



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:33 AM UTC

PDB ID : 5XRT / pdb_00005xrt
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

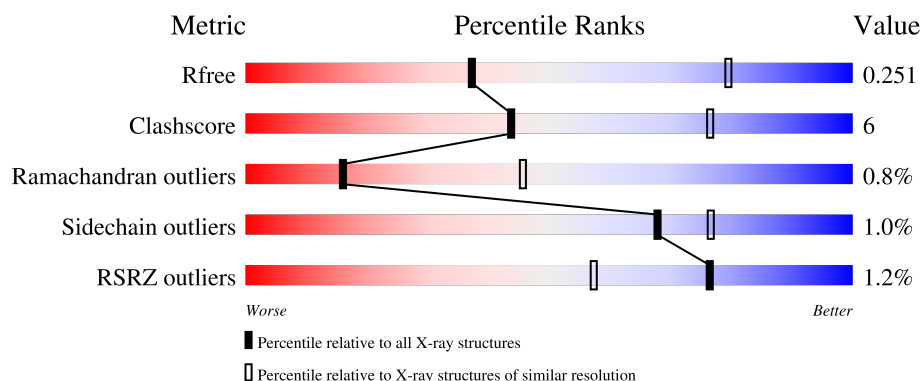
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (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	81% 13% ..
1	C	329	85% 11% ..
1	E	329	82% 14% .
1	G	329	78% 17% ..
2	B	174	82% 16% ..

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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	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 16943 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

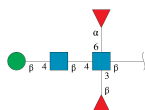
- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2506	1571	438	484	13			
1	C	319	Total	C	N	O	S	0	0	0
			2506	1571	438	484	13			
1	E	319	Total	C	N	O	S	0	0	0
			2506	1571	438	484	13			
1	G	319	Total	C	N	O	S	0	0	0
			2506	1571	438	484	13			

- Molecule 2 is a protein called Hemagglutinin.

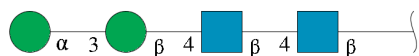
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1409	876	252	275	6			
2	D	174	Total	C	N	O	S	0	0	0
			1404	873	251	274	6			
2	F	174	Total	C	N	O	S	0	0	0
			1409	876	252	275	6			
2	H	174	Total	C	N	O	S	0	0	0
			1409	876	252	275	6			

- Molecule 3 is an oligosaccharide called 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.



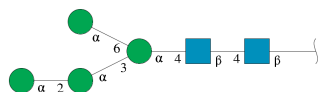
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	5	Total	C	N	O	0	0	0
			59	34	2	23			

- 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.



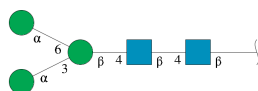
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

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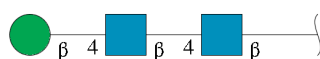
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	U	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	X	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	e	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



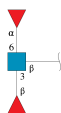
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	b	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



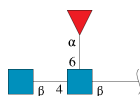
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	T	3	Total	C	N	O	0	0	0
			34	20	1	13			

- 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.



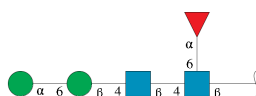
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	V	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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.



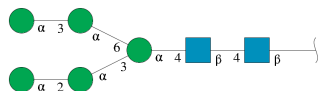
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	Y	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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.



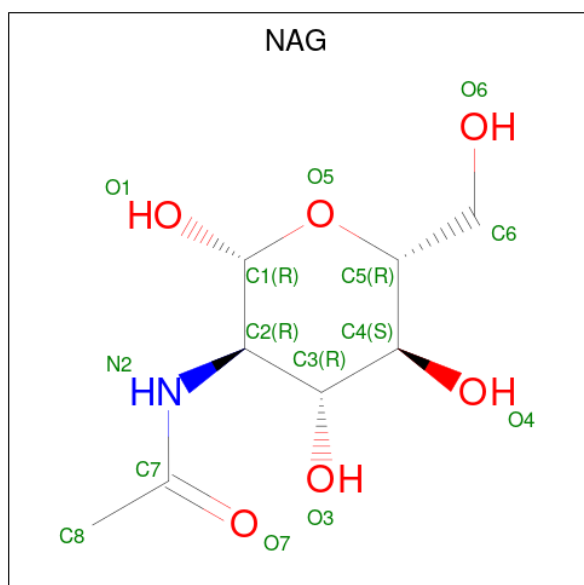
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	c	7	Total	C	N	O	0	0	0
			83	46	2	35			

- 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.



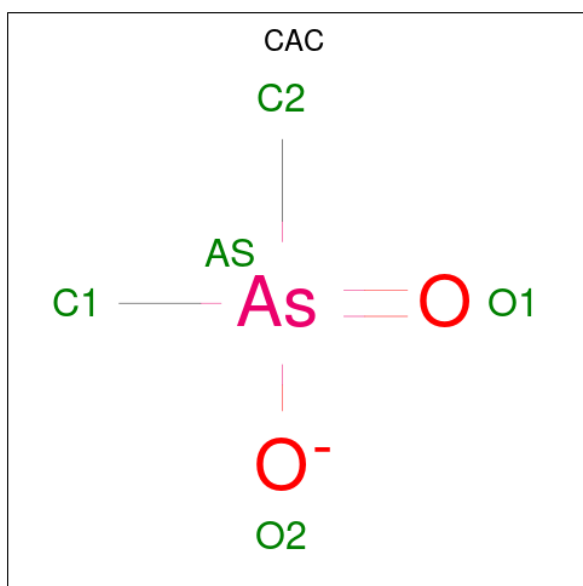
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	d	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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 (CCD ID: CAC) (formula: $C_2H_6AsO_2$).

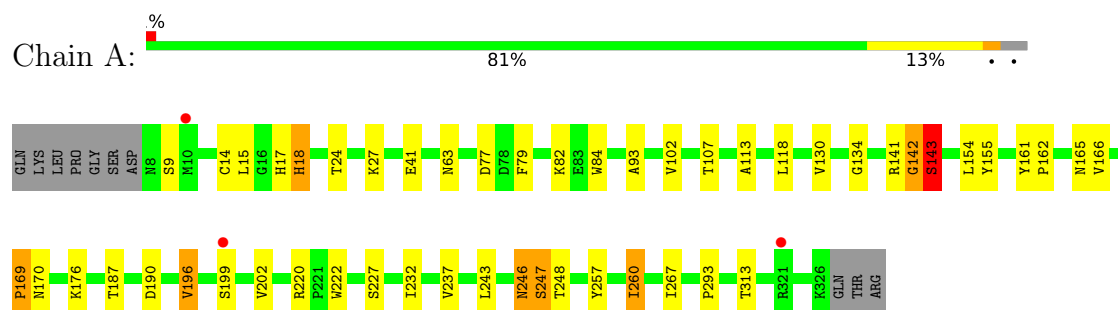


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	B	1	Total	As	C	O	0	0
			5	1	2	2		

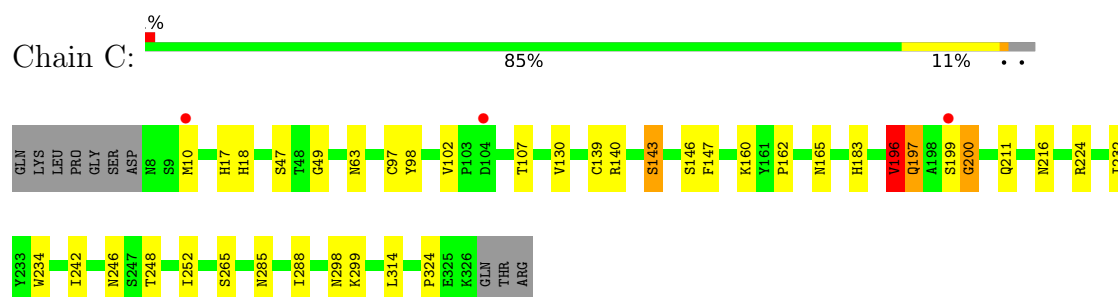
3 Residue-property plots [i](#)

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.

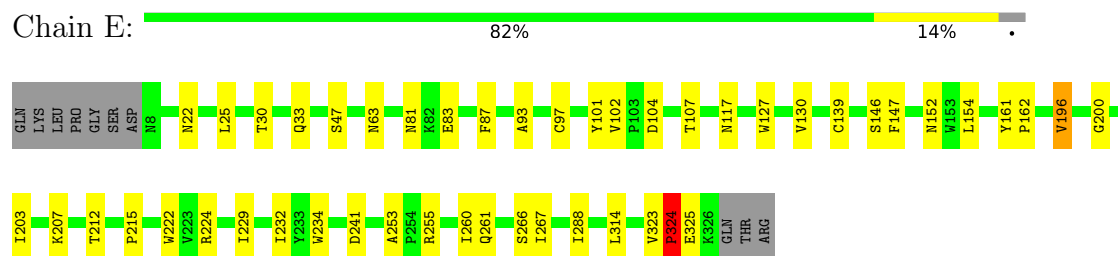
• Molecule 1: Hemagglutinin



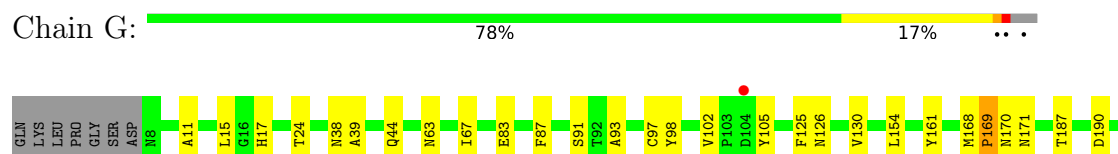
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin

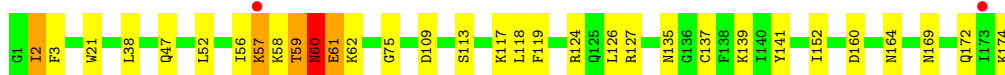
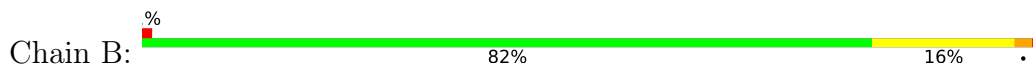


• Molecule 1: Hemagglutinin

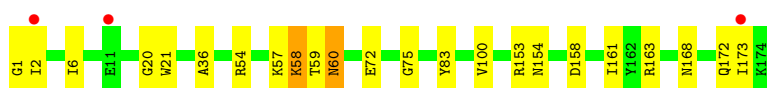
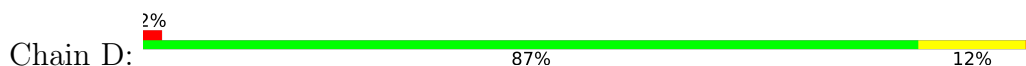




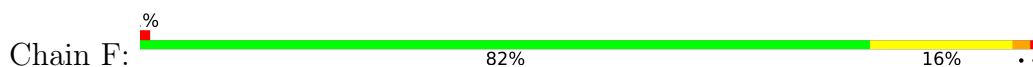
• Molecule 2: Hemagglutinin



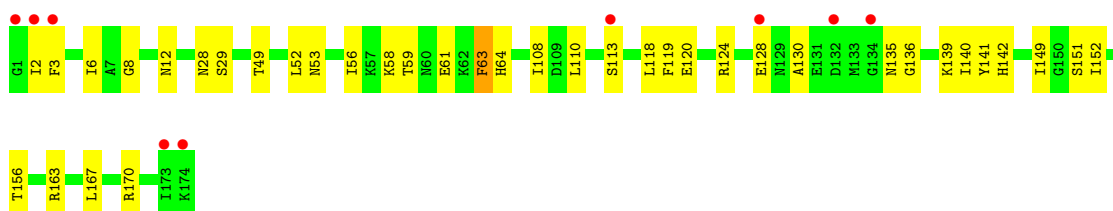
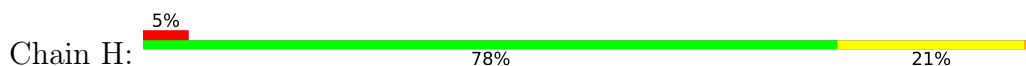
• Molecule 2: Hemagglutinin



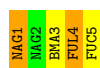
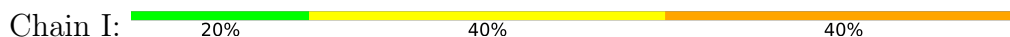
• Molecule 2: Hemagglutinin



• 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



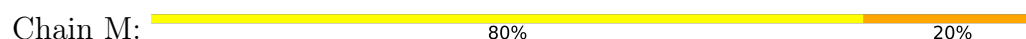
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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

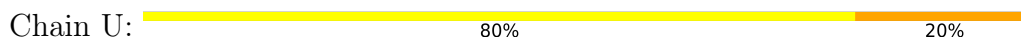


- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- 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: 

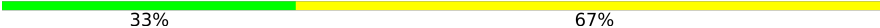


- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 

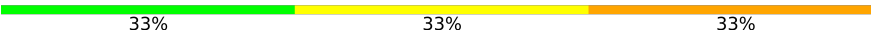


- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 

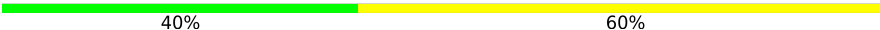


- Molecule 9: beta-L-fucopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 

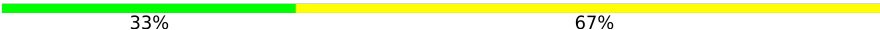


- Molecule 10: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 



- 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: 

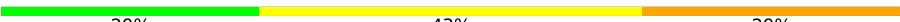


- Molecule 12: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  20% 80%

MAN1	MAN2	MAN3	MAN4	FUC5
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- 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% 43% 29%

MAN1	MAN2	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:  50% 50%

MAN1	MAN2	MAN3	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 0.205 , 0.251	Depositor DCC
R_{free} test set	3513 reflections (4.89%)	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)	0.29 , 59.1	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: MAN, CAC, FUC, NAG, BMA, FUL

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	0.26	2/2565 (0.1%)	0.61	10/3492 (0.3%)
1	C	0.17	0/2565	0.57	10/3492 (0.3%)
1	E	0.23	1/2565 (0.0%)	0.57	6/3492 (0.2%)
1	G	0.44	2/2565 (0.1%)	0.72	18/3492 (0.5%)
2	B	0.20	0/1433	0.75	8/1924 (0.4%)
2	D	0.18	0/1428	0.66	6/1917 (0.3%)
2	F	0.20	0/1433	0.76	9/1924 (0.5%)
2	H	0.17	0/1433	0.89	9/1924 (0.5%)
All	All	0.26	5/15987 (0.0%)	0.68	76/21657 (0.4%)

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	125	PHE	C-N	17.24	1.58	1.33
1	G	169	PRO	N-CD	11.59	1.64	1.47
1	E	162	PRO	N-CD	7.97	1.58	1.47
1	A	169	PRO	N-CD	7.55	1.58	1.47
1	A	162	PRO	N-CD	6.87	1.57	1.47

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	63	PHE	N-CA-C	15.36	134.07	114.56
2	B	61	GLU	N-CA-C	14.02	131.61	111.56
1	G	196	VAL	CB-CA-C	-12.72	90.43	111.29
2	H	64	HIS	N-CA-C	-11.83	87.78	108.13
2	H	63	PHE	CB-CA-C	-11.71	90.86	109.13
1	G	225	GLY	N-CA-C	11.45	128.32	114.69
2	H	64	HIS	N-CA-CB	11.32	129.27	110.59
1	G	197	GLN	N-CA-C	-10.80	93.85	109.18
2	H	136	GLY	N-CA-C	10.60	132.94	115.66
2	D	60	ASN	N-CA-C	9.97	125.48	111.52
2	H	135	ASN	N-CA-C	-9.94	89.62	110.80
1	E	324	PRO	N-CA-C	9.90	132.86	112.47
2	D	154	ASN	N-CA-CB	-9.76	95.29	111.49
1	C	196	VAL	CB-CA-C	-9.50	95.72	111.29
2	B	57	LYS	N-CA-C	9.49	122.49	111.11
2	F	63	PHE	N-CA-C	8.91	124.66	113.43
2	F	66	ILE	N-CA-C	8.87	120.23	110.21
2	F	64	HIS	N-CA-C	-8.61	93.96	108.26
1	A	142	GLY	N-CA-C	8.51	133.35	113.18
1	G	197	GLN	N-CA-CB	8.34	124.39	111.22
1	G	126	ASN	O-C-N	-8.16	111.38	122.48
2	F	64	HIS	N-CA-CB	7.86	123.58	110.77
2	B	61	GLU	CB-CA-C	-7.80	101.83	111.82
1	C	197	GLN	N-CA-CB	7.74	124.69	110.99
1	G	195	TYR	CB-CA-C	7.40	121.45	109.02
1	C	200	GLY	N-CA-C	-7.39	102.98	111.85
2	B	62	LYS	N-CA-C	7.32	121.32	110.48
1	A	199	SER	CB-CA-C	7.28	124.90	110.42
1	E	325	GLU	N-CA-CB	7.25	122.62	111.46
2	D	172	GLN	N-CA-C	-7.04	95.80	110.80
1	C	165	ASN	N-CA-C	-6.98	96.88	108.32
2	D	173	ILE	N-CA-C	6.66	123.19	109.34
1	G	169	PRO	N-CA-CB	6.64	110.22	103.25
2	H	156	THR	N-CA-C	6.51	120.53	112.59
1	G	325	GLU	N-CA-C	-6.50	94.89	107.44
1	E	324	PRO	CB-CA-C	-6.39	101.01	111.56
2	D	153	ARG	CB-CA-C	6.38	124.19	110.21
1	G	226	VAL	N-CA-C	-6.16	98.83	108.86
1	C	63	ASN	N-CA-C	6.09	120.32	113.02
1	A	246	ASN	N-CA-C	-6.03	97.95	110.80
1	A	199	SER	N-CA-C	-6.01	98.01	110.80
2	B	59	THR	N-CA-C	-5.98	100.91	108.45
1	E	161	TYR	N-CA-C	-5.96	96.65	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	169	PRO	CA-N-CD	-5.95	103.67	112.00
2	B	59	THR	CB-CA-C	-5.92	99.45	113.02
2	B	62	LYS	N-CA-CB	-5.92	101.30	110.29
2	H	156	THR	N-CA-CB	-5.90	101.48	110.92
1	G	38	ASN	CB-CA-C	5.83	120.23	110.43
2	F	63	PHE	CB-CA-C	-5.81	99.89	109.65
1	C	165	ASN	CB-CA-C	5.76	119.63	109.89
1	G	171	ASN	N-CA-C	-5.71	106.21	112.72
2	D	58	LYS	CB-CA-C	5.67	116.77	109.80
1	G	168	MET	N-CA-C	-5.67	97.29	109.81
1	G	226	VAL	N-CA-CB	5.66	122.41	111.93
1	C	143	SER	CB-CA-C	-5.66	102.56	111.51
2	B	60	ASN	N-CA-C	-5.66	98.75	110.80
1	A	247	SER	N-CA-CB	5.55	119.95	110.57
2	H	3	PHE	N-CA-CB	5.52	118.66	110.49
2	F	27	GLN	CB-CA-C	5.50	118.28	110.24
1	G	170	ASN	N-CA-C	-5.46	98.11	107.23
1	A	143	SER	CB-CA-C	-5.45	99.57	110.42
1	G	326	LYS	N-CA-CB	-5.45	101.24	110.50
1	C	143	SER	N-CA-C	-5.44	105.28	112.24
2	F	154	ASN	N-CA-C	-5.41	100.91	108.96
1	A	166	VAL	N-CA-CB	5.37	118.44	111.19
1	A	162	PRO	N-CA-C	-5.33	101.49	112.47
1	G	169	PRO	N-CA-C	-5.32	101.50	112.47
2	F	56	ILE	N-CA-C	-5.32	98.27	109.34
1	C	197	GLN	N-CA-C	-5.29	99.97	108.55
1	E	162	PRO	N-CA-C	-5.27	101.62	112.47
1	A	161	TYR	N-CA-C	-5.27	98.17	109.81
1	E	147	PHE	N-CA-CB	-5.25	101.41	110.87
1	C	147	PHE	N-CA-CB	-5.25	101.41	110.87
1	A	169	PRO	N-CA-CB	5.15	108.66	103.25
2	F	57	LYS	N-CA-C	-5.14	99.86	110.80
1	G	168	MET	CB-CA-C	5.02	120.07	110.17

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

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	24	0
1	E	2506	0	2421	26	0
1	G	2506	0	2421	34	0
2	B	1409	0	1347	35	0
2	D	1404	0	1341	26	0
2	F	1409	0	1348	41	0
2	H	1409	0	1350	21	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	2	0
7	N	28	0	25	1	0
7	S	28	0	25	1	0
7	Z	28	0	25	2	0
7	b	28	0	25	3	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	2	0
14	d	50	0	43	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	H	14	0	13	1	0
16	B	5	0	0	0	0
All	All	16943	0	16183	202	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 (202) 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:D:60:ASN:CG	2:D:60:ASN:O	2.29	0.74
2:H:140:ILE:HG22	2:H:142:HIS:H	1.54	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:e:1:NAG:H83	6:e:1:NAG:H3	1.83	0.61
1:G:187:THR:OG1	1:G:190:ASP:OD2	2.17	0.61
2:F:120:GLU:CD	2:F:123:ARG:HH12	2.07	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
7:b:1:NAG:H83	7:b:1:NAG:H3	1.85	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:201:ARG:HH21	7:b:1:NAG:H81	1.73	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: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
2:D:60:ASN:O	2:D:60:ASN:ND2	2.43	0.50
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:c:6:MAN:H4	13:c:7:MAN:H5	1.96	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:G:201:ARG:NH2	7:b:1:NAG:H81	2.31	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
13:c:6:MAN:H3	13:c:7:MAN:H2	1.60	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:G:325:GLU:O	1:G:326:LYS:C	2.61	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
6:e:5:MAN:O6	6:e:5:MAN:O4	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:57:LYS:O	2:D:58:LYS:C	2.63	0.41
2:D:83:TYR:OH	2:F:85:GLU:OE1	2.34	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:B:2:ILE:HG12	2:B:109:ASP:CG	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:160:LYS:HG2	1:C:162:PRO:HD3	2.04	0.40
2:H:28:ASN:OD1	2:H:28:ASN:C	2.64	0.40
1:C:216:ASN:CG	1:E:212:THR:HG21	2.46	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%)	7	32
1	C	317/329 (96%)	296 (93%)	20 (6%)	1 (0%)	36	64
1	E	317/329 (96%)	294 (93%)	21 (7%)	2 (1%)	21	52
1	G	317/329 (96%)	295 (93%)	19 (6%)	3 (1%)	14	43
2	B	172/174 (99%)	162 (94%)	8 (5%)	2 (1%)	10	37
2	D	172/174 (99%)	164 (95%)	8 (5%)	0	100	100
2	F	172/174 (99%)	164 (95%)	7 (4%)	1 (1%)	21	52
2	H	172/174 (99%)	159 (92%)	12 (7%)	1 (1%)	21	52
All	All	1956/2012 (97%)	1828 (94%)	113 (6%)	15 (1%)	16	46

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	18	HIS
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%)	76	80
1	C	284/293 (97%)	279 (98%)	5 (2%)	51	70
1	E	284/293 (97%)	281 (99%)	3 (1%)	65	75
1	G	284/293 (97%)	283 (100%)	1 (0%)	84	84
2	B	148/148 (100%)	146 (99%)	2 (1%)	59	73
2	D	147/148 (99%)	145 (99%)	2 (1%)	59	73
2	F	148/148 (100%)	148 (100%)	0	100	100
2	H	148/148 (100%)	145 (98%)	3 (2%)	48	68
All	All	1727/1764 (98%)	1709 (99%)	18 (1%)	68	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	VAL
1	A	260	ILE
2	B	2	ILE
2	B	38	LEU
1	C	10	MET
1	C	130	VAL
1	C	196	VAL
1	C	242	ILE
1	C	265	SER
2	D	72	GLU
2	D	168	ASN
1	E	81	ASN
1	E	196	VAL
1	E	260	ILE
1	G	195	TYR
2	H	29	SER
2	H	108	ILE
2	H	110	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	33	GLN
1	A	197	GLN
1	A	312	ASN
2	B	12	ASN
2	B	78	GLN
1	C	17	HIS
1	C	18	HIS
1	C	56	HIS
1	C	216	ASN
1	C	278	ASN
2	D	47	GLN
2	D	60	ASN
2	D	65	GLN
2	D	159	HIS
1	E	33	GLN
1	E	261	GLN
1	E	296	ASN
2	F	60	ASN
1	G	210	GLN
1	G	278	ASN

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Mol	Chain	Res	Type
2	H	12	ASN
2	H	60	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.77	1 (7%)	17,19,21	0.56	0
3	NAG	I	2	3	14,14,15	0.38	0	17,19,21	0.42	0
3	BMA	I	3	3	11,11,12	0.76	0	15,15,17	1.15	2 (13%)
3	FUL	I	4	3	10,10,11	1.78	2 (20%)	14,14,16	2.05	3 (21%)
3	FUC	I	5	3	10,10,11	0.73	0	14,14,16	0.89	1 (7%)
4	NAG	J	1	1,4	14,14,15	0.45	0	17,19,21	0.71	0
4	NAG	J	2	4	14,14,15	0.33	0	17,19,21	0.55	0
4	BMA	J	3	4	11,11,12	0.56	0	15,15,17	0.70	0
4	MAN	J	4	4	11,11,12	0.85	0	15,15,17	1.14	1 (6%)
4	NAG	K	1	1,4	14,14,15	0.70	1 (7%)	17,19,21	0.66	0
4	NAG	K	2	4	14,14,15	0.20	0	17,19,21	0.87	1 (5%)
4	BMA	K	3	4	11,11,12	0.80	0	15,15,17	0.93	0
4	MAN	K	4	4	11,11,12	0.97	1 (9%)	15,15,17	1.73	3 (20%)
5	NAG	L	1	1,5	14,14,15	0.41	0	17,19,21	0.69	0
5	NAG	L	2	5	14,14,15	0.42	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	L	3	5	11,11,12	1.45	2 (18%)	15,15,17	1.45	2 (13%)
5	MAN	L	4	5	11,11,12	1.97	3 (27%)	15,15,17	2.53	6 (40%)
5	MAN	L	5	5	11,11,12	1.05	1 (9%)	15,15,17	1.50	3 (20%)
5	MAN	L	6	5	11,11,12	1.40	3 (27%)	15,15,17	2.22	1 (6%)
6	NAG	M	1	1,6	14,14,15	0.60	0	17,19,21	1.00	1 (5%)
6	NAG	M	2	6	14,14,15	0.43	0	17,19,21	1.48	2 (11%)
6	BMA	M	3	6	11,11,12	1.33	2 (18%)	15,15,17	1.85	2 (13%)
6	MAN	M	4	6	11,11,12	1.00	1 (9%)	15,15,17	1.53	1 (6%)
6	MAN	M	5	6	11,11,12	0.89	1 (9%)	15,15,17	1.56	1 (6%)
7	NAG	N	1	7,1	14,14,15	0.35	0	17,19,21	1.31	2 (11%)
7	NAG	N	2	7	14,14,15	0.16	0	17,19,21	0.66	0
8	NAG	O	1	8,1	14,14,15	0.48	0	17,19,21	0.61	0
8	NAG	O	2	8	14,14,15	0.66	0	17,19,21	0.77	0
8	BMA	O	3	8	11,11,12	1.06	2 (18%)	15,15,17	0.66	0
4	NAG	P	1	1,4	14,14,15	0.62	1 (7%)	17,19,21	0.75	0
4	NAG	P	2	4	14,14,15	0.27	0	17,19,21	0.57	0
4	BMA	P	3	4	11,11,12	0.87	0	15,15,17	0.81	0
4	MAN	P	4	4	11,11,12	1.26	2 (18%)	15,15,17	1.85	3 (20%)
5	NAG	Q	1	1,5	14,14,15	0.38	0	17,19,21	0.60	0
5	NAG	Q	2	5	14,14,15	0.49	0	17,19,21	0.96	1 (5%)
5	MAN	Q	3	5	11,11,12	1.09	1 (9%)	15,15,17	1.72	4 (26%)
5	MAN	Q	4	5	11,11,12	1.90	1 (9%)	15,15,17	1.40	3 (20%)
5	MAN	Q	5	5	11,11,12	1.44	2 (18%)	15,15,17	1.98	5 (33%)
5	MAN	Q	6	5	11,11,12	1.43	2 (18%)	15,15,17	1.37	3 (20%)
8	NAG	R	1	8,1	14,14,15	0.53	0	17,19,21	1.41	2 (11%)
8	NAG	R	2	8	14,14,15	0.73	0	17,19,21	0.61	0
8	BMA	R	3	8	11,11,12	0.81	1 (9%)	15,15,17	0.85	0
7	NAG	S	1	7,1	14,14,15	0.37	0	17,19,21	1.43	2 (11%)
7	NAG	S	2	7	14,14,15	0.96	1 (7%)	17,19,21	0.80	0
9	NAG	T	1	9,1	14,14,15	0.25	0	17,19,21	0.46	0
9	FUL	T	2	9	10,10,11	2.05	3 (30%)	14,14,16	1.96	4 (28%)
9	FUC	T	3	9	10,10,11	0.74	0	14,14,16	0.86	0
6	NAG	U	1	1,6	14,14,15	0.66	1 (7%)	17,19,21	0.84	1 (5%)
6	NAG	U	2	6	14,14,15	1.13	1 (7%)	17,19,21	1.79	1 (5%)
6	BMA	U	3	6	11,11,12	0.90	0	15,15,17	1.07	2 (13%)
6	MAN	U	4	6	11,11,12	1.38	2 (18%)	15,15,17	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	U	5	6	11,11,12	0.94	1 (9%)	15,15,17	1.14	2 (13%)
10	NAG	V	1	10,1	14,14,15	0.35	0	17,19,21	0.63	0
10	NAG	V	2	10	14,14,15	0.35	0	17,19,21	0.54	0
10	BMA	V	3	10	11,11,12	0.72	0	15,15,17	0.73	0
10	MAN	V	4	10	11,11,12	1.10	1 (9%)	15,15,17	1.76	4 (26%)
10	MAN	V	5	10	11,11,12	0.95	0	15,15,17	1.48	1 (6%)
5	NAG	W	1	1,5	14,14,15	0.39	0	17,19,21	0.45	0
5	NAG	W	2	5	14,14,15	0.30	0	17,19,21	0.70	0
5	MAN	W	3	5	11,11,12	1.12	1 (9%)	15,15,17	1.22	2 (13%)
5	MAN	W	4	5	11,11,12	1.96	3 (27%)	15,15,17	1.62	2 (13%)
5	MAN	W	5	5	11,11,12	1.43	2 (18%)	15,15,17	1.70	3 (20%)
5	MAN	W	6	5	11,11,12	0.81	0	15,15,17	1.26	1 (6%)
6	NAG	X	1	1,6	14,14,15	0.24	0	17,19,21	0.75	0
6	NAG	X	2	6	14,14,15	0.42	0	17,19,21	0.70	0
6	BMA	X	3	6	11,11,12	1.11	1 (9%)	15,15,17	1.10	0
6	MAN	X	4	6	11,11,12	1.62	1 (9%)	15,15,17	1.73	2 (13%)
6	MAN	X	5	6	11,11,12	1.37	2 (18%)	15,15,17	1.95	3 (20%)
11	NAG	Y	1	11,1	14,14,15	0.58	1 (7%)	17,19,21	0.57	0
11	NAG	Y	2	11	14,14,15	0.31	0	17,19,21	0.37	0
11	FUC	Y	3	11	10,10,11	0.95	1 (10%)	14,14,16	1.20	2 (14%)
7	NAG	Z	1	7,1	14,14,15	0.41	0	17,19,21	1.39	2 (11%)
7	NAG	Z	2	7	14,14,15	0.50	0	17,19,21	1.29	1 (5%)
12	NAG	a	1	1,12	14,14,15	1.26	1 (7%)	17,19,21	1.44	4 (23%)
12	NAG	a	2	12	14,14,15	0.37	0	17,19,21	0.80	0
12	BMA	a	3	12	11,11,12	1.87	3 (27%)	15,15,17	1.43	3 (20%)
12	MAN	a	4	12	11,11,12	1.42	2 (18%)	15,15,17	2.05	4 (26%)
12	FUC	a	5	12	10,10,11	1.05	1 (10%)	14,14,16	1.25	3 (21%)
7	NAG	b	1	7,1	14,14,15	0.64	0	17,19,21	1.67	2 (11%)
7	NAG	b	2	7	14,14,15	0.37	0	17,19,21	0.80	1 (5%)
13	NAG	c	1	1,13	14,14,15	0.48	0	17,19,21	0.50	0
13	NAG	c	2	13	14,14,15	0.51	0	17,19,21	0.52	0
13	MAN	c	3	13	11,11,12	1.70	3 (27%)	15,15,17	1.40	3 (20%)
13	MAN	c	4	13	11,11,12	1.93	3 (27%)	15,15,17	1.81	4 (26%)
13	MAN	c	5	13	11,11,12	1.21	1 (9%)	15,15,17	1.59	2 (13%)
13	MAN	c	6	13	11,11,12	1.16	1 (9%)	15,15,17	1.38	3 (20%)
13	MAN	c	7	13	11,11,12	1.72	3 (27%)	15,15,17	1.55	2 (13%)
14	NAG	d	1	1,14	14,14,15	0.53	0	17,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	d	2	14	14,14,15	0.38	0	17,19,21	0.75	0
14	BMA	d	3	14	11,11,12	0.71	0	15,15,17	0.89	1 (6%)
14	MAN	d	4	14	11,11,12	0.74	0	15,15,17	1.05	2 (13%)
6	NAG	e	1	1,6	14,14,15	0.61	0	17,19,21	1.25	1 (5%)
6	NAG	e	2	6	14,14,15	0.17	0	17,19,21	0.70	0
6	BMA	e	3	6	11,11,12	0.98	0	15,15,17	0.95	0
6	MAN	e	4	6	11,11,12	1.22	1 (9%)	15,15,17	1.88	2 (13%)
6	MAN	e	5	6	11,11,12	1.03	1 (9%)	15,15,17	2.03	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	-	2/6/23/26	0/1/1/1
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	1,5	-	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	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	4/6/23/26	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	N	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
8	NAG	O	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	O	2	8	-	2/6/23/26	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	1,5	-	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	8,1	-	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	7,1	-	6/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
9	NAG	T	1	9,1	-	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	10,1	-	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	1,5	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	4/6/23/26	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	7,1	-	6/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	4/6/23/26	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	7,1	-	6/6/23/26	0/1/1/1
7	NAG	b	2	7	-	4/6/23/26	0/1/1/1
13	NAG	c	1	1,13	-	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	-	6/6/23/26	0/1/1/1
6	NAG	e	2	6	-	2/6/23/26	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 (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	4	MAN	C2-C3	4.95	1.60	1.52
6	X	4	MAN	C1-C2	4.82	1.63	1.52
9	T	2	FUL	O5-C1	4.42	1.51	1.43
3	I	4	FUL	O5-C1	4.41	1.51	1.43
5	L	4	MAN	O2-C2	4.22	1.52	1.43
12	a	1	NAG	O5-C1	-4.15	1.36	1.43
5	W	4	MAN	C2-C3	4.13	1.58	1.52
6	U	2	NAG	O5-C1	4.09	1.50	1.43
5	W	5	MAN	C1-C2	4.07	1.61	1.52
13	c	4	MAN	C2-C3	3.92	1.58	1.52
13	c	4	MAN	O2-C2	3.86	1.51	1.43
5	W	4	MAN	O2-C2	3.79	1.51	1.43
13	c	7	MAN	O5-C1	3.68	1.49	1.43
12	a	3	BMA	C2-C3	3.64	1.58	1.52
12	a	4	MAN	C1-C2	3.55	1.60	1.52
5	L	4	MAN	C2-C3	3.52	1.57	1.52
9	T	2	FUL	C2-C3	-3.49	1.47	1.52
13	c	7	MAN	O5-C5	3.37	1.50	1.43
4	P	4	MAN	C1-C2	3.33	1.60	1.52
13	c	5	MAN	C1-C2	3.28	1.60	1.52
5	L	3	MAN	C2-C3	3.21	1.57	1.52
5	Q	5	MAN	C1-C2	3.19	1.59	1.52
6	X	5	MAN	C1-C2	3.18	1.59	1.52
13	c	3	MAN	C1-C2	3.13	1.59	1.52
5	L	5	MAN	C1-C2	3.12	1.59	1.52
6	e	4	MAN	C1-C2	3.04	1.59	1.52
6	e	5	MAN	C1-C2	2.94	1.59	1.52
6	U	4	MAN	O5-C5	2.92	1.49	1.43
12	a	3	BMA	C4-C3	2.91	1.59	1.52
6	X	3	BMA	O5-C5	2.88	1.49	1.43
10	V	4	MAN	C1-C2	2.82	1.58	1.52
5	Q	6	MAN	C1-C2	2.82	1.58	1.52
5	L	6	MAN	O5-C5	2.81	1.48	1.43
5	Q	6	MAN	O5-C5	2.77	1.48	1.43
13	c	3	MAN	O5-C5	2.67	1.48	1.43
6	M	4	MAN	C1-C2	2.67	1.58	1.52
7	S	2	NAG	C1-C2	2.63	1.55	1.52
6	X	5	MAN	O5-C1	2.63	1.48	1.43
9	T	2	FUL	O5-C5	2.59	1.48	1.43
4	K	4	MAN	C1-C2	2.54	1.58	1.52
5	L	3	MAN	O5-C5	2.54	1.48	1.43
12	a	4	MAN	O5-C1	2.54	1.48	1.43
12	a	3	BMA	O5-C1	-2.54	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	6	MAN	C1-C2	2.51	1.58	1.52
3	I	1	NAG	C1-C2	2.50	1.55	1.52
5	W	3	MAN	C1-C2	2.47	1.58	1.52
5	W	4	MAN	C1-C2	2.45	1.58	1.52
5	L	6	MAN	O5-C1	2.43	1.47	1.43
4	K	1	NAG	O5-C1	-2.43	1.39	1.43
6	U	4	MAN	C1-C2	2.37	1.57	1.52
13	c	3	MAN	O5-C1	2.37	1.47	1.43
6	U	1	NAG	O5-C1	-2.35	1.39	1.43
6	M	3	BMA	O5-C5	2.31	1.47	1.43
8	O	3	BMA	C1-C2	2.25	1.57	1.52
13	c	4	MAN	C1-C2	2.24	1.57	1.52
5	Q	5	MAN	O2-C2	2.23	1.48	1.43
13	c	6	MAN	C4-C5	2.23	1.57	1.53
6	M	5	MAN	C1-C2	2.23	1.57	1.52
4	P	1	NAG	O5-C1	-2.23	1.40	1.43
5	Q	3	MAN	O5-C5	2.21	1.47	1.43
6	M	3	BMA	C4-C5	2.20	1.57	1.53
6	U	5	MAN	C1-C2	2.18	1.57	1.52
3	I	4	FUL	C2-C3	-2.17	1.49	1.52
8	R	3	BMA	C1-C2	2.15	1.57	1.52
13	c	7	MAN	C1-C2	2.15	1.57	1.52
4	P	4	MAN	O5-C1	2.14	1.47	1.43
5	L	4	MAN	C4-C3	2.13	1.57	1.52
12	a	5	FUC	O5-C5	2.12	1.47	1.43
5	W	5	MAN	C2-C3	2.09	1.55	1.52
11	Y	3	FUC	C1-C2	2.05	1.57	1.52
8	O	3	BMA	C2-C3	2.04	1.55	1.52
11	Y	1	NAG	C1-C2	2.03	1.55	1.52

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	6	MAN	C1-O5-C5	7.73	122.55	112.19
5	L	4	MAN	C1-O5-C5	7.50	122.23	112.19
6	U	2	NAG	C1-O5-C5	6.68	121.13	112.19
6	X	5	MAN	C1-O5-C5	6.21	120.51	112.19
6	e	4	MAN	C1-O5-C5	6.06	120.31	112.19
6	e	5	MAN	C1-O5-C5	6.00	120.23	112.19
3	I	4	FUL	C1-C2-C3	5.99	118.37	109.64
6	M	3	BMA	C1-O5-C5	5.76	119.91	112.19
12	a	4	MAN	C1-O5-C5	5.74	119.87	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	4	MAN	C1-O5-C5	5.61	119.70	112.19
5	Q	5	MAN	C1-O5-C5	5.17	119.11	112.19
6	M	5	MAN	C1-O5-C5	5.16	119.11	112.19
13	c	4	MAN	C1-O5-C5	5.01	118.90	112.19
13	c	7	MAN	C1-O5-C5	4.96	118.84	112.19
4	K	4	MAN	C1-O5-C5	4.93	118.79	112.19
9	T	2	FUL	O5-C5-C4	4.86	118.30	109.55
6	X	4	MAN	C1-O5-C5	4.77	118.58	112.19
7	S	1	NAG	C2-N2-C7	4.72	129.23	122.90
6	M	4	MAN	C1-O5-C5	4.72	118.51	112.19
6	M	2	NAG	C2-N2-C7	4.71	129.21	122.90
10	V	5	MAN	C1-O5-C5	4.71	118.50	112.19
7	Z	1	NAG	C2-N2-C7	4.71	129.21	122.90
7	Z	2	NAG	C2-N2-C7	4.59	129.05	122.90
7	N	1	NAG	C2-N2-C7	4.50	128.93	122.90
5	W	4	MAN	C1-O5-C5	4.45	118.15	112.19
7	b	1	NAG	C1-O5-C5	4.40	118.08	112.19
5	L	5	MAN	C1-O5-C5	4.35	118.01	112.19
7	b	1	NAG	C2-N2-C7	4.33	128.70	122.90
6	e	1	NAG	C2-N2-C7	4.29	128.64	122.90
5	Q	3	MAN	C1-O5-C5	4.25	117.88	112.19
5	W	5	MAN	C1-C2-C3	4.16	115.70	109.64
13	c	5	MAN	C1-O5-C5	4.10	117.68	112.19
10	V	4	MAN	C1-C2-C3	4.07	115.57	109.64
5	W	3	MAN	C1-O5-C5	3.84	117.33	112.19
5	W	6	MAN	C1-O5-C5	3.78	117.26	112.19
6	X	4	MAN	C1-C2-C3	3.77	115.13	109.64
5	L	3	MAN	C1-O5-C5	3.52	116.91	112.19
12	a	4	MAN	C1-C2-C3	3.47	114.70	109.64
8	R	1	NAG	C1-O5-C5	3.47	116.83	112.19
10	V	4	MAN	C1-O5-C5	3.46	116.83	112.19
5	W	5	MAN	C1-O5-C5	3.41	116.75	112.19
4	J	4	MAN	C1-O5-C5	3.36	116.69	112.19
12	a	3	BMA	C2-C3-C4	3.31	116.69	110.86
12	a	3	BMA	C3-C4-C5	3.30	116.21	110.23
12	a	1	NAG	C2-N2-C7	3.22	127.22	122.90
12	a	1	NAG	C1-O5-C5	-3.21	107.88	112.19
9	T	2	FUL	C3-C4-C5	3.09	114.50	109.81
5	Q	4	MAN	C1-O5-C5	2.98	116.18	112.19
13	c	5	MAN	C1-C2-C3	2.92	113.89	109.64
9	T	2	FUL	C1-O5-C5	2.92	119.84	112.97
6	e	5	MAN	C1-C2-C3	2.91	113.88	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	c	3	MAN	O2-C2-C3	-2.87	104.20	110.15
5	Q	5	MAN	O2-C2-C1	2.82	115.67	109.22
3	I	4	FUL	C2-C3-C4	2.81	115.80	110.86
5	Q	4	MAN	O3-C3-C2	2.80	115.76	110.05
5	Q	3	MAN	O5-C5-C6	2.79	113.10	107.66
11	Y	3	FUC	C1-O5-C5	2.78	119.53	112.97
5	L	3	MAN	O3-C3-C2	2.78	115.72	110.05
4	P	4	MAN	C1-C2-C3	2.77	113.68	109.64
5	L	4	MAN	C2-C3-C4	2.77	115.73	110.86
13	c	3	MAN	C1-C2-C3	-2.74	105.66	109.64
14	d	4	MAN	C1-O5-C5	2.70	115.81	112.19
12	a	5	FUC	C1-O5-C5	2.70	119.33	112.97
5	L	4	MAN	O5-C1-C2	2.68	117.18	110.79
8	R	1	NAG	C2-N2-C7	2.67	126.47	122.90
6	U	5	MAN	C1-O5-C5	2.64	115.72	112.19
13	c	7	MAN	O2-C2-C3	-2.62	104.73	110.15
10	V	4	MAN	O2-C2-C3	-2.61	104.75	110.15
5	Q	5	MAN	O2-C2-C3	-2.60	104.77	110.15
13	c	4	MAN	O2-C2-C3	2.60	115.53	110.15
13	c	6	MAN	O2-C2-C3	-2.59	104.80	110.15
6	M	2	NAG	C1-C2-N2	2.58	114.50	110.43
6	e	5	MAN	O5-C1-C2	2.57	116.92	110.79
5	Q	6	MAN	O2-C2-C3	-2.56	104.84	110.15
5	Q	6	MAN	O5-C5-C6	2.54	112.61	107.66
12	a	5	FUC	O5-C5-C4	2.54	114.12	109.55
7	b	2	NAG	C1-O5-C5	2.50	115.54	112.19
5	L	4	MAN	O2-C2-C1	2.46	114.86	109.22
12	a	4	MAN	O5-C1-C2	2.44	116.62	110.79
9	T	2	FUL	C6-C5-C4	-2.41	108.67	113.08
6	M	3	BMA	C3-C4-C5	2.40	114.59	110.23
5	Q	4	MAN	O2-C2-C3	2.37	115.06	110.15
13	c	6	MAN	C3-C4-C5	2.37	114.53	110.23
6	X	5	MAN	C1-C2-C3	2.36	113.08	109.64
5	Q	6	MAN	C1-O5-C5	2.36	115.35	112.19
6	e	5	MAN	O2-C2-C3	-2.36	105.27	110.15
4	K	4	MAN	C1-C2-C3	2.36	113.07	109.64
14	d	4	MAN	O2-C2-C3	-2.36	105.27	110.15
11	Y	3	FUC	O5-C5-C4	2.34	113.76	109.55
3	I	4	FUL	O5-C1-C2	2.34	116.36	110.79
4	K	4	MAN	O2-C2-C3	-2.33	105.32	110.15
13	c	3	MAN	O2-C2-C1	2.33	114.55	109.22
6	U	3	BMA	C1-O5-C5	2.33	115.31	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	4	MAN	C3-C4-C5	2.32	114.44	110.23
7	S	1	NAG	C1-C2-N2	2.32	114.08	110.43
5	L	4	MAN	O2-C2-C3	2.29	114.89	110.15
5	Q	2	NAG	C1-O5-C5	2.26	115.22	112.19
5	Q	5	MAN	C1-C2-C3	2.26	112.93	109.64
12	a	1	NAG	C4-C3-C2	2.24	114.30	111.02
7	Z	1	NAG	C1-C2-N2	2.23	113.94	110.43
5	Q	5	MAN	O5-C1-C2	2.22	116.08	110.79
5	Q	3	MAN	O2-C2-C3	-2.20	105.60	110.15
6	e	4	MAN	O5-C1-C2	2.16	115.95	110.79
5	W	3	MAN	O2-C2-C3	-2.16	105.67	110.15
3	I	3	BMA	C1-O5-C5	2.13	115.05	112.19
3	I	5	FUC	C1-O5-C5	2.10	117.93	112.97
6	U	5	MAN	O2-C2-C3	-2.10	105.81	110.15
13	c	6	MAN	C2-C3-C4	2.09	114.53	110.86
12	a	4	MAN	O2-C2-C3	-2.09	105.83	110.15
10	V	4	MAN	O5-C1-C2	2.08	115.75	110.79
5	Q	3	MAN	O6-C6-C5	-2.07	104.28	111.33
12	a	3	BMA	C1-C2-C3	2.07	112.66	109.64
3	I	3	BMA	C1-C2-C3	2.06	112.65	109.64
5	W	4	MAN	O2-C2-C3	2.06	114.42	110.15
12	a	1	NAG	C1-C2-N2	2.06	113.67	110.43
12	a	5	FUC	C1-C2-C3	2.05	112.64	109.64
13	c	4	MAN	O3-C3-C2	2.05	114.25	110.05
5	L	5	MAN	C1-C2-C3	2.05	112.63	109.64
6	U	3	BMA	C1-C2-C3	2.05	112.62	109.64
4	K	2	NAG	C1-O5-C5	2.04	114.92	112.19
6	U	1	NAG	O4-C4-C3	-2.03	105.59	110.38
13	c	4	MAN	O2-C2-C1	2.03	113.86	109.22
4	P	4	MAN	O2-C2-C3	-2.02	105.96	110.15
7	N	1	NAG	C1-C2-N2	2.02	113.61	110.43
5	L	5	MAN	O2-C2-C3	-2.02	105.97	110.15
6	X	5	MAN	O5-C1-C2	2.01	115.57	110.79
14	d	3	BMA	C1-O5-C5	2.00	114.87	112.19
5	W	5	MAN	O2-C2-C3	-2.00	106.00	110.15
6	M	1	NAG	C3-C4-C5	2.00	113.86	110.23

There are no chirality outliers.

All (167) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	U	2	NAG	C1-C2-N2-C7

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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
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
13	c	5	MAN	O5-C5-C6-O6
6	X	5	MAN	C4-C5-C6-O6
6	e	1	NAG	C4-C5-C6-O6
6	e	3	BMA	C4-C5-C6-O6
8	O	1	NAG	C4-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
14	d	1	NAG	O5-C5-C6-O6
14	d	1	NAG	C4-C5-C6-O6
6	X	4	MAN	O5-C5-C6-O6
6	e	5	MAN	O5-C5-C6-O6
14	d	4	MAN	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
5	L	4	MAN	O5-C5-C6-O6
5	L	5	MAN	O5-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
8	R	1	NAG	O5-C5-C6-O6
12	a	3	BMA	O5-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
6	X	4	MAN	C4-C5-C6-O6
12	a	1	NAG	C4-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
4	P	3	BMA	O5-C5-C6-O6
13	c	4	MAN	C4-C5-C6-O6
6	U	5	MAN	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
12	a	1	NAG	O5-C5-C6-O6
13	c	4	MAN	O5-C5-C6-O6
13	c	6	MAN	O5-C5-C6-O6
7	Z	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	V	5	MAN	C4-C5-C6-O6
5	Q	6	MAN	O5-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
13	c	5	MAN	C4-C5-C6-O6
5	L	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	L	4	MAN	C4-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6
5	Q	4	MAN	O5-C5-C6-O6
6	U	5	MAN	C4-C5-C6-O6
4	P	1	NAG	C4-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
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
10	V	4	MAN	O5-C5-C6-O6

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

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Mol	Chain	Res	Type	Atoms
7	S	1	NAG	C1-C2-N2-C7
7	Z	2	NAG	C1-C2-N2-C7
7	b	2	NAG	C1-C2-N2-C7
12	a	2	NAG	C1-C2-N2-C7
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	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
4	J	4	MAN	C4-C5-C6-O6
5	L	3	MAN	C4-C5-C6-O6
6	M	5	MAN	O5-C5-C6-O6
4	J	2	NAG	C1-C2-N2-C7
6	M	1	NAG	C1-C2-N2-C7
6	M	2	NAG	C1-C2-N2-C7
6	X	1	NAG	C1-C2-N2-C7
6	e	1	NAG	C1-C2-N2-C7
6	e	2	NAG	C1-C2-N2-C7
7	N	1	NAG	C1-C2-N2-C7
7	Z	1	NAG	C1-C2-N2-C7
7	b	1	NAG	C1-C2-N2-C7
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
7	b	1	NAG	C4-C5-C6-O6
5	W	4	MAN	O5-C5-C6-O6
5	L	3	MAN	O5-C5-C6-O6
8	O	2	NAG	O5-C5-C6-O6

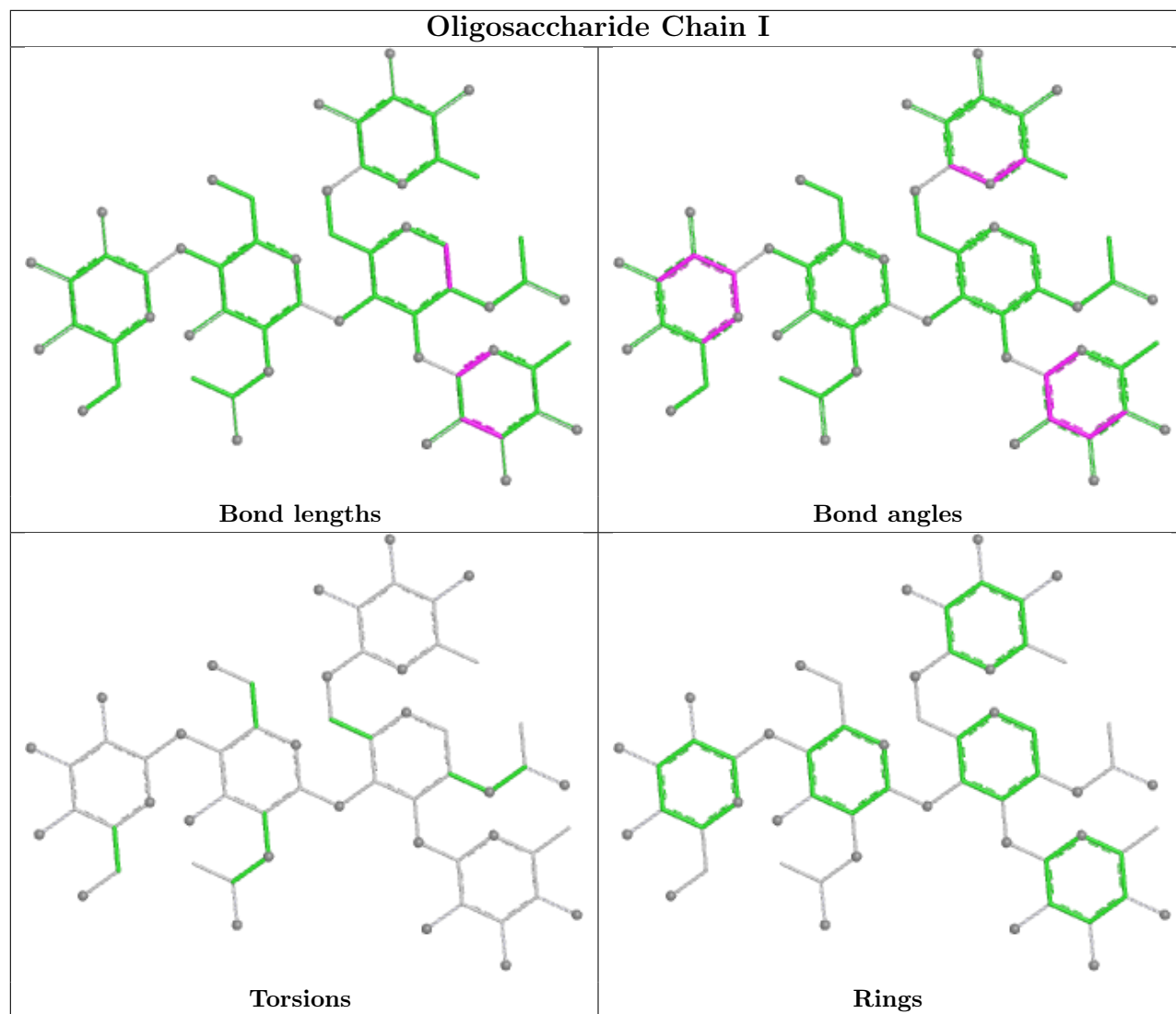
All (9) ring outliers are listed below:

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

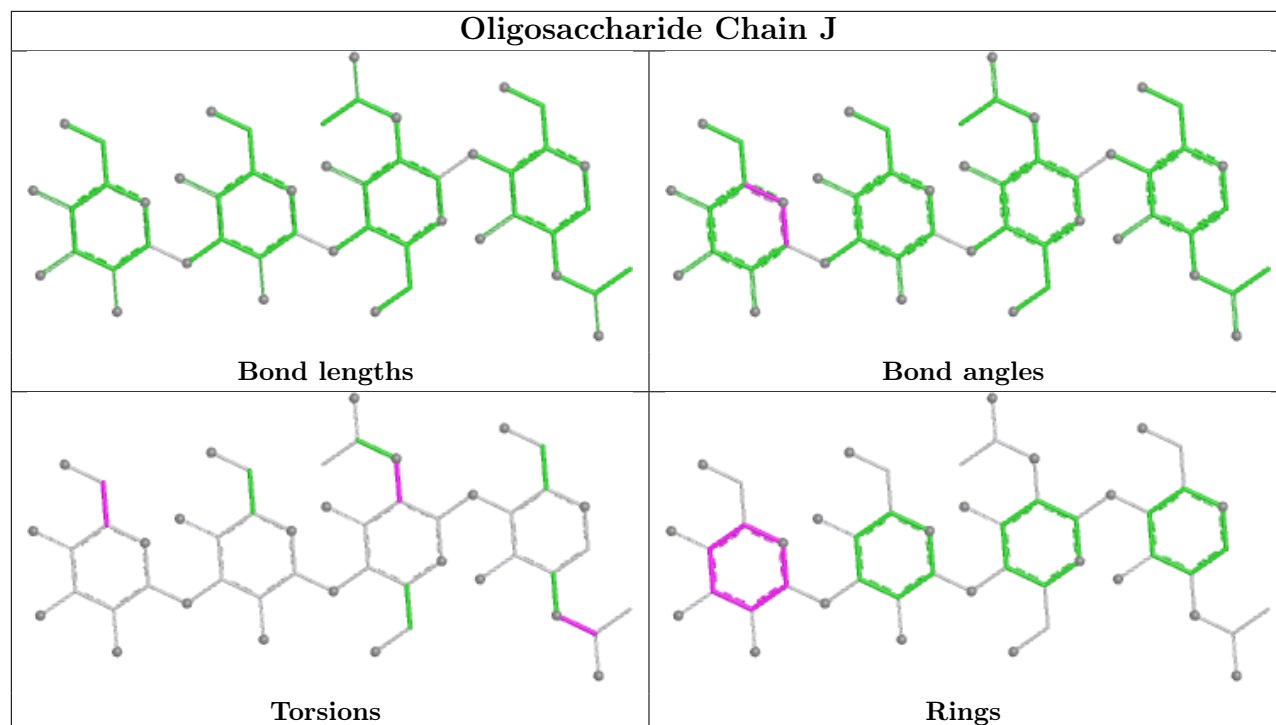
27 monomers are involved in 26 short contacts:

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

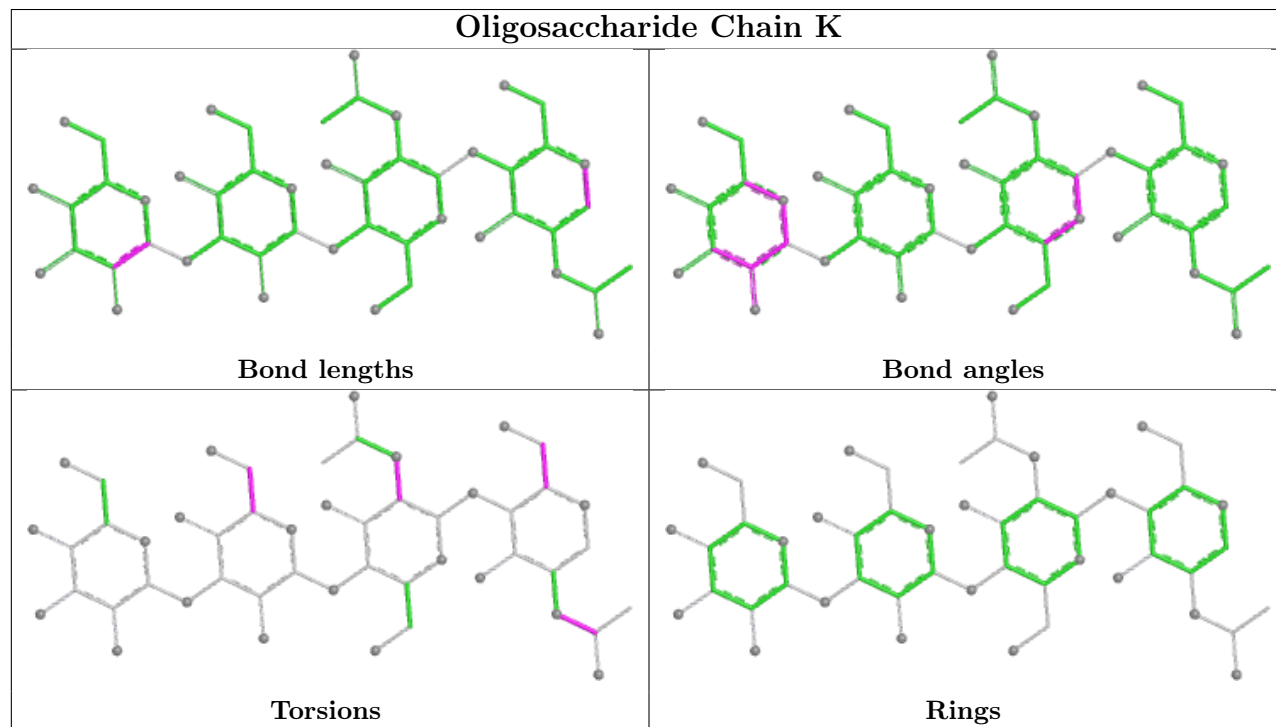
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

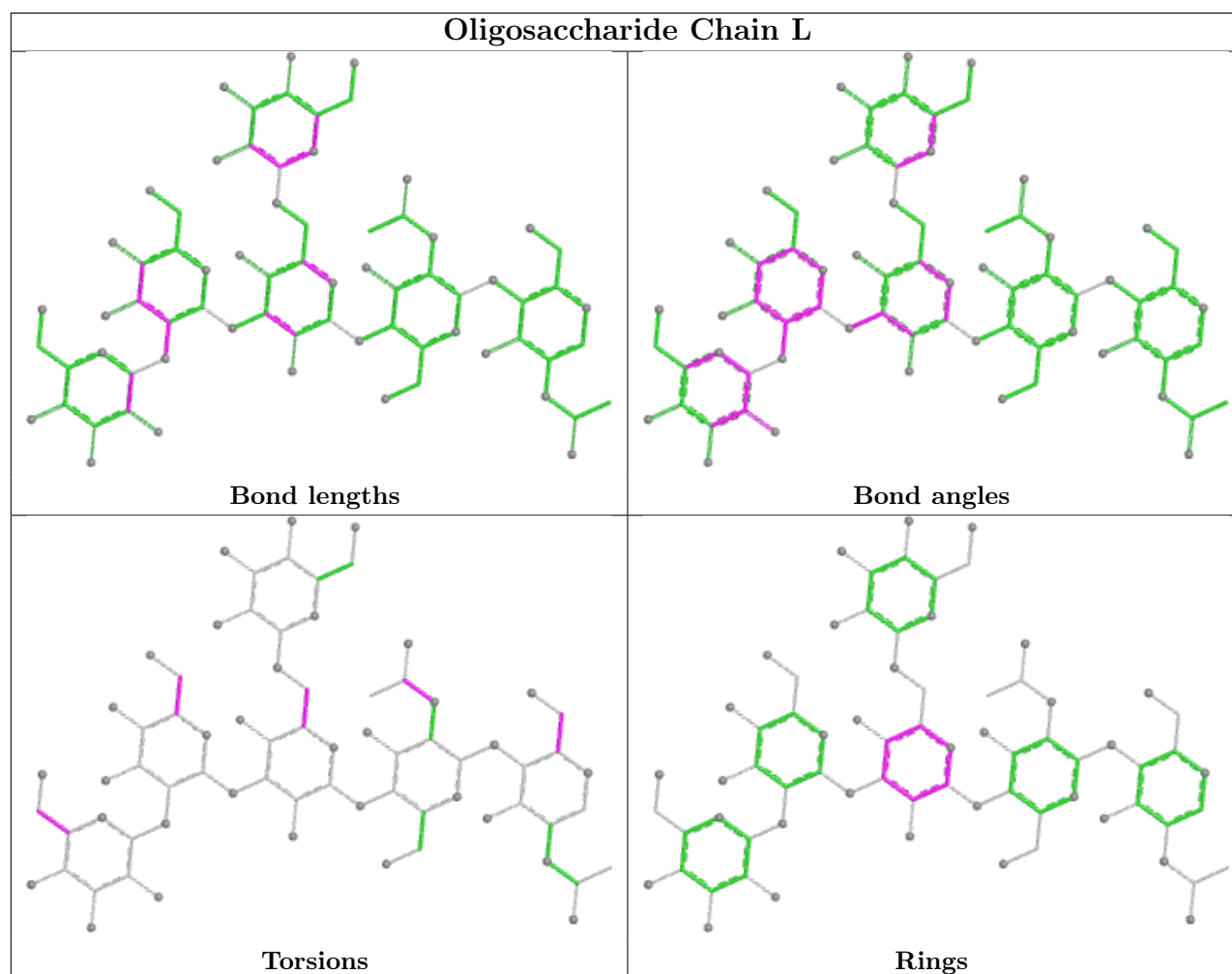
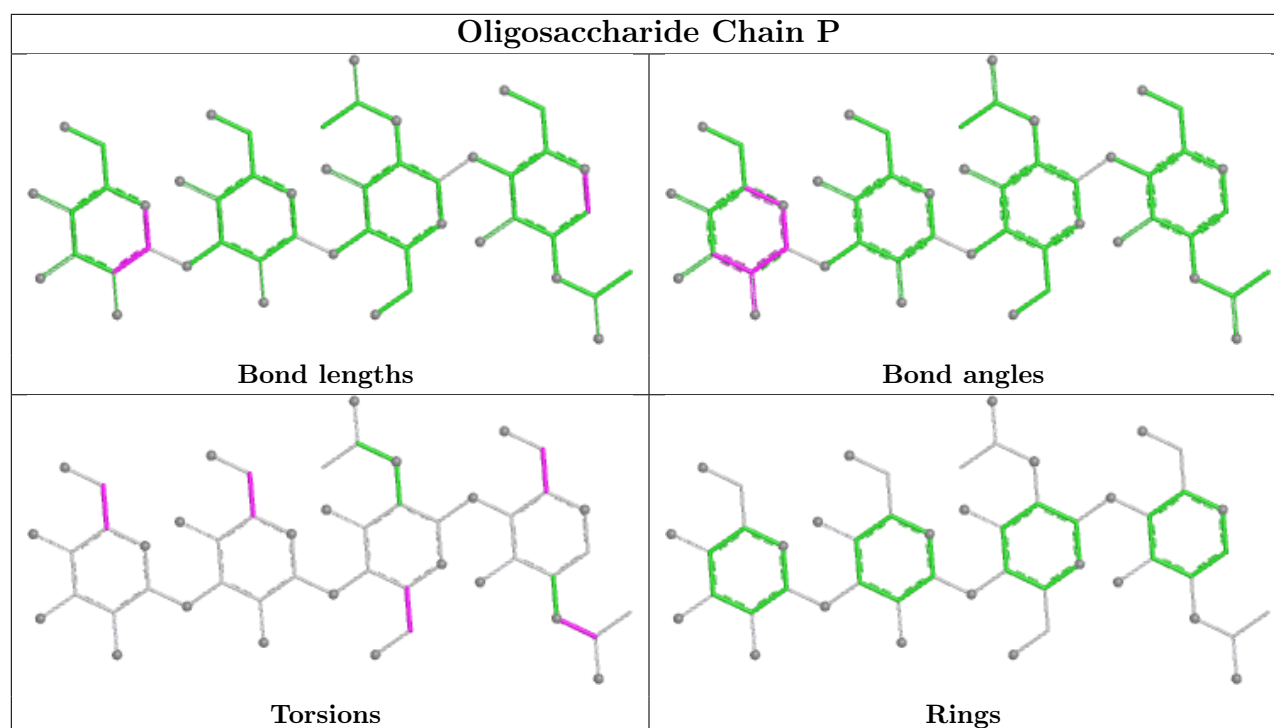


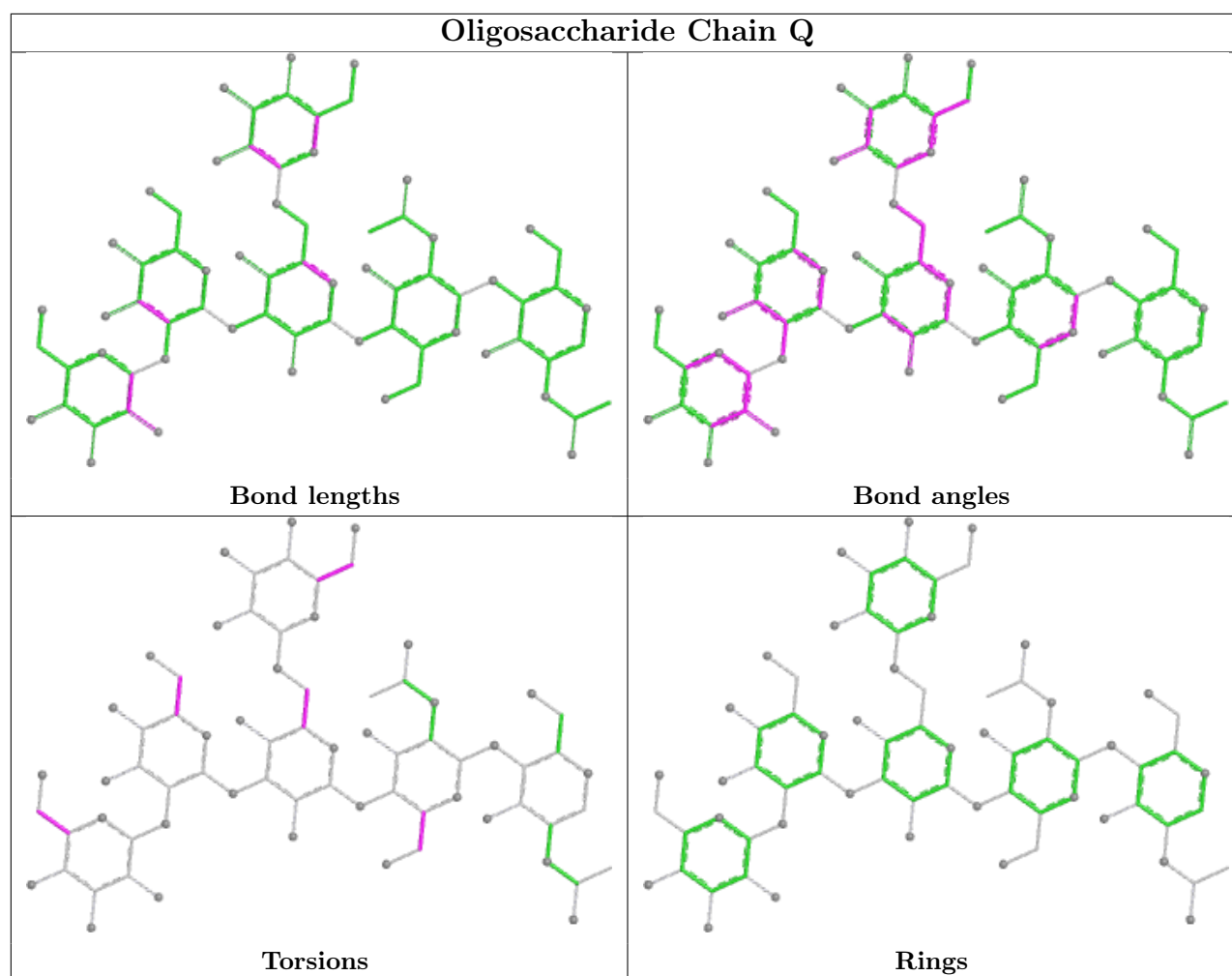
Oligosaccharide Chain J



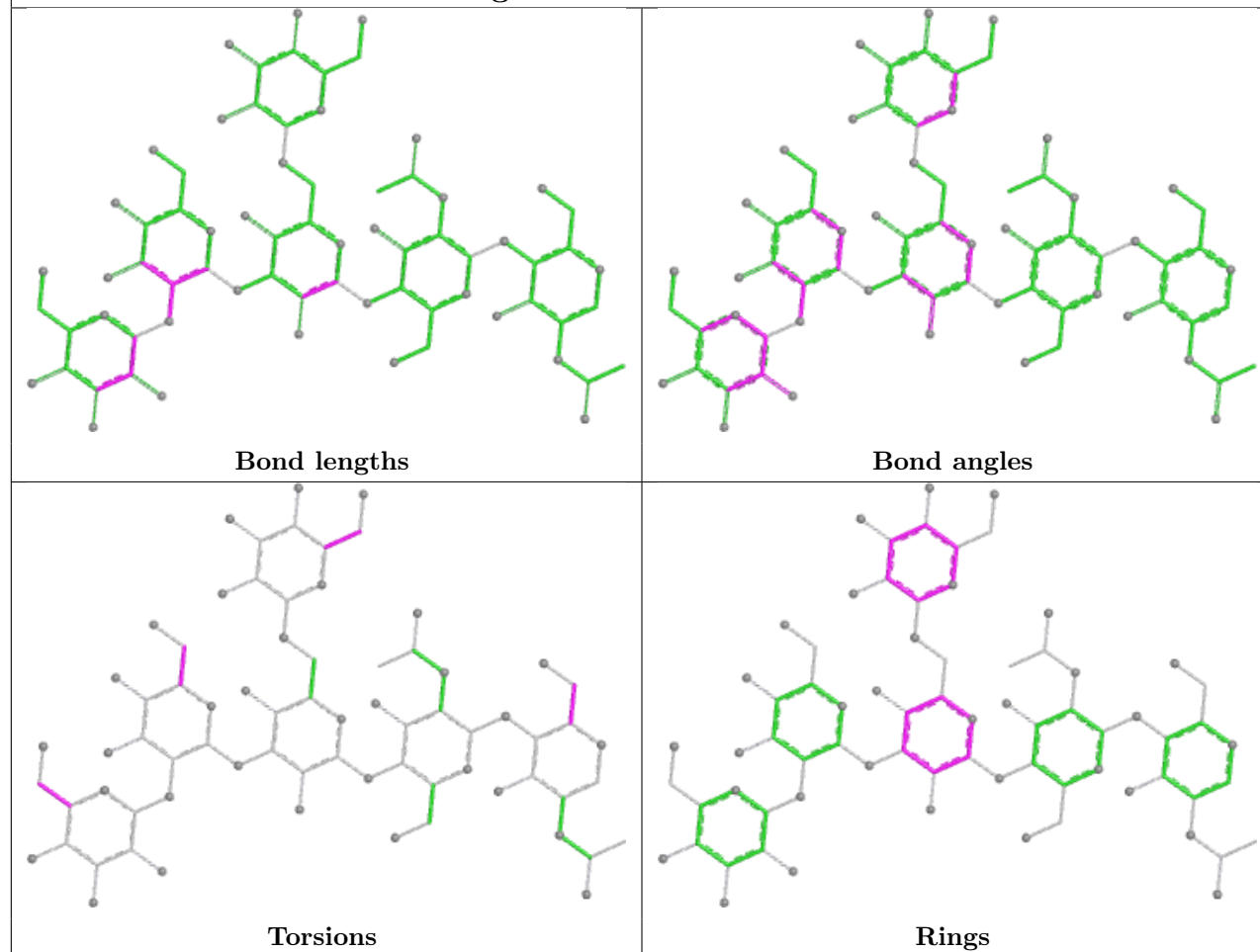
Oligosaccharide Chain K

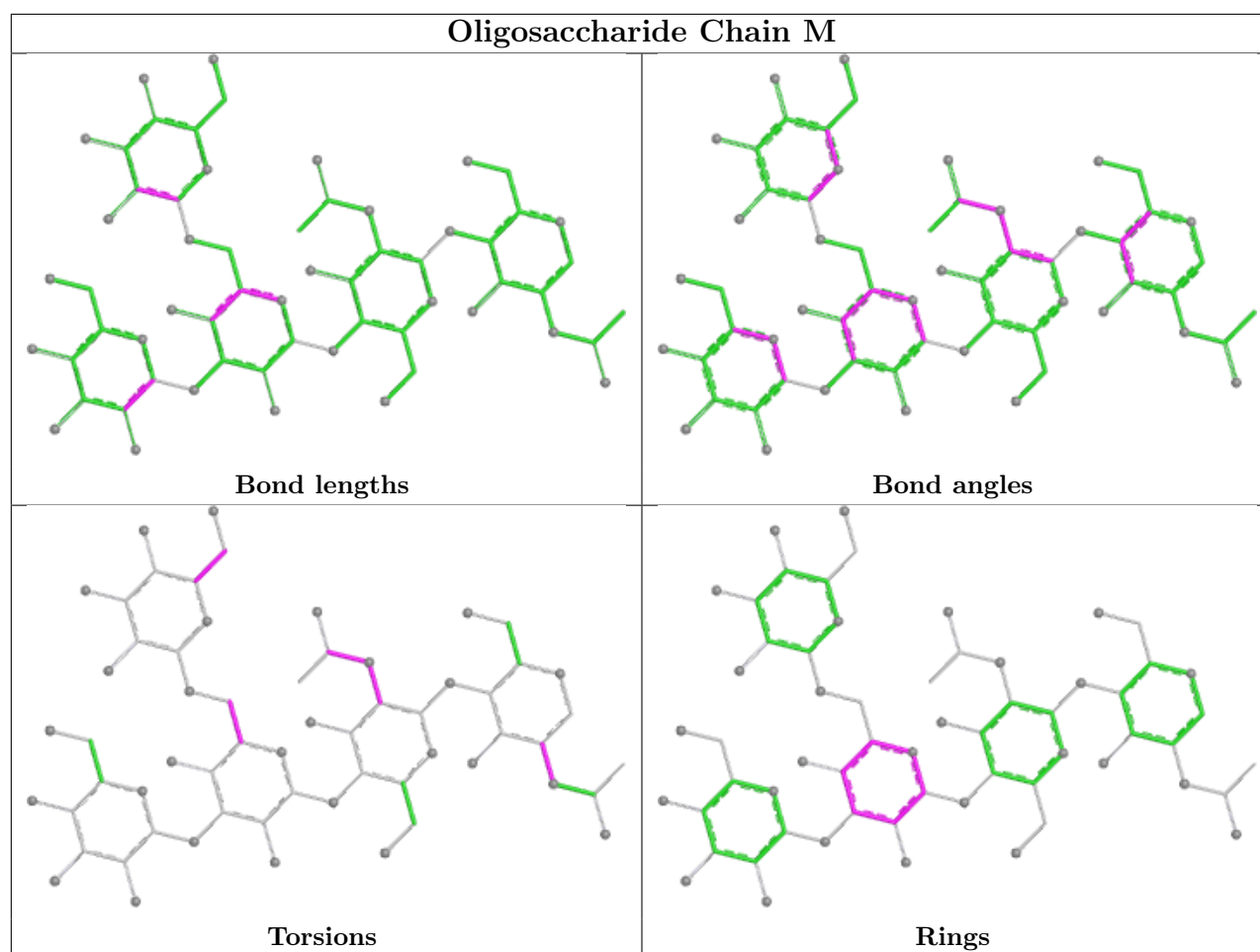


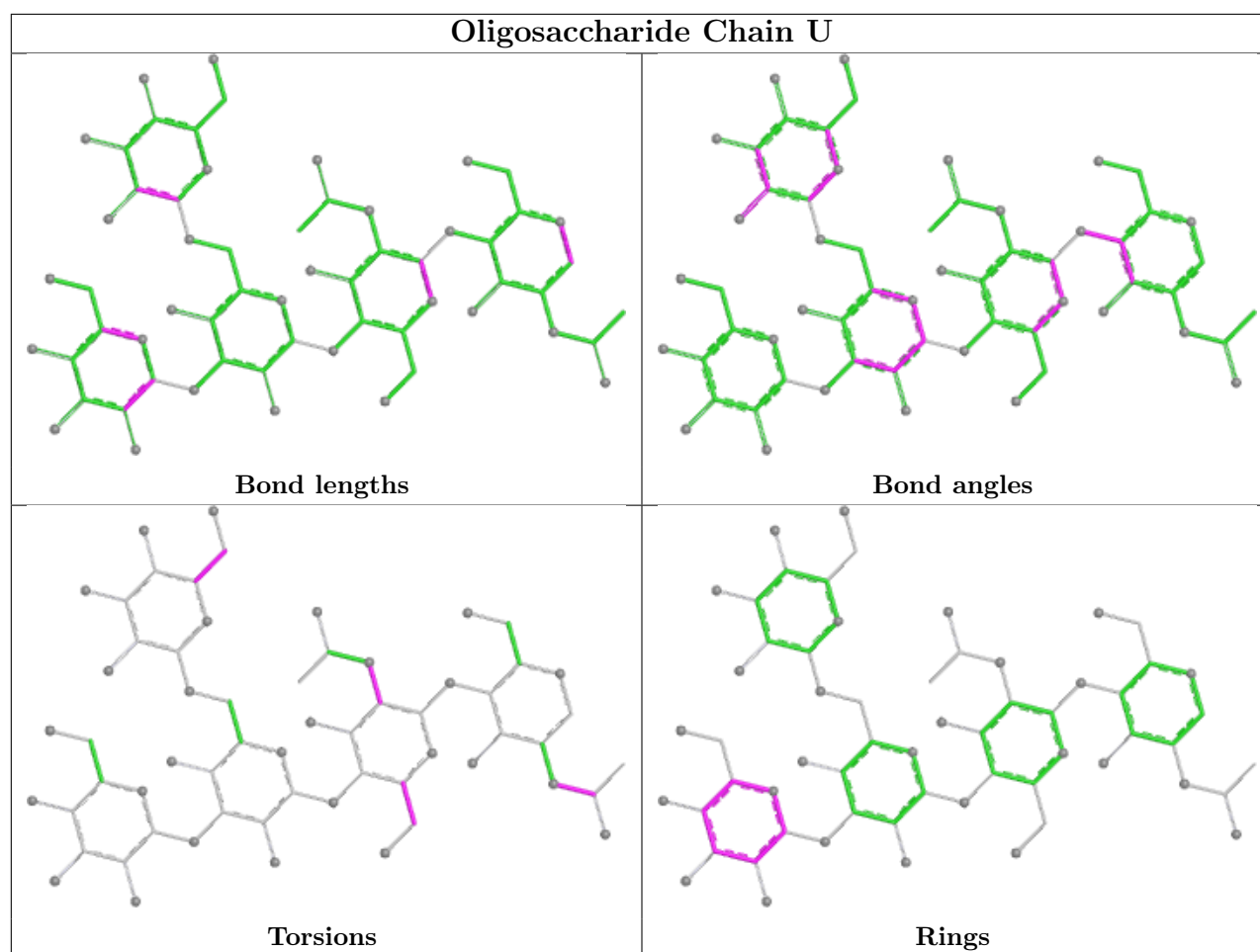


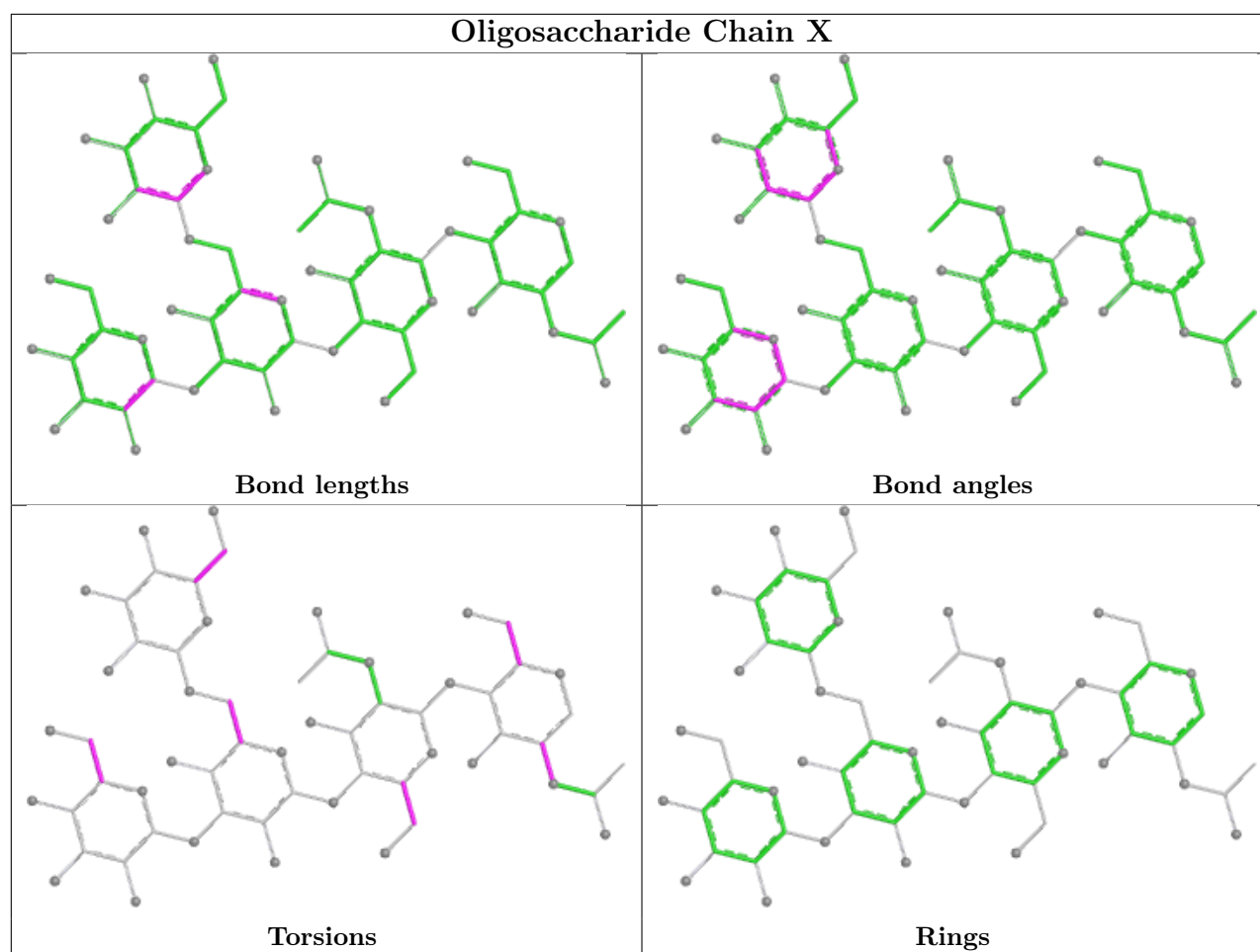


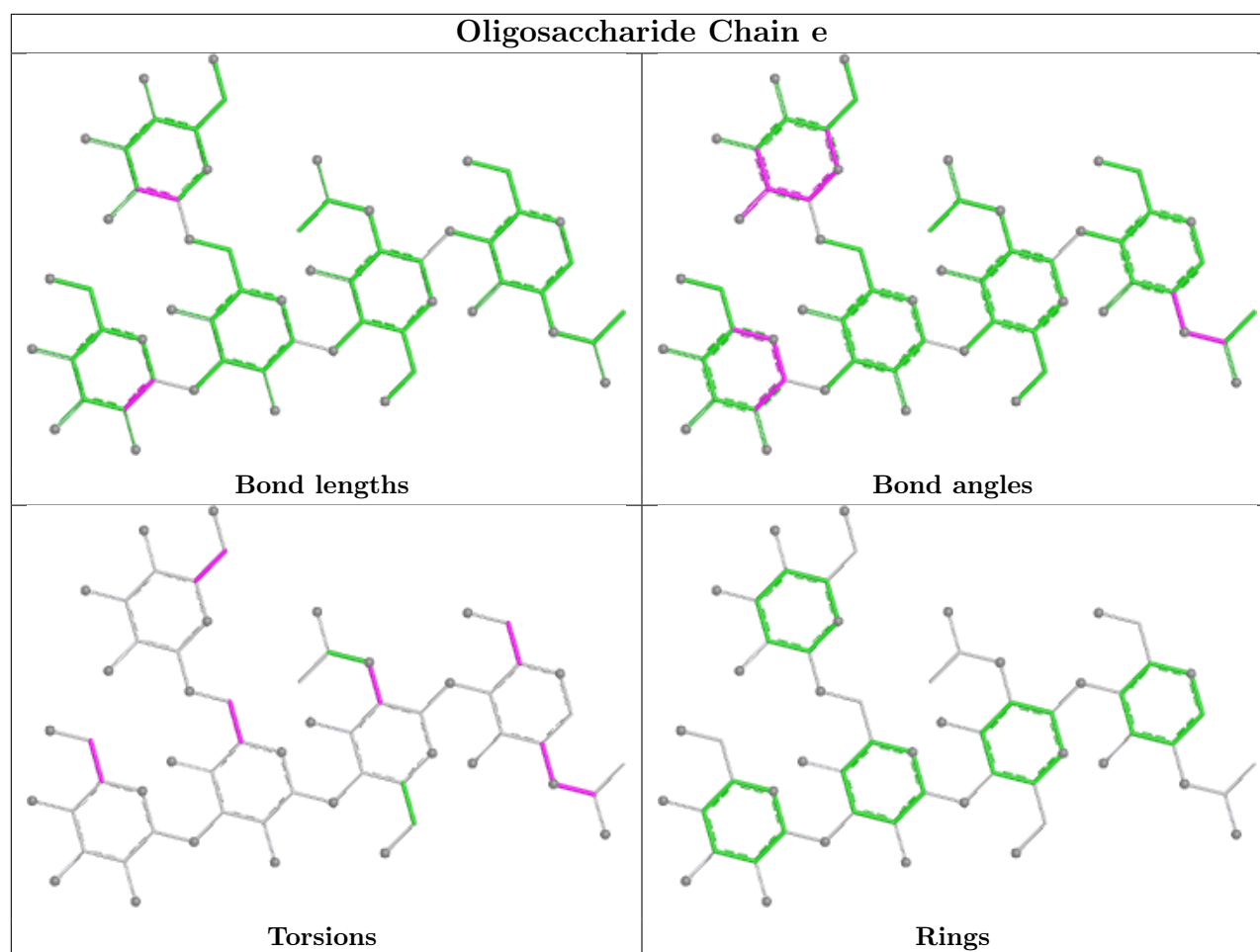
Oligosaccharide Chain W

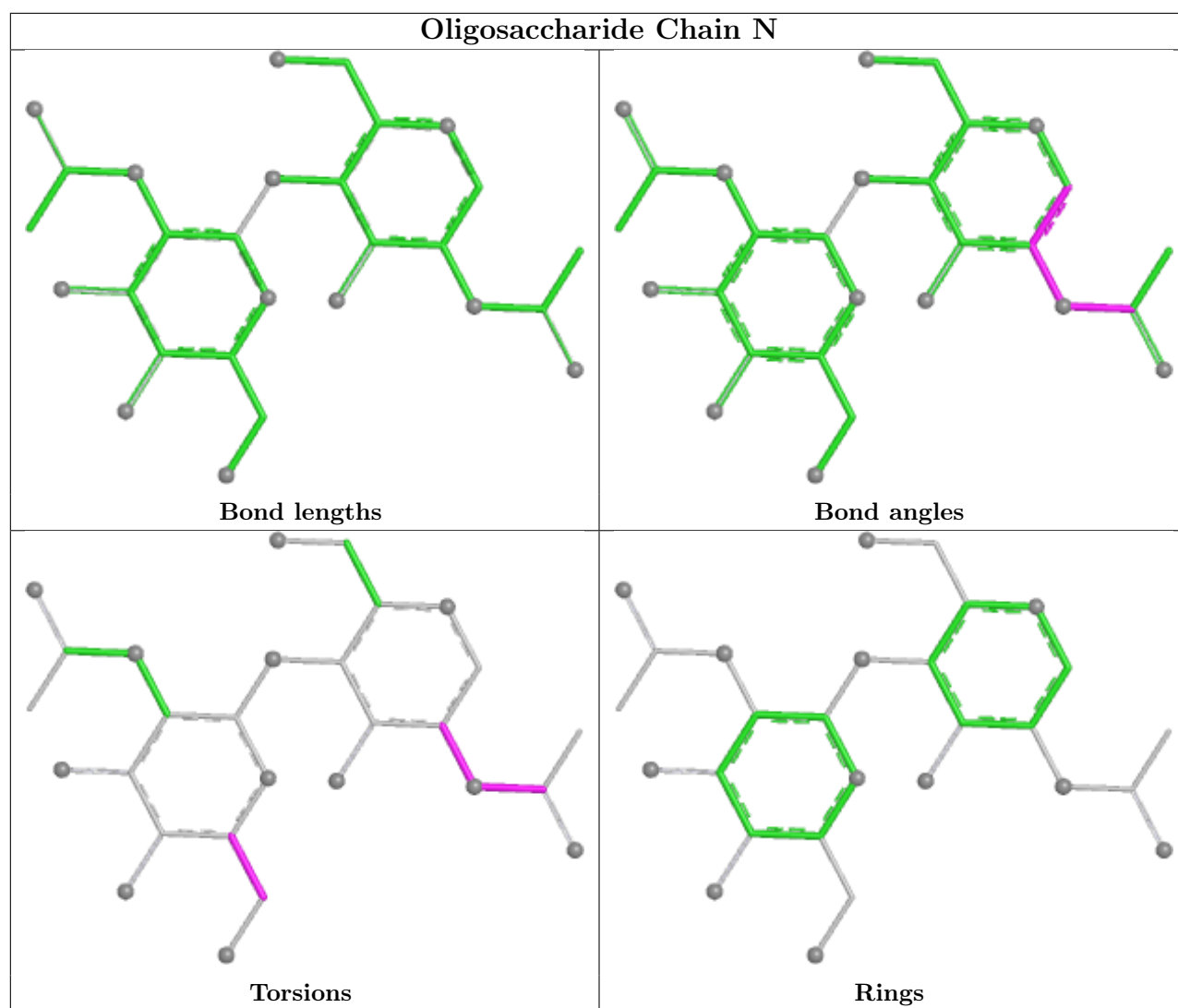


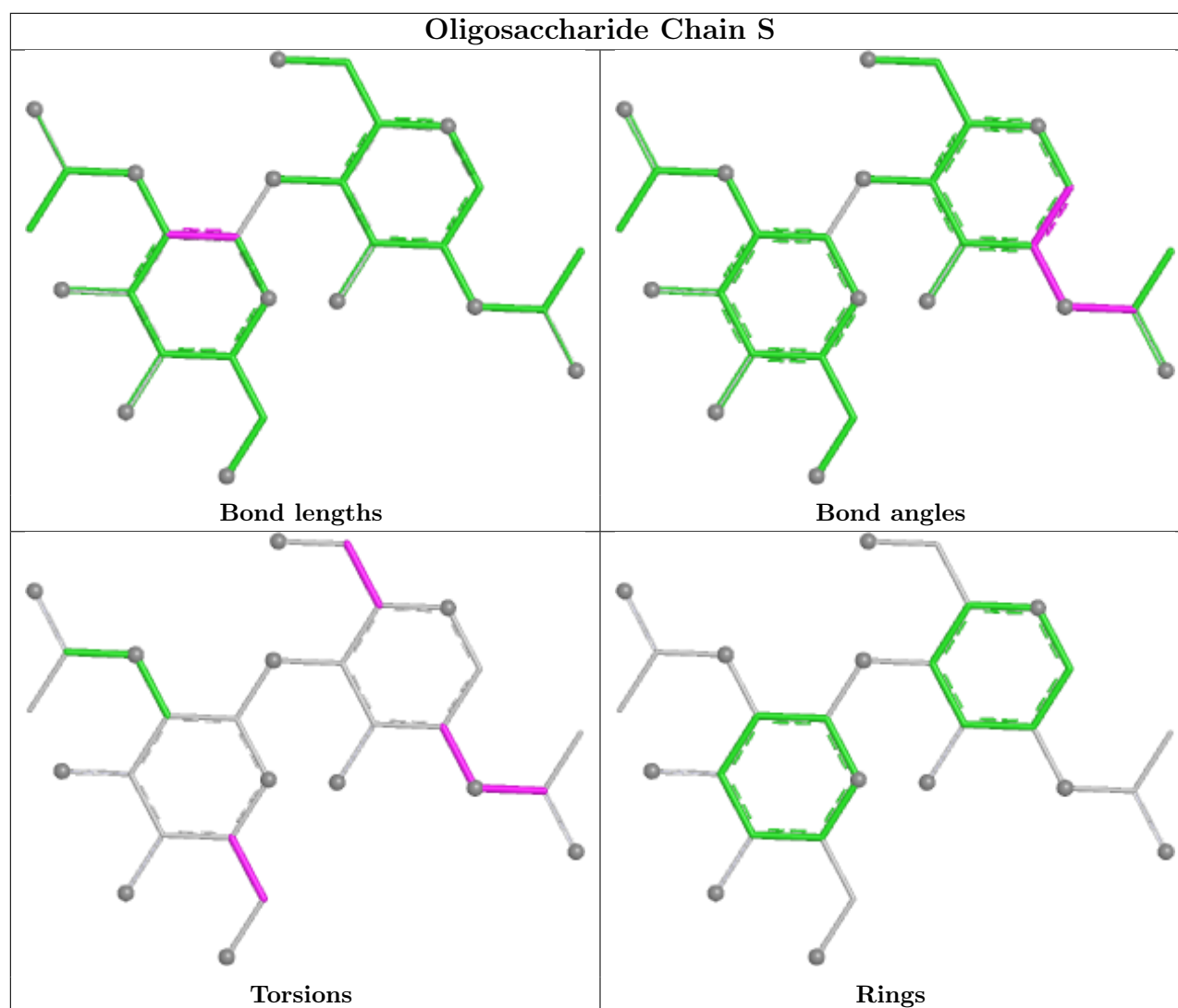


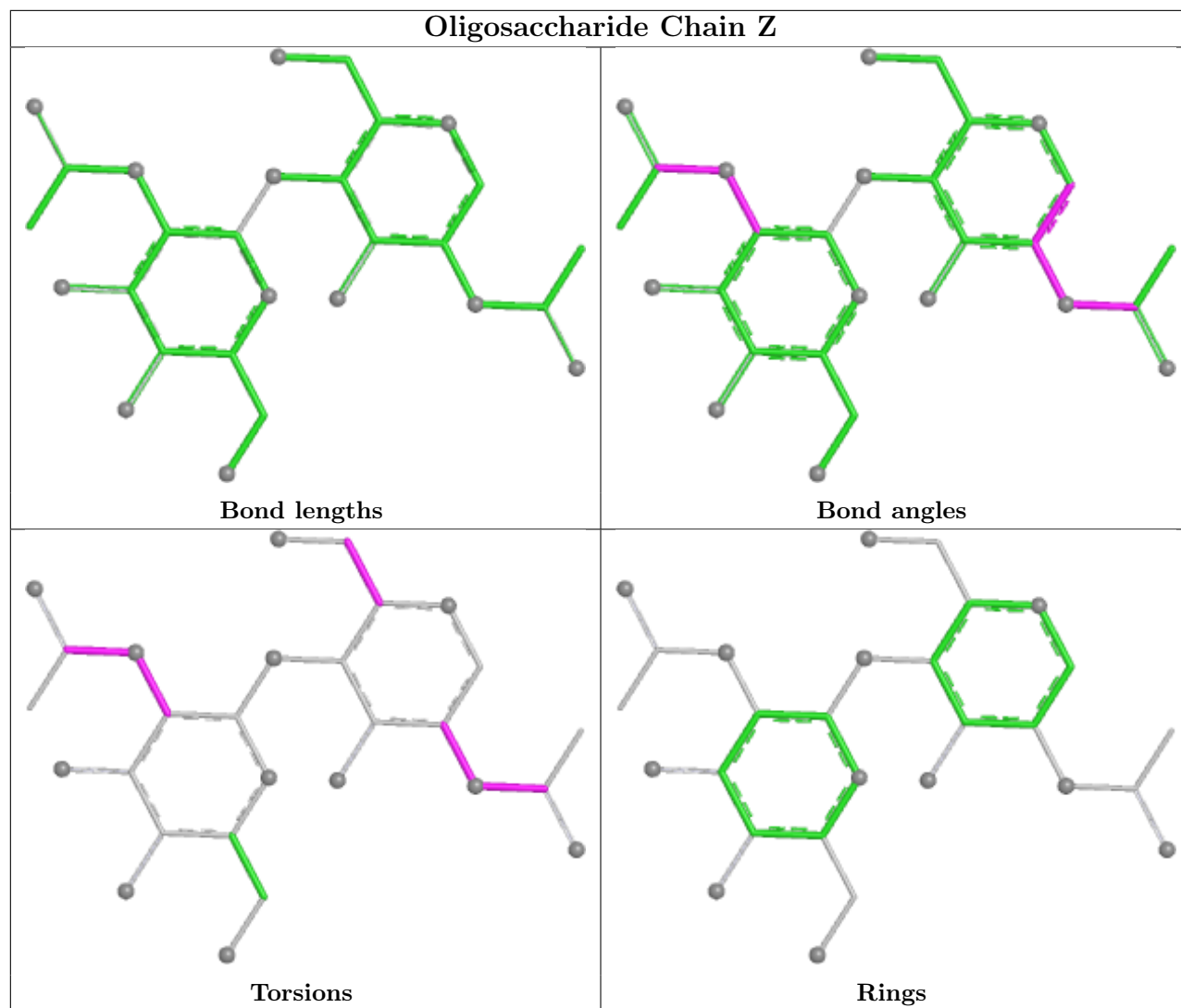


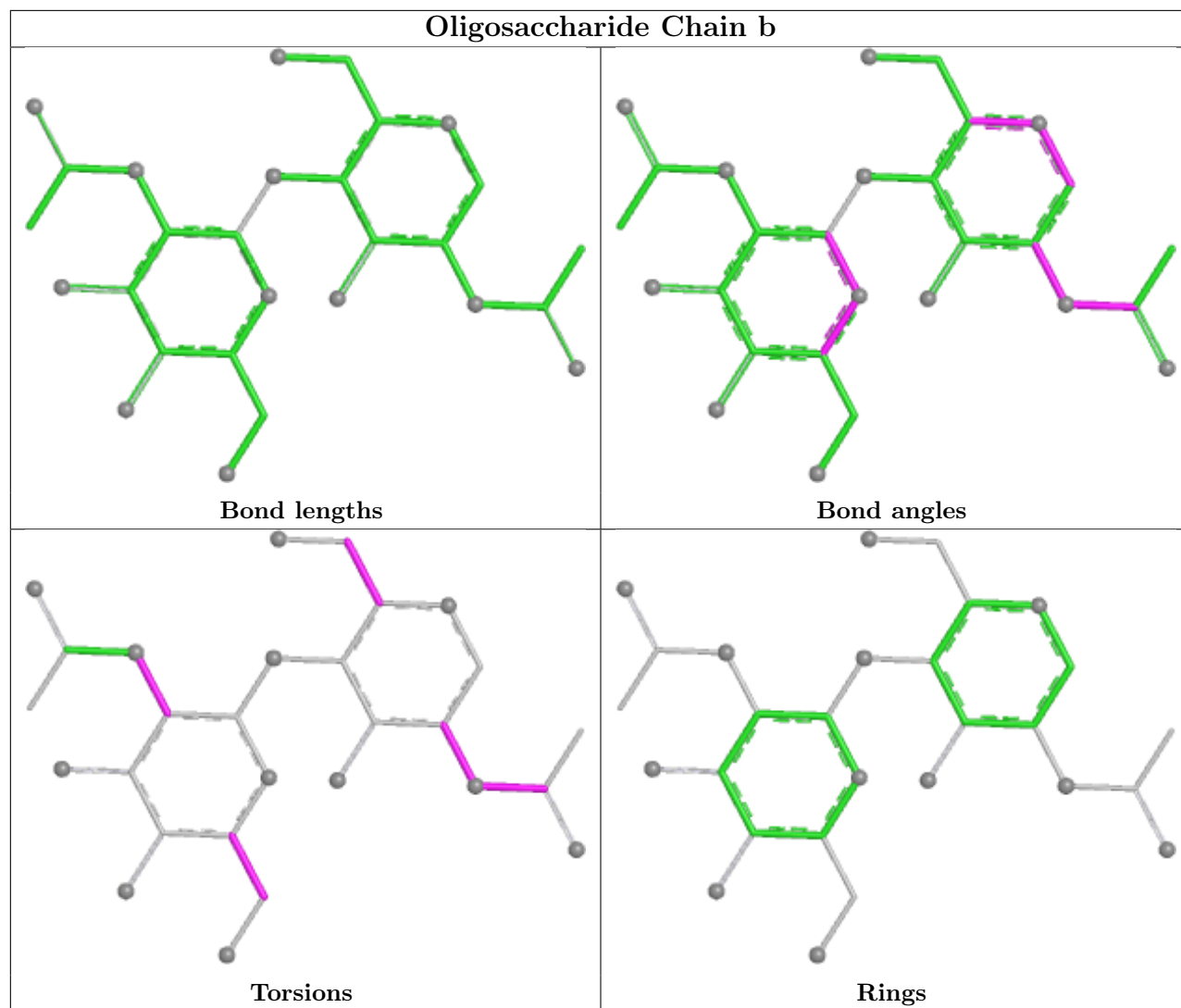


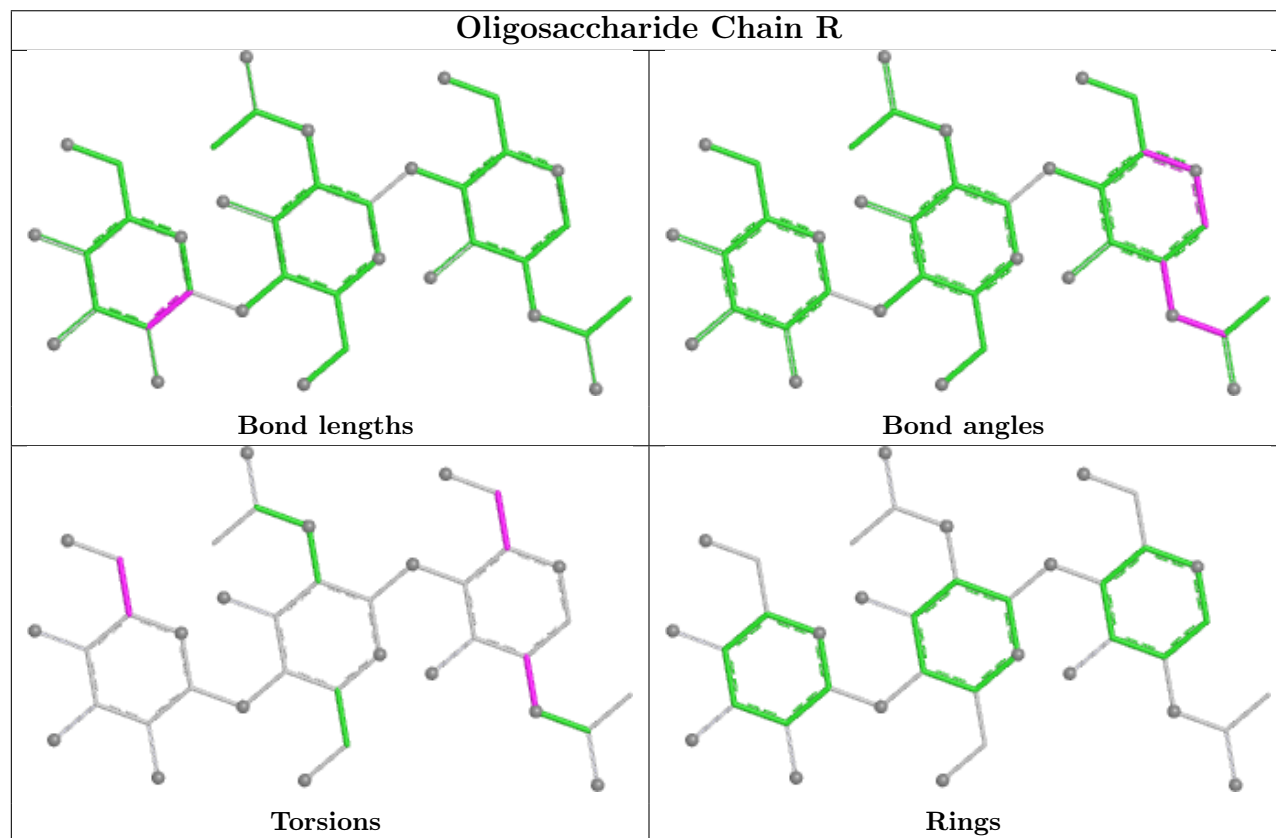
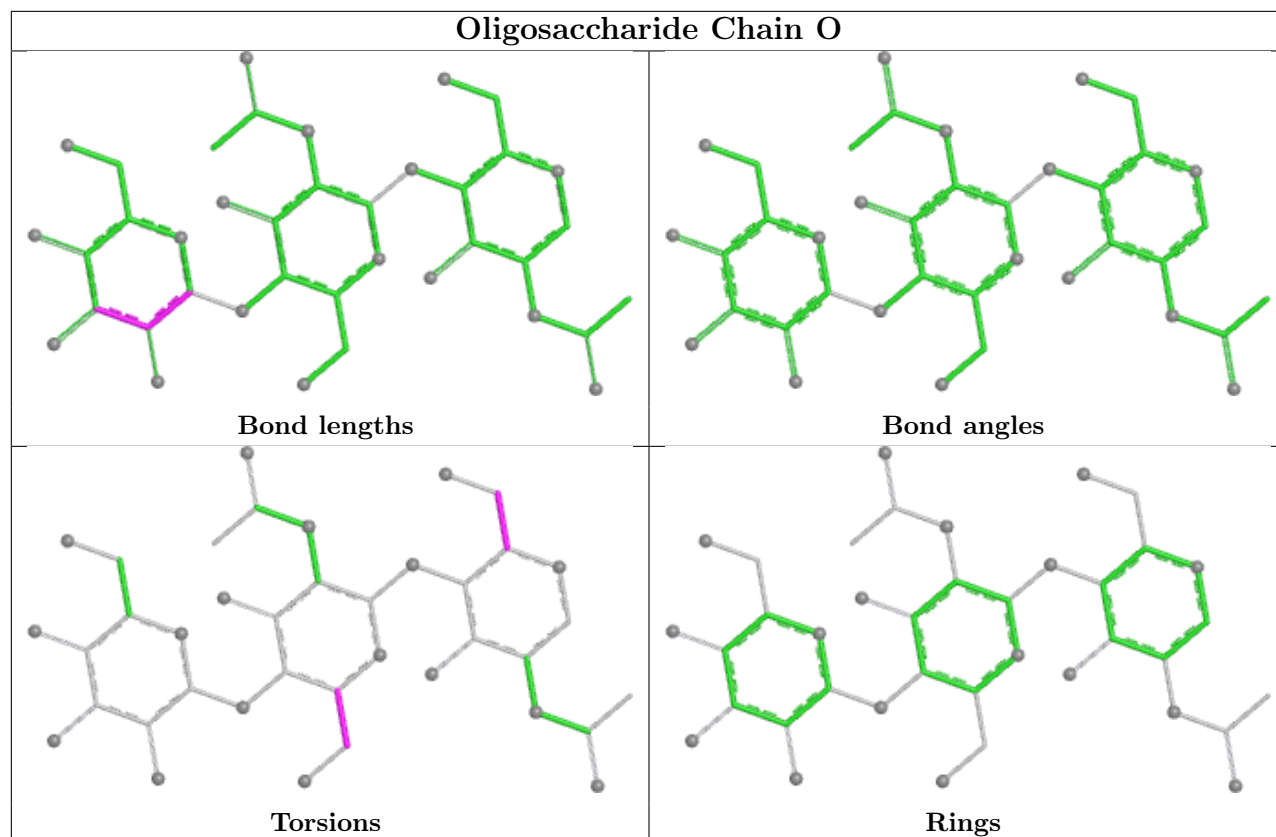


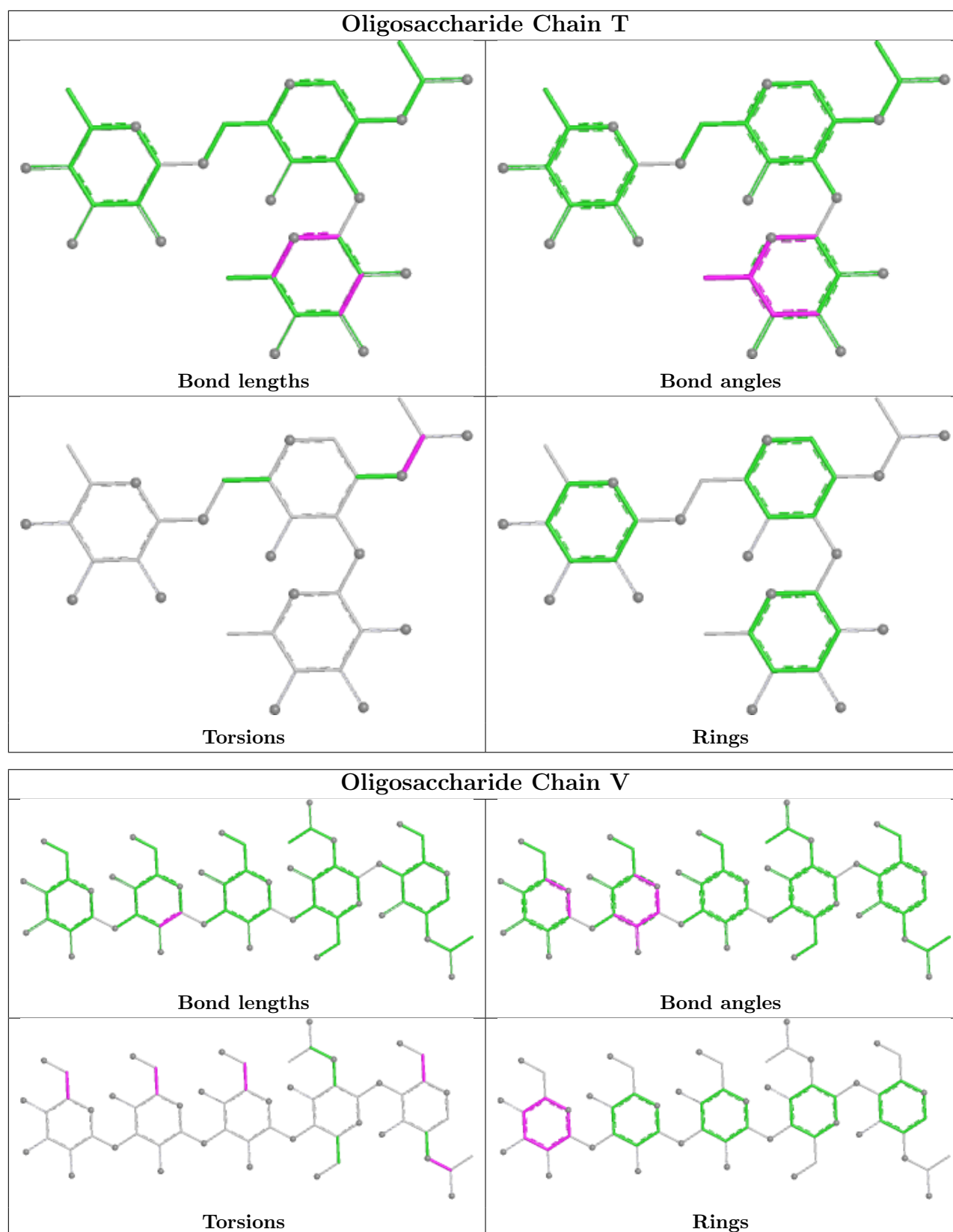


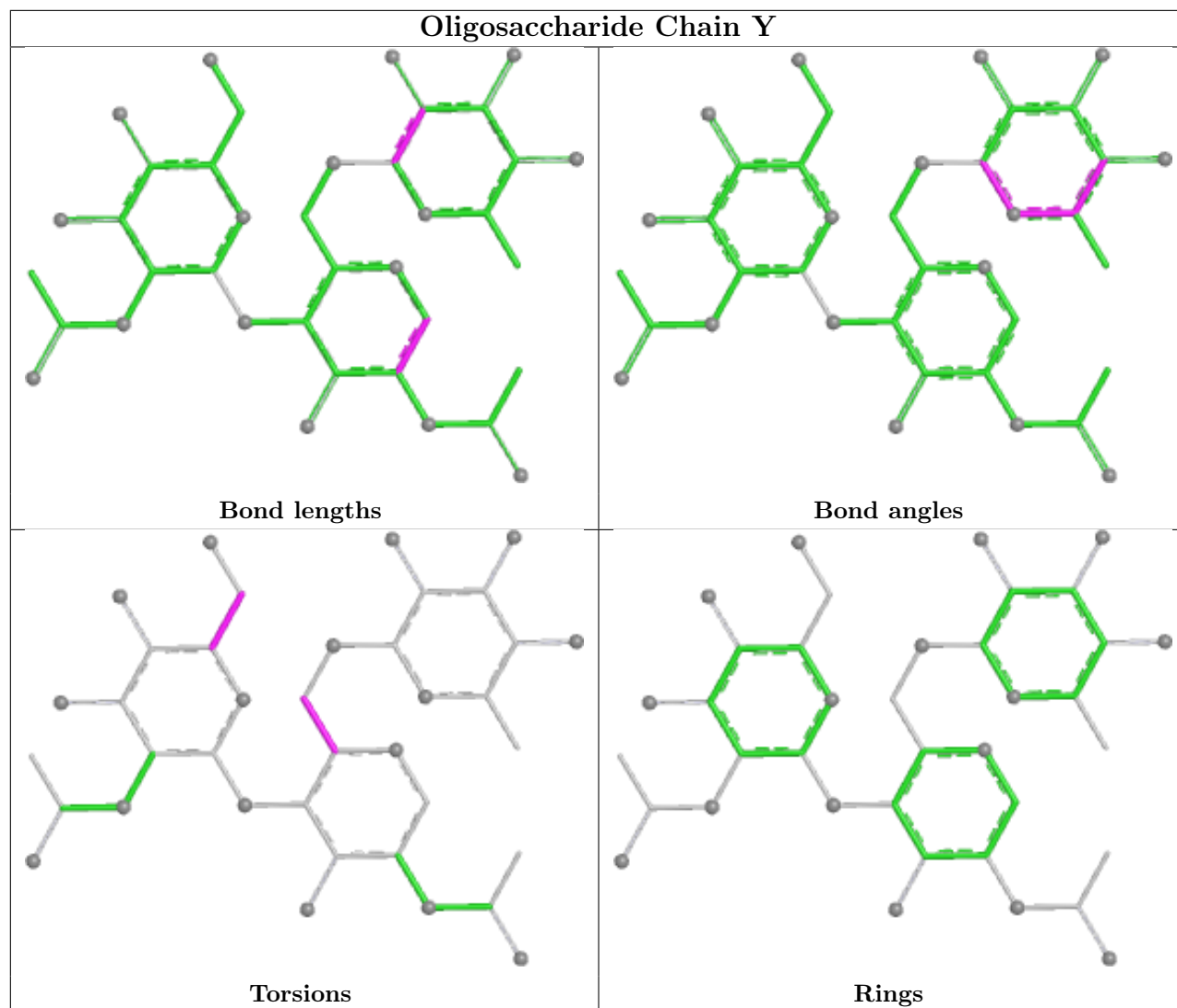


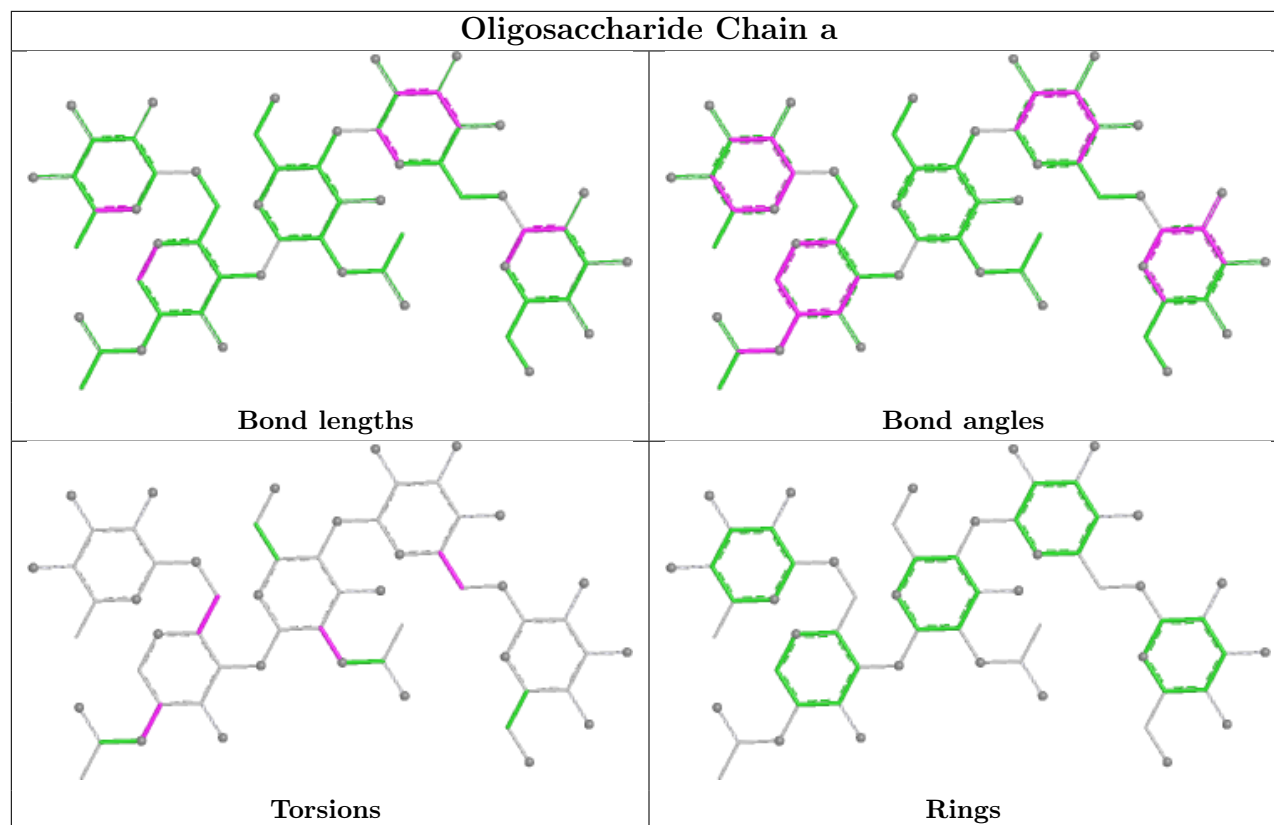


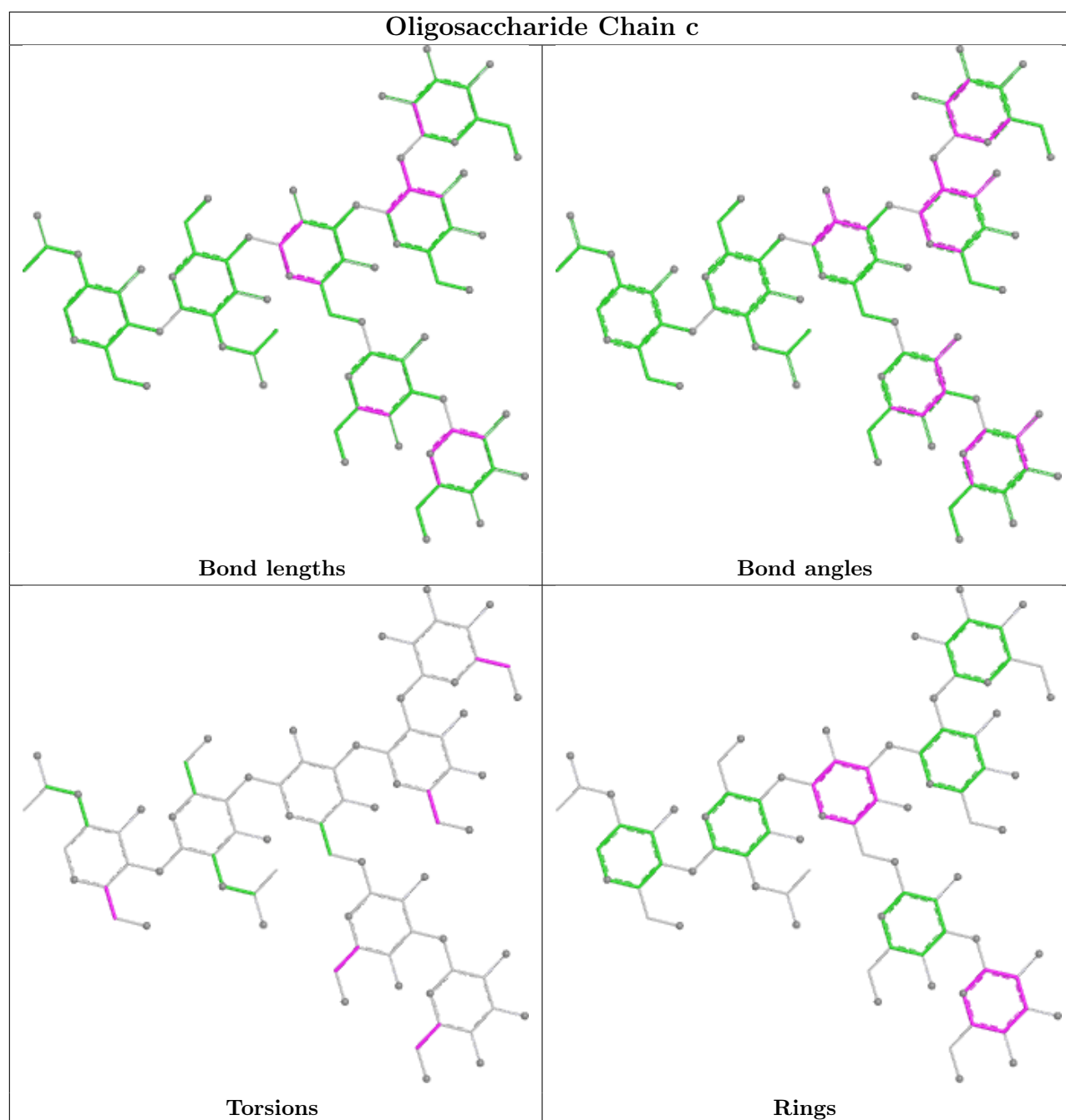


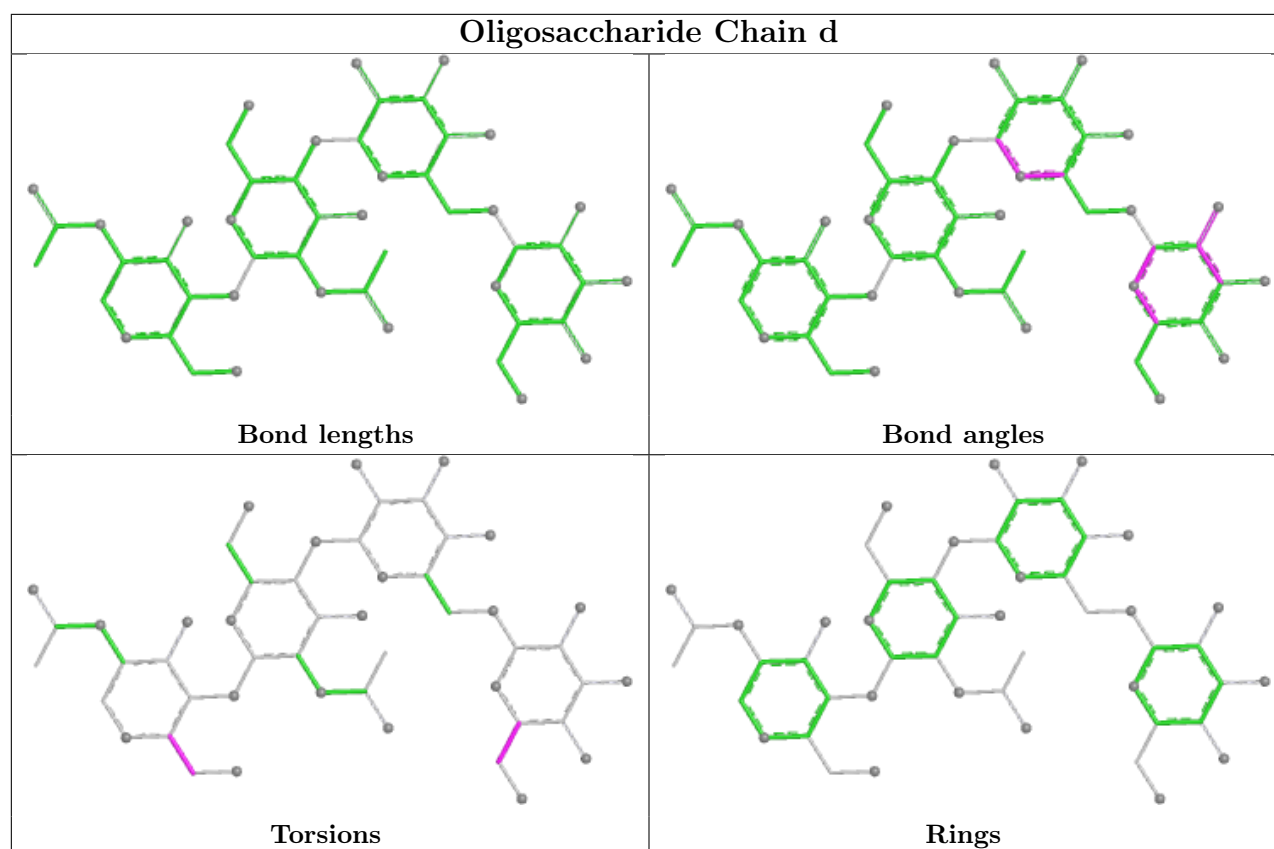












5.6 Ligand geometry [i](#)

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	B	201	2	14,14,15	0.44	0	17,19,21	0.44	0
15	NAG	H	201	2	14,14,15	0.84	2 (14%)	17,19,21	0.45	0
15	NAG	G	419	1	14,14,15	1.00	1 (7%)	17,19,21	3.52	5 (29%)
15	NAG	C	417	1	14,14,15	0.30	0	17,19,21	0.93	1 (5%)
15	NAG	A	525	1	14,14,15	0.43	0	17,19,21	0.57	0
15	NAG	F	201	2	14,14,15	0.67	1 (7%)	17,19,21	1.18	2 (11%)
16	CAC	B	202	-	2,4,4	2.74	2 (100%)	4,6,6	1.70	1 (25%)
15	NAG	D	201	2	14,14,15	0.86	1 (7%)	17,19,21	1.27	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	B	201	2	-	2/6/23/26	0/1/1/1
15	NAG	H	201	2	-	2/6/23/26	0/1/1/1
15	NAG	G	419	1	-	5/6/23/26	0/1/1/1
15	NAG	C	417	1	-	2/6/23/26	0/1/1/1
15	NAG	A	525	1	-	2/6/23/26	0/1/1/1
15	NAG	F	201	2	-	0/6/23/26	0/1/1/1
15	NAG	D	201	2	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	419	NAG	C1-C2	-3.02	1.48	1.52
15	D	201	NAG	O5-C1	2.92	1.48	1.43
16	B	202	CAC	AS-C1	2.79	1.96	1.90
16	B	202	CAC	AS-C2	2.69	1.96	1.90
15	H	201	NAG	C1-C2	2.20	1.55	1.52
15	H	201	NAG	O5-C1	2.10	1.47	1.43
15	F	201	NAG	O5-C1	-2.05	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	G	419	NAG	C2-N2-C7	12.36	139.46	122.90
15	D	201	NAG	C1-O5-C5	4.91	118.76	112.19
15	G	419	NAG	C1-O5-C5	4.57	118.31	112.19
15	C	417	NAG	C1-O5-C5	3.34	116.66	112.19
15	G	419	NAG	C4-C3-C2	-3.32	106.15	111.02
15	F	201	NAG	C3-C4-C5	3.17	115.97	110.23
15	F	201	NAG	C1-O5-C5	2.79	115.92	112.19
15	G	419	NAG	C3-C4-C5	2.57	114.88	110.23
16	B	202	CAC	O2-AS-C1	2.31	111.43	105.84
15	G	419	NAG	C8-C7-N2	-2.26	112.37	116.12

There are no chirality outliers.

All (15) 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
15	G	419	NAG	O5-C5-C6-O6
15	G	419	NAG	C8-C7-N2-C2
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	H	201	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	B	201	NAG	O5-C5-C6-O6
15	A	525	NAG	O5-C5-C6-O6
15	D	201	NAG	O5-C5-C6-O6
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%)	-0.50	3 (0%) 81 64	44, 71, 122, 167	0
1	C	319/329 (96%)	-0.48	3 (0%) 81 64	58, 82, 123, 170	0
1	E	319/329 (96%)	-0.35	0 100 100	55, 89, 134, 187	0
1	G	319/329 (96%)	-0.27	1 (0%) 90 81	59, 100, 171, 247	0
2	B	174/174 (100%)	-0.49	2 (1%) 78 60	43, 68, 114, 170	0
2	D	174/174 (100%)	-0.43	3 (1%) 69 48	51, 79, 116, 193	0
2	F	174/174 (100%)	-0.42	2 (1%) 78 60	44, 86, 135, 187	0
2	H	174/174 (100%)	0.23	9 (5%) 33 19	58, 169, 226, 264	0
All	All	1972/2012 (98%)	-0.36	23 (1%) 76 57	43, 86, 172, 264	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	2	ILE	5.4
1	A	10	MET	3.5
1	C	10	MET	3.3
2	H	128	GLU	3.2
2	D	2	ILE	3.2
2	F	2	ILE	3.0
1	G	104	ASP	3.0
2	B	57	LYS	2.7
2	B	173	ILE	2.6
2	D	11	GLU	2.6
2	H	113	SER	2.5
1	C	199	SER	2.4
1	A	199	SER	2.4
2	H	132	ASP	2.4
2	D	173	ILE	2.4
2	F	173	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	173	ILE	2.3
2	H	134	GLY	2.2
1	C	104	ASP	2.2
2	H	3	PHE	2.1
2	H	1	GLY	2.1
2	H	174	LYS	2.1
1	A	321	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

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
8	BMA	R	3	11/12	0.16	0.12	188,200,207,209	0
6	MAN	X	5	11/12	0.21	0.15	156,193,203,204	0
11	NAG	Y	1	14/15	0.23	0.13	157,183,203,210	0
4	MAN	J	4	11/12	0.24	0.11	171,188,194,199	0
6	MAN	X	4	11/12	0.31	0.12	196,207,218,227	0
5	MAN	L	6	11/12	0.32	0.10	165,187,191,192	0
5	MAN	W	6	11/12	0.35	0.11	171,184,190,194	0
6	MAN	M	5	11/12	0.36	0.11	177,187,192,196	0
9	FUC	T	3	10/11	0.37	0.13	160,188,194,198	0
9	NAG	T	1	14/15	0.37	0.13	144,164,177,187	0
3	NAG	I	2	14/15	0.39	0.12	167,189,206,208	0
6	MAN	U	4	11/12	0.39	0.10	171,194,200,204	0
5	MAN	Q	4	11/12	0.40	0.09	182,195,198,202	0
4	BMA	K	3	11/12	0.41	0.10	167,194,204,206	0
4	BMA	J	3	11/12	0.43	0.11	140,163,175,187	0
6	BMA	U	3	11/12	0.45	0.10	180,190,198,199	0
8	BMA	O	3	11/12	0.45	0.10	154,196,201,203	0
8	NAG	O	2	14/15	0.46	0.14	167,184,195,197	0
4	MAN	P	4	11/12	0.46	0.14	163,183,189,193	0
3	BMA	I	3	11/12	0.47	0.12	171,197,207,207	0
6	MAN	U	5	11/12	0.47	0.10	132,178,193,195	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BMA	M	3	11/12	0.48	0.09	194,207,215,215	0
6	MAN	M	4	11/12	0.51	0.08	142,185,198,201	0
5	MAN	Q	5	11/12	0.52	0.11	146,188,198,202	0
6	BMA	X	3	11/12	0.53	0.11	195,200,208,212	0
8	NAG	O	1	14/15	0.56	0.14	122,142,163,179	0
8	NAG	R	2	14/15	0.56	0.12	142,176,193,201	0
5	MAN	W	5	11/12	0.56	0.09	155,176,188,191	0
4	BMA	P	3	11/12	0.57	0.14	133,166,175,176	0
3	FUC	I	5	10/11	0.58	0.11	149,165,179,186	0
4	NAG	P	2	14/15	0.58	0.15	133,157,163,172	0
5	MAN	Q	6	11/12	0.59	0.11	173,182,193,203	0
11	NAG	Y	2	14/15	0.59	0.11	158,178,195,199	0
7	NAG	N	2	14/15	0.61	0.13	140,174,185,188	0
3	FUL	I	4	10/11	0.61	0.15	148,166,173,180	0
9	FUL	T	2	10/11	0.62	0.12	144,164,171,176	0
6	NAG	M	2	14/15	0.62	0.12	130,155,178,199	0
5	MAN	L	5	11/12	0.63	0.08	177,180,196,202	0
7	NAG	S	2	14/15	0.63	0.10	128,183,200,214	0
10	MAN	V	5	11/12	0.65	0.16	177,196,209,209	0
10	MAN	V	4	11/12	0.66	0.10	181,202,211,214	0
6	NAG	U	2	14/15	0.69	0.11	117,173,184,191	0
11	FUC	Y	3	10/11	0.69	0.13	156,173,176,180	0
7	NAG	Z	2	14/15	0.71	0.10	137,165,181,185	0
4	NAG	K	2	14/15	0.72	0.09	100,153,166,184	0
5	MAN	L	4	11/12	0.72	0.08	148,170,174,177	0
4	MAN	K	4	11/12	0.73	0.09	154,175,188,191	0
10	BMA	V	3	11/12	0.74	0.07	130,159,174,194	0
5	MAN	W	4	11/12	0.74	0.08	155,182,188,189	0
7	NAG	S	1	14/15	0.74	0.10	114,125,169,177	0
6	NAG	e	1	14/15	-	-	121,157,191,205	0
6	NAG	e	2	14/15	-	-	145,202,207,226	0
6	BMA	e	3	11/12	-	-	206,224,233,235	0
6	MAN	e	4	11/12	-	-	183,211,217,218	0
6	MAN	e	5	11/12	-	-	165,199,203,204	0
5	MAN	Q	3	11/12	0.75	0.08	140,152,179,186	0
4	NAG	J	1	14/15	0.75	0.13	68,101,115,124	0
6	NAG	U	1	14/15	0.77	0.12	111,125,148,165	0
7	NAG	Z	1	14/15	0.78	0.13	129,143,164,180	0
7	NAG	N	1	14/15	0.80	0.14	106,134,165,185	0
4	NAG	P	1	14/15	0.80	0.15	102,135,153,158	0
7	NAG	b	1	14/15	-	-	132,156,171,180	0
7	NAG	b	2	14/15	-	-	150,168,176,177	0

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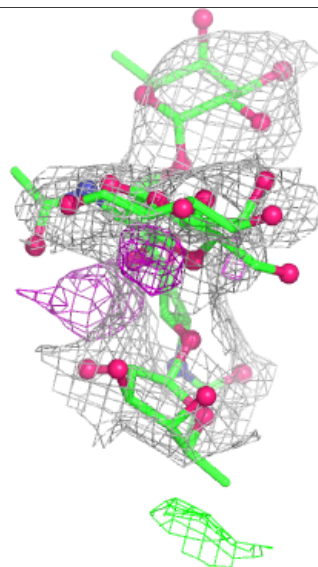
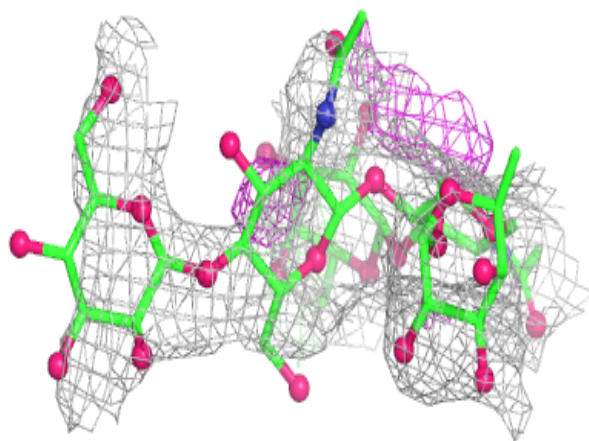
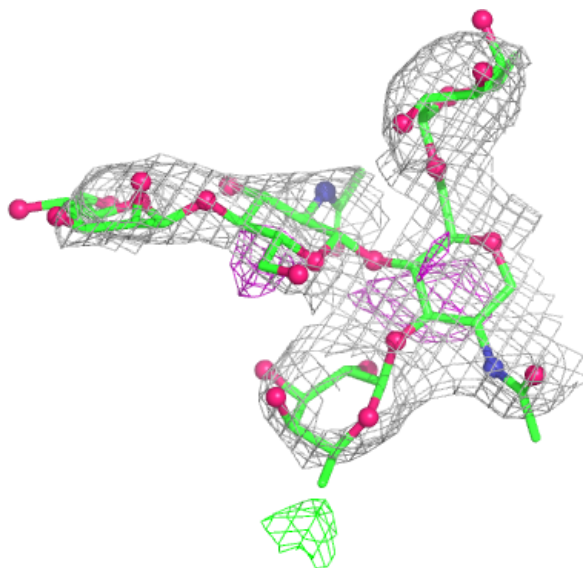
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	R	1	14/15	0.81	0.12	110,128,147,153	0
6	NAG	X	2	14/15	0.83	0.11	117,163,176,189	0
4	NAG	J	2	14/15	0.84	0.12	98,139,149,161	0
5	MAN	W	3	11/12	0.85	0.08	120,138,171,175	0
3	NAG	I	1	14/15	0.85	0.09	132,158,177,179	0
10	NAG	V	1	14/15	0.85	0.12	112,144,154,161	0
10	NAG	V	2	14/15	0.86	0.09	128,151,158,159	0
6	NAG	X	1	14/15	0.87	0.12	89,108,122,140	0
5	MAN	L	3	11/12	0.87	0.06	145,153,169,176	0
6	NAG	M	1	14/15	0.88	0.10	74,103,116,137	0
4	NAG	K	1	14/15	0.89	0.10	108,124,135,148	0
5	NAG	L	2	14/15	0.89	0.11	118,141,149,159	0
5	NAG	W	1	14/15	0.89	0.12	78,100,128,134	0
5	NAG	L	1	14/15	0.90	0.09	98,110,128,131	0
5	NAG	W	2	14/15	0.92	0.09	103,118,126,139	0
5	NAG	Q	1	14/15	0.93	0.10	93,101,118,123	0
5	NAG	Q	2	14/15	0.93	0.08	71,98,120,139	0
12	NAG	a	1	14/15	-	-	150,172,193,195	0
12	NAG	a	2	14/15	-	-	138,186,200,202	0
12	BMA	a	3	11/12	-	-	191,204,210,213	0
12	MAN	a	4	11/12	-	-	172,191,203,204	0
12	FUC	a	5	10/11	-	-	166,186,194,196	0
13	NAG	c	1	14/15	-	-	99,115,134,136	0
13	NAG	c	2	14/15	-	-	127,140,159,177	0
13	MAN	c	3	11/12	-	-	147,174,182,187	0
13	MAN	c	4	11/12	-	-	173,182,191,194	0
13	MAN	c	5	11/12	-	-	156,182,195,199	0
13	MAN	c	6	11/12	-	-	183,196,204,205	0
13	MAN	c	7	11/12	-	-	133,170,186,188	0
14	NAG	d	1	14/15	-	-	107,131,145,163	0
14	NAG	d	2	14/15	-	-	109,167,190,202	0
14	BMA	d	3	11/12	-	-	210,216,220,221	0
14	MAN	d	4	11/12	-	-	198,204,215,216	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

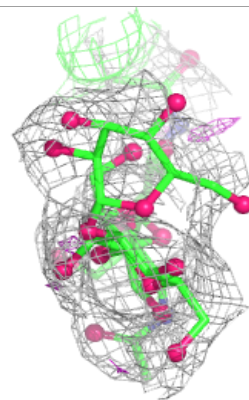
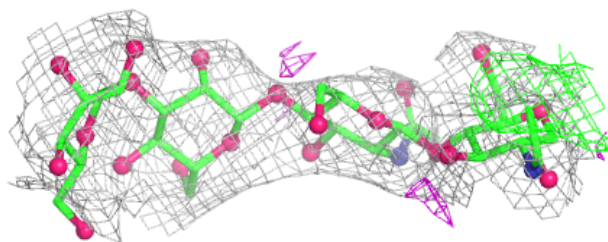
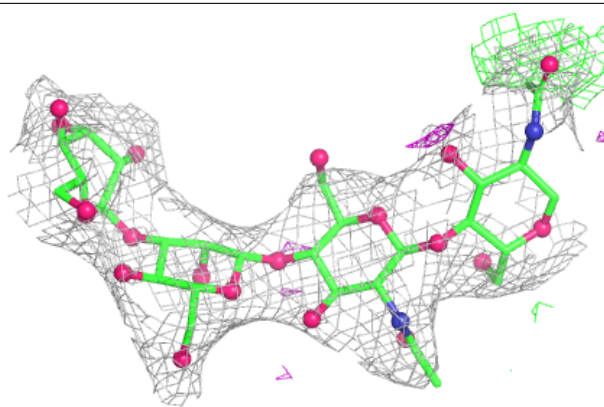
Electron density around Chain I:

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



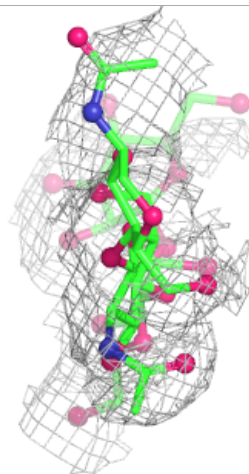
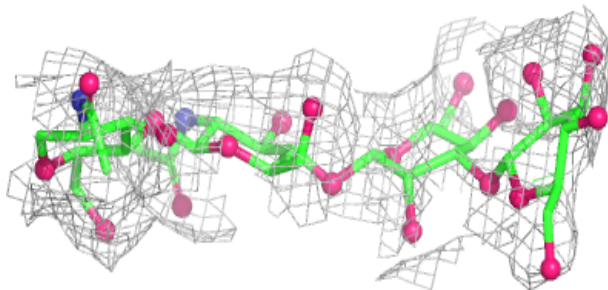
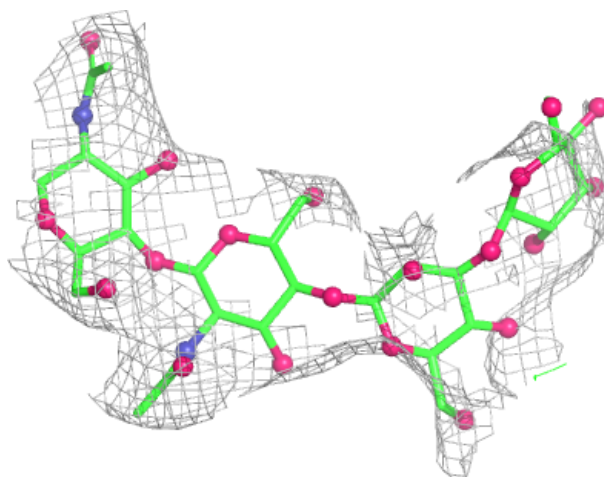
Electron density around Chain J:

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



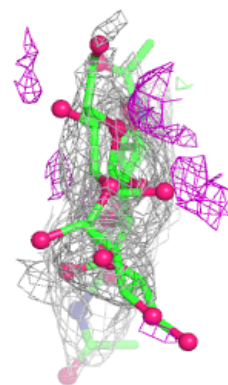
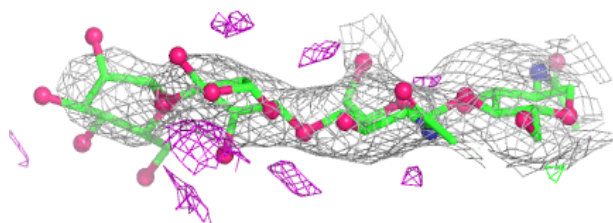
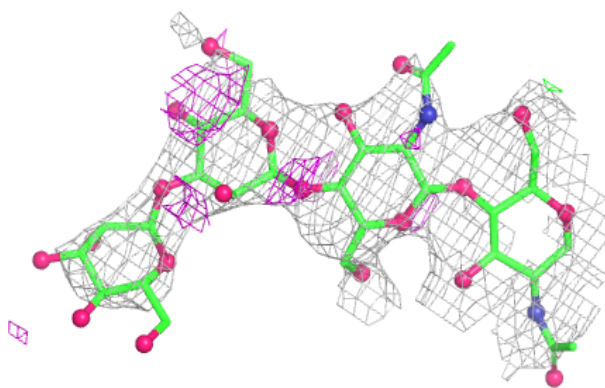
Electron density around Chain K:

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

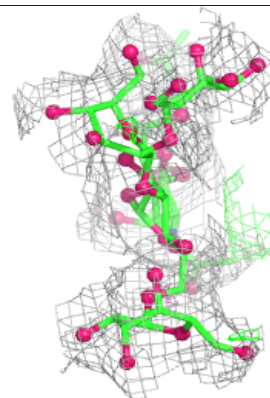
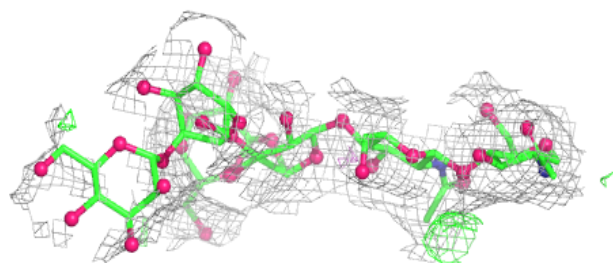
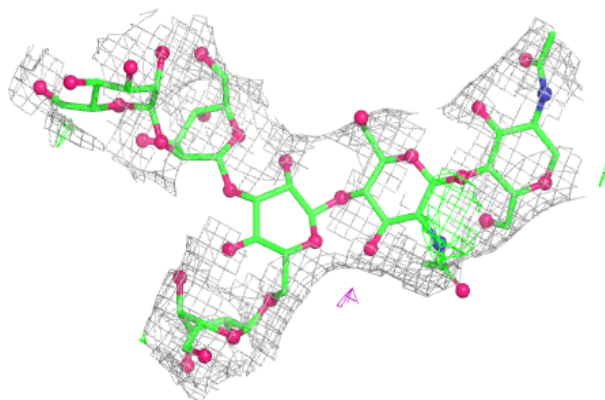


Electron density around Chain P:

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

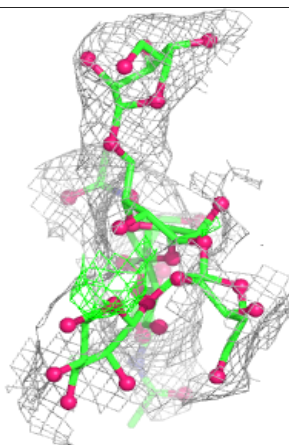
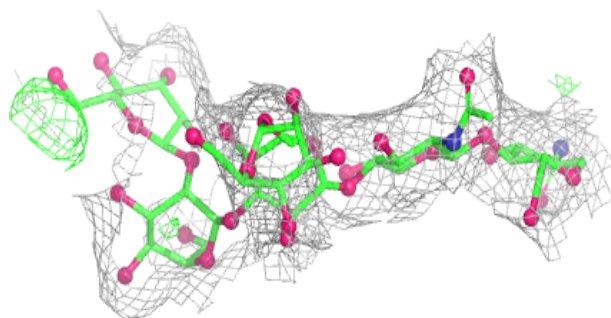
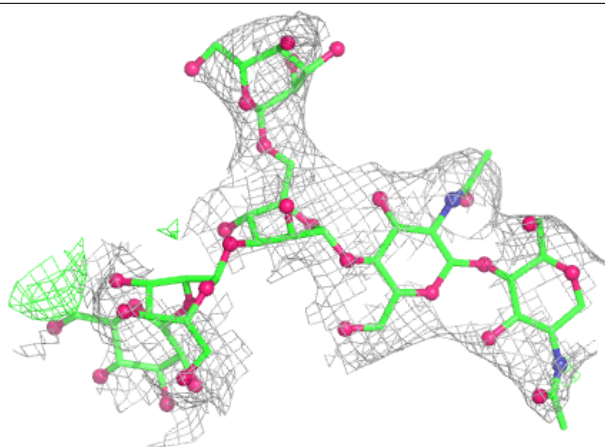
**Electron density around Chain L:**

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

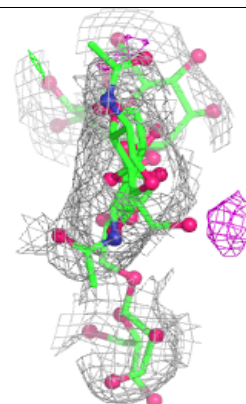
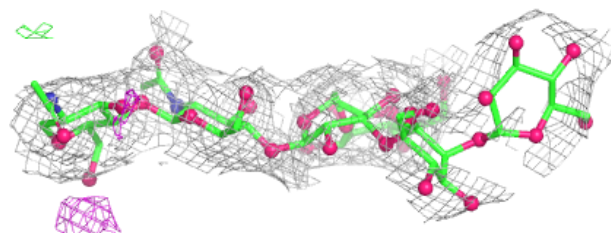
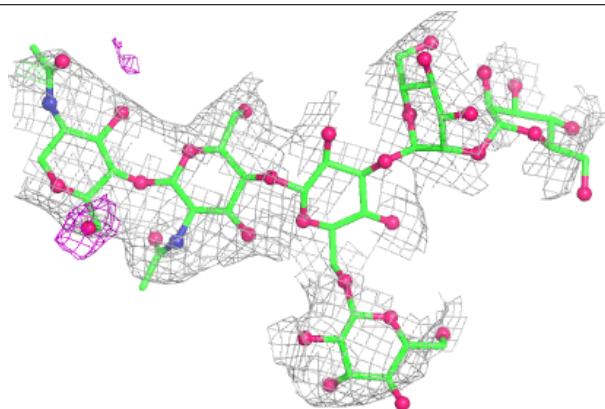


Electron density around Chain Q:

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

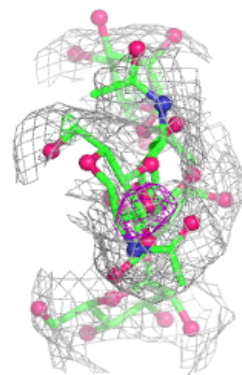
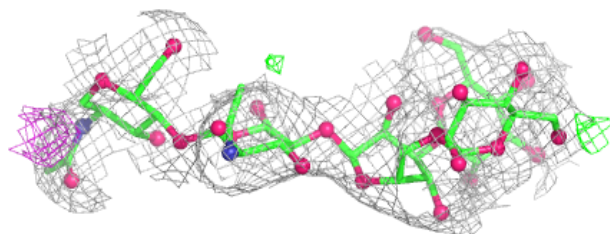
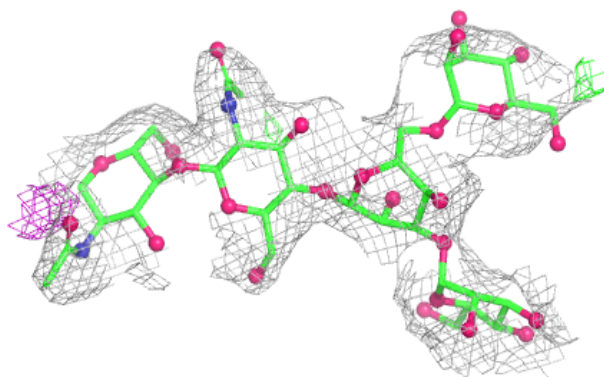
**Electron density around Chain W:**

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



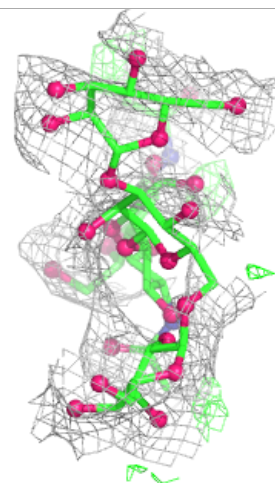
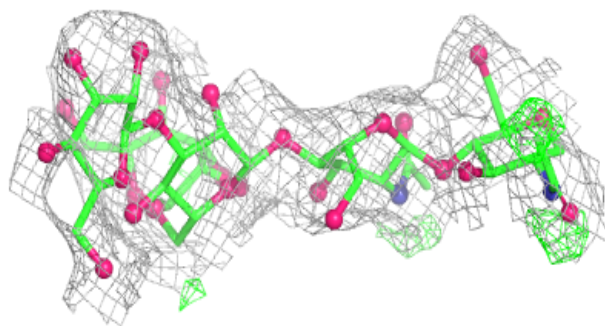
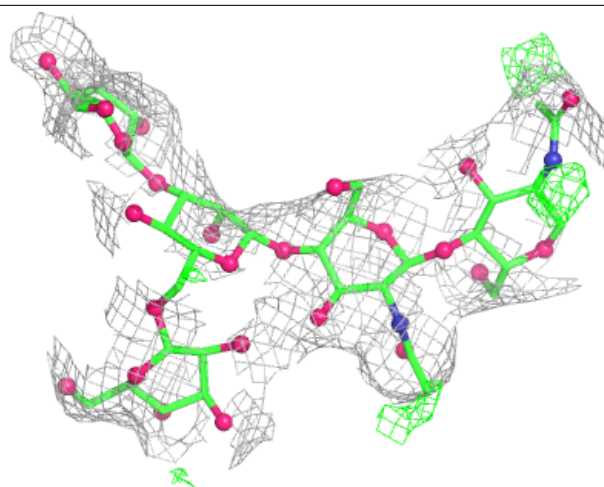
Electron density around Chain M:

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



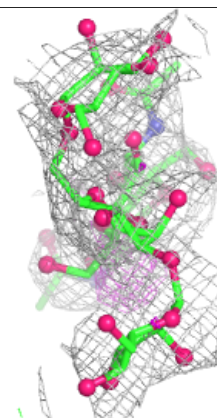
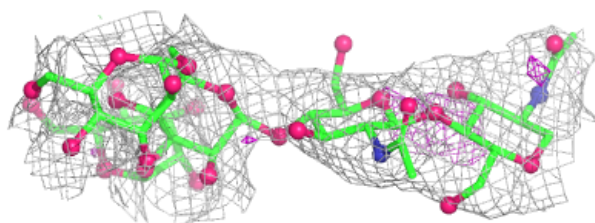
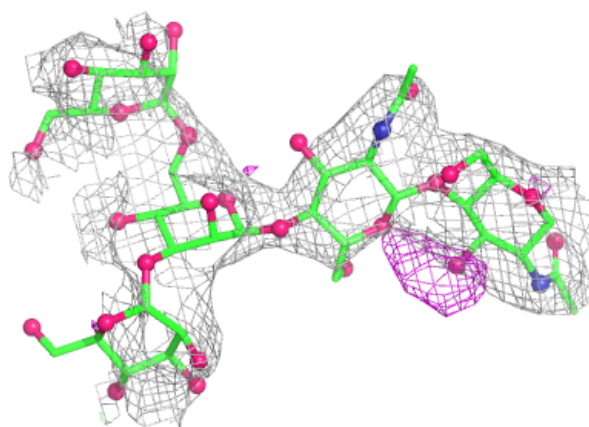
Electron density around Chain U:

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



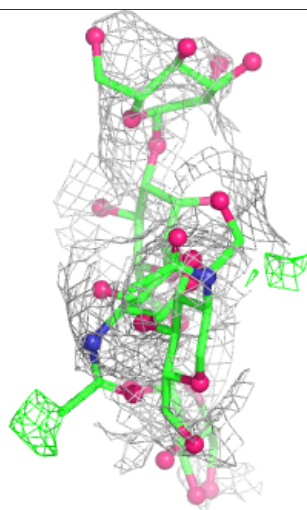
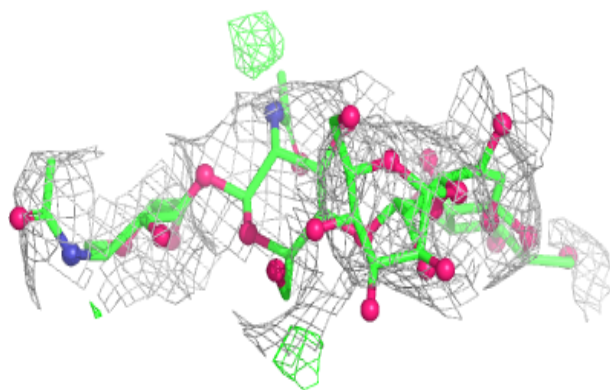
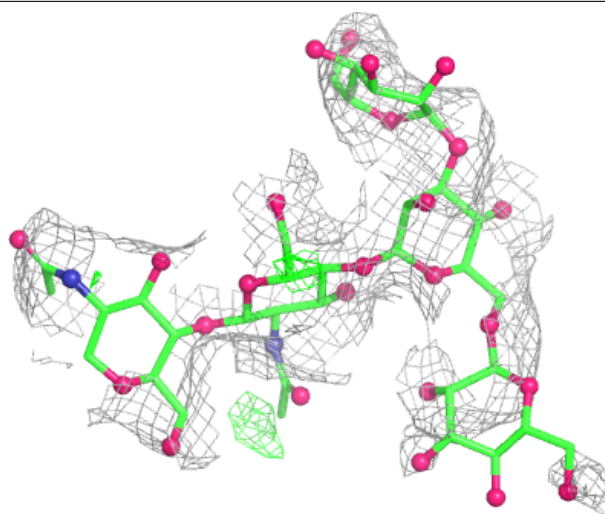
Electron density around Chain X:

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



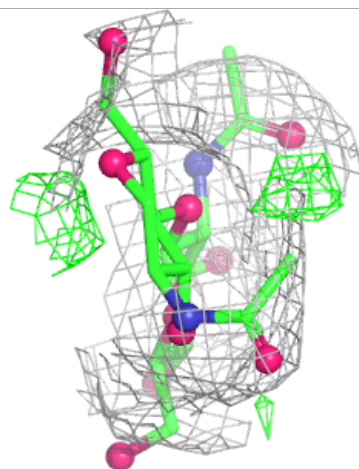
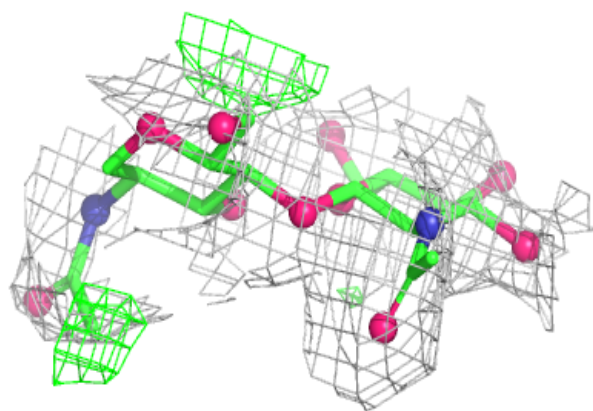
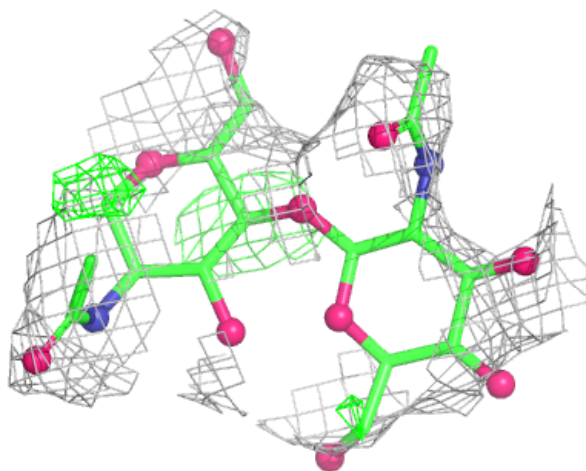
Electron density around Chain e:

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



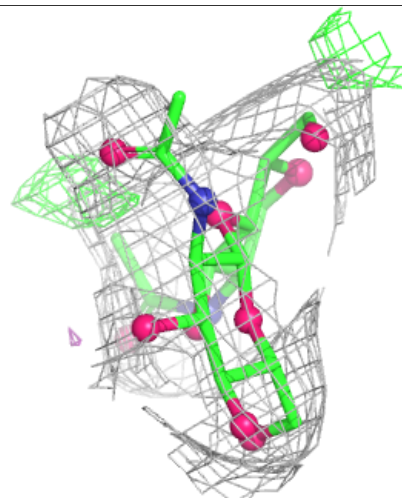
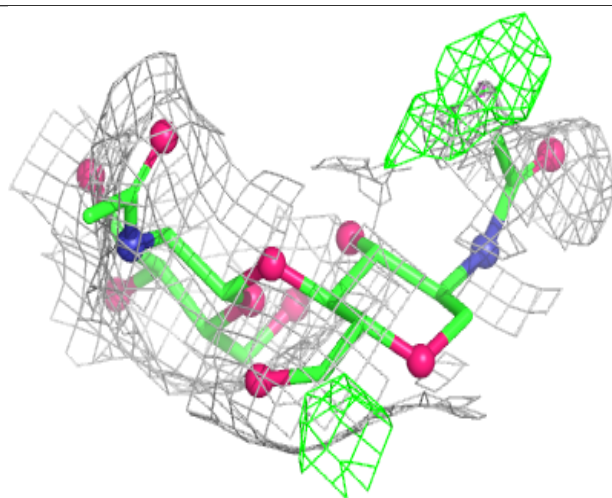
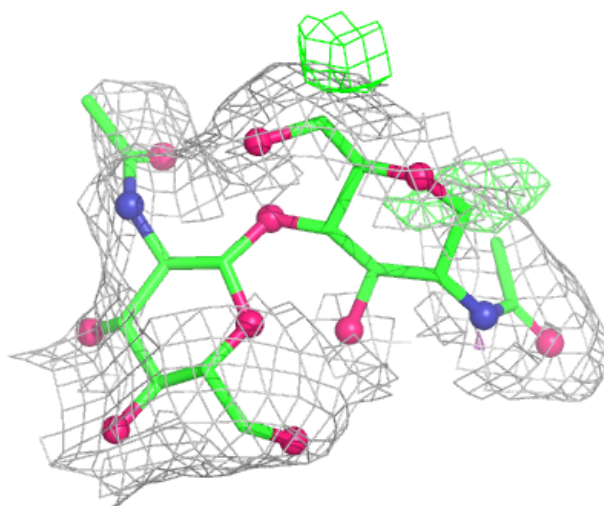
Electron density around Chain N:

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



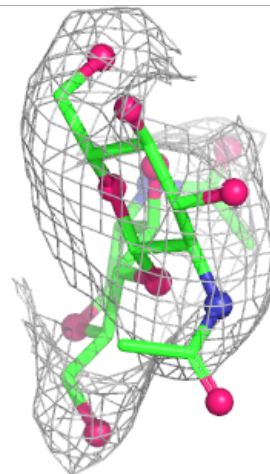
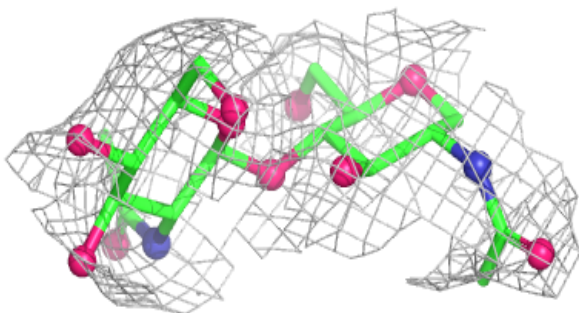
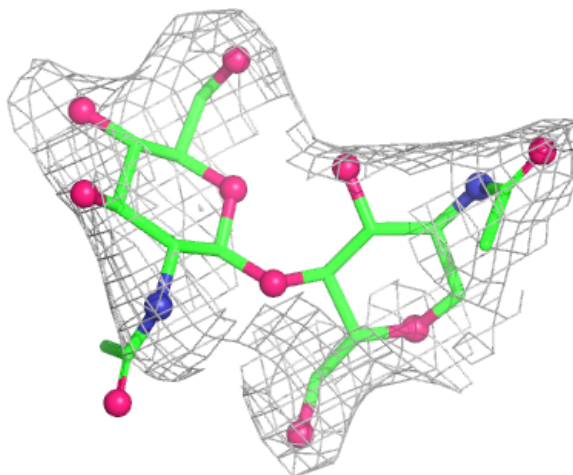
Electron density around Chain S:

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



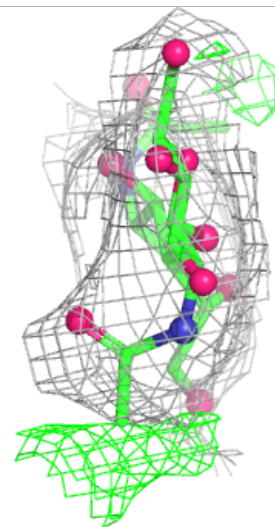
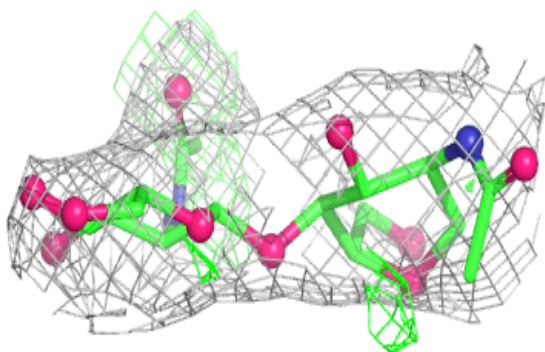
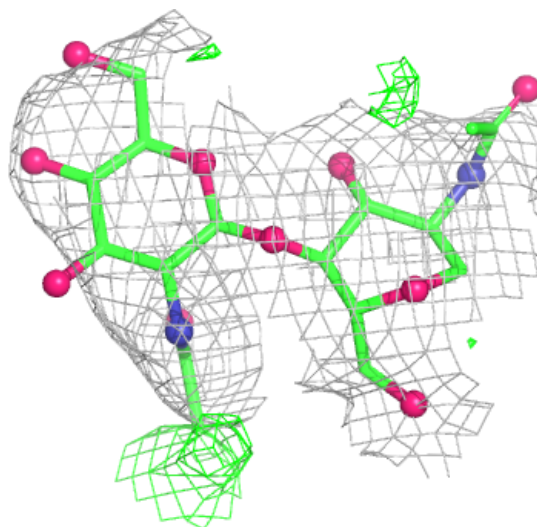
Electron density around Chain Z:

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



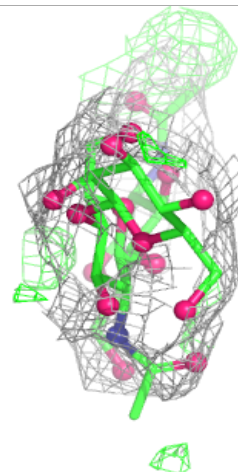
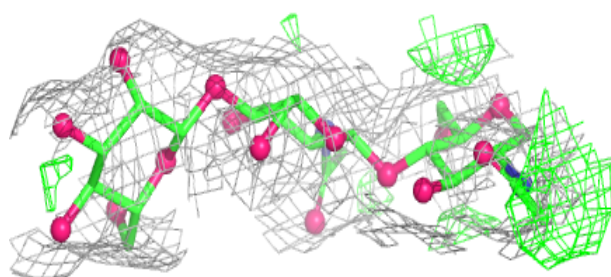
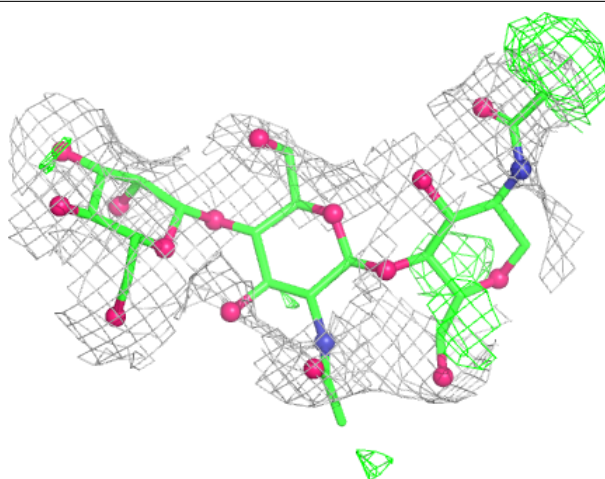
Electron density around Chain b:

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



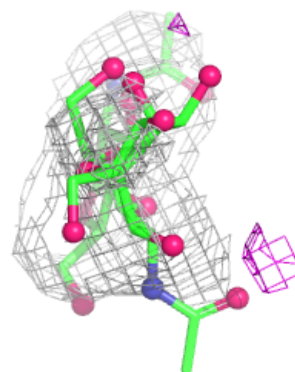
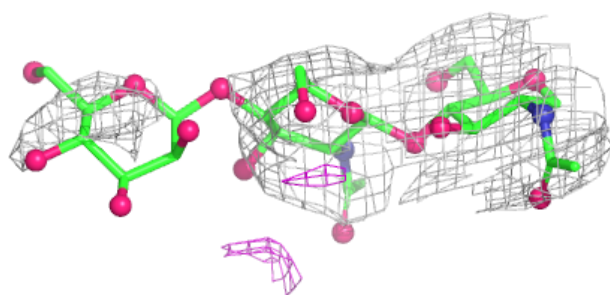
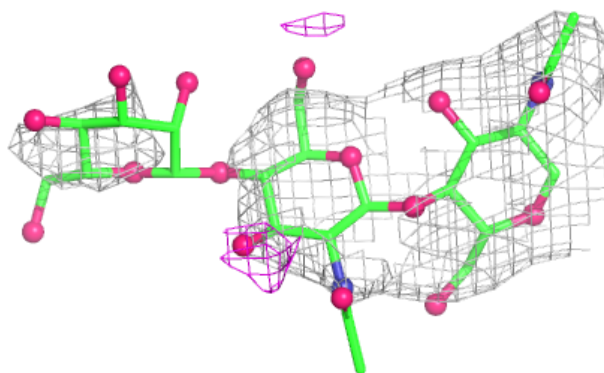
Electron density around Chain O:

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

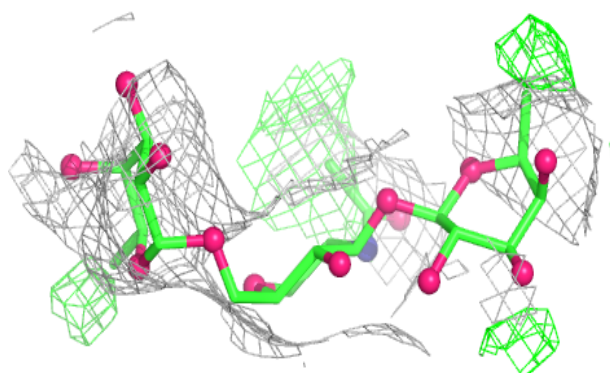
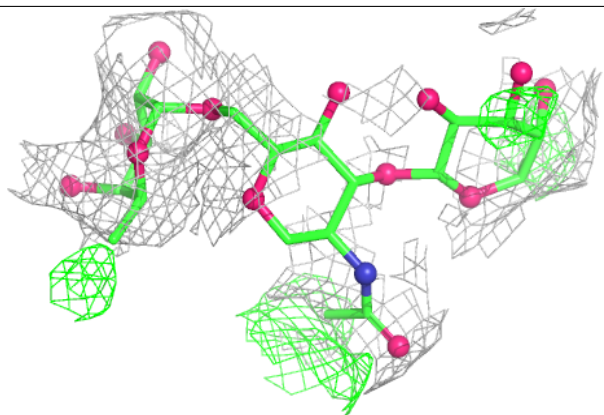


Electron density around Chain R:

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

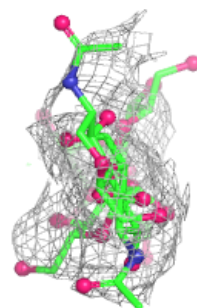
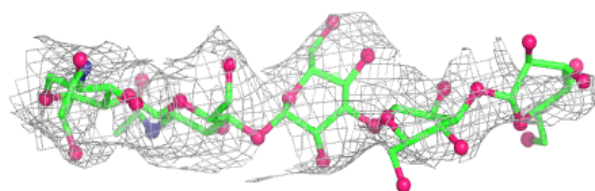
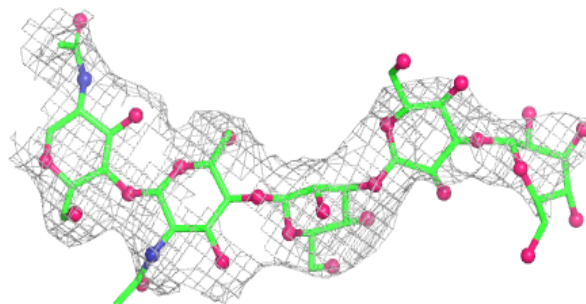
**Electron density around Chain T:**

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

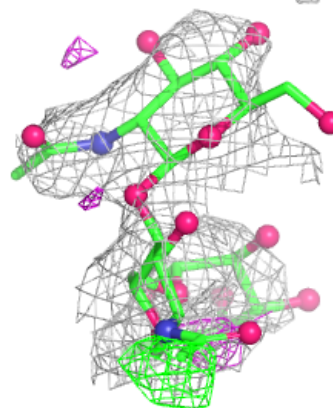
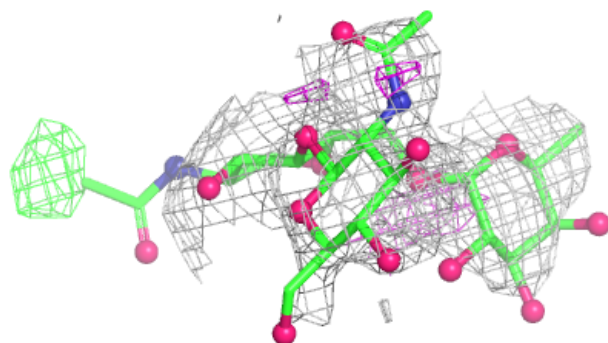
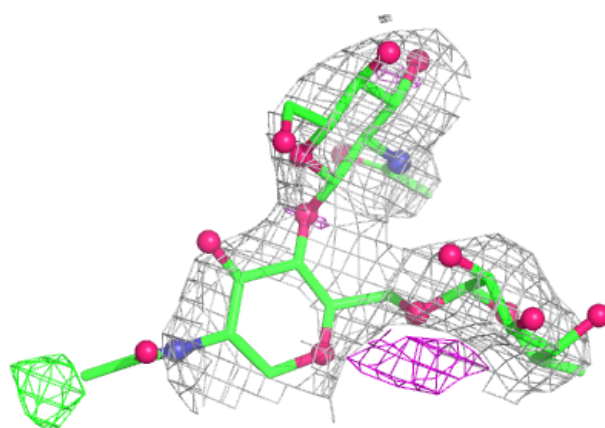


Electron density around Chain V:

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

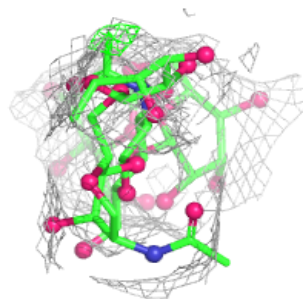
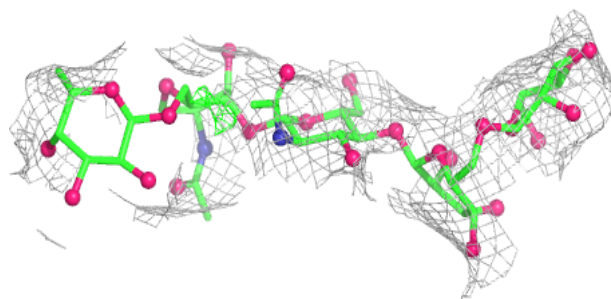
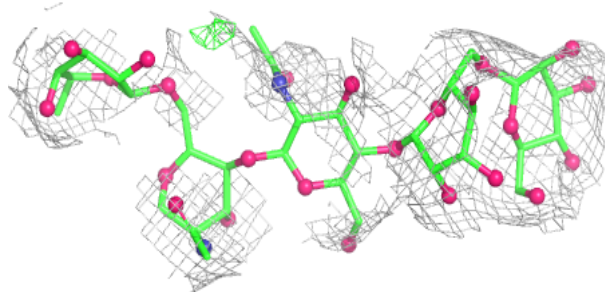
**Electron density around Chain Y:**

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



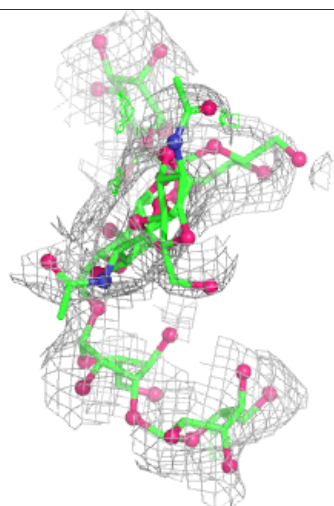
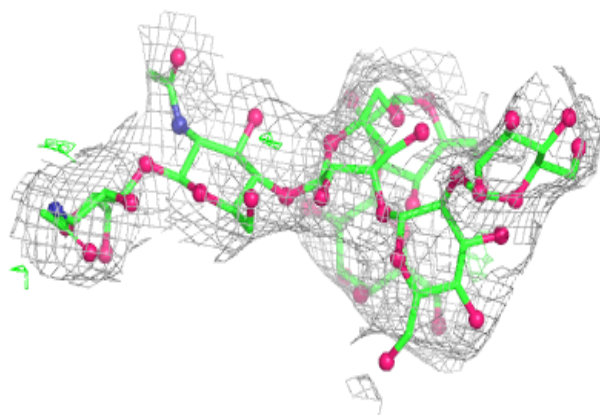
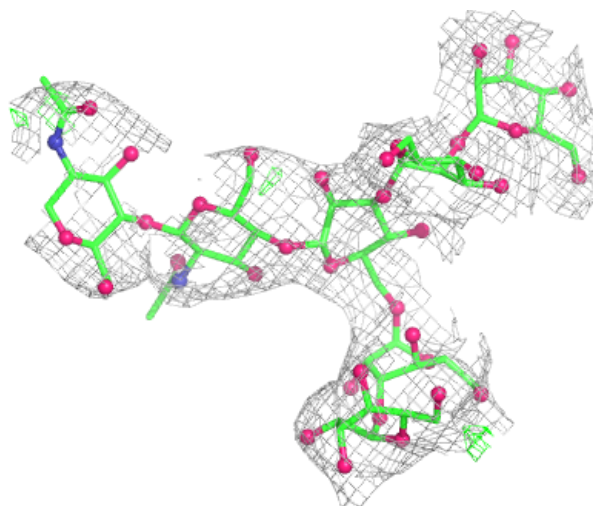
Electron density around Chain a:

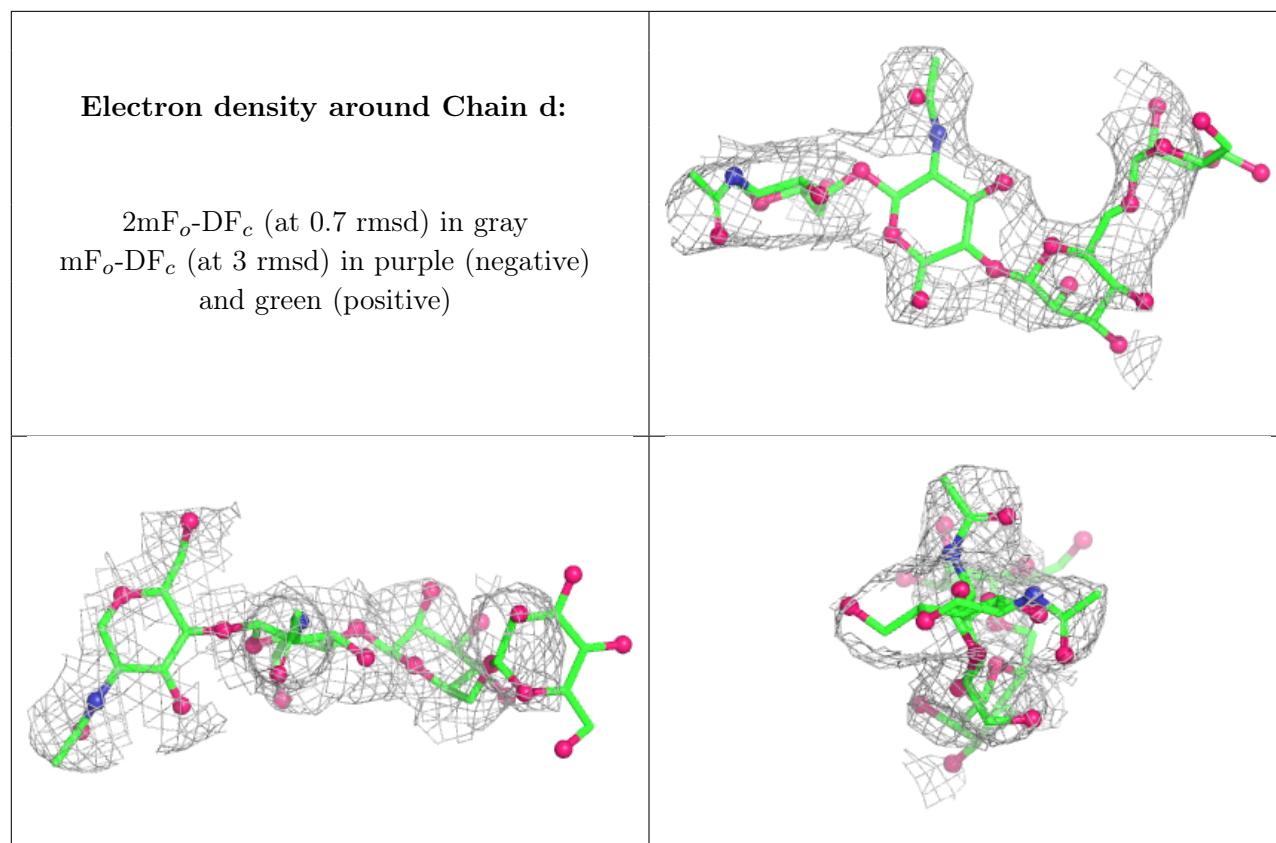
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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	H	201	14/15	0.40	0.11	158,169,184,186	0
15	NAG	A	525	14/15	0.43	0.12	113,179,197,200	0
15	NAG	G	419	14/15	0.45	0.16	124,161,178,179	0
15	NAG	C	417	14/15	0.48	0.12	126,165,183,186	0
15	NAG	F	201	14/15	0.50	0.14	124,167,179,187	0
15	NAG	D	201	14/15	0.56	0.13	103,153,184,194	0
15	NAG	B	201	14/15	0.66	0.12	141,183,190,199	0
16	CAC	B	202	5/5	0.75	0.28	113,128,156,158	0

6.5 Other polymers [i](#)

There are no such residues in this entry.