



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2022 – 06:14 AM EST

PDB ID : 5XRT
Title : Crystal structure of A/Minnesota/11/2010 (H3N2) influenza virus hemagglutinin
Authors : Zhang, H.; Wilson, I.A.
Deposited on : 2017-06-09
Resolution : 3.15 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

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>.

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

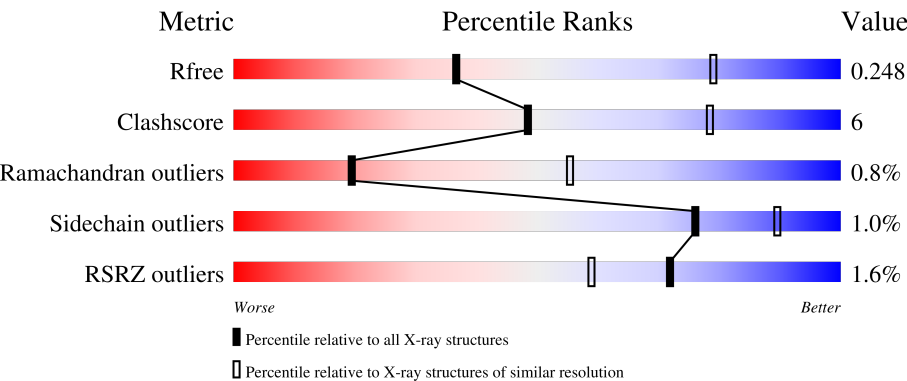
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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.






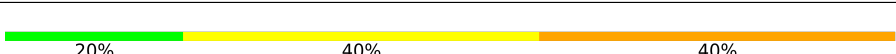
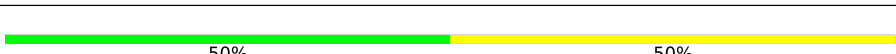
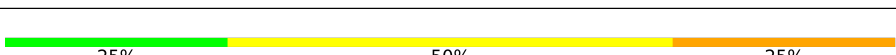
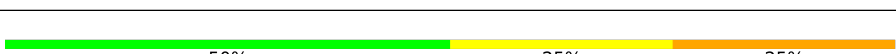
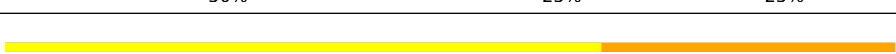
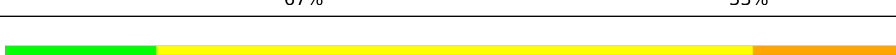
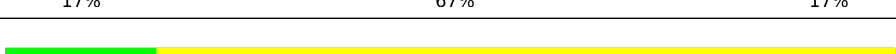
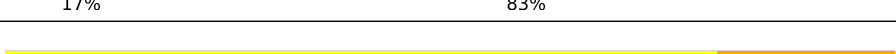
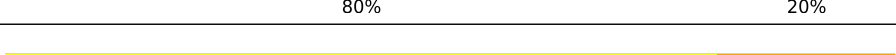
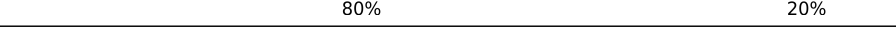
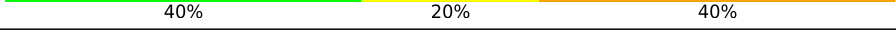


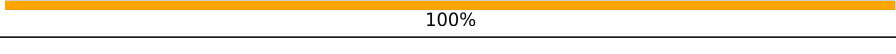
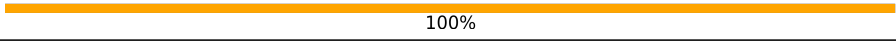
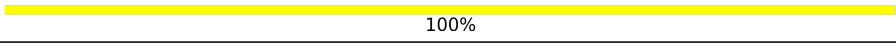
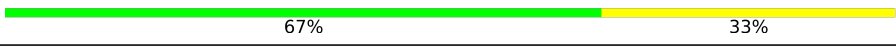
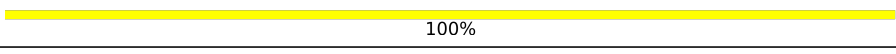
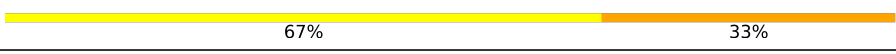



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	
1	C	329	
1	E	329	
1	G	329	
2	B	174	


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Mol	Chain	Length	Quality of chain
2	D	174	
2	F	174	
2	H	174	
3	I	5	
4	J	4	
4	K	4	
4	P	4	
5	L	6	
5	Q	6	
5	W	6	
6	M	5	
6	U	5	
6	X	5	
6	e	5	
7	N	2	
7	S	2	
7	Z	2	
7	b	2	
8	O	3	
8	R	3	
9	T	3	
10	V	5	
11	Y	3	
12	a	5	
13	c	7	

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Mol	Chain	Length	Quality of chain
14	d	4	 <div>75% 25%</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:

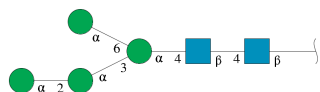
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MAN	V	5	-	-	-	X
11	NAG	Y	1	-	-	-	X
3	NAG	I	2	-	-	-	X
3	BMA	I	3	-	-	-	X
3	FUC	I	5	-	-	-	X
4	MAN	P	4	-	-	-	X
6	MAN	e	4	-	-	-	X
6	MAN	e	5	-	-	-	X
8	BMA	R	3	-	-	-	X

- Molecule 4 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.



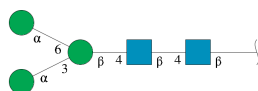
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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	L	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	Q	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	W	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 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
6	M	5	Total	C	N	O	0	0	0
			61	34	2	25			

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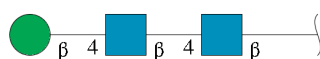
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	U	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	X	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	e	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



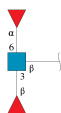
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	b	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 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
8	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
8	R	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



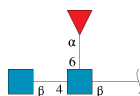
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	T	3	Total	C	N	O	0	0	0
			34	20	1	13			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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.



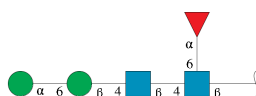
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	V	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



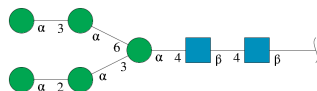
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	Y	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	a	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



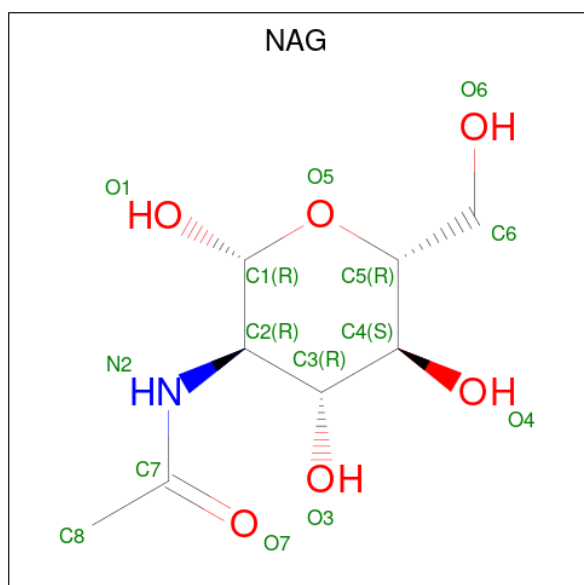
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	c	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



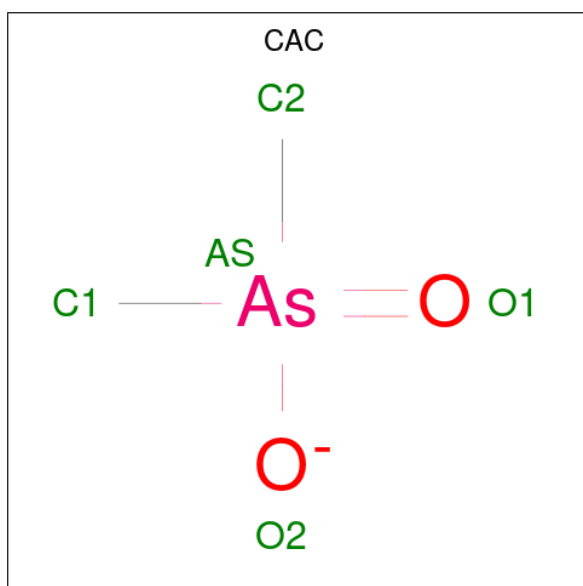
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	d	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	A	1	Total	C	N	O	0	0
			14	8	1	5		
15	B	1	Total	C	N	O	0	0
			14	8	1	5		
15	C	1	Total	C	N	O	0	0
			14	8	1	5		
15	D	1	Total	C	N	O	0	0
			14	8	1	5		
15	F	1	Total	C	N	O	0	0
			14	8	1	5		
15	G	1	Total	C	N	O	0	0
			14	8	1	5		
15	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 16 is CACODYLATE ION (three-letter code: CAC) (formula: $\text{C}_2\text{H}_6\text{AsO}_2$).

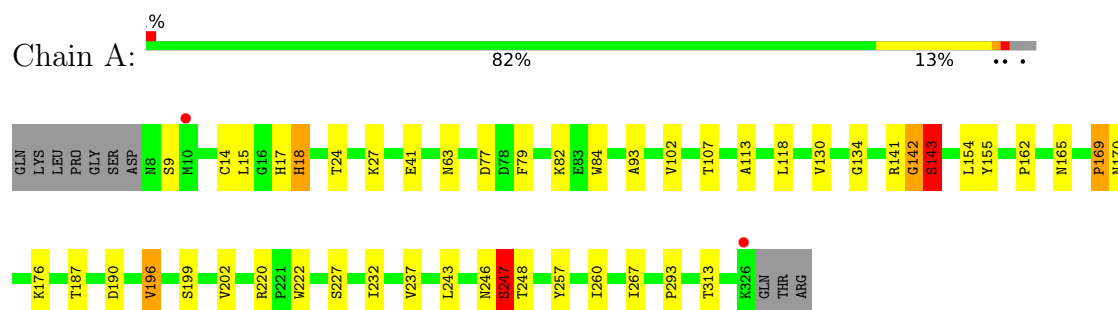


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	B	1	Total	As	C	O	0	0
			5	1	2	2		

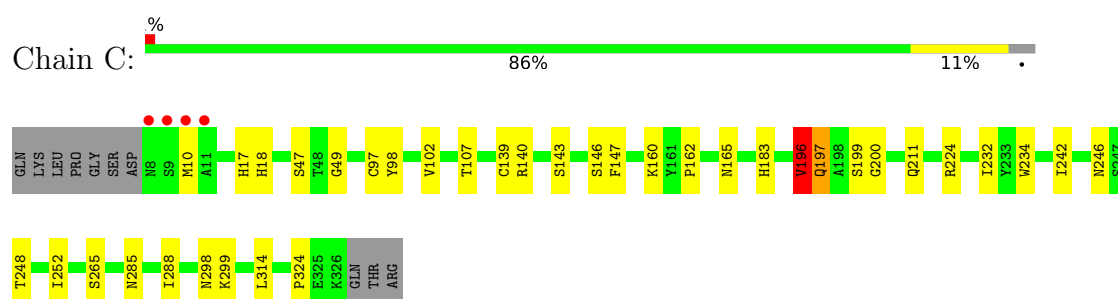
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

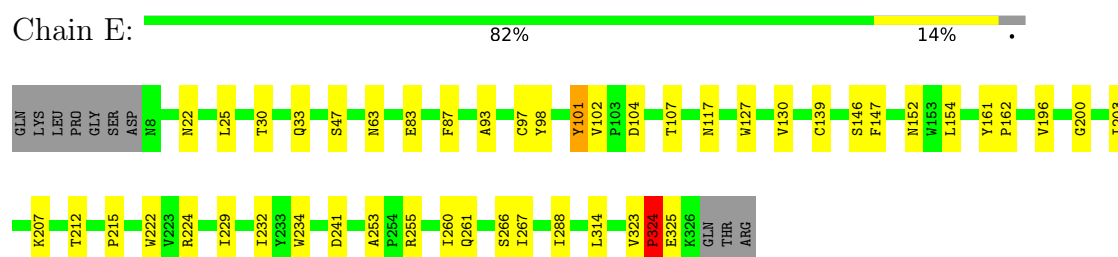
• Molecule 1: Hemagglutinin



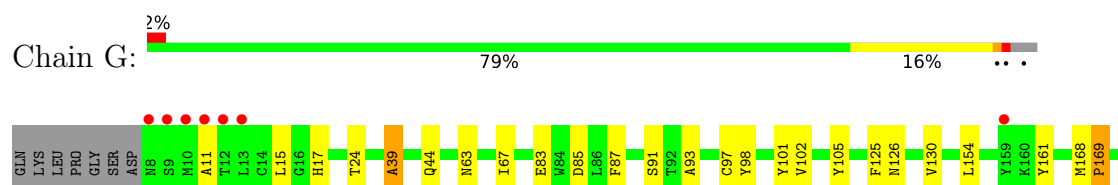
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin

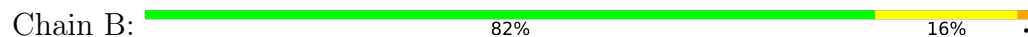


• Molecule 1: Hemagglutinin

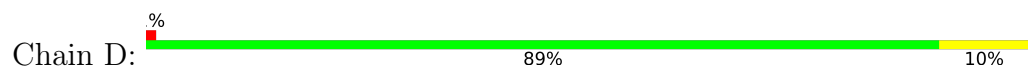




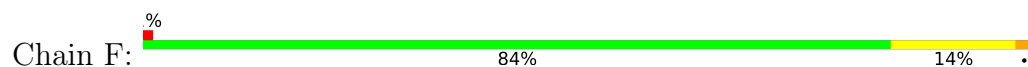
• Molecule 2: Hemagglutinin



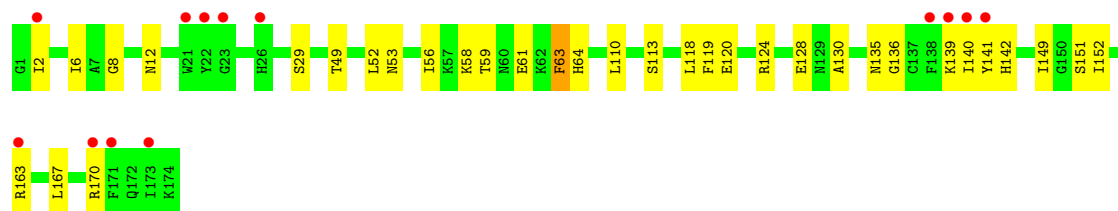
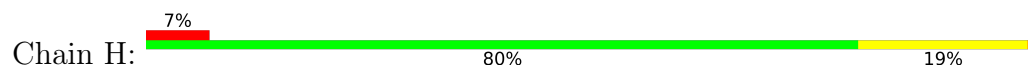
• Molecule 2: Hemagglutinin



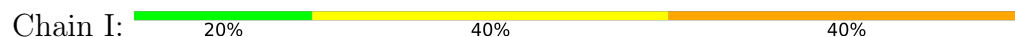
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



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



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





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



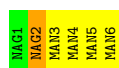
- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



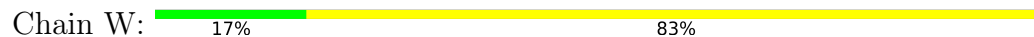
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



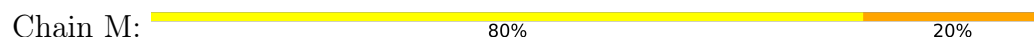
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

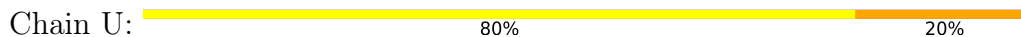


- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





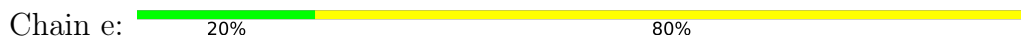
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 100%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 67% 33%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 100%



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

Chain T: 67% 33%



- Molecule 10: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 40% 60%




- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 67% 33%



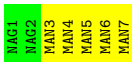
- Molecule 12: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  20% 80%

 MAG1
MAG2
BMJ3
MAN4
FUC5

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

Chain c:  29% 71%

 MAG1
MAG2
MAN3
MAN4
MAN5
MAN6
MAN7

- Molecule 14: 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:  75% 25%

 MAG1
MAG2
BMJ3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	292.78Å 292.78Å 292.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.21 – 3.15 50.21 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.21-3.15) 99.9 (50.21-3.15)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.199 , 0.246 0.204 , 0.248	Depositor DCC
R_{free} test set	3513 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	87.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16943	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: FUL, FUC, BMA, CAC, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.34	2/2565 (0.1%)	0.63	5/3492 (0.1%)
1	C	0.26	0/2565	0.57	4/3492 (0.1%)
1	E	0.31	1/2565 (0.0%)	0.58	4/3492 (0.1%)
1	G	0.40	2/2565 (0.1%)	0.67	12/3492 (0.3%)
2	B	0.27	0/1433	0.62	2/1924 (0.1%)
2	D	0.26	0/1428	0.60	4/1917 (0.2%)
2	F	0.26	0/1433	0.67	5/1924 (0.3%)
2	H	0.25	0/1433	0.73	6/1924 (0.3%)
All	All	0.31	5/15987 (0.0%)	0.63	42/21657 (0.2%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	169	PRO	N-CD	11.52	1.64	1.47
1	G	125	PHE	C-N	10.46	1.58	1.34
1	E	162	PRO	N-CD	7.90	1.58	1.47
1	A	169	PRO	N-CD	7.48	1.58	1.47
1	A	162	PRO	N-CD	6.80	1.57	1.47

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	196	VAL	CB-CA-C	-11.04	90.43	111.40
2	H	64	HIS	N-CA-CB	10.38	129.27	110.60
2	H	63	PHE	CB-CA-C	-9.77	90.86	110.40
2	H	64	HIS	N-CA-C	-8.60	87.78	111.00
2	H	63	PHE	N-CA-C	8.54	134.07	111.00
2	D	154	ASN	N-CA-CB	-8.51	95.29	110.60
1	C	196	VAL	CB-CA-C	-8.26	95.72	111.40
1	A	142	GLY	N-CA-C	8.10	133.35	113.10
1	E	324	PRO	N-CA-C	7.98	132.86	112.10
2	H	136	GLY	N-CA-C	7.93	132.94	113.10
2	H	135	ASN	N-CA-C	-7.92	89.62	111.00
1	C	197	GLN	N-CA-CB	7.83	124.69	110.60
1	A	199	SER	CB-CA-C	7.79	124.90	110.10
1	G	197	GLN	N-CA-CB	7.66	124.39	110.60
2	B	61	GLU	N-CA-C	7.63	131.61	111.00
2	F	64	HIS	N-CA-CB	7.21	123.58	110.60
1	G	126	ASN	O-C-N	-7.07	111.38	122.70
2	D	153	ARG	CB-CA-C	6.89	124.19	110.40
1	E	325	GLU	N-CA-CB	6.68	122.62	110.60
1	G	197	GLN	N-CA-C	-6.35	93.85	111.00
2	F	64	HIS	N-CA-C	-6.31	93.96	111.00
1	A	247	SER	N-CA-CB	6.30	119.95	110.50
1	G	225	GLY	N-CA-C	6.09	128.32	113.10
2	F	154	ASN	CB-CA-C	6.01	122.42	110.40
1	G	325	GLU	N-CA-C	-5.97	94.89	111.00
1	G	169	PRO	N-CA-CB	5.77	110.22	103.30
1	G	39	ALA	N-CA-CB	5.65	118.00	110.10
2	D	172	GLN	N-CA-C	-5.63	95.80	111.00
1	G	169	PRO	CA-N-CD	-5.59	103.67	111.50
1	A	143	SER	CB-CA-C	-5.54	99.57	110.10
1	G	195	TYR	CB-CA-C	5.53	121.45	110.40
2	D	60	ASN	N-CA-C	5.36	125.48	111.00
1	E	161	TYR	N-CA-C	-5.32	96.65	111.00
2	F	63	PHE	CB-CA-C	-5.26	99.89	110.40
1	C	165	ASN	N-CA-C	-5.23	96.88	111.00
1	G	326	LYS	N-CA-CB	-5.20	101.24	110.60
1	A	143	SER	N-CA-CB	5.18	118.27	110.50
2	B	62	LYS	N-CA-CB	-5.17	101.30	110.60
1	E	147	PHE	N-CA-CB	-5.11	101.41	110.60
1	C	147	PHE	N-CA-CB	-5.10	101.41	110.60
1	G	168	MET	N-CA-C	-5.08	97.29	111.00
2	F	63	PHE	N-CA-C	5.06	124.66	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2506	0	2421	31	0
1	C	2506	0	2422	23	0
1	E	2506	0	2421	25	0
1	G	2506	0	2421	31	0
2	B	1409	0	1347	34	0
2	D	1404	0	1341	24	0
2	F	1409	0	1348	40	0
2	H	1409	0	1350	20	3
3	I	59	0	52	2	0
4	J	50	0	43	1	0
4	K	50	0	43	3	0
4	P	50	0	43	2	0
5	L	72	0	61	3	0
5	Q	72	0	61	1	0
5	W	72	0	61	1	0
6	M	61	0	52	1	0
6	U	61	0	52	1	0
6	X	61	0	52	1	0
6	e	61	0	52	0	0
7	N	28	0	25	1	0
7	S	28	0	25	2	0
7	Z	28	0	25	2	0
7	b	28	0	25	0	0
8	O	39	0	34	0	0
8	R	39	0	34	0	0
9	T	34	0	31	2	0
10	V	61	0	52	1	0
11	Y	38	0	34	0	0
12	a	60	0	52	0	0
13	c	83	0	70	0	0
14	d	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	14	0	13	0	0
15	B	14	0	13	0	0
15	C	14	0	13	0	0
15	D	14	0	13	0	0
15	F	14	0	13	0	0
15	G	14	0	12	0	0
15	H	14	0	13	1	0
16	B	5	0	0	0	0
All	All	16943	0	16183	190	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (190) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:PHE:CZ	2:F:2:ILE:CG2	2.24	1.20
2:B:3:PHE:CZ	2:F:2:ILE:HG22	1.78	1.19
1:C:196:VAL:HG23	1:C:196:VAL:O	1.31	1.07
2:B:61:GLU:HG2	2:B:61:GLU:O	1.46	1.06
1:G:195:TYR:O	1:G:196:VAL:HG22	1.58	1.03
1:C:196:VAL:O	1:C:196:VAL:CG2	2.06	0.99
1:G:11:ALA:HB3	2:H:140:ILE:HB	1.46	0.98
1:E:200:GLY:O	1:E:215:PRO:HD2	1.69	0.93
1:C:18:HIS:HD2	2:D:21:TRP:HA	1.33	0.93
2:D:2:ILE:HG22	2:F:3:PHE:CZ	2.04	0.92
2:B:3:PHE:HZ	2:F:2:ILE:CG2	1.77	0.92
2:B:3:PHE:CZ	2:F:2:ILE:HG21	2.04	0.91
2:B:3:PHE:HZ	2:F:2:ILE:HG22	1.34	0.90
2:B:61:GLU:O	2:B:61:GLU:CG	2.16	0.86
1:E:139:CYS:O	1:E:146:SER:O	1.95	0.84
2:D:2:ILE:CG2	2:F:3:PHE:CZ	2.62	0.82
2:F:58:LYS:HB3	2:F:59:THR:HA	1.61	0.82
2:D:2:ILE:HG22	2:F:3:PHE:HZ	1.44	0.80
2:H:58:LYS:HB3	2:H:59:THR:HA	1.63	0.80
2:B:113:SER:HB2	2:F:2:ILE:HG23	1.65	0.79
1:C:18:HIS:CD2	2:D:21:TRP:HA	2.19	0.77
1:G:195:TYR:O	1:G:196:VAL:CG2	2.33	0.76
2:B:3:PHE:CE1	2:F:2:ILE:CG2	2.70	0.74
2:D:2:ILE:HG22	2:D:2:ILE:O	1.85	0.74
2:H:140:ILE:HG22	2:H:142:HIS:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:PHE:CE1	2:F:2:ILE:HG21	2.24	0.72
4:K:1:NAG:H5	5:L:1:NAG:H82	1.72	0.72
1:E:117:ASN:ND2	1:E:261:GLN:HE22	1.89	0.70
2:D:2:ILE:CG2	2:F:3:PHE:HZ	2.01	0.70
1:E:97:CYS:O	1:E:224:ARG:NH1	2.26	0.69
2:D:60:ASN:CG	2:D:60:ASN:O	2.29	0.69
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.74	0.69
2:B:75:GLY:HA3	1:C:107:THR:HG23	1.76	0.68
1:A:107:THR:HG23	2:F:75:GLY:HA3	1.74	0.68
1:A:202:VAL:HG22	1:A:247:SER:HB2	1.77	0.67
1:C:139:CYS:O	1:C:146:SER:O	2.15	0.65
2:F:2:ILE:HG22	2:F:2:ILE:O	1.97	0.65
1:A:130:VAL:HG11	1:A:154:LEU:HB3	1.79	0.63
1:C:248:THR:HB	4:P:1:NAG:H82	1.81	0.63
2:H:151:SER:HA	15:H:201:NAG:H61	1.81	0.63
1:E:200:GLY:O	1:E:215:PRO:CD	2.44	0.63
1:C:97:CYS:O	1:C:224:ARG:NH1	2.32	0.62
1:A:24:THR:HG23	3:I:1:NAG:H81	1.80	0.62
2:D:2:ILE:CG2	2:D:2:ILE:O	2.47	0.62
1:C:199:SER:OG	1:C:200:GLY:N	2.33	0.62
2:F:56:ILE:O	2:F:57:LYS:CB	2.48	0.62
2:F:56:ILE:HG22	2:F:57:LYS:H	1.64	0.62
2:B:113:SER:CB	2:F:2:ILE:HG23	2.28	0.62
2:D:2:ILE:HG23	2:F:113:SER:HB2	1.81	0.62
1:G:187:THR:OG1	1:G:190:ASP:OD2	2.17	0.61
2:B:59:THR:O	2:B:60:ASN:HB2	2.00	0.61
1:G:102:VAL:HG22	1:G:232:ILE:HB	1.82	0.60
6:M:2:NAG:H83	6:M:2:NAG:H3	1.83	0.60
2:H:149:ILE:HD13	2:H:152:ILE:HD12	1.84	0.60
1:A:15:LEU:HD23	2:B:118:LEU:HG	1.83	0.58
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.86	0.58
1:A:220:ARG:HB2	1:A:227:SER:O	2.04	0.58
2:F:56:ILE:O	2:F:57:LYS:HB3	2.04	0.58
1:A:248:THR:HG23	4:K:1:NAG:H81	1.86	0.57
1:G:161:TYR:HB3	1:G:195:TYR:O	2.04	0.57
1:A:77:ASP:OD2	1:A:141:ARG:NH1	2.37	0.57
1:C:47:SER:HB3	1:C:288:ILE:HG22	1.87	0.57
7:N:1:NAG:H83	7:N:1:NAG:H3	1.86	0.57
2:F:120:GLU:CD	2:F:123:ARG:HH12	2.07	0.56
2:D:20:GLY:HA3	2:D:36:ALA:HB1	1.88	0.56
7:Z:1:NAG:H3	7:Z:1:NAG:H83	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.88	0.56
2:B:59:THR:O	2:B:60:ASN:CB	2.54	0.56
2:F:2:ILE:CG2	2:F:2:ILE:O	2.55	0.55
1:A:165:ASN:HB2	4:K:1:NAG:O5	2.07	0.55
2:F:52:LEU:O	2:F:56:ILE:HG12	2.07	0.55
1:G:11:ALA:HB3	2:H:140:ILE:CB	2.30	0.55
3:I:4:FUL:H3	4:J:1:NAG:H3	1.87	0.55
7:Z:2:NAG:H3	7:Z:2:NAG:H83	1.89	0.55
1:G:199:SER:OG	1:G:215:PRO:O	2.25	0.54
1:E:22:ASN:HD22	9:T:1:NAG:H83	1.72	0.54
2:F:154:ASN:N	2:F:154:ASN:OD1	2.40	0.54
1:A:260:ILE:HD11	2:F:73:VAL:HG21	1.90	0.54
1:E:101:TYR:HB3	1:E:229:ILE:HD11	1.90	0.53
1:A:27:LYS:HD3	2:D:54:ARG:NH2	2.24	0.52
2:B:135:ASN:OD1	2:B:135:ASN:N	2.42	0.52
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.91	0.52
2:D:60:ASN:O	2:D:60:ASN:ND2	2.43	0.52
2:H:130:ALA:HA	2:H:139:LYS:O	2.10	0.51
1:G:241:ASP:OD1	1:G:242:ILE:N	2.37	0.51
1:E:222:TRP:H	5:L:2:NAG:H83	1.74	0.51
1:E:104:ASP:OD1	1:E:234:TRP:HZ3	1.93	0.51
2:D:2:ILE:HG23	2:F:113:SER:CB	2.41	0.51
1:G:15:LEU:HD23	2:H:118:LEU:HG	1.92	0.50
1:G:266:SER:HB2	2:H:63:PHE:O	2.11	0.50
2:B:141:TYR:O	2:B:169:ASN:ND2	2.44	0.50
2:H:128:GLU:O	2:H:170:ARG:NH1	2.45	0.50
1:C:97:CYS:SG	1:C:98:TYR:N	2.82	0.50
2:D:75:GLY:HA3	1:E:107:THR:HG23	1.93	0.49
10:V:1:NAG:H5	5:W:1:NAG:H82	1.94	0.49
1:G:24:THR:HG21	1:G:39:ALA:HB3	1.94	0.49
1:E:127:TRP:CZ2	1:E:253:ALA:HB1	2.48	0.49
2:B:47:GLN:HA	1:E:30:THR:HG23	1.96	0.48
1:A:27:LYS:HD3	2:D:54:ARG:HH21	1.77	0.48
1:G:87:PHE:HB3	1:G:267:ILE:HG13	1.96	0.48
2:F:24:PHE:CD1	2:F:153:ARG:HD3	2.47	0.48
1:C:140:ARG:HD2	1:C:143:SER:HA	1.95	0.48
1:E:87:PHE:HB3	1:E:267:ILE:HG13	1.96	0.48
1:G:91:SER:OG	1:G:271:ASP:OD2	2.29	0.48
1:E:130:VAL:HG11	1:E:154:LEU:HB3	1.96	0.47
2:H:140:ILE:HG22	2:H:141:TYR:N	2.29	0.47
1:A:41:GLU:OE2	1:A:313:THR:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:PRO:HD3	2:B:56:ILE:HG22	1.96	0.47
2:H:2:ILE:O	2:H:2:ILE:HG13	2.13	0.47
1:A:142:GLY:O	1:A:143:SER:CB	2.63	0.47
1:G:200:GLY:HA3	1:G:248:THR:OG1	2.15	0.47
1:C:196:VAL:O	1:C:197:GLN:HG3	2.14	0.47
2:F:5:ALA:O	2:F:10:ILE:HB	2.14	0.47
2:F:128:GLU:O	2:F:170:ARG:NH1	2.48	0.46
7:S:1:NAG:H3	7:S:1:NAG:H83	1.96	0.46
1:G:63:ASN:HA	1:G:93:ALA:HA	1.98	0.46
1:G:280:GLU:HB2	1:G:290:ASN:ND2	2.30	0.46
1:G:67:ILE:HG13	1:G:105:TYR:CZ	2.50	0.46
1:C:49:GLY:HA2	1:C:285:ASN:O	2.15	0.46
2:B:52:LEU:O	2:B:56:ILE:HG12	2.15	0.46
5:L:3:MAN:O2	5:L:4:MAN:O5	2.25	0.46
1:G:301:THR:HB	1:G:305:CYS:SG	2.56	0.46
1:A:63:ASN:HA	1:A:93:ALA:HA	1.98	0.45
6:X:3:BMA:C2	6:X:4:MAN:H2	2.47	0.45
2:B:160:ASP:OD1	2:F:174:LYS:HE3	2.17	0.45
1:C:17:HIS:CD2	2:D:6:ILE:HG12	2.52	0.45
1:A:176:LYS:HD2	1:A:257:TYR:CD2	2.51	0.45
1:G:97:CYS:O	1:G:224:ARG:NH1	2.36	0.45
1:A:18:HIS:HB2	2:B:21:TRP:HA	1.98	0.45
2:B:113:SER:O	2:B:117:LYS:HG3	2.16	0.45
1:E:266:SER:HB2	2:F:63:PHE:O	2.16	0.45
1:G:15:LEU:HD22	2:H:119:PHE:HA	1.98	0.45
1:G:304:ALA:HA	2:H:61:GLU:HA	1.98	0.45
9:T:2:FUL:O3	6:U:1:NAG:H3	2.16	0.45
1:A:14:CYS:HA	2:B:137:CYS:HA	1.98	0.44
1:E:83:GLU:OE2	1:G:83:GLU:OE2	2.35	0.44
1:G:243:LEU:HD21	1:G:245:ILE:HD11	1.99	0.44
1:G:44:GLN:HB2	1:G:292:LYS:HG3	1.98	0.44
1:E:47:SER:HB2	1:E:288:ILE:HG22	2.00	0.44
1:E:207:LYS:HB2	1:E:241:ASP:OD2	2.17	0.44
1:G:130:VAL:HG11	1:G:154:LEU:HB3	2.00	0.44
2:B:124:ARG:HD3	2:F:134:GLY:HA2	1.98	0.44
1:C:298:ASN:OD1	1:C:299:LYS:N	2.50	0.44
2:B:164:ASN:OD1	2:B:164:ASN:N	2.50	0.44
2:B:174:LYS:HD2	2:D:163:ARG:HD3	1.99	0.43
2:D:58:LYS:O	2:D:59:THR:HG23	2.18	0.43
1:E:25:LEU:HD13	1:E:33:GLN:HB3	2.00	0.43
1:G:211:GLN:OE1	1:G:235:THR:OG1	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:LYS:HB2	2:B:58:LYS:HA	2.01	0.43
1:G:323:VAL:HG12	2:H:12:ASN:HD22	1.84	0.43
1:A:79:PHE:HA	1:A:82:LYS:HG3	2.00	0.42
1:A:84:TRP:HZ3	1:A:118:LEU:HG	1.84	0.42
1:C:17:HIS:CE1	2:D:6:ILE:HG23	2.54	0.42
1:C:183:HIS:HB2	1:C:252:ILE:HD11	2.01	0.42
1:E:323:VAL:HA	1:E:324:PRO:HD3	1.87	0.42
1:E:203:ILE:HG12	1:E:212:THR:HG23	2.00	0.42
2:H:49:THR:O	2:H:53:ASN:ND2	2.52	0.42
2:H:163:ARG:O	2:H:167:LEU:HG	2.20	0.42
2:F:56:ILE:HG22	2:F:57:LYS:N	2.33	0.42
1:A:222:TRP:HB2	5:Q:2:NAG:H2	2.02	0.41
2:F:127:ARG:HD3	2:F:159:HIS:CE1	2.55	0.41
1:C:314:LEU:HB3	2:D:100:VAL:HG21	2.02	0.41
1:E:63:ASN:HA	1:E:93:ALA:HA	2.02	0.41
2:B:139:LYS:HE3	2:B:139:LYS:HB2	1.89	0.41
1:A:134:GLY:HA2	1:A:155:TYR:HE2	1.85	0.41
2:B:164:ASN:HB3	2:F:174:LYS:HB3	2.03	0.41
1:E:152:ASN:HB2	1:E:255:ARG:HD3	2.01	0.41
1:G:97:CYS:SG	1:G:98:TYR:N	2.91	0.41
2:B:127:ARG:NH1	2:F:133:MET:HA	2.36	0.41
2:H:120:GLU:O	2:H:124:ARG:HG3	2.21	0.41
1:A:176:LYS:HD2	1:A:257:TYR:CG	2.55	0.41
1:A:246:ASN:HD22	1:A:246:ASN:HA	1.79	0.41
2:B:2:ILE:H	2:B:2:ILE:HG12	1.59	0.41
2:B:126:LEU:HD21	2:B:152:ILE:HD13	2.02	0.41
1:C:246:ASN:HD22	4:P:1:NAG:H83	1.86	0.41
2:D:158:ASP:O	2:D:161:ILE:HG12	2.21	0.41
1:A:170:ASN:ND2	1:A:237:VAL:O	2.47	0.41
2:D:1:GLY:O	2:F:117:LYS:NZ	2.51	0.41
2:D:2:ILE:HG21	2:F:3:PHE:CZ	2.52	0.41
1:G:17:HIS:NE2	2:H:6:ILE:HG23	2.36	0.41
7:S:1:NAG:O3	7:S:2:NAG:O5	2.35	0.41
1:A:113:ALA:HB1	1:A:267:ILE:HB	2.04	0.40
1:A:187:THR:OG1	1:A:190:ASP:OD2	2.33	0.40
1:A:237:VAL:HG21	1:A:243:LEU:HB2	2.03	0.40
1:E:314:LEU:HB3	2:F:100:VAL:HG21	2.03	0.40
1:G:284:PRO:HG2	1:G:298:ASN:ND2	2.36	0.40
1:C:211:GLN:NE2	1:C:234:TRP:O	2.54	0.40
2:F:58:LYS:CB	2:F:59:THR:HA	2.40	0.40
2:H:52:LEU:HG	2:H:56:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LYS:HG2	1:C:162:PRO:HD3	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:ILE:CD1	2:H:113:SER:OG[5_555]	1.70	0.50
2:H:2:ILE:CD1	2:H:113:SER:CB[5_555]	1.79	0.41
2:H:2:ILE:CG1	2:H:113:SER:OG[5_555]	1.99	0.21

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	317/329 (96%)	294 (93%)	18 (6%)	5 (2%)	9	40
1	C	317/329 (96%)	296 (93%)	20 (6%)	1 (0%)	41	73
1	E	317/329 (96%)	294 (93%)	21 (7%)	2 (1%)	25	62
1	G	317/329 (96%)	295 (93%)	19 (6%)	3 (1%)	17	53
2	B	172/174 (99%)	162 (94%)	8 (5%)	2 (1%)	13	46
2	D	172/174 (99%)	164 (95%)	8 (5%)	0	100	100
2	F	172/174 (99%)	164 (95%)	7 (4%)	1 (1%)	25	62
2	H	172/174 (99%)	159 (92%)	12 (7%)	1 (1%)	25	62
All	All	1956/2012 (97%)	1828 (94%)	113 (6%)	15 (1%)	19	55

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	18	HIS

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Mol	Chain	Res	Type
2	B	60	ASN
2	F	57	LYS
1	E	324	PRO
1	G	324	PRO
1	A	143	SER
2	B	172	GLN
1	E	196	VAL
1	A	196	VAL
1	G	169	PRO
1	G	196	VAL
2	H	8	GLY
1	A	169	PRO
1	C	324	PRO

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	284/293 (97%)	282 (99%)	2 (1%)	84	93
1	C	284/293 (97%)	280 (99%)	4 (1%)	67	85
1	E	284/293 (97%)	281 (99%)	3 (1%)	73	88
1	G	284/293 (97%)	281 (99%)	3 (1%)	73	88
2	B	148/148 (100%)	146 (99%)	2 (1%)	67	85
2	D	147/148 (99%)	146 (99%)	1 (1%)	84	93
2	F	148/148 (100%)	148 (100%)	0	100	100
2	H	148/148 (100%)	146 (99%)	2 (1%)	67	85
All	All	1727/1764 (98%)	1710 (99%)	17 (1%)	76	89

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	VAL
1	A	247	SER

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Mol	Chain	Res	Type
2	B	2	ILE
2	B	38	LEU
1	C	10	MET
1	C	196	VAL
1	C	242	ILE
1	C	265	SER
2	D	168	ASN
1	E	98	TYR
1	E	101	TYR
1	E	260	ILE
1	G	85	ASP
1	G	101	TYR
1	G	195	TYR
2	H	29	SER
2	H	110	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	18	HIS
1	E	117	ASN
2	H	12	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](#)

96 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	$\# Z > 2$
3	NAG	I	1	1,3	14,14,15	0.72	1 (7%)	17,19,21	0.55	0
3	NAG	I	2	3	14,14,15	0.35	0	17,19,21	0.41	0
3	BMA	I	3	3	11,11,12	0.79	1 (9%)	15,15,17	1.30	3 (20%)
3	FUL	I	4	3	10,10,11	1.84	2 (20%)	14,14,16	2.41	3 (21%)
3	FUC	I	5	3	10,10,11	0.71	0	14,14,16	0.96	1 (7%)
4	NAG	J	1	1,4	14,14,15	0.47	0	17,19,21	0.69	0
4	NAG	J	2	4	14,14,15	0.32	0	17,19,21	0.52	0
4	BMA	J	3	4	11,11,12	0.58	0	15,15,17	0.73	0
4	MAN	J	4	4	11,11,12	0.86	0	15,15,17	1.17	1 (6%)
4	NAG	K	1	1,4	14,14,15	0.73	1 (7%)	17,19,21	0.65	0
4	NAG	K	2	4	14,14,15	0.20	0	17,19,21	0.83	1 (5%)
4	BMA	K	3	4	11,11,12	0.83	0	15,15,17	0.96	0
4	MAN	K	4	4	11,11,12	1.00	1 (9%)	15,15,17	1.87	4 (26%)
5	NAG	L	1	5,1	14,14,15	0.42	0	17,19,21	0.68	0
5	NAG	L	2	5	14,14,15	0.43	0	17,19,21	0.58	0
5	MAN	L	3	5	11,11,12	1.47	2 (18%)	15,15,17	1.52	2 (13%)
5	MAN	L	4	5	11,11,12	1.99	3 (27%)	15,15,17	2.70	6 (40%)
5	MAN	L	5	5	11,11,12	1.10	1 (9%)	15,15,17	1.59	4 (26%)
5	MAN	L	6	5	11,11,12	1.42	3 (27%)	15,15,17	2.27	3 (20%)
6	NAG	M	1	1,6	14,14,15	0.61	0	17,19,21	0.96	1 (5%)
6	NAG	M	2	6	14,14,15	0.40	0	17,19,21	1.40	2 (11%)
6	BMA	M	3	6	11,11,12	1.34	3 (27%)	15,15,17	1.96	4 (26%)
6	MAN	M	4	6	11,11,12	1.03	1 (9%)	15,15,17	1.61	4 (26%)
6	MAN	M	5	6	11,11,12	0.92	1 (9%)	15,15,17	1.61	3 (20%)
7	NAG	N	1	1,7	14,14,15	0.35	0	17,19,21	1.23	1 (5%)
7	NAG	N	2	7	14,14,15	0.16	0	17,19,21	0.64	0
8	NAG	O	1	1,8	14,14,15	0.45	0	17,19,21	0.61	0
8	NAG	O	2	8	14,14,15	0.63	0	17,19,21	0.78	0
8	BMA	O	3	8	11,11,12	1.09	2 (18%)	15,15,17	0.74	0
4	NAG	P	1	1,4	14,14,15	0.66	1 (7%)	17,19,21	0.73	0
4	NAG	P	2	4	14,14,15	0.26	0	17,19,21	0.55	0
4	BMA	P	3	4	11,11,12	0.89	0	15,15,17	0.85	0
4	MAN	P	4	4	11,11,12	1.31	2 (18%)	15,15,17	1.97	4 (26%)
5	NAG	Q	1	5,1	14,14,15	0.40	0	17,19,21	0.58	0
5	NAG	Q	2	5	14,14,15	0.49	0	17,19,21	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	Q	3	5	11,11,12	1.10	2 (18%)	15,15,17	1.87	5 (33%)
5	MAN	Q	4	5	11,11,12	1.95	1 (9%)	15,15,17	1.48	3 (20%)
5	MAN	Q	5	5	11,11,12	1.48	3 (27%)	15,15,17	2.16	5 (33%)
5	MAN	Q	6	5	11,11,12	1.44	2 (18%)	15,15,17	1.55	4 (26%)
8	NAG	R	1	1,8	14,14,15	0.52	0	17,19,21	1.37	3 (17%)
8	NAG	R	2	8	14,14,15	0.73	1 (7%)	17,19,21	0.61	0
8	BMA	R	3	8	11,11,12	0.85	1 (9%)	15,15,17	0.91	0
7	NAG	S	1	1,7	14,14,15	0.36	0	17,19,21	1.36	2 (11%)
7	NAG	S	2	7	14,14,15	0.93	2 (14%)	17,19,21	0.79	0
9	NAG	T	1	1,9	14,14,15	0.24	0	17,19,21	0.44	0
9	FUL	T	2	9	10,10,11	2.11	3 (30%)	14,14,16	2.00	4 (28%)
9	FUC	T	3	9	10,10,11	0.74	0	14,14,16	0.92	1 (7%)
6	NAG	U	1	1,6	14,14,15	0.70	1 (7%)	17,19,21	0.83	1 (5%)
6	NAG	U	2	6	14,14,15	1.18	1 (7%)	17,19,21	1.76	1 (5%)
6	BMA	U	3	6	11,11,12	0.93	0	15,15,17	1.12	2 (13%)
6	MAN	U	4	6	11,11,12	1.38	2 (18%)	15,15,17	0.87	0
6	MAN	U	5	6	11,11,12	0.97	1 (9%)	15,15,17	1.19	2 (13%)
10	NAG	V	1	1,10	14,14,15	0.37	0	17,19,21	0.61	0
10	NAG	V	2	10	14,14,15	0.36	0	17,19,21	0.53	0
10	BMA	V	3	10	11,11,12	0.74	0	15,15,17	0.79	0
10	MAN	V	4	10	11,11,12	1.15	1 (9%)	15,15,17	1.99	4 (26%)
10	MAN	V	5	10	11,11,12	0.95	0	15,15,17	1.51	1 (6%)
5	NAG	W	1	5,1	14,14,15	0.37	0	17,19,21	0.44	0
5	NAG	W	2	5	14,14,15	0.30	0	17,19,21	0.68	0
5	MAN	W	3	5	11,11,12	1.15	1 (9%)	15,15,17	1.24	2 (13%)
5	MAN	W	4	5	11,11,12	2.00	3 (27%)	15,15,17	1.67	3 (20%)
5	MAN	W	5	5	11,11,12	1.49	2 (18%)	15,15,17	1.91	4 (26%)
5	MAN	W	6	5	11,11,12	0.82	0	15,15,17	1.28	1 (6%)
6	NAG	X	1	1,6	14,14,15	0.24	0	17,19,21	0.71	0
6	NAG	X	2	6	14,14,15	0.43	0	17,19,21	0.69	0
6	BMA	X	3	6	11,11,12	1.09	1 (9%)	15,15,17	1.24	2 (13%)
6	MAN	X	4	6	11,11,12	1.70	1 (9%)	15,15,17	1.86	2 (13%)
6	MAN	X	5	6	11,11,12	1.42	2 (18%)	15,15,17	2.08	3 (20%)
11	NAG	Y	1	11,1	14,14,15	0.54	0	17,19,21	0.58	0
11	NAG	Y	2	11	14,14,15	0.30	0	17,19,21	0.34	0
11	FUC	Y	3	11	10,10,11	0.97	1 (10%)	14,14,16	1.28	2 (14%)
7	NAG	Z	1	1,7	14,14,15	0.42	0	17,19,21	1.30	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	Z	2	7	14,14,15	0.47	0	17,19,21	1.22	1 (5%)
12	NAG	a	1	1,12	14,14,15	1.30	1 (7%)	17,19,21	1.39	3 (17%)
12	NAG	a	2	12	14,14,15	0.35	0	17,19,21	0.79	0
12	BMA	a	3	12	11,11,12	1.93	3 (27%)	15,15,17	1.50	3 (20%)
12	MAN	a	4	12	11,11,12	1.48	2 (18%)	15,15,17	2.25	4 (26%)
12	FUC	a	5	12	10,10,11	1.04	0	14,14,16	1.38	3 (21%)
7	NAG	b	1	1,7	14,14,15	0.62	0	17,19,21	1.62	2 (11%)
7	NAG	b	2	7	14,14,15	0.37	0	17,19,21	0.77	1 (5%)
13	NAG	c	1	13,1	14,14,15	0.50	0	17,19,21	0.48	0
13	NAG	c	2	13	14,14,15	0.53	0	17,19,21	0.50	0
13	MAN	c	3	13	11,11,12	1.73	3 (27%)	15,15,17	1.64	5 (33%)
13	MAN	c	4	13	11,11,12	1.97	3 (27%)	15,15,17	1.93	5 (33%)
13	MAN	c	5	13	11,11,12	1.26	2 (18%)	15,15,17	1.71	4 (26%)
13	MAN	c	6	13	11,11,12	1.18	1 (9%)	15,15,17	1.44	3 (20%)
13	MAN	c	7	13	11,11,12	1.75	3 (27%)	15,15,17	1.58	2 (13%)
14	NAG	d	1	1,14	14,14,15	0.55	0	17,19,21	0.68	0
14	NAG	d	2	14	14,14,15	0.40	0	17,19,21	0.74	0
14	BMA	d	3	14	11,11,12	0.73	0	15,15,17	0.90	0
14	MAN	d	4	14	11,11,12	0.75	0	15,15,17	1.08	2 (13%)
6	NAG	e	1	1,6	14,14,15	0.57	0	17,19,21	1.18	1 (5%)
6	NAG	e	2	6	14,14,15	0.18	0	17,19,21	0.68	0
6	BMA	e	3	6	11,11,12	1.00	1 (9%)	15,15,17	1.02	0
6	MAN	e	4	6	11,11,12	1.25	1 (9%)	15,15,17	2.01	3 (20%)
6	MAN	e	5	6	11,11,12	1.07	1 (9%)	15,15,17	2.23	4 (26%)

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
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	FUL	I	4	3	-	-	0/1/1/1
3	FUC	I	5	3	-	-	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	1/2/19/22	1/1/1/1
4	NAG	K	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
4	MAN	K	4	4	-	0/2/19/22	0/1/1/1
5	NAG	L	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	MAN	L	3	5	-	2/2/19/22	1/1/1/1
5	MAN	L	4	5	-	2/2/19/22	0/1/1/1
5	MAN	L	5	5	-	2/2/19/22	0/1/1/1
5	MAN	L	6	5	-	0/2/19/22	0/1/1/1
6	NAG	M	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	M	2	6	-	3/6/23/26	0/1/1/1
6	BMA	M	3	6	-	2/2/19/22	1/1/1/1
6	MAN	M	4	6	-	0/2/19/22	0/1/1/1
6	MAN	M	5	6	-	1/2/19/22	0/1/1/1
7	NAG	N	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
8	NAG	O	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	O	2	8	-	1/6/23/26	0/1/1/1
8	BMA	O	3	8	-	0/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	BMA	P	3	4	-	2/2/19/22	0/1/1/1
4	MAN	P	4	4	-	1/2/19/22	0/1/1/1
5	NAG	Q	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	1/6/23/26	0/1/1/1
5	MAN	Q	3	5	-	1/2/19/22	0/1/1/1
5	MAN	Q	4	5	-	2/2/19/22	0/1/1/1
5	MAN	Q	5	5	-	1/2/19/22	0/1/1/1
5	MAN	Q	6	5	-	2/2/19/22	0/1/1/1
8	NAG	R	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	R	2	8	-	0/6/23/26	0/1/1/1
8	BMA	R	3	8	-	2/2/19/22	0/1/1/1
7	NAG	S	1	1,7	-	5/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	T	1	1,9	-	2/6/23/26	0/1/1/1
9	FUL	T	2	9	-	-	0/1/1/1
9	FUC	T	3	9	-	-	0/1/1/1
6	NAG	U	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	4/6/23/26	0/1/1/1
6	BMA	U	3	6	-	0/2/19/22	0/1/1/1
6	MAN	U	4	6	-	0/2/19/22	1/1/1/1
6	MAN	U	5	6	-	2/2/19/22	0/1/1/1
10	NAG	V	1	1,10	-	4/6/23/26	0/1/1/1
10	NAG	V	2	10	-	0/6/23/26	0/1/1/1
10	BMA	V	3	10	-	1/2/19/22	0/1/1/1
10	MAN	V	4	10	-	2/2/19/22	0/1/1/1
10	MAN	V	5	10	-	2/2/19/22	1/1/1/1
5	NAG	W	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	0/6/23/26	0/1/1/1
5	MAN	W	3	5	-	0/2/19/22	1/1/1/1
5	MAN	W	4	5	-	2/2/19/22	0/1/1/1
5	MAN	W	5	5	-	2/2/19/22	0/1/1/1
5	MAN	W	6	5	-	2/2/19/22	1/1/1/1
6	NAG	X	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	BMA	X	3	6	-	2/2/19/22	0/1/1/1
6	MAN	X	4	6	-	2/2/19/22	0/1/1/1
6	MAN	X	5	6	-	2/2/19/22	0/1/1/1
11	NAG	Y	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	Y	2	11	-	2/6/23/26	0/1/1/1
11	FUC	Y	3	11	-	-	0/1/1/1
7	NAG	Z	1	1,7	-	5/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	3/6/23/26	0/1/1/1
12	NAG	a	1	1,12	-	3/6/23/26	0/1/1/1
12	NAG	a	2	12	-	2/6/23/26	0/1/1/1
12	BMA	a	3	12	-	2/2/19/22	0/1/1/1
12	MAN	a	4	12	-	0/2/19/22	0/1/1/1
12	FUC	a	5	12	-	-	0/1/1/1
7	NAG	b	1	1,7	-	5/6/23/26	0/1/1/1
7	NAG	b	2	7	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	c	1	13,1	-	2/6/23/26	0/1/1/1
13	NAG	c	2	13	-	0/6/23/26	0/1/1/1
13	MAN	c	3	13	-	0/2/19/22	1/1/1/1
13	MAN	c	4	13	-	2/2/19/22	0/1/1/1
13	MAN	c	5	13	-	2/2/19/22	0/1/1/1
13	MAN	c	6	13	-	2/2/19/22	0/1/1/1
13	MAN	c	7	13	-	1/2/19/22	1/1/1/1
14	NAG	d	1	1,14	-	2/6/23/26	0/1/1/1
14	NAG	d	2	14	-	0/6/23/26	0/1/1/1
14	BMA	d	3	14	-	0/2/19/22	0/1/1/1
14	MAN	d	4	14	-	2/2/19/22	0/1/1/1
6	NAG	e	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	e	2	6	-	1/6/23/26	0/1/1/1
6	BMA	e	3	6	-	2/2/19/22	0/1/1/1
6	MAN	e	4	6	-	2/2/19/22	0/1/1/1
6	MAN	e	5	6	-	2/2/19/22	0/1/1/1

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	4	MAN	C2-C3	5.13	1.60	1.52
6	X	4	MAN	C1-C2	5.05	1.63	1.52
9	T	2	FUL	O5-C1	4.64	1.51	1.43
3	I	4	FUL	O5-C1	4.63	1.51	1.43
12	a	1	NAG	O5-C1	-4.37	1.36	1.43
6	U	2	NAG	O5-C1	4.29	1.50	1.43
5	W	4	MAN	C2-C3	4.28	1.58	1.52
5	W	5	MAN	C1-C2	4.27	1.61	1.52
5	L	4	MAN	O2-C2	4.17	1.52	1.43
13	c	4	MAN	C2-C3	4.06	1.58	1.52
13	c	7	MAN	O5-C1	3.86	1.49	1.43
13	c	4	MAN	O2-C2	3.81	1.51	1.43
12	a	3	BMA	C2-C3	3.76	1.58	1.52
5	W	4	MAN	O2-C2	3.74	1.51	1.43
12	a	4	MAN	C1-C2	3.72	1.60	1.52
9	T	2	FUL	C2-C3	-3.64	1.47	1.52
5	L	4	MAN	C2-C3	3.64	1.57	1.52
4	P	4	MAN	C1-C2	3.49	1.60	1.52
13	c	5	MAN	C1-C2	3.43	1.60	1.52
5	Q	5	MAN	C1-C2	3.35	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	5	MAN	C1-C2	3.33	1.59	1.52
5	L	3	MAN	C2-C3	3.32	1.57	1.52
13	c	3	MAN	C1-C2	3.28	1.59	1.52
5	L	5	MAN	C1-C2	3.27	1.59	1.52
13	c	7	MAN	O5-C5	3.24	1.50	1.43
6	e	4	MAN	C1-C2	3.19	1.59	1.52
6	e	5	MAN	C1-C2	3.08	1.59	1.52
12	a	3	BMA	C4-C3	2.97	1.59	1.52
10	V	4	MAN	C1-C2	2.96	1.58	1.52
5	Q	6	MAN	C1-C2	2.95	1.58	1.52
6	U	4	MAN	O5-C5	2.80	1.49	1.43
6	M	4	MAN	C1-C2	2.79	1.58	1.52
6	X	3	BMA	O5-C5	2.76	1.49	1.43
6	X	5	MAN	O5-C1	2.75	1.48	1.43
5	L	6	MAN	O5-C5	2.70	1.48	1.43
12	a	3	BMA	O5-C1	-2.68	1.39	1.43
4	K	4	MAN	C1-C2	2.67	1.58	1.52
12	a	4	MAN	O5-C1	2.66	1.48	1.43
5	Q	6	MAN	O5-C5	2.65	1.48	1.43
5	L	6	MAN	C1-C2	2.63	1.58	1.52
5	W	3	MAN	C1-C2	2.59	1.58	1.52
4	K	1	NAG	O5-C1	-2.57	1.39	1.43
5	W	4	MAN	C1-C2	2.56	1.58	1.52
13	c	3	MAN	O5-C5	2.56	1.48	1.43
5	L	6	MAN	O5-C1	2.54	1.47	1.43
6	U	4	MAN	C1-C2	2.48	1.57	1.52
6	U	1	NAG	O5-C1	-2.48	1.39	1.43
13	c	3	MAN	O5-C1	2.48	1.47	1.43
5	L	3	MAN	O5-C5	2.44	1.48	1.43
9	T	2	FUL	O5-C5	2.41	1.48	1.43
7	S	2	NAG	C1-C2	2.41	1.55	1.52
8	O	3	BMA	C1-C2	2.36	1.57	1.52
4	P	1	NAG	O5-C1	-2.35	1.40	1.43
13	c	4	MAN	C1-C2	2.35	1.57	1.52
6	M	5	MAN	C1-C2	2.33	1.57	1.52
6	U	5	MAN	C1-C2	2.29	1.57	1.52
3	I	1	NAG	C1-C2	2.29	1.55	1.52
3	I	4	FUL	C2-C3	-2.27	1.49	1.52
8	R	3	BMA	C1-C2	2.25	1.57	1.52
13	c	6	MAN	C4-C5	2.25	1.57	1.53
13	c	7	MAN	C1-C2	2.25	1.57	1.52
4	P	4	MAN	O5-C1	2.24	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	3	BMA	C4-C5	2.22	1.57	1.53
6	M	3	BMA	O5-C5	2.22	1.47	1.43
5	Q	5	MAN	O2-C2	2.20	1.48	1.43
5	L	4	MAN	C4-C3	2.17	1.57	1.52
5	W	5	MAN	C2-C3	2.16	1.55	1.52
11	Y	3	FUC	C1-C2	2.15	1.57	1.52
5	Q	3	MAN	O5-C5	2.12	1.47	1.43
8	O	3	BMA	C2-C3	2.10	1.55	1.52
8	R	2	NAG	O5-C1	-2.09	1.40	1.43
6	M	3	BMA	C1-C2	2.08	1.56	1.52
3	I	3	BMA	C1-C2	2.07	1.56	1.52
5	Q	3	MAN	C1-C2	2.03	1.56	1.52
5	Q	5	MAN	O5-C1	2.03	1.47	1.43
13	c	5	MAN	C2-C3	2.03	1.55	1.52
7	S	2	NAG	O5-C1	-2.01	1.40	1.43
6	e	3	BMA	C4-C3	2.01	1.57	1.52

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	6	MAN	C1-O5-C5	7.64	122.55	112.19
5	L	4	MAN	C1-O5-C5	7.41	122.23	112.19
3	I	4	FUL	C1-C2-C3	7.08	118.37	109.67
6	U	2	NAG	C1-O5-C5	6.60	121.13	112.19
6	X	5	MAN	C1-O5-C5	6.14	120.51	112.19
6	e	4	MAN	C1-O5-C5	5.99	120.31	112.19
6	e	5	MAN	C1-O5-C5	5.93	120.23	112.19
6	M	3	BMA	C1-O5-C5	5.70	119.91	112.19
12	a	4	MAN	C1-O5-C5	5.67	119.87	112.19
4	P	4	MAN	C1-O5-C5	5.55	119.70	112.19
5	Q	5	MAN	C1-O5-C5	5.11	119.11	112.19
6	M	5	MAN	C1-O5-C5	5.10	119.11	112.19
13	c	4	MAN	C1-O5-C5	4.95	118.90	112.19
5	W	5	MAN	C1-C2-C3	4.91	115.70	109.67
13	c	7	MAN	C1-O5-C5	4.91	118.84	112.19
9	T	2	FUL	O5-C5-C4	4.89	118.30	109.52
4	K	4	MAN	C1-O5-C5	4.87	118.79	112.19
10	V	4	MAN	C1-C2-C3	4.80	115.57	109.67
6	X	4	MAN	C1-O5-C5	4.72	118.58	112.19
6	M	4	MAN	C1-O5-C5	4.66	118.51	112.19
10	V	5	MAN	C1-O5-C5	4.65	118.50	112.19
6	X	4	MAN	C1-C2-C3	4.44	115.13	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	1	NAG	C2-N2-C7	4.44	129.23	122.90
6	M	2	NAG	C2-N2-C7	4.43	129.21	122.90
7	Z	1	NAG	C2-N2-C7	4.43	129.21	122.90
5	W	4	MAN	C1-O5-C5	4.39	118.15	112.19
7	b	1	NAG	C1-O5-C5	4.34	118.08	112.19
7	Z	2	NAG	C2-N2-C7	4.32	129.05	122.90
5	L	5	MAN	C1-O5-C5	4.30	118.01	112.19
7	N	1	NAG	C2-N2-C7	4.23	128.93	122.90
5	Q	3	MAN	C1-O5-C5	4.20	117.88	112.19
5	L	4	MAN	O5-C1-C2	4.15	117.18	110.77
12	a	4	MAN	C1-C2-C3	4.10	114.70	109.67
7	b	1	NAG	C2-N2-C7	4.07	128.70	122.90
13	c	5	MAN	C1-O5-C5	4.05	117.68	112.19
6	e	1	NAG	C2-N2-C7	4.03	128.64	122.90
6	e	5	MAN	O5-C1-C2	3.98	116.92	110.77
5	W	3	MAN	C1-O5-C5	3.79	117.33	112.19
12	a	4	MAN	O5-C1-C2	3.79	116.62	110.77
5	Q	3	MAN	O5-C5-C6	3.76	113.10	107.20
5	W	6	MAN	C1-O5-C5	3.74	117.26	112.19
3	I	4	FUL	O5-C1-C2	3.62	116.36	110.77
5	L	3	MAN	C1-O5-C5	3.48	116.91	112.19
5	Q	6	MAN	O5-C5-C6	3.45	112.61	107.20
5	Q	5	MAN	O5-C1-C2	3.44	116.08	110.77
13	c	5	MAN	C1-C2-C3	3.44	113.89	109.67
6	e	5	MAN	C1-C2-C3	3.43	113.88	109.67
8	R	1	NAG	C1-O5-C5	3.42	116.83	112.19
10	V	4	MAN	C1-O5-C5	3.42	116.83	112.19
5	W	5	MAN	C1-O5-C5	3.37	116.75	112.19
6	e	4	MAN	O5-C1-C2	3.36	115.95	110.77
12	a	3	BMA	C3-C4-C5	3.35	116.21	110.24
12	a	3	BMA	C2-C3-C4	3.35	116.69	110.89
4	J	4	MAN	C1-O5-C5	3.32	116.69	112.19
4	P	4	MAN	C1-C2-C3	3.26	113.68	109.67
13	c	3	MAN	C1-C2-C3	-3.26	105.66	109.67
10	V	4	MAN	O5-C1-C2	3.22	115.75	110.77
5	Q	5	MAN	O2-C2-C1	3.19	115.67	109.15
12	a	1	NAG	C1-O5-C5	-3.18	107.88	112.19
9	T	2	FUL	C1-O5-C5	3.12	119.84	112.78
6	X	5	MAN	O5-C1-C2	3.11	115.57	110.77
9	T	2	FUL	C3-C4-C5	3.04	114.50	109.77
12	a	1	NAG	C2-N2-C7	3.03	127.22	122.90
5	Q	4	MAN	O3-C3-C2	3.01	115.76	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	3	MAN	O3-C3-C2	2.99	115.72	109.99
11	Y	3	FUC	C1-O5-C5	2.98	119.53	112.78
13	c	3	MAN	O2-C2-C3	-2.96	104.20	110.14
4	K	4	MAN	O5-C1-C2	2.95	115.32	110.77
5	Q	4	MAN	C1-O5-C5	2.94	116.18	112.19
12	a	5	FUC	C1-O5-C5	2.89	119.33	112.78
3	I	4	FUL	C2-C3-C4	2.84	115.80	110.89
5	L	4	MAN	C2-C3-C4	2.79	115.73	110.89
5	L	4	MAN	O2-C2-C1	2.79	114.86	109.15
6	X	5	MAN	C1-C2-C3	2.78	113.08	109.67
4	K	4	MAN	C1-C2-C3	2.77	113.07	109.67
4	P	4	MAN	O5-C1-C2	2.75	115.02	110.77
13	c	7	MAN	O2-C2-C3	-2.70	104.73	110.14
10	V	4	MAN	O2-C2-C3	-2.69	104.75	110.14
13	c	4	MAN	O2-C2-C3	2.69	115.53	110.14
5	Q	5	MAN	O2-C2-C3	-2.68	104.77	110.14
14	d	4	MAN	C1-O5-C5	2.67	115.81	112.19
13	c	6	MAN	O2-C2-C3	-2.67	104.80	110.14
5	Q	5	MAN	C1-C2-C3	2.66	112.93	109.67
5	Q	6	MAN	O2-C2-C3	-2.64	104.84	110.14
13	c	3	MAN	O2-C2-C1	2.64	114.55	109.15
13	c	4	MAN	O5-C1-C2	2.62	114.82	110.77
6	U	5	MAN	C1-O5-C5	2.60	115.72	112.19
12	a	5	FUC	O5-C5-C4	2.56	114.12	109.52
5	W	5	MAN	O5-C1-C2	2.55	114.70	110.77
8	R	1	NAG	C2-N2-C7	2.51	126.47	122.90
7	b	2	NAG	C1-O5-C5	2.47	115.54	112.19
5	Q	4	MAN	O2-C2-C3	2.46	115.06	110.14
6	M	3	BMA	C3-C4-C5	2.44	114.59	110.24
12	a	3	BMA	C1-C2-C3	2.43	112.66	109.67
6	e	5	MAN	O2-C2-C3	-2.43	105.27	110.14
14	d	4	MAN	O2-C2-C3	-2.43	105.27	110.14
6	M	3	BMA	O5-C1-C2	2.43	114.52	110.77
3	I	3	BMA	C1-C2-C3	2.43	112.65	109.67
12	a	5	FUC	C1-C2-C3	2.42	112.64	109.67
13	c	3	MAN	O5-C1-C2	-2.42	107.04	110.77
5	L	5	MAN	C1-C2-C3	2.41	112.63	109.67
4	K	4	MAN	O2-C2-C3	-2.41	105.32	110.14
6	U	3	BMA	C1-C2-C3	2.41	112.62	109.67
13	c	6	MAN	C3-C4-C5	2.40	114.53	110.24
9	T	2	FUL	C6-C5-C4	-2.38	108.67	113.07
5	L	4	MAN	O2-C2-C3	2.37	114.89	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	3	BMA	O5-C1-C2	2.37	114.43	110.77
11	Y	3	FUC	O5-C5-C4	2.36	113.76	109.52
5	L	4	MAN	C3-C4-C5	2.36	114.44	110.24
6	M	2	NAG	C1-C2-N2	2.35	114.50	110.49
5	Q	6	MAN	C1-O5-C5	2.33	115.35	112.19
13	c	4	MAN	O2-C2-C1	2.30	113.86	109.15
6	U	3	BMA	C1-O5-C5	2.30	115.31	112.19
3	I	5	FUC	C1-O5-C5	2.27	117.93	112.78
5	Q	3	MAN	O2-C2-C3	-2.27	105.60	110.14
6	M	3	BMA	O5-C5-C6	2.26	110.75	107.20
12	a	1	NAG	C4-C3-C2	2.24	114.30	111.02
5	Q	2	NAG	C1-O5-C5	2.23	115.22	112.19
5	W	3	MAN	O2-C2-C3	-2.23	105.67	110.14
13	c	4	MAN	O3-C3-C2	2.22	114.25	109.99
5	Q	6	MAN	C1-C2-C3	2.21	112.39	109.67
6	M	4	MAN	C1-C2-C3	2.20	112.38	109.67
5	Q	3	MAN	C1-C2-C3	2.17	112.34	109.67
6	U	5	MAN	O2-C2-C3	-2.16	105.81	110.14
12	a	4	MAN	O2-C2-C3	-2.15	105.83	110.14
5	W	4	MAN	O3-C3-C2	2.15	114.11	109.99
13	c	5	MAN	O5-C1-C2	2.14	114.08	110.77
5	W	4	MAN	O2-C2-C3	2.14	114.42	110.14
5	L	6	MAN	O5-C1-C2	2.12	114.05	110.77
9	T	3	FUC	C1-O5-C5	2.12	117.58	112.78
3	I	3	BMA	C1-O5-C5	2.11	115.05	112.19
7	S	1	NAG	C1-C2-N2	2.11	114.08	110.49
6	X	3	BMA	C1-C2-C3	-2.10	107.08	109.67
13	c	6	MAN	C2-C3-C4	2.10	114.53	110.89
4	P	4	MAN	O2-C2-C3	-2.08	105.96	110.14
5	L	5	MAN	O2-C2-C3	-2.08	105.97	110.14
13	c	3	MAN	O5-C5-C6	2.06	110.44	107.20
5	W	5	MAN	O2-C2-C3	-2.06	106.00	110.14
6	U	1	NAG	O4-C4-C3	-2.06	105.59	110.35
6	e	4	MAN	C1-C2-C3	2.05	112.19	109.67
5	Q	3	MAN	O6-C6-C5	-2.04	104.28	111.29
6	M	4	MAN	O5-C1-C2	2.04	113.92	110.77
6	M	5	MAN	C1-C2-C3	2.04	112.17	109.67
13	c	5	MAN	O2-C2-C3	-2.03	106.06	110.14
6	M	4	MAN	O2-C2-C3	-2.03	106.07	110.14
6	M	1	NAG	C3-C4-C5	2.03	113.86	110.24
5	L	6	MAN	O2-C2-C3	-2.02	106.09	110.14
7	Z	1	NAG	C1-C2-N2	2.02	113.94	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	1	NAG	C3-C4-C5	2.02	113.84	110.24
4	K	2	NAG	C1-O5-C5	2.01	114.92	112.19
5	L	5	MAN	O5-C1-C2	2.01	113.87	110.77
6	X	3	BMA	O5-C5-C6	2.01	110.35	107.20
6	M	5	MAN	O2-C2-C3	-2.00	106.13	110.14

There are no chirality outliers.

All (154) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	a	1	NAG	C1-C2-N2-C7
14	d	4	MAN	O5-C5-C6-O6
6	e	3	BMA	O5-C5-C6-O6
4	P	3	BMA	C4-C5-C6-O6
6	e	1	NAG	O5-C5-C6-O6
6	X	5	MAN	O5-C5-C6-O6
7	Z	1	NAG	O5-C5-C6-O6
8	O	1	NAG	O5-C5-C6-O6
10	V	5	MAN	O5-C5-C6-O6
13	c	5	MAN	O5-C5-C6-O6
6	M	3	BMA	C4-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
6	M	3	BMA	O5-C5-C6-O6
6	X	5	MAN	C4-C5-C6-O6
6	e	1	NAG	C4-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
5	L	4	MAN	O5-C5-C6-O6
14	d	1	NAG	O5-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
6	e	3	BMA	C4-C5-C6-O6
8	O	1	NAG	C4-C5-C6-O6
14	d	1	NAG	C4-C5-C6-O6
4	P	3	BMA	O5-C5-C6-O6
6	X	4	MAN	O5-C5-C6-O6
6	e	5	MAN	O5-C5-C6-O6
8	R	1	NAG	O5-C5-C6-O6
13	c	6	MAN	O5-C5-C6-O6
6	X	4	MAN	C4-C5-C6-O6
14	d	4	MAN	C4-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	L	5	MAN	O5-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
6	U	5	MAN	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
12	a	3	BMA	O5-C5-C6-O6
12	a	1	NAG	C4-C5-C6-O6
13	c	4	MAN	C4-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
12	a	1	NAG	O5-C5-C6-O6
13	c	4	MAN	O5-C5-C6-O6
5	L	5	MAN	C4-C5-C6-O6
7	Z	1	NAG	C4-C5-C6-O6
10	V	5	MAN	C4-C5-C6-O6
5	Q	6	MAN	O5-C5-C6-O6
5	L	4	MAN	C4-C5-C6-O6
13	c	5	MAN	C4-C5-C6-O6
12	a	3	BMA	C4-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
5	Q	4	MAN	O5-C5-C6-O6
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	P	1	NAG	C8-C7-N2-C2
4	P	1	NAG	O7-C7-N2-C2
5	L	2	NAG	C8-C7-N2-C2
5	L	2	NAG	O7-C7-N2-C2
6	M	2	NAG	C8-C7-N2-C2
6	M	2	NAG	O7-C7-N2-C2
6	U	1	NAG	C8-C7-N2-C2
6	U	1	NAG	O7-C7-N2-C2
6	e	1	NAG	C8-C7-N2-C2
6	e	1	NAG	O7-C7-N2-C2
7	N	1	NAG	C8-C7-N2-C2
7	N	1	NAG	O7-C7-N2-C2
7	S	1	NAG	C8-C7-N2-C2
7	S	1	NAG	O7-C7-N2-C2
7	Z	1	NAG	C8-C7-N2-C2
7	Z	1	NAG	O7-C7-N2-C2
7	Z	2	NAG	C8-C7-N2-C2
7	Z	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	b	1	NAG	C8-C7-N2-C2
7	b	1	NAG	O7-C7-N2-C2
9	T	1	NAG	C8-C7-N2-C2
9	T	1	NAG	O7-C7-N2-C2
10	V	1	NAG	C8-C7-N2-C2
10	V	1	NAG	O7-C7-N2-C2
5	W	1	NAG	C4-C5-C6-O6
8	R	3	BMA	C4-C5-C6-O6
10	V	4	MAN	O5-C5-C6-O6
6	X	1	NAG	C4-C5-C6-O6
5	W	5	MAN	C4-C5-C6-O6
6	U	5	MAN	C4-C5-C6-O6
7	N	2	NAG	C4-C5-C6-O6
5	W	6	MAN	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
5	Q	3	MAN	O5-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
8	R	3	BMA	O5-C5-C6-O6
11	Y	1	NAG	O5-C5-C6-O6
7	b	1	NAG	O5-C5-C6-O6
13	c	1	NAG	O5-C5-C6-O6
5	W	6	MAN	C4-C5-C6-O6
5	W	5	MAN	O5-C5-C6-O6
11	Y	1	NAG	C4-C5-C6-O6
13	c	1	NAG	C4-C5-C6-O6
4	K	3	BMA	C4-C5-C6-O6
6	e	5	MAN	C4-C5-C6-O6
6	X	3	BMA	C4-C5-C6-O6
11	Y	2	NAG	C4-C5-C6-O6
6	X	1	NAG	O5-C5-C6-O6
6	X	3	BMA	O5-C5-C6-O6
10	V	1	NAG	C4-C5-C6-O6
10	V	4	MAN	C4-C5-C6-O6
8	R	1	NAG	C4-C5-C6-O6
7	N	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
5	Q	6	MAN	C4-C5-C6-O6
4	P	4	MAN	O5-C5-C6-O6
13	c	7	MAN	O5-C5-C6-O6
10	V	3	BMA	O5-C5-C6-O6
7	b	2	NAG	C4-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	Q	5	MAN	O5-C5-C6-O6
10	V	1	NAG	O5-C5-C6-O6
5	Q	4	MAN	C4-C5-C6-O6
11	Y	2	NAG	O5-C5-C6-O6
8	R	1	NAG	C3-C2-N2-C7
13	c	6	MAN	C4-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
6	X	2	NAG	C4-C5-C6-O6
6	e	4	MAN	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
6	e	4	MAN	O5-C5-C6-O6
5	W	4	MAN	C4-C5-C6-O6
8	O	2	NAG	C4-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
4	J	4	MAN	C4-C5-C6-O6
6	U	2	NAG	C1-C2-N2-C7
4	J	2	NAG	C3-C2-N2-C7
4	K	2	NAG	C3-C2-N2-C7
6	M	1	NAG	C3-C2-N2-C7
6	M	2	NAG	C3-C2-N2-C7
6	X	1	NAG	C3-C2-N2-C7
6	e	2	NAG	C3-C2-N2-C7
7	S	1	NAG	C3-C2-N2-C7
7	Z	2	NAG	C3-C2-N2-C7
7	b	1	NAG	C3-C2-N2-C7
12	a	2	NAG	C3-C2-N2-C7
5	L	3	MAN	C4-C5-C6-O6
6	M	5	MAN	O5-C5-C6-O6
12	a	2	NAG	C1-C2-N2-C7
7	b	1	NAG	C4-C5-C6-O6
5	W	4	MAN	O5-C5-C6-O6
6	U	2	NAG	C3-C2-N2-C7
6	e	1	NAG	C3-C2-N2-C7
7	N	1	NAG	C3-C2-N2-C7
7	Z	1	NAG	C3-C2-N2-C7
7	b	2	NAG	C3-C2-N2-C7
5	L	3	MAN	O5-C5-C6-O6

All (9) ring outliers are listed below:

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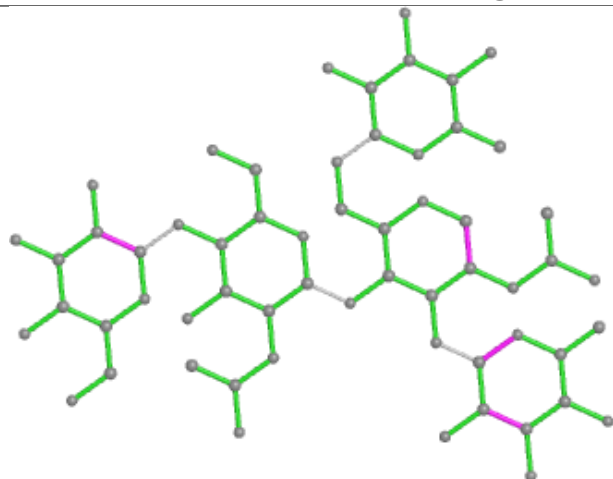
Mol	Chain	Res	Type	Atoms
6	M	3	BMA	C1-C2-C3-C4-C5-O5
13	c	7	MAN	C1-C2-C3-C4-C5-O5
10	V	5	MAN	C1-C2-C3-C4-C5-O5
5	W	3	MAN	C1-C2-C3-C4-C5-O5
5	L	3	MAN	C1-C2-C3-C4-C5-O5
5	W	6	MAN	C1-C2-C3-C4-C5-O5
6	U	4	MAN	C1-C2-C3-C4-C5-O5
4	J	4	MAN	C1-C2-C3-C4-C5-O5
13	c	3	MAN	C1-C2-C3-C4-C5-O5

23 monomers are involved in 20 short contacts:

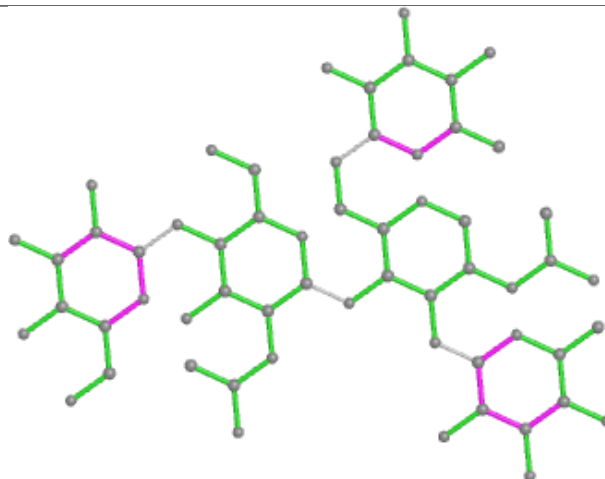
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	S	1	NAG	2	0
3	I	1	NAG	1	0
4	K	1	NAG	3	0
7	S	2	NAG	1	0
6	U	1	NAG	1	0
6	X	4	MAN	1	0
7	N	1	NAG	1	0
9	T	2	FUL	1	0
10	V	1	NAG	1	0
7	Z	1	NAG	1	0
4	J	1	NAG	1	0
5	L	4	MAN	1	0
5	L	1	NAG	1	0
5	W	1	NAG	1	0
6	X	3	BMA	1	0
5	Q	2	NAG	1	0
7	Z	2	NAG	1	0
5	L	3	MAN	1	0
4	P	1	NAG	2	0
5	L	2	NAG	1	0
3	I	4	FUL	1	0
9	T	1	NAG	1	0
6	M	2	NAG	1	0

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

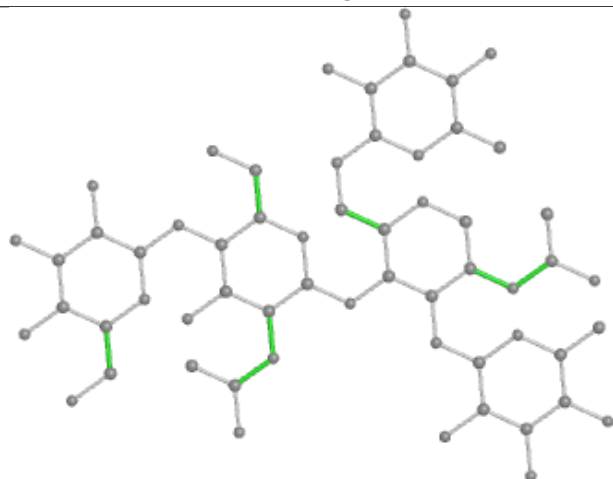
Oligosaccharide Chain I



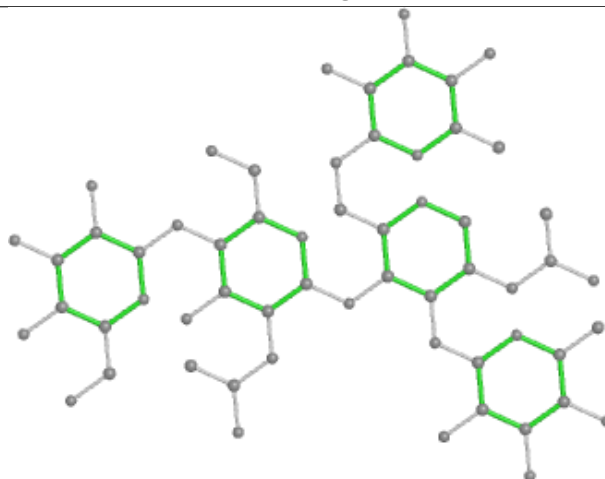
Bond lengths



Bond angles

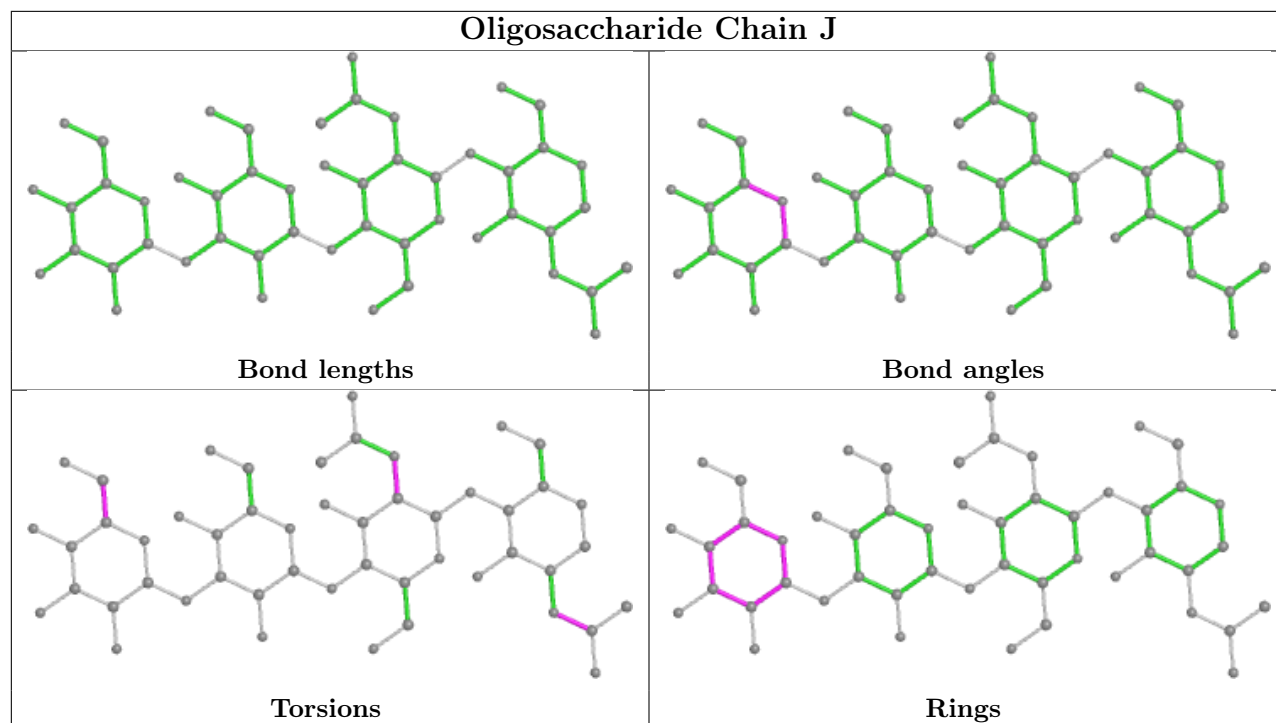


Torsions

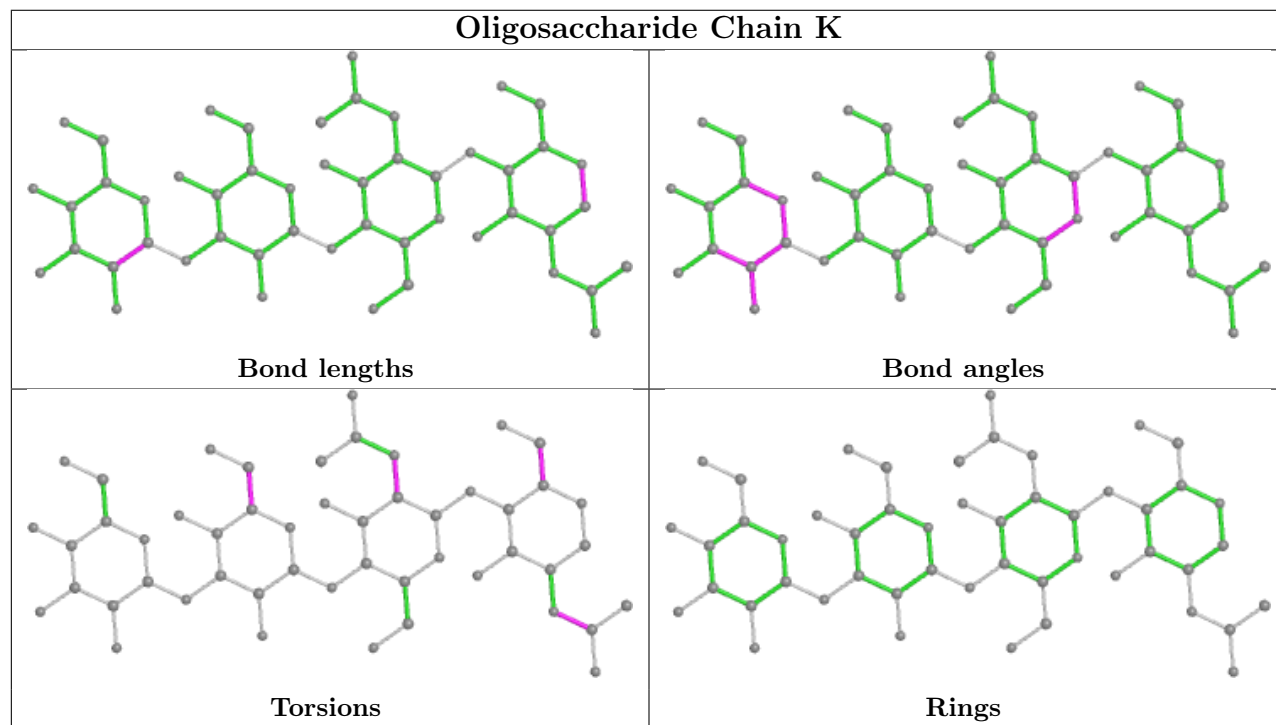


Rings

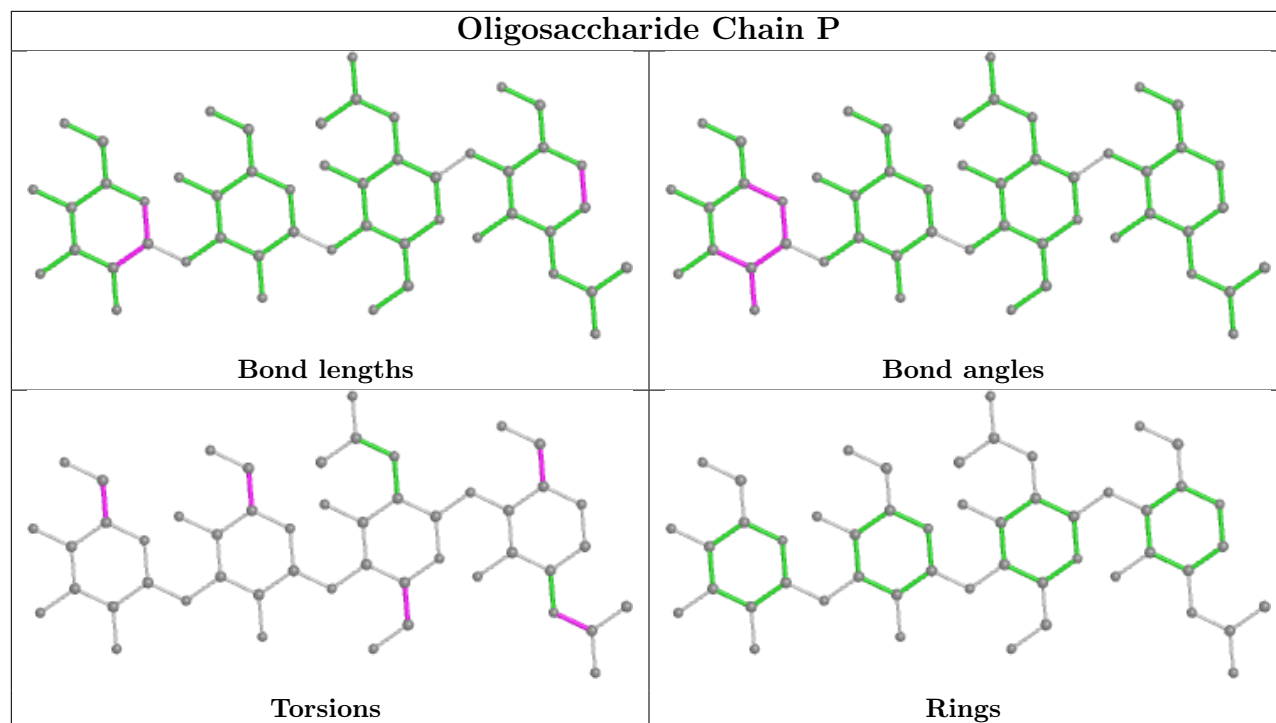
Oligosaccharide Chain J



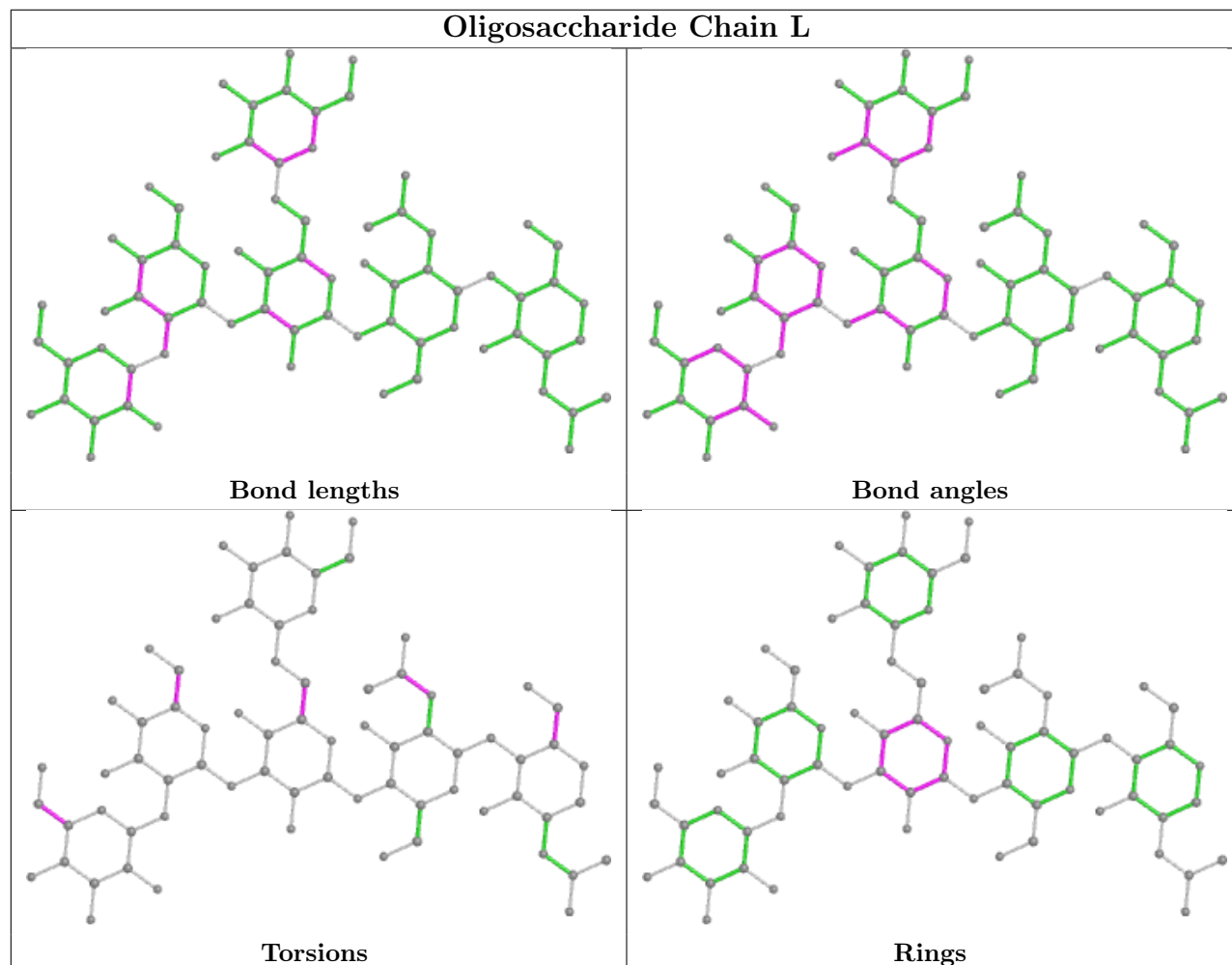
Oligosaccharide Chain K

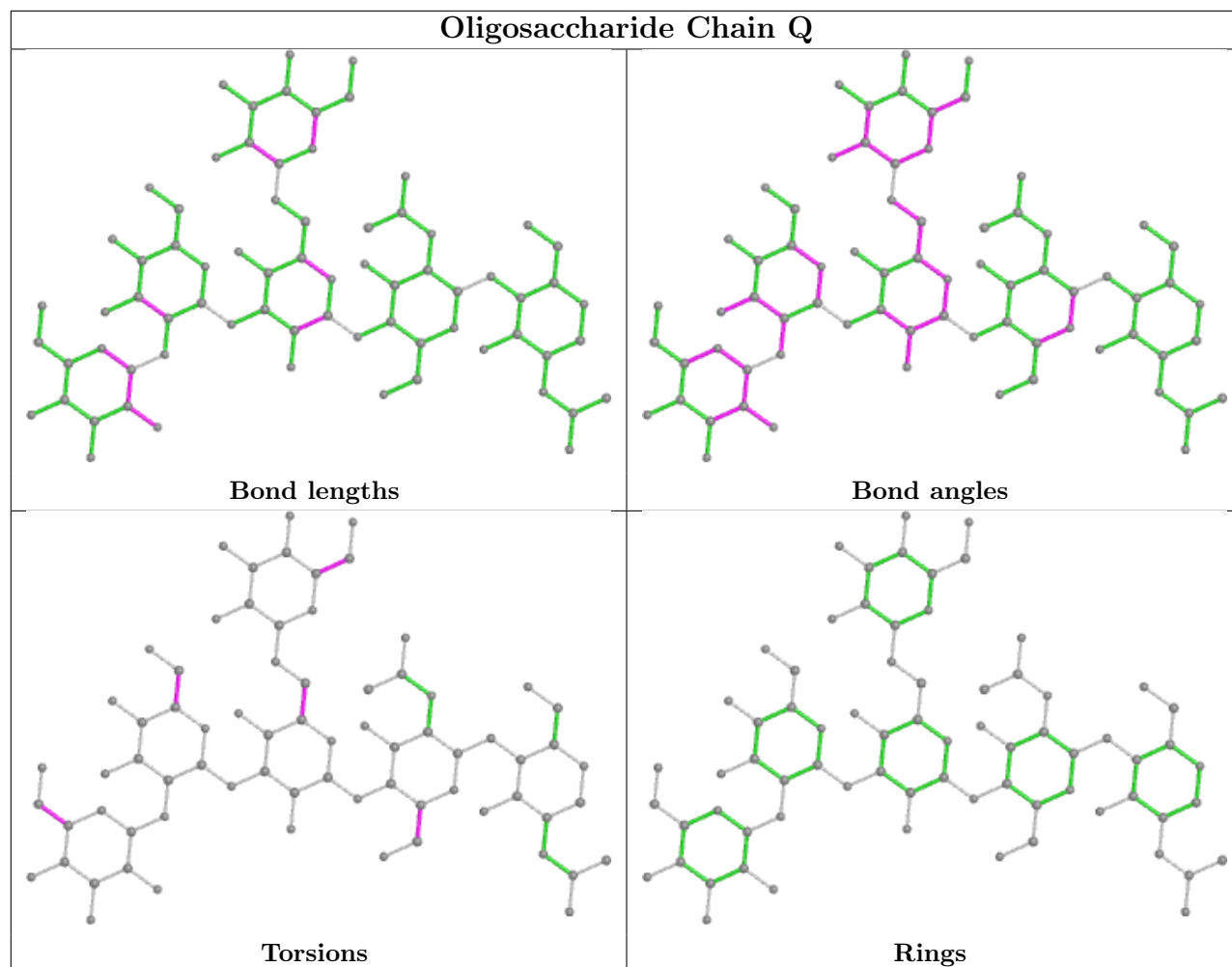


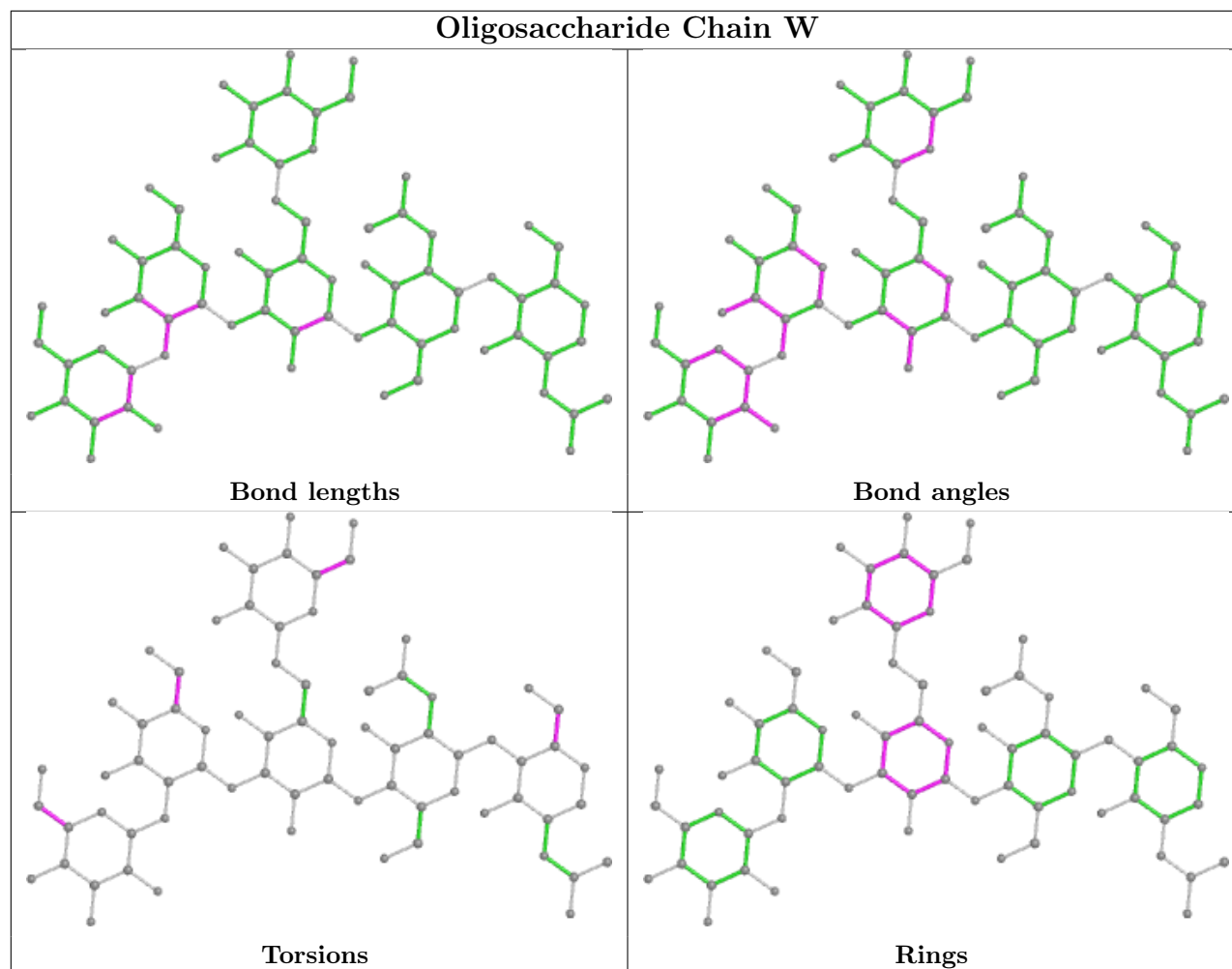
Oligosaccharide Chain P

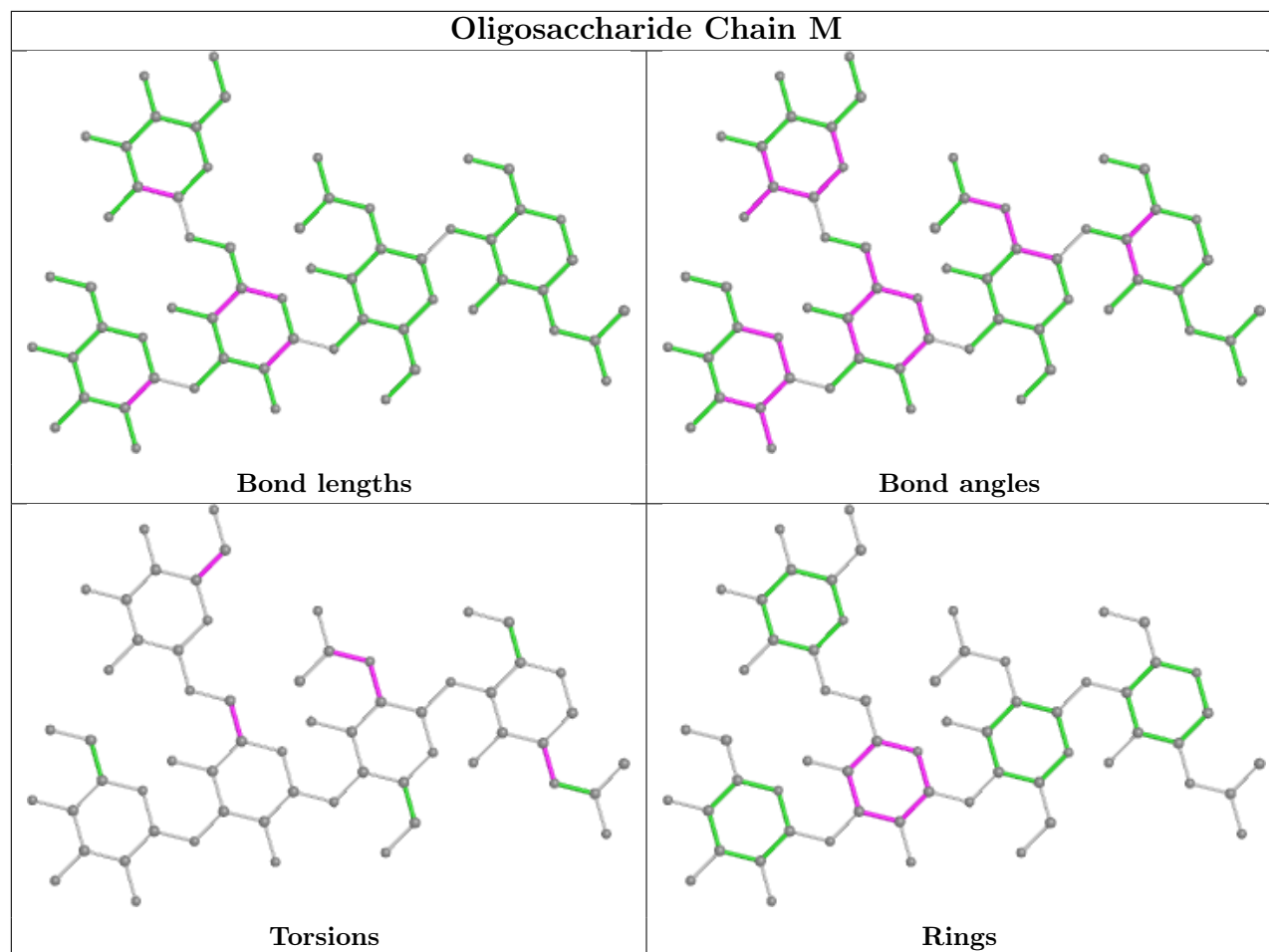


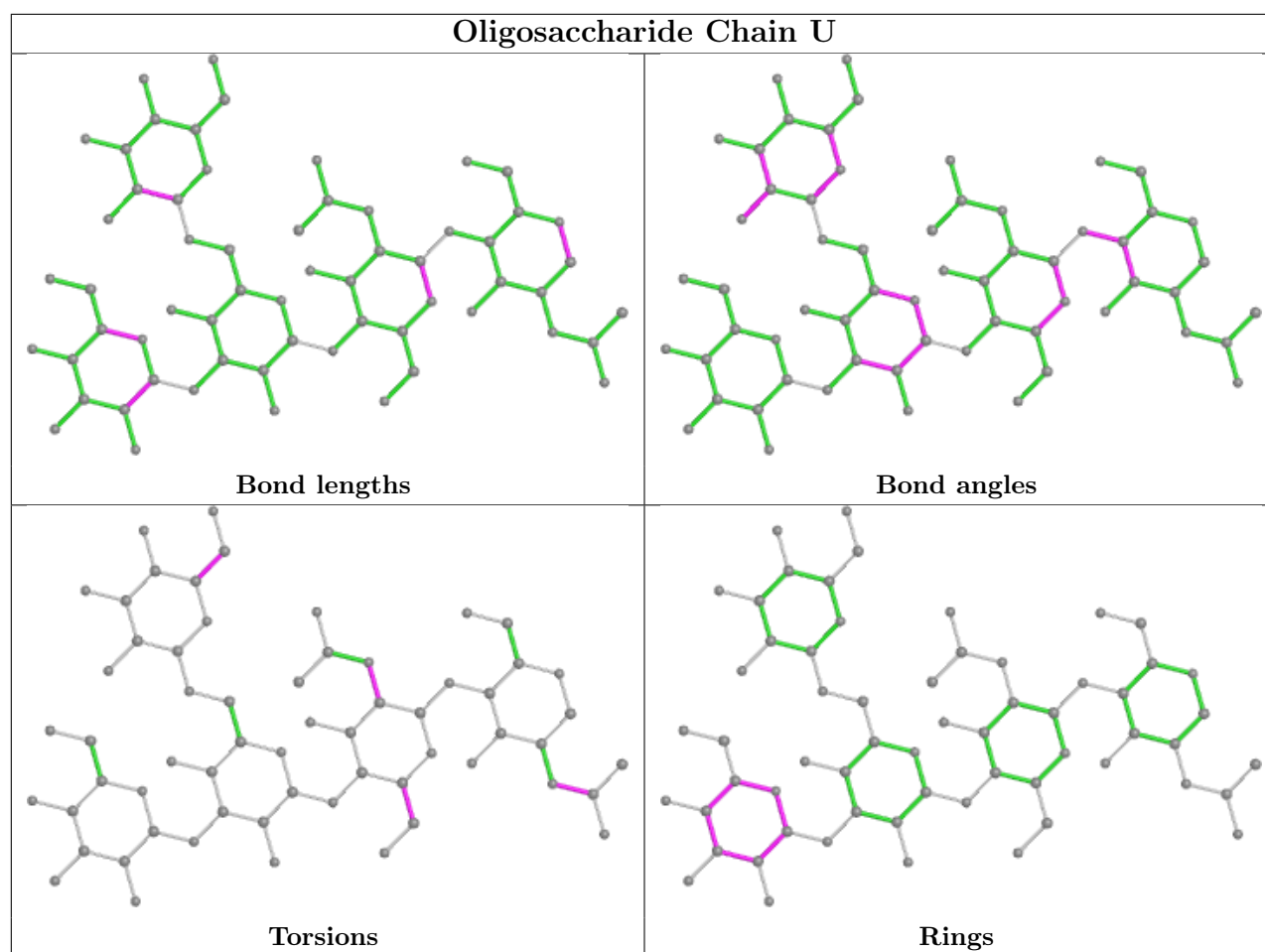
Oligosaccharide Chain L

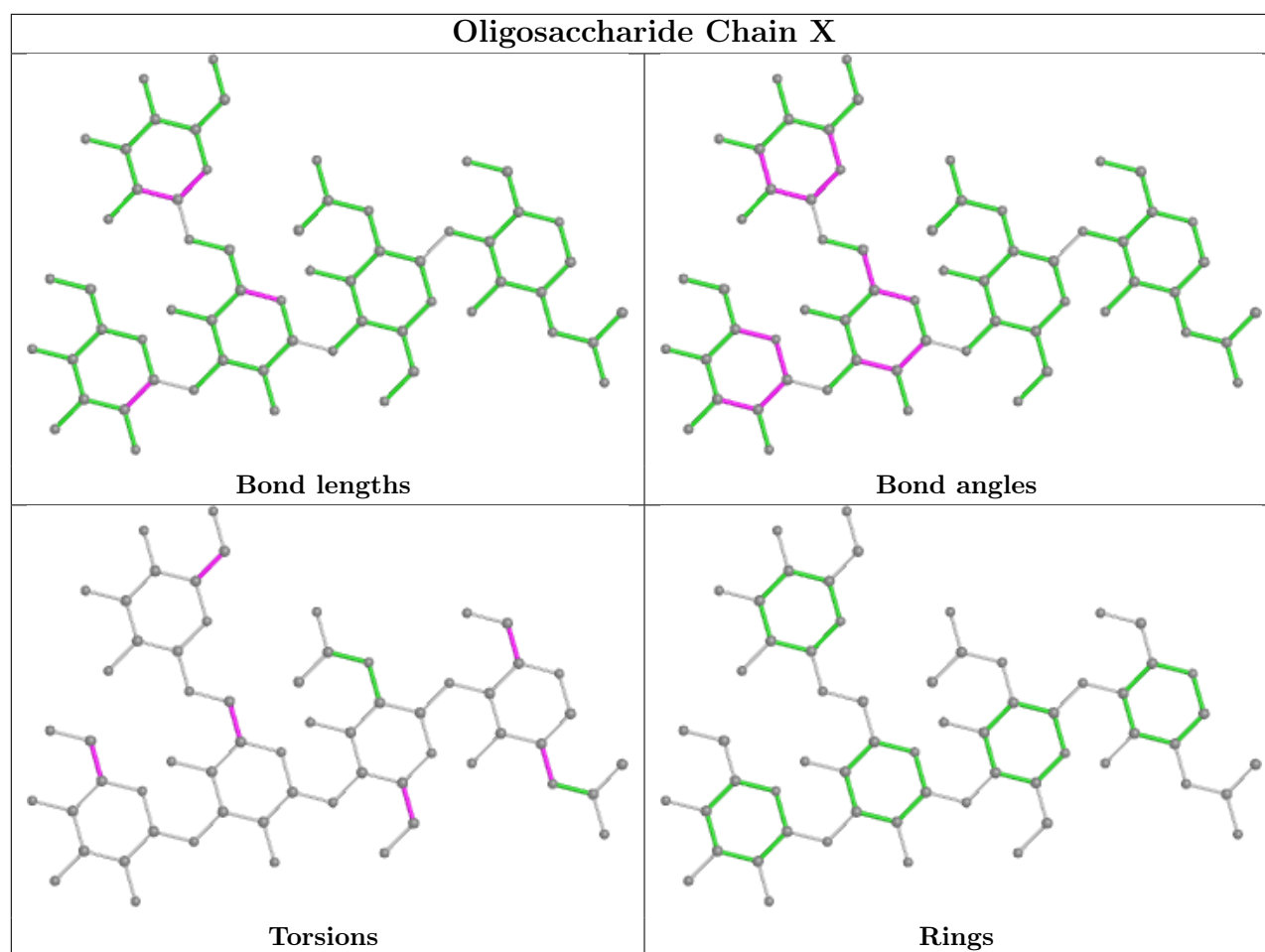


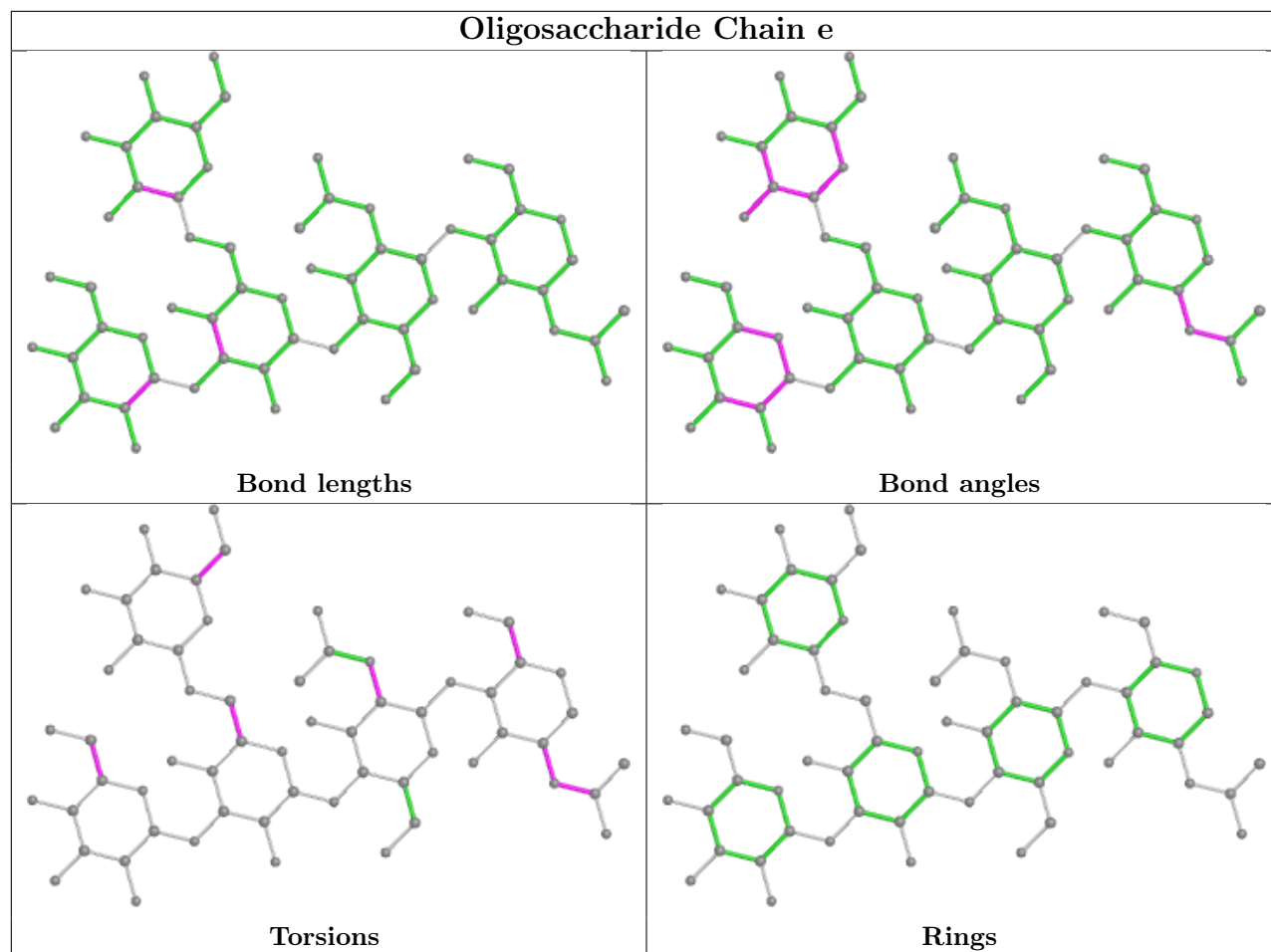


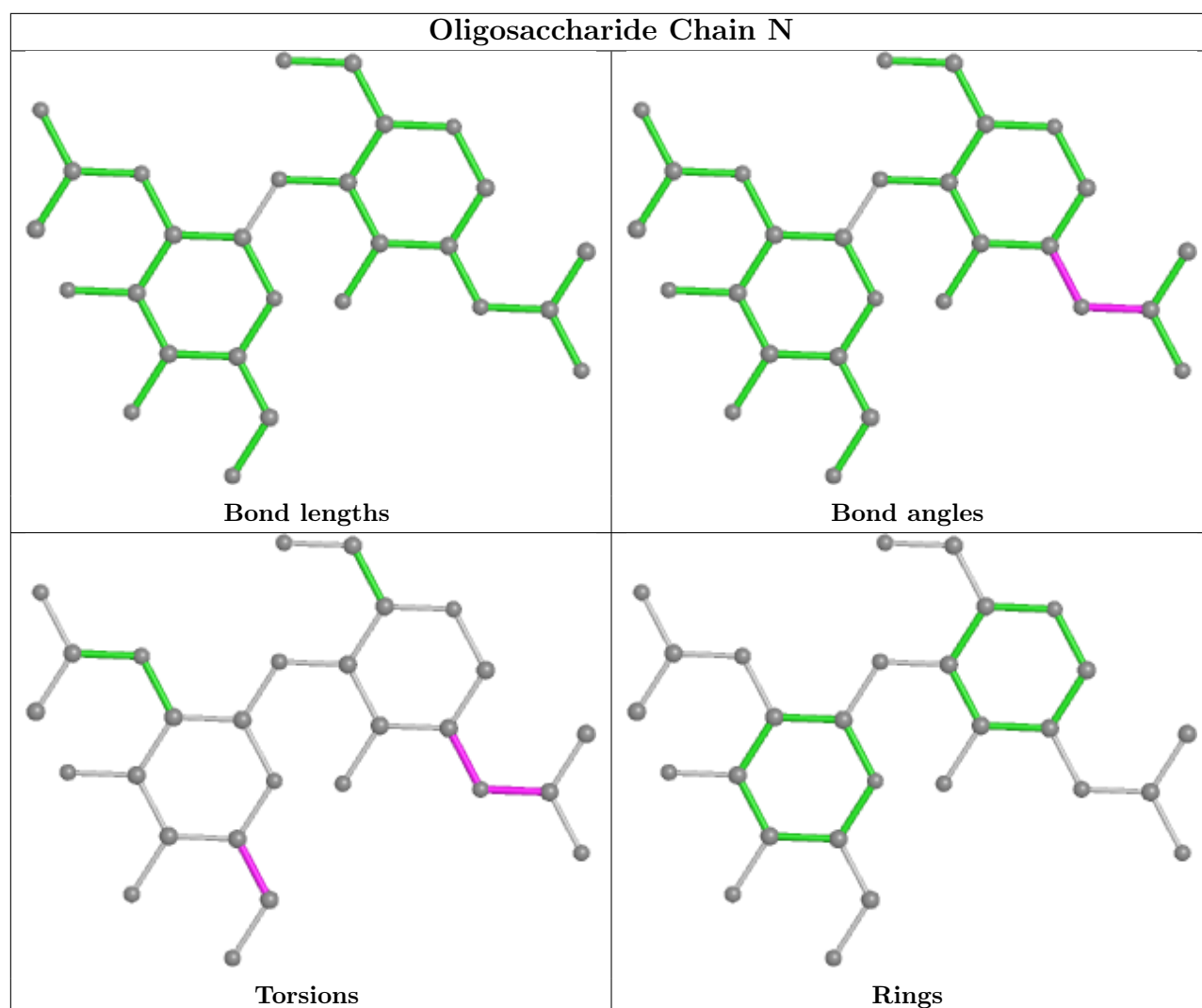


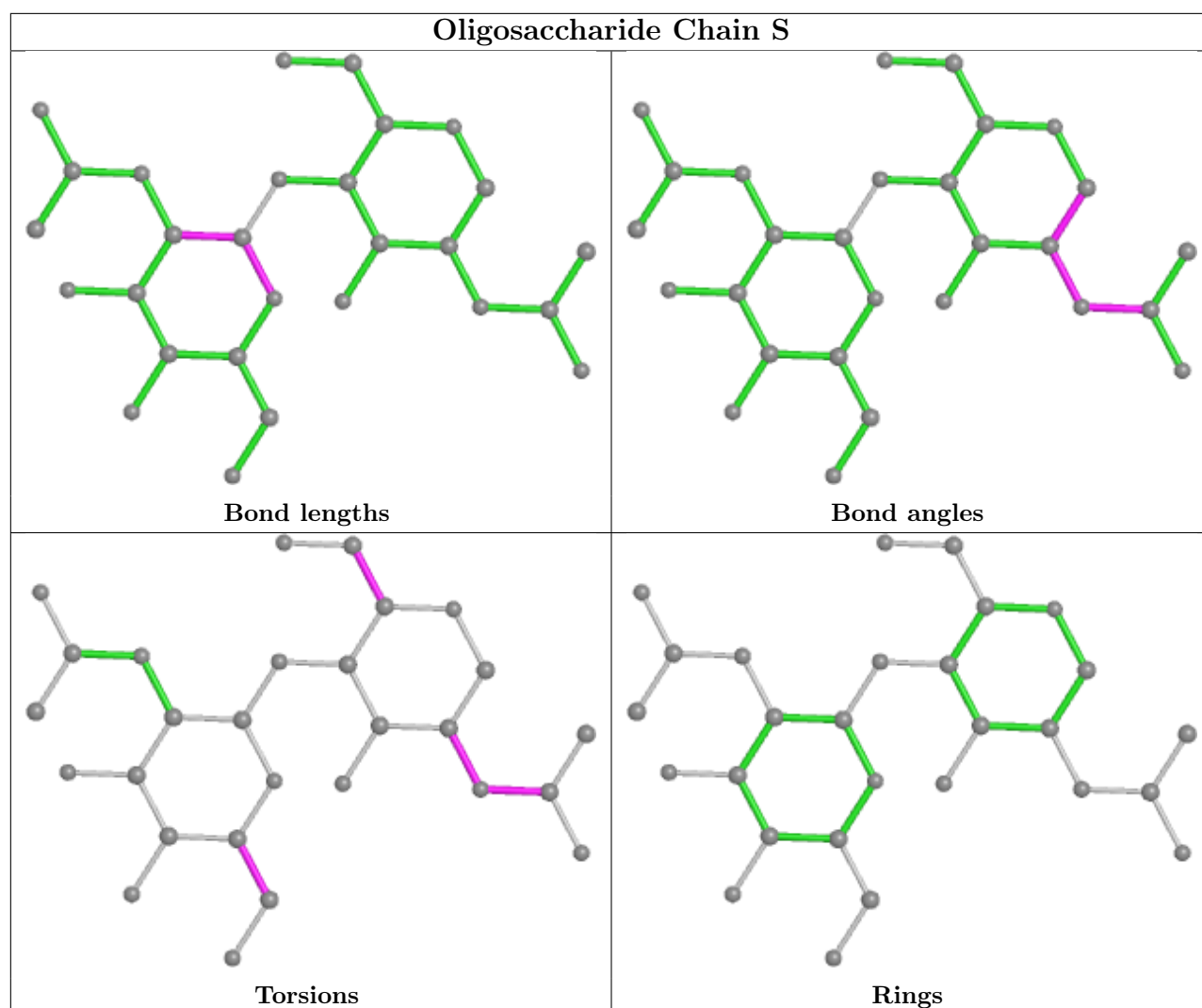


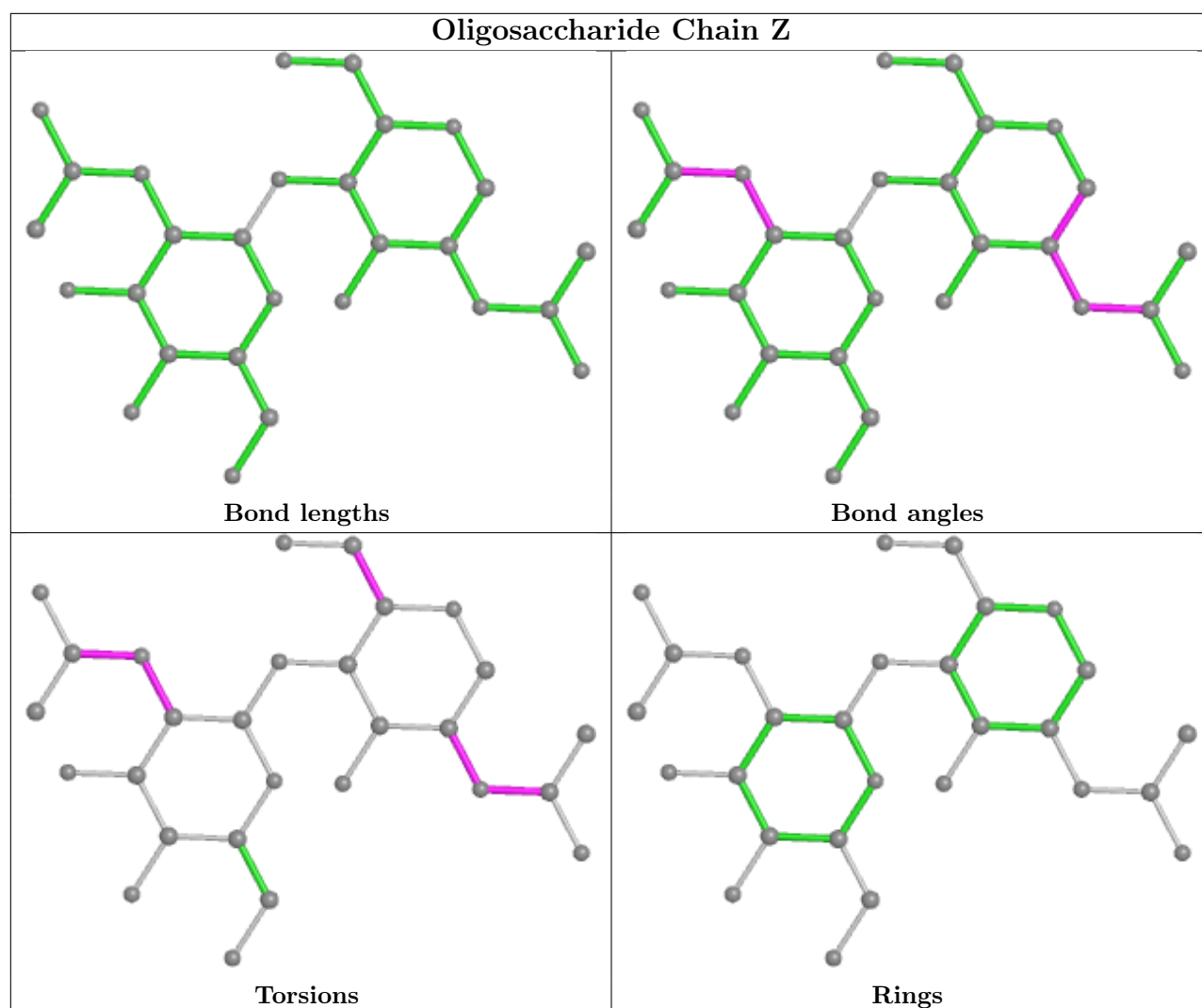


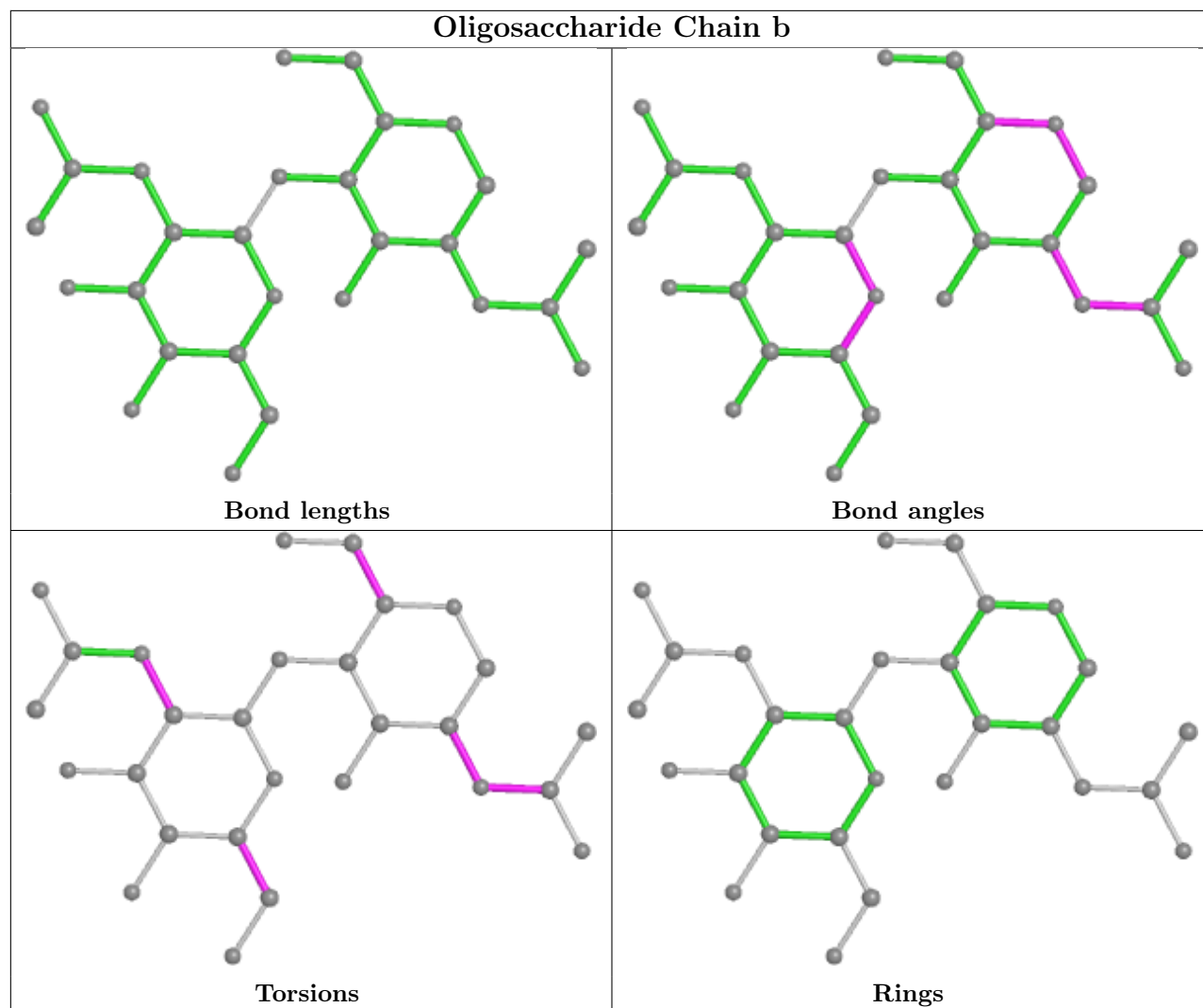


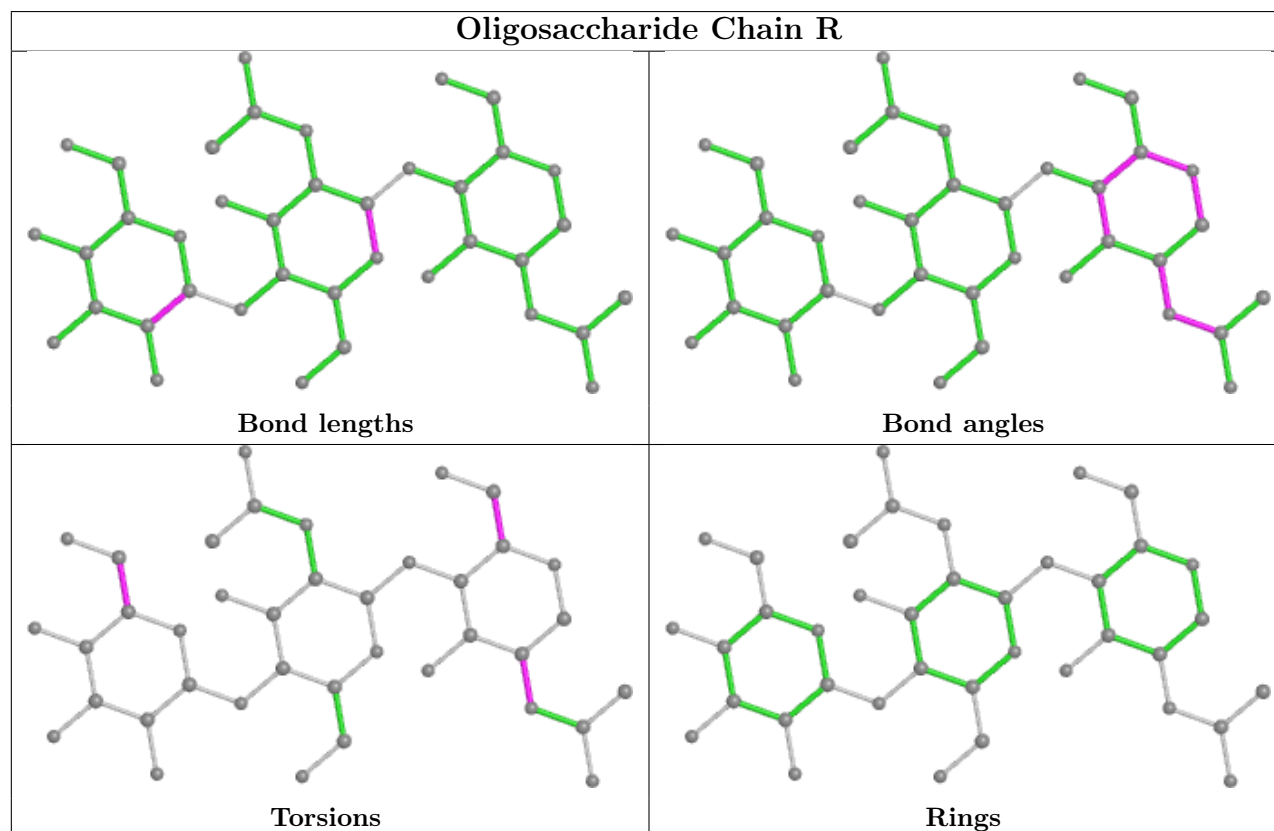
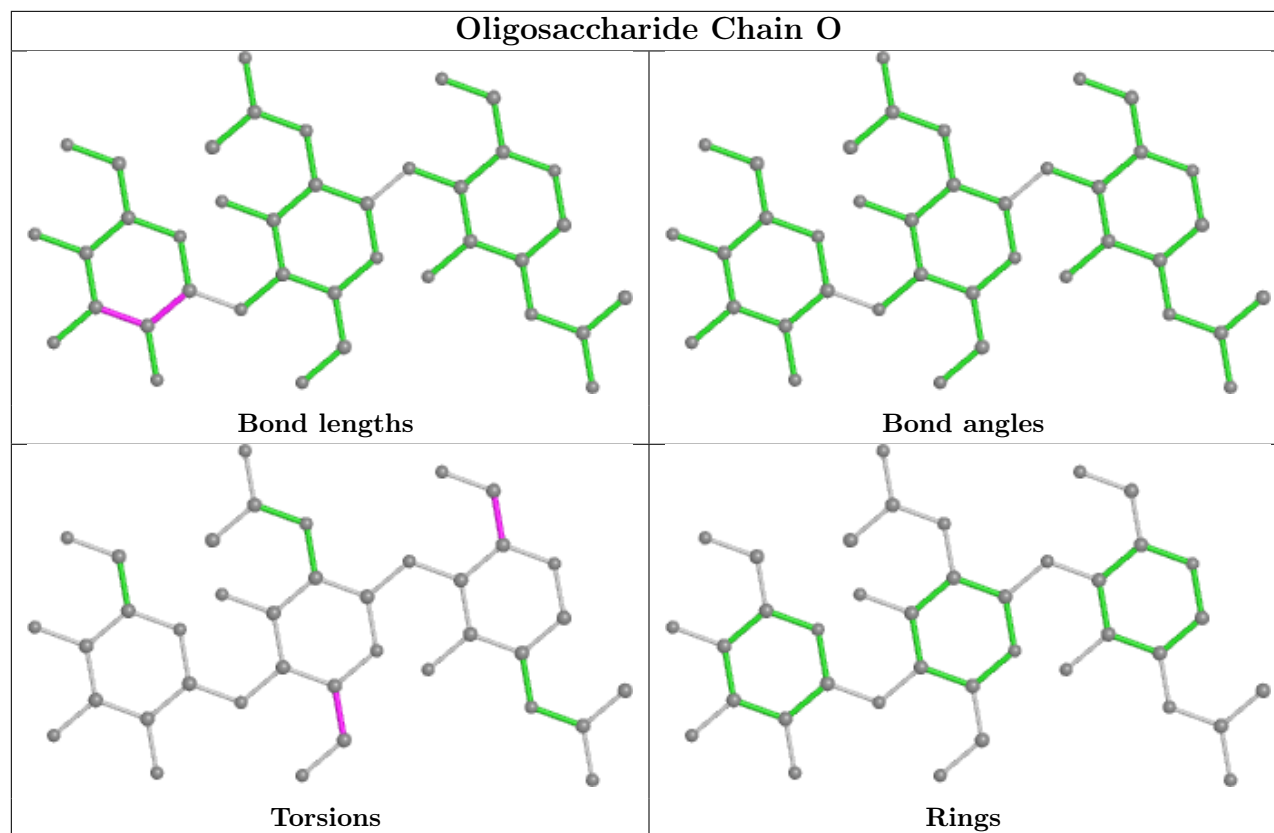


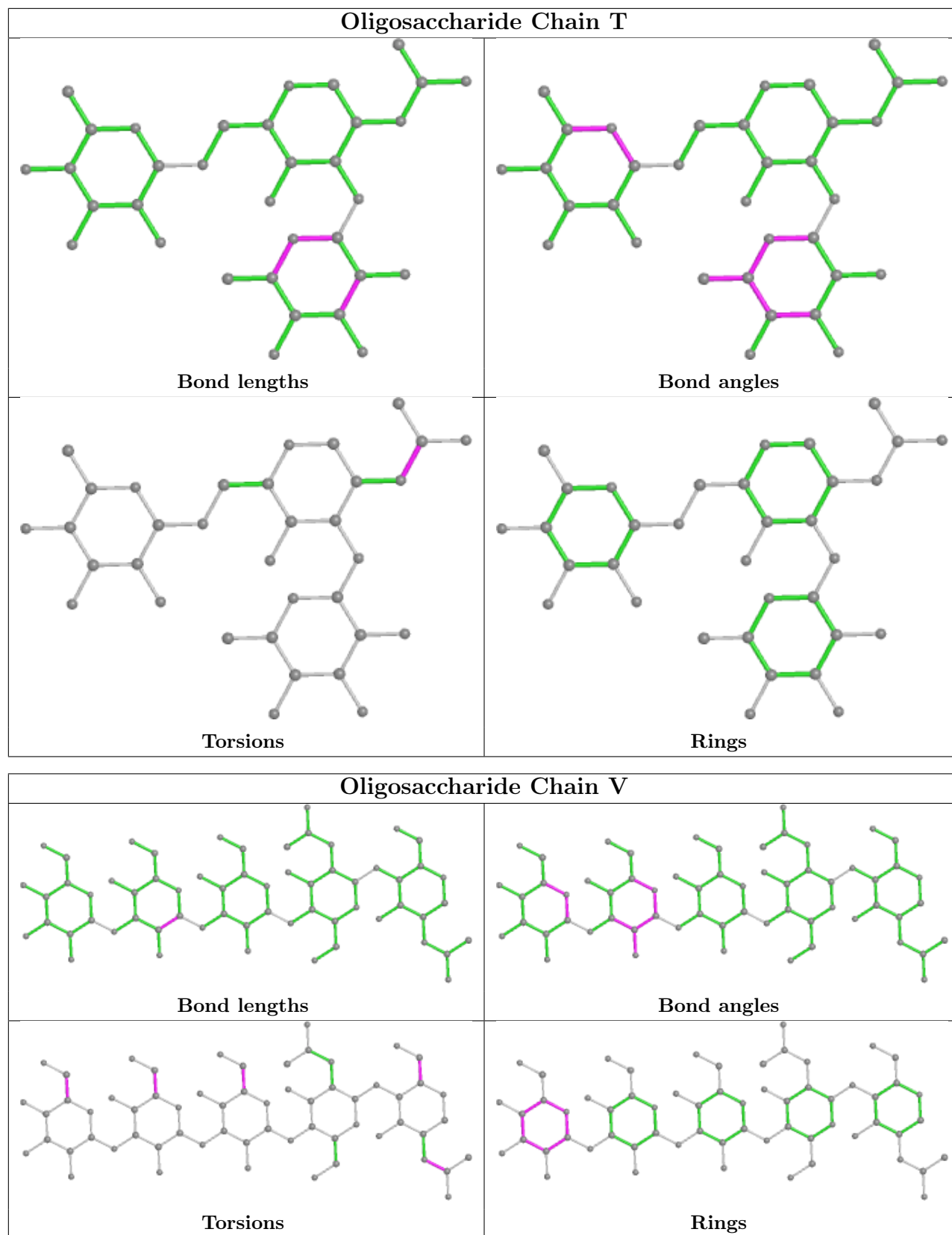


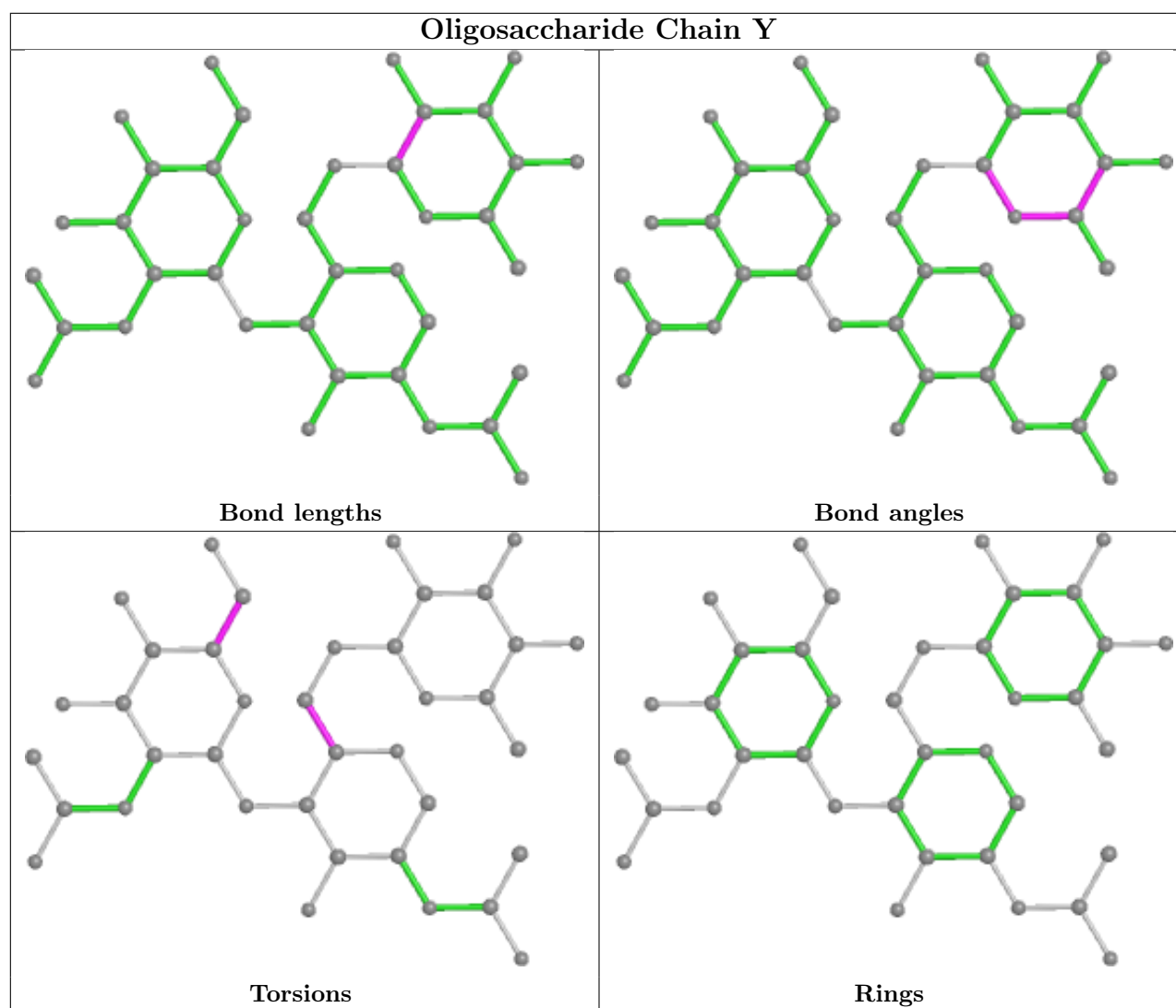


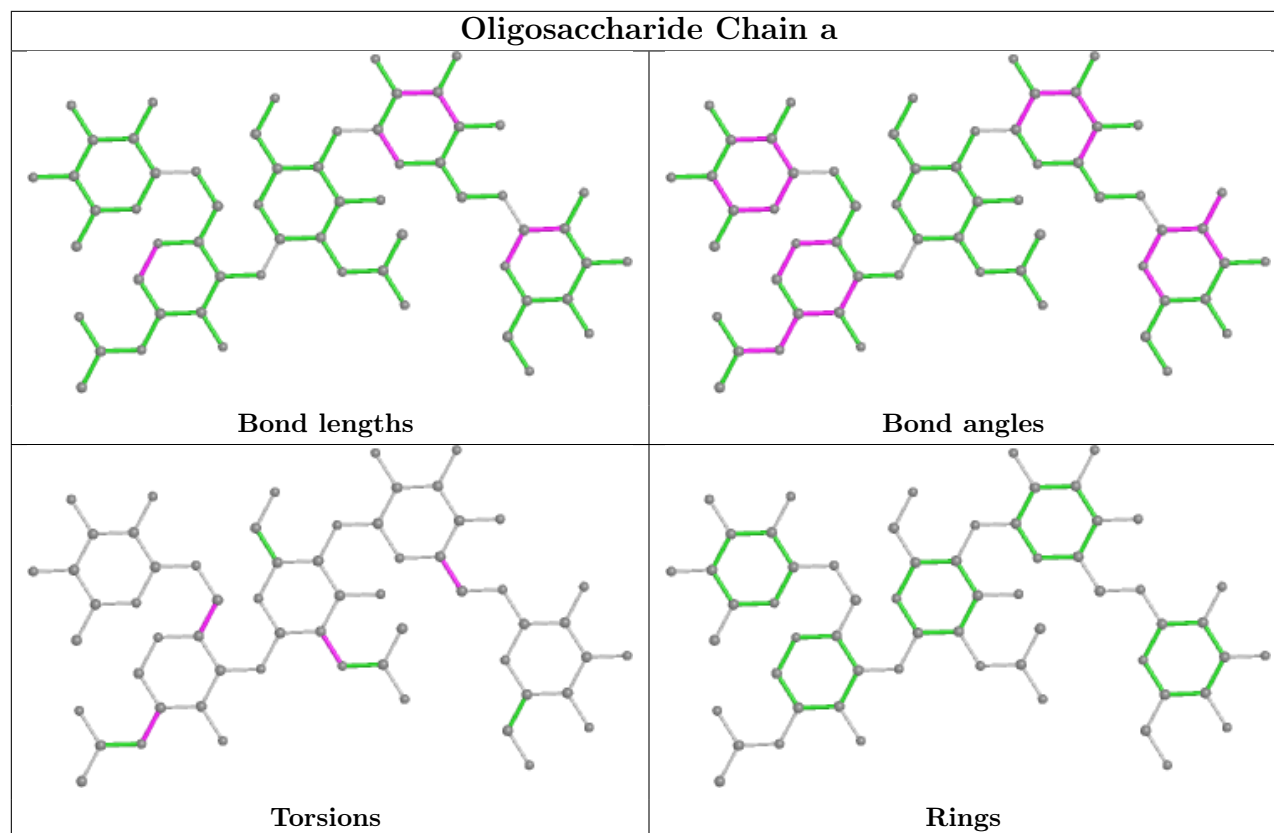


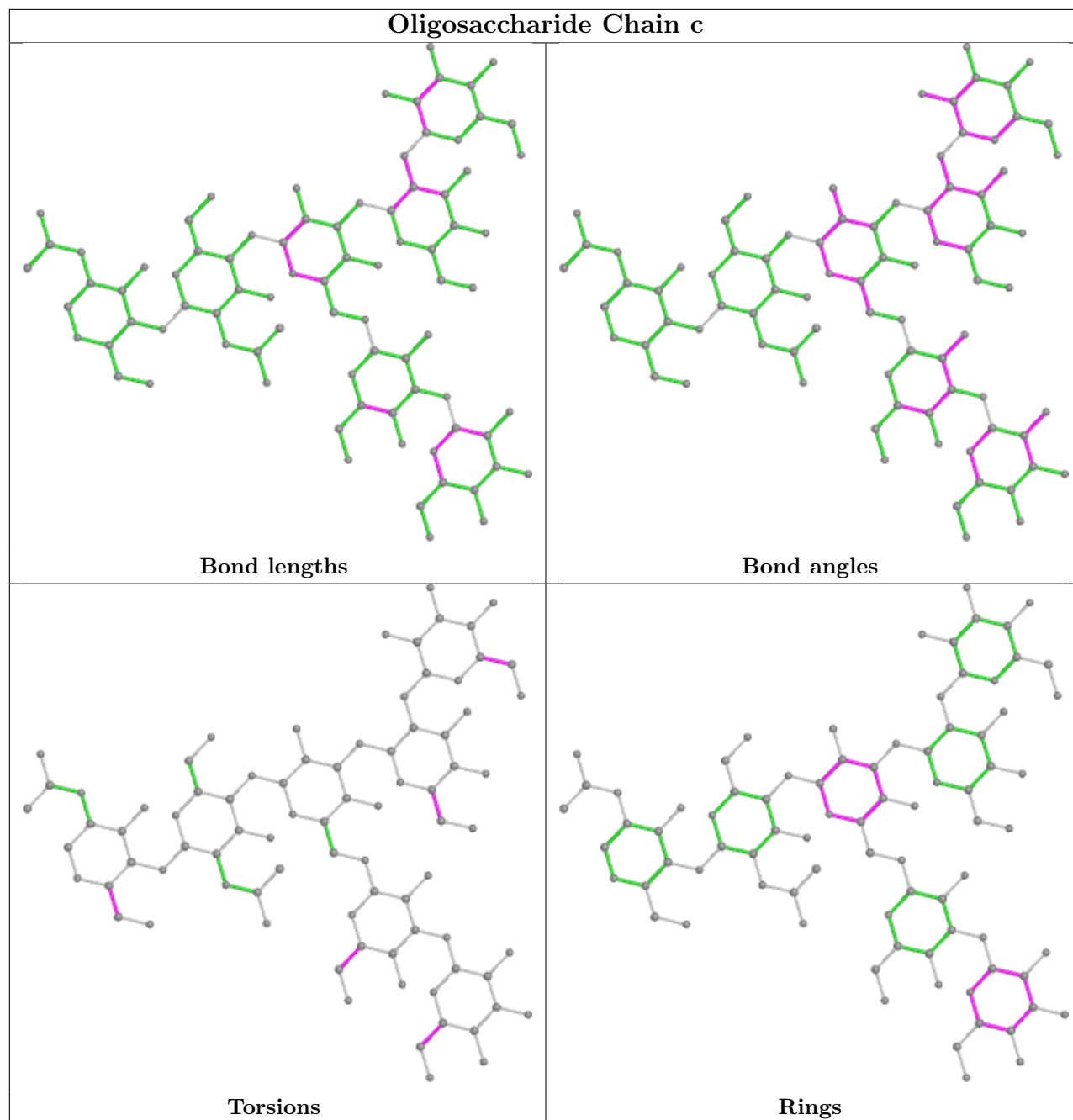


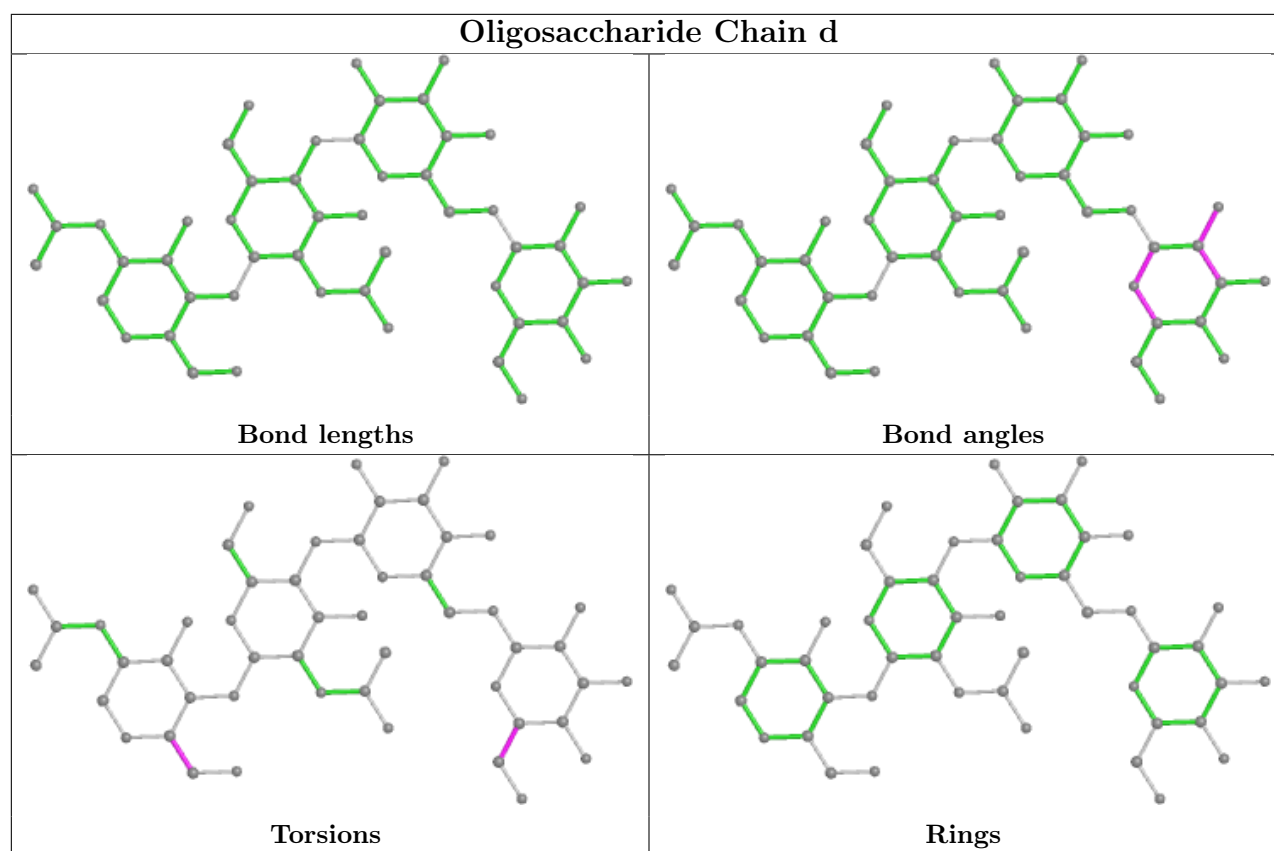












5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	NAG	H	201	2	14,14,15	0.82	2 (14%)	17,19,21	0.48	0
15	NAG	C	417	1	14,14,15	0.30	0	17,19,21	0.91	1 (5%)
15	NAG	D	201	2	14,14,15	0.88	1 (7%)	17,19,21	1.26	1 (5%)
15	NAG	B	201	2	14,14,15	0.43	0	17,19,21	0.42	0
15	NAG	F	201	2	14,14,15	0.69	1 (7%)	17,19,21	1.17	2 (11%)
15	NAG	G	419	1	14,14,15	0.95	1 (7%)	17,19,21	3.36	5 (29%)
15	NAG	A	525	1	14,14,15	0.41	0	17,19,21	0.55	0
16	CAC	B	202	-	0,4,4	-	-	0,6,6	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	H	201	2	-	2/6/23/26	0/1/1/1
15	NAG	C	417	1	-	2/6/23/26	0/1/1/1
15	NAG	D	201	2	-	3/6/23/26	0/1/1/1
15	NAG	B	201	2	-	3/6/23/26	0/1/1/1
15	NAG	F	201	2	-	0/6/23/26	0/1/1/1
15	NAG	G	419	1	-	6/6/23/26	0/1/1/1
15	NAG	A	525	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	201	NAG	O5-C1	3.06	1.48	1.43
15	G	419	NAG	C1-C2	-2.74	1.48	1.52
15	H	201	NAG	O5-C1	2.20	1.47	1.43
15	F	201	NAG	O5-C1	-2.17	1.40	1.43
15	H	201	NAG	C1-C2	2.01	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	G	419	NAG	C2-N2-C7	11.63	139.46	122.90
15	D	201	NAG	C1-O5-C5	4.85	118.76	112.19
15	G	419	NAG	C1-O5-C5	4.52	118.31	112.19
15	G	419	NAG	C4-C3-C2	-3.32	106.15	111.02
15	C	417	NAG	C1-O5-C5	3.29	116.66	112.19
15	F	201	NAG	C3-C4-C5	3.21	115.97	110.24
15	F	201	NAG	C1-O5-C5	2.75	115.92	112.19
15	G	419	NAG	C3-C4-C5	2.60	114.88	110.24
15	G	419	NAG	C8-C7-N2	-2.20	112.37	116.10

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	G	419	NAG	C3-C2-N2-C7
15	G	419	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
15	G	419	NAG	C8-C7-N2-C2
15	G	419	NAG	O5-C5-C6-O6
15	H	201	NAG	O5-C5-C6-O6
15	B	201	NAG	C4-C5-C6-O6
15	G	419	NAG	C4-C5-C6-O6
15	C	417	NAG	C8-C7-N2-C2
15	C	417	NAG	O7-C7-N2-C2
15	A	525	NAG	C4-C5-C6-O6
15	H	201	NAG	C4-C5-C6-O6
15	B	201	NAG	O5-C5-C6-O6
15	A	525	NAG	O5-C5-C6-O6
15	G	419	NAG	C1-C2-N2-C7
15	D	201	NAG	C1-C2-N2-C7
15	D	201	NAG	O5-C5-C6-O6
15	B	201	NAG	C1-C2-N2-C7
15	D	201	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	201	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	A	319/329 (96%)	-0.43	2 (0%) 89 84	44, 71, 122, 167	0
1	C	319/329 (96%)	-0.36	4 (1%) 77 66	58, 82, 123, 170	0
1	E	319/329 (96%)	-0.33	0 100 100	55, 89, 134, 187	0
1	G	319/329 (96%)	-0.13	8 (2%) 57 42	59, 100, 171, 247	0
2	B	174/174 (100%)	-0.37	0 100 100	43, 68, 114, 170	0
2	D	174/174 (100%)	-0.27	2 (1%) 80 70	51, 79, 116, 193	0
2	F	174/174 (100%)	-0.24	2 (1%) 80 70	44, 86, 135, 187	0
2	H	174/174 (100%)	0.33	13 (7%) 14 7	58, 169, 226, 264	0
All	All	1972/2012 (98%)	-0.25	31 (1%) 72 59	43, 86, 172, 264	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	174	LYS	6.5
2	D	173	ILE	4.7
2	H	140	ILE	4.6
1	G	11	ALA	4.4
2	H	141	TYR	4.1
2	H	26	HIS	3.9
2	H	2	ILE	3.8
2	H	21	TRP	3.7
1	G	10	MET	3.7
1	G	13	LEU	3.7
2	H	170	ARG	3.6
1	G	12	THR	3.6
2	F	173	ILE	3.4
2	H	173	ILE	3.4
2	F	174	LYS	3.0
2	H	22	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	23	GLY	2.9
2	H	139	LYS	2.8
2	H	171	PHE	2.8
2	H	163	ARG	2.7
1	G	320	MET	2.6
1	G	9	SER	2.5
1	C	9	SER	2.5
1	C	10	MET	2.4
1	G	8	ASN	2.4
2	H	138	PHE	2.3
1	G	159	TYR	2.2
1	C	11	ALA	2.2
1	A	326	LYS	2.1
1	A	10	MET	2.1
1	C	8	ASN	2.1

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](#)

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, 95th 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(Å ²)	Q<0.9
6	BMA	e	3	11/12	0.49	0.31	206,224,233,235	0
3	BMA	I	3	11/12	0.54	0.44	171,197,207,207	0
9	FUC	T	3	10/11	0.56	0.35	160,188,194,198	0
10	MAN	V	5	11/12	0.56	0.54	177,196,209,209	0
6	MAN	X	4	11/12	0.57	0.35	196,207,218,227	0
8	BMA	R	3	11/12	0.58	0.54	188,200,207,209	0
6	MAN	e	5	11/12	0.59	0.52	165,199,203,204	0
6	MAN	U	4	11/12	0.59	0.29	171,194,200,204	0
6	NAG	e	2	14/15	0.60	0.38	145,202,207,226	0
6	BMA	X	3	11/12	0.61	0.23	195,200,208,212	0
14	BMA	d	3	11/12	0.61	0.29	210,216,220,221	0
4	BMA	K	3	11/12	0.62	0.31	167,194,204,206	0
5	MAN	Q	5	11/12	0.62	0.17	146,188,198,202	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MAN	X	5	11/12	0.63	0.31	156,193,203,204	0
9	NAG	T	1	14/15	0.65	0.23	144,164,177,187	0
4	MAN	P	4	11/12	0.66	0.43	163,183,189,193	0
6	BMA	M	3	11/12	0.68	0.27	194,207,215,215	0
6	BMA	U	3	11/12	0.68	0.30	180,190,198,199	0
6	MAN	U	5	11/12	0.70	0.32	132,178,193,195	0
14	MAN	d	4	11/12	0.70	0.32	198,204,215,216	0
12	BMA	a	3	11/12	0.71	0.20	191,204,210,213	0
13	MAN	c	6	11/12	0.71	0.21	183,196,204,205	0
12	MAN	a	4	11/12	0.72	0.22	172,191,203,204	0
8	BMA	O	3	11/12	0.72	0.22	154,196,201,203	0
6	NAG	e	1	14/15	0.72	0.29	121,157,191,205	0
7	NAG	N	2	14/15	0.72	0.23	140,174,185,188	0
13	MAN	c	5	11/12	0.73	0.26	156,182,195,199	0
5	MAN	W	5	11/12	0.74	0.28	155,176,188,191	0
5	MAN	W	6	11/12	0.77	0.25	171,184,190,194	0
5	MAN	L	5	11/12	0.77	0.24	177,180,196,202	0
6	MAN	M	4	11/12	0.77	0.30	142,185,198,201	0
12	FUC	a	5	10/11	0.77	0.21	166,186,194,196	0
7	NAG	Z	2	14/15	0.78	0.31	137,165,181,185	0
6	MAN	e	4	11/12	0.78	0.44	183,211,217,218	0
11	NAG	Y	1	14/15	0.78	0.41	157,183,203,210	0
3	FUC	I	5	10/11	0.78	0.56	149,165,179,186	0
3	NAG	I	2	14/15	0.78	0.49	167,189,206,208	0
11	NAG	Y	2	14/15	0.79	0.38	158,178,195,199	0
4	MAN	K	4	11/12	0.79	0.29	154,175,188,191	0
14	NAG	d	1	14/15	0.79	0.19	107,131,145,163	0
5	MAN	L	6	11/12	0.79	0.26	165,187,191,192	0
7	NAG	b	2	14/15	0.79	0.24	150,168,176,177	0
13	MAN	c	4	11/12	0.80	0.22	173,182,191,194	0
5	MAN	Q	6	11/12	0.80	0.36	173,182,193,203	0
13	MAN	c	3	11/12	0.80	0.20	147,174,182,187	0
7	NAG	S	2	14/15	0.81	0.31	128,183,200,214	0
4	MAN	J	4	11/12	0.81	0.25	171,188,194,199	0
4	NAG	P	1	14/15	0.81	0.21	102,135,153,158	0
10	NAG	V	2	14/15	0.81	0.18	128,151,158,159	0
10	MAN	V	4	11/12	0.81	0.21	181,202,211,214	0
4	BMA	P	3	11/12	0.81	0.42	133,166,175,176	0
8	NAG	O	2	14/15	0.82	0.18	167,184,195,197	0
6	NAG	M	2	14/15	0.82	0.26	130,155,178,199	0
8	NAG	R	2	14/15	0.82	0.37	142,176,193,201	0
9	FUL	T	2	10/11	0.83	0.14	144,164,171,176	0

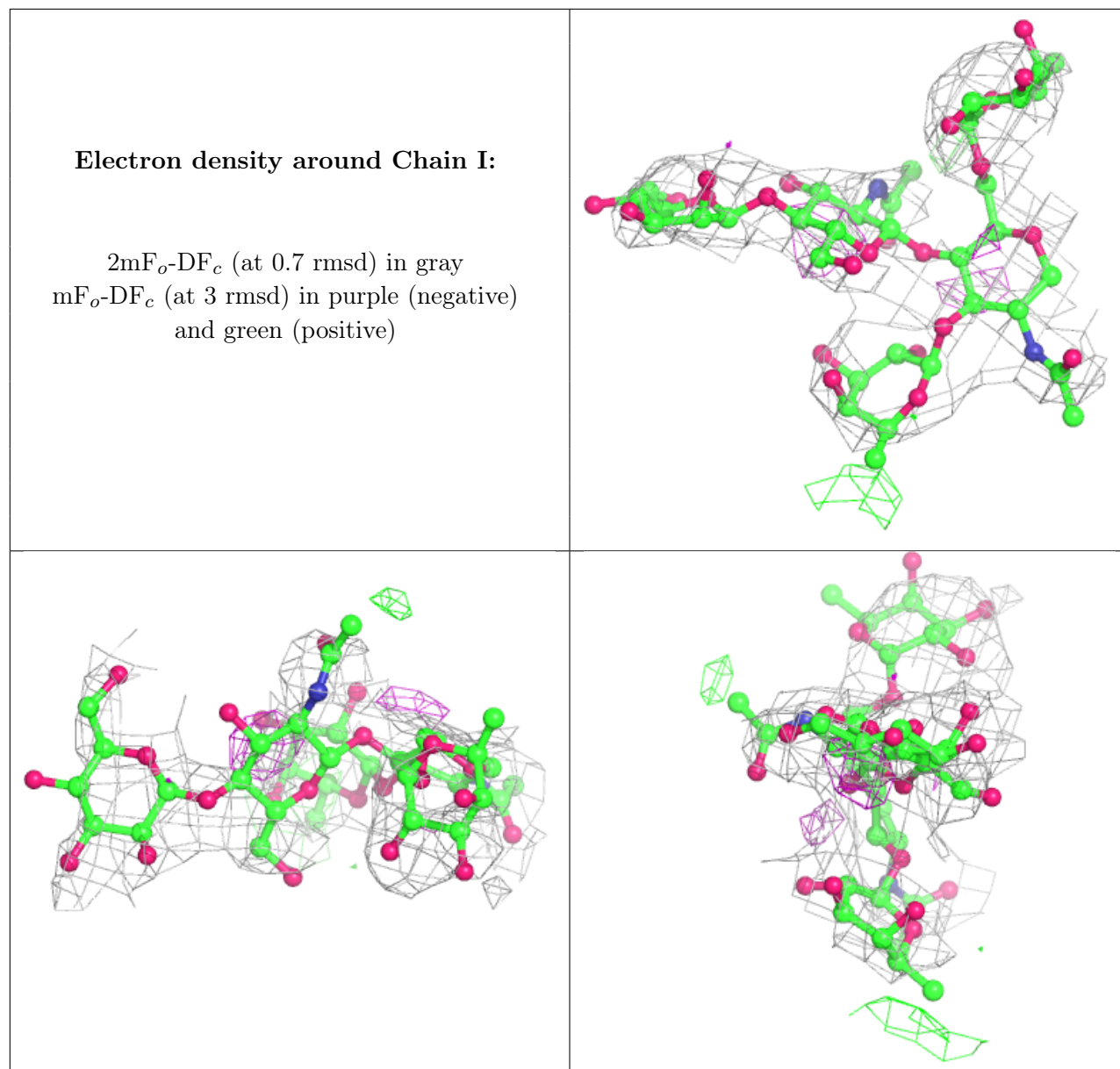
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	NAG	a	2	14/15	0.83	0.25	138,186,200,202	0
6	MAN	M	5	11/12	0.84	0.20	177,187,192,196	0
5	MAN	W	4	11/12	0.84	0.27	155,182,188,189	0
11	FUC	Y	3	10/11	0.84	0.38	156,173,176,180	0
10	NAG	V	1	14/15	0.84	0.19	112,144,154,161	0
4	BMA	J	3	11/12	0.84	0.21	140,163,175,187	0
5	MAN	L	4	11/12	0.84	0.20	148,170,174,177	0
8	NAG	O	1	14/15	0.84	0.14	122,142,163,179	0
13	MAN	c	7	11/12	0.85	0.22	133,170,186,188	0
6	NAG	X	2	14/15	0.85	0.31	117,163,176,189	0
6	NAG	U	2	14/15	0.85	0.27	117,173,184,191	0
6	NAG	M	1	14/15	0.85	0.17	74,103,116,137	0
4	NAG	P	2	14/15	0.86	0.41	133,157,163,172	0
4	NAG	K	2	14/15	0.86	0.18	100,153,166,184	0
5	MAN	Q	4	11/12	0.86	0.16	182,195,198,202	0
6	NAG	U	1	14/15	0.87	0.14	111,125,148,165	0
5	MAN	Q	3	11/12	0.87	0.16	140,152,179,186	0
7	NAG	N	1	14/15	0.87	0.14	106,134,165,185	0
14	NAG	d	2	14/15	0.87	0.20	109,167,190,202	0
5	MAN	W	3	11/12	0.87	0.14	120,138,171,175	0
7	NAG	S	1	14/15	0.87	0.18	114,125,169,177	0
12	NAG	a	1	14/15	0.88	0.14	150,172,193,195	0
3	FUL	I	4	10/11	0.88	0.28	148,166,173,180	0
7	NAG	Z	1	14/15	0.89	0.18	129,143,164,180	0
10	BMA	V	3	11/12	0.90	0.13	130,159,174,194	0
3	NAG	I	1	14/15	0.90	0.31	132,158,177,179	0
8	NAG	R	1	14/15	0.90	0.21	110,128,147,153	0
4	NAG	K	1	14/15	0.90	0.17	108,124,135,148	0
13	NAG	c	2	14/15	0.91	0.19	127,140,159,177	0
5	NAG	L	1	14/15	0.91	0.20	98,110,128,131	0
7	NAG	b	1	14/15	0.92	0.21	132,156,171,180	0
4	NAG	J	2	14/15	0.92	0.23	98,139,149,161	0
5	NAG	Q	2	14/15	0.93	0.12	71,98,120,139	0
13	NAG	c	1	14/15	0.93	0.12	99,115,134,136	0
5	MAN	L	3	11/12	0.93	0.14	145,153,169,176	0
5	NAG	L	2	14/15	0.93	0.18	118,141,149,159	0
4	NAG	J	1	14/15	0.94	0.14	68,101,115,124	0
6	NAG	X	1	14/15	0.94	0.24	89,108,122,140	0
5	NAG	W	2	14/15	0.94	0.20	103,118,126,139	0
5	NAG	Q	1	14/15	0.94	0.18	93,101,118,123	0
5	NAG	W	1	14/15	0.96	0.18	78,100,128,134	0

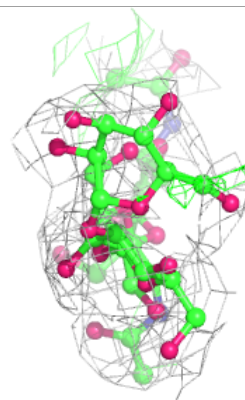
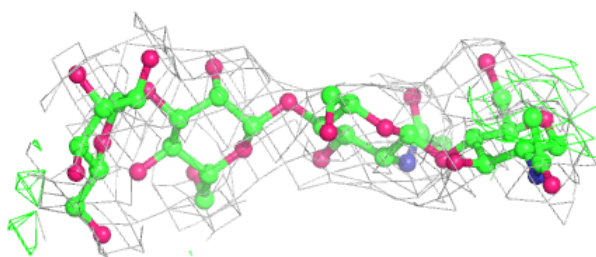
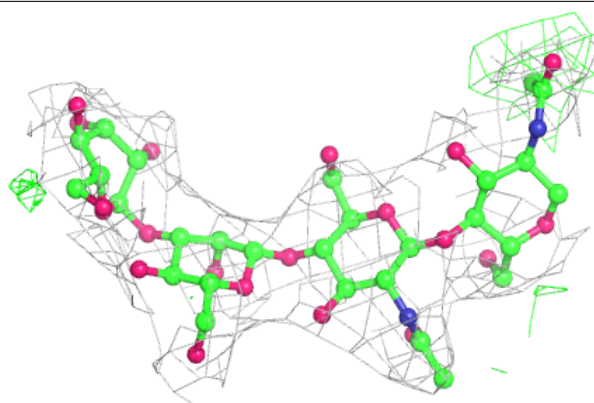
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

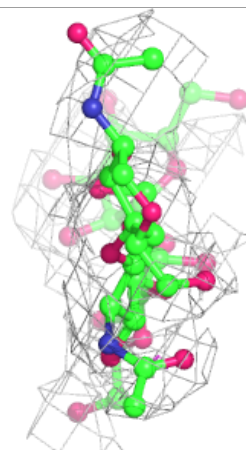
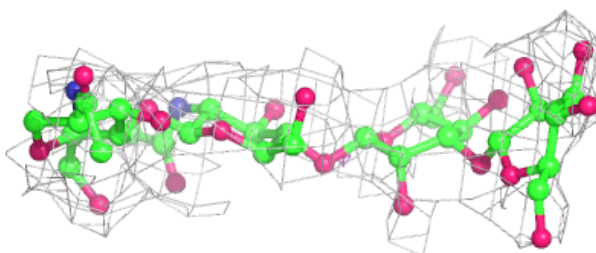
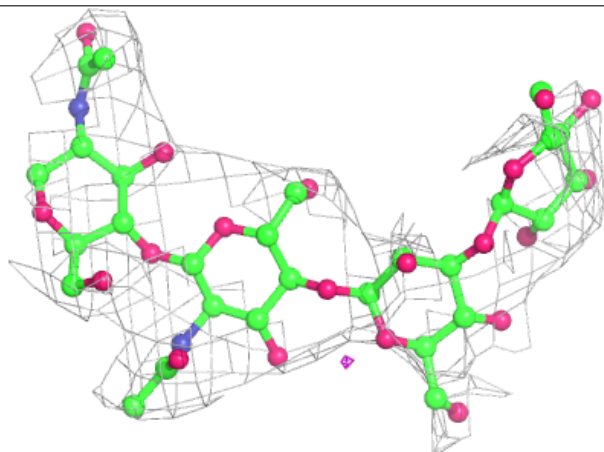


Electron density around Chain J:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

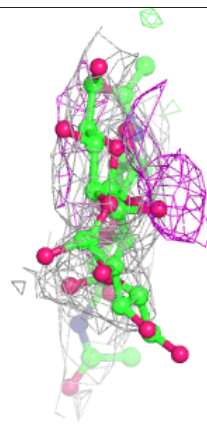
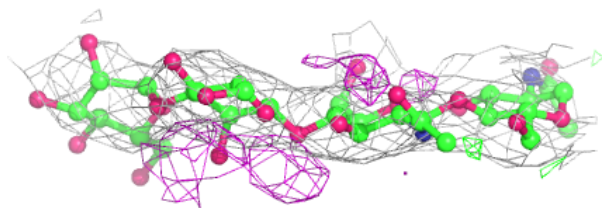
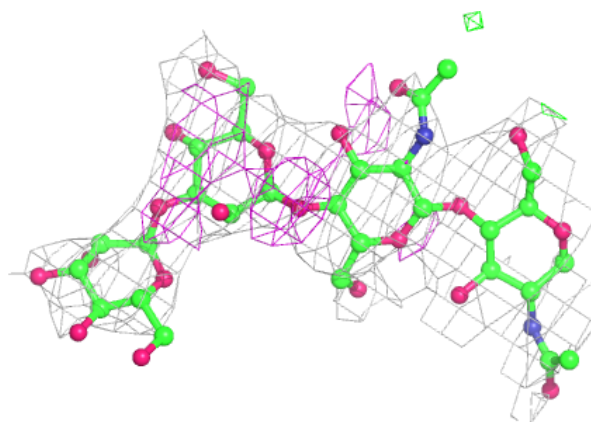
**Electron density around Chain K:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

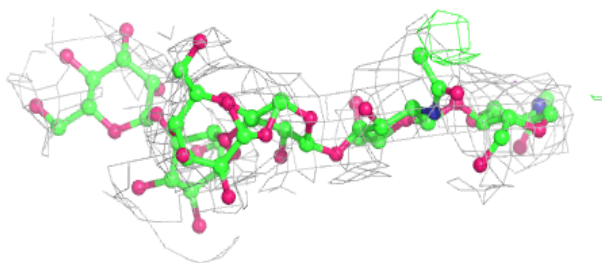
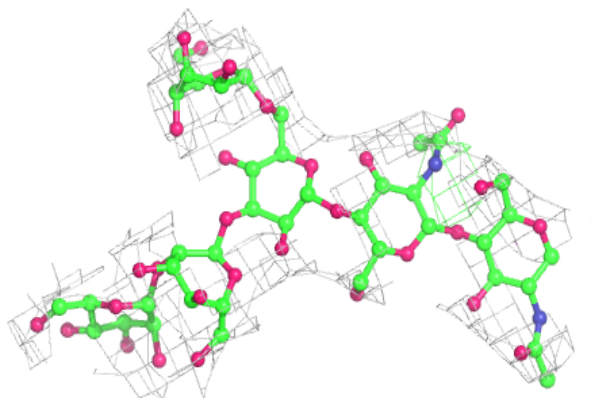


Electron density around Chain P:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

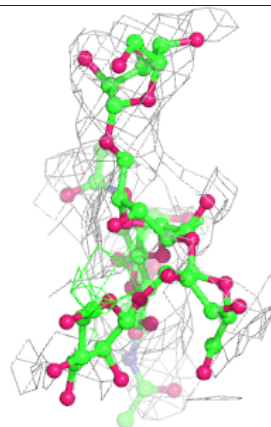
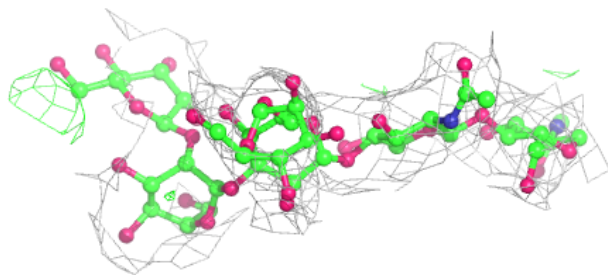
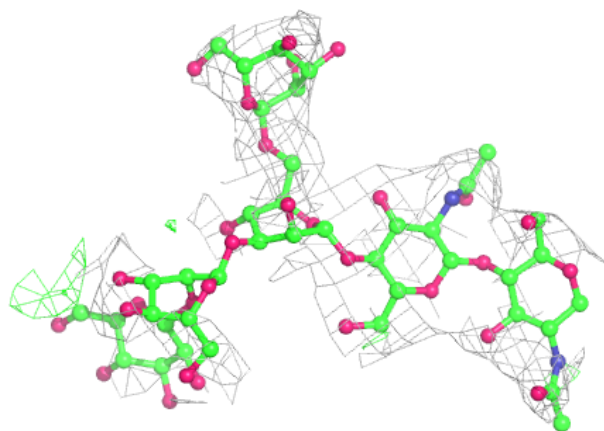
**Electron density around Chain L:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

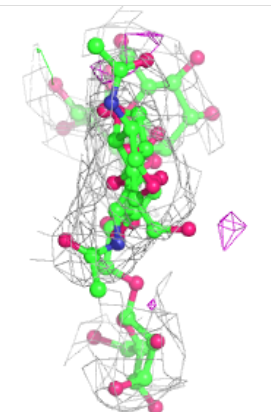
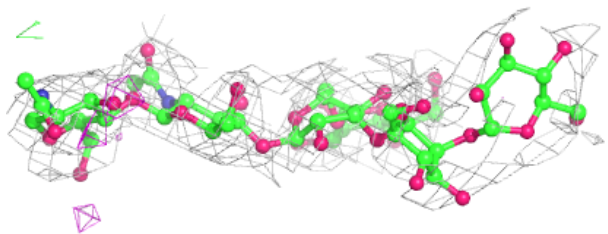
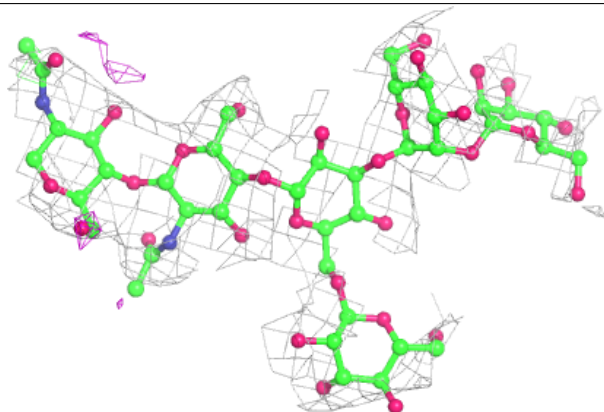


Electron density around Chain Q:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

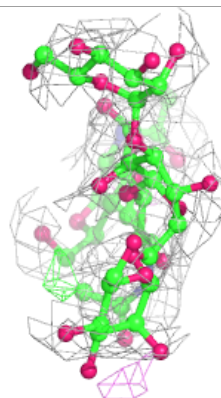
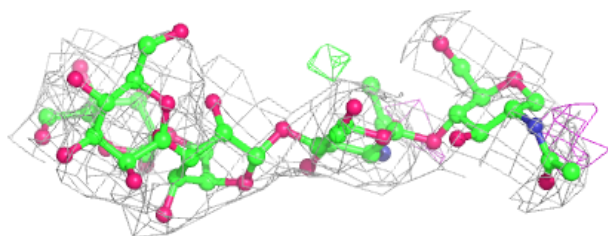
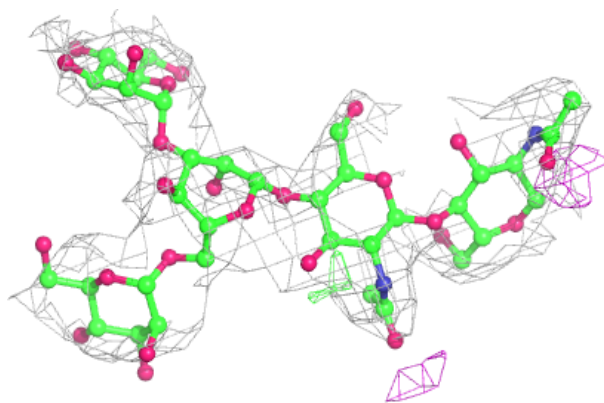
**Electron density around Chain W:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

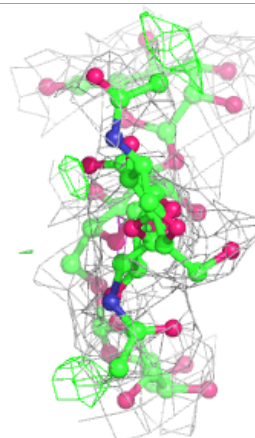
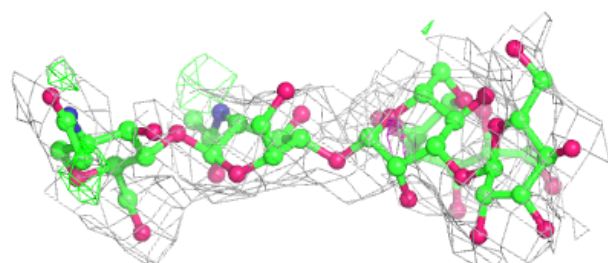
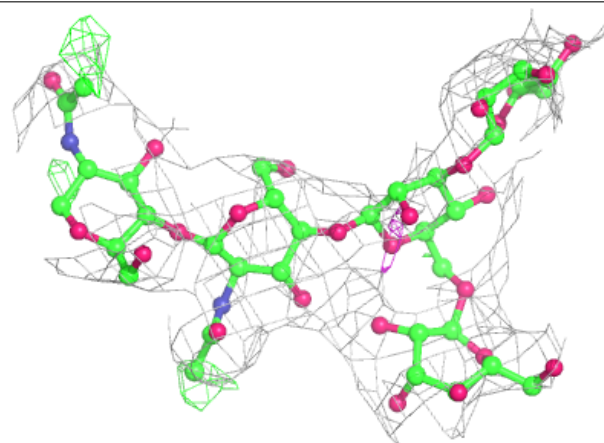


Electron density around Chain M:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

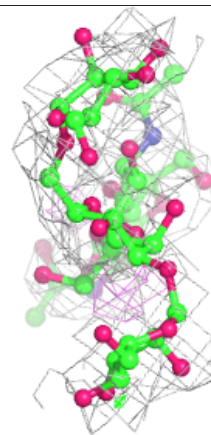
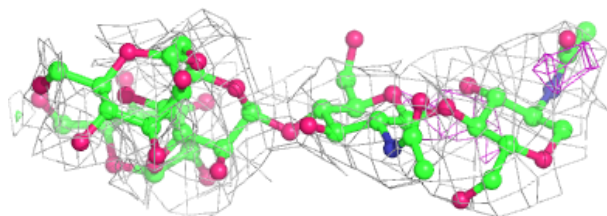
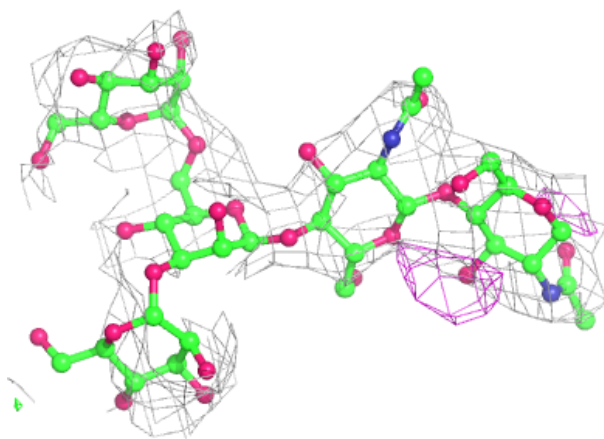
**Electron density around Chain U:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



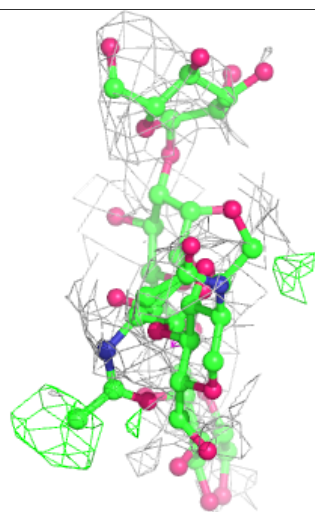
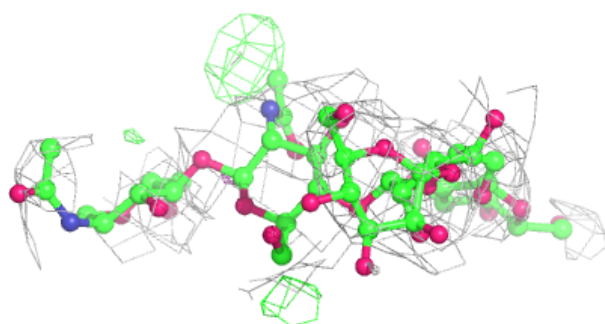
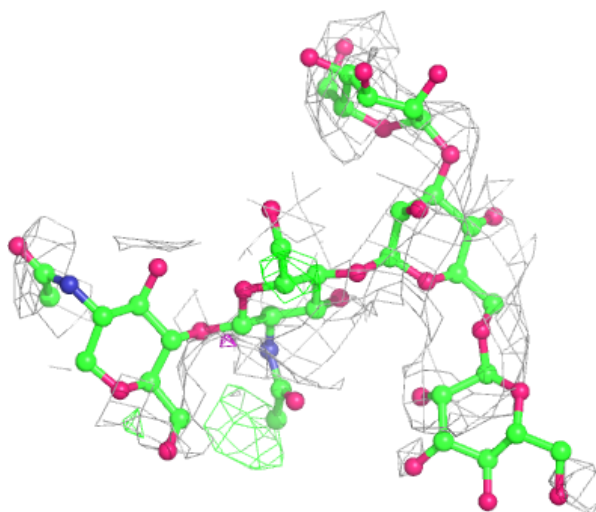
Electron density around Chain X:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



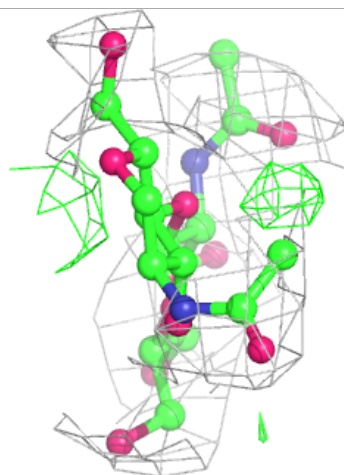
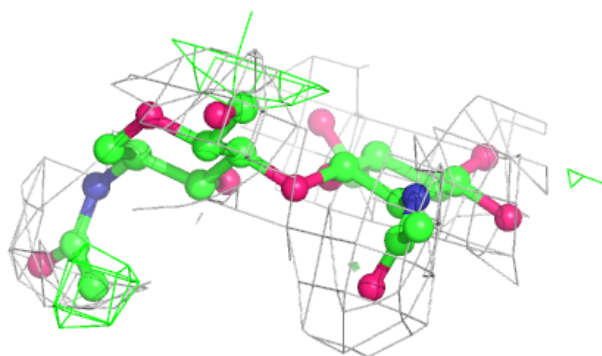
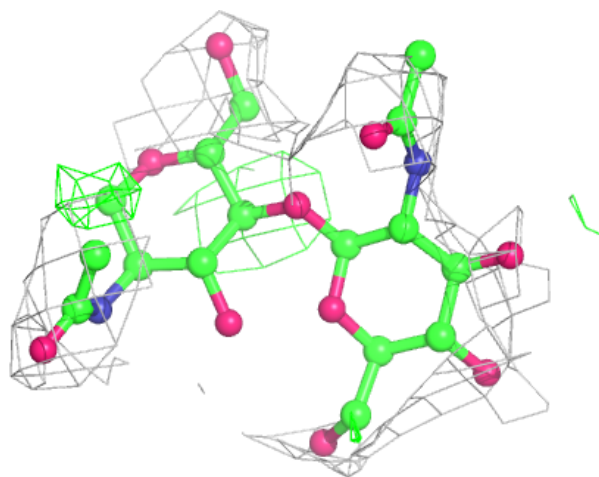
Electron density around Chain e:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



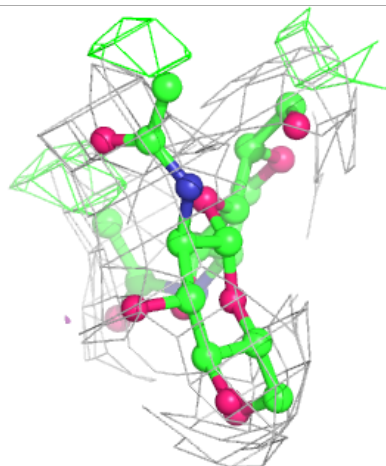
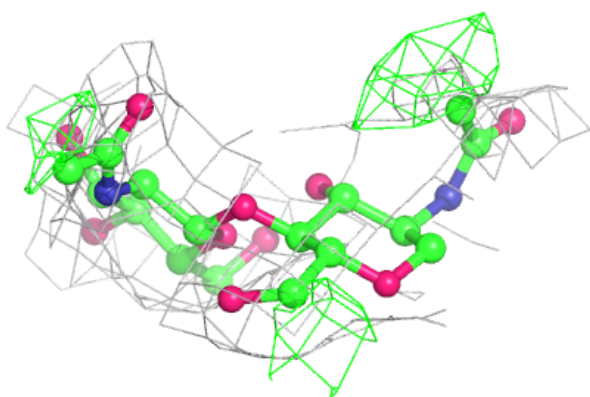
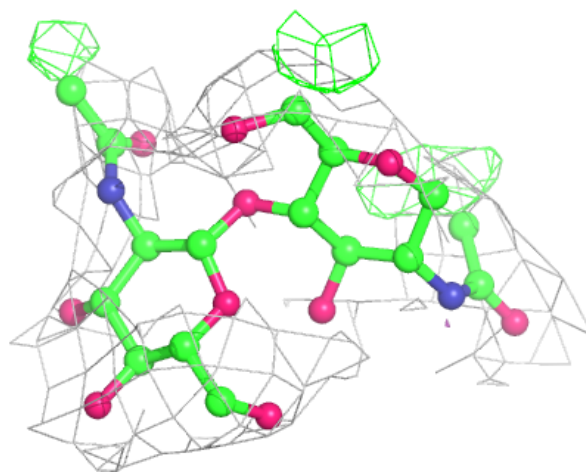
Electron density around Chain N:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



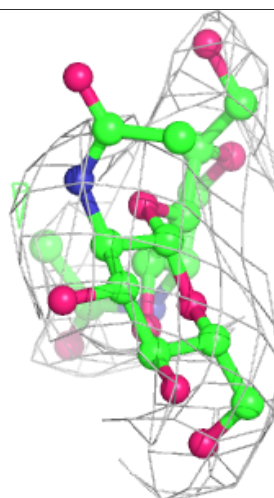
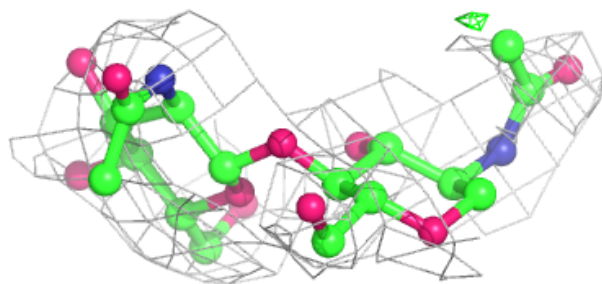
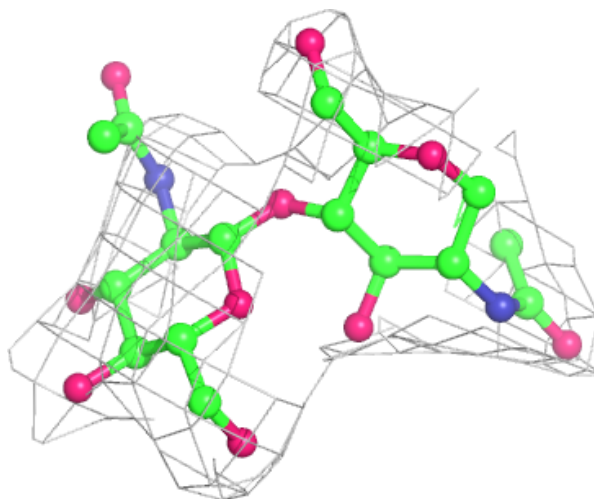
Electron density around Chain S:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



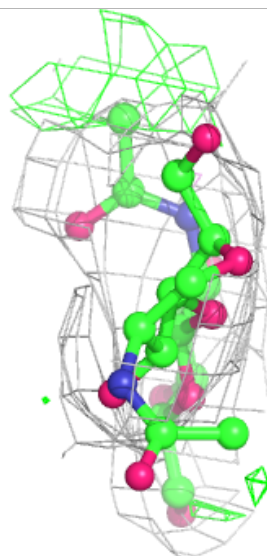
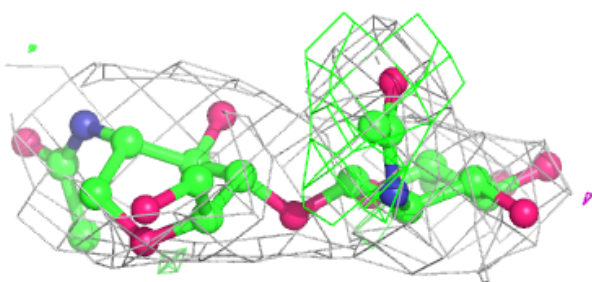
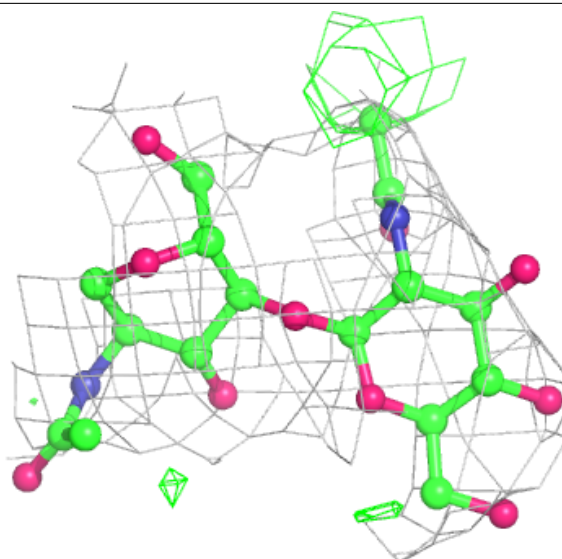
Electron density around Chain Z:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



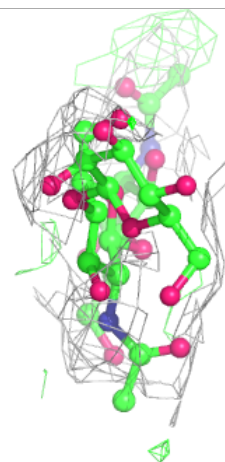
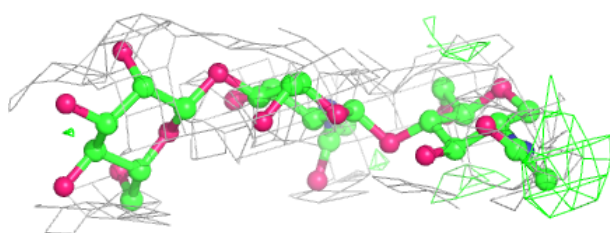
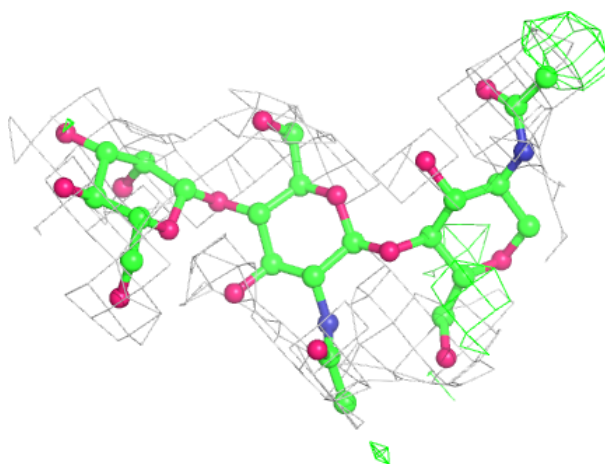
Electron density around Chain b:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



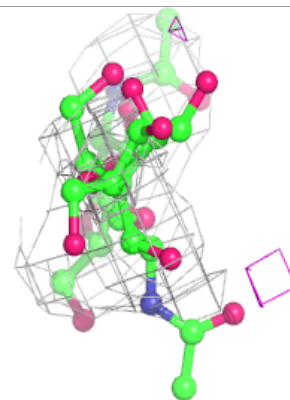
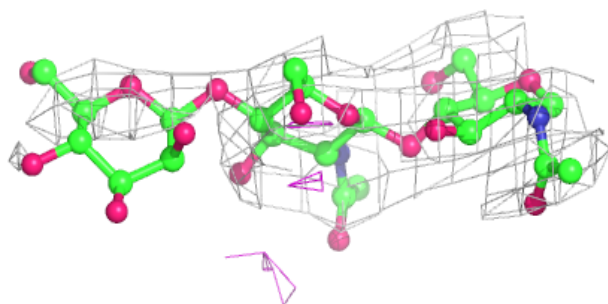
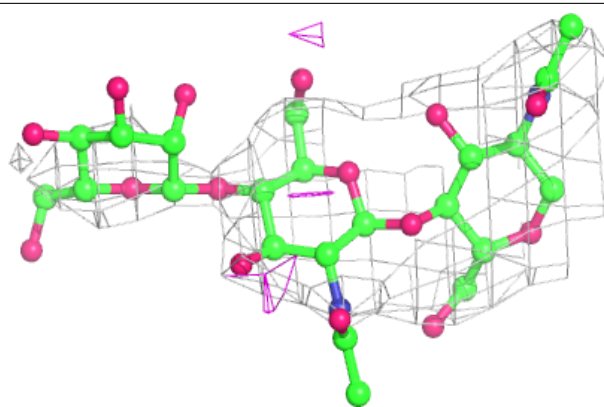
Electron density around Chain O:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

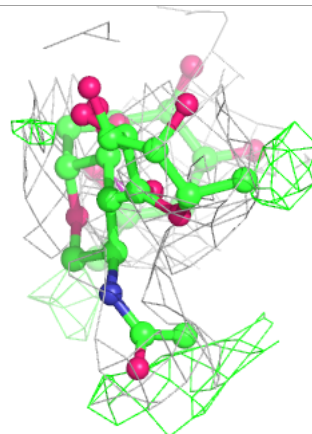
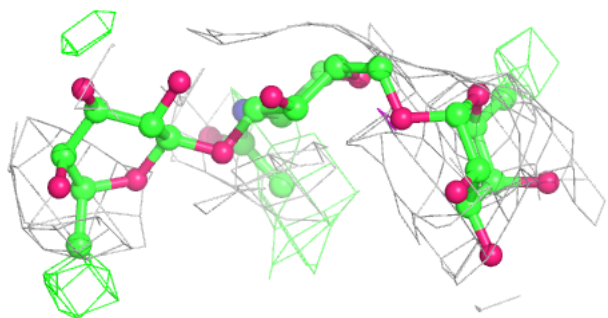
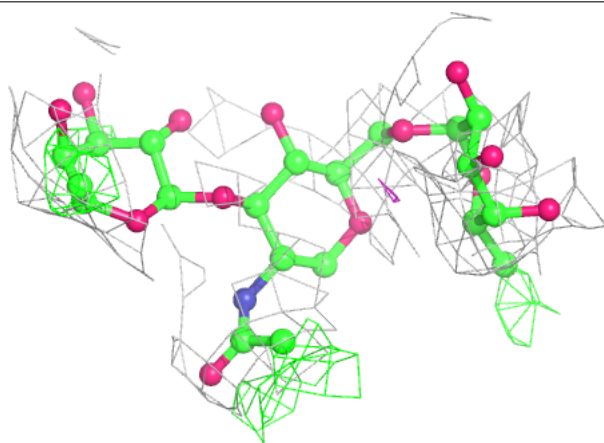


Electron density around Chain R:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

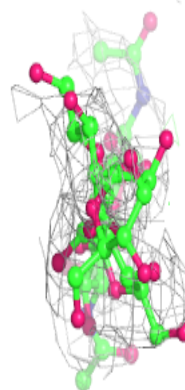
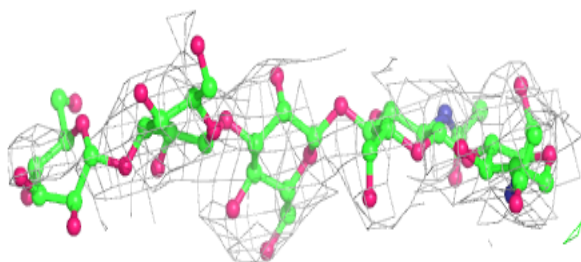
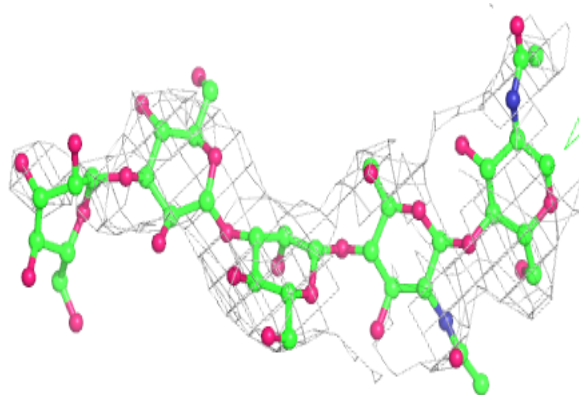
**Electron density around Chain T:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

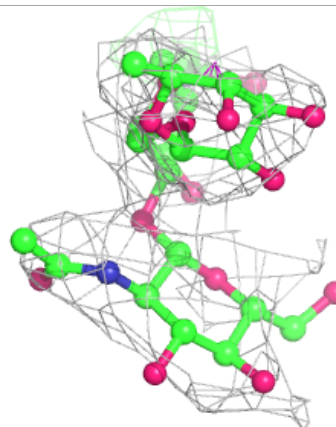
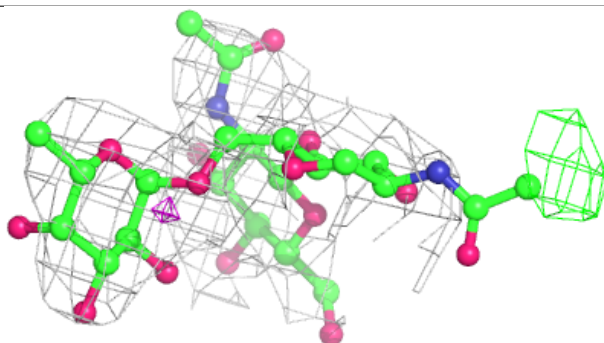
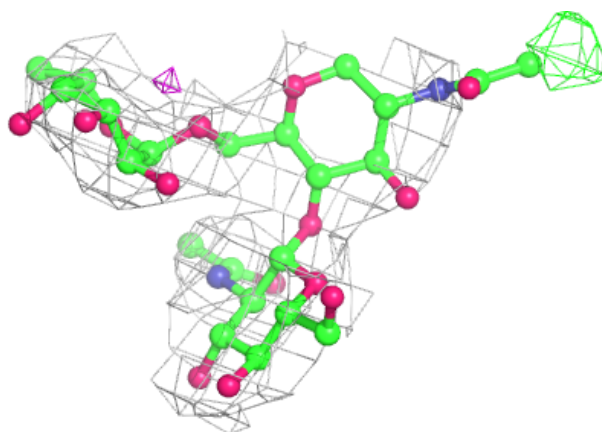


Electron density around Chain V:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

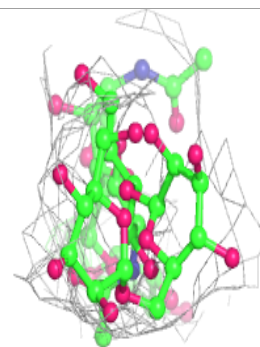
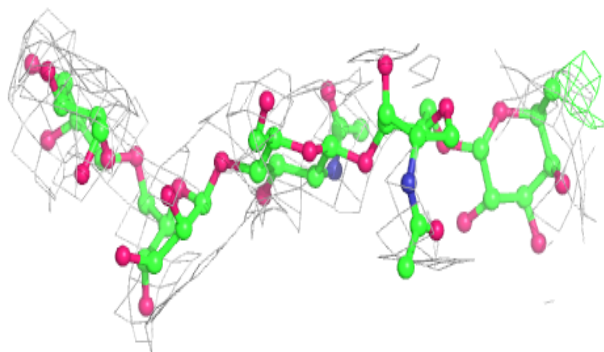
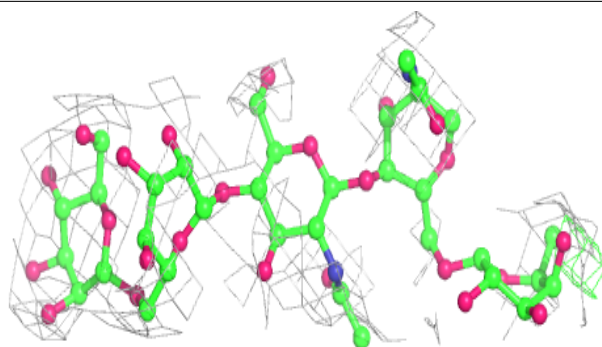
**Electron density around Chain Y:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



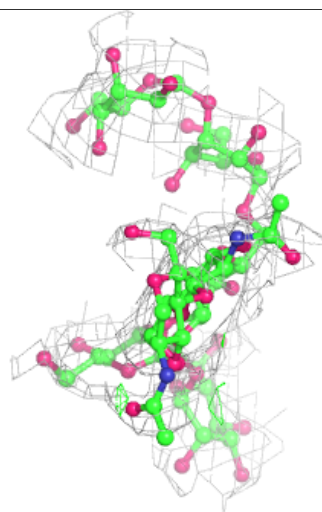
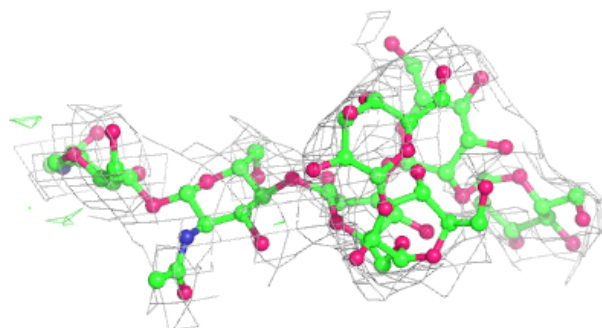
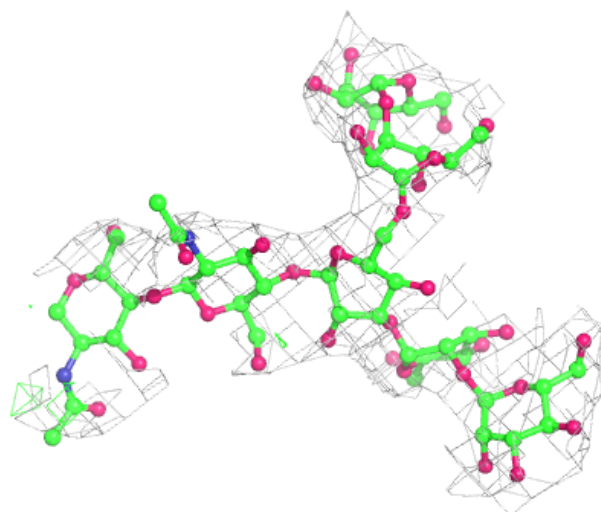
Electron density around Chain a:

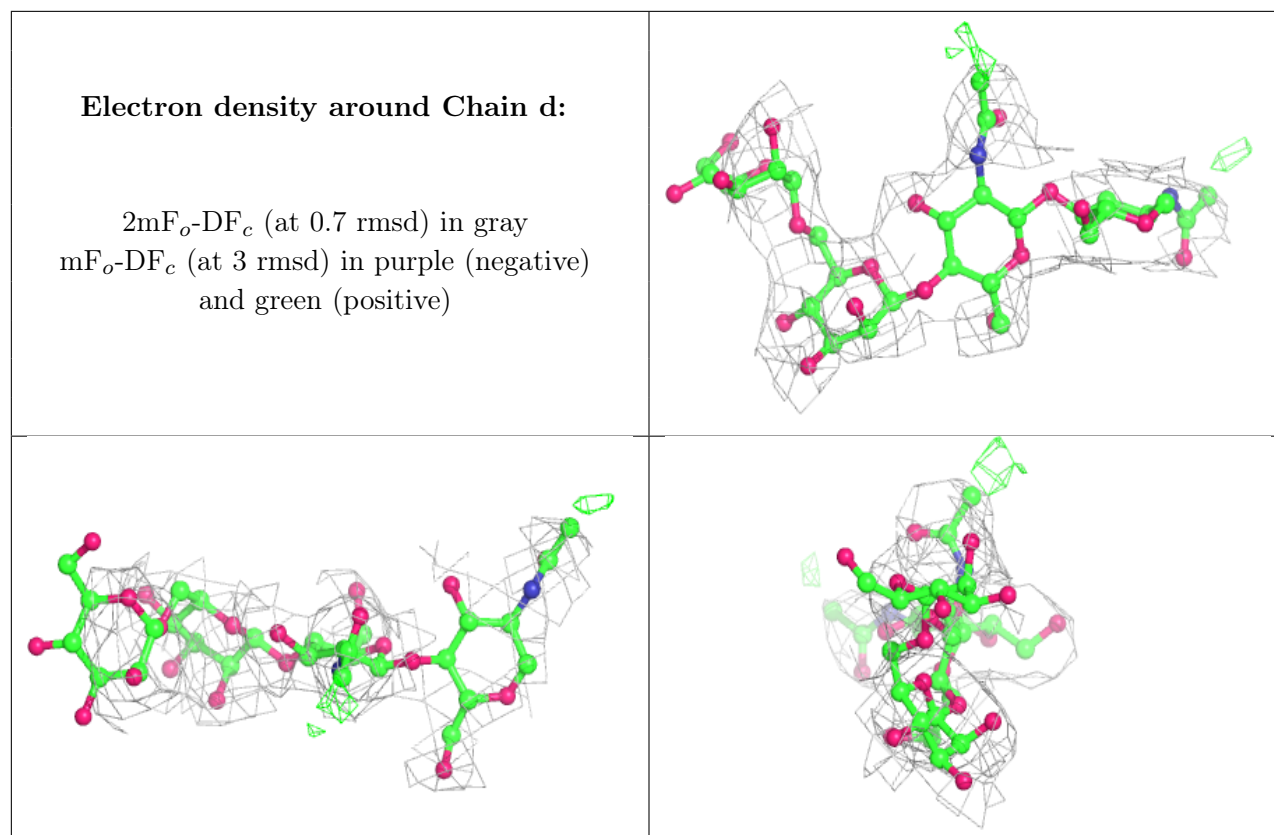
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain c:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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, 95th 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(Å ²)	Q<0.9
15	NAG	G	419	14/15	0.50	0.38	124,161,178,179	0
15	NAG	A	525	14/15	0.58	0.38	113,179,197,200	0
15	NAG	H	201	14/15	0.67	0.33	158,169,184,186	0
15	NAG	D	201	14/15	0.72	0.22	103,153,184,194	0
15	NAG	F	201	14/15	0.72	0.28	124,167,179,187	0
15	NAG	B	201	14/15	0.75	0.32	141,183,190,199	0
15	NAG	C	417	14/15	0.76	0.31	126,165,183,186	0
16	CAC	B	202	5/5	0.92	0.37	113,128,156,158	0

6.5 Other polymers [i](#)

There are no such residues in this entry.