H	6	MAN	C4-C5-C6-O6
2	k	4	MAN	C4-C5-C6-O6
3	j	2	NAG	C4-C5-C6-O6
5	l	3	BMA	C4-C5-C6-O6
7	T	6	MAN	C4-C5-C6-O6
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
5	h	1	NAG	C8-C7-N2-C2
5	h	1	NAG	O7-C7-N2-C2
7	T	1	NAG	O7-C7-N2-C2
2	U	5	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	L	3	BMA	C4-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
7	e	7	MAN	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	j	4	MAN	C4-C5-C6-O6
2	G	5	MAN	O5-C5-C6-O6
2	a	4	MAN	O5-C5-C6-O6
3	j	6	MAN	O5-C5-C6-O6
2	O	3	BMA	C4-C5-C6-O6
3	Z	5	MAN	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
2	f	5	MAN	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
3	j	4	MAN	O5-C5-C6-O6
2	G	4	MAN	C4-C5-C6-O6
5	h	3	BMA	C4-C5-C6-O6
7	e	4	MAN	C4-C5-C6-O6
7	e	2	NAG	C4-C5-C6-O6
2	a	3	BMA	O5-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
2	k	1	NAG	C4-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
2	U	3	BMA	O5-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	a	5	MAN	C4-C5-C6-O6
2	f	3	BMA	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	M	4	MAN	O5-C5-C6-O6
5	l	3	BMA	O5-C5-C6-O6
3	j	2	NAG	O5-C5-C6-O6
3	Z	5	MAN	O5-C5-C6-O6
7	T	7	MAN	C4-C5-C6-O6
2	i	2	NAG	C8-C7-N2-C2
4	P	2	NAG	C8-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
2	O	4	MAN	O5-C5-C6-O6
2	S	5	MAN	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	f	1	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
2	M	5	MAN	O5-C5-C6-O6
4	P	2	NAG	O7-C7-N2-C2
2	Y	5	MAN	O5-C5-C6-O6
2	J	5	MAN	O5-C5-C6-O6
2	U	5	MAN	O5-C5-C6-O6
5	W	1	NAG	O7-C7-N2-C2
2	i	5	MAN	O5-C5-C6-O6
7	e	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
3	N	4	MAN	O5-C5-C6-O6
5	l	1	NAG	C8-C7-N2-C2
2	J	2	NAG	C3-C2-N2-C7
2	f	4	MAN	O5-C5-C6-O6
2	S	4	MAN	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
2	i	2	NAG	O7-C7-N2-C2
5	c	2	NAG	C8-C7-N2-C2
2	G	3	BMA	O5-C5-C6-O6
2	f	3	BMA	O5-C5-C6-O6
2	k	2	NAG	C4-C5-C6-O6
4	g	1	NAG	C4-C5-C6-O6
7	e	1	NAG	C4-C5-C6-O6
4	g	1	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
5	l	1	NAG	O7-C7-N2-C2
5	c	2	NAG	O7-C7-N2-C2
2	a	1	NAG	C4-C5-C6-O6
5	K	2	NAG	C8-C7-N2-C2
4	P	1	NAG	C4-C5-C6-O6
3	H	4	MAN	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
3	H	4	MAN	O5-C5-C6-O6
3	j	2	NAG	C3-C2-N2-C7
4	b	1	NAG	C3-C2-N2-C7
5	K	1	NAG	C3-C2-N2-C7
7	e	7	MAN	C4-C5-C6-O6
2	a	3	BMA	C4-C5-C6-O6
3	j	5	MAN	C4-C5-C6-O6
3	j	6	MAN	C4-C5-C6-O6

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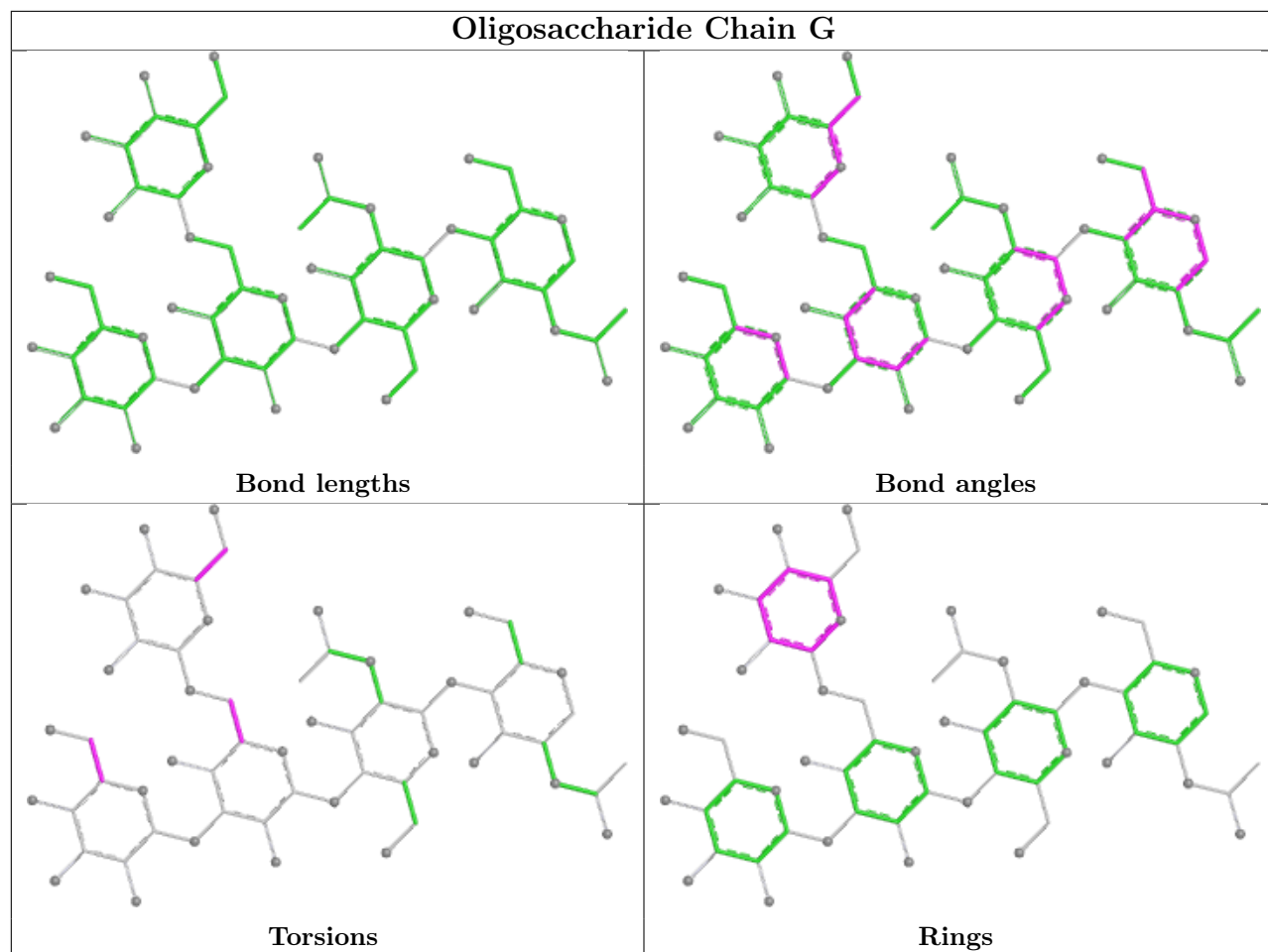
Mol	Chain	Res	Type	Atoms
5	K	2	NAG	O7-C7-N2-C2
2	i	2	NAG	C1-C2-N2-C7
4	b	1	NAG	C1-C2-N2-C7
2	G	5	MAN	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
6	R	4	MAN	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	d	2	NAG	C4-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
2	O	4	MAN	C4-C5-C6-O6
7	e	6	MAN	C4-C5-C6-O6
2	U	3	BMA	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
2	k	2	NAG	O5-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6

All (5) ring outliers are listed below:

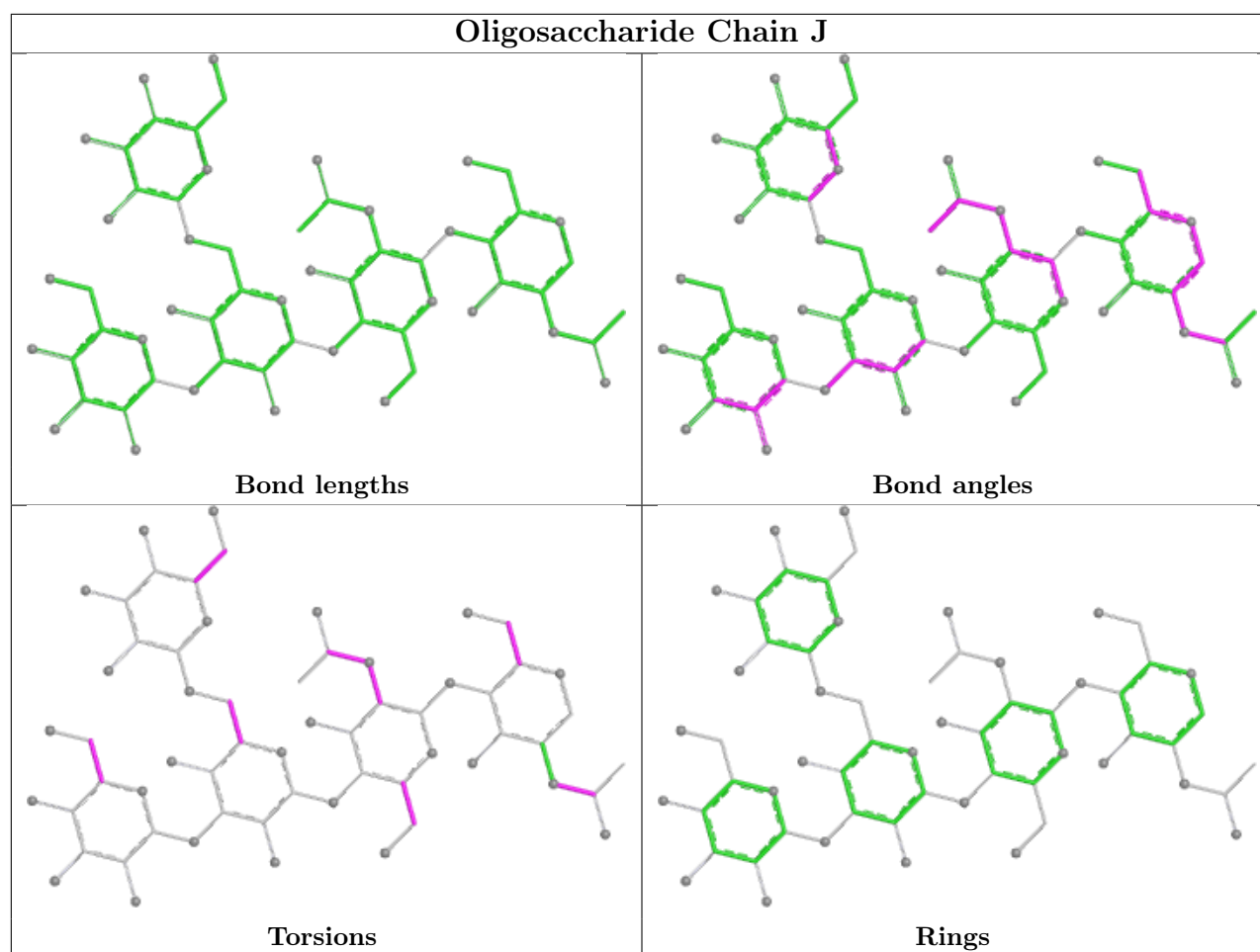
Mol	Chain	Res	Type	Atoms
2	G	5	MAN	C1-C2-C3-C4-C5-O5
2	k	5	MAN	C1-C2-C3-C4-C5-O5
2	f	4	MAN	C1-C2-C3-C4-C5-O5
2	i	5	MAN	C1-C2-C3-C4-C5-O5
2	M	5	MAN	C1-C2-C3-C4-C5-O5

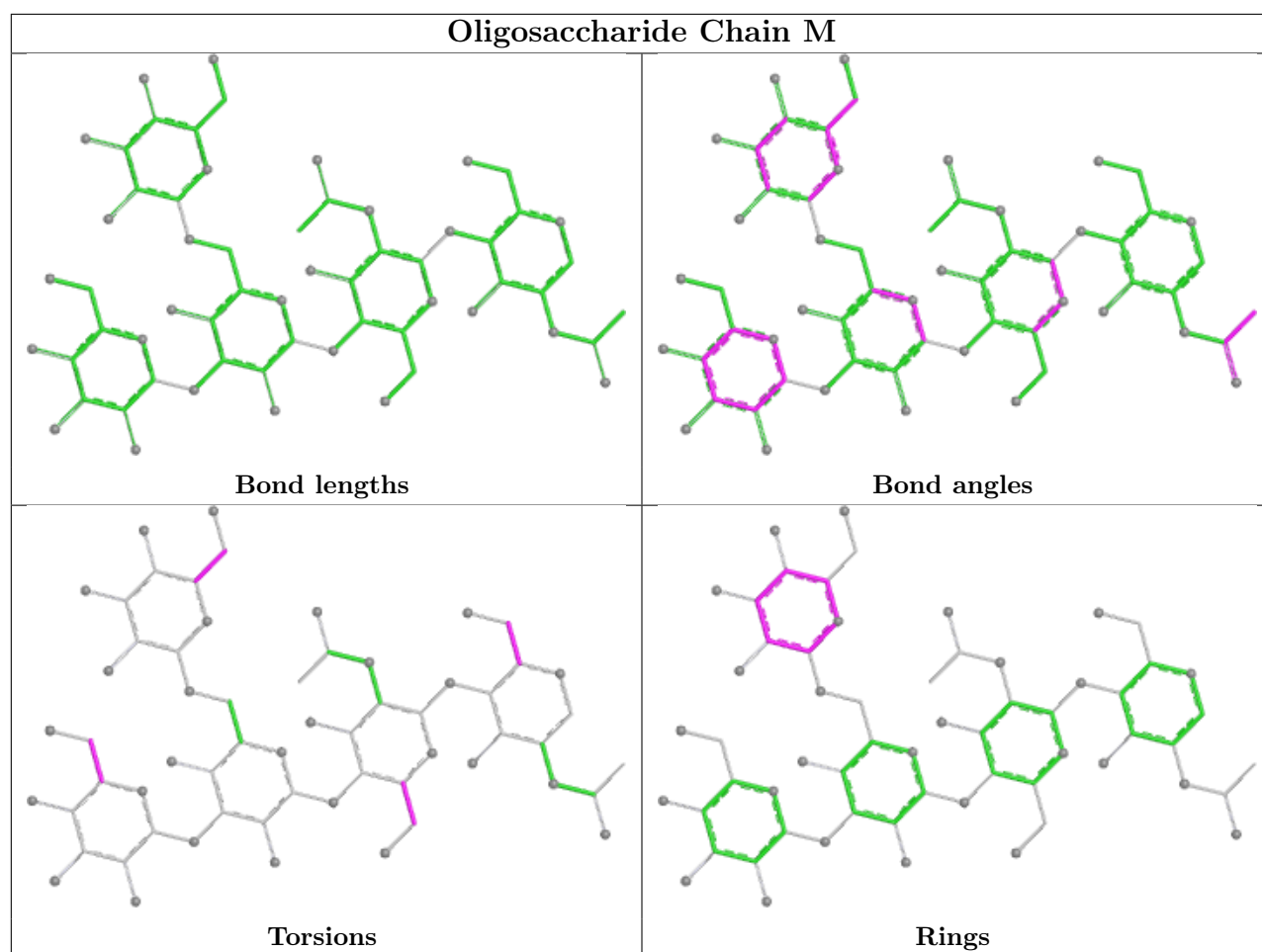
No monomer is involved in short contacts.

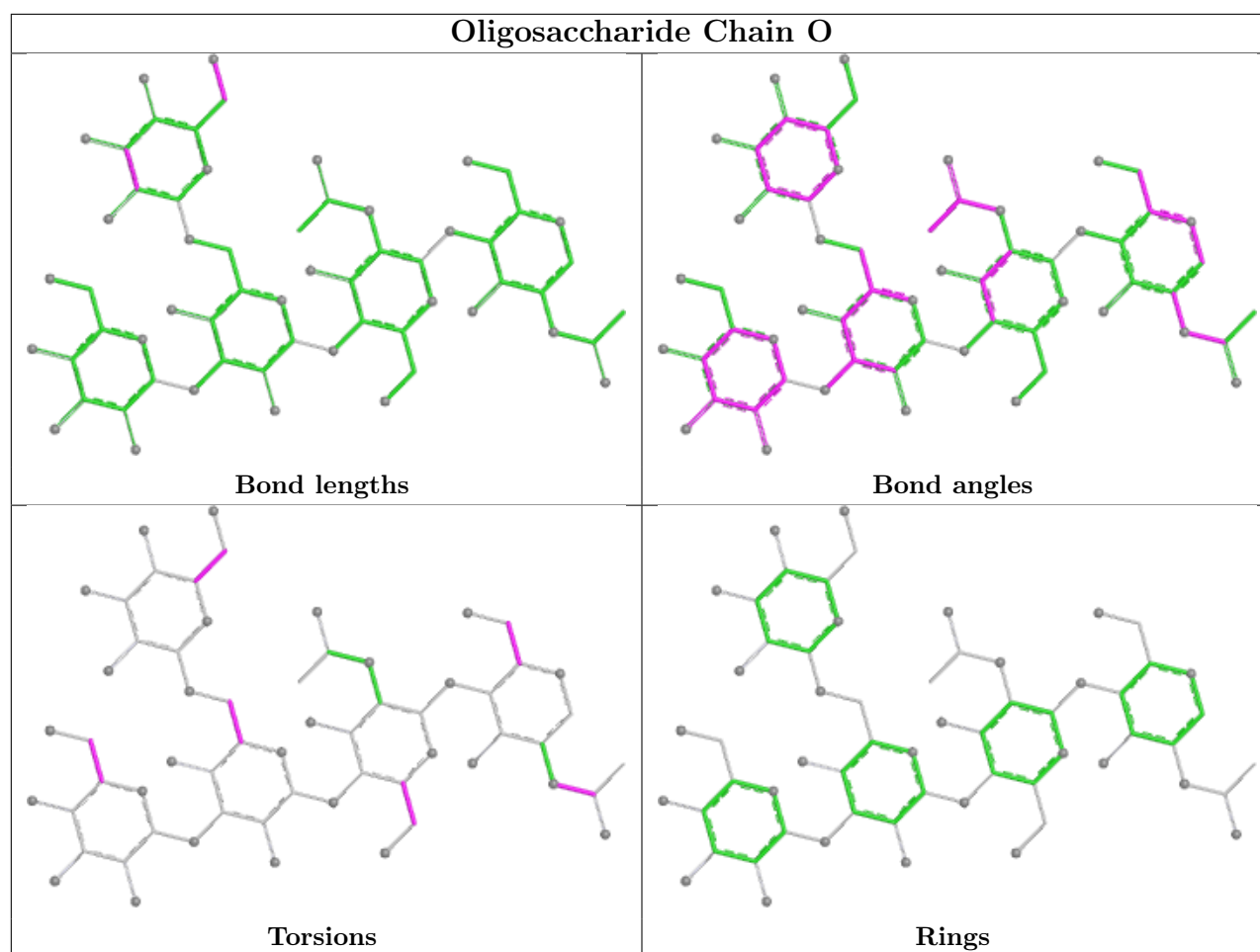
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

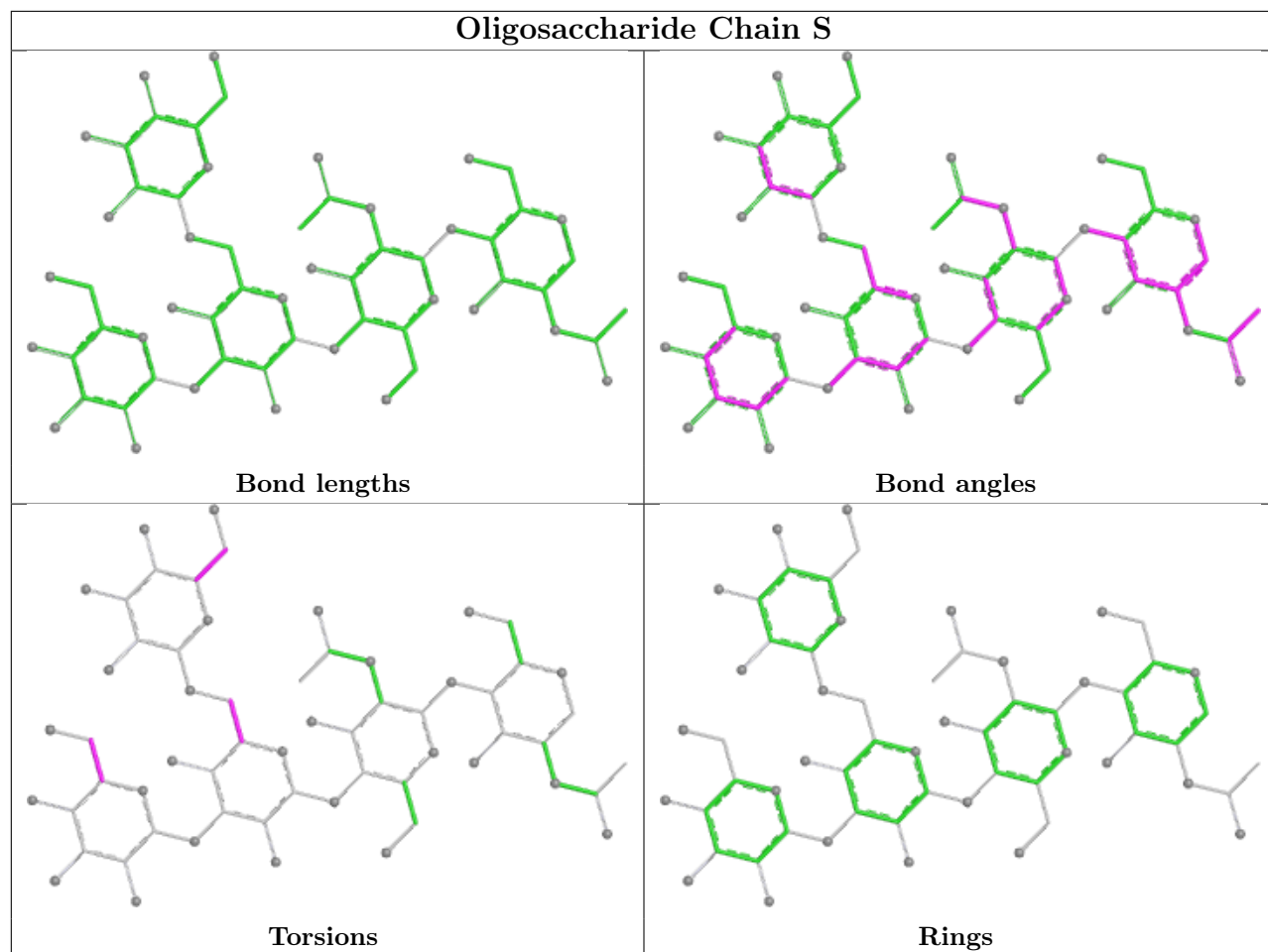


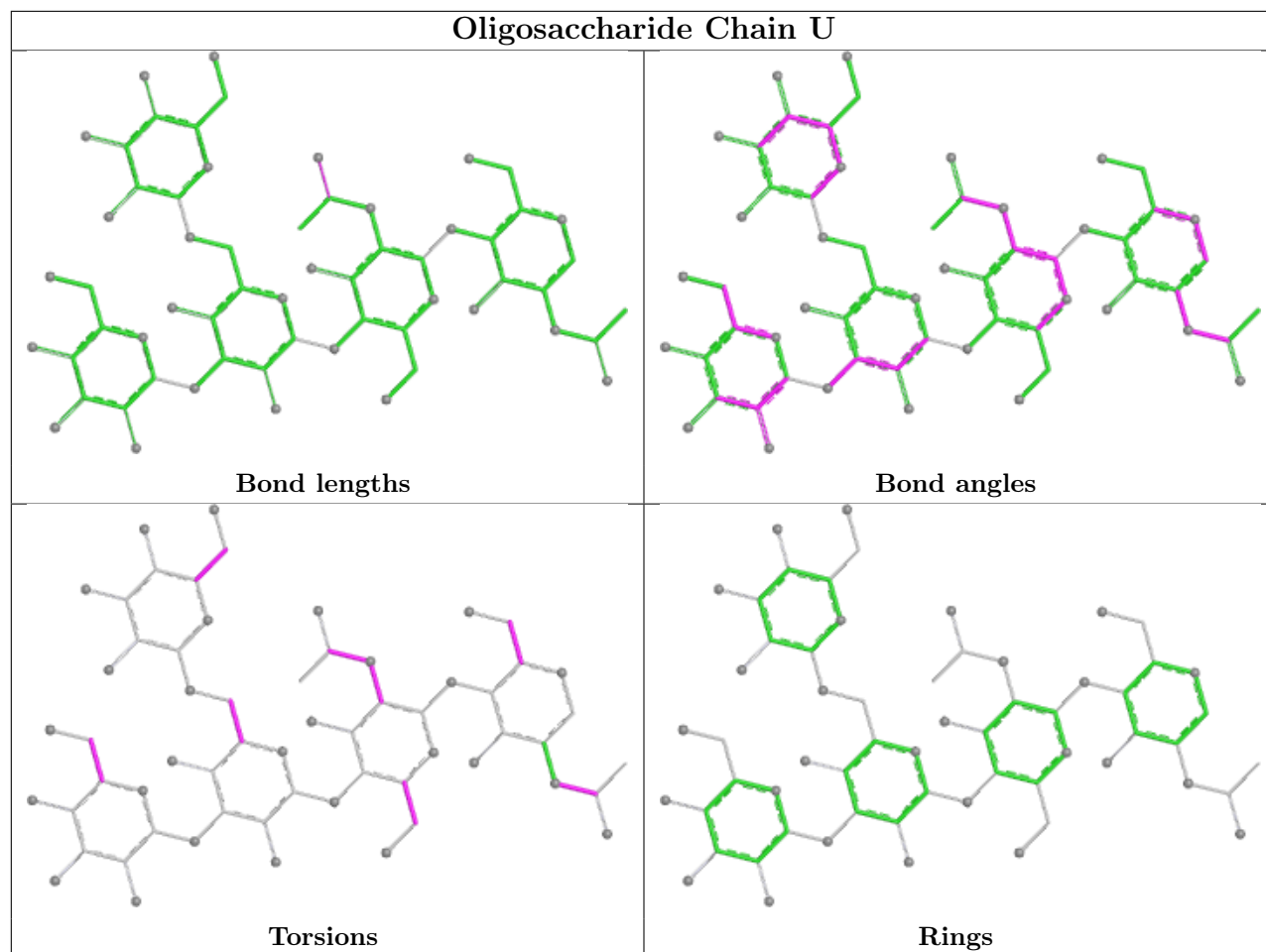


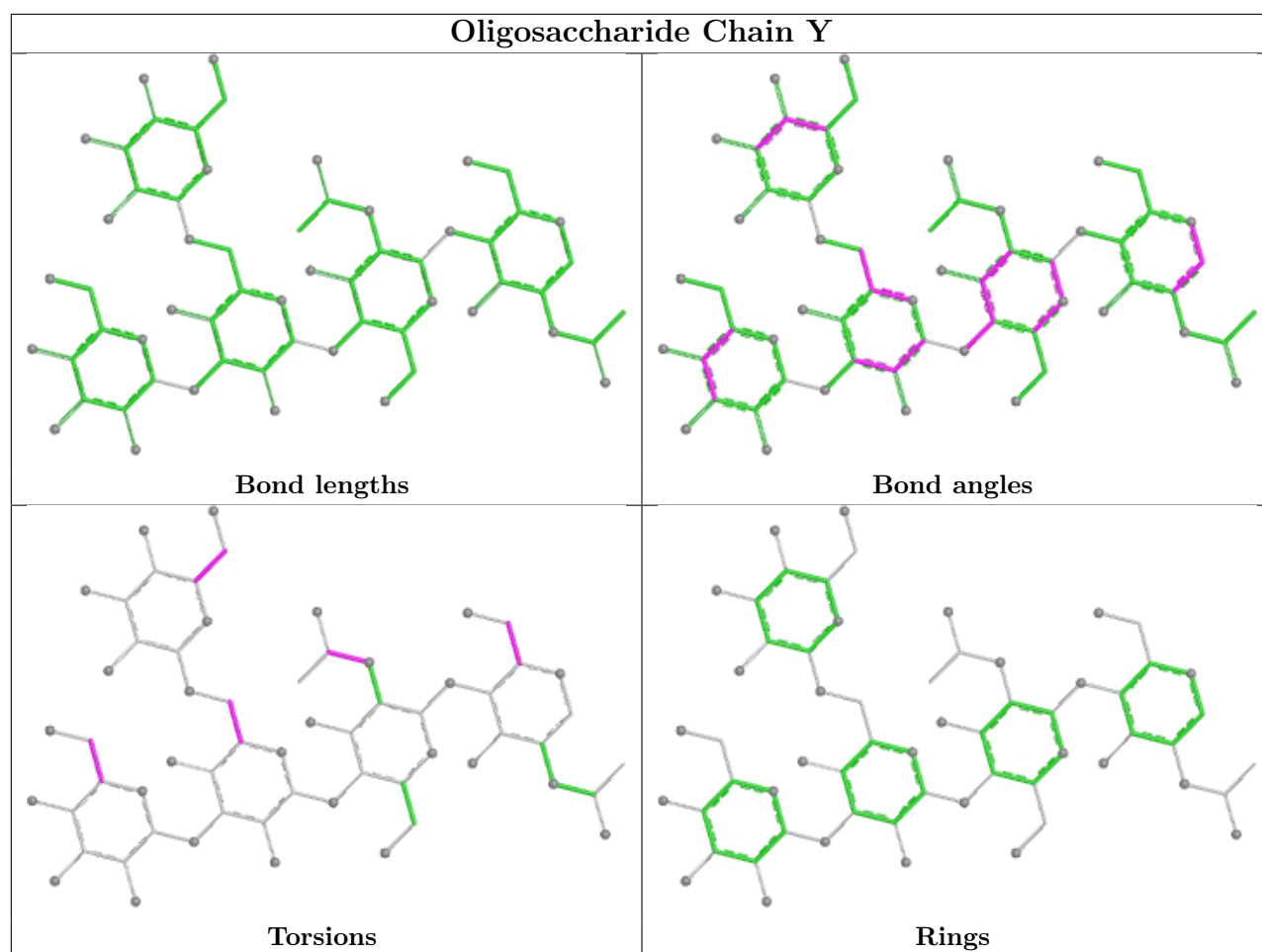


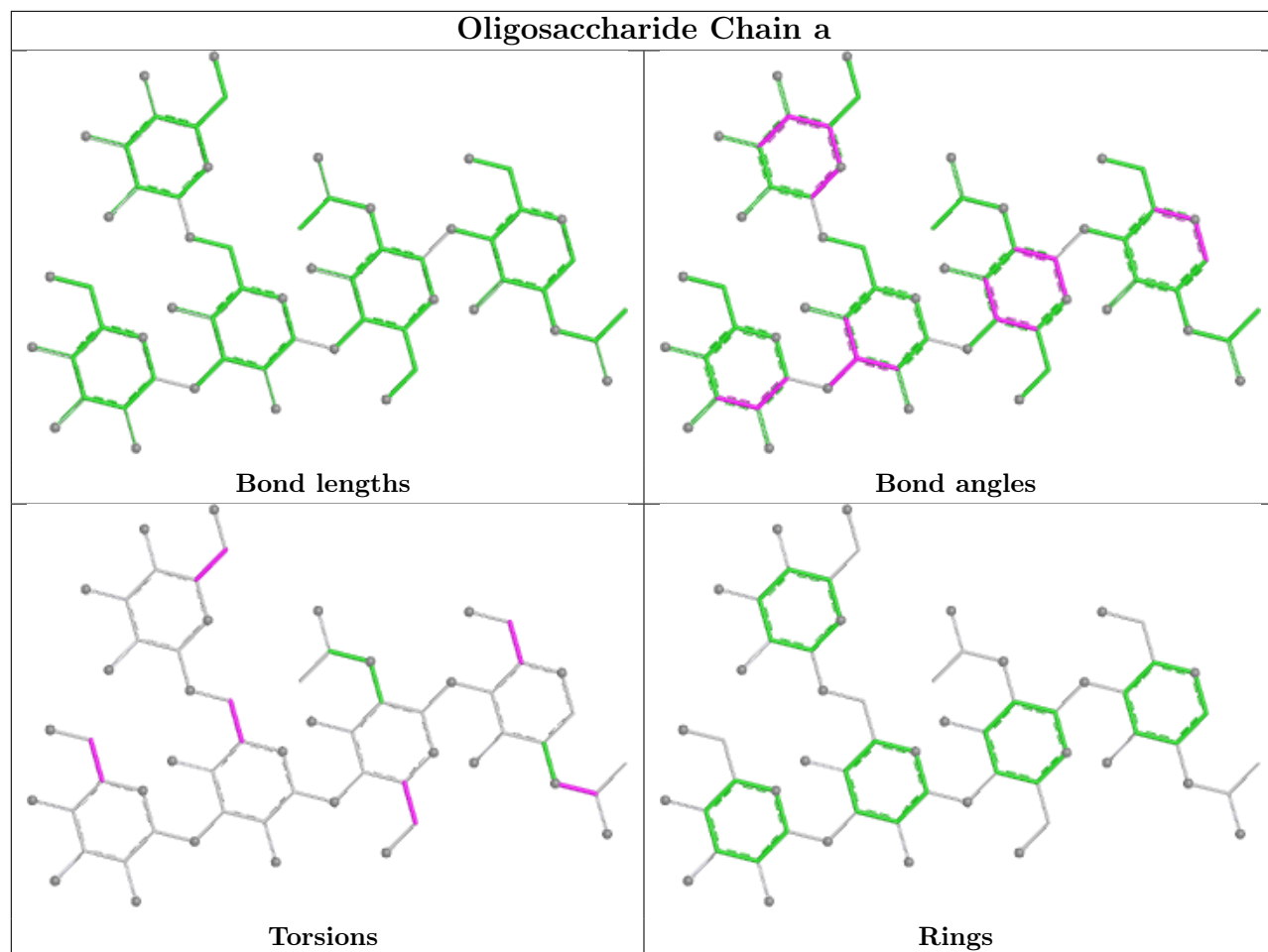


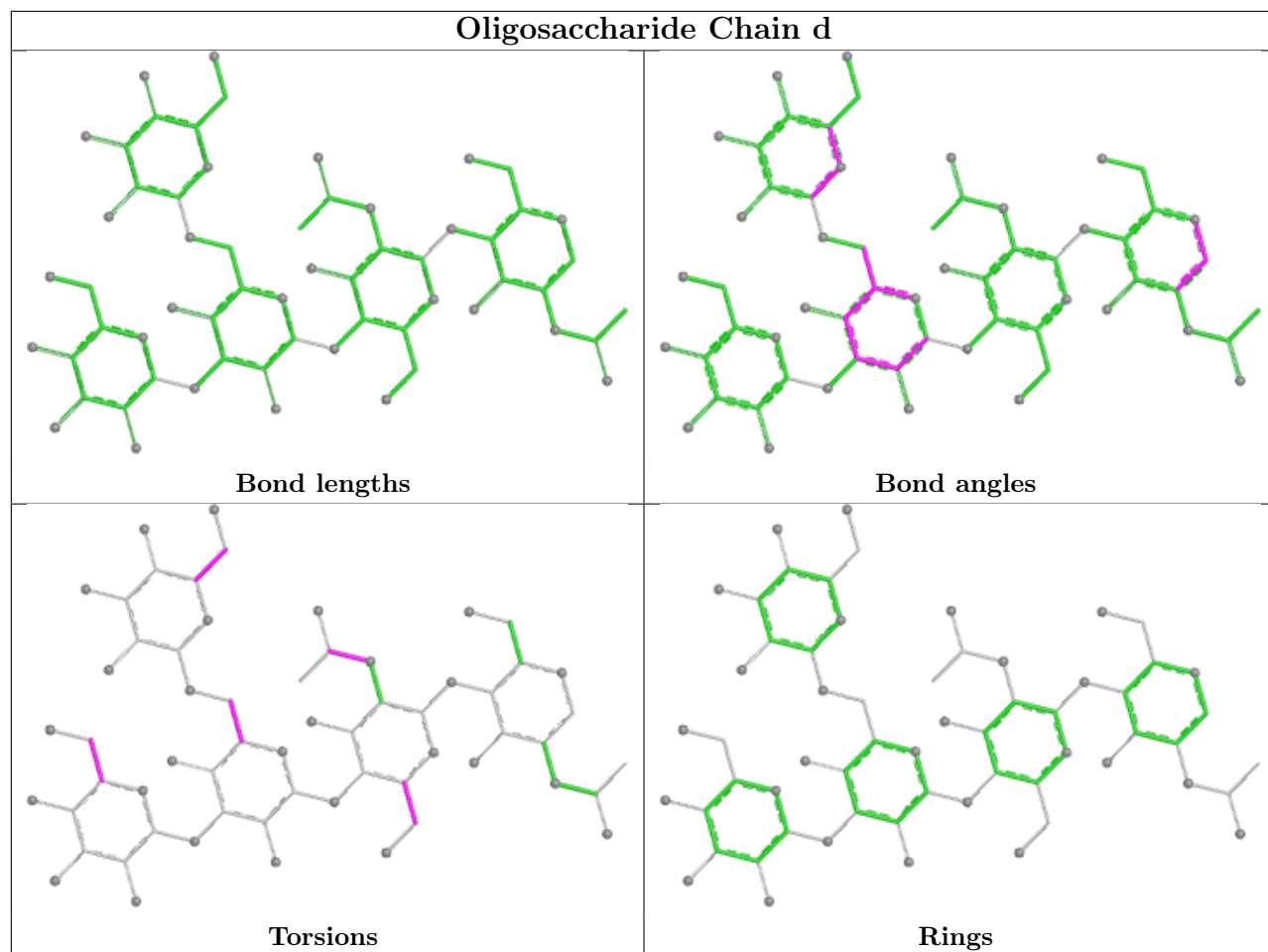




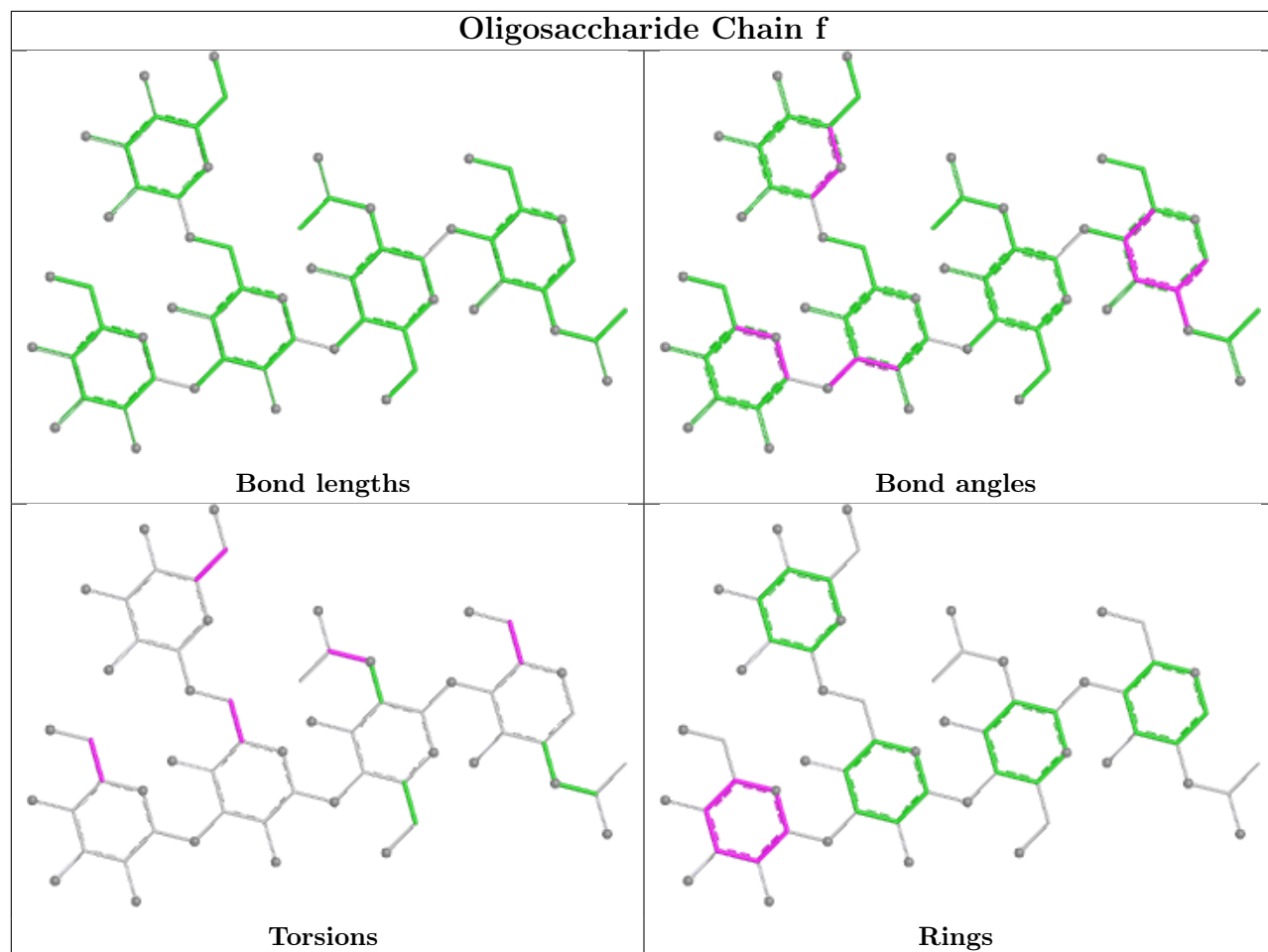


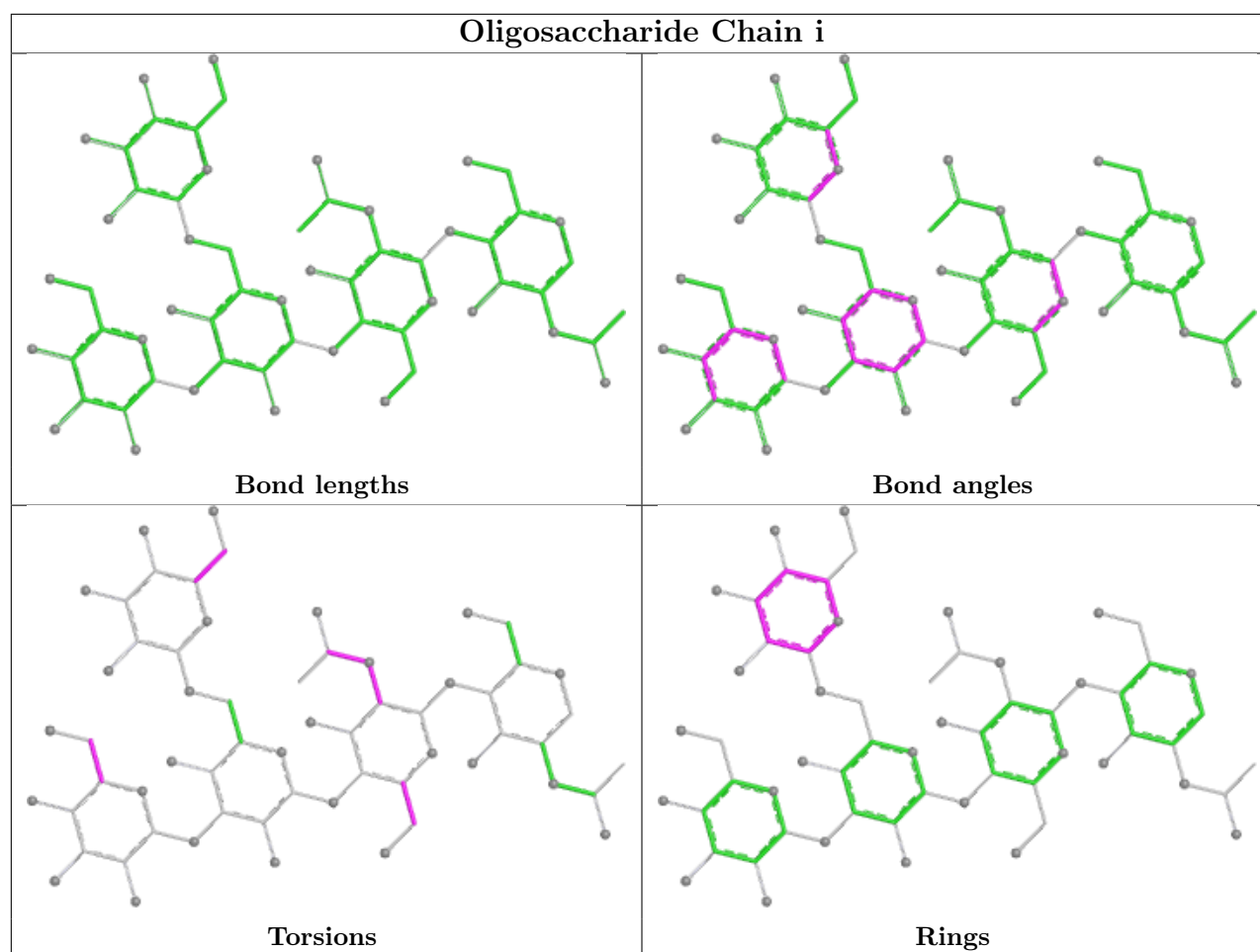


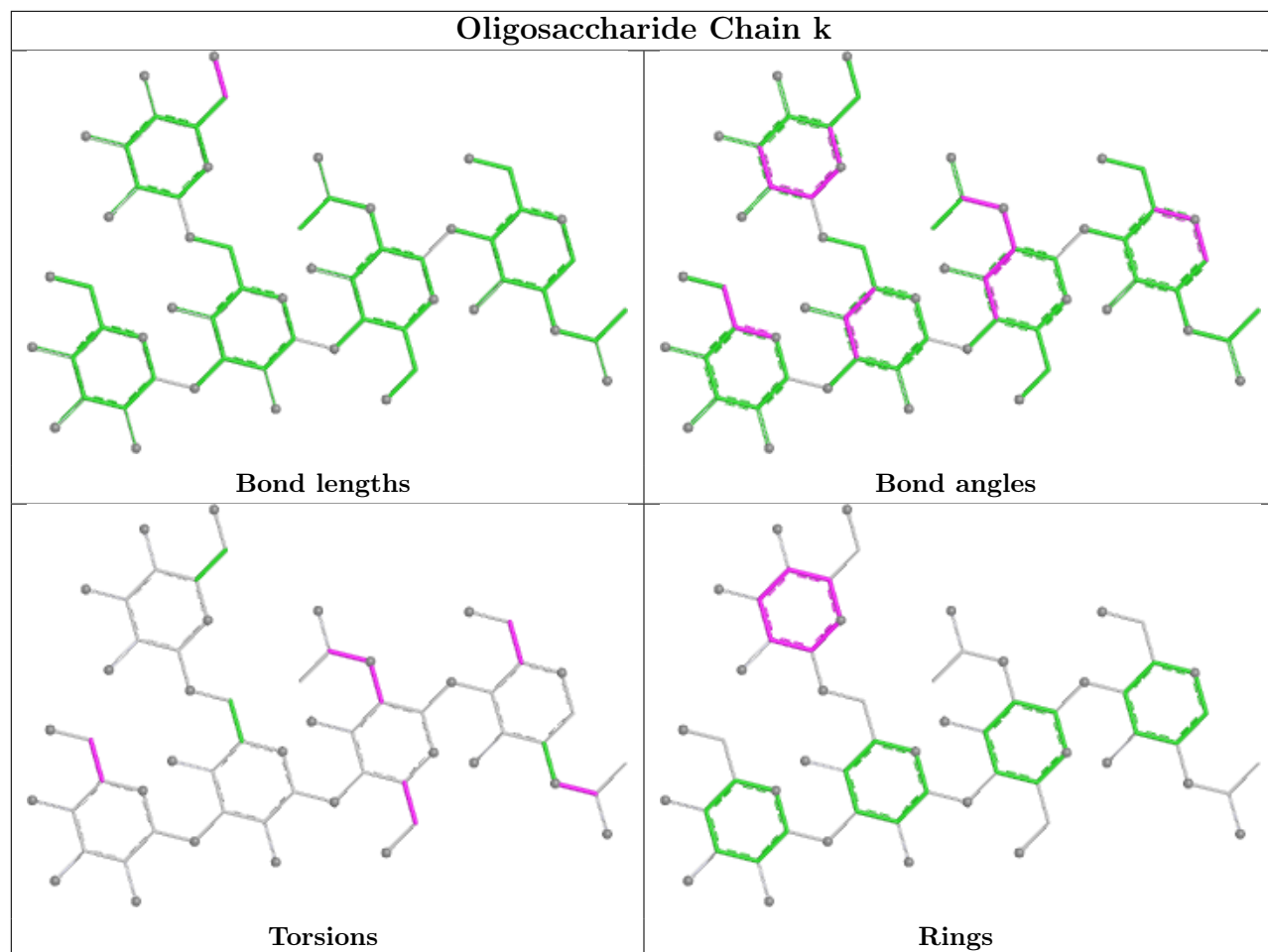


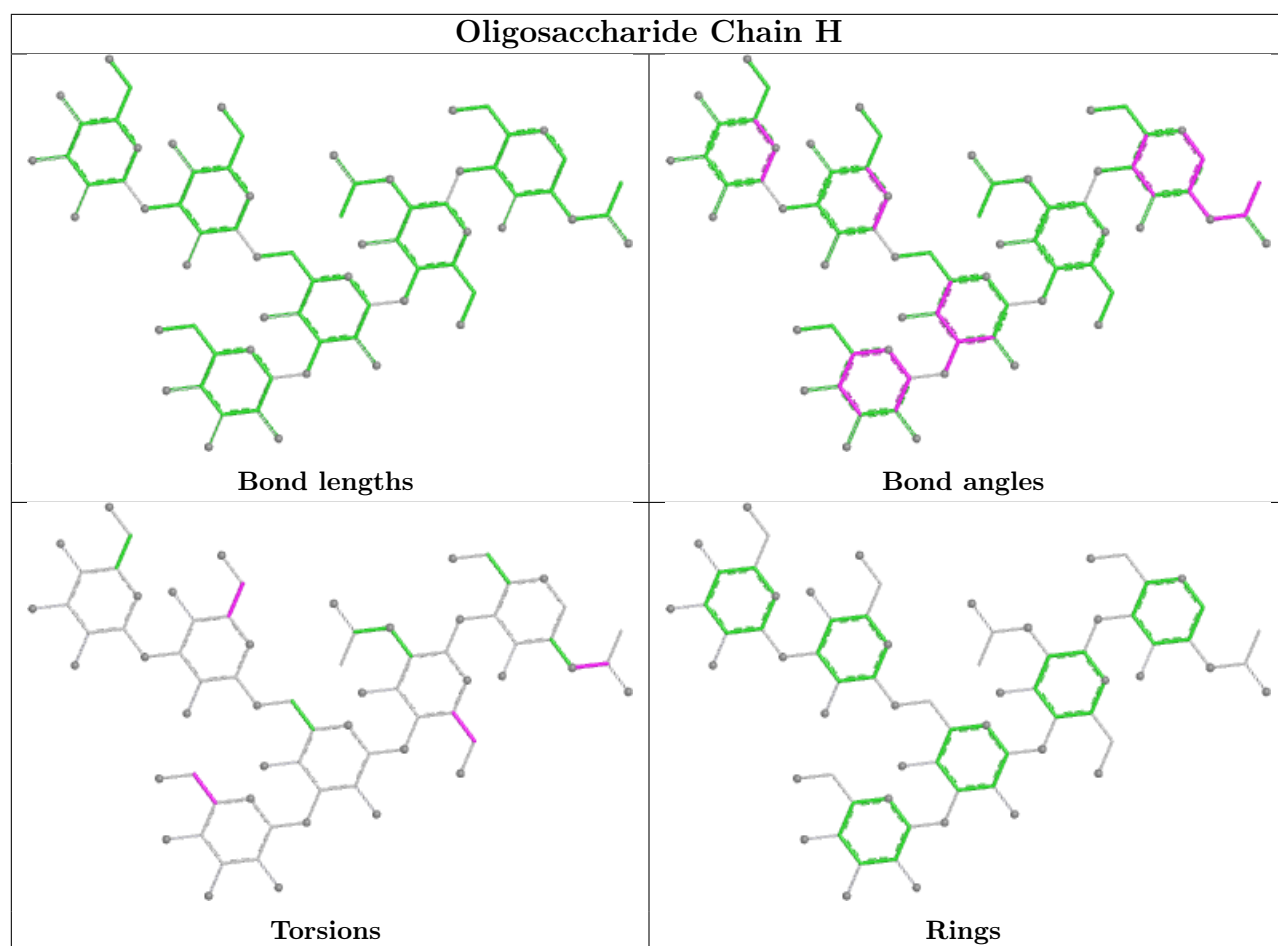


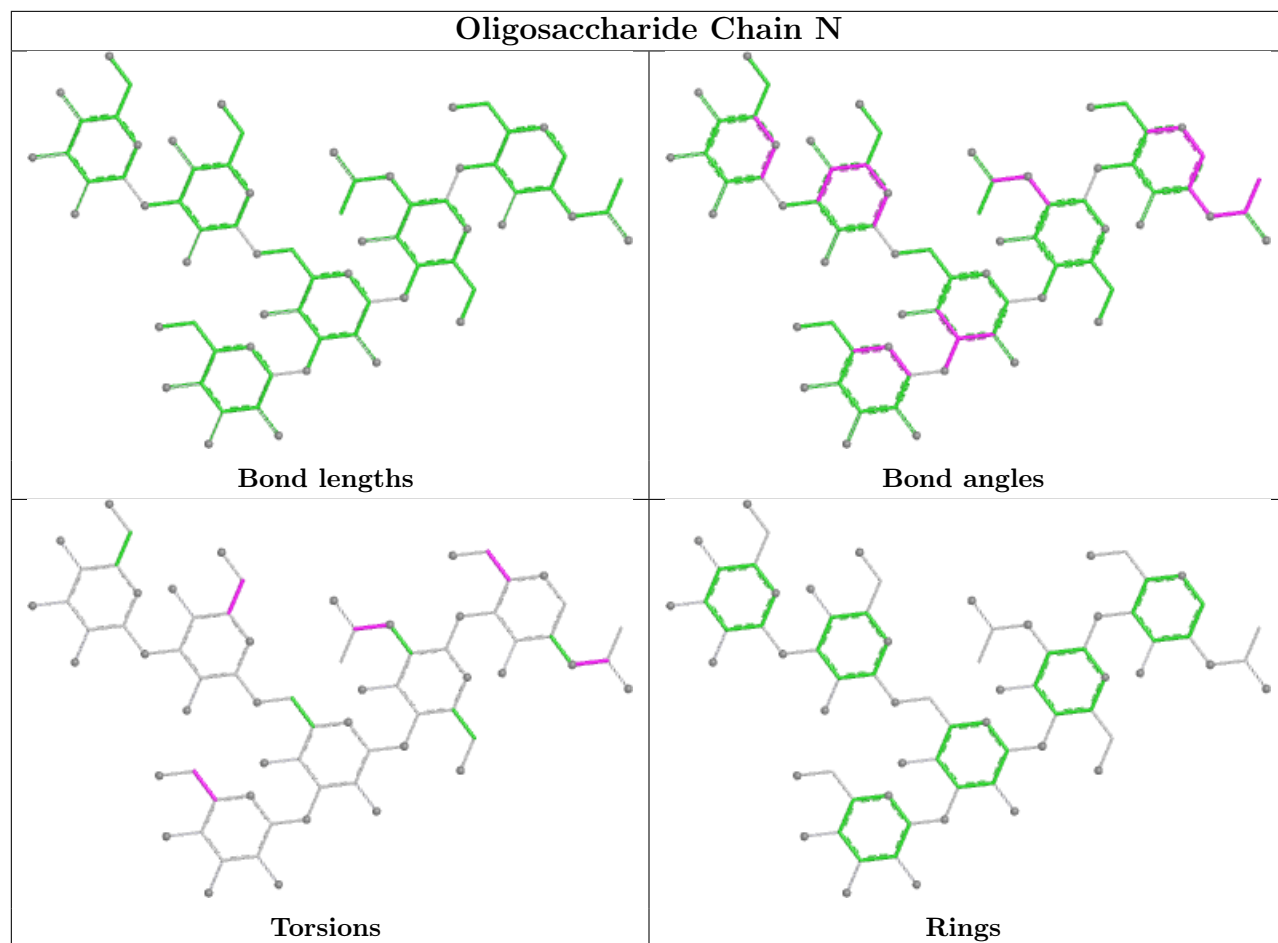


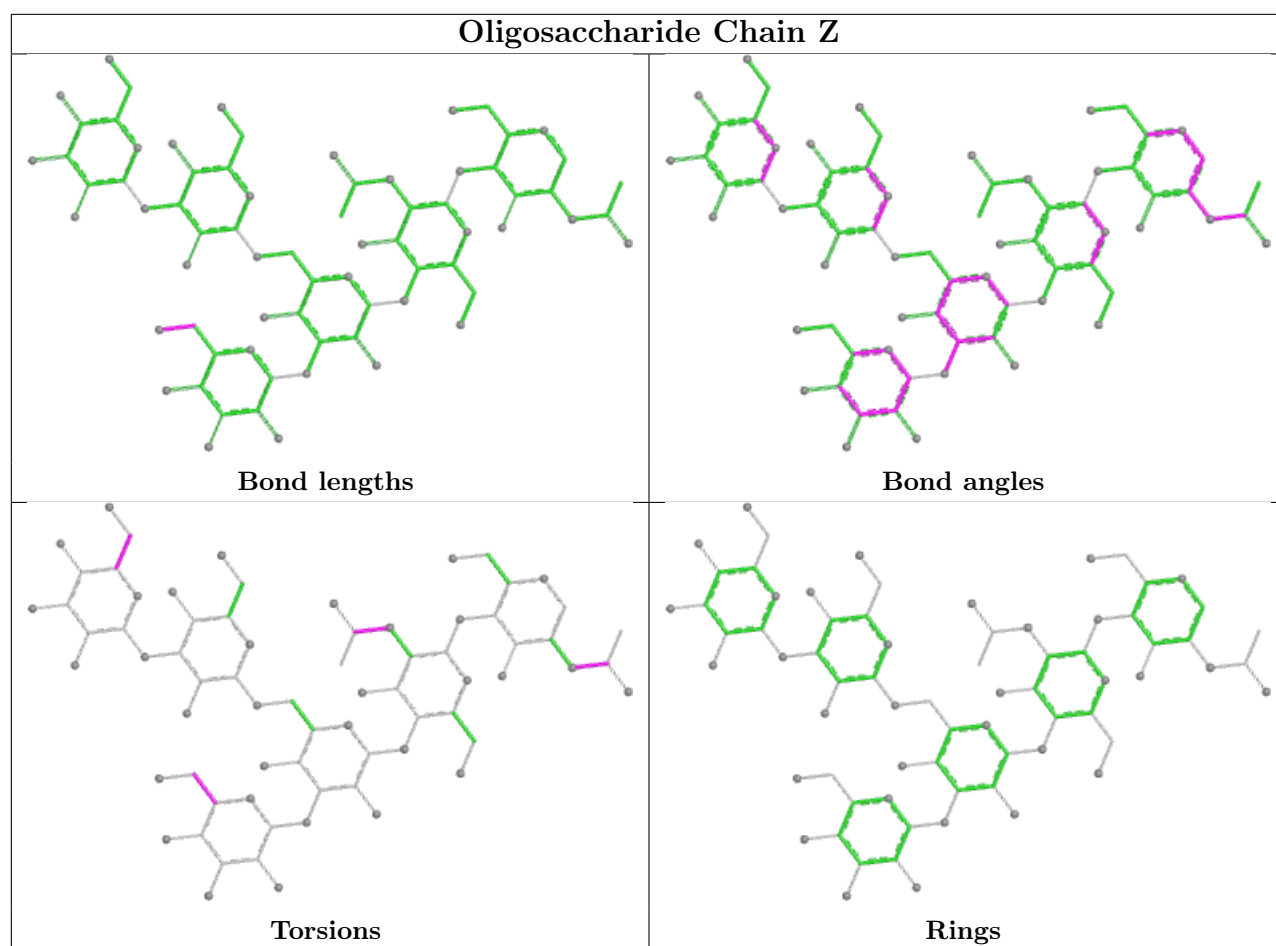


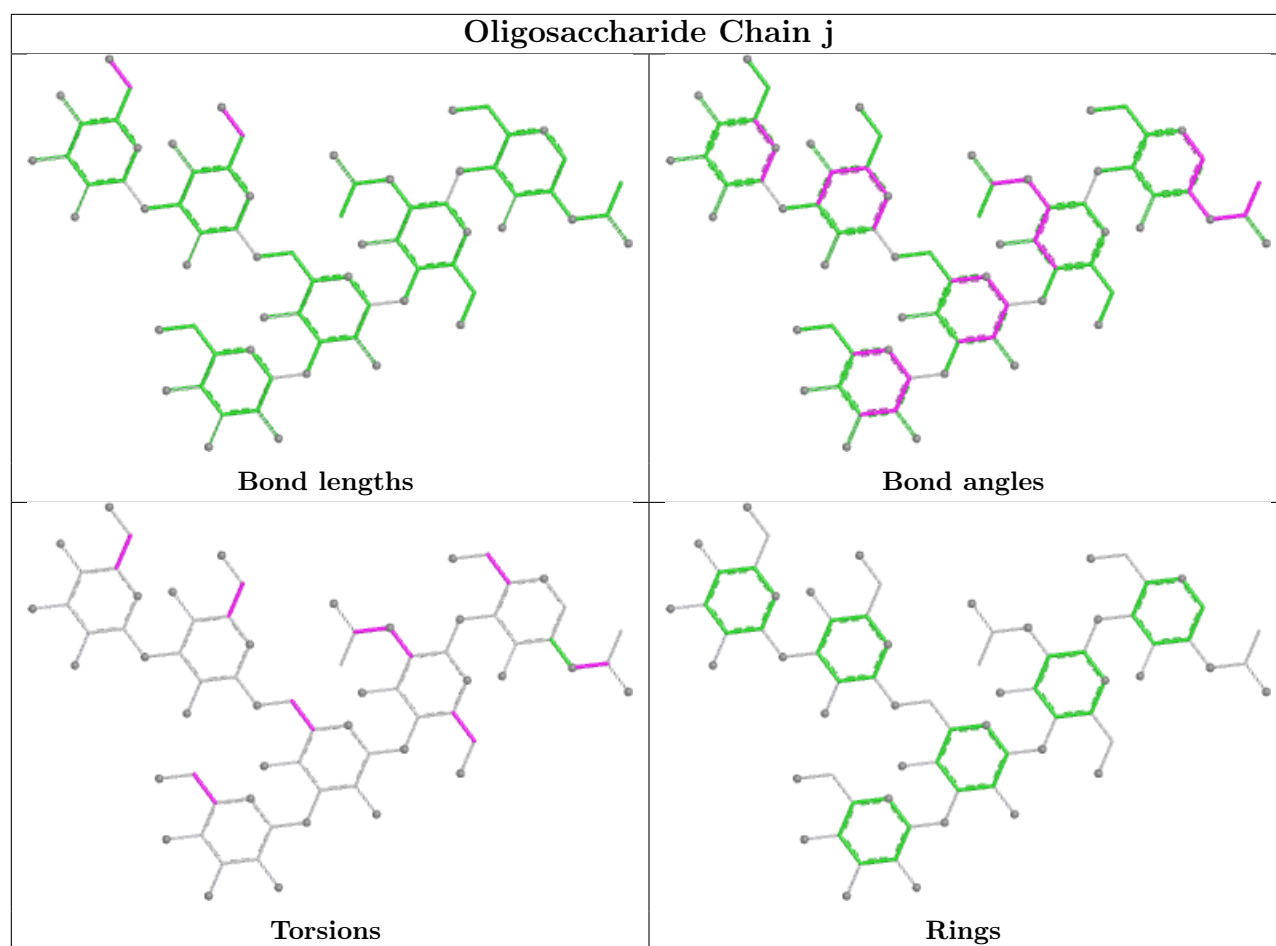


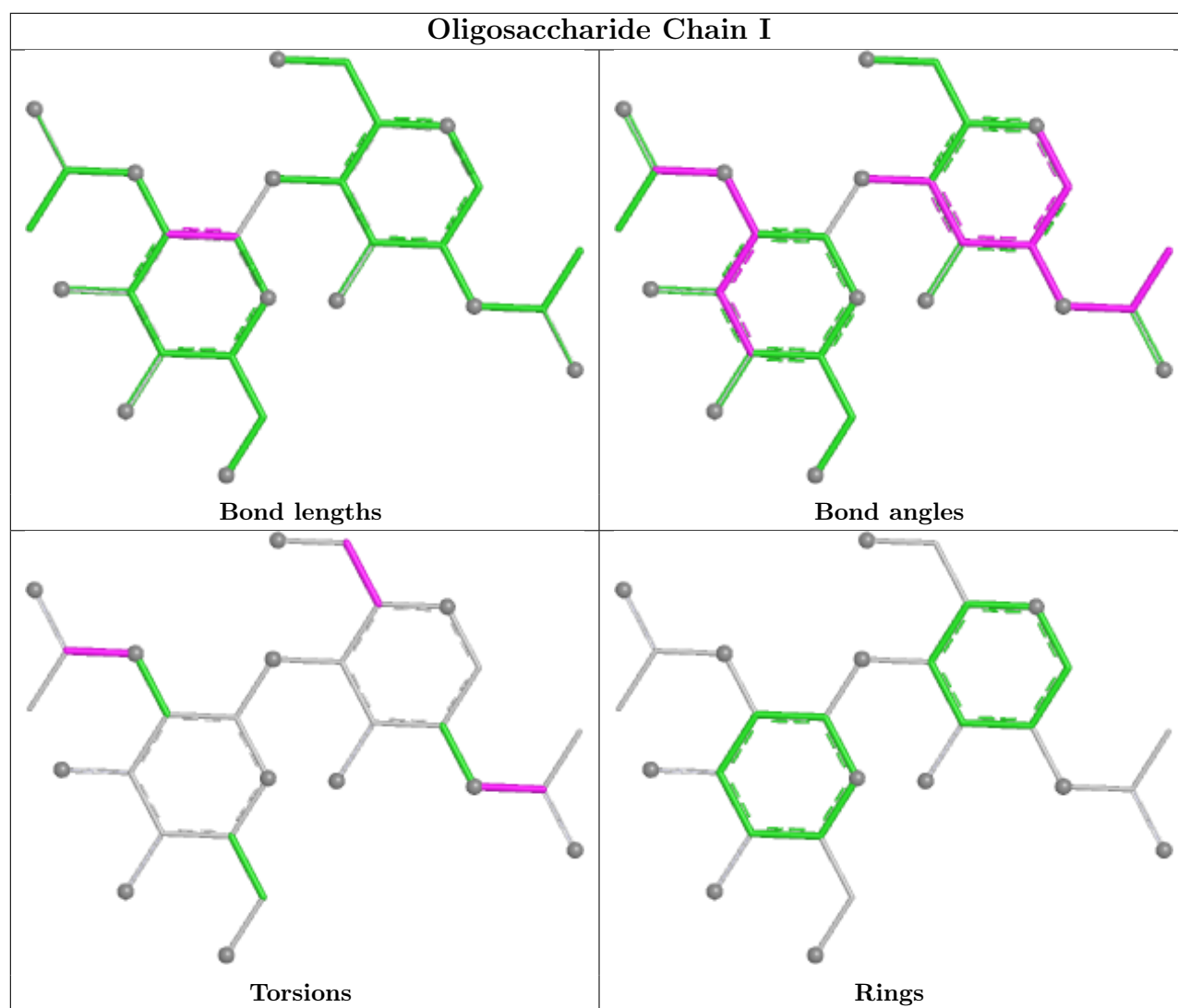




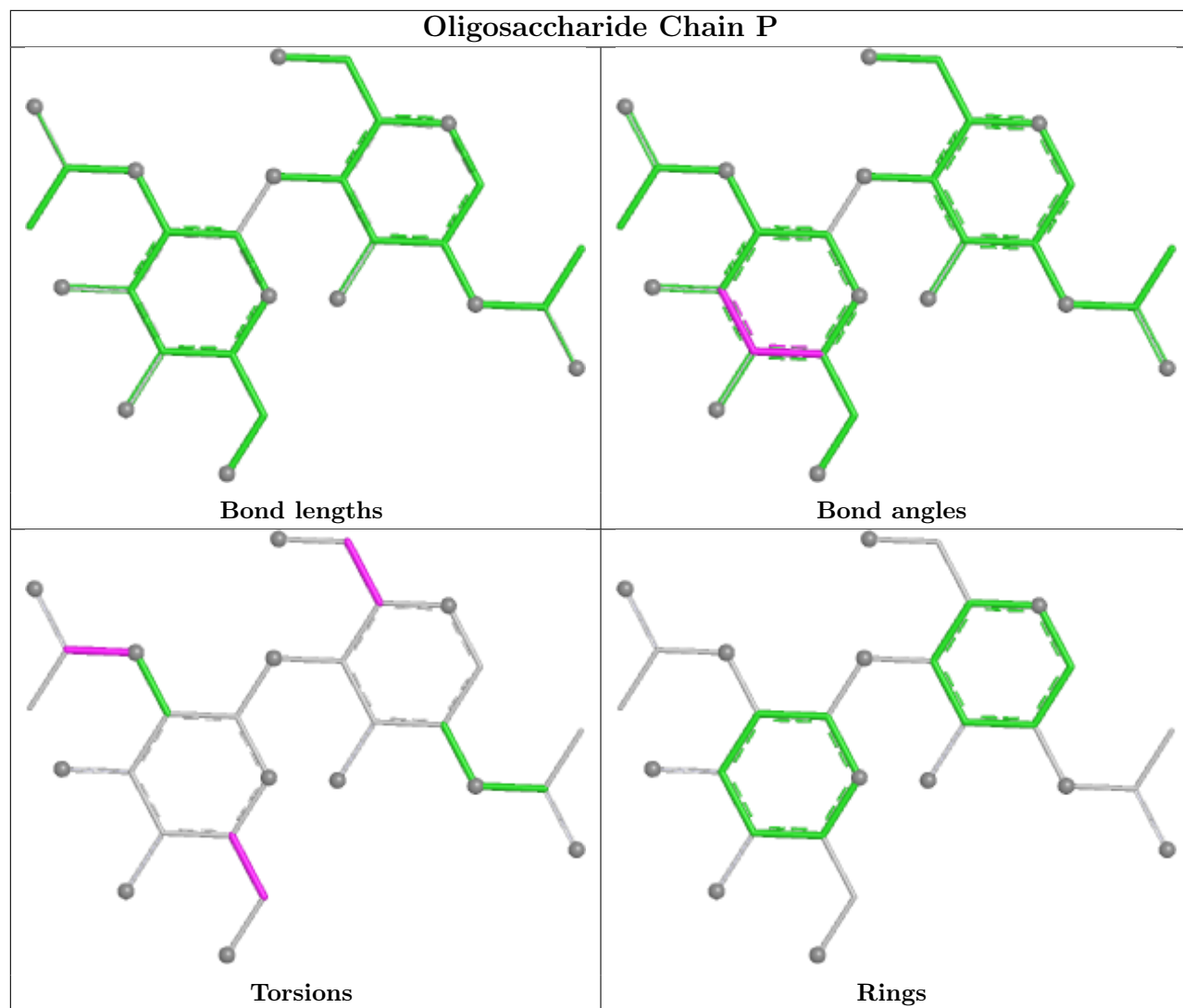


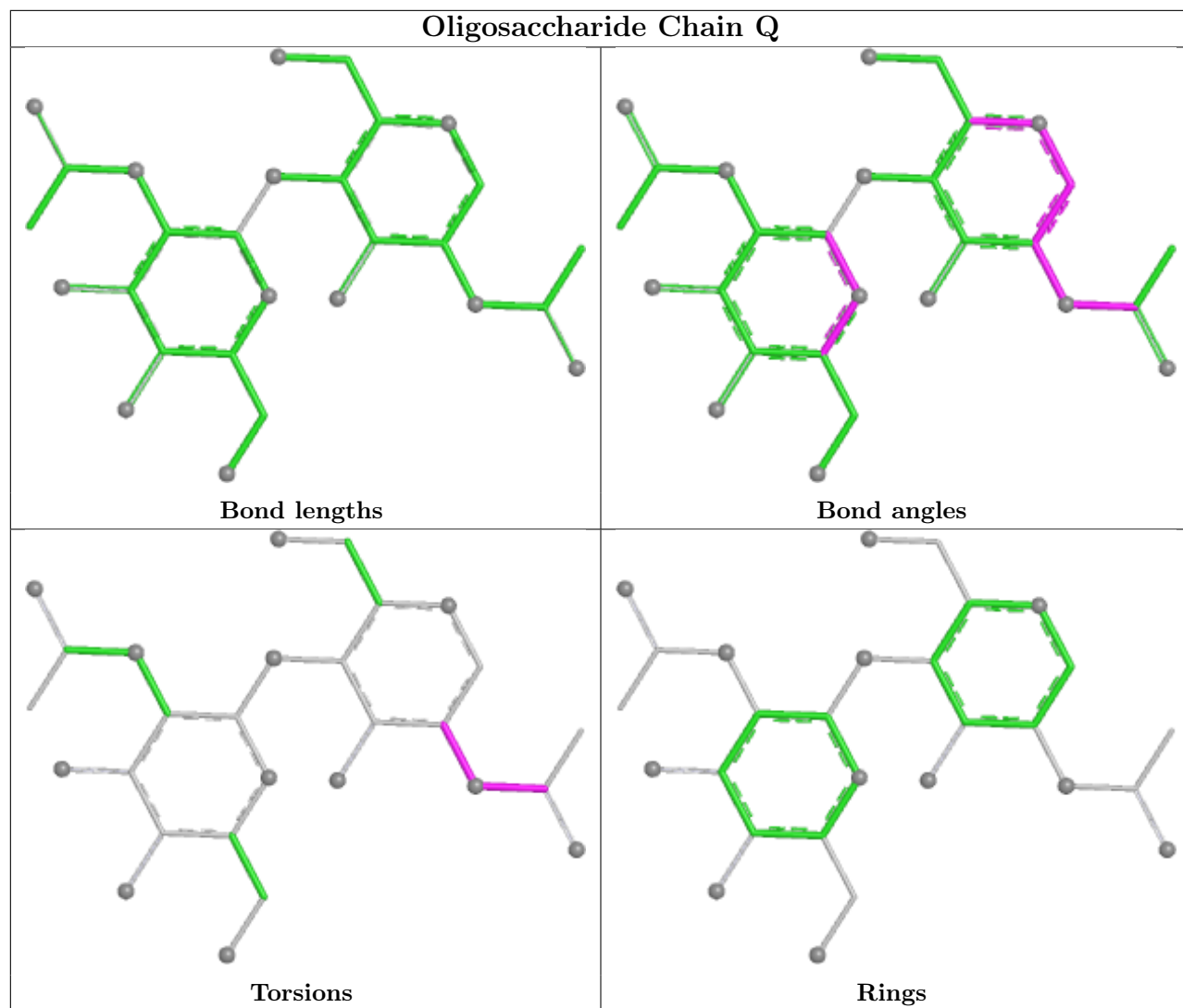


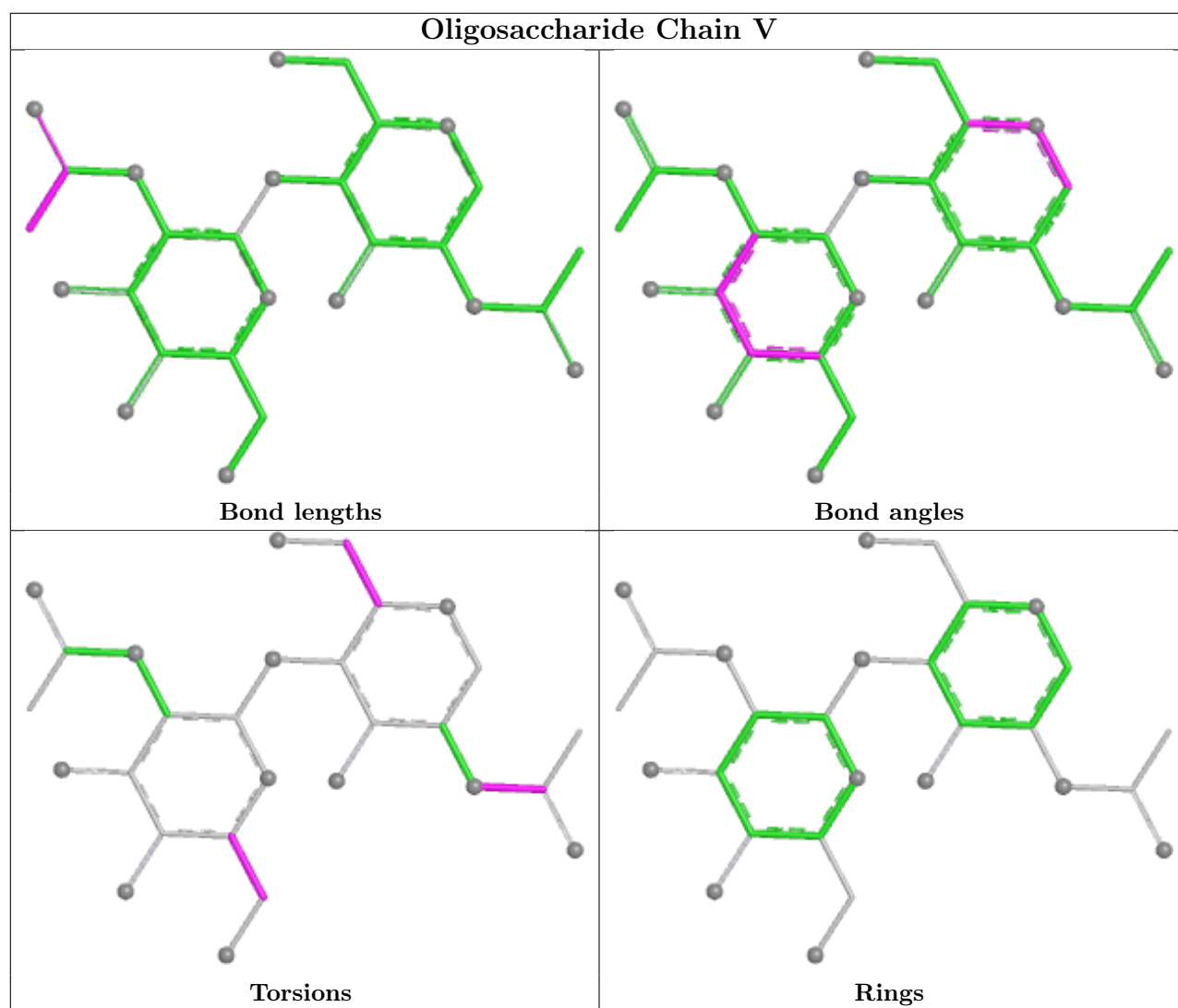


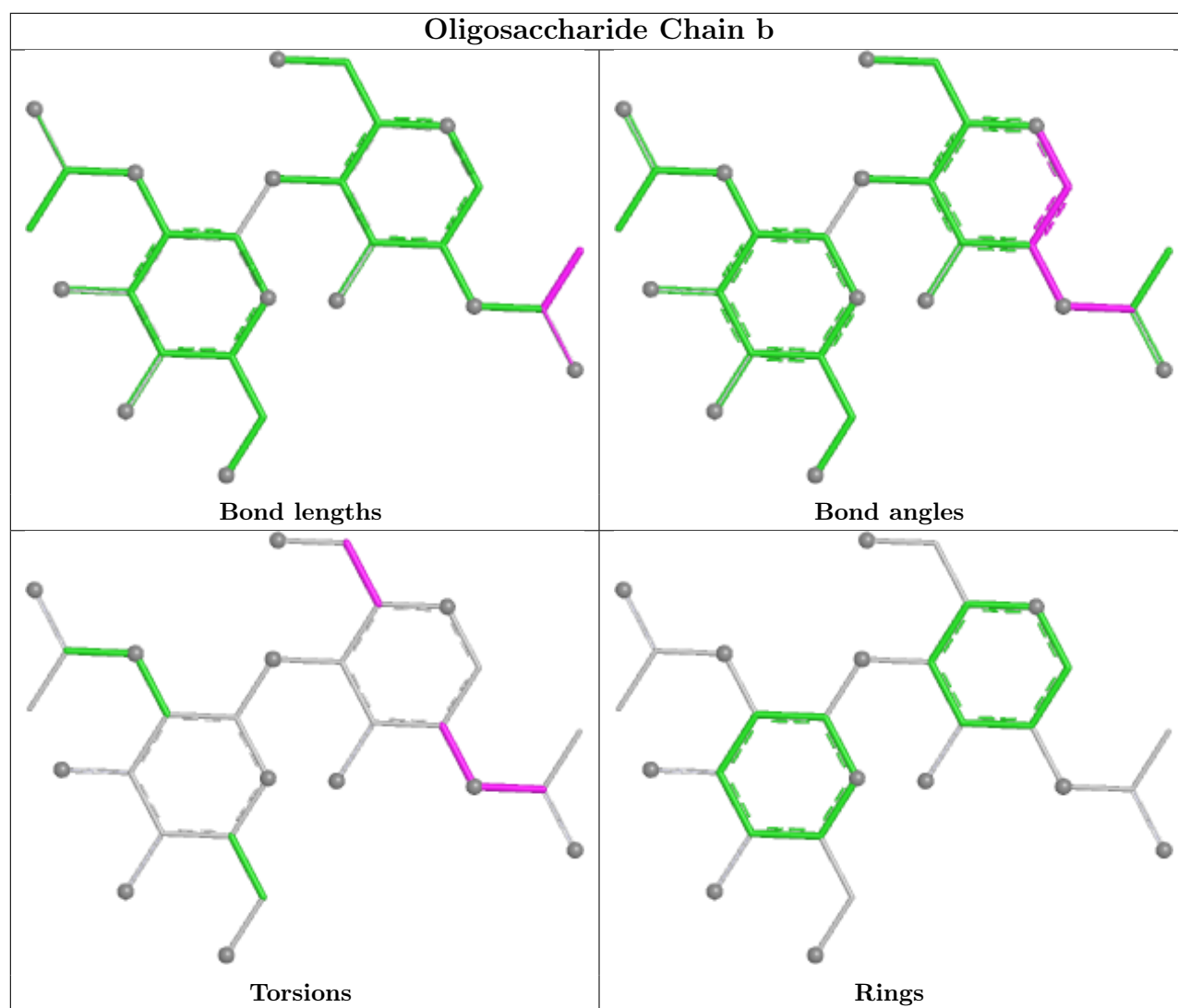


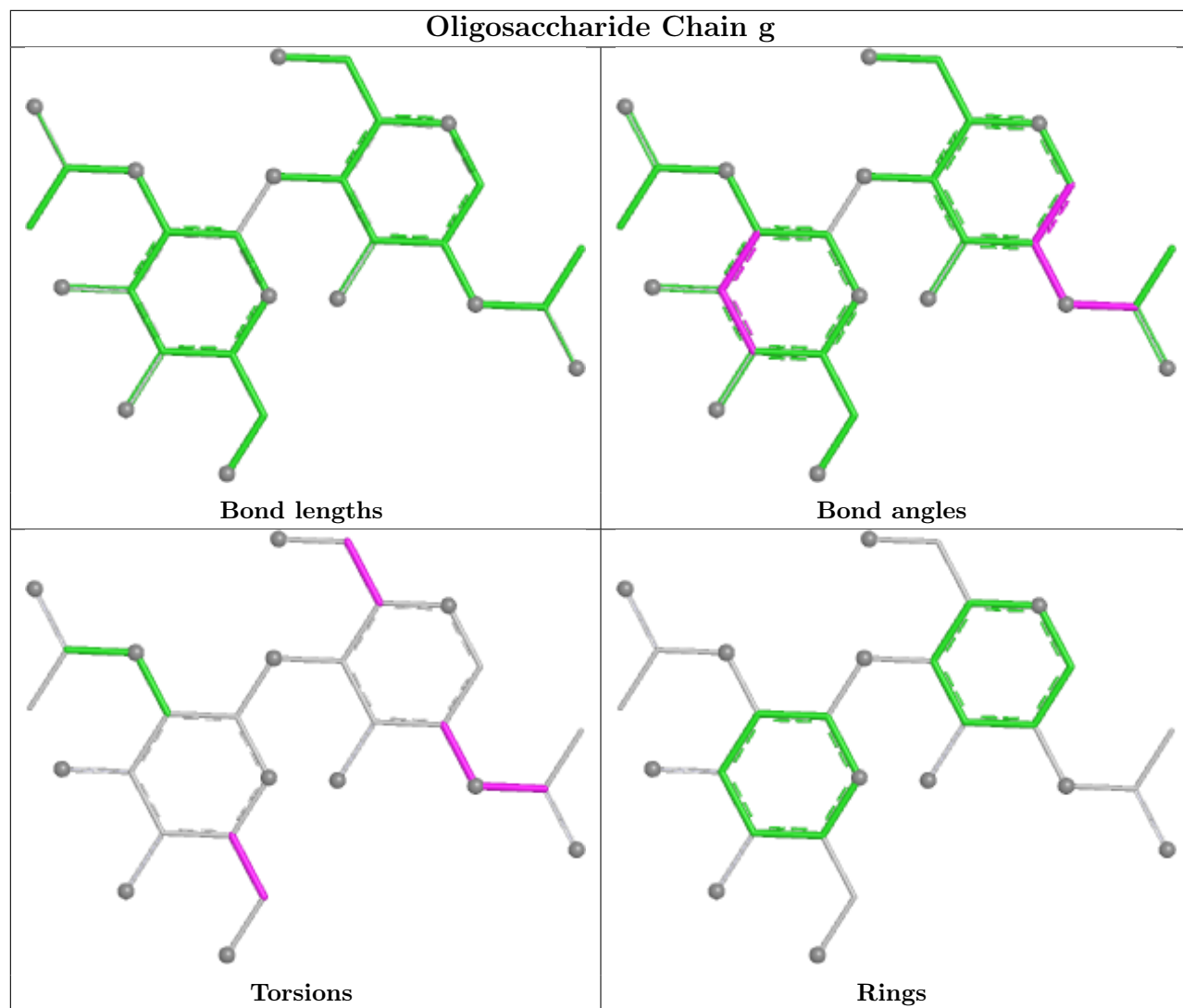


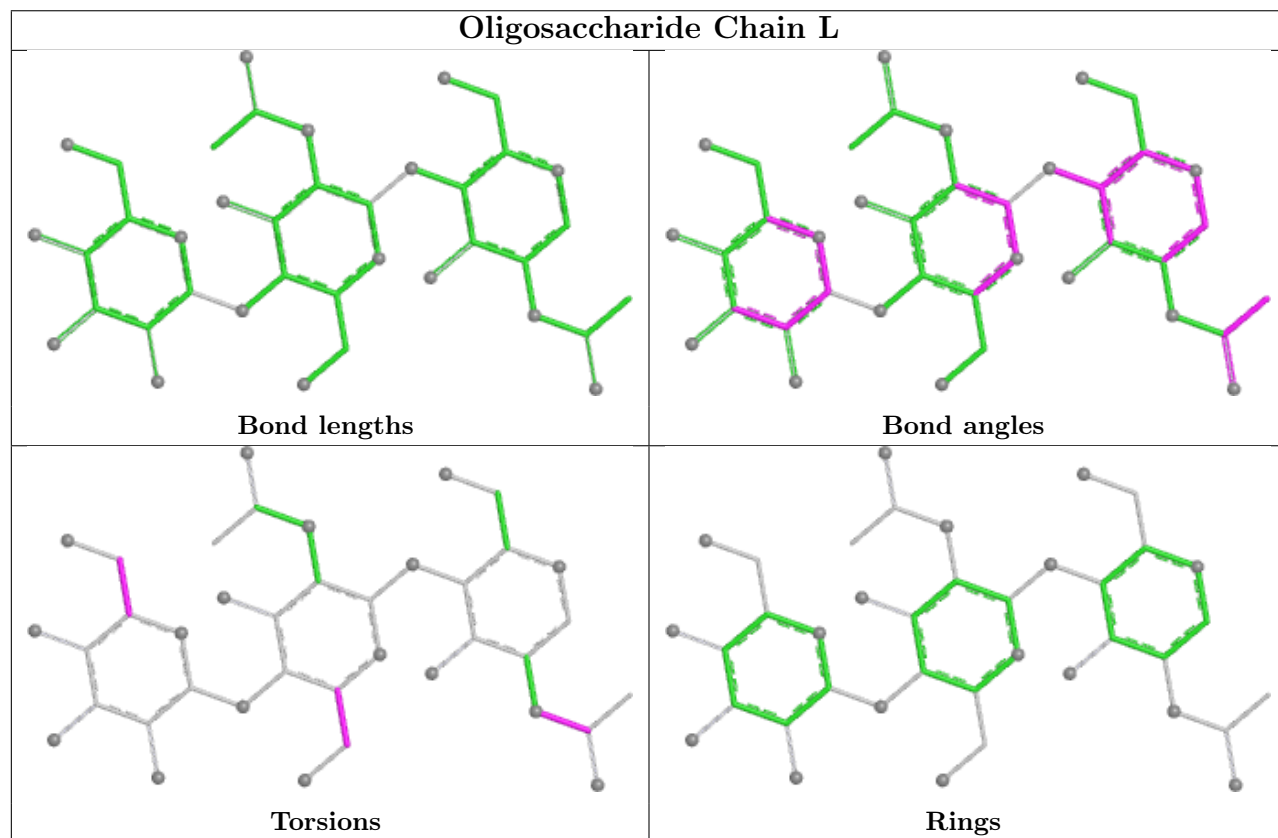
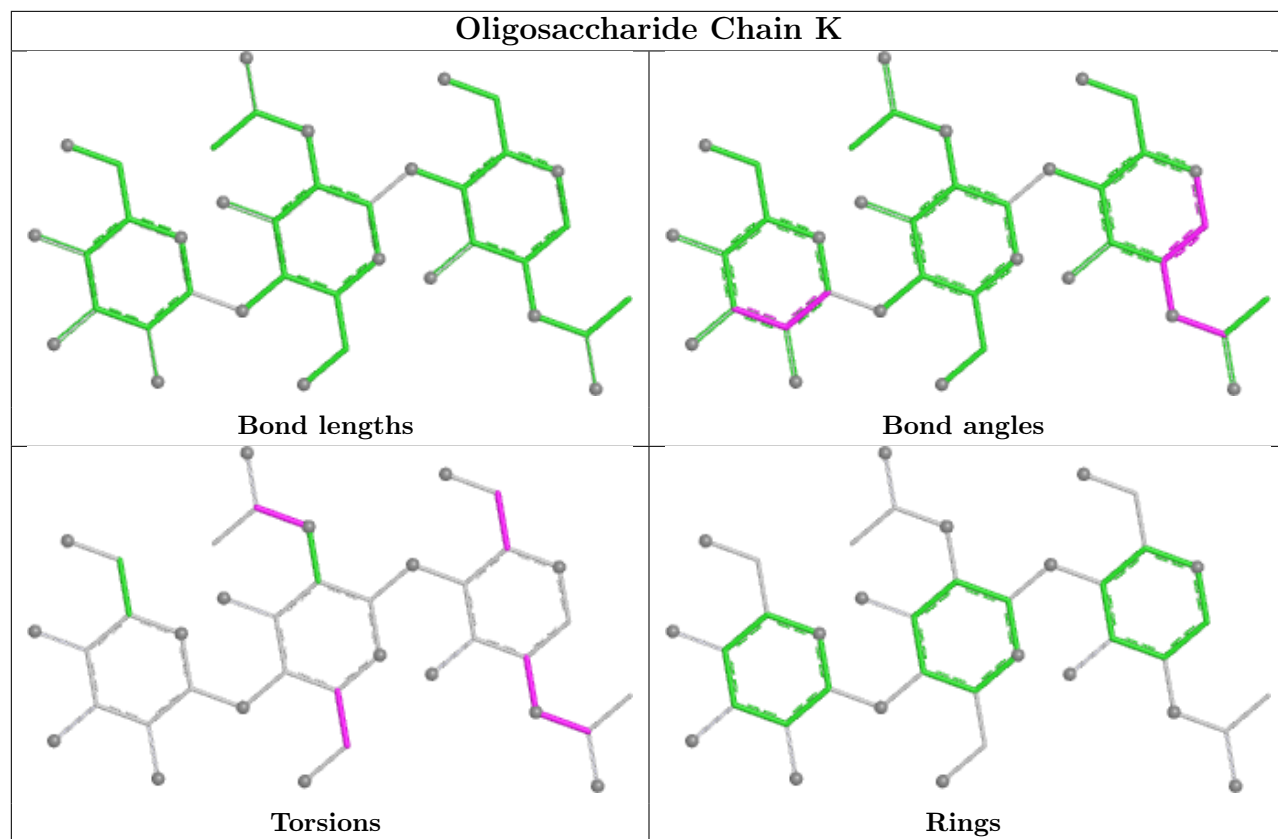


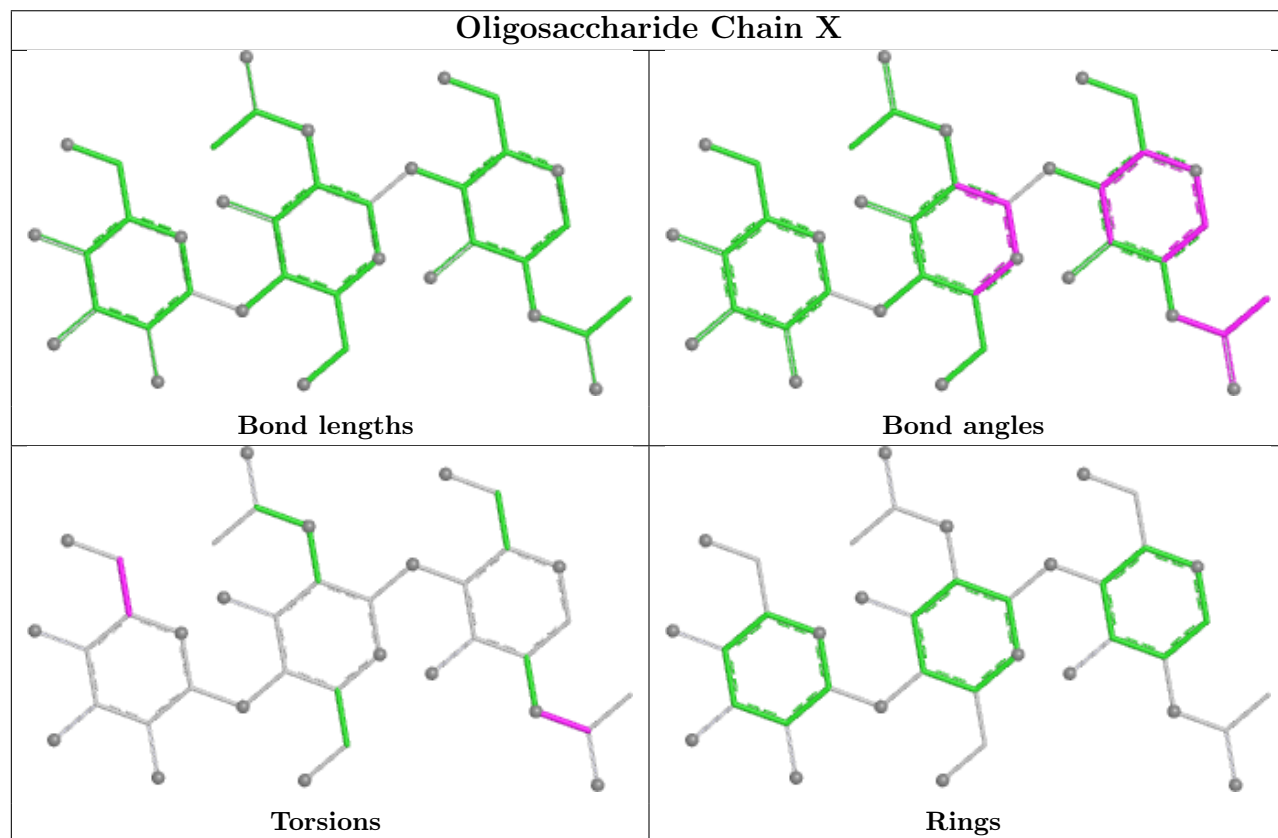
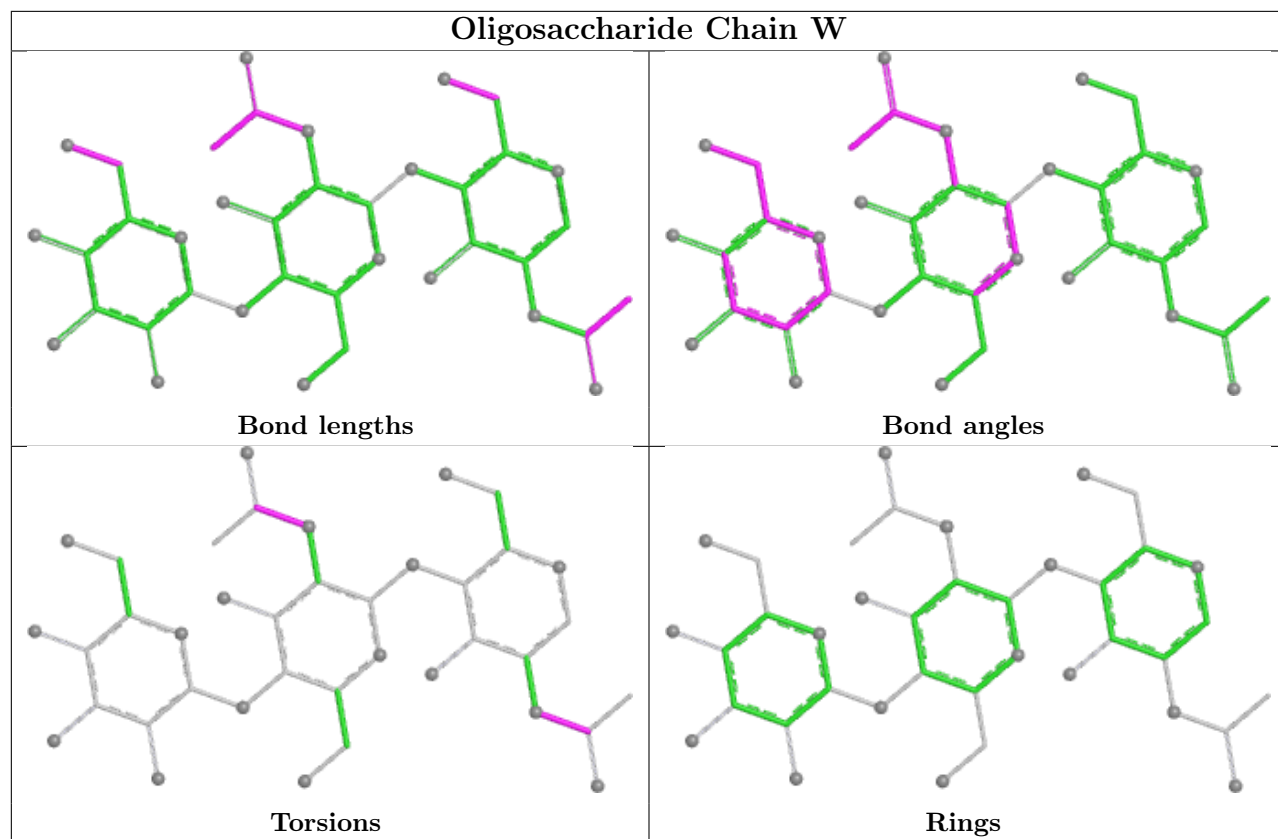


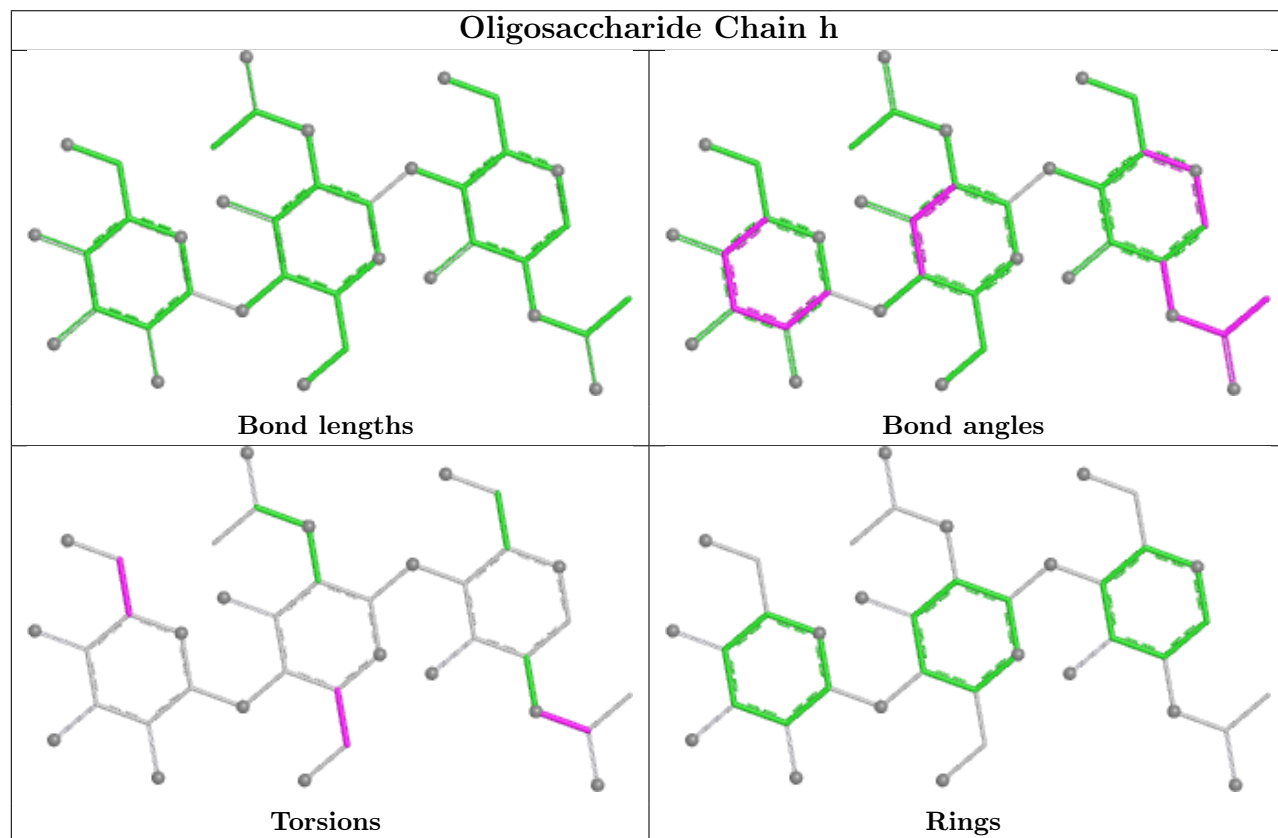
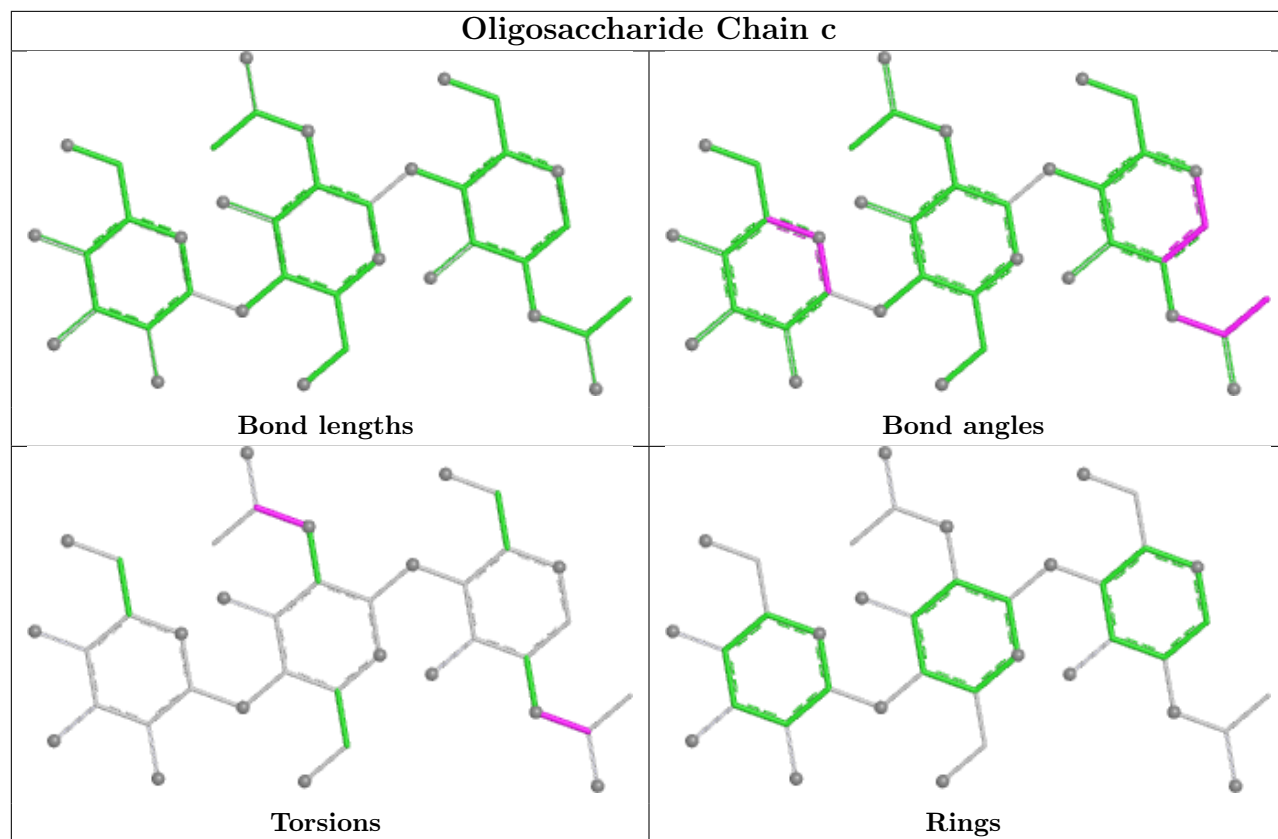




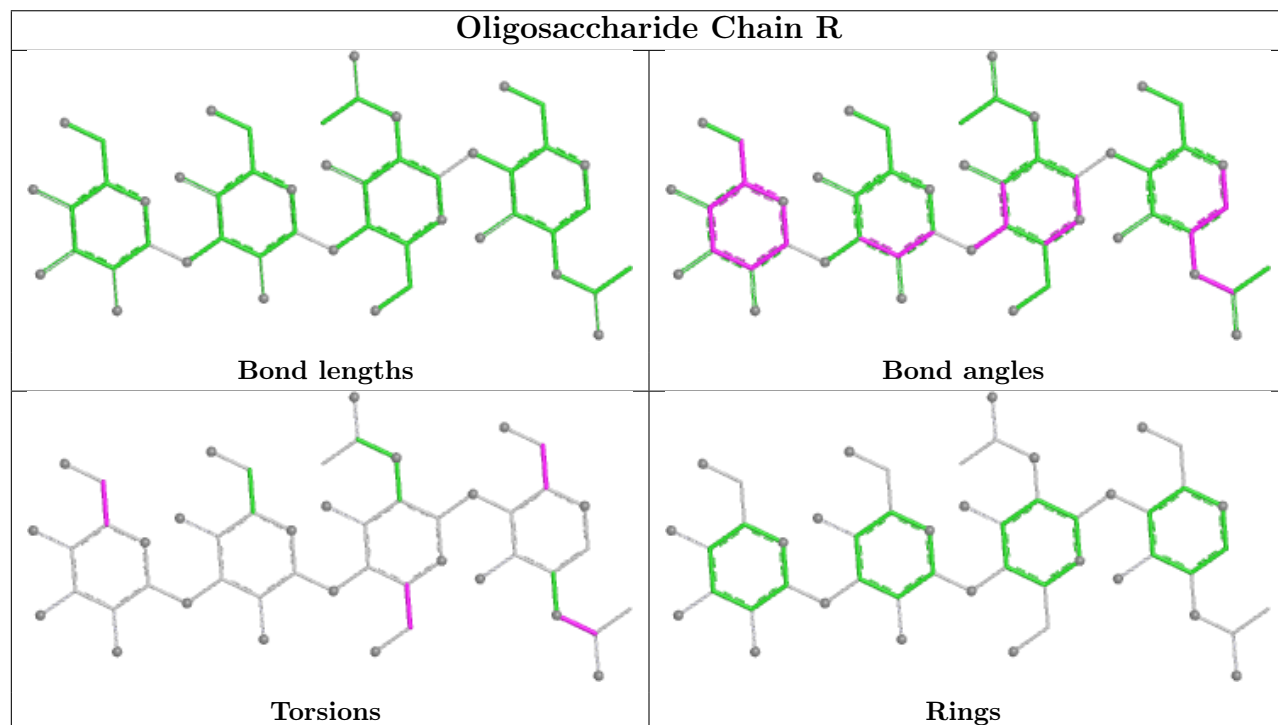
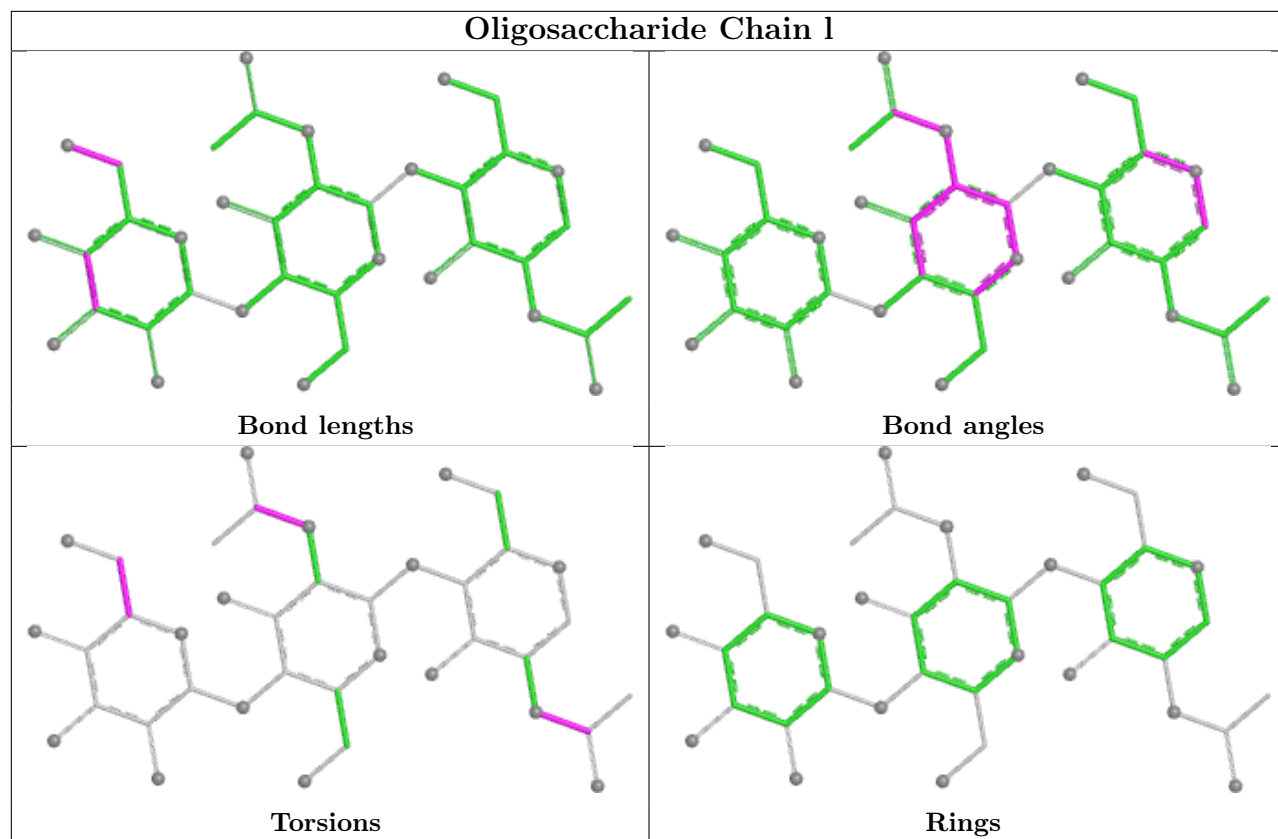


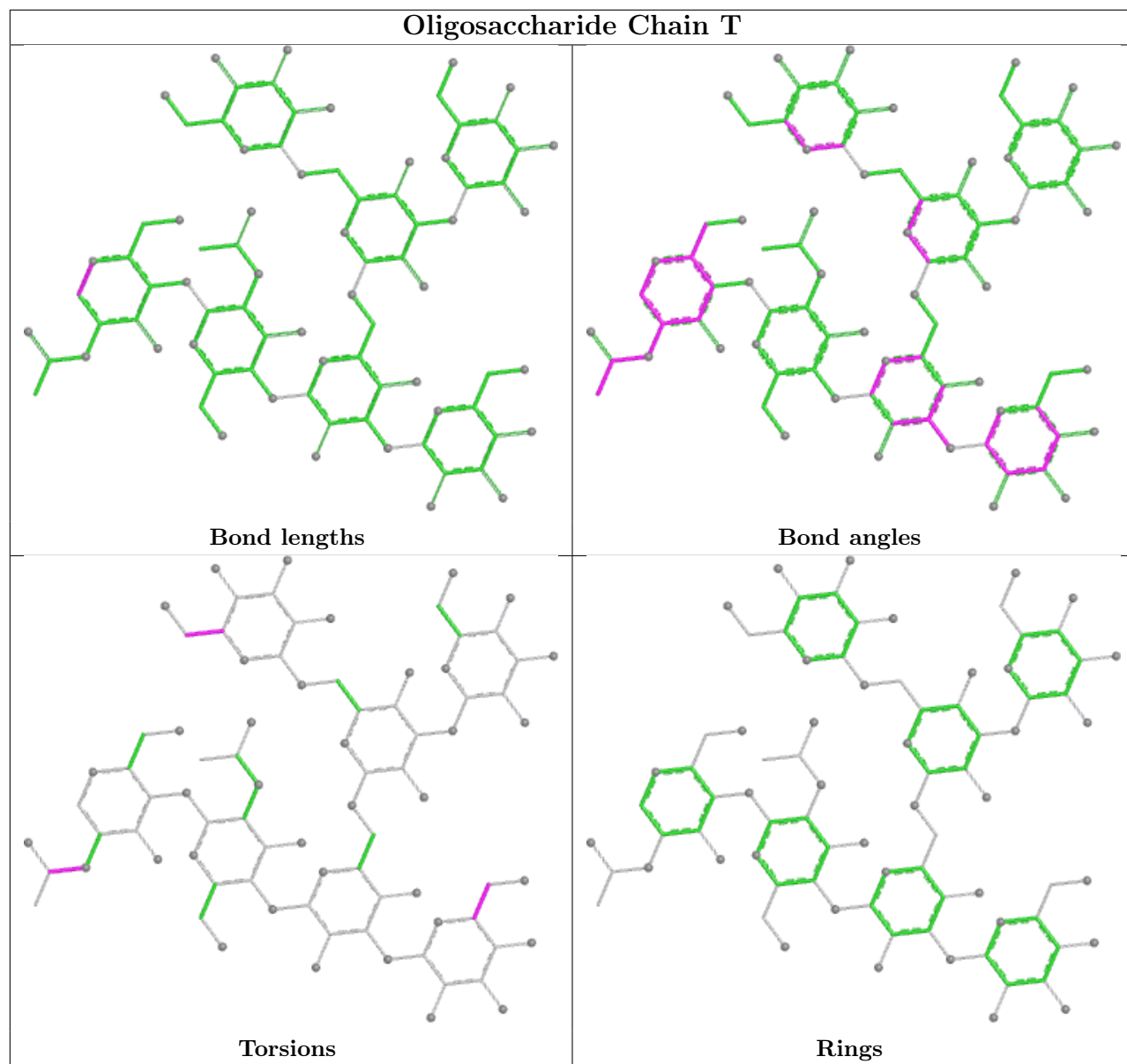


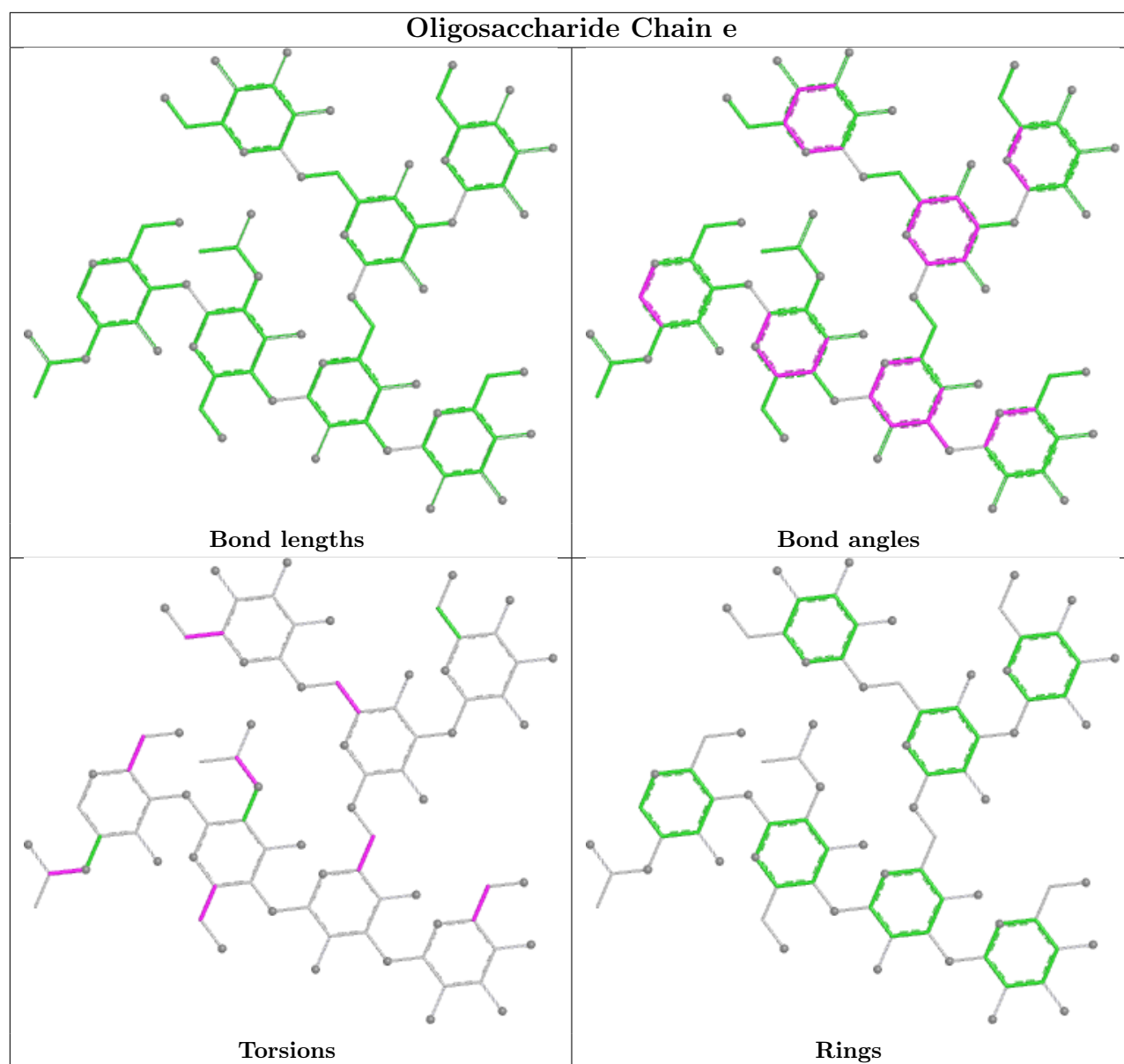












## 5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 24 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	D	2008	1	14,14,15	0.48	0	17,19,21	1.09	1 (5%)
8	NAG	A	2018	1	14,14,15	0.70	0	17,19,21	1.55	2 (11%)
8	NAG	F	2012	1	14,14,15	0.48	0	17,19,21	1.39	2 (11%)
8	NAG	B	2005	1	14,14,15	0.58	0	17,19,21	1.00	2 (11%)
8	NAG	A	2006	1	14,14,15	0.88	0	17,19,21	1.17	3 (17%)
8	NAG	F	2014	1	14,14,15	0.46	0	17,19,21	1.28	2 (11%)
8	NAG	B	2006	1	14,14,15	0.67	0	17,19,21	1.01	1 (5%)
8	NAG	F	2008	1	14,14,15	0.55	0	17,19,21	1.13	1 (5%)
8	NAG	F	2005	1	14,14,15	4.26	4 (28%)	17,19,21	1.96	4 (23%)
8	NAG	E	2012	1	14,14,15	3.43	2 (14%)	17,19,21	1.50	3 (17%)
8	NAG	F	2009	1	14,14,15	0.88	0	17,19,21	1.59	4 (23%)
8	NAG	C	2018	1	14,14,15	5.07	3 (21%)	17,19,21	2.19	4 (23%)
8	NAG	F	2006	1	14,14,15	4.11	4 (28%)	17,19,21	1.98	4 (23%)
8	NAG	C	2005	1	14,14,15	0.54	0	17,19,21	1.70	4 (23%)
8	NAG	B	2014	1	14,14,15	0.46	0	17,19,21	2.00	3 (17%)
8	NAG	C	2014	1	14,14,15	0.54	0	17,19,21	1.82	3 (17%)
8	NAG	D	2006	1	14,14,15	3.86	3 (21%)	17,19,21	2.07	4 (23%)
8	NAG	D	2014	1	14,14,15	0.52	0	17,19,21	0.91	0
8	NAG	C	2006	1	14,14,15	0.47	0	17,19,21	1.45	1 (5%)
8	NAG	E	2005	1	14,14,15	0.55	0	17,19,21	0.88	1 (5%)
8	NAG	A	2014	1	14,14,15	0.64	0	17,19,21	1.08	0
8	NAG	E	2006	1	14,14,15	0.68	0	17,19,21	1.88	4 (23%)
8	NAG	E	2014	1	14,14,15	0.47	0	17,19,21	1.86	2 (11%)
8	NAG	B	2012	1	14,14,15	0.53	0	17,19,21	1.21	1 (5%)
8	NAG	A	2008	1	14,14,15	0.48	0	17,19,21	0.92	1 (5%)
8	NAG	B	2018	1	14,14,15	0.80	1 (7%)	17,19,21	1.26	1 (5%)
8	NAG	D	2012	1	14,14,15	0.67	0	17,19,21	1.02	1 (5%)
8	NAG	C	2012	1	14,14,15	0.54	0	17,19,21	1.60	2 (11%)
8	NAG	D	2005	1	14,14,15	0.52	0	17,19,21	1.17	2 (11%)
8	NAG	E	2008	1	14,14,15	0.52	0	17,19,21	0.94	0
8	NAG	A	2012	1	14,14,15	0.54	0	17,19,21	1.21	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	D	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	A	2018	1	1/1/5/7	3/6/23/26	0/1/1/1
8	NAG	F	2012	1	1/1/5/7	5/6/23/26	0/1/1/1
8	NAG	B	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	A	2006	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	F	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	B	2006	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	F	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	F	2005	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	E	2012	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	F	2009	1	1/1/5/7	5/6/23/26	0/1/1/1
8	NAG	C	2018	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	F	2006	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	C	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	D	2006	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	B	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	C	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	D	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
8	NAG	E	2005	1	-	2/6/23/26	0/1/1/1
8	NAG	A	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	E	2006	1	-	3/6/23/26	0/1/1/1
8	NAG	E	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	B	2012	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	B	2018	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	D	2012	1	-	5/6/23/26	0/1/1/1
8	NAG	C	2012	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	D	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	E	2008	1	-	2/6/23/26	0/1/1/1
8	NAG	A	2012	1	1/1/5/7	3/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2018	NAG	O7-C7	14.52	1.55	1.23
8	F	2006	NAG	C8-C7	14.37	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2006	NAG	O7-C7	11.91	1.49	1.23
8	C	2018	NAG	C8-C7	11.45	1.74	1.50
8	E	2012	NAG	C8-C7	10.37	1.72	1.50
8	F	2005	NAG	C8-C7	9.16	1.69	1.50
8	F	2005	NAG	C1-C2	8.45	1.63	1.52
8	F	2005	NAG	O6-C6	7.65	1.74	1.42
8	E	2012	NAG	O7-C7	7.31	1.39	1.23
8	D	2006	NAG	C8-C7	6.64	1.64	1.50
8	F	2005	NAG	C2-N2	5.27	1.55	1.46
8	F	2006	NAG	O7-C7	-3.42	1.15	1.23
8	F	2006	NAG	C7-N2	2.99	1.44	1.34
8	C	2018	NAG	O6-C6	2.99	1.55	1.42
8	D	2006	NAG	C1-C2	2.49	1.55	1.52
8	B	2018	NAG	C1-C2	2.28	1.55	1.52
8	F	2006	NAG	C1-C2	2.22	1.55	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	2014	NAG	C1-O5-C5	6.36	120.71	112.19
8	C	2014	NAG	C1-O5-C5	5.97	120.19	112.19
8	F	2005	NAG	C1-O5-C5	5.46	119.51	112.19
8	D	2006	NAG	C8-C7-N2	-5.31	107.31	116.12
8	B	2014	NAG	C1-O5-C5	5.25	119.22	112.19
8	C	2018	NAG	O7-C7-N2	-5.14	112.90	121.98
8	C	2012	NAG	C1-O5-C5	4.65	118.41	112.19
8	F	2006	NAG	O7-C7-N2	-4.62	113.82	121.98
8	A	2018	NAG	C4-C3-C2	4.60	117.77	111.02
8	E	2006	NAG	C1-O5-C5	4.55	118.28	112.19
8	C	2018	NAG	C4-C3-C2	4.45	117.54	111.02
8	C	2018	NAG	O7-C7-C8	4.38	129.86	122.05
8	F	2006	NAG	C2-N2-C7	-4.22	117.24	122.90
8	C	2006	NAG	C1-O5-C5	4.05	117.61	112.19
8	B	2018	NAG	C4-C3-C2	4.01	116.89	111.02
8	F	2012	NAG	C2-N2-C7	3.93	128.17	122.90
8	C	2005	NAG	C2-N2-C7	3.90	128.13	122.90
8	B	2014	NAG	O5-C1-C2	-3.65	105.64	111.29
8	E	2012	NAG	O7-C7-C8	3.61	128.48	122.05
8	F	2009	NAG	C2-N2-C7	3.55	127.66	122.90
8	F	2008	NAG	C1-O5-C5	3.54	116.92	112.19
8	C	2005	NAG	C8-C7-N2	3.47	121.88	116.12
8	F	2005	NAG	O6-C6-C5	-3.46	99.55	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	2006	NAG	O5-C1-C2	3.44	116.61	111.29
8	B	2012	NAG	C1-O5-C5	3.40	116.75	112.19
8	D	2006	NAG	C2-N2-C7	-3.33	118.44	122.90
8	C	2005	NAG	C1-O5-C5	3.32	116.64	112.19
8	F	2014	NAG	C1-O5-C5	3.24	116.53	112.19
8	F	2009	NAG	C1-C2-N2	3.18	115.44	110.43
8	A	2012	NAG	C1-O5-C5	3.16	116.42	112.19
8	B	2006	NAG	O5-C1-C2	-3.13	106.45	111.29
8	F	2005	NAG	O7-C7-N2	-3.05	116.59	121.98
8	F	2006	NAG	O5-C1-C2	-3.03	106.60	111.29
8	F	2006	NAG	O7-C7-C8	3.02	127.43	122.05
8	E	2006	NAG	C2-N2-C7	3.00	126.93	122.90
8	F	2009	NAG	C1-O5-C5	2.88	116.05	112.19
8	C	2018	NAG	C3-C4-C5	2.86	115.42	110.23
8	D	2008	NAG	O5-C1-C2	-2.66	107.18	111.29
8	D	2006	NAG	C1-O5-C5	2.60	115.67	112.19
8	E	2006	NAG	C4-C3-C2	2.59	114.81	111.02
8	C	2012	NAG	C4-C3-C2	2.59	114.81	111.02
8	F	2012	NAG	C1-O5-C5	2.58	115.64	112.19
8	E	2012	NAG	C8-C7-N2	-2.53	111.91	116.12
8	E	2012	NAG	C1-O5-C5	2.53	115.58	112.19
8	D	2006	NAG	O5-C1-C2	-2.47	107.46	111.29
8	B	2005	NAG	O5-C1-C2	-2.47	107.47	111.29
8	A	2006	NAG	O5-C5-C4	-2.44	104.90	110.83
8	A	2018	NAG	C3-C4-C5	2.40	114.58	110.23
8	F	2005	NAG	O5-C1-C2	-2.32	107.70	111.29
8	B	2014	NAG	C1-C2-N2	2.29	114.05	110.43
8	C	2014	NAG	O5-C5-C4	2.28	116.38	110.83
8	A	2008	NAG	O5-C1-C2	-2.27	107.78	111.29
8	D	2005	NAG	C8-C7-N2	2.27	119.88	116.12
8	A	2006	NAG	C4-C3-C2	2.23	114.29	111.02
8	D	2005	NAG	O5-C1-C2	-2.21	107.87	111.29
8	F	2014	NAG	O5-C1-C2	-2.20	107.88	111.29
8	C	2014	NAG	C6-C5-C4	-2.16	107.71	113.02
8	A	2006	NAG	O5-C1-C2	-2.16	107.96	111.29
8	C	2005	NAG	O7-C7-C8	-2.15	118.22	122.05
8	E	2014	NAG	C6-C5-C4	-2.13	107.79	113.02
8	F	2009	NAG	O5-C1-C2	-2.11	108.03	111.29
8	B	2005	NAG	C8-C7-N2	2.09	119.58	116.12
8	E	2005	NAG	C8-C7-N2	2.04	119.51	116.12
8	D	2012	NAG	O5-C1-C2	2.02	114.41	111.29

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	2006	NAG	C1
8	A	2012	NAG	C1
8	A	2018	NAG	C1
8	B	2006	NAG	C1
8	B	2012	NAG	C1
8	B	2018	NAG	C1
8	C	2012	NAG	C1
8	C	2018	NAG	C1
8	D	2006	NAG	C1
8	E	2012	NAG	C1
8	F	2005	NAG	C1
8	F	2006	NAG	C1
8	F	2009	NAG	C1
8	F	2012	NAG	C1

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2012	NAG	C8-C7-N2-C2
8	A	2012	NAG	O7-C7-N2-C2
8	A	2014	NAG	O7-C7-N2-C2
8	B	2005	NAG	C8-C7-N2-C2
8	B	2005	NAG	O7-C7-N2-C2
8	B	2012	NAG	O7-C7-N2-C2
8	B	2014	NAG	C8-C7-N2-C2
8	B	2014	NAG	O7-C7-N2-C2
8	B	2018	NAG	C8-C7-N2-C2
8	B	2018	NAG	O7-C7-N2-C2
8	C	2018	NAG	C8-C7-N2-C2
8	C	2018	NAG	O7-C7-N2-C2
8	D	2005	NAG	C8-C7-N2-C2
8	D	2005	NAG	O7-C7-N2-C2
8	D	2006	NAG	C8-C7-N2-C2
8	D	2012	NAG	C8-C7-N2-C2
8	D	2012	NAG	O7-C7-N2-C2
8	D	2014	NAG	C8-C7-N2-C2
8	D	2014	NAG	O7-C7-N2-C2
8	E	2005	NAG	C8-C7-N2-C2
8	E	2005	NAG	O7-C7-N2-C2
8	E	2006	NAG	C1-C2-N2-C7
8	E	2006	NAG	C8-C7-N2-C2
8	E	2006	NAG	O7-C7-N2-C2
8	F	2005	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
8	F	2005	NAG	C8-C7-N2-C2
8	F	2005	NAG	O7-C7-N2-C2
8	F	2006	NAG	C8-C7-N2-C2
8	F	2006	NAG	O7-C7-N2-C2
8	F	2009	NAG	C8-C7-N2-C2
8	F	2009	NAG	O7-C7-N2-C2
8	F	2012	NAG	C3-C2-N2-C7
8	F	2012	NAG	C8-C7-N2-C2
8	F	2012	NAG	O7-C7-N2-C2
8	F	2014	NAG	C8-C7-N2-C2
8	F	2014	NAG	O7-C7-N2-C2
8	A	2006	NAG	O7-C7-N2-C2
8	A	2014	NAG	C8-C7-N2-C2
8	B	2012	NAG	C8-C7-N2-C2
8	D	2006	NAG	O7-C7-N2-C2
8	C	2018	NAG	O5-C5-C6-O6
8	C	2012	NAG	O5-C5-C6-O6
8	E	2014	NAG	O5-C5-C6-O6
8	A	2006	NAG	C8-C7-N2-C2
8	B	2006	NAG	C8-C7-N2-C2
8	B	2006	NAG	O7-C7-N2-C2
8	C	2006	NAG	C8-C7-N2-C2
8	C	2006	NAG	O7-C7-N2-C2
8	E	2012	NAG	O7-C7-N2-C2
8	B	2005	NAG	O5-C5-C6-O6
8	D	2014	NAG	C4-C5-C6-O6
8	F	2009	NAG	C4-C5-C6-O6
8	C	2005	NAG	O5-C5-C6-O6
8	D	2005	NAG	O5-C5-C6-O6
8	F	2012	NAG	O5-C5-C6-O6
8	B	2014	NAG	O5-C5-C6-O6
8	B	2018	NAG	O5-C5-C6-O6
8	E	2012	NAG	O5-C5-C6-O6
8	C	2012	NAG	C4-C5-C6-O6
8	C	2018	NAG	C4-C5-C6-O6
8	C	2014	NAG	O5-C5-C6-O6
8	B	2005	NAG	C4-C5-C6-O6
8	E	2012	NAG	C8-C7-N2-C2
8	E	2014	NAG	C4-C5-C6-O6
8	F	2009	NAG	O5-C5-C6-O6
8	C	2005	NAG	C4-C5-C6-O6
8	D	2005	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	B	2014	NAG	C4-C5-C6-O6
8	D	2014	NAG	O5-C5-C6-O6
8	B	2018	NAG	C4-C5-C6-O6
8	C	2014	NAG	C4-C5-C6-O6
8	C	2005	NAG	C8-C7-N2-C2
8	C	2005	NAG	O7-C7-N2-C2
8	E	2008	NAG	O5-C5-C6-O6
8	B	2012	NAG	O5-C5-C6-O6
8	F	2012	NAG	C4-C5-C6-O6
8	A	2006	NAG	O5-C5-C6-O6
8	A	2006	NAG	C4-C5-C6-O6
8	A	2012	NAG	O5-C5-C6-O6
8	F	2005	NAG	C3-C2-N2-C7
8	F	2006	NAG	C4-C5-C6-O6
8	E	2012	NAG	C4-C5-C6-O6
8	A	2018	NAG	C8-C7-N2-C2
8	E	2008	NAG	C4-C5-C6-O6
8	A	2018	NAG	O7-C7-N2-C2
8	C	2014	NAG	C8-C7-N2-C2
8	F	2009	NAG	C3-C2-N2-C7
8	F	2006	NAG	O5-C5-C6-O6
8	C	2014	NAG	O7-C7-N2-C2
8	D	2012	NAG	C3-C2-N2-C7
8	A	2018	NAG	C4-C5-C6-O6
8	D	2012	NAG	O5-C5-C6-O6
8	B	2012	NAG	C4-C5-C6-O6
8	D	2012	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

**Warning:** The R factor obtained from EDS is 0.3081, which does not match the depositor's R factor of 0.22563. Please interpret the results in this section carefully.

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	529/534 (99%)	1.54	140 (26%)	2 2	67, 69, 71, 74	0
1	B	529/534 (99%)	1.08	55 (10%)	13 10	67, 69, 71, 74	0
1	C	529/534 (99%)	1.72	193 (36%)	1 1	67, 69, 71, 74	0
1	D	529/534 (99%)	1.45	112 (21%)	3 3	67, 69, 71, 73	0
1	E	529/534 (99%)	1.51	122 (23%)	2 3	68, 69, 71, 73	0
1	F	529/534 (99%)	2.56	342 (64%)	0 0	68, 69, 71, 73	0
All	All	3174/3204 (99%)	1.64	964 (30%)	1 1	67, 69, 71, 74	0

All (964) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	550	ALA	7.6
1	F	436	GLY	7.2
1	D	533	ALA	6.5
1	F	533	ALA	6.4
1	F	454	PRO	6.3
1	A	397	LYS	6.3
1	F	376	SER	5.9
1	A	533	ALA	5.9
1	F	435	LEU	5.9
1	F	87	GLN	5.9
1	F	313	SER	5.9
1	F	549	HIS	5.8
1	F	108	SER	5.8
1	F	38	ASP	5.7
1	F	105	ALA	5.7
1	F	266	ASP	5.7

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Mol	Chain	Res	Type	RSRZ
1	F	446	ASN	5.7
1	F	109	THR	5.5
1	F	372	THR	5.5
1	C	540	THR	5.4
1	F	503	PHE	5.4
1	F	96	VAL	5.3
1	F	526	VAL	5.3
1	C	533	ALA	5.3
1	C	493	GLY	5.3
1	F	307	THR	5.2
1	D	312	ASP	5.2
1	F	444	PRO	5.2
1	F	291	LEU	5.2
1	F	99	LEU	5.1
1	C	177	SER	5.1
1	F	504	GLY	5.1
1	D	535	ASN	5.0
1	F	306	PRO	5.0
1	B	535	ASN	5.0
1	F	536	THR	5.0
1	B	540	THR	4.9
1	F	294	THR	4.9
1	F	188	PRO	4.9
1	F	355	ALA	4.9
1	F	453	TYR	4.9
1	F	302	THR	4.9
1	F	543	THR	4.9
1	A	272	ALA	4.9
1	F	287	SER	4.8
1	C	352	VAL	4.8
1	F	309	ASN	4.8
1	D	290	GLN	4.8
1	F	286	PRO	4.8
1	F	385	ILE	4.8
1	D	534	ALA	4.8
1	F	206	ASP	4.7
1	E	184	ALA	4.7
1	F	514	SER	4.7
1	F	312	ASP	4.7
1	B	529	GLU	4.7
1	A	540	THR	4.7
1	F	428	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	474	ALA	4.6
1	C	196	THR	4.6
1	F	347	ASN	4.5
1	F	178	VAL	4.5
1	D	241	THR	4.5
1	F	164	TYR	4.5
1	F	325	PRO	4.5
1	F	303	ALA	4.4
1	F	542	LEU	4.4
1	E	535	ASN	4.4
1	A	302	THR	4.4
1	F	508	ALA	4.4
1	F	290	GLN	4.3
1	A	549	HIS	4.3
1	F	529	GLU	4.3
1	E	540	THR	4.3
1	E	269	LYS	4.3
1	F	425	ILE	4.3
1	A	228	ASP	4.3
1	C	102	CYS	4.3
1	F	451	PRO	4.3
1	C	179	TYR	4.3
1	C	39	GLY	4.3
1	F	84	GLY	4.3
1	F	530	GLY	4.3
1	F	520	VAL	4.2
1	F	59	VAL	4.2
1	F	361	THR	4.2
1	C	198	ASN	4.2
1	F	353	ASN	4.2
1	E	454	PRO	4.2
1	F	103	PRO	4.2
1	B	533	ALA	4.2
1	C	304	ALA	4.2
1	F	184	ALA	4.2
1	A	372	THR	4.2
1	F	28	TRP	4.2
1	A	198	ASN	4.2
1	F	349	LYS	4.2
1	C	538	ASP	4.2
1	C	38	ASP	4.1
1	C	178	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	465	GLN	4.1
1	F	308	GLN	4.1
1	C	40	LEU	4.1
1	F	305	LEU	4.1
1	B	146	ASP	4.1
1	D	549	HIS	4.1
1	A	303	ALA	4.1
1	A	299	TYR	4.1
1	F	359	ASN	4.1
1	F	400	ILE	4.1
1	F	539	LEU	4.0
1	E	333	GLY	4.0
1	C	515	GLU	4.0
1	A	245	VAL	4.0
1	F	131	GLY	4.0
1	F	462	VAL	4.0
1	E	549	HIS	4.0
1	E	113	ASN	4.0
1	F	265	ASN	4.0
1	F	507	ASP	4.0
1	E	262	HIS	4.0
1	F	513	LEU	4.0
1	E	400	ILE	4.0
1	F	181	PRO	3.9
1	A	270	ASN	3.9
1	F	443	ASP	3.9
1	C	524	CYS	3.9
1	F	301	LYS	3.9
1	C	539	LEU	3.9
1	F	118	TYR	3.9
1	A	36	ASN	3.9
1	C	300	ASN	3.9
1	F	227	GLU	3.8
1	F	237	ASP	3.8
1	F	445	ASP	3.8
1	C	370	LEU	3.8
1	A	534	ALA	3.8
1	B	205	PRO	3.8
1	F	548	GLN	3.8
1	E	435	LEU	3.8
1	F	100	THR	3.8
1	A	311	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	298	VAL	3.8
1	C	36	ASN	3.8
1	C	292	ASN	3.8
1	D	307	THR	3.8
1	A	378	ASP	3.8
1	F	136	GLY	3.8
1	F	322	TYR	3.8
1	A	298	VAL	3.8
1	E	261	VAL	3.8
1	F	244	ASN	3.8
1	F	434	ALA	3.8
1	F	342	ASP	3.8
1	F	431	TYR	3.8
1	D	272	ALA	3.7
1	F	493	GLY	3.7
1	F	323	LEU	3.7
1	A	294	THR	3.7
1	F	475	ASP	3.7
1	F	101	GLN	3.7
1	E	299	TYR	3.7
1	E	547	VAL	3.7
1	F	209	TYR	3.7
1	F	296	TYR	3.7
1	A	292	ASN	3.7
1	A	536	THR	3.7
1	F	360	ILE	3.7
1	F	98	PHE	3.7
1	D	71	ASN	3.7
1	F	191	LEU	3.7
1	B	42	SER	3.6
1	C	531	ASN	3.6
1	F	270	ASN	3.6
1	A	550	ALA	3.6
1	F	388	SER	3.6
1	F	540	THR	3.6
1	F	180	ASN	3.6
1	F	345	MET	3.6
1	F	505	ILE	3.6
1	B	228	ASP	3.6
1	E	130	ASP	3.6
1	C	34	TYR	3.6
1	C	169	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	29	THR	3.6
1	F	77	ASN	3.6
1	F	476	ASN	3.6
1	A	130	ASP	3.6
1	E	378	ASP	3.6
1	F	534	ALA	3.6
1	F	310	TYR	3.6
1	A	226	ILE	3.5
1	F	48	CYS	3.5
1	F	104	ILE	3.5
1	E	51	GLN	3.5
1	B	292	ASN	3.5
1	F	406	ASN	3.5
1	E	304	ALA	3.5
1	C	501	ASP	3.5
1	A	227	GLU	3.5
1	F	419	GLY	3.5
1	D	503	PHE	3.5
1	D	539	LEU	3.5
1	D	38	ASP	3.4
1	F	338	VAL	3.4
1	D	540	THR	3.4
1	C	175	PHE	3.4
1	C	289	LEU	3.4
1	D	254	ALA	3.4
1	D	380	ALA	3.4
1	E	431	TYR	3.4
1	C	33	ASP	3.4
1	F	31	GLY	3.4
1	F	288	ASP	3.4
1	F	346	ASP	3.4
1	E	455	MET	3.4
1	C	508	ALA	3.4
1	D	508	ALA	3.4
1	C	163	TRP	3.4
1	A	71	ASN	3.4
1	E	497	VAL	3.4
1	E	526	VAL	3.4
1	F	311	VAL	3.4
1	F	437	GLU	3.4
1	E	544	GLY	3.4
1	F	179	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	445	ASP	3.4
1	F	374	LEU	3.4
1	F	205	PRO	3.4
1	F	525	SER	3.4
1	C	513	LEU	3.3
1	F	405	LEU	3.3
1	F	70	THR	3.3
1	A	535	ASN	3.3
1	C	190	ASN	3.3
1	D	329	GLU	3.3
1	F	496	LEU	3.3
1	B	130	ASP	3.3
1	A	207	THR	3.3
1	D	506	GLN	3.3
1	C	262	HIS	3.3
1	E	384	GLU	3.3
1	A	105	ALA	3.3
1	A	304	ALA	3.3
1	F	429	ARG	3.3
1	F	340	THR	3.3
1	F	46	ILE	3.3
1	D	367	VAL	3.3
1	E	154	GLU	3.3
1	F	518	LEU	3.3
1	F	34	TYR	3.3
1	F	510	SER	3.3
1	C	29	THR	3.3
1	C	100	THR	3.3
1	D	390	THR	3.3
1	C	549	HIS	3.3
1	C	529	GLU	3.3
1	F	356	PHE	3.2
1	D	180	ASN	3.2
1	E	527	ALA	3.2
1	F	78	THR	3.2
1	A	537	LEU	3.2
1	C	305	LEU	3.2
1	A	309	ASN	3.2
1	A	200	THR	3.2
1	F	116	VAL	3.2
1	F	248	MET	3.2
1	C	41	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	389	ASN	3.2
1	A	47	THR	3.2
1	A	39	GLY	3.2
1	C	31	GLY	3.2
1	D	400	ILE	3.2
1	E	265	ASN	3.2
1	F	420	HIS	3.2
1	A	196	THR	3.2
1	D	258	THR	3.2
1	F	521	CYS	3.2
1	A	532	ALA	3.1
1	F	455	MET	3.1
1	D	292	ASN	3.1
1	B	549	HIS	3.1
1	C	291	LEU	3.1
1	F	65	VAL	3.1
1	D	466	SER	3.1
1	E	207	THR	3.1
1	D	538	ASP	3.1
1	E	503	PHE	3.1
1	F	482	PHE	3.1
1	F	448	PRO	3.1
1	F	67	ILE	3.1
1	F	298	VAL	3.1
1	F	531	ASN	3.1
1	C	302	THR	3.1
1	D	313	SER	3.1
1	D	530	GLY	3.1
1	E	183	GLY	3.1
1	F	241	THR	3.1
1	C	402	GLU	3.1
1	D	306	PRO	3.1
1	E	150	TYR	3.1
1	F	27	ASN	3.1
1	F	71	ASN	3.1
1	F	492	GLN	3.1
1	F	412	THR	3.1
1	B	117	ASP	3.1
1	F	40	LEU	3.1
1	A	269	LYS	3.1
1	E	389	ASN	3.1
1	F	43	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	89	GLY	3.1
1	F	471	ARG	3.1
1	F	182	THR	3.1
1	A	295	SER	3.1
1	C	254	ALA	3.1
1	E	550	ALA	3.1
1	F	494	LEU	3.0
1	F	413	HIS	3.0
1	F	133	TYR	3.0
1	C	107	GLY	3.0
1	C	377	GLY	3.0
1	A	30	THR	3.0
1	C	536	THR	3.0
1	F	30	THR	3.0
1	F	449	ALA	3.0
1	F	452	GLU	3.0
1	F	32	TRP	3.0
1	A	38	ASP	3.0
1	D	130	ASP	3.0
1	A	203	VAL	3.0
1	C	43	ARG	3.0
1	C	164	TYR	3.0
1	F	50	GLY	3.0
1	E	90	THR	3.0
1	F	358	ASN	3.0
1	F	186	PRO	3.0
1	C	253	VAL	3.0
1	F	501	ASP	3.0
1	F	64	ARG	3.0
1	D	310	TYR	3.0
1	C	439	PRO	3.0
1	D	259	VAL	3.0
1	D	373	VAL	3.0
1	D	342	ASP	3.0
1	F	26	PHE	3.0
1	F	321	PHE	3.0
1	C	306	PRO	3.0
1	C	99	LEU	3.0
1	D	78	THR	3.0
1	F	49	ASN	3.0
1	B	329	GLU	3.0
1	F	173	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	102	CYS	2.9
1	A	146	ASP	2.9
1	C	170	ASP	2.9
1	D	428	ASP	2.9
1	F	130	ASP	2.9
1	F	260	LEU	2.9
1	A	115	THR	2.9
1	A	154	GLU	2.9
1	C	77	ASN	2.9
1	F	230	GLU	2.9
1	D	311	VAL	2.9
1	F	233	VAL	2.9
1	E	440	HIS	2.9
1	C	356	PHE	2.9
1	D	288	ASP	2.9
1	F	279	ASP	2.9
1	F	450	PHE	2.9
1	F	51	GLN	2.9
1	F	187	ILE	2.9
1	C	299	TYR	2.9
1	C	307	THR	2.9
1	F	430	THR	2.9
1	F	83	HIS	2.9
1	A	512	GLN	2.9
1	E	408	GLN	2.9
1	F	289	LEU	2.9
1	A	446	ASN	2.9
1	D	300	ASN	2.9
1	D	476	ASN	2.9
1	A	271	PHE	2.9
1	C	165	HIS	2.9
1	F	480	TRP	2.9
1	C	530	GLY	2.9
1	A	342	ASP	2.9
1	C	507	ASP	2.9
1	F	537	LEU	2.9
1	F	197	MET	2.9
1	C	351	GLY	2.8
1	D	121	GLY	2.8
1	D	493	GLY	2.8
1	C	44	PRO	2.8
1	F	541	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	293	ALA	2.8
1	E	272	ALA	2.8
1	A	129	THR	2.8
1	A	107	GLY	2.8
1	E	385	ILE	2.8
1	F	368	PRO	2.8
1	C	145	ASP	2.8
1	F	247	ASP	2.8
1	C	272	ALA	2.8
1	C	303	ALA	2.8
1	A	233	VAL	2.8
1	F	68	TYR	2.8
1	C	30	THR	2.8
1	D	543	THR	2.8
1	A	273	ILE	2.8
1	C	353	ASN	2.8
1	E	537	LEU	2.8
1	B	419	GLY	2.8
1	C	201	TRP	2.8
1	C	130	ASP	2.8
1	D	550	ALA	2.8
1	F	532	ALA	2.8
1	F	404	VAL	2.8
1	F	463	ARG	2.8
1	F	442	PHE	2.8
1	E	239	ILE	2.8
1	C	408	GLN	2.8
1	C	421	ALA	2.8
1	E	108	SER	2.8
1	E	533	ALA	2.8
1	D	146	ASP	2.8
1	E	38	ASP	2.8
1	F	315	ASP	2.8
1	A	34	TYR	2.8
1	C	453	TYR	2.8
1	C	47	THR	2.8
1	E	524	CYS	2.8
1	F	240	THR	2.8
1	A	509	HIS	2.8
1	D	477	PRO	2.7
1	C	71	ASN	2.7
1	C	105	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	220	VAL	2.7
1	F	272	ALA	2.7
1	B	206	ASP	2.7
1	B	312	ASP	2.7
1	C	117	ASP	2.7
1	D	144	LYS	2.7
1	F	269	LYS	2.7
1	B	539	LEU	2.7
1	C	543	THR	2.7
1	E	536	THR	2.7
1	F	165	HIS	2.7
1	F	95	GLY	2.7
1	F	477	PRO	2.7
1	A	274	MET	2.7
1	D	309	ASN	2.7
1	F	488	TRP	2.7
1	A	264	LYS	2.7
1	C	42	SER	2.7
1	A	539	LEU	2.7
1	C	342	ASP	2.7
1	F	402	GLU	2.7
1	C	104	ILE	2.7
1	F	461	TYR	2.7
1	F	410	THR	2.7
1	D	84	GLY	2.7
1	C	309	ASN	2.7
1	C	37	VAL	2.7
1	E	245	VAL	2.7
1	E	397	LYS	2.7
1	F	69	LEU	2.7
1	F	460	LEU	2.7
1	A	42	SER	2.7
1	E	466	SER	2.7
1	A	278	ASP	2.7
1	E	361	THR	2.7
1	F	115	THR	2.7
1	F	392	THR	2.7
1	E	451	PRO	2.7
1	A	382	ASN	2.7
1	C	270	ASN	2.7
1	F	426	GLN	2.7
1	B	435	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	114	PHE	2.7
1	A	296	TYR	2.7
1	A	507	ASP	2.7
1	B	78	THR	2.7
1	F	232	THR	2.7
1	F	299	TYR	2.7
1	F	424	THR	2.7
1	F	517	HIS	2.7
1	C	218	GLY	2.7
1	C	544	GLY	2.7
1	F	243	LYS	2.6
1	C	522	GLN	2.6
1	C	395	LEU	2.6
1	F	111	LEU	2.6
1	F	370	LEU	2.6
1	E	334	GLU	2.6
1	F	137	MET	2.6
1	E	514	SER	2.6
1	A	451	PRO	2.6
1	E	495	GLY	2.6
1	F	112	TYR	2.6
1	F	326	TYR	2.6
1	F	351	GLY	2.6
1	C	284	VAL	2.6
1	F	45	VAL	2.6
1	B	380	ALA	2.6
1	A	229	HIS	2.6
1	A	147	SER	2.6
1	C	514	SER	2.6
1	D	338	VAL	2.6
1	E	253	VAL	2.6
1	E	462	VAL	2.6
1	C	527	ALA	2.6
1	D	474	ALA	2.6
1	F	148	PHE	2.6
1	F	175	PHE	2.6
1	C	350	ASN	2.6
1	F	467	ASN	2.6
1	F	335	PRO	2.6
1	A	366	LYS	2.6
1	C	411	GLY	2.6
1	D	397	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	530	GLY	2.6
1	F	377	GLY	2.6
1	C	294	THR	2.6
1	F	246	THR	2.6
1	E	441	SER	2.6
1	F	42	SER	2.6
1	F	161	SER	2.6
1	F	174	SER	2.6
1	F	319	ASP	2.6
1	F	438	VAL	2.6
1	E	40	LEU	2.6
1	F	271	PHE	2.6
1	B	74	ASN	2.6
1	F	242	GLU	2.6
1	D	544	GLY	2.6
1	A	310	TYR	2.6
1	B	241	THR	2.6
1	D	392	THR	2.6
1	F	200	THR	2.6
1	F	280	THR	2.6
1	A	261	VAL	2.6
1	C	79	SER	2.6
1	B	542	LEU	2.6
1	C	167	LEU	2.6
1	D	235	GLU	2.5
1	D	411	GLY	2.5
1	F	544	GLY	2.5
1	B	34	TYR	2.5
1	C	310	TYR	2.5
1	C	520	VAL	2.5
1	D	25	THR	2.5
1	C	490	LEU	2.5
1	A	145	ASP	2.5
1	A	409	ASP	2.5
1	D	170	ASP	2.5
1	F	268	ASP	2.5
1	E	481	PHE	2.5
1	B	531	ASN	2.5
1	D	74	ASN	2.5
1	E	62	GLY	2.5
1	A	169	THR	2.5
1	A	199	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	220	VAL	2.5
1	A	367	VAL	2.5
1	E	294	THR	2.5
1	F	76	THR	2.5
1	F	110	MET	2.5
1	F	357	PHE	2.5
1	C	473	LYS	2.5
1	F	81	HIS	2.5
1	C	399	GLU	2.5
1	C	311	VAL	2.5
1	F	85	LEU	2.5
1	A	208	THR	2.5
1	E	322	TYR	2.5
1	D	226	ILE	2.5
1	F	277	PHE	2.5
1	A	106	PRO	2.5
1	C	286	PRO	2.5
1	A	262	HIS	2.5
1	B	22	GLU	2.5
1	F	102	CYS	2.5
1	A	190	ASN	2.5
1	E	406	ASN	2.5
1	F	401	VAL	2.5
1	F	479	VAL	2.5
1	A	241	THR	2.5
1	C	532	ALA	2.5
1	E	196	THR	2.5
1	F	143	ILE	2.5
1	F	239	ILE	2.5
1	F	144	LYS	2.4
1	B	288	ASP	2.4
1	C	161	SER	2.4
1	F	465	GLN	2.4
1	C	188	PRO	2.4
1	F	502	PRO	2.4
1	A	183	GLY	2.4
1	F	333	GLY	2.4
1	A	384	GLU	2.4
1	D	435	LEU	2.4
1	C	45	VAL	2.4
1	C	367	VAL	2.4
1	C	547	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	298	VAL	2.4
1	F	93	MET	2.4
1	F	341	VAL	2.4
1	A	244	ASN	2.4
1	C	180	ASN	2.4
1	E	270	ASN	2.4
1	F	381	ASN	2.4
1	D	184	ALA	2.4
1	D	532	ALA	2.4
1	F	304	ALA	2.4
1	C	173	LYS	2.4
1	C	263	THR	2.4
1	C	397	LYS	2.4
1	E	148	PHE	2.4
1	E	267	THR	2.4
1	E	271	PHE	2.4
1	F	317	PHE	2.4
1	C	326	TYR	2.4
1	F	457	ARG	2.4
1	A	108	SER	2.4
1	C	268	ASP	2.4
1	E	283	ASP	2.4
1	F	97	PRO	2.4
1	F	432	ASP	2.4
1	C	28	TRP	2.4
1	C	139	GLY	2.4
1	E	377	GLY	2.4
1	F	121	GLY	2.4
1	C	274	MET	2.4
1	D	529	GLU	2.4
1	E	499	VAL	2.4
1	F	176	MET	2.4
1	D	104	ILE	2.4
1	A	300	ASN	2.4
1	B	36	ASN	2.4
1	B	397	LYS	2.4
1	C	184	ALA	2.4
1	C	269	LYS	2.4
1	E	303	ALA	2.4
1	D	528	THR	2.4
1	F	47	THR	2.4
1	A	522	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	205	PRO	2.4
1	C	477	PRO	2.4
1	D	151	ASP	2.4
1	D	171	LEU	2.4
1	D	289	LEU	2.4
1	E	432	ASP	2.4
1	F	63	ASP	2.4
1	F	398	ASP	2.4
1	F	498	LEU	2.4
1	B	352	VAL	2.4
1	C	384	GLU	2.4
1	A	184	ALA	2.4
1	F	36	ASN	2.4
1	F	113	ASN	2.4
1	F	292	ASN	2.4
1	C	267	THR	2.4
1	D	302	THR	2.4
1	F	256	ARG	2.4
1	F	332	TYR	2.4
1	B	66	GLN	2.4
1	F	66	GLN	2.4
1	F	371	MET	2.4
1	A	157	SER	2.4
1	A	268	ASP	2.4
1	C	32	TRP	2.4
1	C	398	ASP	2.4
1	D	127	SER	2.4
1	E	151	ASP	2.4
1	F	170	ASP	2.4
1	C	202	GLU	2.4
1	E	227	GLU	2.4
1	F	515	GLU	2.4
1	D	27	ASN	2.4
1	E	390	THR	2.4
1	F	300	ASN	2.4
1	F	316	ASN	2.4
1	F	257	TYR	2.3
1	C	325	PRO	2.3
1	C	297	MET	2.3
1	F	522	GLN	2.3
1	A	544	GLY	2.3
1	A	221	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	336	ASP	2.3
1	D	159	SER	2.3
1	E	61	LYS	2.3
1	F	344	VAL	2.3
1	D	105	ALA	2.3
1	D	303	ALA	2.3
1	A	194	ASN	2.3
1	A	389	ASN	2.3
1	E	198	ASN	2.3
1	F	23	THR	2.3
1	E	374	LEU	2.3
1	A	308	GLN	2.3
1	C	379	GLN	2.3
1	C	465	GLN	2.3
1	D	419	GLY	2.3
1	E	95	GLY	2.3
1	E	469	VAL	2.3
1	F	245	VAL	2.3
1	C	226	ILE	2.3
1	A	170	ASP	2.3
1	A	399	GLU	2.3
1	A	538	ASP	2.3
1	D	507	ASP	2.3
1	D	510	SER	2.3
1	E	437	GLU	2.3
1	C	550	ALA	2.3
1	E	254	ALA	2.3
1	A	280	THR	2.3
1	C	129	THR	2.3
1	C	410	THR	2.3
1	A	167	LEU	2.3
1	D	531	ASN	2.3
1	D	296	TYR	2.3
1	A	379	GLN	2.3
1	C	84	GLY	2.3
1	C	436	GLY	2.3
1	F	337	HIS	2.3
1	F	373	VAL	2.3
1	F	411	GLY	2.3
1	F	547	VAL	2.3
1	C	486	ILE	2.3
1	A	443	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	38	ASP	2.3
1	B	145	ASP	2.3
1	B	449	ALA	2.3
1	F	177	SER	2.3
1	C	171	LEU	2.3
1	D	274	MET	2.3
1	E	231	MET	2.3
1	F	348	LEU	2.3
1	A	528	THR	2.3
1	B	543	THR	2.3
1	D	23	THR	2.3
1	F	267	THR	2.3
1	A	381	ASN	2.3
1	A	546	ASN	2.3
1	C	308	GLN	2.3
1	F	408	GLN	2.3
1	C	95	GLY	2.3
1	E	517	HIS	2.3
1	F	120	VAL	2.3
1	F	238	GLY	2.3
1	C	480	TRP	2.3
1	F	334	GLU	2.3
1	D	378	ASP	2.3
1	E	342	ASP	2.3
1	F	283	ASP	2.3
1	B	99	LEU	2.3
1	D	260	LEU	2.3
1	A	502	PRO	2.3
1	C	280	THR	2.3
1	F	369	THR	2.3
1	E	467	ASN	2.2
1	A	192	ILE	2.2
1	C	192	ILE	2.2
1	C	373	VAL	2.2
1	E	66	GLN	2.2
1	F	314	ILE	2.2
1	A	225	TRP	2.2
1	B	434	ALA	2.2
1	B	534	ALA	2.2
1	C	225	TRP	2.2
1	C	545	GLU	2.2
1	F	330	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	221	SER	2.2
1	D	383	SER	2.2
1	F	278	ASP	2.2
1	F	538	ASP	2.2
1	D	464	PRO	2.2
1	E	464	PRO	2.2
1	E	412	THR	2.2
1	F	172	THR	2.2
1	C	46	ILE	2.2
1	C	419	GLY	2.2
1	D	401	VAL	2.2
1	E	425	ILE	2.2
1	F	183	GLY	2.2
1	F	535	ASN	2.2
1	E	256	ARG	2.2
1	C	162	GLU	2.2
1	D	304	ALA	2.2
1	E	402	GLU	2.2
1	F	380	ALA	2.2
1	A	291	LEU	2.2
1	C	146	ASP	2.2
1	F	145	ASP	2.2
1	F	336	ASP	2.2
1	C	466	SER	2.2
1	C	368	PRO	2.2
1	F	414	PRO	2.2
1	E	47	THR	2.2
1	A	31	GLY	2.2
1	B	311	VAL	2.2
1	C	273	ILE	2.2
1	F	213	ILE	2.2
1	F	469	VAL	2.2
1	A	204	GLN	2.2
1	B	512	GLN	2.2
1	C	509	HIS	2.2
1	A	467	ASN	2.2
1	C	516	ASN	2.2
1	D	198	ASN	2.2
1	F	350	ASN	2.2
1	A	43	ARG	2.2
1	D	271	PHE	2.2
1	F	52	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	393	PHE	2.2
1	C	293	ALA	2.2
1	C	327	GLU	2.2
1	E	529	GLU	2.2
1	D	85	LEU	2.2
1	E	318	LEU	2.2
1	E	490	LEU	2.2
1	A	541	ASP	2.2
1	B	501	ASP	2.2
1	B	528	THR	2.2
1	C	401	VAL	2.2
1	F	90	THR	2.2
1	C	183	GLY	2.2
1	C	189	GLN	2.2
1	F	324	GLN	2.2
1	C	354	TYR	2.2
1	E	215	ASN	2.2
1	E	386	TYR	2.2
1	F	254	ALA	2.2
1	A	519	GLU	2.2
1	C	106	PRO	2.2
1	F	409	ASP	2.2
1	A	313	SER	2.2
1	F	441	SER	2.2
1	A	526	VAL	2.2
1	B	341	VAL	2.2
1	E	344	VAL	2.2
1	F	261	VAL	2.2
1	E	302	THR	2.1
1	D	416	HIS	2.1
1	A	297	MET	2.1
1	D	34	TYR	2.1
1	D	118	TYR	2.1
1	B	550	ALA	2.1
1	E	264	LYS	2.1
1	D	384	GLU	2.1
1	F	384	GLU	2.1
1	E	28	TRP	2.1
1	B	314	ILE	2.1
1	C	166	ASP	2.1
1	E	313	SER	2.1
1	A	232	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	267	THR	2.1
1	E	436	GLY	2.1
1	E	337	HIS	2.1
1	C	511	GLN	2.1
1	D	204	GLN	2.1
1	F	222	GLN	2.1
1	A	210	LEU	2.1
1	C	366	LYS	2.1
1	F	395	LEU	2.1
1	F	162	GLU	2.1
1	A	306	PRO	2.1
1	C	451	PRO	2.1
1	C	193	VAL	2.1
1	D	547	VAL	2.1
1	A	279	ASP	2.1
1	E	145	ASP	2.1
1	F	107	GLY	2.1
1	B	302	THR	2.1
1	D	418	HIS	2.1
1	E	376	SER	2.1
1	E	543	THR	2.1
1	F	447	HIS	2.1
1	B	260	LEU	2.1
1	C	69	LEU	2.1
1	F	250	TYR	2.1
1	B	227	GLU	2.1
1	F	382	ASN	2.1
1	F	365	PRO	2.1
1	F	524	CYS	2.1
1	C	261	VAL	2.1
1	D	404	VAL	2.1
1	E	367	VAL	2.1
1	C	197	MET	2.1
1	B	409	ASP	2.1
1	E	366	LYS	2.1
1	F	416	HIS	2.1
1	C	200	THR	2.1
1	C	348	LEU	2.1
1	D	280	THR	2.1
1	E	323	LEU	2.1
1	F	249	LEU	2.1
1	F	263	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	290	GLN	2.1
1	A	510	SER	2.1
1	D	66	GLN	2.1
1	D	525	SER	2.1
1	C	380	ALA	2.1
1	A	431	TYR	2.1
1	D	150	TYR	2.1
1	E	223	TYR	2.1
1	C	505	ILE	2.1
1	D	32	TRP	2.1
1	A	168	VAL	2.1
1	B	547	VAL	2.1
1	E	59	VAL	2.1
1	F	168	VAL	2.1
1	A	136	GLY	2.1
1	A	440	HIS	2.1
1	A	450	PHE	2.1
1	C	271	PHE	2.1
1	C	494	LEU	2.0
1	A	390	THR	2.0
1	A	465	GLN	2.0
1	B	23	THR	2.0
1	C	278	ASP	2.0
1	D	100	THR	2.0
1	E	423	GLN	2.0
1	F	146	ASP	2.0
1	C	296	TYR	2.0
1	A	27	ASN	2.0
1	C	407	ASN	2.0
1	D	143	ILE	2.0
1	E	476	ASN	2.0
1	A	163	TRP	2.0
1	C	35	ARG	2.0
1	E	341	VAL	2.0
1	E	401	VAL	2.0
1	A	50	GLY	2.0
1	B	544	GLY	2.0
1	F	139	GLY	2.0
1	D	542	LEU	2.0
1	F	140	LEU	2.0
1	A	87	GLN	2.0
1	B	115	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	51	GLN	2.0
1	C	207	THR	2.0
1	D	232	THR	2.0
1	E	263	THR	2.0
1	F	511	GLN	2.0
1	F	378	ASP	2.0
1	C	157	SER	2.0
1	A	209	TYR	2.0
1	C	332	TYR	2.0
1	F	125	TYR	2.0
1	B	451	PRO	2.0
1	F	285	ILE	2.0
1	C	281	MET	2.0
1	D	347	ASN	2.0
1	B	462	VAL	2.0
1	C	212	ARG	2.0
1	F	328	LYS	2.0
1	D	480	TRP	2.0
1	E	201	TRP	2.0
1	C	495	GLY	2.0
1	E	411	GLY	2.0
1	F	39	GLY	2.0
1	F	318	LEU	2.0
1	F	128	HIS	2.0

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

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

## 6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	E	2005	14/15	0.29	0.23	70,71,71,71	0
8	NAG	E	2012	14/15	0.35	0.23	73,74,77,77	0
8	NAG	F	2012	14/15	0.35	0.22	72,73,75,75	0
8	NAG	F	2006	14/15	0.37	0.23	67,68,70,70	0
8	NAG	C	2018	14/15	0.52	0.19	74,76,77,78	0
8	NAG	E	2008	14/15	0.53	0.22	72,72,73,73	0
8	NAG	A	2018	14/15	0.53	0.20	78,80,82,82	0
8	NAG	D	2014	14/15	0.54	0.21	65,66,67,67	0
8	NAG	E	2006	14/15	0.55	0.22	73,74,75,76	0
8	NAG	F	2008	14/15	0.56	0.23	71,71,72,72	0
8	NAG	B	2014	14/15	0.56	0.22	67,70,71,71	0
8	NAG	B	2018	14/15	0.60	0.18	80,83,83,83	0
8	NAG	F	2005	14/15	0.61	0.18	67,70,71,72	0
8	NAG	F	2009	14/15	0.61	0.19	66,69,69,69	0
8	NAG	C	2006	14/15	0.61	0.19	74,76,77,78	0
8	NAG	D	2006	14/15	0.63	0.18	65,68,70,71	0
8	NAG	A	2006	14/15	0.64	0.19	71,73,74,74	0
8	NAG	C	2012	14/15	0.69	0.18	75,77,79,80	0
8	NAG	A	2012	14/15	0.71	0.18	76,79,80,81	0
8	NAG	D	2012	14/15	0.72	0.16	73,74,76,77	0
8	NAG	D	2008	14/15	0.73	0.19	70,71,73,73	0
8	NAG	D	2005	14/15	0.73	0.18	71,72,74,75	0
8	NAG	F	2014	14/15	0.74	0.16	59,62,63,64	0
8	NAG	B	2006	14/15	0.76	0.14	74,76,78,79	0
8	NAG	A	2014	14/15	0.79	0.16	67,67,71,72	0
8	NAG	B	2012	14/15	0.79	0.15	74,75,79,79	0
8	NAG	B	2005	14/15	0.83	0.14	64,67,69,70	0
8	NAG	C	2005	14/15	0.83	0.16	64,68,70,70	0
8	NAG	E	2014	14/15	0.84	0.13	52,56,57,58	0
8	NAG	A	2008	14/15	0.86	0.15	68,69,70,70	0
8	NAG	C	2014	14/15	0.88	0.12	53,55,57,58	0
9	CU1	F	1001	1/1	0.89	0.19	90,90,90,90	0
9	CU1	D	1004	1/1	0.92	0.18	100,100,100,100	0
9	CU1	F	1004	1/1	0.94	0.17	100,100,100,100	0
9	CU1	C	1004	1/1	0.95	0.16	100,100,100,100	0
9	CU1	F	1003	1/1	0.95	0.14	91,91,91,91	0
9	CU1	A	1004	1/1	0.95	0.12	100,100,100,100	0
9	CU1	E	1004	1/1	0.96	0.15	100,100,100,100	0
9	CU1	C	1001	1/1	0.96	0.08	85,85,85,85	0
9	CU1	F	1002	1/1	0.96	0.11	96,96,96,96	0
9	CU1	E	1001	1/1	0.96	0.14	88,88,88,88	0
9	CU1	E	1003	1/1	0.96	0.14	99,99,99,99	0
9	CU1	D	1002	1/1	0.97	0.07	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	CU1	E	1002	1/1	0.97	0.16	93,93,93,93	0
9	CU1	D	1003	1/1	0.97	0.07	89,89,89,89	0
9	CU1	B	1004	1/1	0.97	0.08	100,100,100,100	0
9	CU1	D	1001	1/1	0.98	0.05	86,86,86,86	0
9	CU1	C	1003	1/1	0.98	0.05	83,83,83,83	0
9	CU1	B	1002	1/1	0.98	0.09	88,88,88,88	0
9	CU1	B	1003	1/1	0.99	0.09	87,87,87,87	0
9	CU1	A	1003	1/1	0.99	0.10	89,89,89,89	0
9	CU1	A	1001	1/1	0.99	0.03	82,82,82,82	0
9	CU1	C	1002	1/1	0.99	0.04	85,85,85,85	0
9	CU1	B	1001	1/1	0.99	0.05	87,87,87,87	0
9	CU1	A	1002	1/1	0.99	0.09	87,87,87,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.