



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:58 PM UTC

PDB ID : 5XRS / pdb_00005xrs
Title : Crystal structure of A/Minnesota/11/2010 (H3N2) influenza virus hemagglutinin in complex with LSTc
Authors : Zhang, H.; Wilson, I.A.
Deposited on : 2017-06-09
Resolution : 2.91 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:

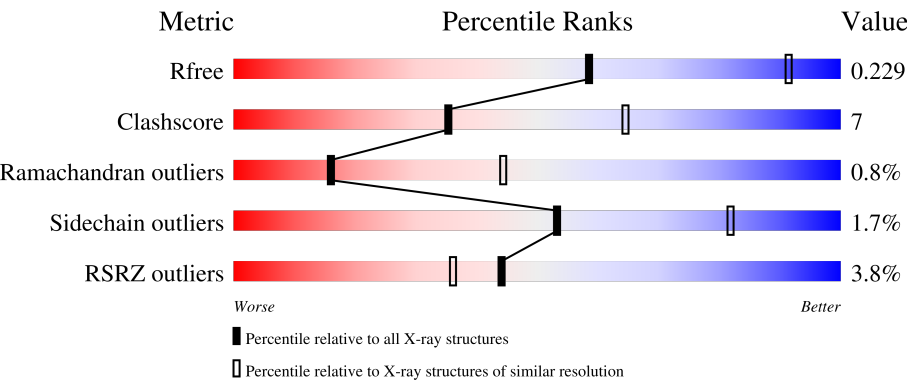
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.91 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	2% 84% 12% ..
1	C	329	2% 84% 12% ..
1	E	329	3% 88% 9% .
1	G	329	2% 81% 15% ..
2	B	174	% 87% 10% ...

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
12	a	2	50% 50%
12	f	2	50% 50%
13	d	5	20% 20% 60%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 16918 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.

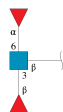
- Molecule 1 is a protein called Hemagglutinin.

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	321	Total	C	N	O	S	0	0	0
			2522	1580	441	488	13			

- Molecule 2 is a protein called Hemagglutinin.

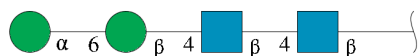
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1392	864	249	273	6			
2	D	172	Total	C	N	O	S	0	0	0
			1392	864	249	273	6			
2	F	172	Total	C	N	O	S	0	0	0
			1392	864	249	273	6			
2	H	172	Total	C	N	O	S	0	0	0
			1392	864	249	273	6			

- Molecule 3 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
3	I	3	Total	C	N	O	0	0	0
			34	20	1	13			

- Molecule 4 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.



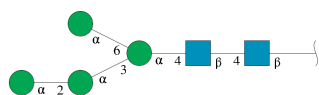
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 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.



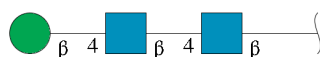
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	R	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	W	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	c	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 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.



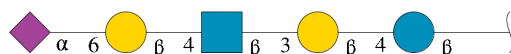
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 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
7	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	b	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	e	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



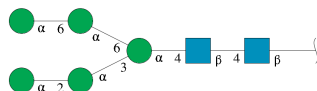
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	O	5	Total	C	N	O	0	0	0
			68	37	2	29			
8	V	5	Total	C	N	O	0	0	0
			68	37	2	29			
8	g	5	Total	C	N	O	0	0	0
			68	37	2	29			

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



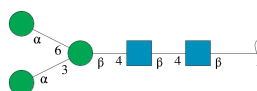
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	P	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-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.



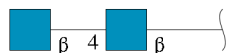
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	S	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 11 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
11	T	5	Total	C	N	O	0	0	0
			61	34	2	25			
11	X	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 12 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



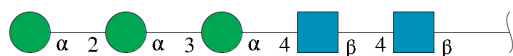
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
12	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

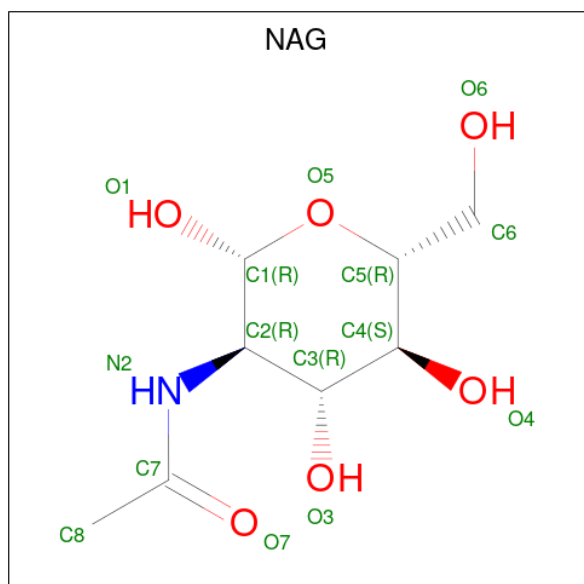
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
12	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
12	f	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-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	d	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



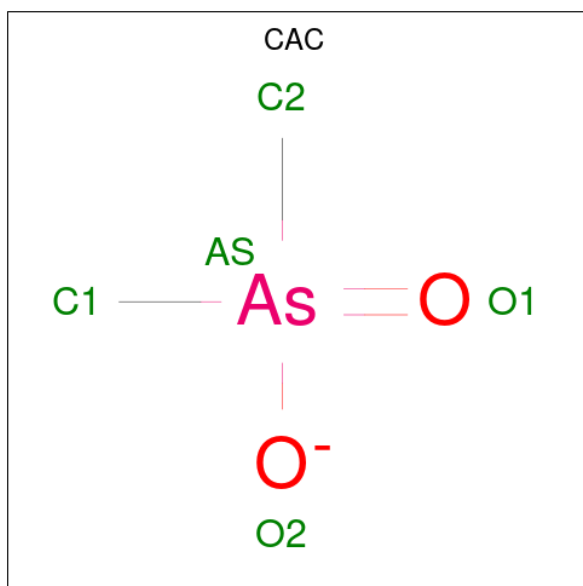
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

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

- Molecule 15 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).

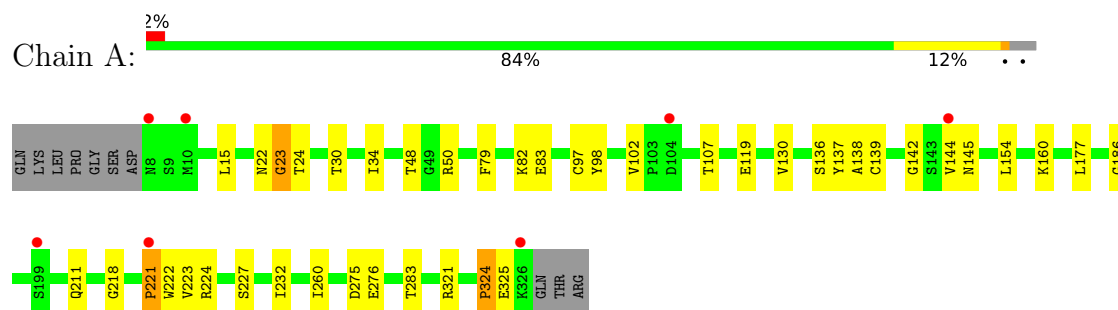


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	D	1	Total	As	C	O	0	0
			5	1	2	2		

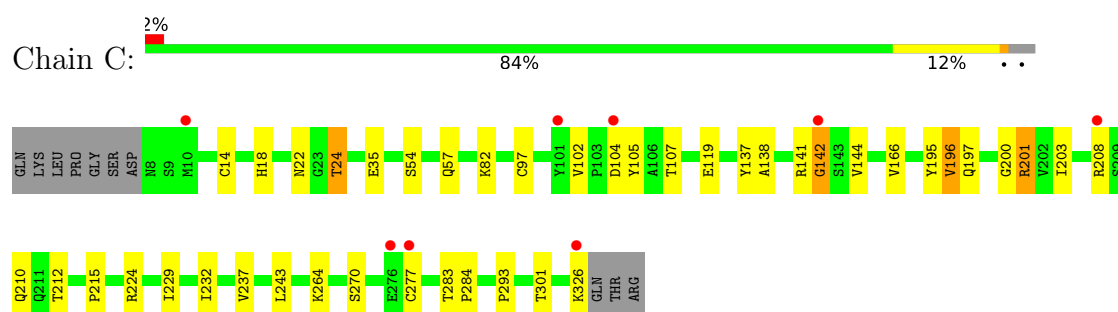
3 Residue-property plots [i](#)

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.

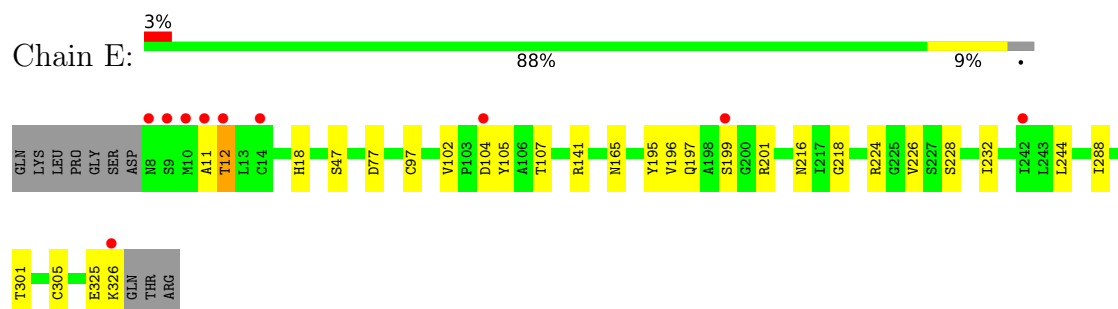
• Molecule 1: Hemagglutinin



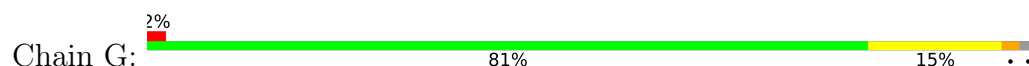
• Molecule 1: Hemagglutinin

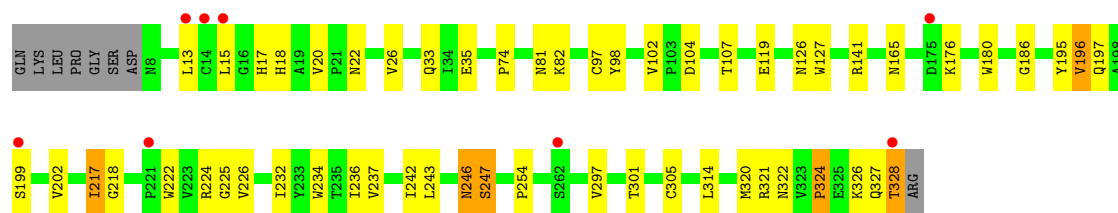


• Molecule 1: Hemagglutinin

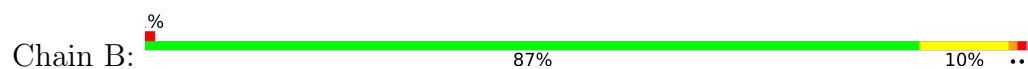


• Molecule 1: Hemagglutinin

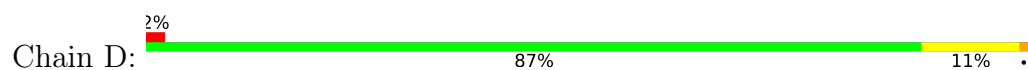




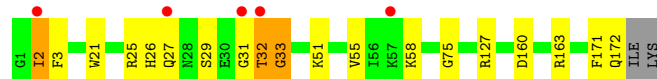
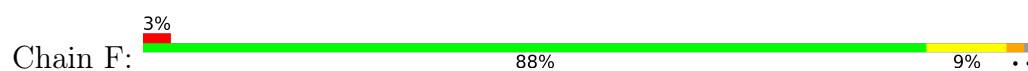
• Molecule 2: Hemagglutinin



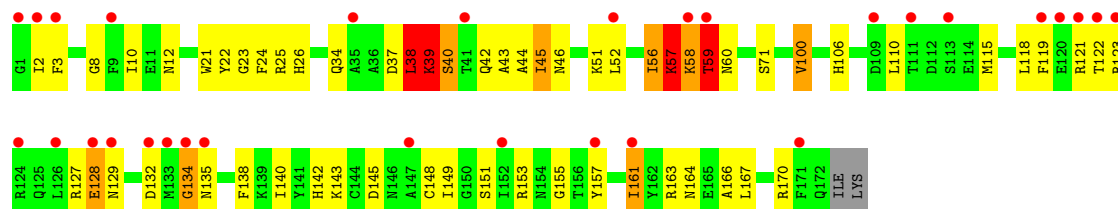
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



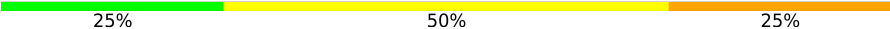
• Molecule 2: Hemagglutinin



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

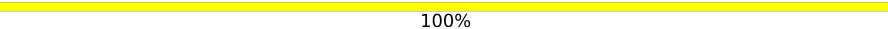


• Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  25% 50% 25%



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

Chain M:  100%

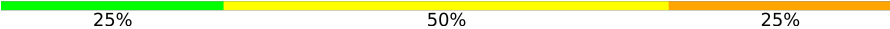


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%



- Molecule 5: 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 Q:  25% 50% 25%

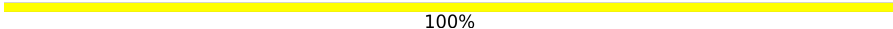


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  25% 25% 50%



- Molecule 5: 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 W:  100%

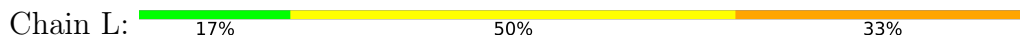


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  75% 25%



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



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



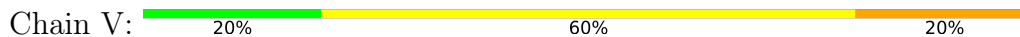
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



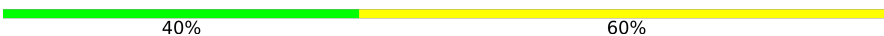
- Molecule 8: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 8: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 8: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain g:  40% 60%

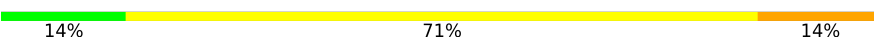
BGC1
GAL2
NAG3
GAL4
SIA5

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

Chain P:  100%

NAG1
FUC2

- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-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 S:  14% 71% 14%

NAG1
NAG2
MAN3
MAN4
MAN5
MAN6
MAN7

- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  40% 60%

NAG1
NAG2
MAN3
MAN4
MAN5

- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  60% 40%

NAG1
NAG2
MAN3
MAN4
MAN5

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

Chain U:  100%

NAG1
NAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain Z:  100%

MAG1
MAG2

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

Chain a:  50% 50%

MAG1
MAG2

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

Chain f:  50% 50%

MAG1
MAG2

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

Chain d:  20% 20% 60%

MAG1
MAG2
MAN3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	292.98Å 292.98Å 292.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.32 – 2.91 46.32 – 2.91	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.32-2.91) 100.0 (46.32-2.91)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.187 , 0.225 0.193 , 0.229	Depositor DCC
R_{free} test set	4471 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16918	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% 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, BMA, FUL, SIA, NAG, FUC, GAL, BGC

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	0.17	0/2565	0.63	7/3492 (0.2%)
1	C	0.15	0/2565	0.52	7/3492 (0.2%)
1	E	0.15	0/2565	0.46	2/3492 (0.1%)
1	G	0.18	0/2581	0.49	5/3514 (0.1%)
2	B	0.21	0/1416	0.55	1/1902 (0.1%)
2	D	0.24	0/1416	0.46	0/1902
2	F	0.18	0/1416	0.69	3/1902 (0.2%)
2	H	0.22	0/1416	1.09	16/1902 (0.8%)
All	All	0.18	0/15940	0.61	41/21598 (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
2	H	0	2

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	32	THR	CB-CA-C	-17.19	77.51	110.35
1	A	22	ASN	N-CA-C	16.98	139.38	111.37
2	H	58	LYS	N-CA-C	-16.15	86.92	108.24
2	F	32	THR	N-CA-C	13.12	139.54	113.29
2	H	57	LYS	CB-CA-C	12.36	135.01	110.42
1	A	22	ASN	CB-CA-C	-11.58	91.52	110.74
2	H	58	LYS	N-CA-CB	11.42	128.79	110.97
2	H	129	ASN	N-CA-C	-10.62	100.37	113.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	39	LYS	N-CA-CB	-9.83	93.88	110.49
2	H	38	LEU	N-CA-C	-9.36	92.13	108.23
2	H	39	LYS	N-CA-C	9.20	130.39	110.80
2	H	59	THR	N-CA-C	-9.07	91.47	110.80
2	F	33	GLY	N-CA-C	8.53	133.39	113.18
2	H	38	LEU	CB-CA-C	7.88	124.36	111.05
1	C	201	ARG	N-CA-CB	-7.70	98.56	110.56
1	E	105	TYR	N-CA-C	-7.49	101.25	112.04
2	H	60	ASN	N-CA-CB	-7.49	97.78	110.50
1	G	246	ASN	N-CA-C	-7.32	96.32	108.32
1	C	105	TYR	N-CA-C	-7.29	102.32	112.45
2	H	170	ARG	N-CA-C	-7.26	103.27	112.93
1	C	201	ARG	N-CA-C	7.25	121.66	110.42
1	A	324	PRO	CA-C-O	-7.15	112.93	122.08
2	H	57	LYS	N-CA-C	-6.88	96.15	110.80
1	C	141	ARG	N-CA-C	-6.68	94.46	107.62
2	H	59	THR	CB-CA-C	6.22	122.80	110.42
1	A	23	GLY	N-CA-C	6.10	127.63	113.18
1	G	127	TRP	N-CA-C	-6.01	99.44	109.24
1	C	142	GLY	N-CA-C	5.93	124.85	114.76
2	H	56	ILE	CB-CA-C	-5.90	101.61	111.29
1	G	246	ASN	CB-CA-C	5.86	119.79	109.89
1	C	208	ARG	CB-CA-C	-5.85	100.00	109.13
1	C	57	GLN	N-CA-C	-5.65	101.54	109.96
1	G	247	SER	N-CA-CB	5.52	119.93	110.77
1	E	12	THR	N-CA-CB	5.25	120.57	111.39
1	A	324	PRO	CA-C-N	5.21	131.08	121.70
1	A	324	PRO	C-N-CA	5.21	131.08	121.70
2	H	40	SER	N-CA-C	-5.17	96.86	107.67
1	A	221	PRO	N-CA-C	-5.13	101.89	112.47
1	G	126	ASN	N-CA-C	-5.10	98.73	108.17
2	H	134	GLY	N-CA-C	5.10	118.97	112.13
2	B	142	HIS	N-CA-CB	-5.01	103.46	111.43

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	38	LEU	Peptide
2	H	39	LYS	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	2420	31	0
1	C	2506	0	2421	24	0
1	E	2506	0	2422	22	0
1	G	2522	0	2439	51	0
2	B	1392	0	1323	17	0
2	D	1392	0	1323	25	0
2	F	1392	0	1324	20	1
2	H	1392	0	1325	63	0
3	I	34	0	31	2	0
4	J	50	0	43	1	0
4	M	50	0	43	0	0
5	K	50	0	43	1	0
5	Q	50	0	43	1	0
5	R	50	0	43	2	0
5	W	50	0	43	0	0
5	c	50	0	43	2	0
6	L	72	0	61	2	0
7	N	39	0	34	1	0
7	b	39	0	34	1	0
7	e	39	0	34	1	0
8	O	68	0	58	1	0
8	V	68	0	58	1	0
8	g	68	0	58	0	0
9	P	24	0	22	2	0
10	S	83	0	70	1	0
11	T	61	0	52	0	0
11	X	61	0	52	2	0
12	U	28	0	25	2	0
12	Y	28	0	25	3	0
12	Z	28	0	25	0	0
12	a	28	0	25	1	0
12	f	28	0	25	1	0
13	d	61	0	52	2	0
14	A	14	0	13	0	0
14	B	14	0	13	0	0
14	C	14	0	13	0	0
14	D	14	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	E	14	0	13	0	0
14	F	14	0	13	0	0
14	G	14	0	13	0	0
15	D	5	0	0	0	0
All	All	16918	0	16130	243	1

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 7.

All (243) 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:F:2:ILE:CD1	2:F:3:PHE:CE1	2.00	1.42
2:F:2:ILE:HD11	2:F:3:PHE:CE1	1.55	1.42
2:F:2:ILE:HD12	2:F:3:PHE:CD1	1.62	1.32
2:F:2:ILE:CD1	2:F:3:PHE:CD1	2.25	1.14
1:G:195:TYR:O	1:G:196:VAL:CG1	1.96	1.14
1:G:196:VAL:HG13	1:G:197:GLN:N	1.60	1.09
2:H:2:ILE:HD11	2:H:3:PHE:HE1	1.10	1.08
2:H:2:ILE:CD1	2:H:3:PHE:HE1	1.66	1.07
2:H:2:ILE:HG13	2:H:3:PHE:CD1	1.91	1.06
2:H:2:ILE:CD1	2:H:3:PHE:CE1	2.38	1.05
1:A:144:VAL:HG22	1:A:145:ASN:H	1.21	1.04
1:G:195:TYR:O	1:G:196:VAL:HG12	1.54	1.04
2:H:2:ILE:HG13	2:H:3:PHE:HD1	1.17	1.03
1:G:196:VAL:CG1	1:G:197:GLN:H	1.65	1.01
2:H:2:ILE:HD11	2:H:3:PHE:CE1	1.96	1.00
1:G:195:TYR:C	1:G:196:VAL:HG12	1.83	0.99
2:F:2:ILE:HD11	2:F:3:PHE:HE1	1.18	0.96
1:G:196:VAL:HG13	1:G:197:GLN:H	0.83	0.95
2:H:161:ILE:CG2	2:H:163:ARG:HB2	1.96	0.95
1:G:195:TYR:O	1:G:196:VAL:HG13	1.72	0.88
5:K:1:NAG:H5	6:L:1:NAG:H82	1.58	0.85
1:A:144:VAL:HG22	1:A:145:ASN:N	1.91	0.84
2:B:58:LYS:O	2:B:58:LYS:HG3	1.82	0.80
1:C:97:CYS:O	1:C:224:ARG:NH1	2.15	0.80
2:H:21:TRP:CG	2:H:22:TYR:H	2.01	0.79
1:G:195:TYR:C	1:G:196:VAL:CG1	2.47	0.77
1:C:200:GLY:O	1:C:215:PRO:HD2	1.84	0.76
2:H:39:LYS:HG2	2:H:40:SER:H	1.51	0.76
1:G:17:HIS:HA	2:H:22:TYR:HB2	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:ILE:CD1	2:D:3:PHE:CE1	2.68	0.75
2:H:2:ILE:HD12	2:H:3:PHE:CE1	2.18	0.75
1:G:195:TYR:O	1:G:197:GLN:N	2.17	0.75
1:A:144:VAL:CG2	1:A:145:ASN:H	1.99	0.75
1:G:20:VAL:HG12	1:G:22:ASN:H	1.51	0.75
1:G:97:CYS:O	1:G:224:ARG:NH1	2.19	0.75
1:C:24:THR:HG23	9:P:1:NAG:H81	1.69	0.74
2:H:161:ILE:HG22	2:H:163:ARG:HB2	1.69	0.74
2:F:2:ILE:HD12	2:F:3:PHE:CE1	1.93	0.73
1:G:196:VAL:CG1	1:G:197:GLN:CD	2.61	0.73
1:A:107:THR:HG23	2:D:75:GLY:HA3	1.71	0.72
1:E:77:ASP:OD2	1:E:141:ARG:NH1	2.23	0.72
1:E:195:TYR:O	1:E:197:GLN:N	2.20	0.72
1:A:97:CYS:O	1:A:224:ARG:NH1	2.23	0.71
2:H:2:ILE:CG1	2:H:3:PHE:CD1	2.70	0.71
2:D:150:GLY:O	2:D:154:ASN:HB2	1.92	0.70
1:G:20:VAL:O	1:G:322:ASN:ND2	2.25	0.70
1:C:107:THR:HG23	2:F:75:GLY:HA3	1.73	0.70
2:H:39:LYS:HG2	2:H:40:SER:N	2.07	0.70
2:H:161:ILE:HG21	2:H:163:ARG:HB2	1.74	0.69
1:A:24:THR:HG23	3:I:1:NAG:H81	1.73	0.69
2:H:151:SER:HB2	2:H:157:TYR:HB2	1.74	0.69
2:D:2:ILE:HD11	2:D:3:PHE:CE1	2.27	0.69
2:B:2:ILE:CG2	2:B:3:PHE:CD1	2.76	0.67
2:H:39:LYS:HE2	2:H:45:ILE:HB	1.76	0.67
1:G:196:VAL:HG13	1:G:197:GLN:CD	2.18	0.67
2:B:2:ILE:HG23	2:B:3:PHE:CD1	2.29	0.67
1:E:97:CYS:O	1:E:224:ARG:NH1	2.28	0.66
2:H:145:ASP:H	2:H:148:CYS:HB2	1.60	0.65
2:H:56:ILE:HG22	2:H:57:LYS:H	1.61	0.64
2:H:132:ASP:HB3	2:H:138:PHE:HB3	1.79	0.64
2:H:21:TRP:CD1	2:H:39:LYS:HG3	2.32	0.64
9:P:2:FUL:H4	5:Q:1:NAG:H3	1.80	0.64
1:G:196:VAL:HG11	1:G:197:GLN:CD	2.22	0.64
12:f:1:NAG:H83	12:f:1:NAG:H3	1.80	0.64
1:G:196:VAL:HG11	1:G:197:GLN:NE2	2.13	0.63
2:F:2:ILE:HD13	2:F:3:PHE:CE1	2.28	0.63
2:H:149:ILE:O	2:H:153:ARG:N	2.28	0.63
2:D:2:ILE:HD12	2:D:3:PHE:CE1	2.33	0.63
2:H:58:LYS:O	2:H:59:THR:O	2.17	0.62
1:C:200:GLY:O	1:C:215:PRO:CD	2.47	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.81	0.61
2:B:127:ARG:NH2	2:D:131:GLU:OE1	2.32	0.61
1:G:102:VAL:HG22	1:G:232:ILE:HB	1.82	0.60
1:G:17:HIS:HA	2:H:22:TYR:CB	2.30	0.60
1:G:297:VAL:HG13	7:e:1:NAG:H82	1.83	0.60
12:Y:2:NAG:O7	12:Y:2:NAG:O3	2.18	0.60
1:E:165:ASN:HB3	11:X:1:NAG:H83	1.84	0.60
1:E:11:ALA:O	1:E:12:THR:HG23	2.01	0.59
2:H:163:ARG:O	2:H:166:ALA:O	2.19	0.59
11:X:2:NAG:H3	12:Y:2:NAG:H62	1.85	0.59
1:A:324:PRO:HA	1:A:325:GLU:HB2	1.83	0.59
2:H:21:TRP:CG	2:H:22:TYR:N	2.69	0.58
1:A:221:PRO:HB3	1:E:244:LEU:HD13	1.85	0.58
1:G:18:HIS:HB2	2:H:21:TRP:O	2.03	0.58
2:H:118:LEU:HA	2:H:121:ARG:O	2.03	0.58
2:B:152:ILE:C	2:B:154:ASN:H	2.12	0.58
1:C:119:GLU:OE2	1:G:82:LYS:HA	2.03	0.57
1:G:196:VAL:CG1	1:G:197:GLN:OE1	2.52	0.57
1:G:165:ASN:HB2	5:c:1:NAG:O5	2.04	0.57
2:H:2:ILE:CD1	2:H:3:PHE:CD1	2.87	0.57
2:F:160:ASP:HA	2:F:163:ARG:HB2	1.88	0.56
2:B:139:LYS:HZ2	2:F:127:ARG:HH22	1.53	0.56
2:B:2:ILE:CG2	2:B:3:PHE:CE1	2.89	0.56
1:C:54:SER:OG	1:C:277:CYS:O	2.23	0.56
1:A:221:PRO:HB3	1:E:244:LEU:CD1	2.36	0.55
7:N:1:NAG:H3	7:N:1:NAG:H83	1.88	0.55
1:G:74:PRO:HB3	1:G:141:ARG:HB2	1.87	0.55
2:H:2:ILE:CG1	2:H:3:PHE:HD1	2.05	0.55
1:G:104:ASP:OD2	1:G:234:TRP:NE1	2.19	0.55
3:I:2:FUL:H63	4:J:1:NAG:H3	1.89	0.55
2:F:26:HIS:NE2	2:F:33:GLY:HA3	2.23	0.54
13:d:4:MAN:H62	13:d:5:MAN:H2	1.90	0.54
2:B:24:PHE:HB2	2:B:153:ARG:HD3	1.91	0.53
2:D:2:ILE:HD11	2:D:3:PHE:HE1	1.72	0.53
2:D:58:LYS:HB3	2:D:59:THR:HA	1.90	0.53
12:U:2:NAG:H3	12:U:2:NAG:H83	1.91	0.53
2:H:106:HIS:O	2:H:110:LEU:HB2	2.08	0.52
1:G:246:ASN:OD1	5:c:1:NAG:N2	2.43	0.52
1:G:314:LEU:HB3	2:H:100:VAL:HG21	1.91	0.52
12:U:1:NAG:H83	12:U:1:NAG:H3	1.90	0.52
2:D:56:ILE:HG13	2:D:56:ILE:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:LYS:CG	2:H:40:SER:H	2.21	0.52
2:B:27:GLN:HG3	2:B:32:THR:HG22	1.92	0.52
1:C:293:PRO:HD3	2:D:56:ILE:HG22	1.91	0.52
1:G:237:VAL:HG21	1:G:243:LEU:HB2	1.92	0.52
2:D:149:ILE:HD12	2:D:153:ARG:CZ	2.40	0.51
2:H:58:LYS:O	2:H:59:THR:OG1	2.26	0.51
2:H:39:LYS:CG	2:H:40:SER:N	2.74	0.51
2:F:2:ILE:CD1	2:F:3:PHE:CZ	2.82	0.51
2:H:123:ARG:CZ	2:H:138:PHE:HB2	2.40	0.51
1:A:137:TYR:C	1:A:139:CYS:H	2.17	0.51
2:H:10:ILE:HG13	2:H:115:MET:HE2	1.92	0.51
2:D:52:LEU:O	2:D:56:ILE:HG12	2.11	0.50
2:F:2:ILE:HD12	2:F:3:PHE:CG	2.33	0.50
2:D:149:ILE:HD12	2:D:153:ARG:NH2	2.27	0.50
8:O:5:SIA:O10	8:O:5:SIA:O4	2.29	0.50
2:B:3:PHE:CZ	2:D:2:ILE:HB	2.46	0.50
1:G:35:GLU:O	1:G:321:ARG:HA	2.12	0.49
1:E:104:ASP:HB2	1:E:107:THR:HB	1.94	0.49
1:A:83:GLU:OE2	1:A:119:GLU:OE2	2.29	0.49
1:C:203:ILE:HD12	1:E:218:GLY:HA3	1.95	0.49
1:C:264:LYS:HB3	2:D:63:PHE:CG	2.47	0.49
13:d:2:NAG:H61	13:d:3:MAN:O2	2.12	0.49
2:H:51:LYS:HG3	2:H:52:LEU:N	2.27	0.48
1:A:15:LEU:HD23	2:B:118:LEU:HG	1.96	0.48
1:G:26:VAL:O	1:G:33:GLN:HA	2.14	0.48
2:H:151:SER:CB	2:H:157:TYR:HB2	2.42	0.48
1:A:275:ASP:OD1	1:A:276:GLU:N	2.47	0.48
2:B:2:ILE:HG22	2:B:3:PHE:CD1	2.49	0.48
2:H:25:ARG:HD3	2:H:34:GLN:HE21	1.77	0.48
2:H:115:MET:O	2:H:119:PHE:N	2.44	0.48
1:G:202:VAL:HG22	1:G:247:SER:HB2	1.95	0.48
1:G:196:VAL:HG13	1:G:197:GLN:OE1	2.13	0.48
1:C:212:THR:HG21	1:E:216:ASN:CG	2.39	0.47
2:B:126:LEU:HD21	2:B:152:ILE:HD13	1.97	0.47
1:C:14:CYS:HA	2:D:137:CYS:HA	1.96	0.47
1:A:218:GLY:HA3	1:E:201:ARG:CZ	2.44	0.47
2:F:31:GLY:O	2:F:32:THR:OG1	2.26	0.47
1:G:196:VAL:CG1	1:G:197:GLN:N	2.33	0.47
2:D:150:GLY:CA	2:D:153:ARG:HH21	2.27	0.47
2:H:58:LYS:C	2:H:59:THR:O	2.57	0.47
1:G:186:GLY:HA2	1:G:218:GLY:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:ASP:O	2:H:39:LYS:N	2.47	0.47
2:H:42:GLN:C	2:H:46:ASN:HB2	2.40	0.47
1:A:218:GLY:HA3	1:E:201:ARG:NH2	2.30	0.47
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.96	0.46
1:E:195:TYR:C	1:E:197:GLN:H	2.18	0.46
1:G:327:GLN:O	1:G:328:THR:O	2.33	0.46
2:H:56:ILE:O	2:H:57:LYS:HG3	2.15	0.46
1:C:142:GLY:C	1:C:144:VAL:H	2.22	0.46
1:G:97:CYS:SG	1:G:98:TYR:N	2.87	0.46
2:F:160:ASP:OD1	2:F:160:ASP:N	2.40	0.46
1:C:195:TYR:O	1:C:197:GLN:N	2.39	0.46
1:G:301:THR:HB	1:G:305:CYS:SG	2.55	0.46
1:A:34:ILE:HD11	1:A:321:ARG:HD2	1.97	0.46
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.97	0.46
2:H:40:SER:HB2	2:H:43:ALA:HB3	1.96	0.46
1:A:222:TRP:CZ2	1:A:227:SER:HB3	2.51	0.45
1:G:13:LEU:CD2	2:H:26:HIS:HB3	2.46	0.45
1:G:222:TRP:CZ2	1:G:225:GLY:HA2	2.51	0.45
1:A:136:SER:OG	1:A:137:TYR:O	2.26	0.45
1:C:201:ARG:NH2	5:R:1:NAG:O7	2.49	0.45
1:C:270:SER:HB2	1:C:284:PRO:HA	1.99	0.45
1:E:11:ALA:O	1:E:12:THR:CG2	2.64	0.45
1:G:176:LYS:O	1:G:236:ILE:HA	2.16	0.45
5:R:3:BMA:H3	5:R:4:MAN:H2	1.73	0.45
1:E:47:SER:HB2	1:E:288:ILE:HG22	1.98	0.44
12:Y:1:NAG:O7	12:Y:1:NAG:O3	2.33	0.44
2:H:132:ASP:CB	2:H:138:PHE:HB3	2.47	0.44
2:H:142:HIS:CG	2:H:143:LYS:H	2.35	0.44
1:C:237:VAL:HG21	1:C:243:LEU:HB2	1.99	0.44
2:F:51:LYS:O	2:F:55:VAL:HG13	2.17	0.44
1:G:15:LEU:HD22	2:H:24:PHE:CD1	2.53	0.44
1:E:226:VAL:HG12	1:E:228:SER:H	1.83	0.44
1:A:48:THR:HG23	1:A:50:ARG:H	1.83	0.44
1:A:144:VAL:CG2	1:A:145:ASN:N	2.63	0.44
1:G:81:ASN:HA	1:G:119:GLU:HA	1.99	0.44
12:a:1:NAG:H83	12:a:1:NAG:H3	2.00	0.44
1:E:12:THR:OG1	2:F:27:GLN:HB3	2.17	0.44
2:F:2:ILE:H	2:F:2:ILE:HG13	1.53	0.44
1:A:79:PHE:HA	1:A:82:LYS:HG3	2.00	0.43
2:B:3:PHE:HZ	2:D:2:ILE:HB	1.83	0.43
2:B:152:ILE:C	2:B:154:ASN:N	2.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:1:NAG:H61	7:b:2:NAG:N2	2.34	0.43
2:H:56:ILE:O	2:H:57:LYS:CB	2.66	0.43
2:B:120:GLU:OE1	2:B:123:ARG:NH2	2.52	0.43
1:G:327:GLN:C	1:G:328:THR:O	2.61	0.43
2:H:25:ARG:NH1	2:H:25:ARG:HA	2.34	0.43
2:H:51:LYS:HG3	2:H:52:LEU:H	1.82	0.43
10:S:2:NAG:O3	10:S:3:MAN:O5	2.31	0.43
2:D:128:GLU:O	2:D:170:ARG:NH1	2.48	0.43
1:A:97:CYS:SG	1:A:98:TYR:N	2.91	0.43
1:A:218:GLY:HA3	1:E:201:ARG:NH1	2.34	0.43
2:H:121:ARG:HA	2:H:122:THR:HA	1.58	0.43
1:A:324:PRO:CA	1:A:325:GLU:HB2	2.46	0.42
1:C:24:THR:O	1:C:35:GLU:HA	2.19	0.42
1:A:160:LYS:HB3	1:A:160:LYS:HE2	1.91	0.42
2:F:171:PHE:O	2:F:172:GLN:NE2	2.44	0.42
1:G:104:ASP:HB2	1:G:107:THR:HB	2.01	0.42
1:C:283:THR:HG22	1:C:301:THR:HG22	2.01	0.42
2:D:58:LYS:HB3	2:D:59:THR:HG22	2.00	0.42
1:A:138:ALA:HB1	1:A:224:ARG:HB3	2.02	0.42
2:D:24:PHE:CD1	2:D:153:ARG:HG2	2.53	0.42
6:L:3:MAN:H62	6:L:6:MAN:H2	1.86	0.42
2:D:145:ASP:O	2:D:148:CYS:SG	2.78	0.42
1:C:137:TYR:N	8:V:5:SIA:O1B	2.44	0.42
1:E:18:HIS:ND1	2:F:21:TRP:HA	2.35	0.42
2:H:40:SER:O	2:H:44:ALA:N	2.45	0.42
1:A:130:VAL:HG11	1:A:154:LEU:HB3	2.01	0.42
1:A:177:LEU:HB2	1:A:260:ILE:HD11	2.00	0.42
2:D:149:ILE:CD1	2:D:153:ARG:NH2	2.82	0.42
1:G:324:PRO:O	2:H:12:ASN:ND2	2.53	0.42
1:G:180:TRP:HB3	1:G:254:PRO:HD3	2.01	0.41
1:E:301:THR:HB	1:E:305:CYS:SG	2.60	0.41
1:G:13:LEU:CD2	2:H:26:HIS:CB	2.98	0.41
1:A:186:GLY:HA2	1:A:218:GLY:O	2.21	0.41
2:H:25:ARG:HD3	2:H:34:GLN:NE2	2.35	0.41
2:H:134:GLY:O	2:H:135:ASN:HB2	2.20	0.41
2:D:150:GLY:HA2	2:D:153:ARG:HH21	1.86	0.41
2:H:21:TRP:CZ3	2:H:23:GLY:HA2	2.55	0.41
2:B:30:GLU:OE2	2:B:145:ASP:HB2	2.20	0.41
2:D:5:ALA:O	2:D:10:ILE:HG12	2.21	0.41
1:C:326:LYS:HE2	1:C:326:LYS:HB2	1.95	0.41
2:H:127:ARG:O	2:H:128:GLU:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:ASN:O	2:H:167:LEU:HB2	2.21	0.41
1:A:137:TYR:O	1:A:138:ALA:HB3	2.20	0.40
1:C:138:ALA:HB1	1:C:224:ARG:HB3	2.03	0.40
1:C:104:ASP:O	1:C:104:ASP:CG	2.64	0.40
1:G:196:VAL:HG22	1:G:197:GLN:N	2.35	0.40
1:E:325:GLU:HG2	1:E:326:LYS:H	1.86	0.40
1:G:199:SER:HB3	1:G:217:ILE:HD11	2.02	0.40
1:G:320:MET:SD	1:G:321:ARG:N	2.86	0.40
2:H:39:LYS:HG2	2:H:40:SER:C	2.47	0.40

All (1) 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:F:25:ARG:NH1	2:F:32:THR:O[14_555]	1.88	0.32

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%)	296 (93%)	19 (6%)	2 (1%)	21	51
1	C	317/329 (96%)	303 (96%)	13 (4%)	1 (0%)	36	65
1	E	317/329 (96%)	300 (95%)	15 (5%)	2 (1%)	21	51
1	G	319/329 (97%)	300 (94%)	16 (5%)	3 (1%)	14	41
2	B	170/174 (98%)	161 (95%)	8 (5%)	1 (1%)	21	51
2	D	170/174 (98%)	163 (96%)	7 (4%)	0	100	100
2	F	170/174 (98%)	160 (94%)	9 (5%)	1 (1%)	21	51
2	H	170/174 (98%)	140 (82%)	24 (14%)	6 (4%)	3	12
All	All	1950/2012 (97%)	1823 (94%)	111 (6%)	16 (1%)	16	44

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLY
2	B	58	LYS
1	E	196	VAL
2	H	39	LYS
2	H	57	LYS
1	A	142	GLY
2	F	58	LYS
1	G	324	PRO
1	G	326	LYS
2	H	155	GLY
2	H	161	ILE
1	G	196	VAL
2	H	59	THR
1	E	199	SER
2	H	8	GLY
1	C	196	VAL

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%)	280 (99%)	4 (1%)	59	85
1	C	284/293 (97%)	276 (97%)	8 (3%)	38	72
1	E	284/293 (97%)	284 (100%)	0	100	100
1	G	286/293 (98%)	282 (99%)	4 (1%)	59	85
2	B	146/148 (99%)	142 (97%)	4 (3%)	39	73
2	D	146/148 (99%)	145 (99%)	1 (1%)	76	92
2	F	146/148 (99%)	144 (99%)	2 (1%)	59	85
2	H	146/148 (99%)	140 (96%)	6 (4%)	27	61
All	All	1722/1764 (98%)	1693 (98%)	29 (2%)	53	82

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	211	GLN
1	A	223	VAL
1	A	283	THR
2	B	10	ILE
2	B	58	LYS
2	B	108	ILE
2	B	154	ASN
1	C	18	HIS
1	C	22	ASN
1	C	24	THR
1	C	82	LYS
1	C	166	VAL
1	C	196	VAL
1	C	210	GLN
1	C	229	ILE
2	D	2	ILE
2	F	2	ILE
2	F	29	SER
1	G	217	ILE
1	G	226	VAL
1	G	242	ILE
1	G	328	THR
2	H	38	LEU
2	H	45	ILE
2	H	71	SER
2	H	100	VAL
2	H	128	GLU
2	H	140	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
2	B	60	ASN
1	C	17	HIS
1	C	33	GLN
1	C	80	GLN
1	C	261	GLN
2	D	12	ASN
2	D	26	HIS
2	D	42	GLN
2	D	60	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	33	GLN
1	E	197	GLN
1	E	261	GLN
2	F	12	ASN
2	F	42	GLN
1	G	156	ASN
1	G	158	ASN
2	H	12	ASN
2	H	28	ASN
2	H	46	ASN
2	H	129	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 ⓘ

95 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	0.27	0	17,19,21	1.14	2 (11%)
3	FUL	I	2	3	10,10,11	2.05	2 (20%)	14,14,16	3.04	7 (50%)
3	FUC	I	3	3	10,10,11	0.80	0	14,14,16	0.83	0
4	NAG	J	1	4,1	14,14,15	0.71	1 (7%)	17,19,21	0.69	0
4	NAG	J	2	4	14,14,15	0.22	0	17,19,21	0.66	0
4	BMA	J	3	4	11,11,12	0.79	1 (9%)	15,15,17	1.45	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	J	4	4	11,11,12	0.85	1 (9%)	15,15,17	1.12	1 (6%)
5	NAG	K	1	5,1	14,14,15	0.58	0	17,19,21	0.86	0
5	NAG	K	2	5	14,14,15	0.22	0	17,19,21	0.79	0
5	BMA	K	3	5	11,11,12	0.41	0	15,15,17	0.87	0
5	MAN	K	4	5	11,11,12	0.69	1 (9%)	15,15,17	1.09	2 (13%)
6	NAG	L	1	1,6	14,14,15	0.22	0	17,19,21	0.59	0
6	NAG	L	2	6	14,14,15	0.35	0	17,19,21	0.54	0
6	MAN	L	3	6	11,11,12	0.94	1 (9%)	15,15,17	2.11	5 (33%)
6	MAN	L	4	6	11,11,12	1.94	3 (27%)	15,15,17	1.80	4 (26%)
6	MAN	L	5	6	11,11,12	1.17	2 (18%)	15,15,17	1.36	1 (6%)
6	MAN	L	6	6	11,11,12	1.50	3 (27%)	15,15,17	1.85	2 (13%)
4	NAG	M	1	4,1	14,14,15	0.22	0	17,19,21	0.90	1 (5%)
4	NAG	M	2	4	14,14,15	0.42	0	17,19,21	0.79	1 (5%)
4	BMA	M	3	4	11,11,12	1.82	4 (36%)	15,15,17	1.41	3 (20%)
4	MAN	M	4	4	11,11,12	1.16	1 (9%)	15,15,17	1.24	3 (20%)
7	NAG	N	1	1,7	14,14,15	0.41	0	17,19,21	1.31	2 (11%)
7	NAG	N	2	7	14,14,15	0.31	0	17,19,21	0.64	0
7	BMA	N	3	7	11,11,12	1.17	2 (18%)	15,15,17	1.61	3 (20%)
8	BGC	O	1	8	12,12,12	1.76	4 (33%)	17,17,17	1.48	4 (23%)
8	GAL	O	2	8	11,11,12	0.63	0	15,15,17	0.78	0
8	NAG	O	3	8	14,14,15	0.36	0	17,19,21	0.43	0
8	GAL	O	4	8	11,11,12	0.41	0	15,15,17	0.92	1 (6%)
8	SIA	O	5	8	20,20,21	1.69	2 (10%)	21,28,31	1.83	5 (23%)
9	NAG	P	1	9,1	14,14,15	0.69	1 (7%)	17,19,21	0.54	0
9	FUL	P	2	9	10,10,11	1.99	3 (30%)	14,14,16	1.90	4 (28%)
5	NAG	Q	1	5,1	14,14,15	0.80	1 (7%)	17,19,21	0.81	0
5	NAG	Q	2	5	14,14,15	0.47	0	17,19,21	0.63	0
5	BMA	Q	3	5	11,11,12	1.04	0	15,15,17	1.04	2 (13%)
5	MAN	Q	4	5	11,11,12	0.98	0	15,15,17	0.91	2 (13%)
5	NAG	R	1	5,1	14,14,15	0.41	0	17,19,21	0.70	0
5	NAG	R	2	5	14,14,15	0.47	0	17,19,21	0.58	0
5	BMA	R	3	5	11,11,12	1.09	1 (9%)	15,15,17	1.18	2 (13%)
5	MAN	R	4	5	11,11,12	1.00	1 (9%)	15,15,17	0.90	1 (6%)
10	NAG	S	1	10,1	14,14,15	0.25	0	17,19,21	0.53	0
10	NAG	S	2	10	14,14,15	0.23	0	17,19,21	0.52	0
10	MAN	S	3	10	11,11,12	0.97	0	15,15,17	1.69	2 (13%)
10	MAN	S	4	10	11,11,12	1.69	2 (18%)	15,15,17	1.61	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	S	5	10	11,11,12	1.11	1 (9%)	15,15,17	2.09	5 (33%)
10	MAN	S	6	10	11,11,12	1.13	1 (9%)	15,15,17	1.29	2 (13%)
10	MAN	S	7	10	11,11,12	0.90	1 (9%)	15,15,17	1.41	2 (13%)
11	NAG	T	1	11,1	14,14,15	0.25	0	17,19,21	0.58	0
11	NAG	T	2	11	14,14,15	0.51	0	17,19,21	0.55	0
11	BMA	T	3	11	11,11,12	0.66	0	15,15,17	1.24	1 (6%)
11	MAN	T	4	11	11,11,12	0.96	0	15,15,17	1.25	2 (13%)
11	MAN	T	5	11	11,11,12	0.89	0	15,15,17	1.02	1 (6%)
12	NAG	U	1	12,1	14,14,15	0.32	0	17,19,21	1.41	2 (11%)
12	NAG	U	2	12	14,14,15	0.46	0	17,19,21	1.35	2 (11%)
8	BGC	V	1	8	12,12,12	1.39	2 (16%)	17,17,17	1.32	1 (5%)
8	GAL	V	2	8	11,11,12	0.83	0	15,15,17	0.88	1 (6%)
8	NAG	V	3	8	14,14,15	0.34	0	17,19,21	0.51	0
8	GAL	V	4	8	11,11,12	0.96	1 (9%)	15,15,17	1.07	1 (6%)
8	SIA	V	5	8	20,20,21	1.62	2 (10%)	21,28,31	1.57	2 (9%)
5	NAG	W	1	5,1	14,14,15	0.76	1 (7%)	17,19,21	0.65	0
5	NAG	W	2	5	14,14,15	1.57	2 (14%)	17,19,21	1.34	2 (11%)
5	BMA	W	3	5	11,11,12	0.70	0	15,15,17	1.13	1 (6%)
5	MAN	W	4	5	11,11,12	0.77	0	15,15,17	0.97	1 (6%)
11	NAG	X	1	11,1	14,14,15	0.61	0	17,19,21	0.98	2 (11%)
11	NAG	X	2	11	14,14,15	0.97	1 (7%)	17,19,21	1.43	1 (5%)
11	BMA	X	3	11	11,11,12	0.89	0	15,15,17	1.08	1 (6%)
11	MAN	X	4	11	11,11,12	0.67	0	15,15,17	1.06	2 (13%)
11	MAN	X	5	11	11,11,12	1.43	2 (18%)	15,15,17	1.47	2 (13%)
12	NAG	Y	1	12,1	14,14,15	0.47	0	17,19,21	0.51	0
12	NAG	Y	2	12	14,14,15	0.44	0	17,19,21	0.67	0
12	NAG	Z	1	12,1	14,14,15	0.21	0	17,19,21	0.49	0
12	NAG	Z	2	12	14,14,15	0.34	0	17,19,21	0.43	0
12	NAG	a	1	12,1	14,14,15	0.50	0	17,19,21	1.65	3 (17%)
12	NAG	a	2	12	14,14,15	0.53	0	17,19,21	0.66	0
7	NAG	b	1	1,7	14,14,15	0.28	0	17,19,21	0.45	0
7	NAG	b	2	7	14,14,15	1.29	2 (14%)	17,19,21	1.27	3 (17%)
7	BMA	b	3	7	11,11,12	0.67	0	15,15,17	0.97	0
5	NAG	c	1	5,1	14,14,15	0.31	0	17,19,21	0.74	1 (5%)
5	NAG	c	2	5	14,14,15	0.32	0	17,19,21	2.36	1 (5%)
5	BMA	c	3	5	11,11,12	0.83	1 (9%)	15,15,17	0.90	0
5	MAN	c	4	5	11,11,12	0.99	1 (9%)	15,15,17	1.71	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	NAG	d	1	13,1	14,14,15	0.52	0	17,19,21	0.60	0
13	NAG	d	2	13	14,14,15	0.46	0	17,19,21	0.57	0
13	MAN	d	3	13	11,11,12	1.71	3 (27%)	15,15,17	1.51	3 (20%)
13	MAN	d	4	13	11,11,12	1.97	2 (18%)	15,15,17	1.89	3 (20%)
13	MAN	d	5	13	11,11,12	1.07	1 (9%)	15,15,17	1.45	2 (13%)
7	NAG	e	1	1,7	14,14,15	0.78	1 (7%)	17,19,21	1.11	1 (5%)
7	NAG	e	2	7	14,14,15	0.39	0	17,19,21	0.65	0
7	BMA	e	3	7	11,11,12	0.93	0	15,15,17	1.02	1 (6%)
12	NAG	f	1	12,1	14,14,15	1.33	2 (14%)	17,19,21	1.38	2 (11%)
12	NAG	f	2	12	14,14,15	0.36	0	17,19,21	0.50	0
8	BGC	g	1	8	12,12,12	1.59	3 (25%)	17,17,17	1.38	2 (11%)
8	GAL	g	2	8	11,11,12	0.57	0	15,15,17	1.03	1 (6%)
8	NAG	g	3	8	14,14,15	0.25	0	17,19,21	0.52	0
8	GAL	g	4	8	11,11,12	0.60	0	15,15,17	0.72	0
8	SIA	g	5	8	20,20,21	1.62	1 (5%)	21,28,31	1.51	2 (9%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	L	6	6	-	2/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1
4	MAN	M	4	4	-	2/2/19/22	0/1/1/1
7	NAG	N	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
8	BGC	O	1	8	-	2/2/22/22	0/1/1/1
8	GAL	O	2	8	-	2/2/19/22	0/1/1/1
8	NAG	O	3	8	-	0/6/23/26	0/1/1/1
8	GAL	O	4	8	-	0/2/19/22	0/1/1/1
8	SIA	O	5	8	-	2/18/34/38	0/1/1/1
9	NAG	P	1	9,1	-	0/6/23/26	0/1/1/1
9	FUL	P	2	9	-	-	0/1/1/1
5	NAG	Q	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	2/2/19/22	0/1/1/1
5	MAN	Q	4	5	-	0/2/19/22	0/1/1/1
5	NAG	R	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	BMA	R	3	5	-	2/2/19/22	0/1/1/1
5	MAN	R	4	5	-	2/2/19/22	0/1/1/1
10	NAG	S	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	S	2	10	-	0/6/23/26	0/1/1/1
10	MAN	S	3	10	-	2/2/19/22	0/1/1/1
10	MAN	S	4	10	-	2/2/19/22	1/1/1/1
10	MAN	S	5	10	-	0/2/19/22	0/1/1/1
10	MAN	S	6	10	-	0/2/19/22	1/1/1/1
10	MAN	S	7	10	-	2/2/19/22	1/1/1/1
11	NAG	T	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	T	2	11	-	0/6/23/26	0/1/1/1
11	BMA	T	3	11	-	2/2/19/22	0/1/1/1
11	MAN	T	4	11	-	1/2/19/22	1/1/1/1
11	MAN	T	5	11	-	2/2/19/22	1/1/1/1
12	NAG	U	1	12,1	-	5/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	U	2	12	-	6/6/23/26	0/1/1/1
8	BGC	V	1	8	-	2/2/22/22	0/1/1/1
8	GAL	V	2	8	-	2/2/19/22	0/1/1/1
8	NAG	V	3	8	-	0/6/23/26	0/1/1/1
8	GAL	V	4	8	-	2/2/19/22	0/1/1/1
8	SIA	V	5	8	-	4/18/34/38	0/1/1/1
5	NAG	W	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	W	2	5	-	1/6/23/26	0/1/1/1
5	BMA	W	3	5	-	0/2/19/22	0/1/1/1
5	MAN	W	4	5	-	2/2/19/22	1/1/1/1
11	NAG	X	1	11,1	-	3/6/23/26	0/1/1/1
11	NAG	X	2	11	-	0/6/23/26	0/1/1/1
11	BMA	X	3	11	-	2/2/19/22	0/1/1/1
11	MAN	X	4	11	-	0/2/19/22	0/1/1/1
11	MAN	X	5	11	-	0/2/19/22	0/1/1/1
12	NAG	Y	1	12,1	-	1/6/23/26	0/1/1/1
12	NAG	Y	2	12	-	3/6/23/26	0/1/1/1
12	NAG	Z	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	Z	2	12	-	0/6/23/26	0/1/1/1
12	NAG	a	1	12,1	-	4/6/23/26	0/1/1/1
12	NAG	a	2	12	-	2/6/23/26	0/1/1/1
7	NAG	b	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	b	2	7	-	4/6/23/26	0/1/1/1
7	BMA	b	3	7	-	1/2/19/22	0/1/1/1
5	NAG	c	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
5	BMA	c	3	5	-	0/2/19/22	0/1/1/1
5	MAN	c	4	5	-	1/2/19/22	0/1/1/1
13	NAG	d	1	13,1	-	2/6/23/26	0/1/1/1
13	NAG	d	2	13	-	4/6/23/26	0/1/1/1
13	MAN	d	3	13	-	2/2/19/22	0/1/1/1
13	MAN	d	4	13	-	1/2/19/22	0/1/1/1
13	MAN	d	5	13	-	2/2/19/22	0/1/1/1
7	NAG	e	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	e	2	7	-	0/6/23/26	0/1/1/1
7	BMA	e	3	7	-	2/2/19/22	0/1/1/1
12	NAG	f	1	12,1	-	5/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	f	2	12	-	0/6/23/26	0/1/1/1
8	BGC	g	1	8	-	2/2/22/22	0/1/1/1
8	GAL	g	2	8	-	0/2/19/22	0/1/1/1
8	NAG	g	3	8	-	2/6/23/26	0/1/1/1
8	GAL	g	4	8	-	2/2/19/22	0/1/1/1
8	SIA	g	5	8	-	2/18/34/38	0/1/1/1

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	O	5	SIA	C2-C1	5.82	1.59	1.52
8	V	5	SIA	C2-C1	5.74	1.59	1.52
8	g	5	SIA	C2-C1	5.69	1.59	1.52
3	I	2	FUL	O5-C1	5.17	1.52	1.43
9	P	2	FUL	O5-C1	4.83	1.51	1.43
5	W	2	NAG	O5-C1	-4.79	1.35	1.43
6	L	4	MAN	C2-C3	4.77	1.59	1.52
13	d	4	MAN	O2-C2	4.08	1.51	1.43
13	d	4	MAN	C2-C3	3.97	1.58	1.52
7	b	2	NAG	O5-C1	-3.89	1.37	1.43
4	M	3	BMA	C4-C5	3.79	1.61	1.53
12	f	1	NAG	O5-C1	-3.69	1.37	1.43
10	S	4	MAN	C2-C3	3.63	1.58	1.52
11	X	2	NAG	O5-C1	3.45	1.49	1.43
11	X	5	MAN	C2-C3	3.31	1.57	1.52
8	O	1	BGC	C4-C3	3.28	1.60	1.52
10	S	4	MAN	O2-C2	3.24	1.50	1.43
13	d	3	MAN	C4-C5	3.18	1.59	1.53
6	L	4	MAN	O2-C2	3.17	1.50	1.43
13	d	5	MAN	C1-C2	3.13	1.59	1.52
10	S	5	MAN	C1-C2	3.01	1.59	1.52
6	L	6	MAN	C1-C2	2.98	1.59	1.52
11	X	5	MAN	C1-C2	2.97	1.59	1.52
5	Q	1	NAG	O5-C1	-2.90	1.38	1.43
4	M	3	BMA	C1-C2	2.88	1.59	1.52
6	L	6	MAN	O5-C1	2.82	1.48	1.43
12	f	1	NAG	C1-C2	2.78	1.56	1.52
5	W	1	NAG	O5-C1	-2.74	1.39	1.43
9	P	2	FUL	C2-C3	-2.73	1.48	1.52
13	d	3	MAN	O5-C5	2.73	1.48	1.43
6	L	6	MAN	O5-C5	2.70	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	3	MAN	C2-C3	2.69	1.56	1.52
3	I	2	FUL	O5-C5	2.69	1.48	1.43
5	W	2	NAG	C1-C2	2.68	1.56	1.52
4	M	3	BMA	O5-C5	2.65	1.48	1.43
5	c	4	MAN	C1-C2	2.63	1.58	1.52
8	O	1	BGC	C3-C2	2.58	1.59	1.52
4	J	1	NAG	O5-C1	-2.58	1.39	1.43
7	N	3	BMA	C1-C2	2.56	1.58	1.52
8	g	1	BGC	C4-C3	2.56	1.59	1.52
6	L	5	MAN	C1-C2	2.51	1.58	1.52
8	g	1	BGC	C3-C2	2.47	1.58	1.52
6	L	5	MAN	C2-C3	2.46	1.56	1.52
8	V	1	BGC	C4-C5	2.44	1.58	1.53
7	N	3	BMA	C2-C3	2.41	1.56	1.52
4	M	3	BMA	C4-C3	2.34	1.58	1.52
10	S	6	MAN	O5-C5	2.34	1.48	1.43
5	R	4	MAN	C1-C2	2.34	1.57	1.52
9	P	2	FUL	O5-C5	2.32	1.48	1.43
8	O	1	BGC	O5-C5	-2.30	1.38	1.44
8	O	1	BGC	C4-C5	2.29	1.57	1.53
8	g	1	BGC	C1-C2	2.29	1.57	1.52
4	M	4	MAN	C4-C3	2.28	1.58	1.52
8	O	5	SIA	O6-C2	2.19	1.47	1.43
7	b	2	NAG	C1-C2	2.19	1.55	1.52
4	J	4	MAN	C1-C2	2.17	1.57	1.52
9	P	1	NAG	O5-C1	-2.15	1.40	1.43
6	L	3	MAN	O5-C5	2.13	1.47	1.43
5	c	3	BMA	C1-C2	2.11	1.57	1.52
8	V	4	GAL	C2-C3	2.09	1.55	1.52
4	J	3	BMA	O5-C1	-2.07	1.40	1.43
7	e	1	NAG	O5-C1	-2.06	1.40	1.43
8	V	5	SIA	O6-C2	2.04	1.47	1.43
5	K	4	MAN	C1-C2	2.02	1.57	1.52
10	S	7	MAN	C1-C2	2.01	1.57	1.52
5	R	3	BMA	C4-C3	2.01	1.57	1.52
6	L	4	MAN	C4-C3	2.01	1.57	1.52
8	V	1	BGC	C4-C3	2.00	1.57	1.52

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	2	NAG	C1-O5-C5	9.16	124.47	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	FUL	C1-C2-C3	6.07	118.49	109.64
10	S	5	MAN	C1-O5-C5	6.00	120.23	112.19
11	X	2	NAG	C1-O5-C5	5.66	119.77	112.19
13	d	4	MAN	C1-O5-C5	5.55	119.63	112.19
6	L	6	MAN	C1-O5-C5	5.48	119.53	112.19
3	I	2	FUL	O5-C5-C4	5.03	118.60	109.55
6	L	3	MAN	C1-O5-C5	4.99	118.87	112.19
12	a	1	NAG	C2-N2-C7	4.85	129.40	122.90
5	c	4	MAN	C1-O5-C5	4.83	118.66	112.19
6	L	4	MAN	C1-O5-C5	4.76	118.56	112.19
12	U	1	NAG	C2-N2-C7	4.67	129.16	122.90
12	U	2	NAG	C2-N2-C7	4.63	129.10	122.90
10	S	3	MAN	C1-O5-C5	4.61	118.36	112.19
8	g	5	SIA	O1A-C1-C2	-4.51	113.10	122.85
7	N	1	NAG	C2-N2-C7	4.50	128.94	122.90
8	V	5	SIA	O1A-C1-C2	-4.46	113.21	122.85
10	S	4	MAN	C1-O5-C5	4.36	118.03	112.19
8	O	5	SIA	O1A-C1-C2	-4.31	113.53	122.85
3	I	2	FUL	C2-C3-C4	4.22	118.29	110.86
9	P	2	FUL	C3-C4-C5	4.22	116.23	109.81
10	S	7	MAN	C1-O5-C5	4.12	117.71	112.19
12	f	1	NAG	C2-N2-C7	4.05	128.33	122.90
10	S	6	MAN	C1-O5-C5	4.04	117.60	112.19
11	T	3	BMA	C1-O5-C5	4.02	117.58	112.19
11	X	5	MAN	C1-C2-C3	3.98	115.44	109.64
5	W	2	NAG	C4-C3-C2	3.93	116.78	111.02
11	T	4	MAN	C1-O5-C5	3.78	117.25	112.19
3	I	2	FUL	C1-O5-C5	3.69	121.67	112.97
3	I	2	FUL	C3-C4-C5	3.69	115.42	109.81
13	d	5	MAN	C1-O5-C5	3.66	117.09	112.19
7	b	2	NAG	C4-C3-C2	3.57	116.25	111.02
7	N	3	BMA	C1-C2-C3	3.52	114.77	109.64
8	O	5	SIA	C5-N5-C10	3.38	131.01	123.11
6	L	5	MAN	C1-C2-C3	3.31	114.47	109.64
7	e	1	NAG	C3-C4-C5	3.26	116.15	110.23
4	J	3	BMA	C1-O5-C5	3.26	116.56	112.19
12	a	1	NAG	C1-C2-N2	3.14	115.38	110.43
8	O	5	SIA	C4-C5-N5	3.13	116.60	110.44
13	d	3	MAN	C1-O5-C5	3.12	116.36	112.19
7	N	3	BMA	C1-O5-C5	3.11	116.35	112.19
6	L	6	MAN	O2-C2-C3	-3.01	103.92	110.15
9	P	2	FUL	O5-C5-C4	3.00	114.96	109.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	X	4	MAN	C1-O5-C5	2.98	116.18	112.19
10	S	5	MAN	C1-C2-C3	2.96	113.95	109.64
13	d	3	MAN	C3-C4-C5	2.95	115.58	110.23
11	T	5	MAN	C1-O5-C5	2.95	116.14	112.19
9	P	2	FUL	C1-C2-C3	2.91	113.88	109.64
6	L	3	MAN	O6-C6-C5	-2.89	101.50	111.33
13	d	3	MAN	O3-C3-C2	2.89	115.95	110.05
6	L	3	MAN	O5-C5-C6	2.83	113.18	107.66
6	L	4	MAN	O2-C2-C3	2.82	116.00	110.15
5	K	4	MAN	C1-O5-C5	2.81	115.95	112.19
8	g	1	BGC	C6-C5-C4	-2.81	106.12	113.02
3	I	1	NAG	O3-C3-C4	2.80	116.98	110.38
10	S	5	MAN	O5-C1-C2	2.79	117.45	110.79
5	W	4	MAN	C1-O5-C5	2.76	115.89	112.19
10	S	4	MAN	O2-C2-C3	2.76	115.87	110.15
8	O	1	BGC	C6-C5-C4	-2.75	106.27	113.02
4	M	3	BMA	C3-C4-C5	2.73	115.19	110.23
6	L	3	MAN	O3-C3-C4	-2.72	103.96	110.38
9	P	2	FUL	C1-O5-C5	2.71	119.36	112.97
10	S	3	MAN	C3-C4-C5	2.70	115.13	110.23
13	d	5	MAN	C1-C2-C3	2.68	113.54	109.64
13	d	4	MAN	O2-C2-C3	2.67	115.69	110.15
10	S	4	MAN	O3-C3-C2	2.63	115.43	110.05
13	d	4	MAN	O3-C3-C2	2.63	115.41	110.05
5	W	2	NAG	C1-O5-C5	-2.58	108.73	112.19
3	I	2	FUL	O5-C1-C2	2.57	116.91	110.79
8	O	1	BGC	C1-O5-C5	-2.56	108.71	113.65
11	X	3	BMA	C3-C4-C5	2.55	114.86	110.23
3	I	2	FUL	C6-C5-C4	-2.55	108.42	113.08
4	M	3	BMA	O2-C2-C3	-2.54	104.89	110.15
10	S	5	MAN	O2-C2-C3	-2.53	104.91	110.15
12	f	1	NAG	C4-C3-C2	2.53	114.72	111.02
8	V	4	GAL	C1-C2-C3	2.52	113.32	109.64
8	g	1	BGC	C1-O5-C5	-2.49	108.84	113.65
4	M	2	NAG	O4-C4-C3	2.45	116.15	110.38
4	M	1	NAG	C2-N2-C7	2.45	126.18	122.90
12	U	1	NAG	C1-C2-N2	2.45	114.29	110.43
5	R	3	BMA	C1-C2-C3	2.43	113.18	109.64
6	L	3	MAN	C1-C2-C3	2.42	113.16	109.64
5	W	3	BMA	C1-C2-C3	2.41	113.15	109.64
6	L	4	MAN	C2-C3-C4	2.40	115.09	110.86
4	J	4	MAN	C1-O5-C5	2.39	115.38	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	4	MAN	C1-C2-C3	2.36	113.08	109.64
4	M	4	MAN	C2-C3-C4	2.34	114.98	110.86
4	M	4	MAN	C3-C4-C5	2.34	114.47	110.23
7	b	2	NAG	C1-O5-C5	-2.34	109.05	112.19
8	V	5	SIA	O1B-C1-O1A	2.33	129.37	124.08
8	O	5	SIA	O10-C10-N5	2.32	126.07	121.98
8	V	2	GAL	C1-C2-C3	2.31	113.01	109.64
7	N	3	BMA	O5-C5-C4	-2.30	105.24	110.83
8	g	5	SIA	O1B-C1-O1A	2.28	129.24	124.08
8	O	1	BGC	O1-C1-C2	-2.28	102.38	108.98
5	Q	4	MAN	C1-O5-C5	2.27	115.23	112.19
5	c	4	MAN	O2-C2-C3	-2.25	105.49	110.15
6	L	4	MAN	O3-C3-C2	2.23	114.60	110.05
8	V	1	BGC	O1-C1-C2	-2.22	102.55	108.98
8	O	1	BGC	C4-C3-C2	2.22	114.72	110.83
4	M	3	BMA	O5-C1-C2	-2.21	105.51	110.79
3	I	1	NAG	O3-C3-C2	2.20	113.97	109.40
11	X	1	NAG	C3-C4-C5	2.17	114.17	110.23
10	S	7	MAN	O2-C2-C3	-2.16	105.67	110.15
8	O	5	SIA	O1B-C1-O1A	2.16	128.98	124.08
7	b	2	NAG	C3-C4-C5	2.16	114.14	110.23
12	U	2	NAG	C1-C2-N2	2.14	113.81	110.43
4	J	3	BMA	C3-C4-C5	2.13	114.10	110.23
5	Q	3	BMA	C1-O5-C5	2.11	115.02	112.19
11	X	4	MAN	O2-C2-C3	-2.10	105.80	110.15
5	c	1	NAG	O4-C4-C5	-2.08	104.19	109.32
7	e	3	BMA	C2-C3-C4	2.08	114.53	110.86
5	Q	4	MAN	O2-C2-C3	-2.07	105.86	110.15
8	g	2	GAL	C1-C2-C3	2.07	112.66	109.64
7	N	1	NAG	C1-C2-N2	2.07	113.70	110.43
12	a	1	NAG	C4-C3-C2	-2.07	107.99	111.02
8	O	4	GAL	C1-O5-C5	2.06	114.95	112.19
4	M	4	MAN	O2-C2-C3	-2.06	105.89	110.15
10	S	6	MAN	O2-C2-C3	-2.06	105.89	110.15
5	K	4	MAN	O2-C2-C3	-2.05	105.91	110.15
5	Q	3	BMA	C1-C2-C3	2.04	112.61	109.64
11	X	1	NAG	C1-O5-C5	2.03	114.91	112.19
5	R	4	MAN	C1-O5-C5	2.02	114.89	112.19
11	T	4	MAN	O2-C2-C3	-2.01	105.98	110.15
11	X	5	MAN	C2-C3-C4	2.01	114.39	110.86
10	S	5	MAN	C3-C4-C5	-2.00	106.60	110.23
5	R	3	BMA	C3-C4-C5	2.00	113.86	110.23

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	O	5	SIA	C4-C5-N5-C10
8	O	5	SIA	O6-C6-C7-O7
8	g	5	SIA	O8-C8-C9-O9
10	S	1	NAG	O5-C5-C6-O6
11	X	3	BMA	C4-C5-C6-O6
8	V	1	BGC	O5-C5-C6-O6
13	d	5	MAN	O5-C5-C6-O6
5	Q	3	BMA	C4-C5-C6-O6
8	g	4	GAL	O5-C5-C6-O6
12	Y	2	NAG	O5-C5-C6-O6
13	d	1	NAG	O5-C5-C6-O6
8	V	4	GAL	O5-C5-C6-O6
8	O	2	GAL	C4-C5-C6-O6
8	V	1	BGC	C4-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6
5	R	3	BMA	O5-C5-C6-O6
7	e	3	BMA	O5-C5-C6-O6
11	X	3	BMA	O5-C5-C6-O6
13	d	5	MAN	C4-C5-C6-O6
7	e	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
10	S	1	NAG	C4-C5-C6-O6
11	T	5	MAN	C4-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
11	T	5	MAN	O5-C5-C6-O6
12	a	2	NAG	O5-C5-C6-O6
6	L	5	MAN	O5-C5-C6-O6
8	O	2	GAL	O5-C5-C6-O6
8	g	1	BGC	O5-C5-C6-O6
10	S	3	MAN	O5-C5-C6-O6
12	U	2	NAG	C4-C5-C6-O6
10	S	7	MAN	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	M	4	MAN	O5-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
11	T	1	NAG	O5-C5-C6-O6
8	g	4	GAL	C4-C5-C6-O6
7	b	1	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
10	S	7	MAN	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	T	1	NAG	C4-C5-C6-O6
6	L	5	MAN	C4-C5-C6-O6
5	K	3	BMA	C4-C5-C6-O6
8	V	4	GAL	C4-C5-C6-O6
12	Y	2	NAG	C4-C5-C6-O6
13	d	1	NAG	C4-C5-C6-O6
4	M	4	MAN	C4-C5-C6-O6
5	Q	3	BMA	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
7	b	1	NAG	C4-C5-C6-O6
7	e	1	NAG	O5-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6
8	O	1	BGC	O5-C5-C6-O6
5	R	3	BMA	C4-C5-C6-O6
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	Q	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
5	R	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
5	W	1	NAG	O7-C7-N2-C2
6	L	2	NAG	C8-C7-N2-C2
6	L	2	NAG	O7-C7-N2-C2
7	N	1	NAG	C8-C7-N2-C2
7	N	1	NAG	O7-C7-N2-C2
11	X	1	NAG	C8-C7-N2-C2
11	X	1	NAG	O7-C7-N2-C2
12	U	1	NAG	C8-C7-N2-C2
12	U	1	NAG	O7-C7-N2-C2
12	U	2	NAG	C8-C7-N2-C2
12	U	2	NAG	O7-C7-N2-C2
12	a	1	NAG	C8-C7-N2-C2
12	a	1	NAG	O7-C7-N2-C2
12	f	1	NAG	C8-C7-N2-C2
12	f	1	NAG	O7-C7-N2-C2
13	d	2	NAG	C8-C7-N2-C2
13	d	2	NAG	O7-C7-N2-C2
8	g	3	NAG	O5-C5-C6-O6
11	T	3	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	g	5	SIA	C7-C8-C9-O9
5	W	4	MAN	O5-C5-C6-O6
5	R	4	MAN	O5-C5-C6-O6
10	S	4	MAN	O5-C5-C6-O6
4	J	4	MAN	C4-C5-C6-O6
13	d	2	NAG	C4-C5-C6-O6
10	S	3	MAN	C4-C5-C6-O6
12	U	2	NAG	O5-C5-C6-O6
12	a	2	NAG	C4-C5-C6-O6
13	d	2	NAG	O5-C5-C6-O6
8	V	5	SIA	C6-C7-C8-O8
6	L	6	MAN	O5-C5-C6-O6
8	g	1	BGC	C4-C5-C6-O6
13	d	3	MAN	O5-C5-C6-O6
13	d	4	MAN	O5-C5-C6-O6
8	V	2	GAL	C4-C5-C6-O6
7	b	3	BMA	O5-C5-C6-O6
7	e	3	BMA	C4-C5-C6-O6
6	L	6	MAN	C4-C5-C6-O6
8	V	2	GAL	O5-C5-C6-O6
8	O	1	BGC	C4-C5-C6-O6
6	L	4	MAN	O5-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
8	g	3	NAG	C4-C5-C6-O6
4	M	1	NAG	C3-C2-N2-C7
12	Y	2	NAG	C3-C2-N2-C7
6	L	3	MAN	O5-C5-C6-O6
11	X	1	NAG	O5-C5-C6-O6
8	V	5	SIA	O7-C7-C8-O8
13	d	3	MAN	C4-C5-C6-O6
11	T	3	BMA	C4-C5-C6-O6
8	V	5	SIA	C6-C7-C8-C9
5	W	1	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
4	J	2	NAG	C1-C2-N2-C7
5	Q	2	NAG	C1-C2-N2-C7
5	W	2	NAG	C1-C2-N2-C7
7	N	1	NAG	C1-C2-N2-C7
7	b	2	NAG	C1-C2-N2-C7
12	a	1	NAG	C1-C2-N2-C7
5	K	1	NAG	C4-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	W	1	NAG	O5-C5-C6-O6
11	T	4	MAN	O5-C5-C6-O6
12	U	1	NAG	C4-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
5	R	2	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
5	R	4	MAN	C4-C5-C6-O6
4	J	2	NAG	C3-C2-N2-C7
5	K	2	NAG	C3-C2-N2-C7
12	U	2	NAG	C3-C2-N2-C7
12	a	1	NAG	C3-C2-N2-C7
5	R	1	NAG	O5-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
7	b	2	NAG	C4-C5-C6-O6
8	V	5	SIA	O7-C7-C8-C9
5	K	4	MAN	C4-C5-C6-O6
5	K	2	NAG	C1-C2-N2-C7
12	U	1	NAG	C1-C2-N2-C7
12	U	2	NAG	C1-C2-N2-C7
12	f	1	NAG	C1-C2-N2-C7
5	Q	2	NAG	C3-C2-N2-C7
7	N	1	NAG	C3-C2-N2-C7
7	b	2	NAG	C3-C2-N2-C7
12	U	1	NAG	C3-C2-N2-C7
12	Y	1	NAG	C3-C2-N2-C7
12	f	1	NAG	C3-C2-N2-C7
4	M	1	NAG	O5-C5-C6-O6
5	c	4	MAN	C4-C5-C6-O6
12	f	1	NAG	C4-C5-C6-O6
10	S	4	MAN	C4-C5-C6-O6
5	W	4	MAN	C4-C5-C6-O6

All (7) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	S	7	MAN	C1-C2-C3-C4-C5-O5
6	L	3	MAN	C1-C2-C3-C4-C5-O5
10	S	4	MAN	C1-C2-C3-C4-C5-O5
11	T	5	MAN	C1-C2-C3-C4-C5-O5
5	W	4	MAN	C1-C2-C3-C4-C5-O5
10	S	6	MAN	C1-C2-C3-C4-C5-O5

Continued on next page...

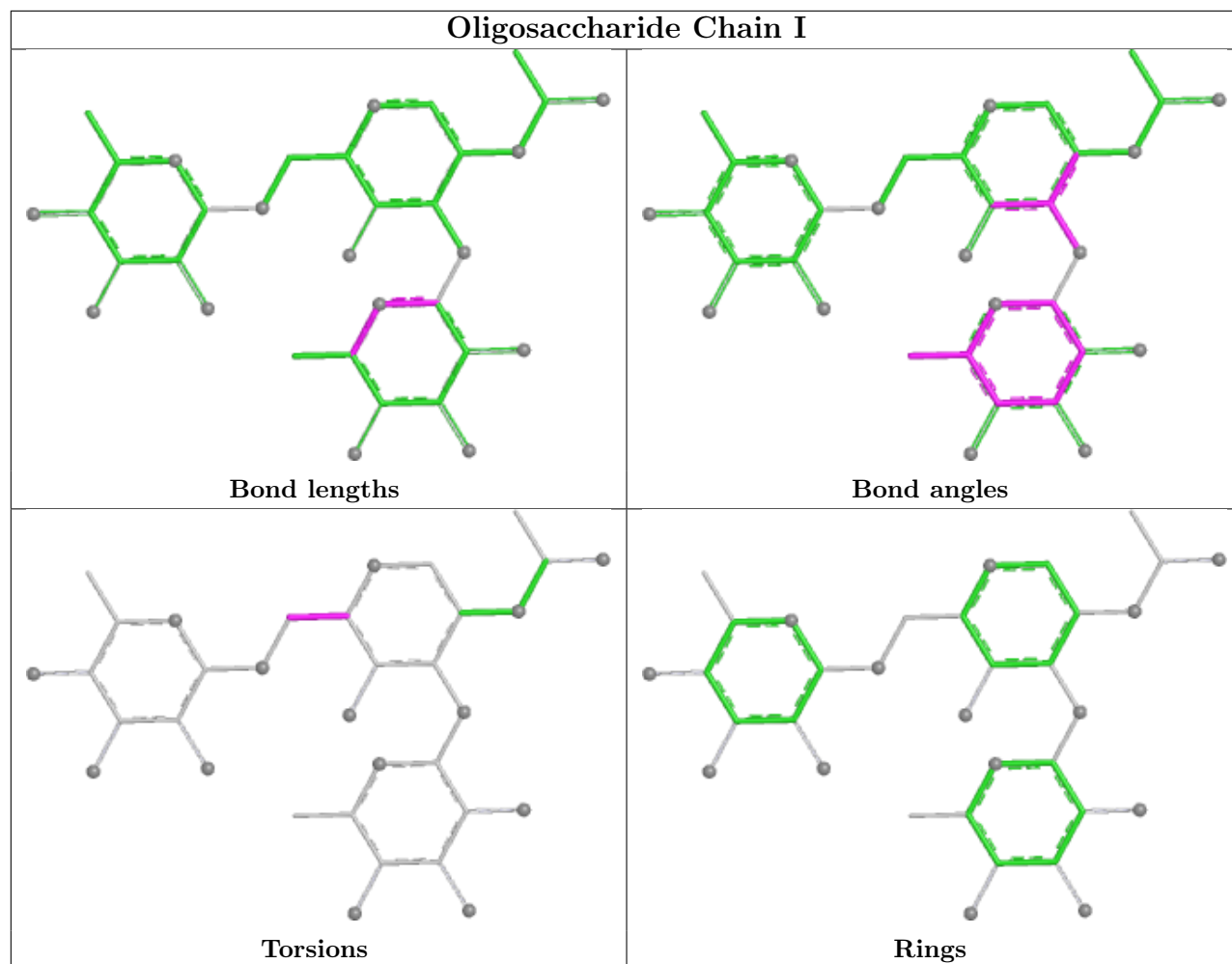
Continued from previous page...

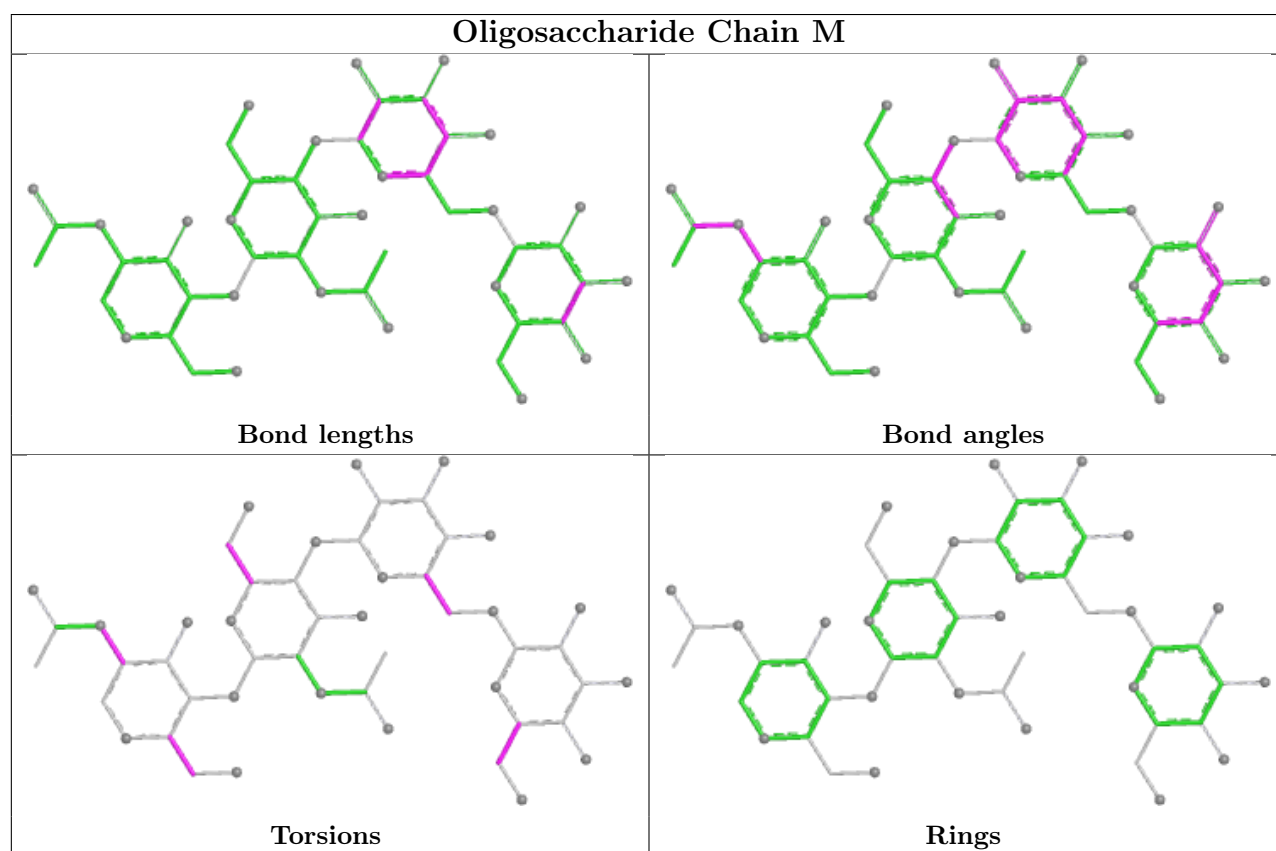
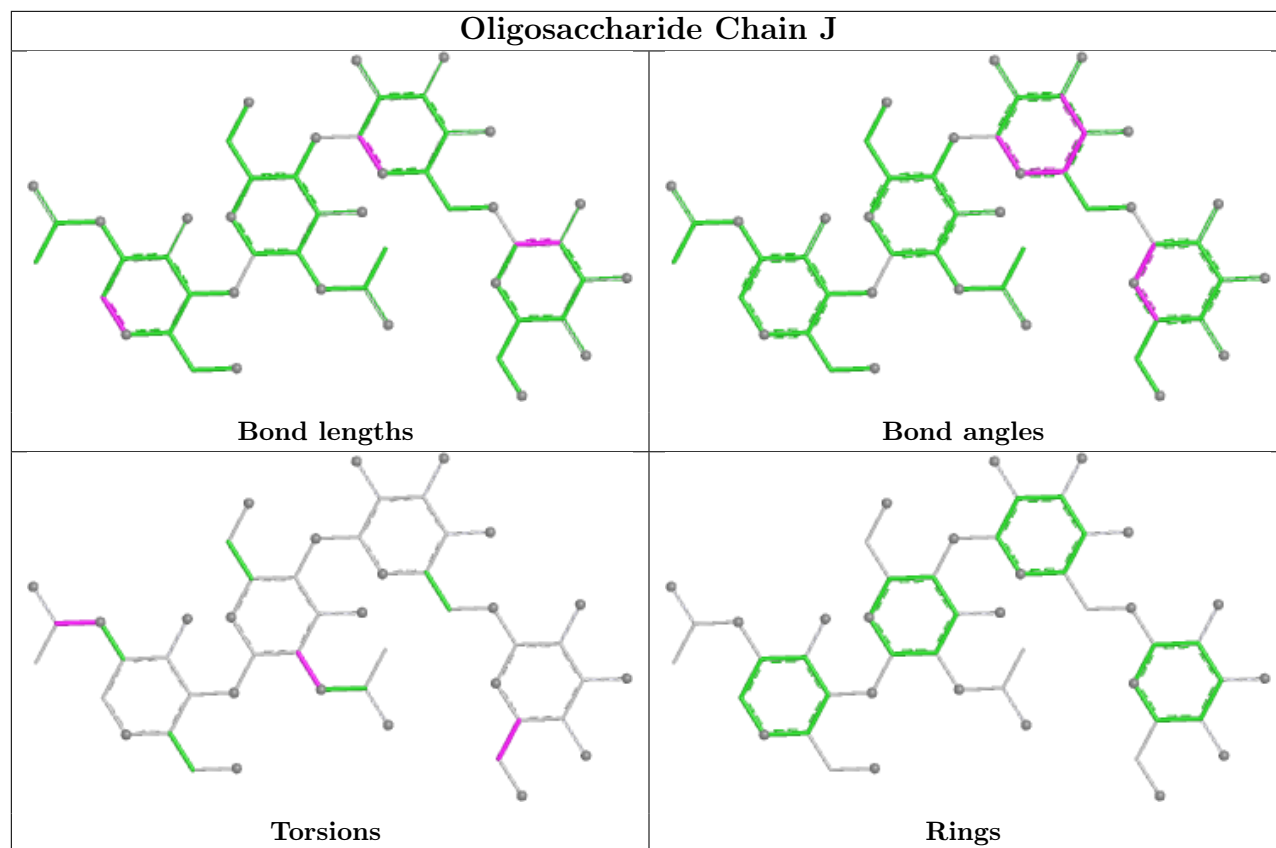
Mol	Chain	Res	Type	Atoms
11	T	4	MAN	C1-C2-C3-C4-C5-O5

34 monomers are involved in 26 short contacts:

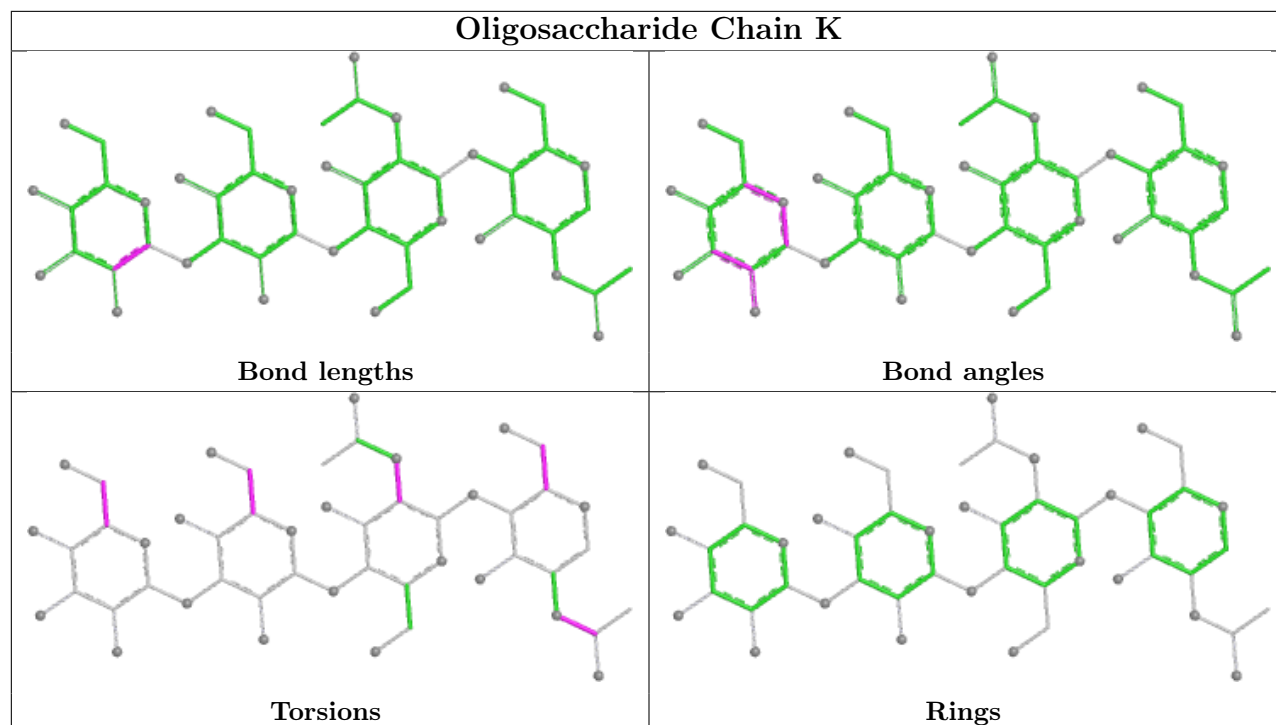
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	P	1	NAG	1	0
5	R	1	NAG	1	0
5	R	4	MAN	1	0
7	b	1	NAG	1	0
8	V	5	SIA	1	0
12	U	1	NAG	1	0
4	J	1	NAG	1	0
12	U	2	NAG	1	0
13	d	5	MAN	1	0
7	e	1	NAG	1	0
5	c	1	NAG	2	0
12	Y	2	NAG	2	0
3	I	1	NAG	1	0
6	L	6	MAN	1	0
11	X	2	NAG	1	0
13	d	4	MAN	1	0
6	L	3	MAN	1	0
5	Q	1	NAG	1	0
8	O	5	SIA	1	0
5	R	3	BMA	1	0
10	S	3	MAN	1	0
9	P	2	FUL	1	0
12	Y	1	NAG	1	0
13	d	3	MAN	1	0
7	N	1	NAG	1	0
3	I	2	FUL	1	0
11	X	1	NAG	1	0
10	S	2	NAG	1	0
13	d	2	NAG	1	0
7	b	2	NAG	1	0
6	L	1	NAG	1	0
5	K	1	NAG	1	0
12	a	1	NAG	1	0
12	f	1	NAG	1	0

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

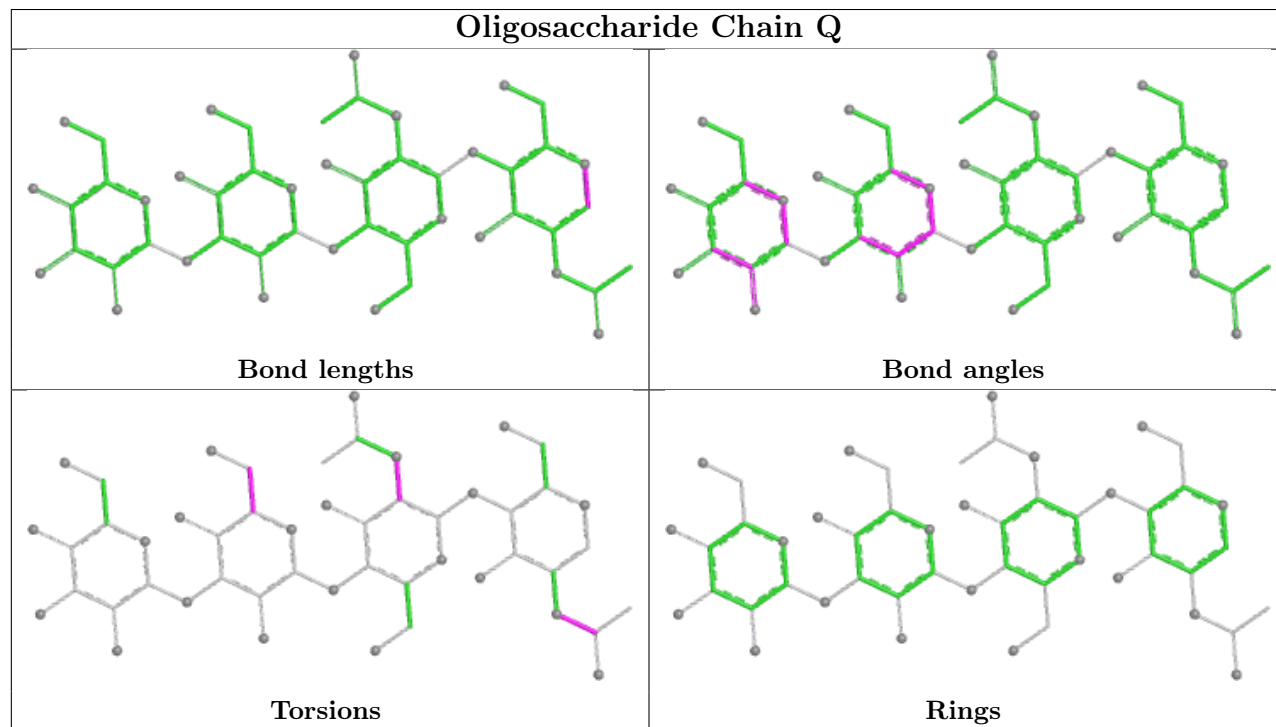


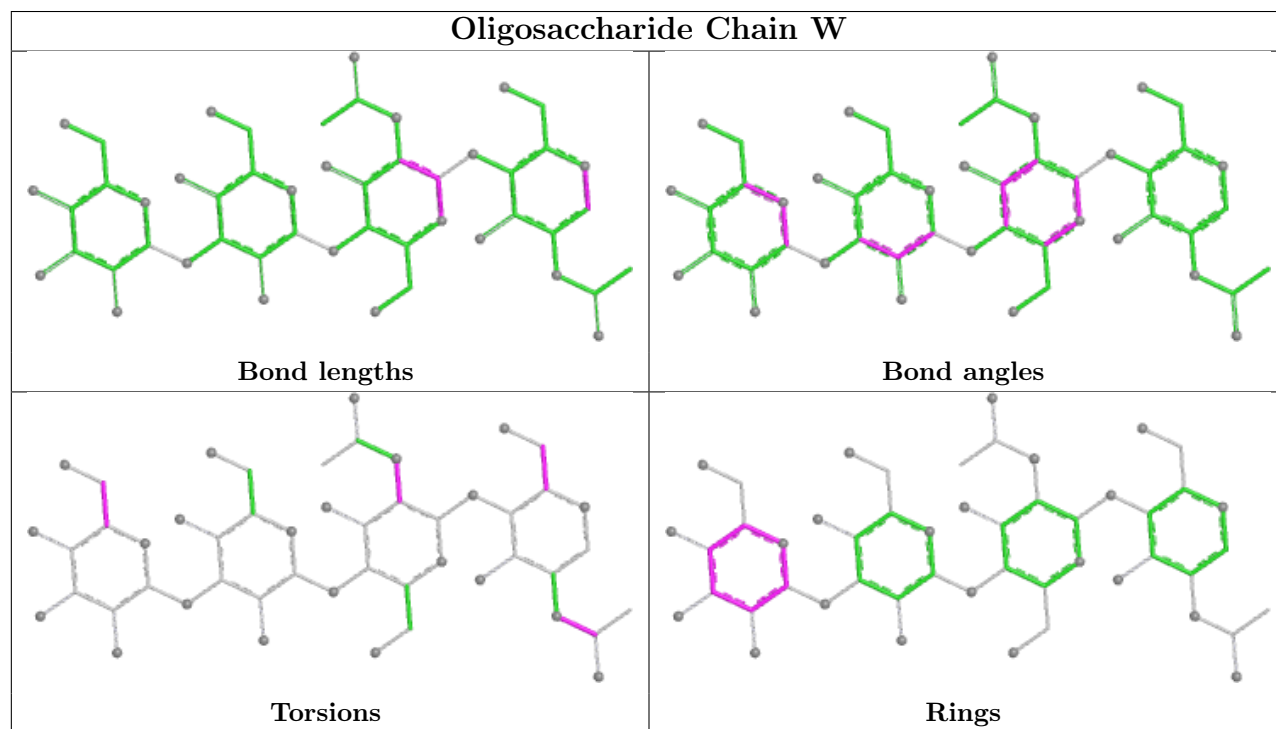
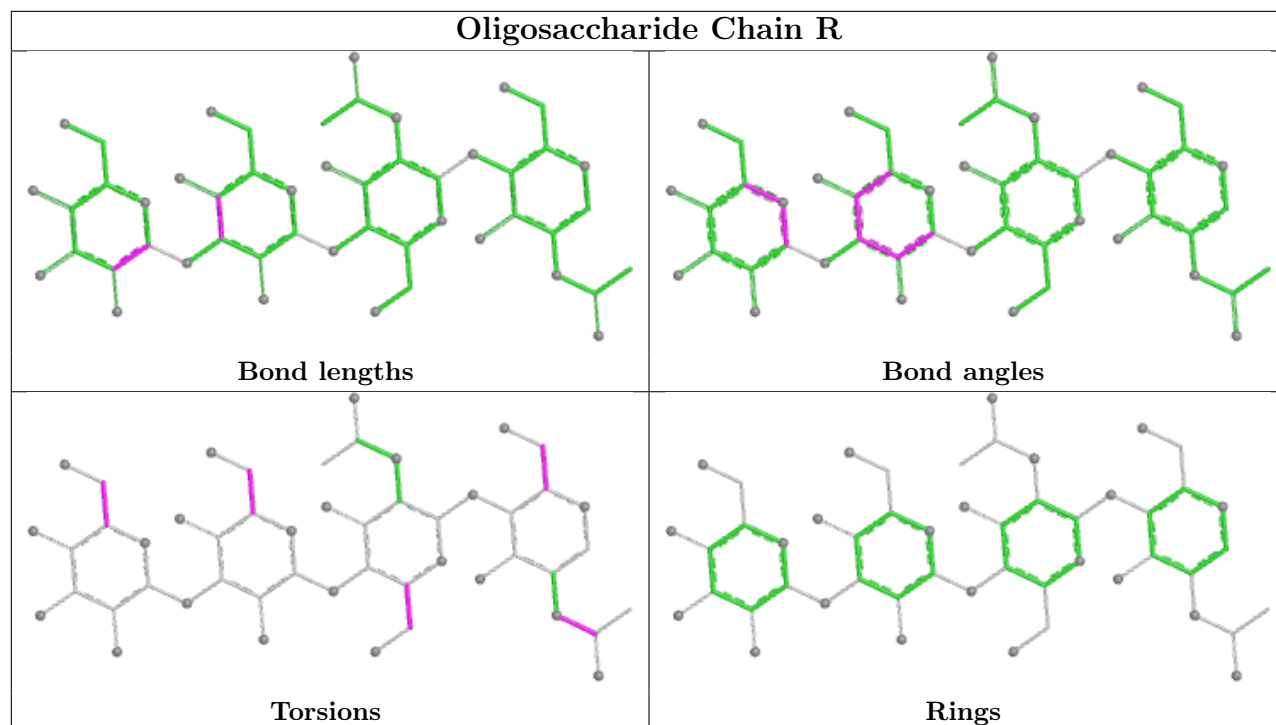


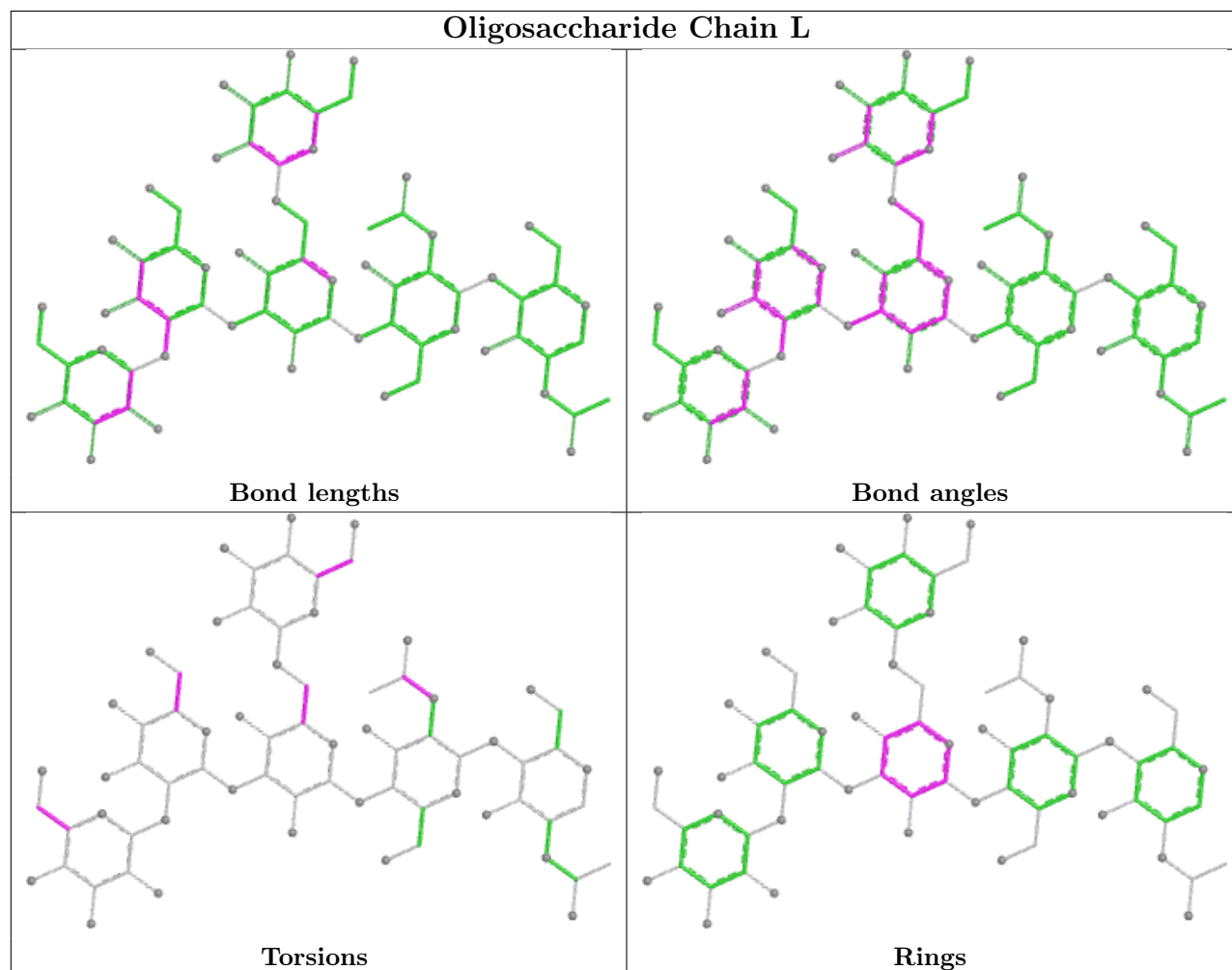
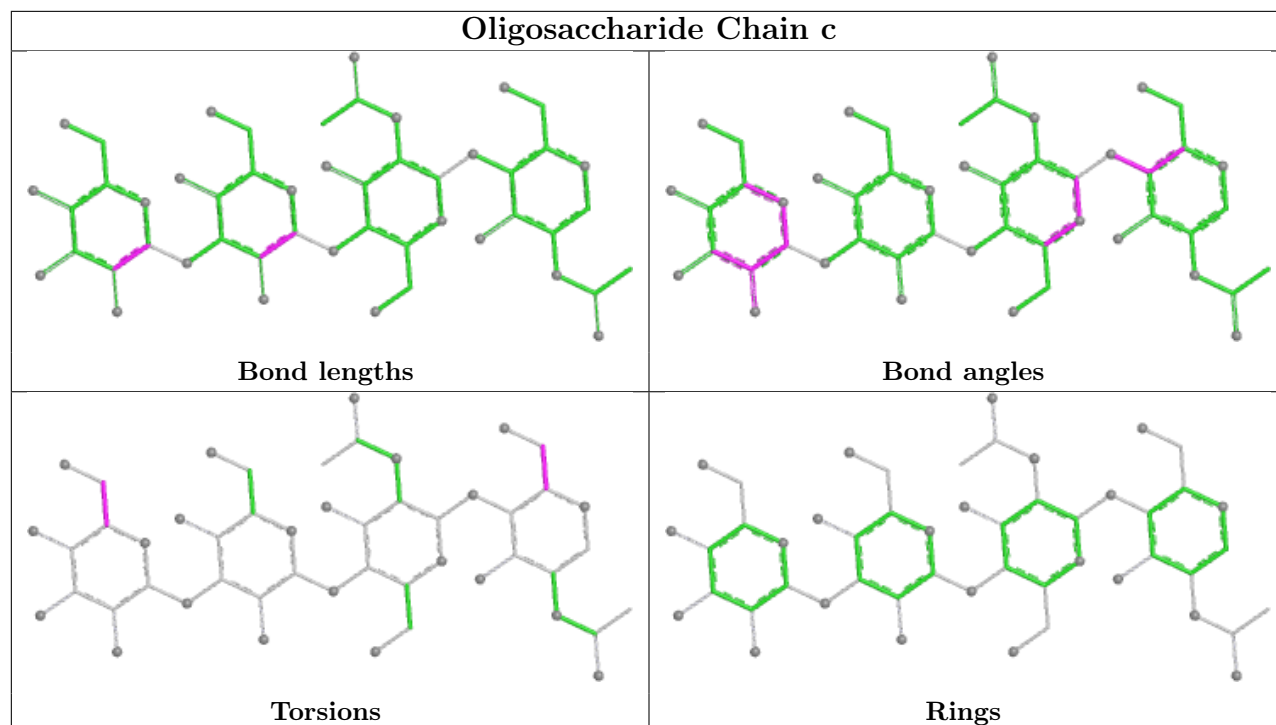
Oligosaccharide Chain K

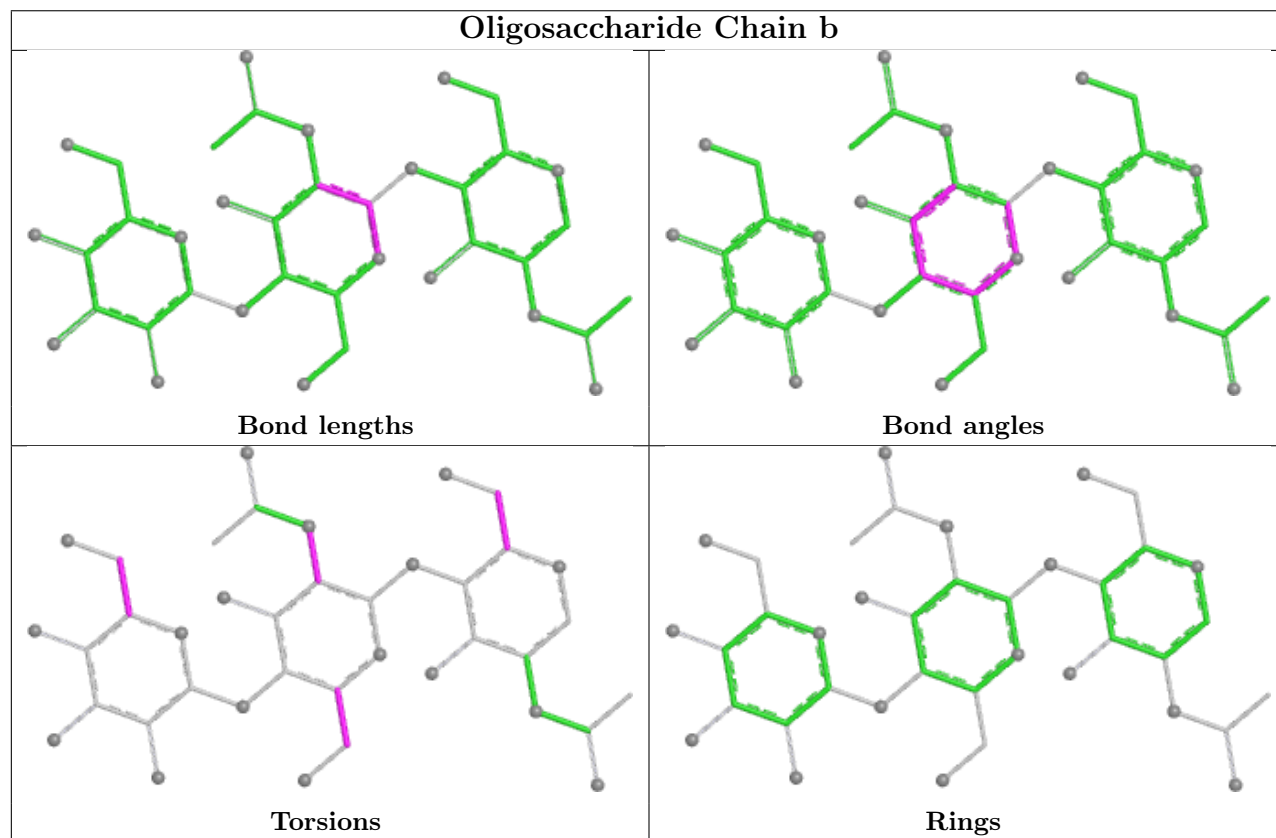
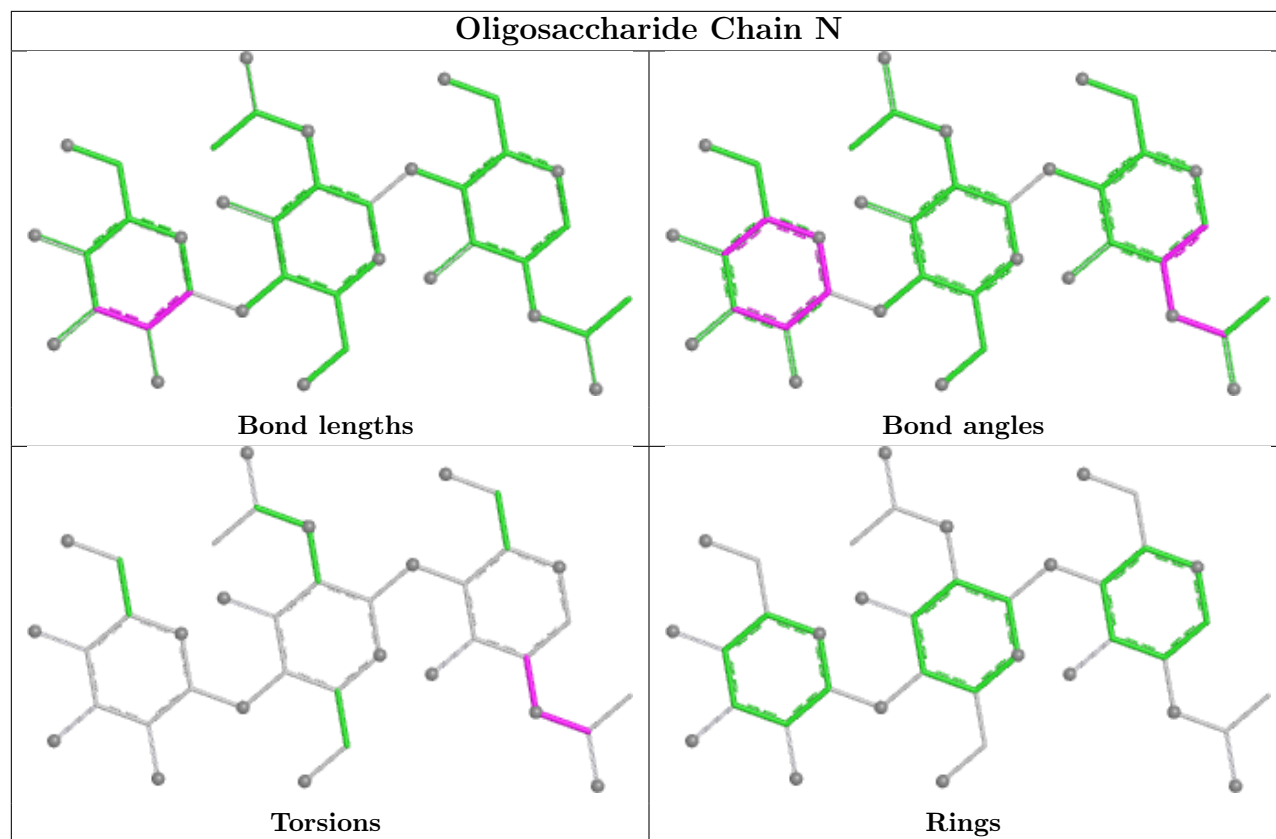


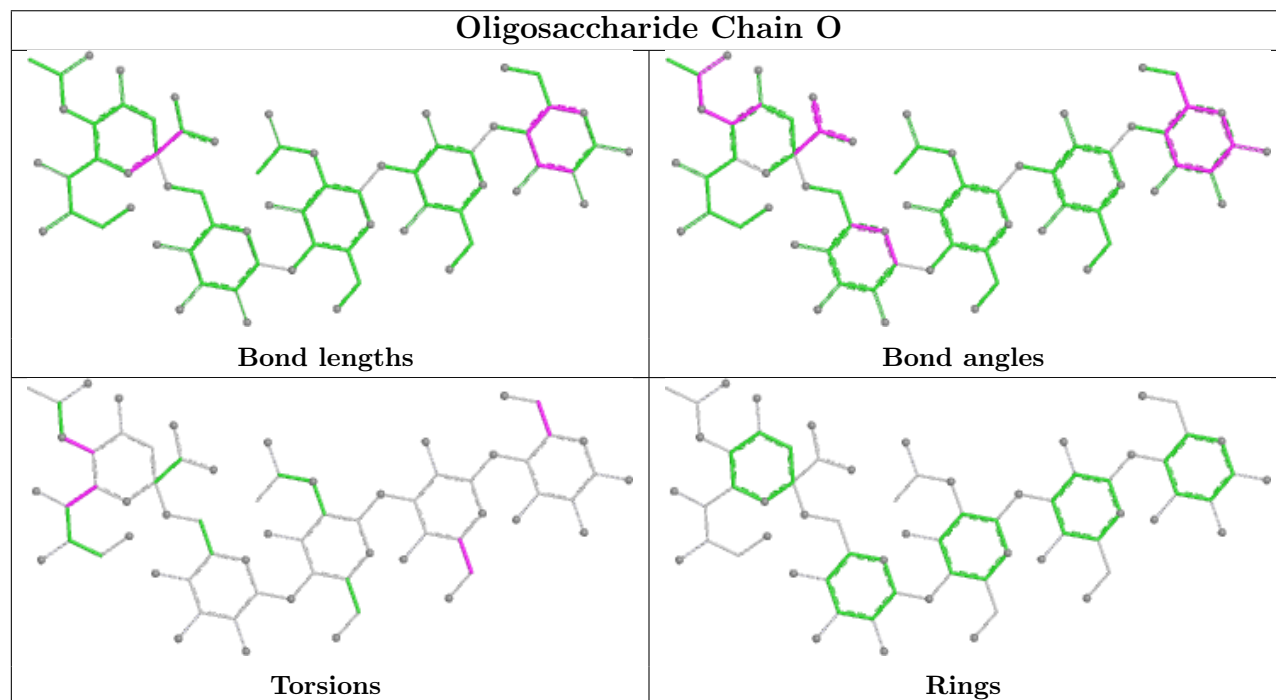
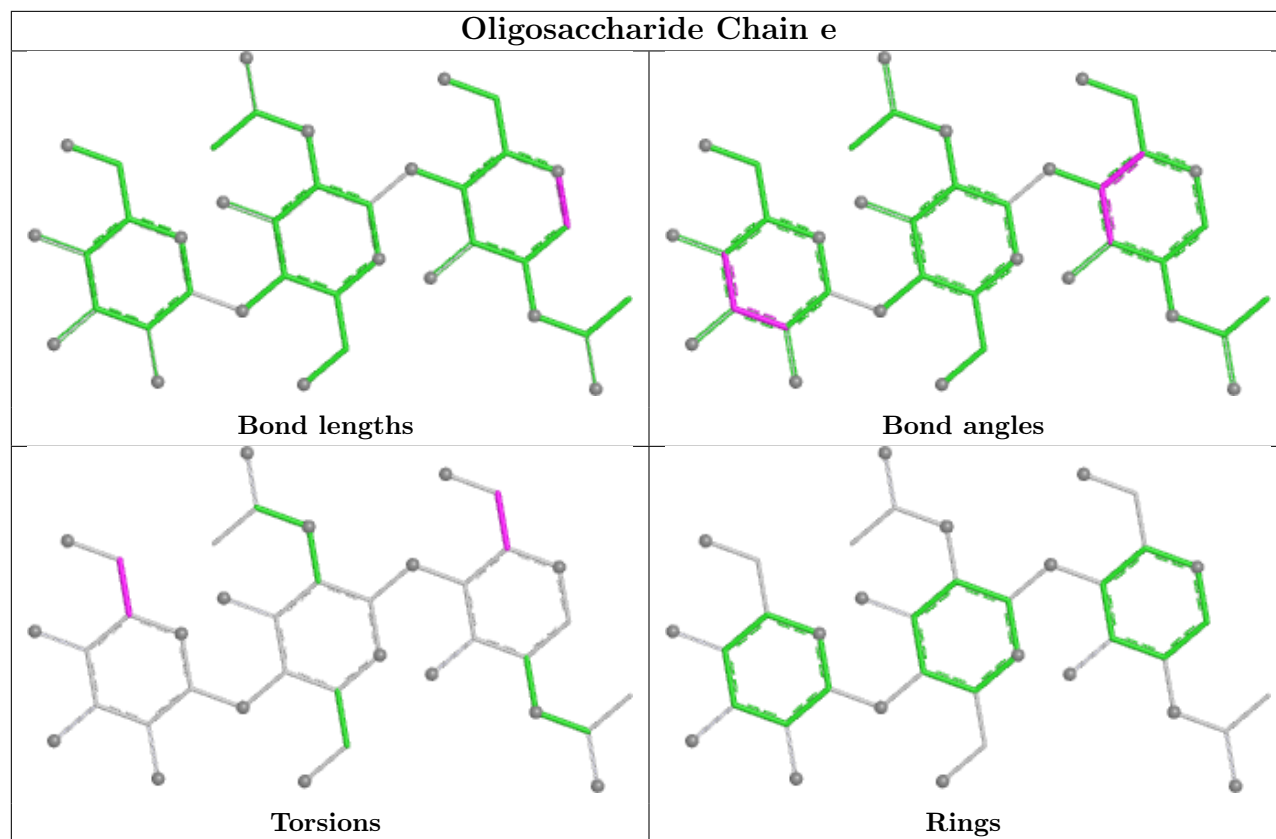
Oligosaccharide Chain Q

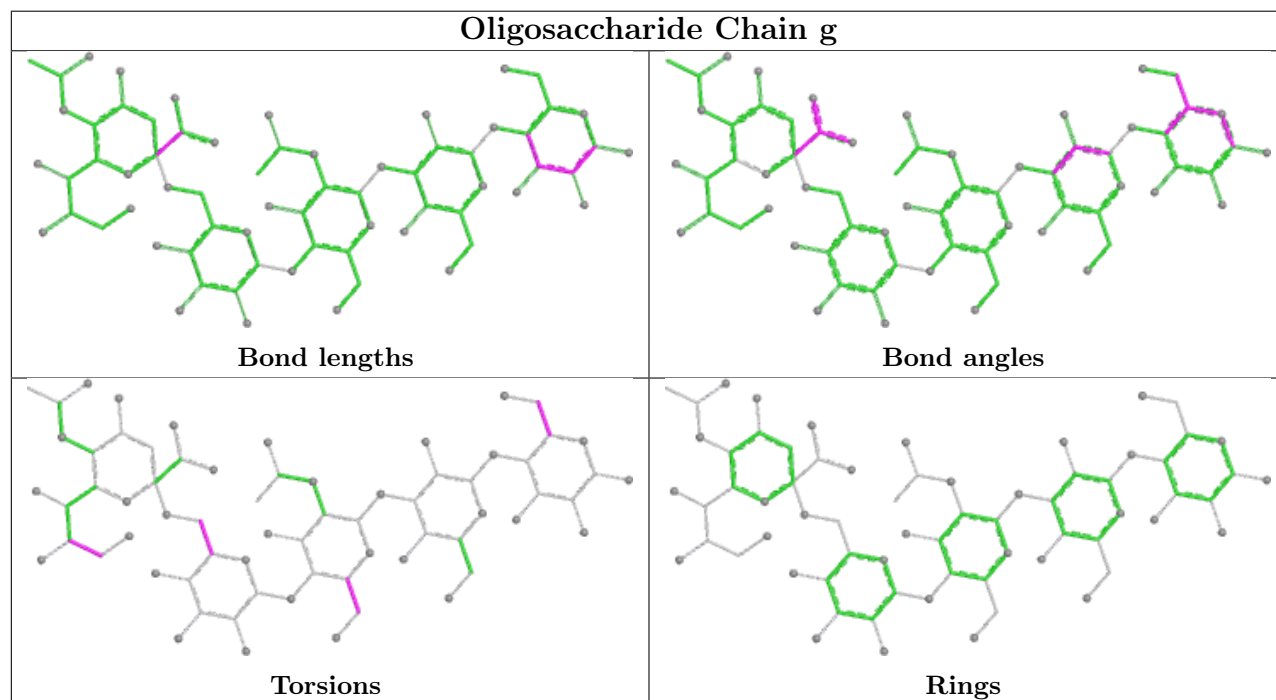
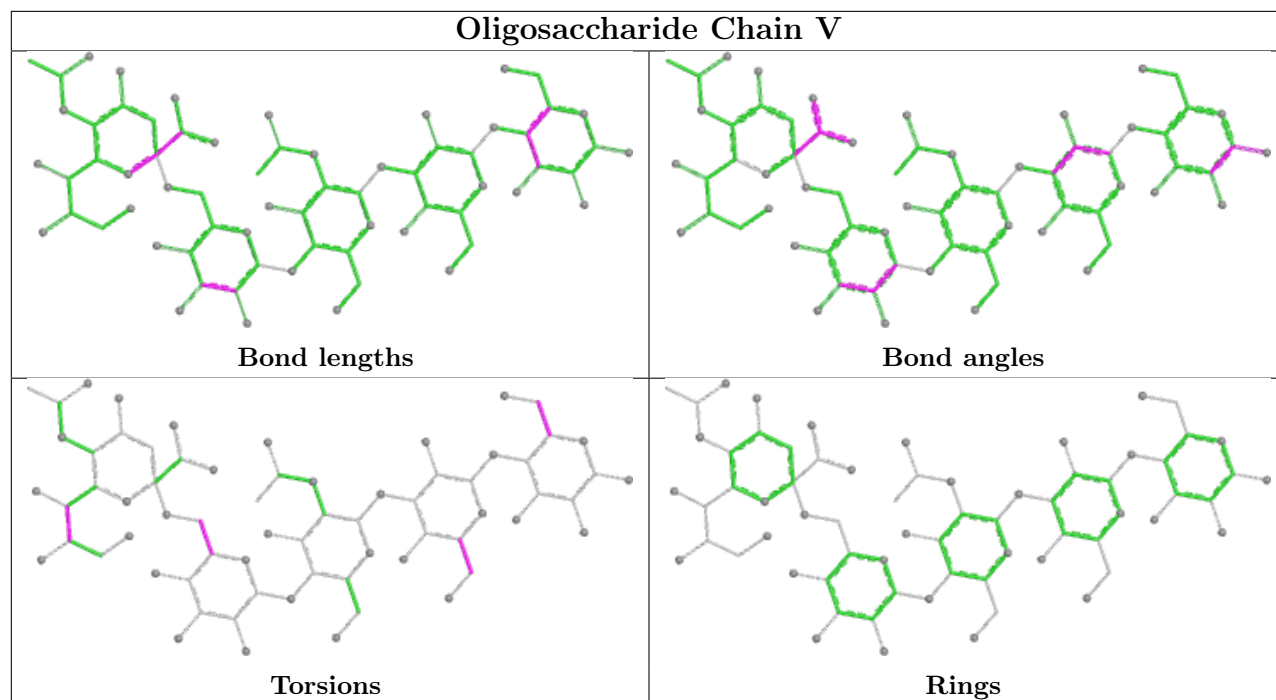


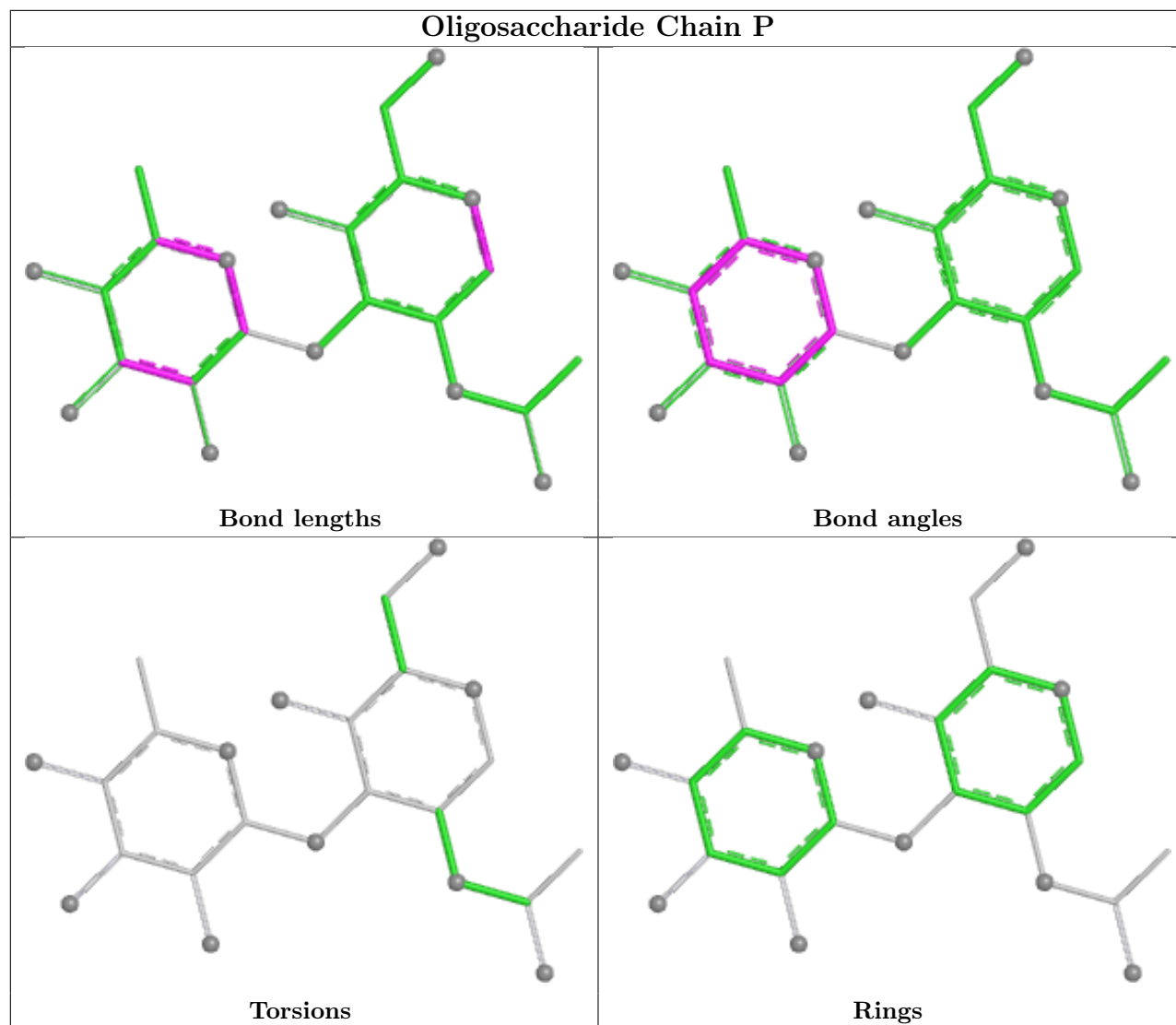


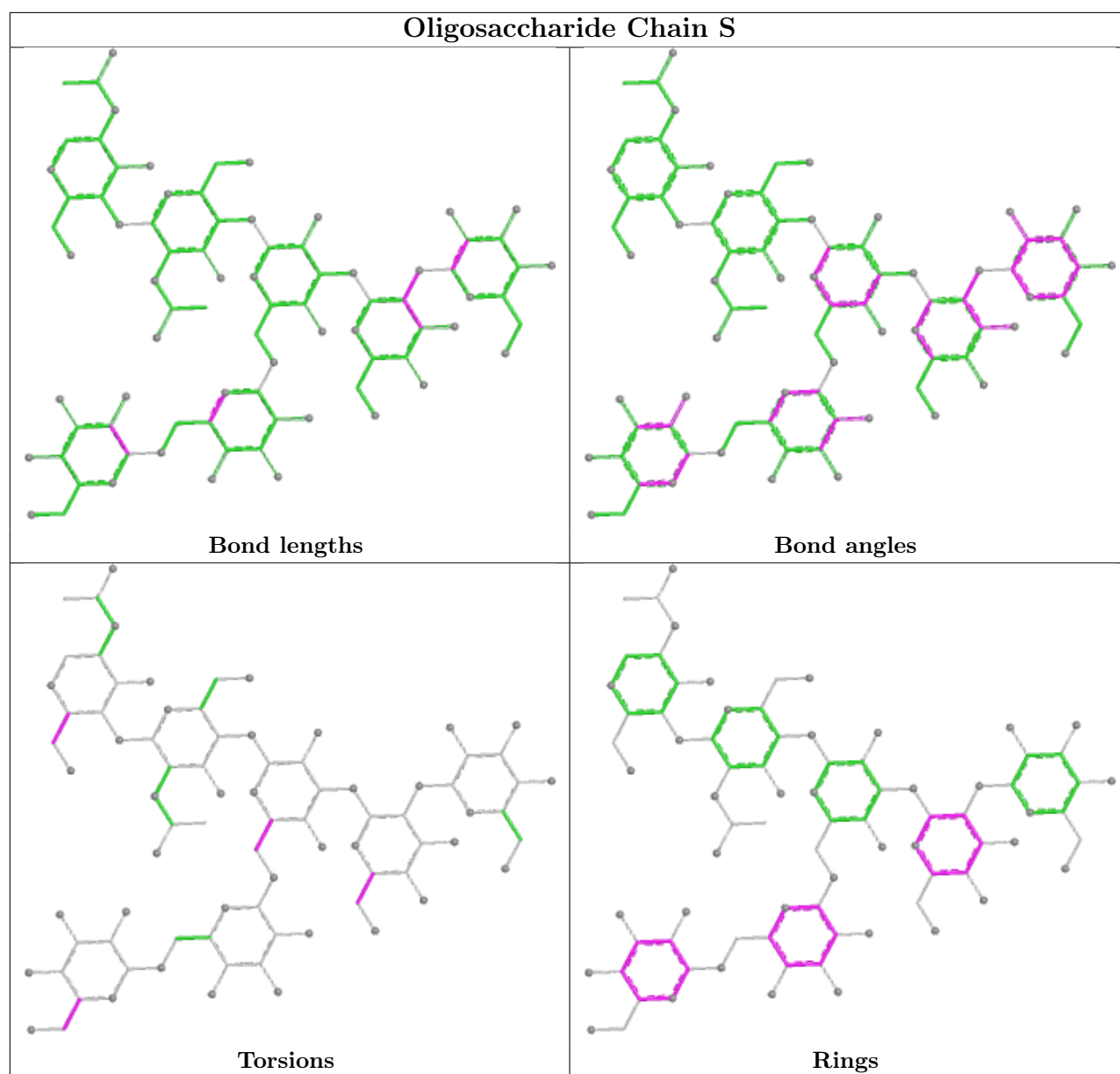


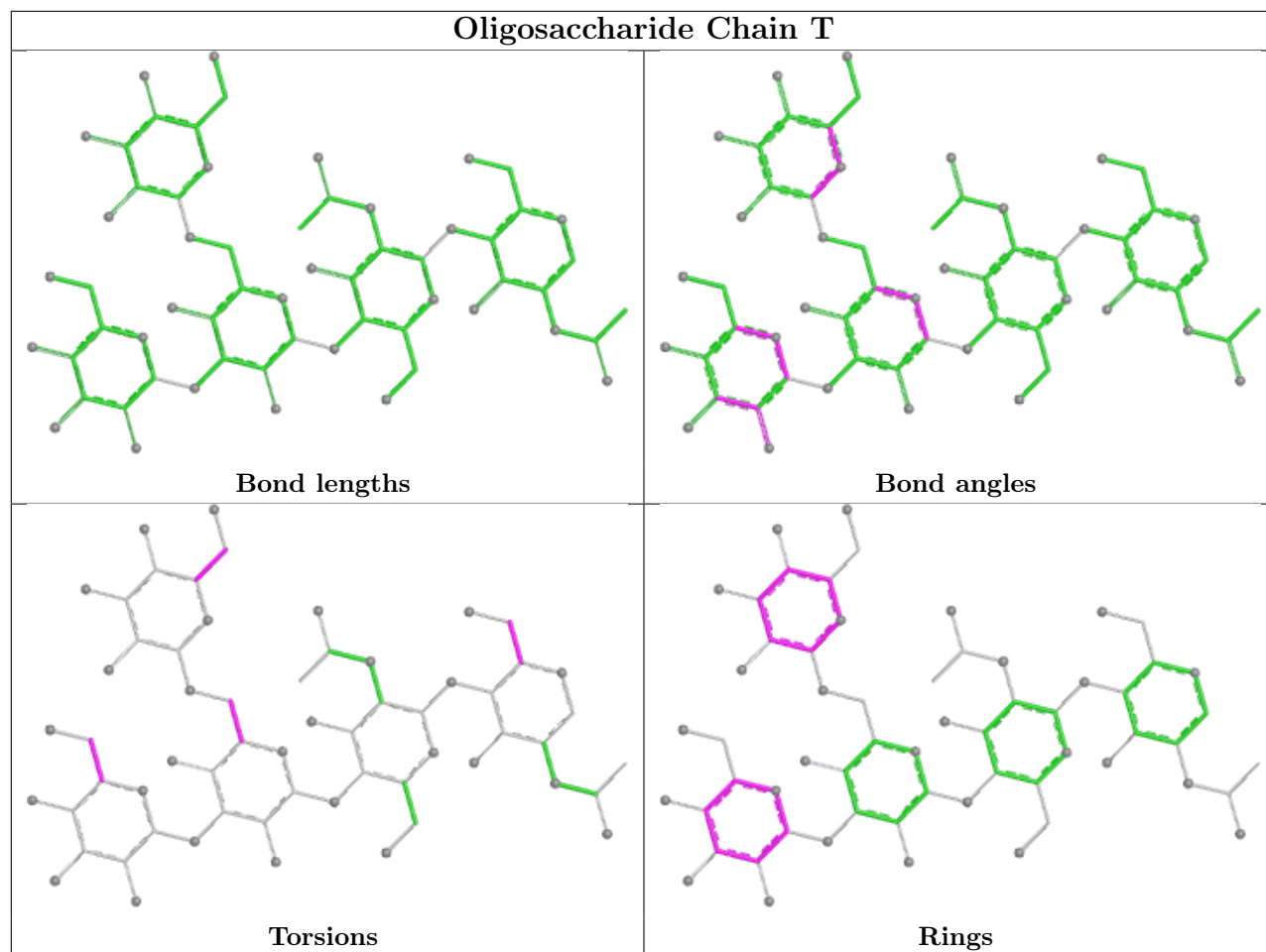


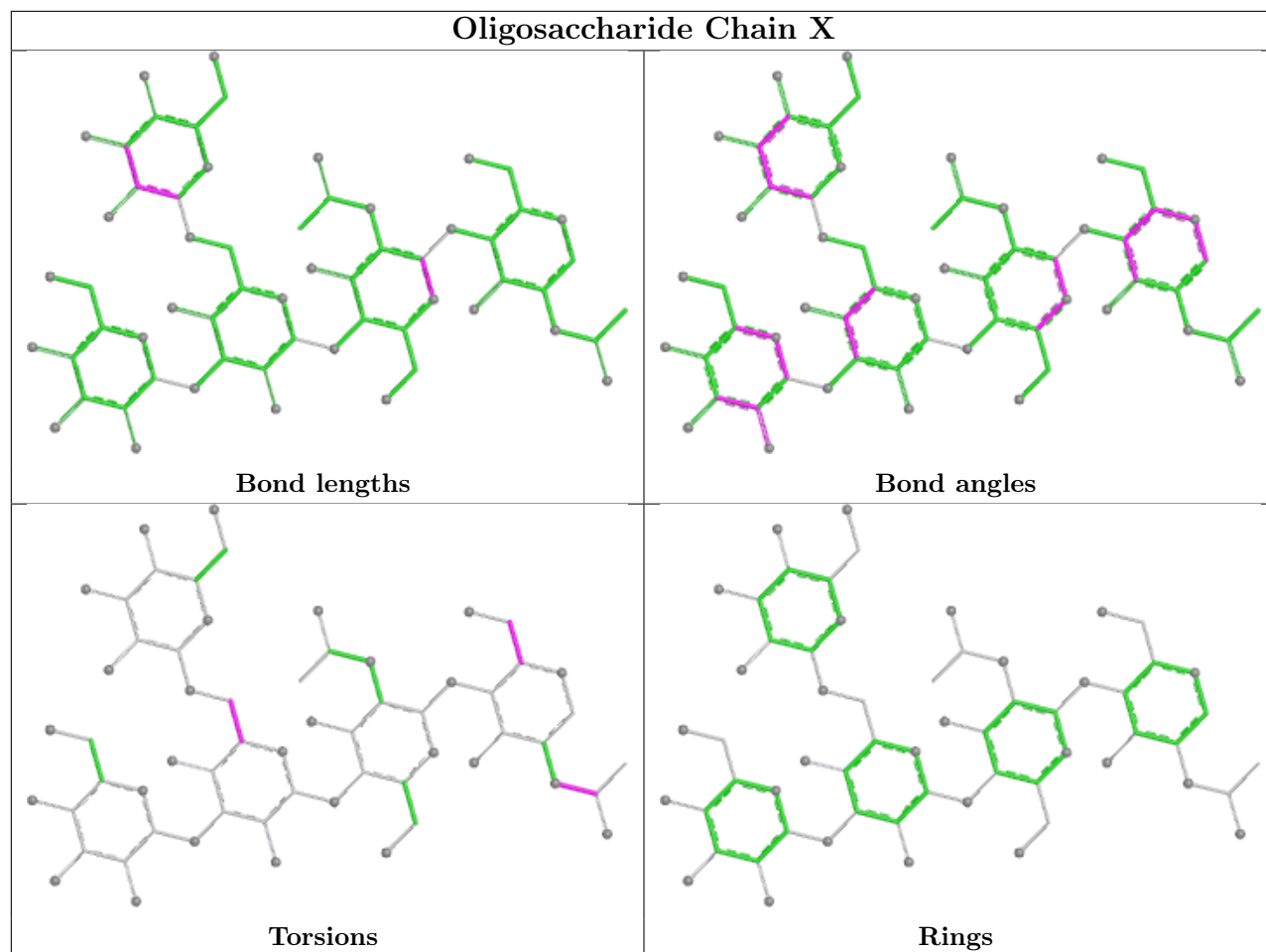


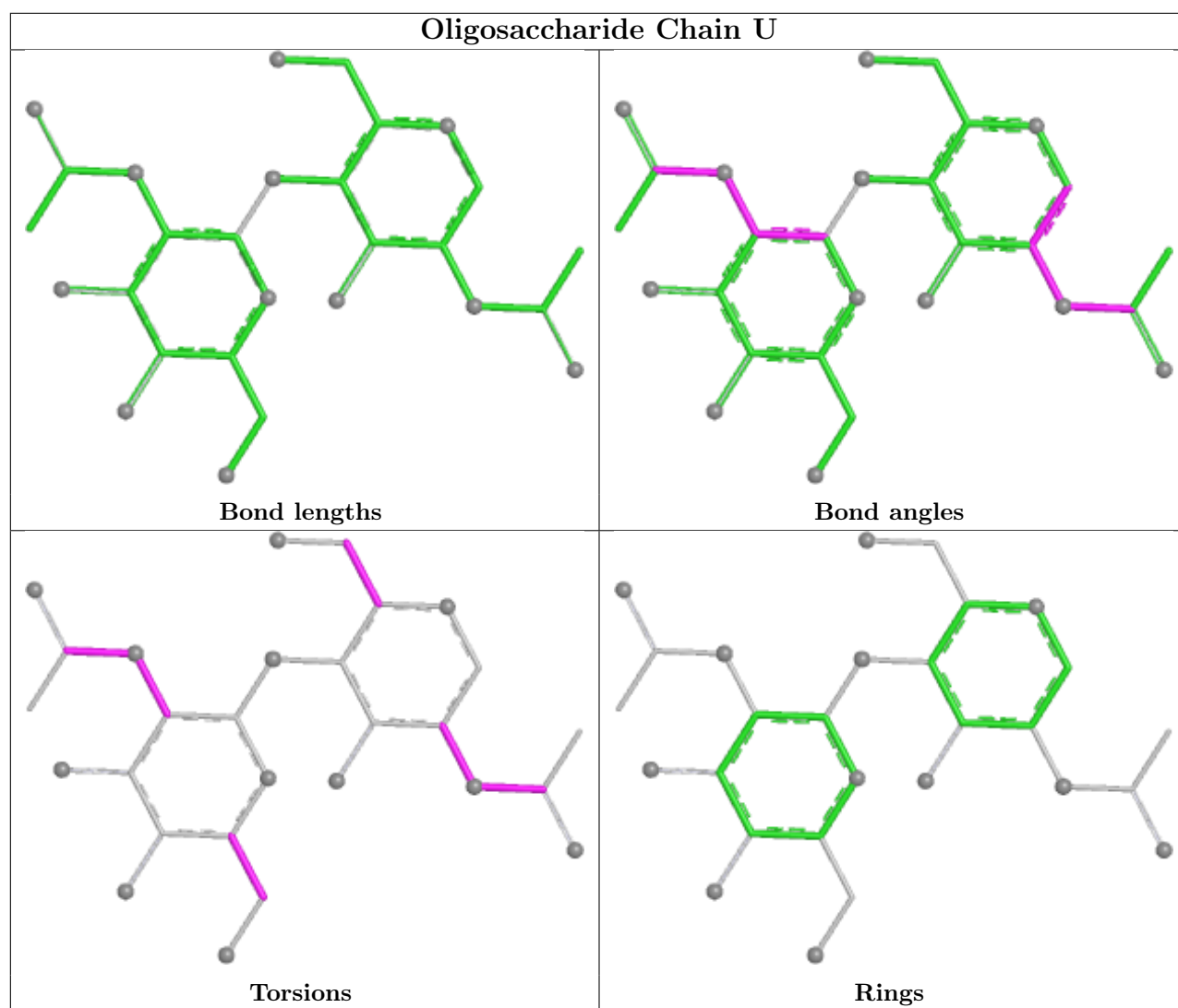


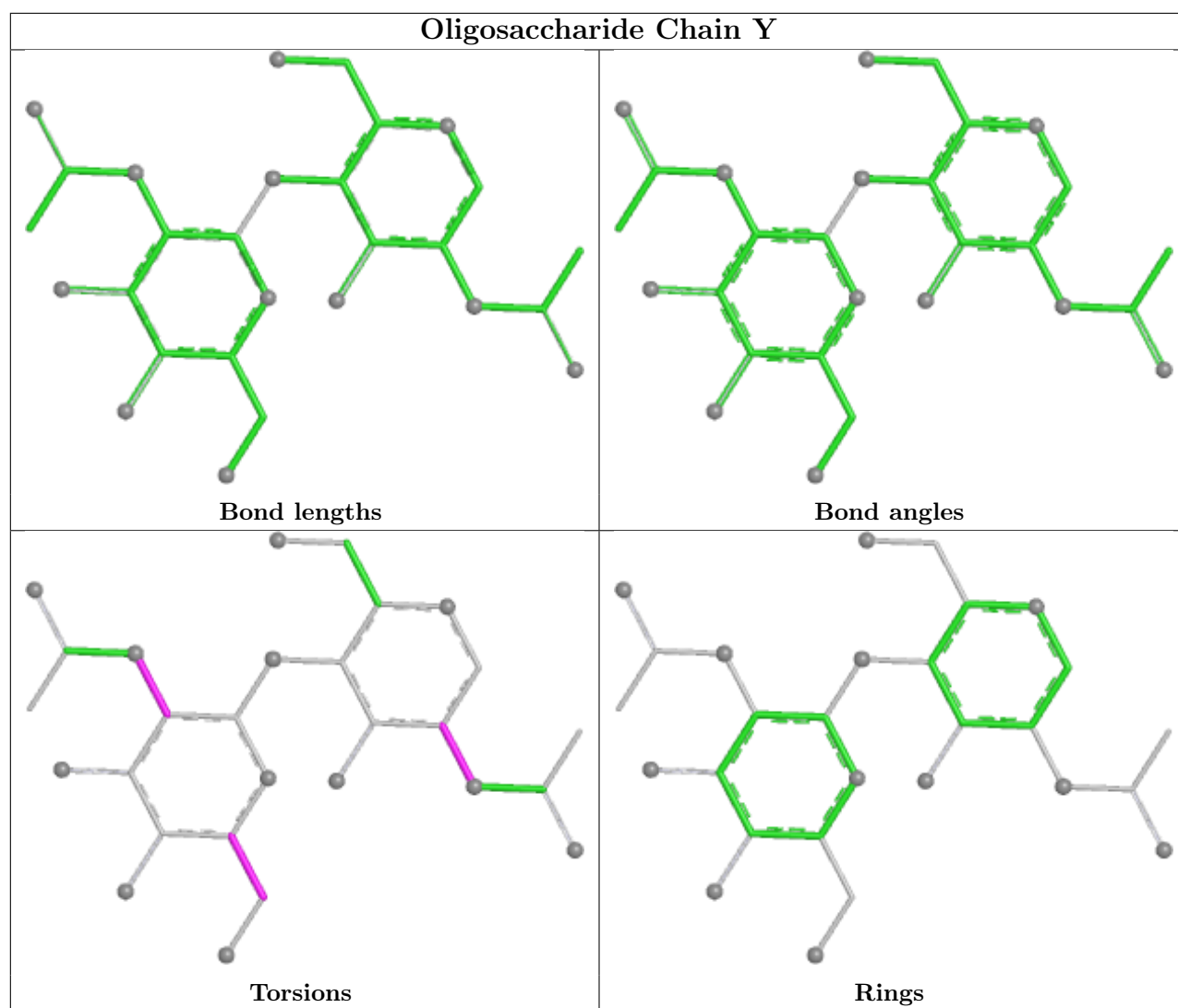


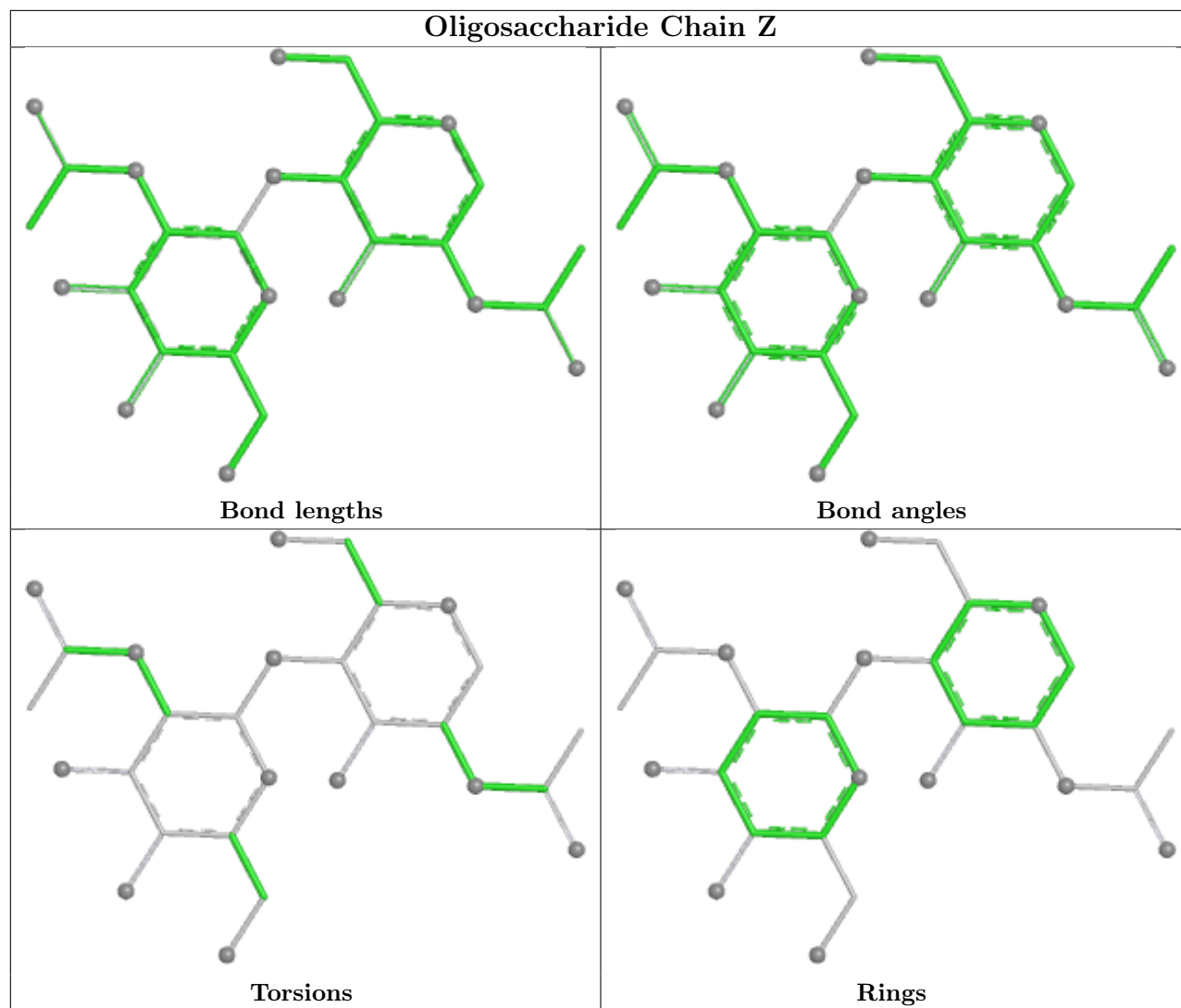


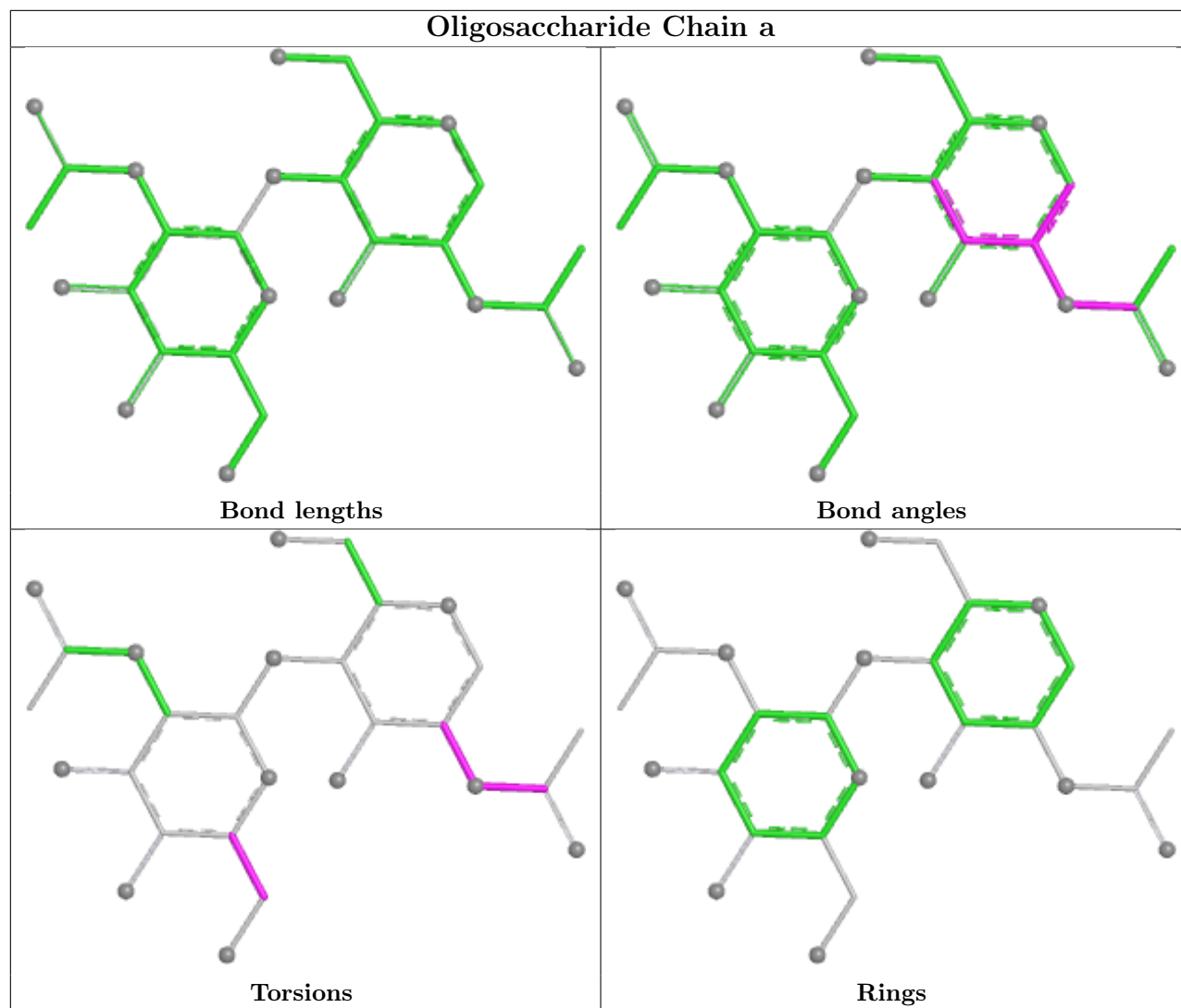


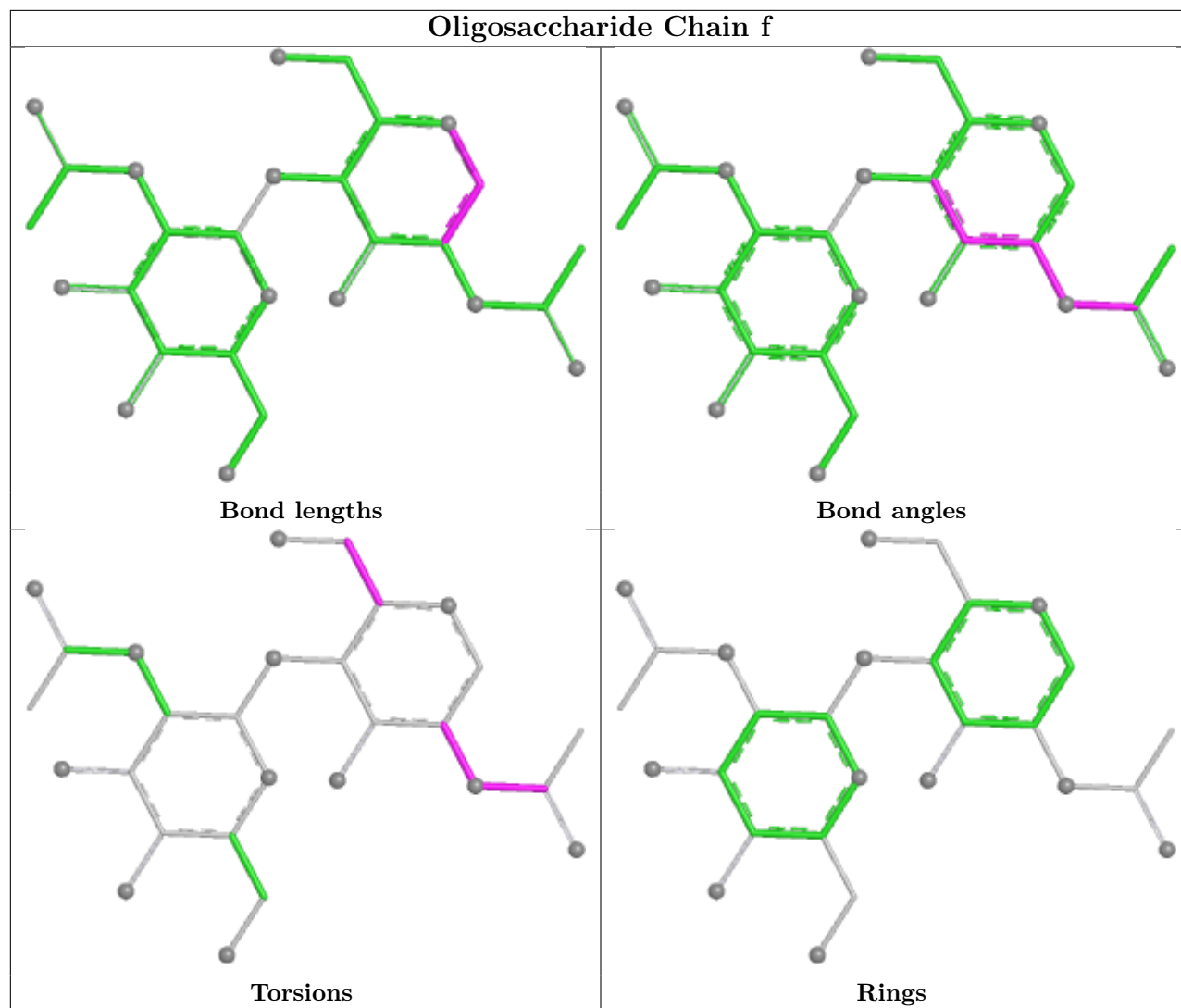


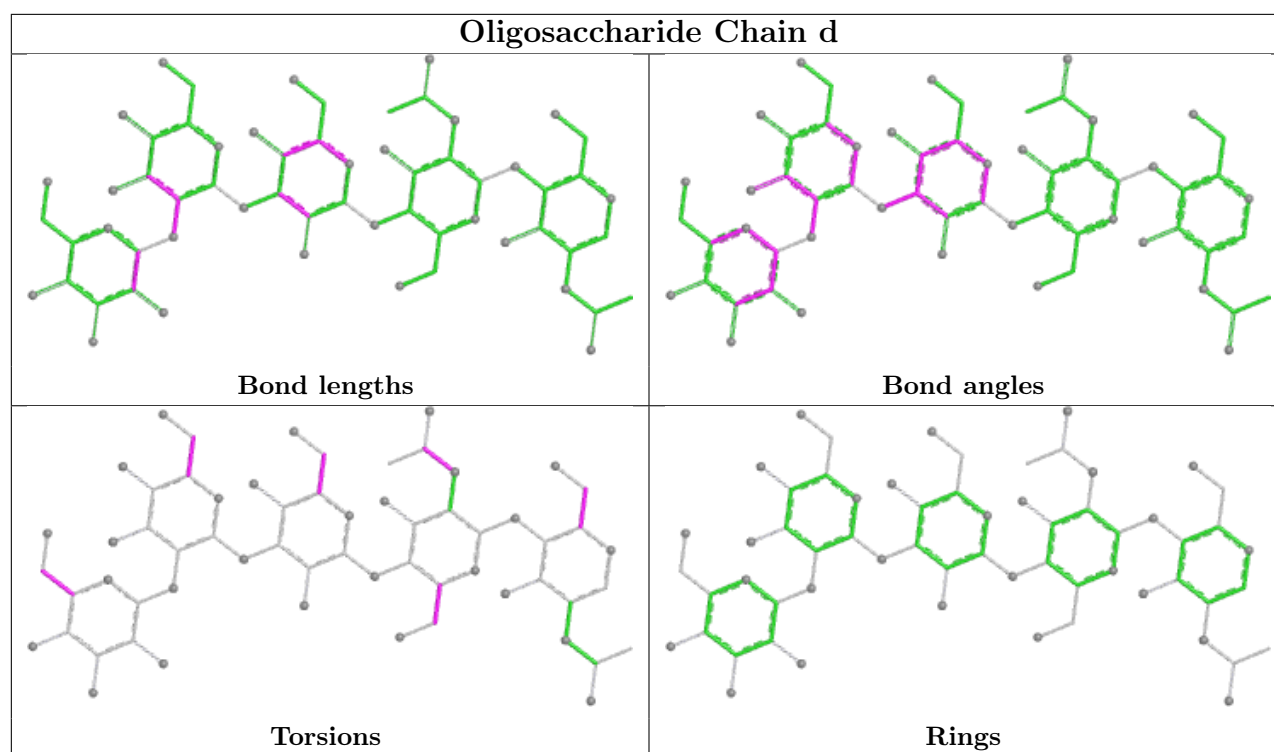












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
14	NAG	C	523	1	14,14,15	0.25	0	17,19,21	1.07	1 (5%)
14	NAG	F	201	2	14,14,15	0.37	0	17,19,21	0.65	1 (5%)
14	NAG	E	414	1	14,14,15	0.38	0	17,19,21	0.53	0
14	NAG	D	202	2	14,14,15	1.09	1 (7%)	17,19,21	0.73	0
14	NAG	A	522	1	14,14,15	0.38	0	17,19,21	0.49	0
15	CAC	D	201	-	2,4,4	2.20	2 (100%)	4,6,6	1.57	1 (25%)
14	NAG	B	201	2	14,14,15	0.51	0	17,19,21	1.26	1 (5%)
14	NAG	G	416	1	14,14,15	1.24	1 (7%)	17,19,21	1.49	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
14	NAG	C	523	1	-	2/6/23/26	0/1/1/1
14	NAG	F	201	2	-	2/6/23/26	0/1/1/1
14	NAG	E	414	1	-	0/6/23/26	0/1/1/1
14	NAG	D	202	2	-	0/6/23/26	0/1/1/1
14	NAG	A	522	1	-	0/6/23/26	0/1/1/1
14	NAG	B	201	2	-	2/6/23/26	0/1/1/1
14	NAG	G	416	1	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	416	NAG	O5-C1	4.44	1.51	1.43
14	D	202	NAG	O5-C1	-3.38	1.38	1.43
15	D	201	CAC	AS-C1	2.34	1.95	1.90
15	D	201	CAC	AS-C2	2.04	1.95	1.90

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	416	NAG	C1-O5-C5	5.90	120.10	112.19
14	B	201	NAG	C1-O5-C5	4.43	118.13	112.19
14	C	523	NAG	C1-O5-C5	3.55	116.95	112.19
15	D	201	CAC	O1-AS-C1	-2.61	108.26	111.50
14	F	201	NAG	C1-O5-C5	2.07	114.97	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	416	NAG	O5-C5-C6-O6
14	B	201	NAG	O5-C5-C6-O6
14	C	523	NAG	O5-C5-C6-O6
14	B	201	NAG	C4-C5-C6-O6
14	G	416	NAG	C4-C5-C6-O6
14	C	523	NAG	C4-C5-C6-O6
14	F	201	NAG	O5-C5-C6-O6
14	F	201	NAG	C4-C5-C6-O6
14	G	416	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 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%)	-0.33	7 (2%) 62 53	36, 63, 116, 177	0
1	C	319/329 (96%)	-0.22	8 (2%) 58 48	46, 76, 116, 186	0
1	E	319/329 (96%)	-0.36	10 (3%) 51 42	52, 74, 111, 178	0
1	G	321/329 (97%)	-0.01	8 (2%) 58 48	53, 92, 173, 245	0
2	B	172/174 (98%)	-0.40	2 (1%) 76 69	38, 60, 100, 139	0
2	D	172/174 (98%)	-0.33	4 (2%) 61 52	25, 76, 116, 163	0
2	F	172/174 (98%)	-0.29	5 (2%) 53 45	40, 71, 109, 160	0
2	H	172/174 (98%)	0.97	30 (17%) 4 3	50, 162, 227, 274	0
All	All	1966/2012 (97%)	-0.15	74 (3%) 44 36	25, 76, 174, 274	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	2	ILE	7.8
2	H	119	PHE	7.4
1	G	13	LEU	6.8
1	A	326	LYS	4.6
2	F	32	THR	4.5
1	G	15	LEU	4.3
2	H	3	PHE	4.1
1	G	328	THR	4.1
2	H	135	ASN	4.1
1	A	10	MET	4.0
2	H	41	THR	3.6
2	D	58	LYS	3.4
1	E	326	LYS	3.3
1	A	8	ASN	3.3
2	H	152	ILE	3.2
1	E	10	MET	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	9	PHE	3.2
1	A	199	SER	3.2
2	B	139	LYS	3.2
2	H	171	PHE	3.1
1	G	221	PRO	3.1
1	E	9	SER	3.0
2	H	121	ARG	3.0
1	E	8	ASN	3.0
2	H	134	GLY	2.9
2	H	161	ILE	2.9
2	H	123	ARG	2.8
2	H	35	ALA	2.8
1	C	142	GLY	2.8
2	D	172	GLN	2.8
1	A	221	PRO	2.8
1	C	276	GLU	2.7
2	D	2	ILE	2.7
2	H	126	LEU	2.7
2	F	31	GLY	2.7
2	H	128	GLU	2.7
2	D	154	ASN	2.7
2	H	122	THR	2.6
2	H	109	ASP	2.6
1	C	10	MET	2.5
1	E	199	SER	2.5
1	G	262	SER	2.5
2	H	1	GLY	2.5
2	H	52	LEU	2.4
2	F	2	ILE	2.4
1	G	199	SER	2.4
2	H	124	ARG	2.4
1	E	11	ALA	2.4
1	C	104	ASP	2.4
2	B	59	THR	2.4
2	H	120	GLU	2.3
2	F	57	LYS	2.3
1	C	101	TYR	2.3
2	H	59	THR	2.3
2	H	157	TYR	2.3
2	H	147	ALA	2.3
1	C	326	LYS	2.3
1	E	14	CYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	133	MET	2.2
1	C	277	CYS	2.2
1	E	242	ILE	2.2
1	A	104	ASP	2.2
1	E	104	ASP	2.1
2	H	111	THR	2.1
2	H	129	ASN	2.1
1	G	175	ASP	2.1
1	G	14	CYS	2.1
2	H	58	LYS	2.1
2	H	132	ASP	2.1
2	H	113	SER	2.0
1	C	208	ARG	2.0
1	E	12	THR	2.0
2	F	27	GLN	2.0
1	A	144	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

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
11	MAN	T	5	11/12	0.08	0.18	150,179,184,186	0
5	BMA	W	3	11/12	0.23	0.13	196,199,202,203	0
6	MAN	L	4	11/12	0.33	0.10	170,179,185,190	0
4	MAN	M	4	11/12	0.33	0.13	142,159,173,180	0
5	BMA	Q	3	11/12	0.41	0.12	197,204,208,208	0
12	NAG	U	2	14/15	0.42	0.14	147,171,181,182	0
5	MAN	W	4	11/12	0.43	0.10	167,187,193,194	0
5	BMA	K	3	11/12	0.44	0.10	144,171,177,178	0
4	BMA	J	3	11/12	0.45	0.12	143,161,171,185	0
4	BMA	M	3	11/12	0.45	0.10	185,198,205,205	0
5	MAN	R	4	11/12	0.47	0.13	164,184,193,194	0
3	FUL	I	2	10/11	0.47	0.16	151,161,168,176	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	BMA	N	3	11/12	0.48	0.11	175,201,208,210	0
10	MAN	S	7	11/12	0.50	0.11	181,183,188,189	0
11	MAN	X	5	11/12	0.54	0.15	114,133,140,141	0
4	MAN	J	4	11/12	0.54	0.12	147,161,172,176	0
7	NAG	N	2	14/15	0.56	0.13	138,187,202,212	0
11	MAN	X	4	11/12	0.57	0.13	104,160,175,176	0
12	NAG	Y	2	14/15	0.57	0.11	178,182,187,189	0
11	BMA	T	3	11/12	0.58	0.10	172,186,187,189	0
5	MAN	Q	4	11/12	0.59	0.08	180,193,203,203	0
11	MAN	T	4	11/12	0.61	0.11	137,173,185,188	0
5	MAN	K	4	11/12	0.61	0.11	140,160,169,170	0
5	NAG	K	2	14/15	0.63	0.11	112,135,147,164	0
10	MAN	S	5	11/12	0.64	0.08	137,162,168,170	0
11	BMA	X	3	11/12	0.64	0.12	138,156,162,164	0
10	MAN	S	6	11/12	0.65	0.11	155,172,181,182	0
5	NAG	c	1	14/15	-	-	108,131,147,155	0
5	NAG	c	2	14/15	-	-	123,161,177,191	0
5	BMA	c	3	11/12	-	-	161,186,195,195	0
5	MAN	c	4	11/12	-	-	153,179,183,185	0
6	MAN	L	6	11/12	0.65	0.09	147,160,167,167	0
12	NAG	Z	2	14/15	0.65	0.12	156,192,207,214	0
12	NAG	Y	1	14/15	0.66	0.12	113,148,163,167	0
9	FUL	P	2	10/11	0.68	0.14	179,182,184,185	0
6	MAN	L	5	11/12	0.68	0.09	132,170,178,178	0
10	MAN	S	4	11/12	0.69	0.08	141,169,172,177	0
5	NAG	Q	2	14/15	0.71	0.12	129,175,188,197	0
9	NAG	P	1	14/15	0.72	0.13	136,162,179,196	0
4	NAG	M	2	14/15	0.72	0.14	112,171,187,198	0
7	NAG	b	1	14/15	-	-	144,171,190,199	0
7	NAG	b	2	14/15	-	-	166,205,210,210	0
7	BMA	b	3	11/12	-	-	167,179,193,193	0
7	NAG	e	1	14/15	-	-	98,114,130,147	0
7	NAG	e	2	14/15	-	-	86,155,172,177	0
7	BMA	e	3	11/12	-	-	153,178,185,186	0
3	FUC	I	3	10/11	0.73	0.12	139,152,159,161	0
8	BGC	V	1	12/12	0.73	0.10	129,146,153,155	0
7	NAG	N	1	14/15	0.76	0.13	100,128,154,176	0
5	NAG	W	1	14/15	0.77	0.14	100,121,145,165	0
11	NAG	T	2	14/15	0.77	0.12	97,158,173,184	0
5	BMA	R	3	11/12	0.78	0.08	122,160,173,187	0
8	NAG	V	3	14/15	0.79	0.09	76,124,140,140	0
3	NAG	I	1	14/15	0.80	0.13	131,141,150,153	0

Continued on next page...

Continued from previous page...

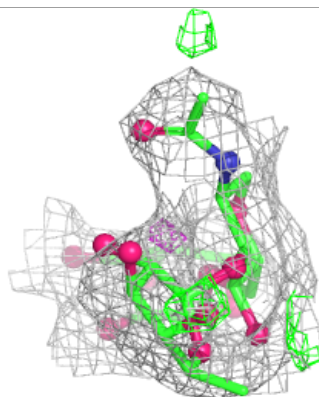
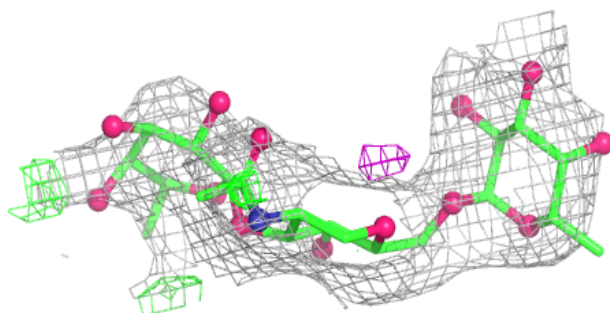
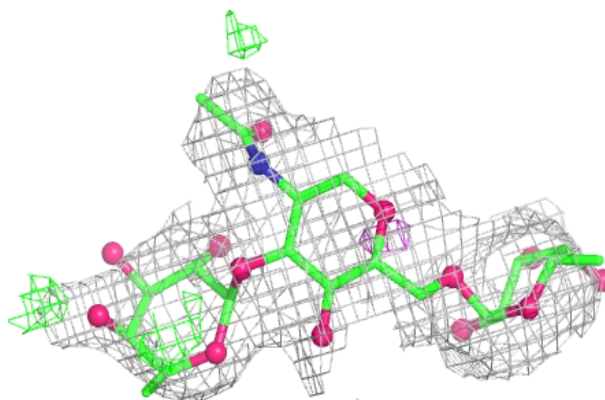
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GAL	V	2	11/12	0.80	0.08	105,138,153,154	0
5	NAG	W	2	14/15	0.82	0.13	132,167,182,192	0
8	BGC	g	1	12/12	-	-	167,182,186,189	0
8	GAL	g	2	11/12	-	-	162,174,179,180	0
8	NAG	g	3	14/15	-	-	150,166,172,173	0
8	GAL	g	4	11/12	-	-	142,149,154,154	0
8	SIA	g	5	20/21	-	-	107,142,149,149	0
12	NAG	U	1	14/15	0.82	0.13	125,135,156,170	0
11	NAG	T	1	14/15	0.82	0.15	85,98,117,132	0
5	NAG	Q	1	14/15	0.83	0.11	82,95,125,148	0
4	NAG	M	1	14/15	0.83	0.11	78,98,119,147	0
8	BGC	O	1	12/12	0.83	0.08	101,129,142,144	0
5	NAG	R	2	14/15	0.83	0.11	102,126,149,158	0
6	NAG	L	2	14/15	0.83	0.13	98,113,136,138	0
11	NAG	X	2	14/15	0.84	0.13	77,107,124,128	0
6	MAN	L	3	11/12	0.85	0.07	153,158,164,175	0
8	GAL	V	4	11/12	0.85	0.08	113,124,135,139	0
10	MAN	S	3	11/12	0.85	0.10	101,135,153,160	0
4	NAG	J	1	14/15	0.86	0.11	66,77,101,114	0
12	NAG	Z	1	14/15	0.87	0.10	104,115,130,152	0
5	NAG	K	1	14/15	0.87	0.12	93,107,114,123	0
4	NAG	J	2	14/15	0.88	0.12	94,121,136,150	0
8	GAL	O	2	11/12	0.88	0.07	97,111,116,118	0
5	NAG	R	1	14/15	0.89	0.14	102,126,141,150	0
6	NAG	L	1	14/15	0.90	0.09	71,83,106,109	0
8	SIA	V	5	20/21	0.90	0.13	86,110,139,139	0
10	NAG	S	1	14/15	0.91	0.18	50,82,109,110	0
11	NAG	X	1	14/15	0.91	0.10	84,103,114,115	0
10	NAG	S	2	14/15	0.92	0.12	87,103,115,137	0
8	NAG	O	3	14/15	0.92	0.08	73,98,108,115	0
8	SIA	O	5	20/21	0.94	0.08	67,89,119,129	0
8	GAL	O	4	11/12	0.95	0.05	71,77,91,99	0
12	NAG	a	1	14/15	-	-	102,121,148,167	0
12	NAG	a	2	14/15	-	-	124,169,182,185	0
12	NAG	f	1	14/15	-	-	110,142,172,184	0
12	NAG	f	2	14/15	-	-	136,171,182,184	0
13	NAG	d	1	14/15	-	-	86,101,119,123	0
13	NAG	d	2	14/15	-	-	108,130,159,166	0
13	MAN	d	3	11/12	-	-	164,177,193,200	0
13	MAN	d	4	11/12	-	-	160,181,191,196	0
13	MAN	d	5	11/12	-	-	163,174,189,190	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.

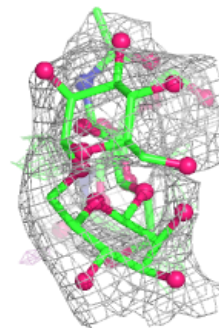
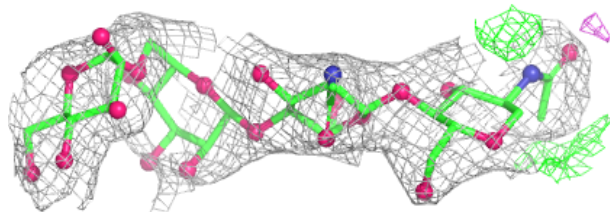
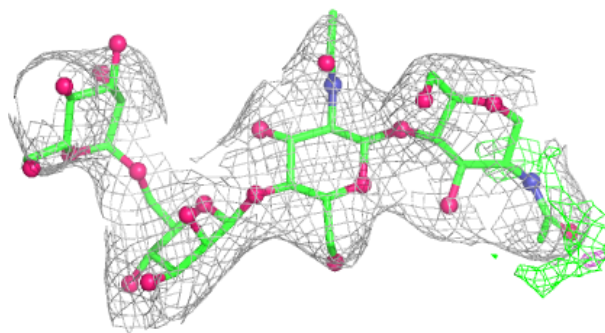
Electron density around Chain I:

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



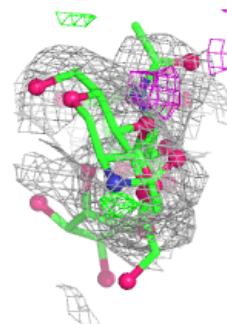
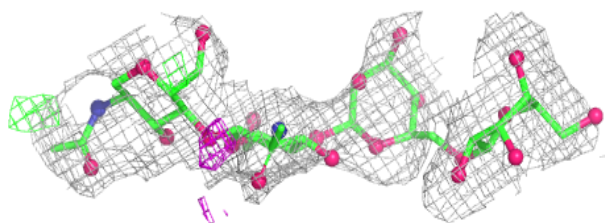
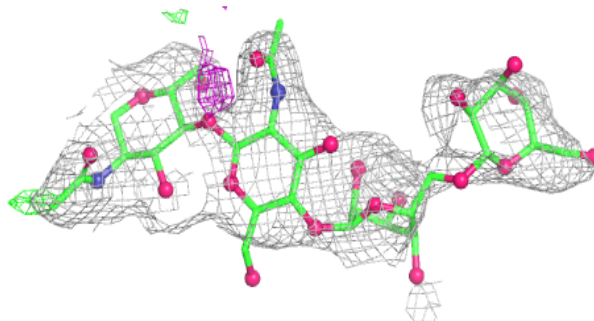
Electron density around Chain J:

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

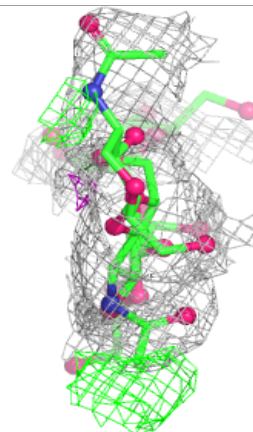
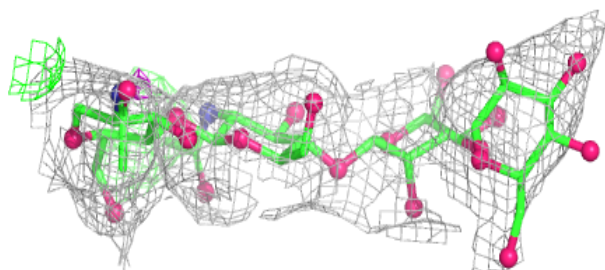
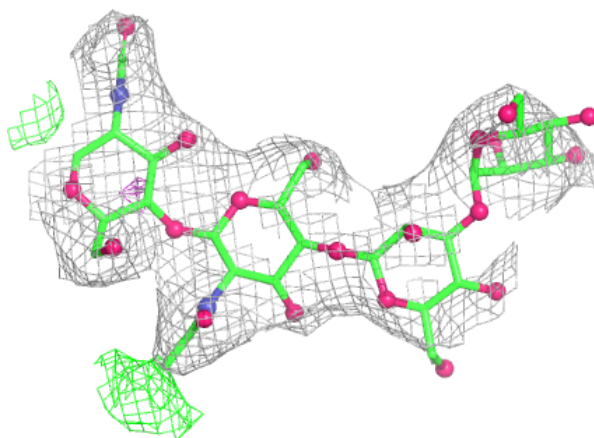


Electron density around Chain M:

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

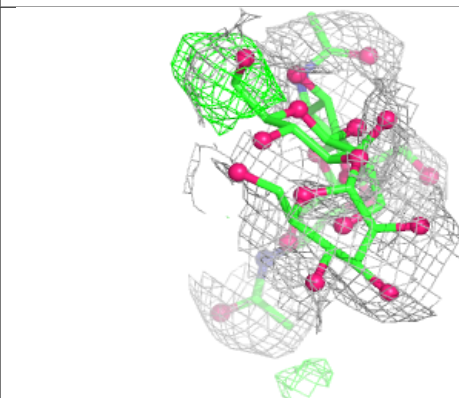
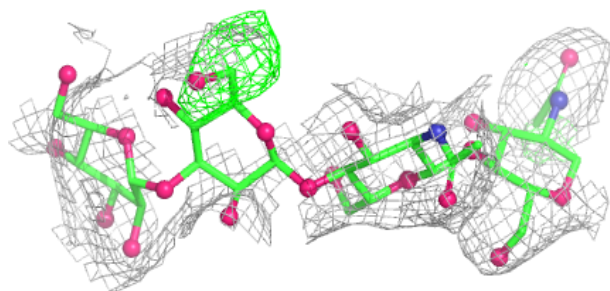
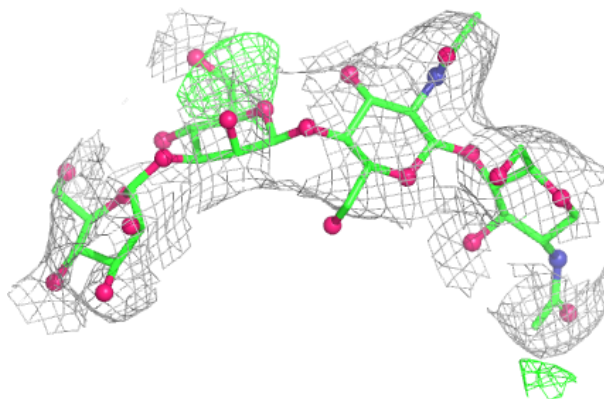
**Electron density around Chain K:**

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

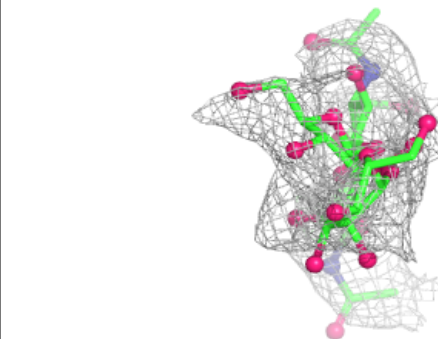
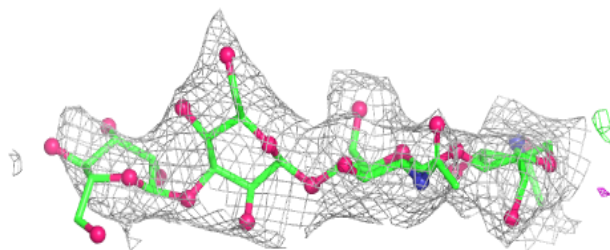
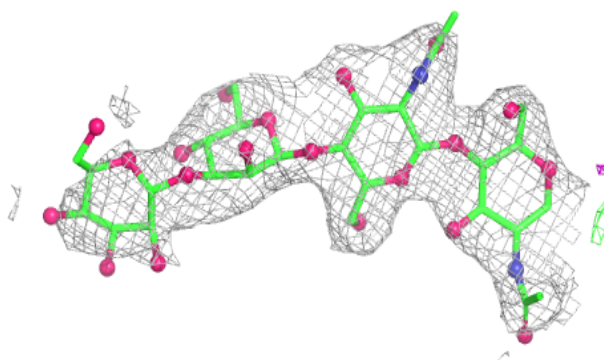


Electron density around Chain Q:

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

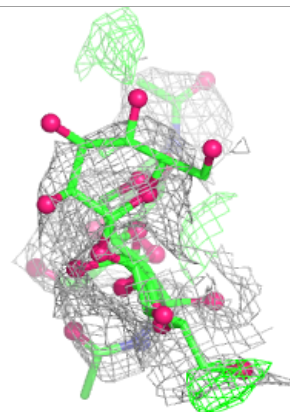
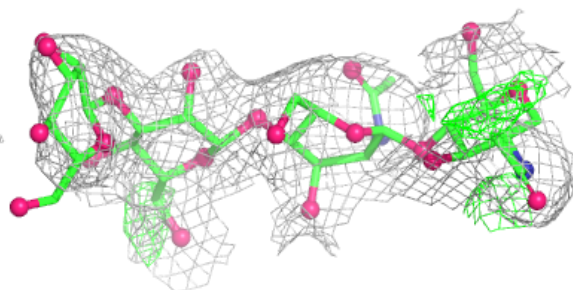
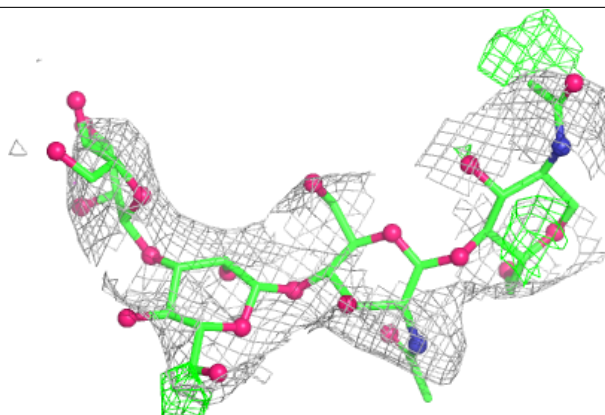
**Electron density around Chain R:**

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

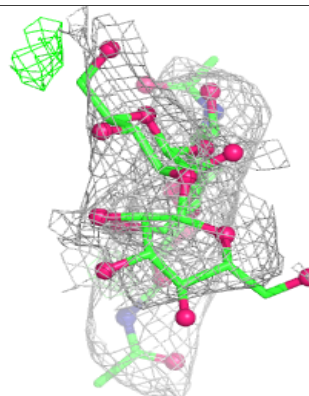
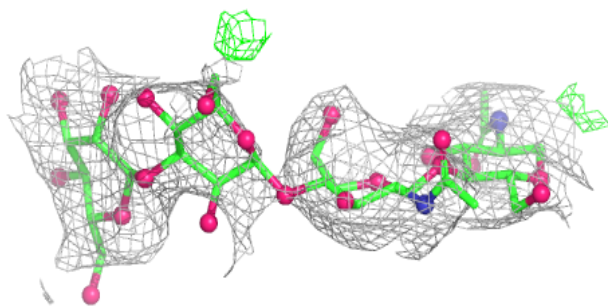
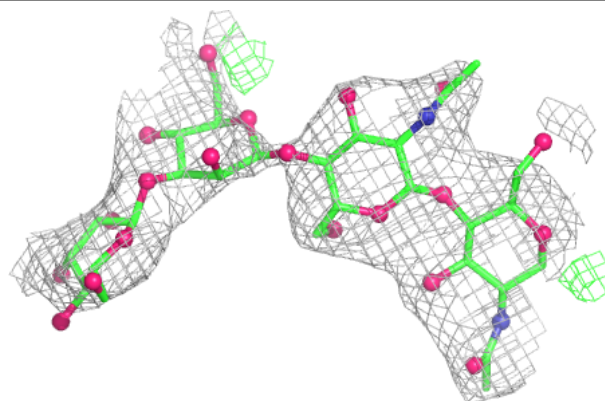


Electron density around Chain W:

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

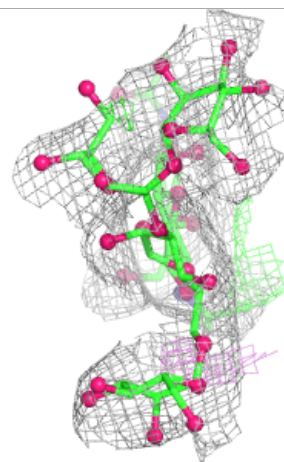
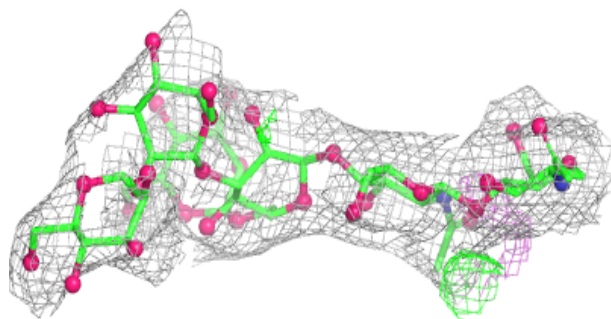
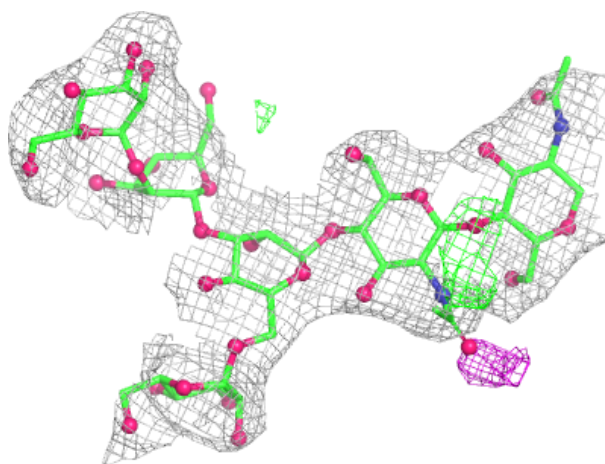
**Electron density around Chain c:**

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



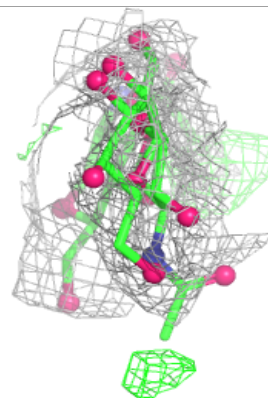
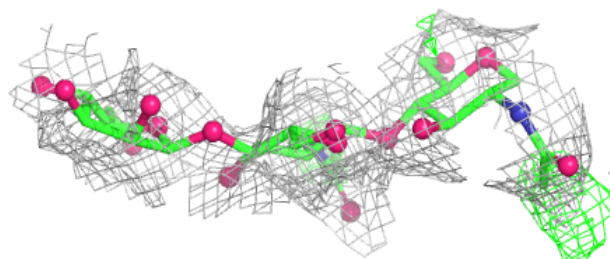
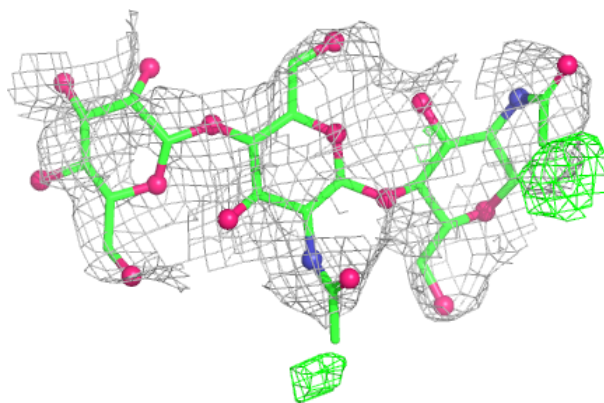
Electron density around Chain L:

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

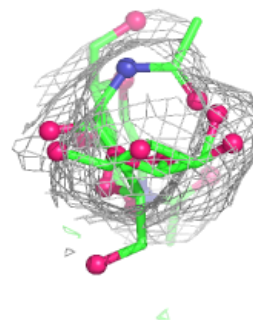
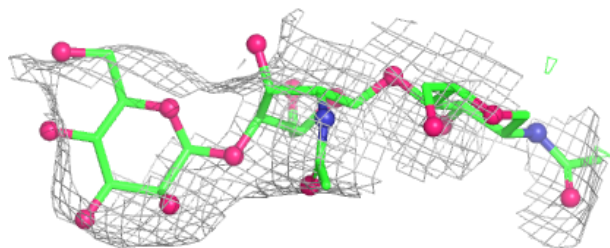
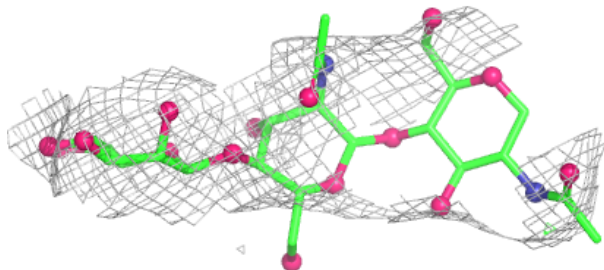


Electron density around Chain N:

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

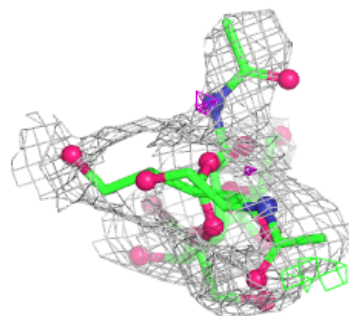
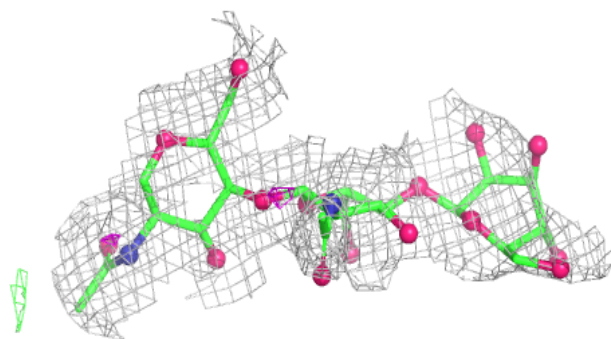
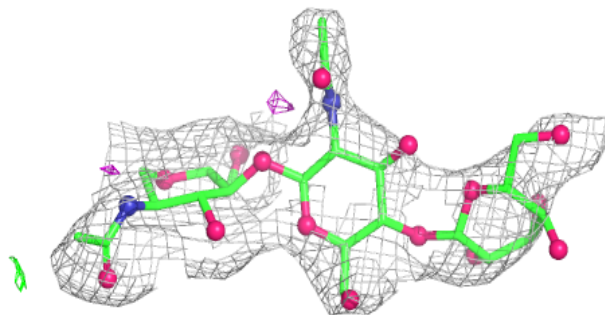
**Electron density around Chain b:**

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

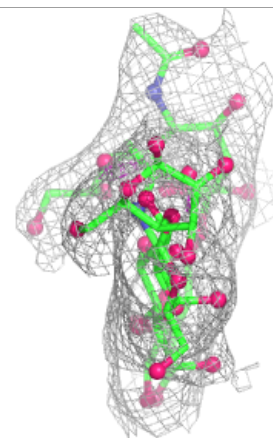
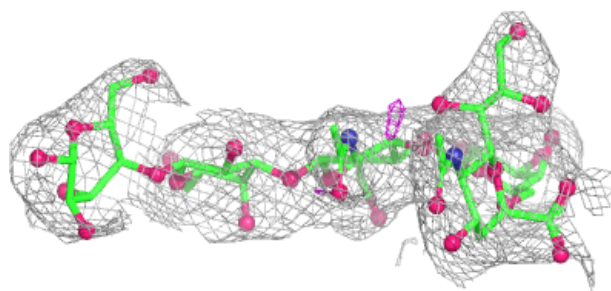
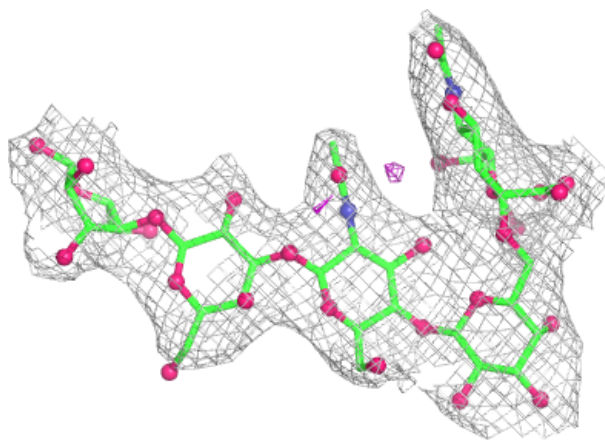


Electron density around Chain e:

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

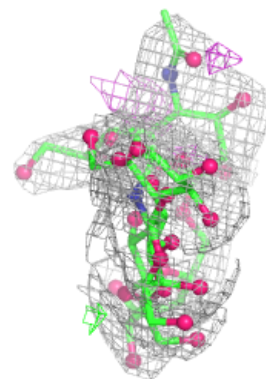
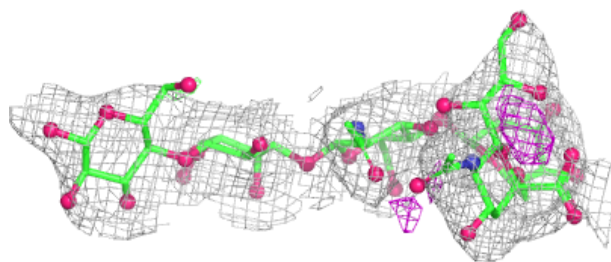
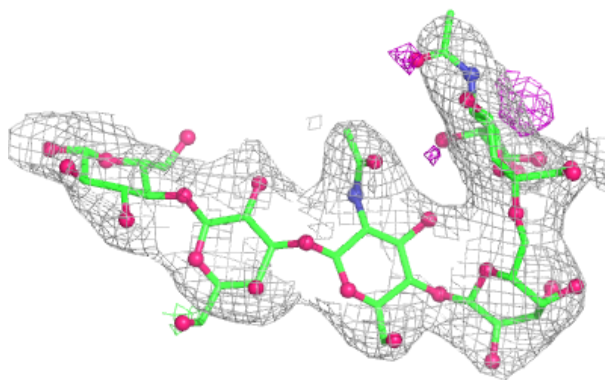
**Electron density around Chain O:**

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

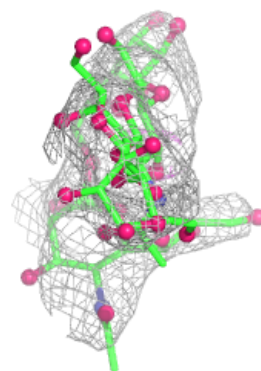
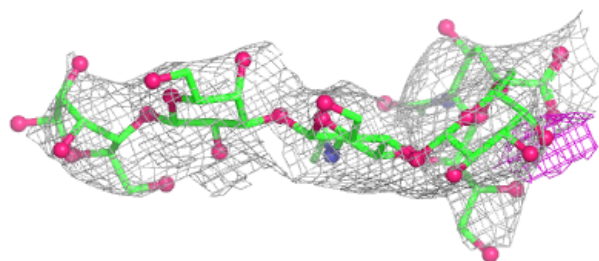
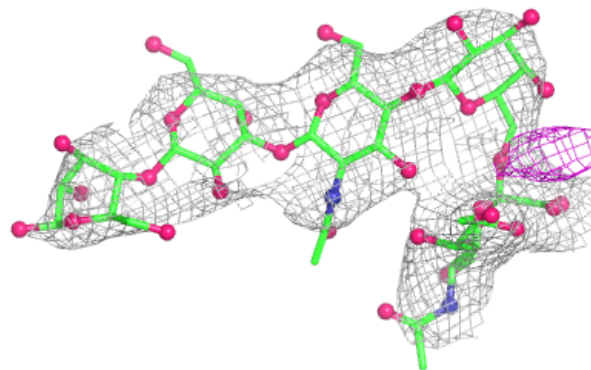


Electron density around Chain V:

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

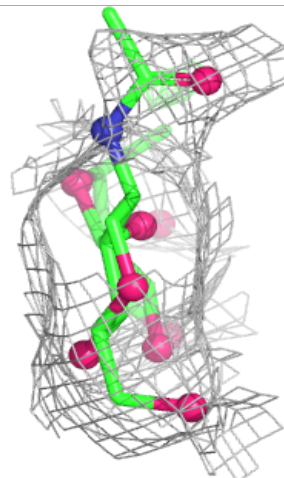
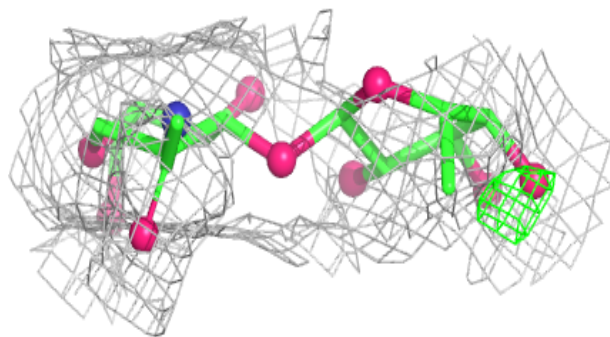
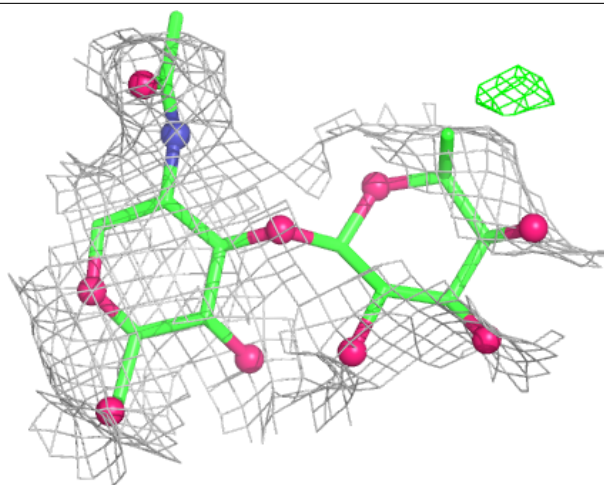
**Electron density around Chain g:**

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



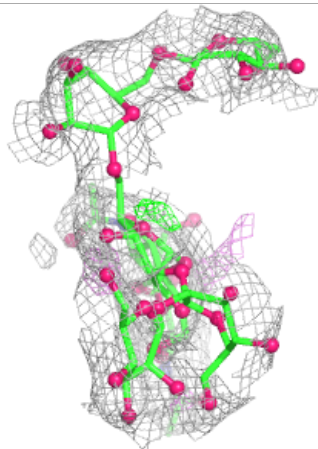
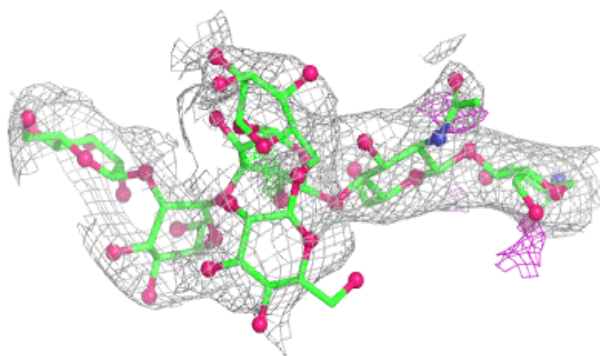
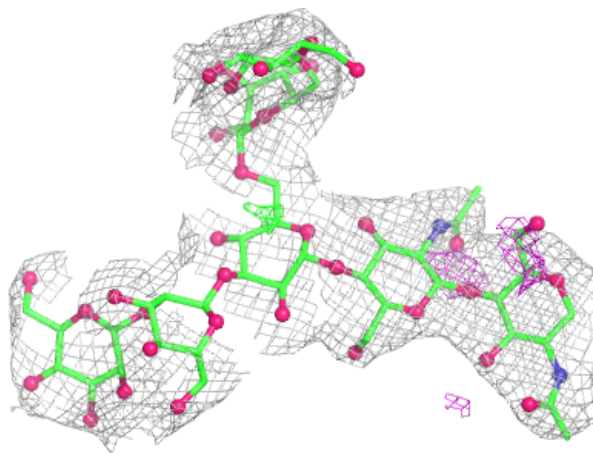
Electron density around Chain P:

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



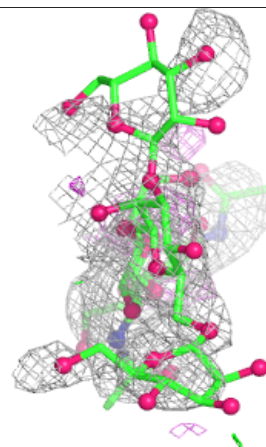
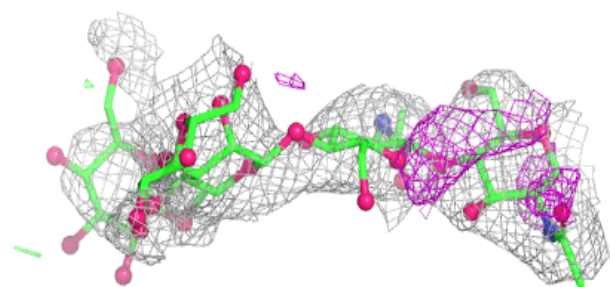
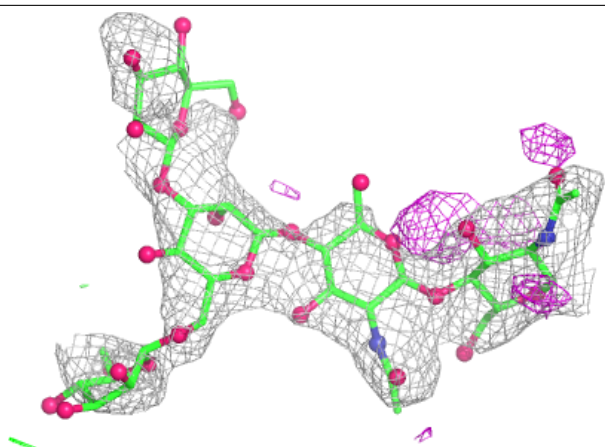
Electron density around Chain S:

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



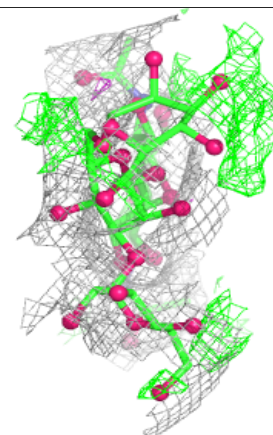
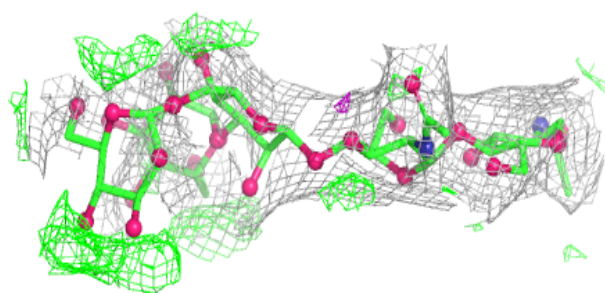
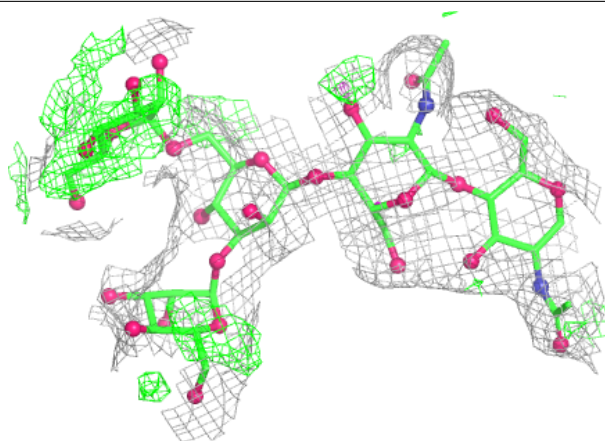
Electron density around Chain T:

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



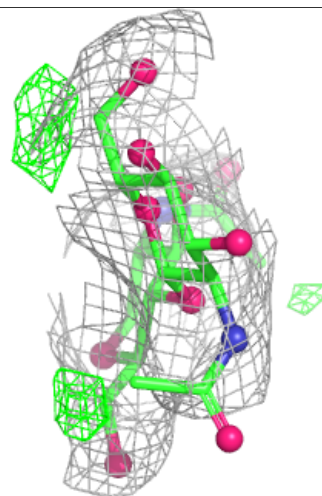
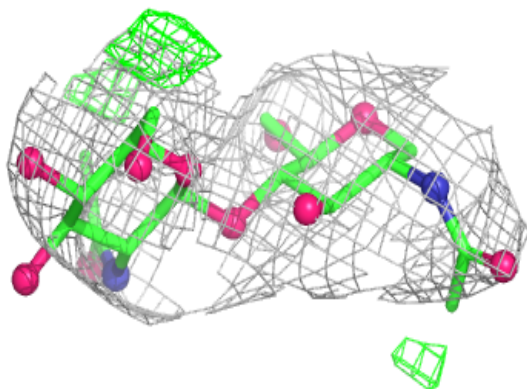
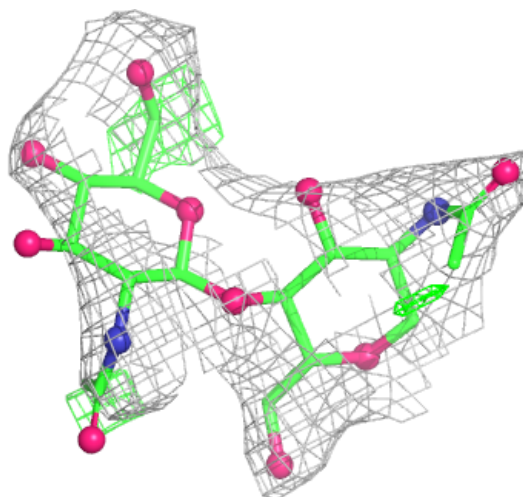
Electron density around Chain X:

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



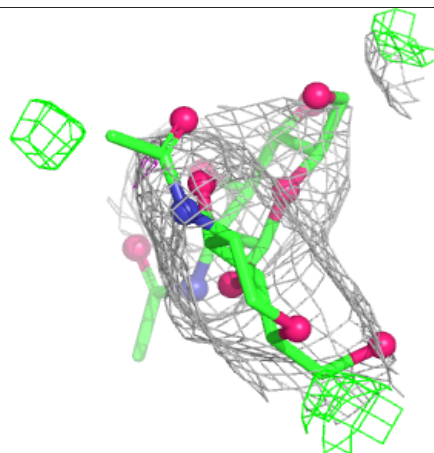
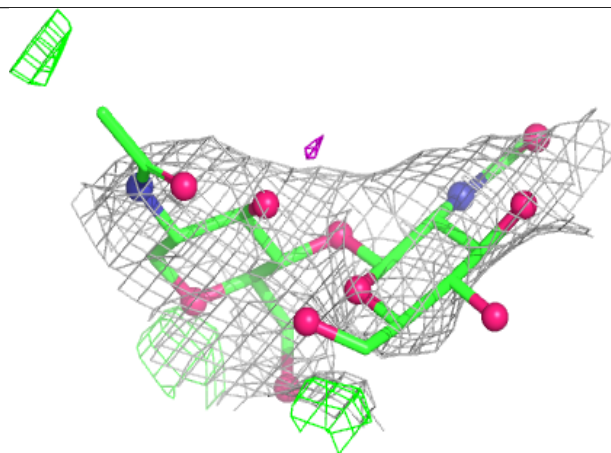
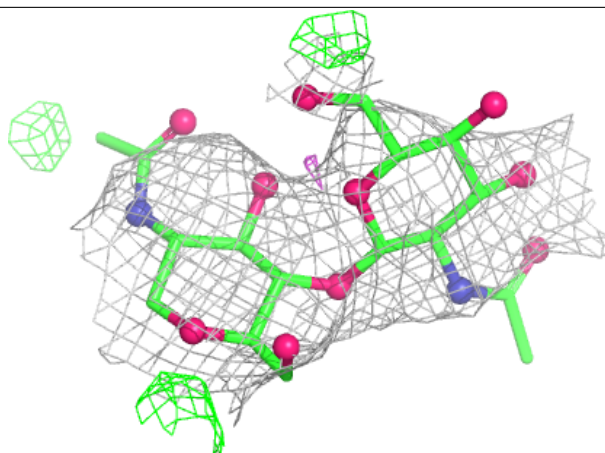
Electron density around Chain U:

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



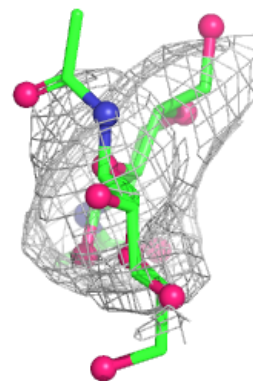
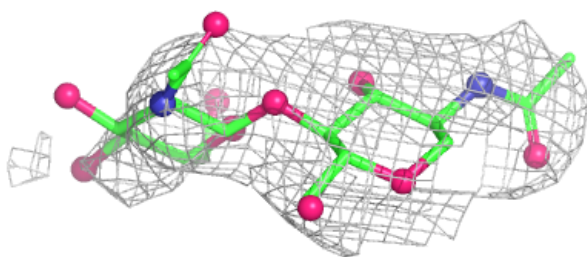
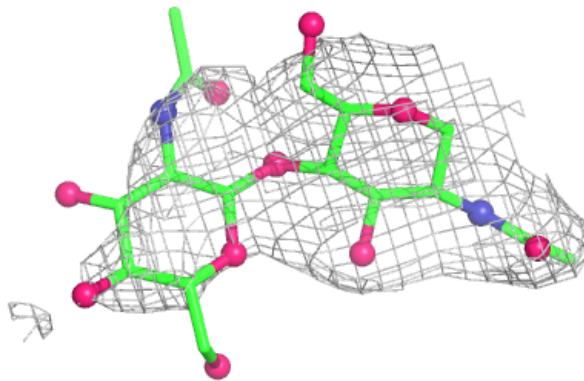
Electron density around Chain Y:

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



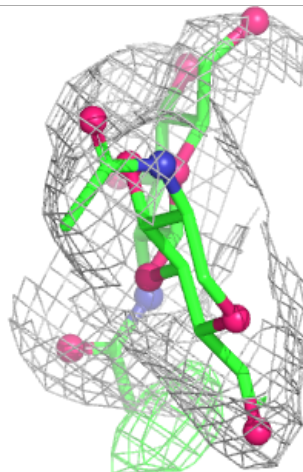
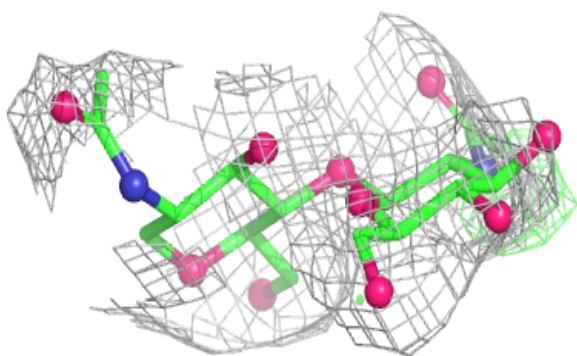
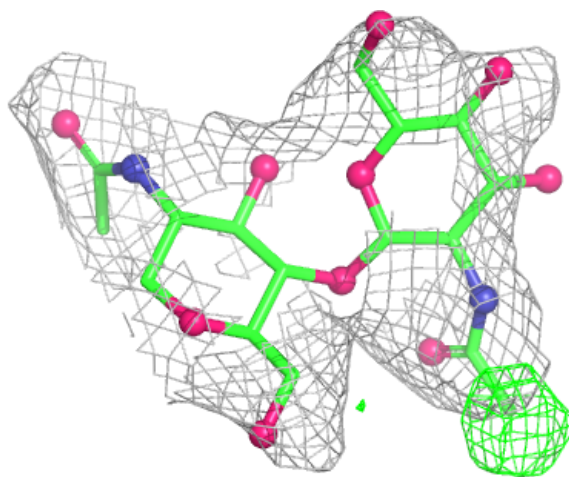
Electron density around Chain Z:

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



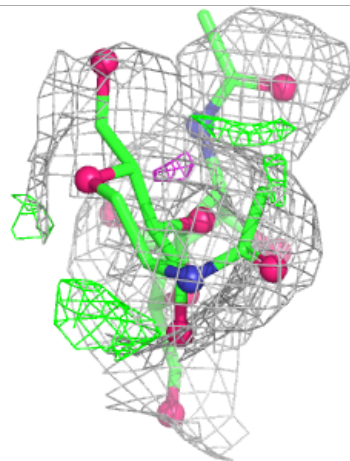
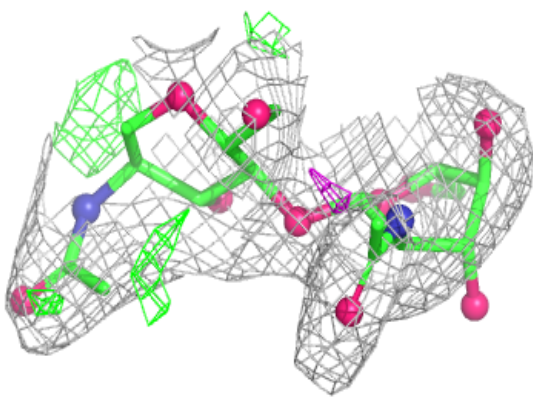
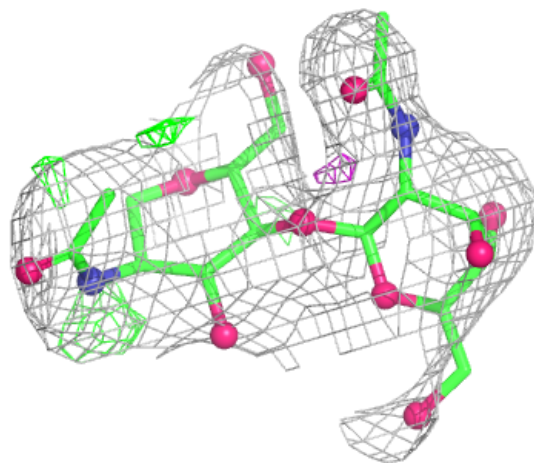
Electron density around Chain a:

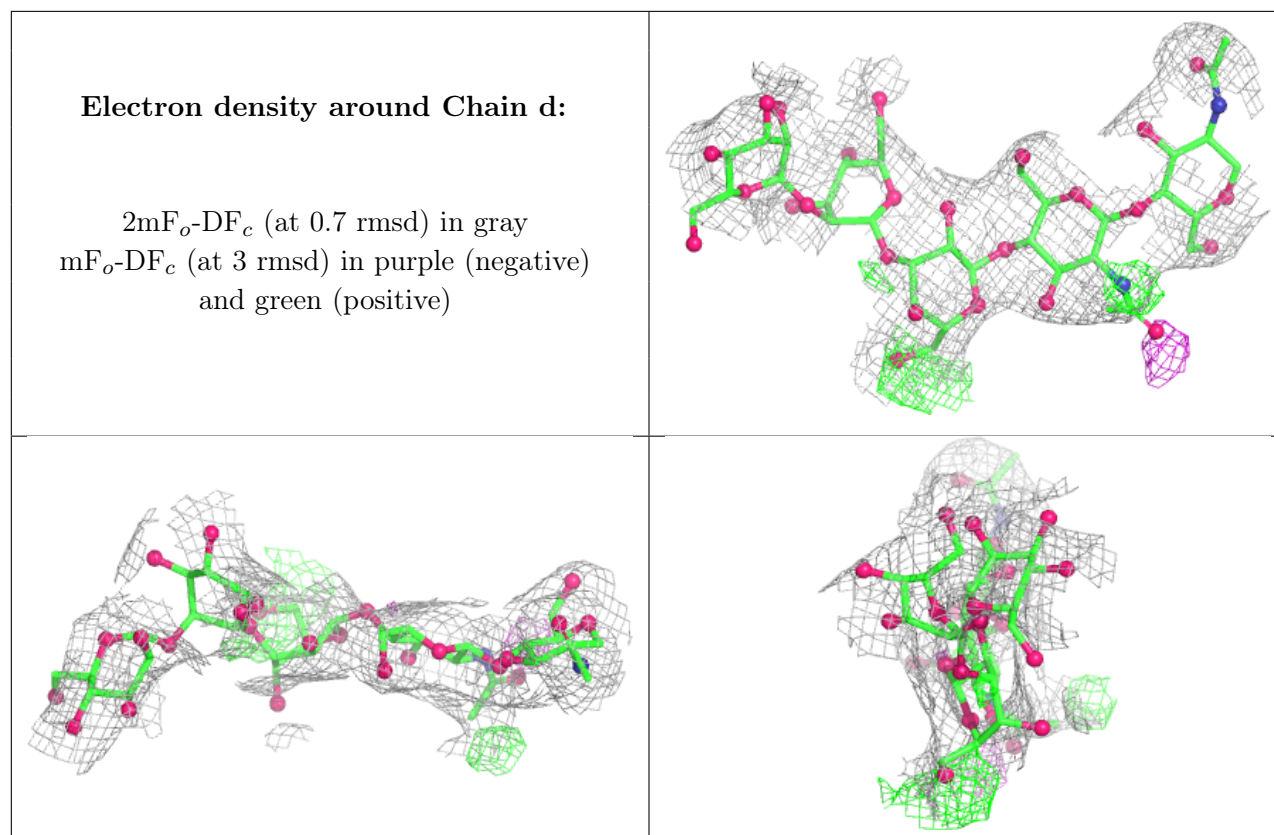
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain f:

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





6.4 Ligands ⓘ

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
14	NAG	A	522	14/15	0.30	0.17	132,160,170,173	0
14	NAG	E	414	14/15	0.31	0.16	120,156,178,183	0
14	NAG	C	523	14/15	0.43	0.14	113,146,151,152	0
14	NAG	B	201	14/15	0.58	0.14	106,165,174,175	0
14	NAG	D	202	14/15	0.67	0.17	117,138,149,156	0
14	NAG	G	416	14/15	0.73	0.13	133,149,163,164	0
14	NAG	F	201	14/15	0.82	0.12	109,130,138,139	0
15	CAC	D	201	5/5	0.84	0.20	145,146,151,160	0

6.5 Other polymers ⓘ

There are no such residues in this entry.