



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 11:38 AM EDT

PDB ID : 4NRL
Title : Structure of hemagglutinin with F95Y mutation of influenza virus B/Lee/40
Authors : Ni, F.; Mbawuike, I.N.; Kondrashkina, E.; Wang, Q.
Deposited on : 2013-11-26
Resolution : 2.72 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

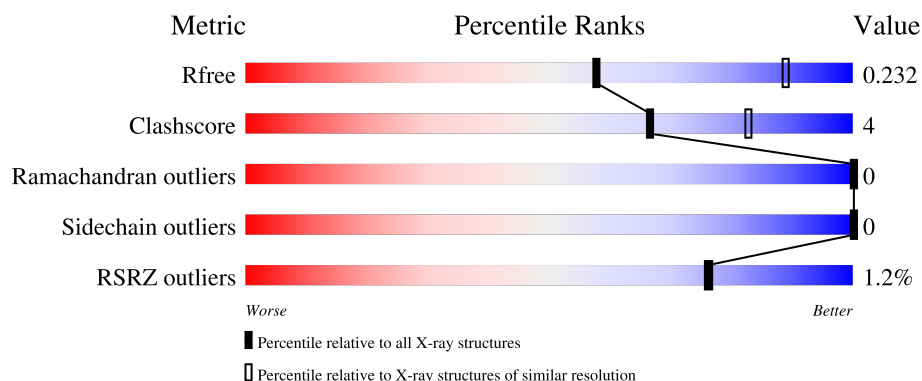
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

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	346	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
1	C	346	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
1	E	346	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
2	B	182	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>5%</div> <div>7%</div> </div> </div>
2	D	182	<div> <div></div> <div> <div></div> <div>86%</div> <div>7%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	182	
3	G	5	
3	L	5	
3	Q	5	
4	H	2	
4	I	2	
4	J	2	
4	K	2	
4	M	2	
4	O	2	
4	P	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	V	2	
5	N	3	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12583 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 HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2600	1631	461	492	16			
1	C	341	Total	C	N	O	S	0	0	0
			2600	1631	461	492	16			
1	E	341	Total	C	N	O	S	0	0	0
			2600	1631	461	492	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ARG	LYS	conflict	UNP P03460
A	76	ILE	THR	conflict	UNP P03460
A	90	VAL	ALA	conflict	UNP P03460
A	95	TYR	PHE	engineered mutation	UNP P03460
A	147	THR	ALA	conflict	UNP P03460
A	167	ILE	THR	conflict	UNP P03460
C	38	ARG	LYS	conflict	UNP P03460
C	76	ILE	THR	conflict	UNP P03460
C	90	VAL	ALA	conflict	UNP P03460
C	95	TYR	PHE	engineered mutation	UNP P03460
C	147	THR	ALA	conflict	UNP P03460
C	167	ILE	THR	conflict	UNP P03460
E	38	ARG	LYS	conflict	UNP P03460
E	76	ILE	THR	conflict	UNP P03460
E	90	VAL	ALA	conflict	UNP P03460
E	95	TYR	PHE	engineered mutation	UNP P03460
E	147	THR	ALA	conflict	UNP P03460
E	167	ILE	THR	conflict	UNP P03460

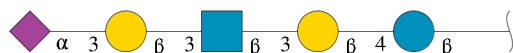
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1289	806	220	257	6			
2	D	169	Total	C	N	O	S	0	0	0
			1281	800	219	256	6			
2	F	169	Total	C	N	O	S	0	0	0
			1281	800	219	256	6			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	54	SER	TYR	conflict	UNP P03460
B	177	GLY	-	expression tag	UNP P03460
B	178	ALA	-	expression tag	UNP P03460
B	179	LEU	-	expression tag	UNP P03460
B	180	VAL	-	expression tag	UNP P03460
B	181	PRO	-	expression tag	UNP P03460
B	182	ARG	-	expression tag	UNP P03460
D	54	SER	TYR	conflict	UNP P03460
D	177	GLY	-	expression tag	UNP P03460
D	178	ALA	-	expression tag	UNP P03460
D	179	LEU	-	expression tag	UNP P03460
D	180	VAL	-	expression tag	UNP P03460
D	181	PRO	-	expression tag	UNP P03460
D	182	ARG	-	expression tag	UNP P03460
F	54	SER	TYR	conflict	UNP P03460
F	177	GLY	-	expression tag	UNP P03460
F	178	ALA	-	expression tag	UNP P03460
F	179	LEU	-	expression tag	UNP P03460
F	180	VAL	-	expression tag	UNP P03460
F	181	PRO	-	expression tag	UNP P03460
F	182	ARG	-	expression tag	UNP P03460

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	5	Total	C	N	O	0	0	0
			68	37	2	29			

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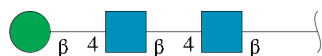
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	L	5	Total	C	N	O	0	0	0
			68	37	2	29			
3	Q	5	Total	C	N	O	0	0	0
			68	37	2	29			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

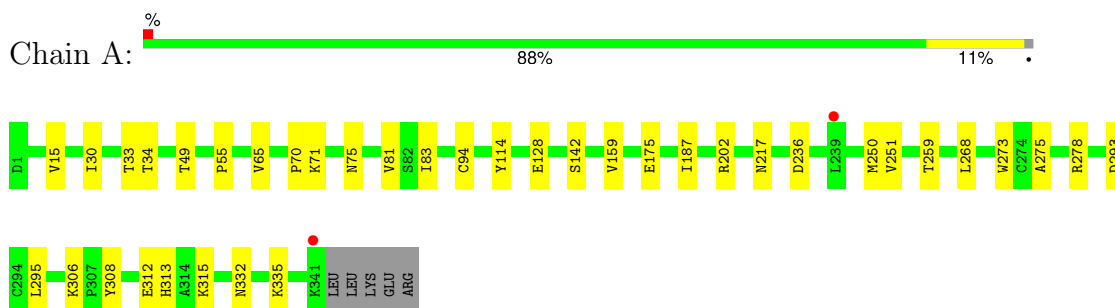
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	66	Total 66	O 66	0	0
7	B	13	Total 13	O 13	0	0
7	C	59	Total 59	O 59	0	0
7	D	29	Total 29	O 29	0	0
7	E	82	Total 82	O 82	0	0
7	F	20	Total 20	O 20	0	0

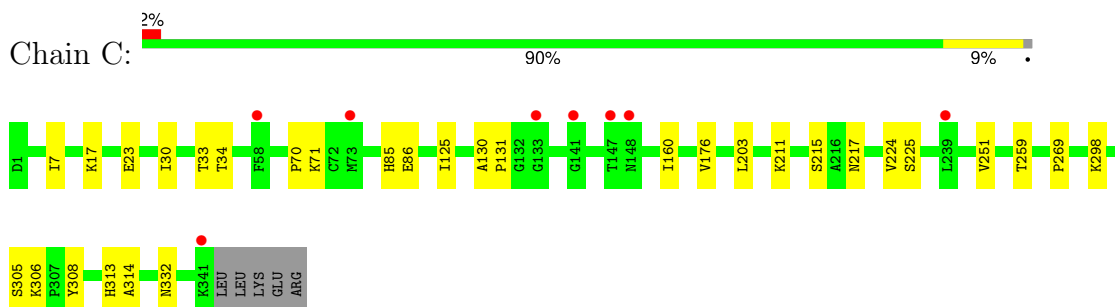
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

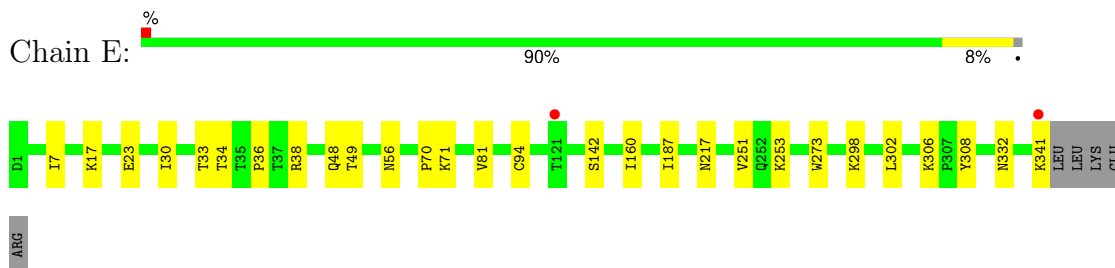
- Molecule 1: Hemagglutinin HA1 chain



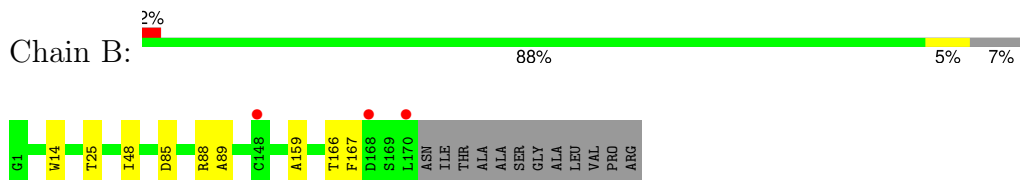
- Molecule 1: Hemagglutinin HA1 chain




- Molecule 1: Hemagglutinin HA1 chain



- Molecule 2: Hemagglutinin HA2 chain




- Molecule 2: Hemagglutinin HA2 chain

Chain D:  86% 7% 7%



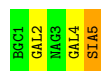
- Molecule 2: Hemagglutinin HA2 chain

Chain F:  2% 87% 5% 7%



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

Chain G:  40% 40% 20%



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

Chain L:  20% 60% 20%



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

Chain Q:  20% 60% 20%



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

Chain H:  100%



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

Chain I:  50% 50%



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

Chain J:  50% 50%



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

Chain K:  50% 50%



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

Chain M:  50% 50%



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

Chain O:  100%



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

Chain P:  50% 50%



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

Chain R:  100%



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

Chain S:  50% 50%

MAG1
MAG2

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

Chain T:  50% 50%

MAG1
MAG2

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

Chain U:  100%

MAG1
MAG2

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

Chain V:  50% 50%

MAG1
MAG2

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

Chain N:  67% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	83.61Å 128.40Å 211.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 – 2.72 47.49 – 2.72	Depositor EDS
% Data completeness (in resolution range)	95.5 (47.49-2.72) 95.5 (47.49-2.72)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1452)	Depositor
R, R_{free}	0.194 , 0.229 0.201 , 0.232	Depositor DCC
R_{free} test set	2946 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.800	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12583	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: NAG, GAL, BMA, BGC, SIA

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	0.23	0/2659	0.44	0/3614
1	C	0.23	0/2659	0.46	1/3614 (0.0%)
1	E	0.23	0/2659	0.45	0/3614
2	B	0.21	0/1308	0.37	0/1763
2	D	0.21	0/1300	0.36	0/1752
2	F	0.22	0/1300	0.37	0/1752
All	All	0.22	0/11885	0.42	1/16109 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	LEU	CB-CG-CD2	-5.90	100.96	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2600	0	2597	27	0
1	C	2600	0	2597	22	0
1	E	2600	0	2596	19	0
2	B	1289	0	1261	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1281	0	1251	10	0
2	F	1281	0	1251	8	0
3	G	68	0	58	1	0
3	L	68	0	58	1	0
3	Q	68	0	58	2	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	M	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	4	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	1	0
4	U	28	0	25	0	0
4	V	28	0	25	1	0
5	N	39	0	34	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
6	D	14	0	13	1	0
6	E	14	0	13	0	0
6	F	14	0	13	0	0
7	A	66	0	0	8	0
7	B	13	0	0	2	0
7	C	59	0	0	9	0
7	D	29	0	0	2	0
7	E	82	0	0	2	0
7	F	20	0	0	2	0
All	All	12583	0	12139	89	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 89 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:GLN:NE2	7:E:559:HOH:O	1.96	0.98
1:A:128:GLU:OE1	7:A:565:HOH:O	1.92	0.88
1:E:56:ASN:OD1	7:E:546:HOH:O	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:SER:O	7:C:551:HOH:O	1.92	0.86
1:A:15:VAL:O	7:A:558:HOH:O	2.03	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/346 (98%)	326 (96%)	13 (4%)	0	100	100
1	C	339/346 (98%)	326 (96%)	13 (4%)	0	100	100
1	E	339/346 (98%)	326 (96%)	13 (4%)	0	100	100
2	B	168/182 (92%)	167 (99%)	1 (1%)	0	100	100
2	D	167/182 (92%)	166 (99%)	1 (1%)	0	100	100
2	F	167/182 (92%)	166 (99%)	1 (1%)	0	100	100
All	All	1519/1584 (96%)	1477 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	293/298 (98%)	293 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	293/298 (98%)	293 (100%)	0	100	100
1	E	293/298 (98%)	293 (100%)	0	100	100
2	B	137/145 (94%)	137 (100%)	0	100	100
2	D	136/145 (94%)	136 (100%)	0	100	100
2	F	136/145 (94%)	136 (100%)	0	100	100
All	All	1288/1329 (97%)	1288 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	27	HIS
1	E	154	ASN
1	E	241	GLN
1	E	217	ASN
1	C	154	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 ⓘ

42 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	BGC	G	1	3	12,12,12	0.51	0	17,17,17	0.45	0
3	GAL	G	2	3	11,11,12	0.96	1 (9%)	15,15,17	1.82	2 (13%)
3	NAG	G	3	3	14,14,15	0.21	0	17,19,21	0.43	0
3	GAL	G	4	3	11,11,12	0.59	0	15,15,17	1.23	1 (6%)
3	SIA	G	5	3	20,20,21	1.18	2 (10%)	21,28,31	2.10	6 (28%)
4	NAG	H	1	1,4	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	H	2	4	14,14,15	0.31	0	17,19,21	0.38	0
4	NAG	I	1	1,4	14,14,15	1.04	1 (7%)	17,19,21	2.12	3 (17%)
4	NAG	I	2	4	14,14,15	0.30	0	17,19,21	0.38	0
4	NAG	J	1	1,4	14,14,15	0.96	1 (7%)	17,19,21	1.33	1 (5%)
4	NAG	J	2	4	14,14,15	0.42	0	17,19,21	0.52	0
4	NAG	K	1	1,4	14,14,15	0.88	1 (7%)	17,19,21	1.07	1 (5%)
4	NAG	K	2	4	14,14,15	0.29	0	17,19,21	0.45	0
3	BGC	L	1	3	12,12,12	0.55	0	17,17,17	0.86	0
3	GAL	L	2	3	11,11,12	0.97	1 (9%)	15,15,17	1.08	2 (13%)
3	NAG	L	3	3	14,14,15	0.61	1 (7%)	17,19,21	1.05	1 (5%)
3	GAL	L	4	3	11,11,12	0.67	0	15,15,17	1.08	2 (13%)
3	SIA	L	5	3	20,20,21	1.34	2 (10%)	21,28,31	2.55	10 (47%)
4	NAG	M	1	1,4	14,14,15	1.25	1 (7%)	17,19,21	1.86	1 (5%)
4	NAG	M	2	4	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	N	1	5,1	14,14,15	0.41	0	17,19,21	0.57	0
5	NAG	N	2	5	14,14,15	0.42	0	17,19,21	0.74	0
5	BMA	N	3	5	11,11,12	0.92	1 (9%)	15,15,17	1.03	1 (6%)
4	NAG	O	1	1,4	14,14,15	0.39	0	17,19,21	0.57	0
4	NAG	O	2	4	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	P	1	1,4	14,14,15	0.59	0	17,19,21	0.59	0
4	NAG	P	2	4	14,14,15	0.37	0	17,19,21	1.33	2 (11%)
3	BGC	Q	1	3	12,12,12	0.55	0	17,17,17	1.62	4 (23%)
3	GAL	Q	2	3	11,11,12	0.73	0	15,15,17	1.00	1 (6%)
3	NAG	Q	3	3	14,14,15	0.24	0	17,19,21	0.53	0
3	GAL	Q	4	3	11,11,12	0.43	0	15,15,17	1.00	1 (6%)
3	SIA	Q	5	3	20,20,21	1.30	3 (15%)	21,28,31	2.16	8 (38%)
4	NAG	R	1	1,4	14,14,15	0.37	0	17,19,21	0.41	0
4	NAG	R	2	4	14,14,15	0.23	0	17,19,21	0.36	0
4	NAG	S	1	1,4	14,14,15	1.21	1 (7%)	17,19,21	1.78	1 (5%)
4	NAG	S	2	4	14,14,15	0.32	0	17,19,21	0.55	0
4	NAG	T	1	1,4	14,14,15	1.54	2 (14%)	17,19,21	1.74	4 (23%)
4	NAG	T	2	4	14,14,15	0.43	0	17,19,21	0.68	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	U	1	1,4	14,14,15	0.35	0	17,19,21	0.52	0
4	NAG	U	2	4	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	V	1	1,4	14,14,15	0.52	0	17,19,21	0.60	0
4	NAG	V	2	4	14,14,15	0.27	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	G	1	3	-	1/2/22/22	0/1/1/1
3	GAL	G	2	3	-	0/2/19/22	0/1/1/1
3	NAG	G	3	3	-	0/6/23/26	0/1/1/1
3	GAL	G	4	3	-	2/2/19/22	0/1/1/1
3	SIA	G	5	3	-	3/18/34/38	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
3	BGC	L	1	3	-	0/2/22/22	0/1/1/1
3	GAL	L	2	3	-	1/2/19/22	0/1/1/1
3	NAG	L	3	3	-	2/6/23/26	0/1/1/1
3	GAL	L	4	3	-	0/2/19/22	0/1/1/1
3	SIA	L	5	3	-	2/18/34/38	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	4/6/23/26	0/1/1/1
5	BMA	N	3	5	-	1/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	Q	1	3	-	1/2/22/22	0/1/1/1
3	GAL	Q	2	3	-	2/2/19/22	0/1/1/1
3	NAG	Q	3	3	-	2/6/23/26	0/1/1/1
3	GAL	Q	4	3	-	0/2/19/22	0/1/1/1
3	SIA	Q	5	3	-	0/18/34/38	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	S	2	4	-	1/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	3/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	1	NAG	O5-C1	-4.99	1.35	1.43
4	M	1	NAG	O5-C1	4.52	1.51	1.43
4	S	1	NAG	O5-C1	4.43	1.51	1.43
4	I	1	NAG	O5-C1	3.67	1.49	1.43
4	J	1	NAG	O5-C1	3.49	1.49	1.43

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	5	SIA	O6-C2-C3	-7.67	100.25	110.56
4	M	1	NAG	C1-O5-C5	7.43	122.15	112.19
4	S	1	NAG	C1-O5-C5	7.05	121.63	112.19
4	I	1	NAG	C1-O5-C5	6.37	120.72	112.19
3	G	5	SIA	O6-C2-C3	-5.82	102.73	110.56

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	3	NAG	C4-C5-C6-O6

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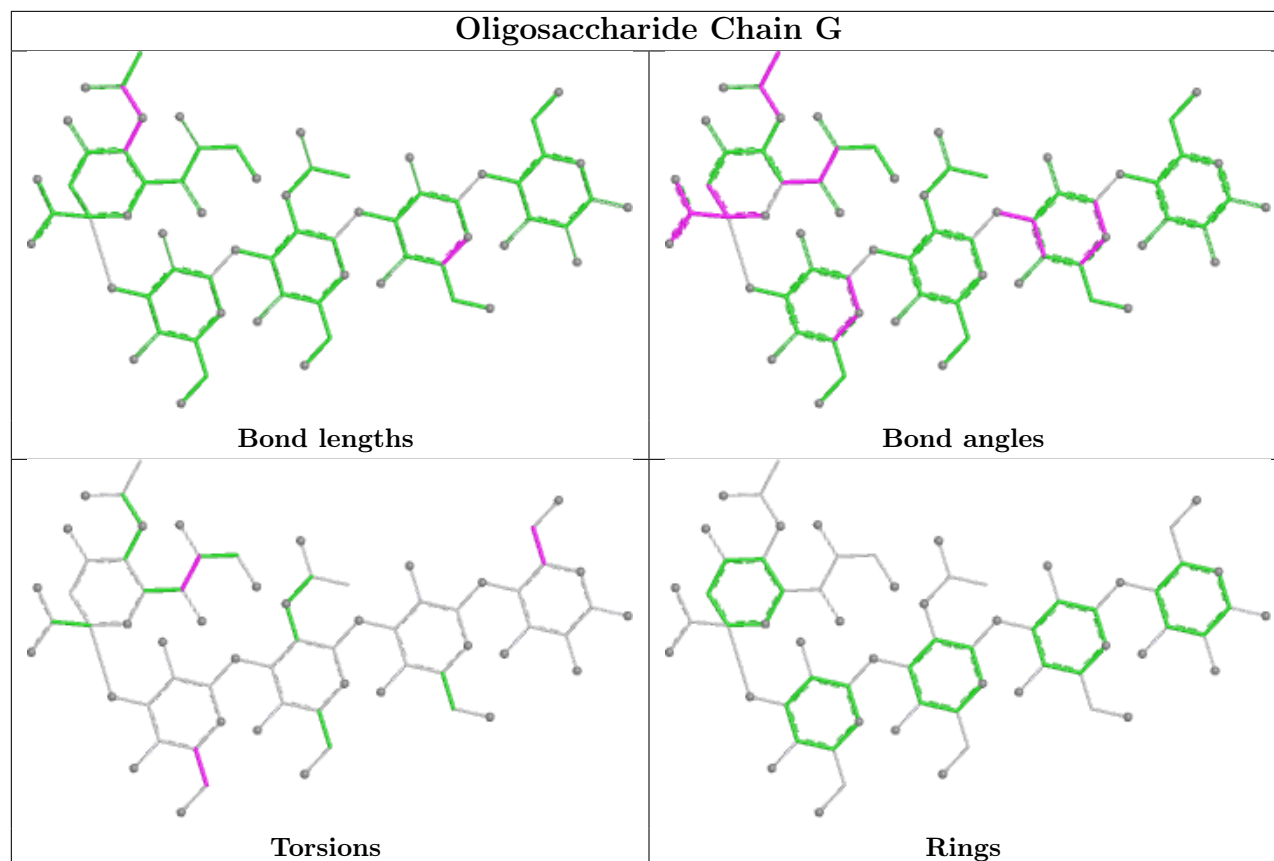
Mol	Chain	Res	Type	Atoms
4	K	1	NAG	O5-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6

There are no ring outliers.

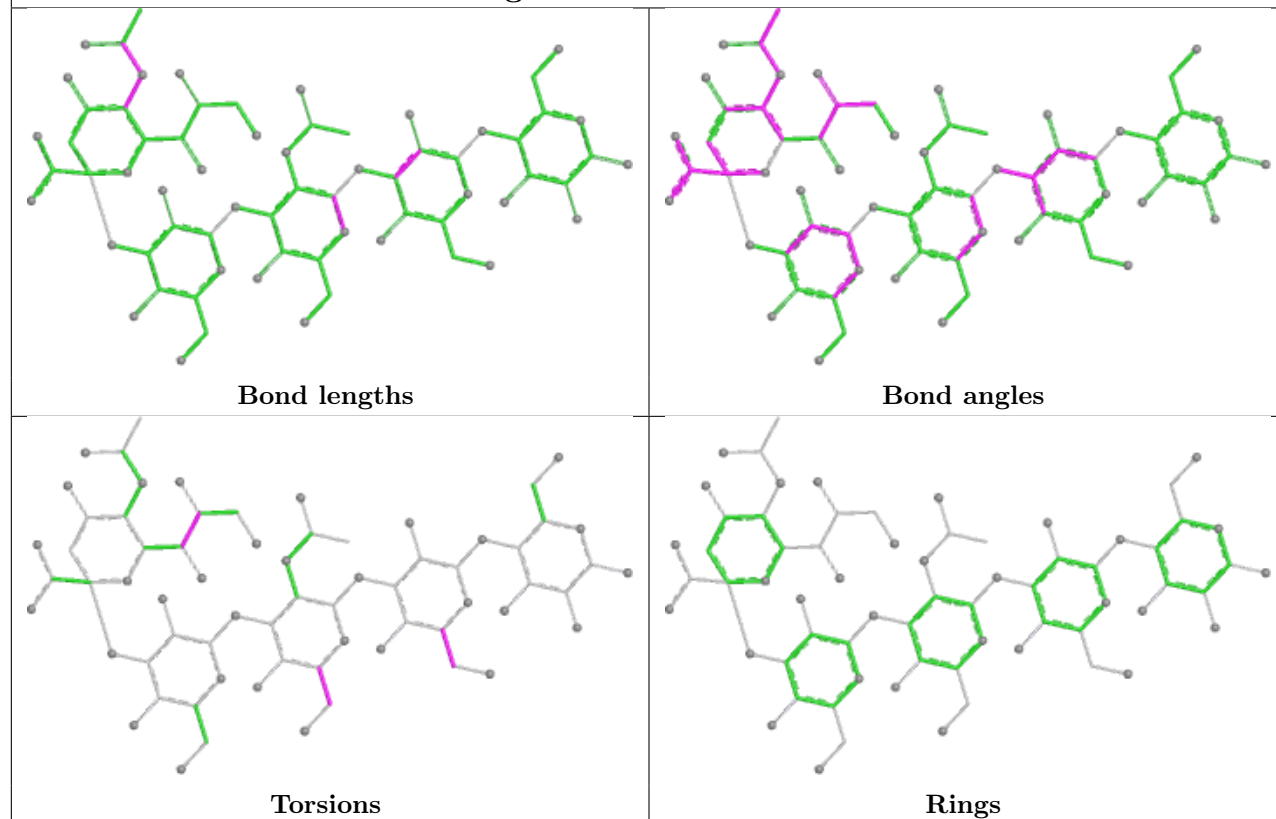
7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	5	SIA	1	0
4	P	2	NAG	2	0
4	V	1	NAG	1	0
3	G	5	SIA	1	0
4	T	1	NAG	1	0
4	P	1	NAG	3	0
3	Q	5	SIA	2	0

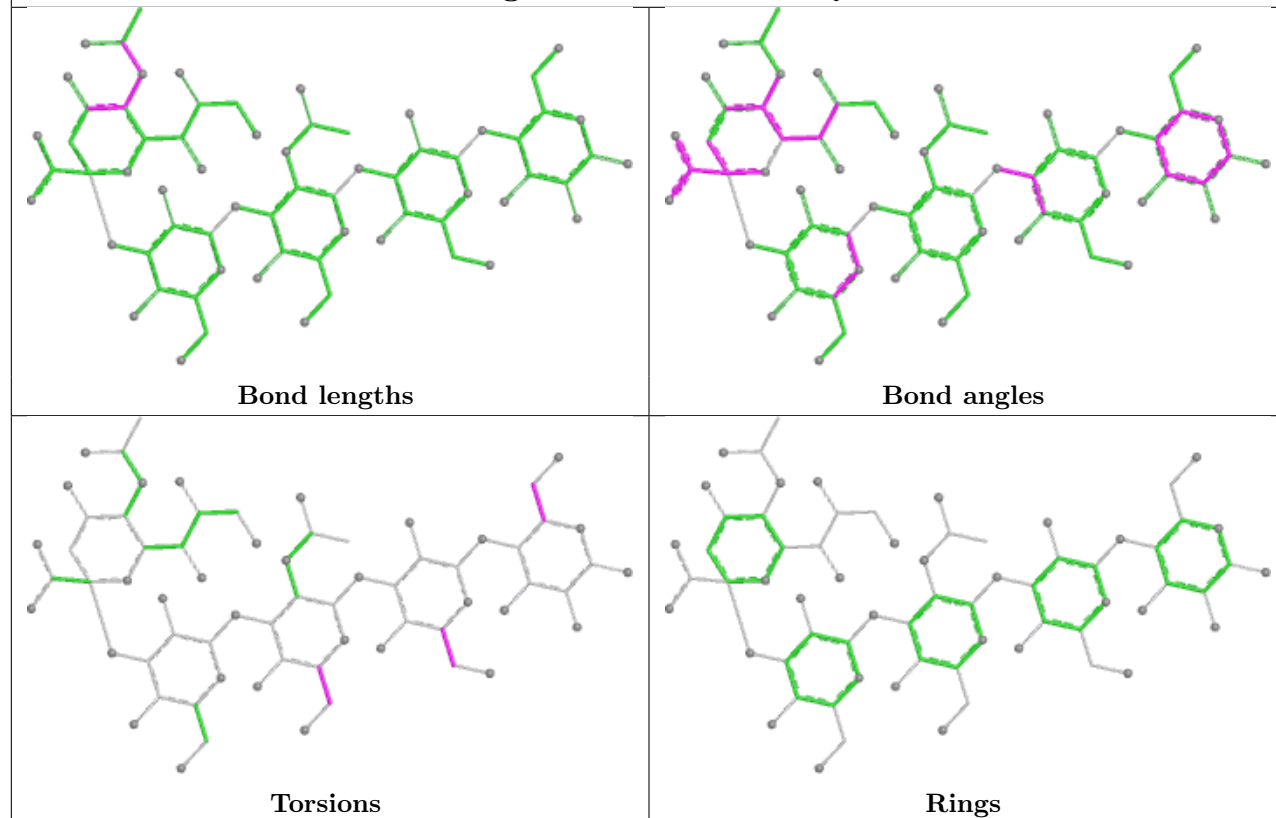
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

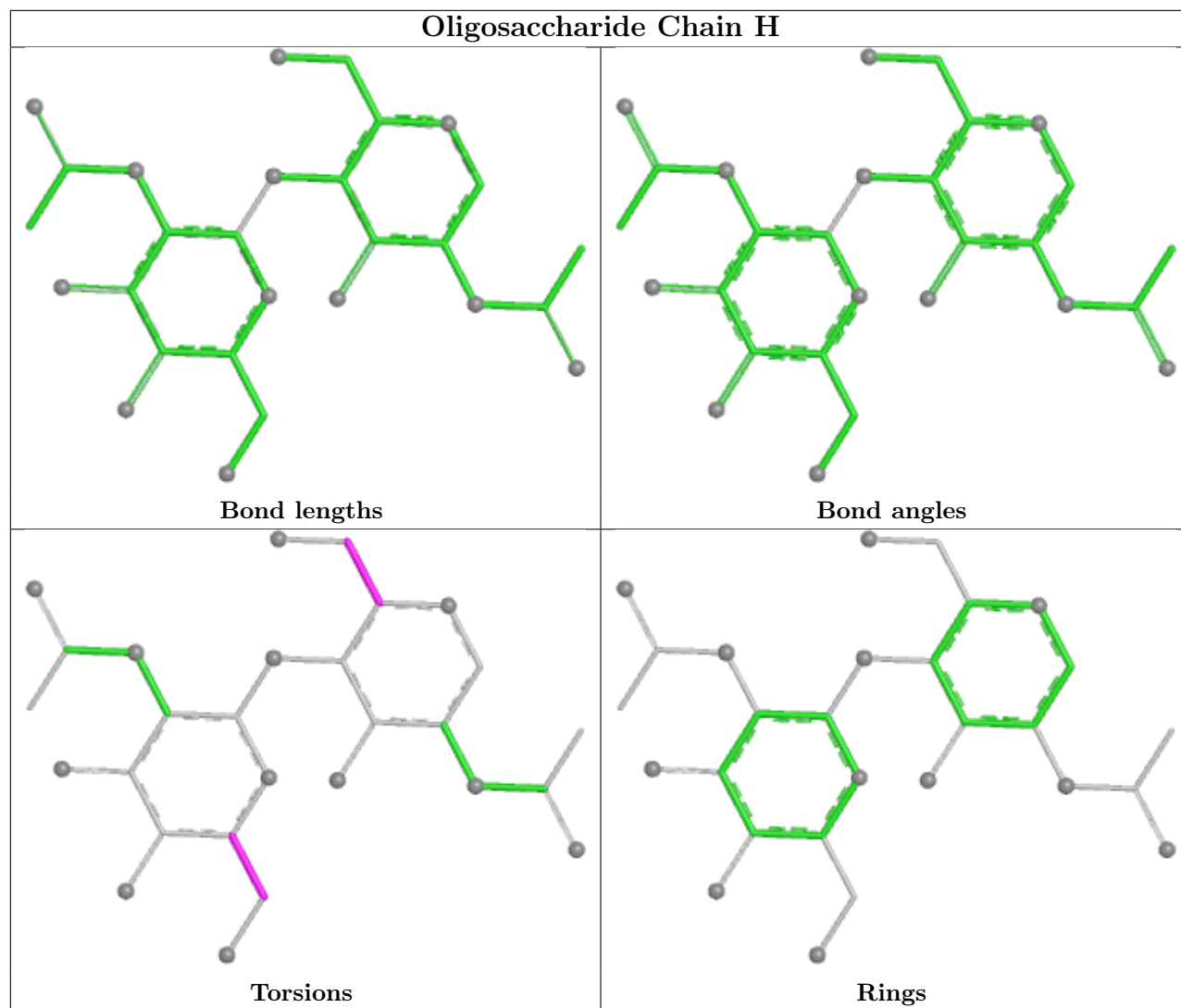


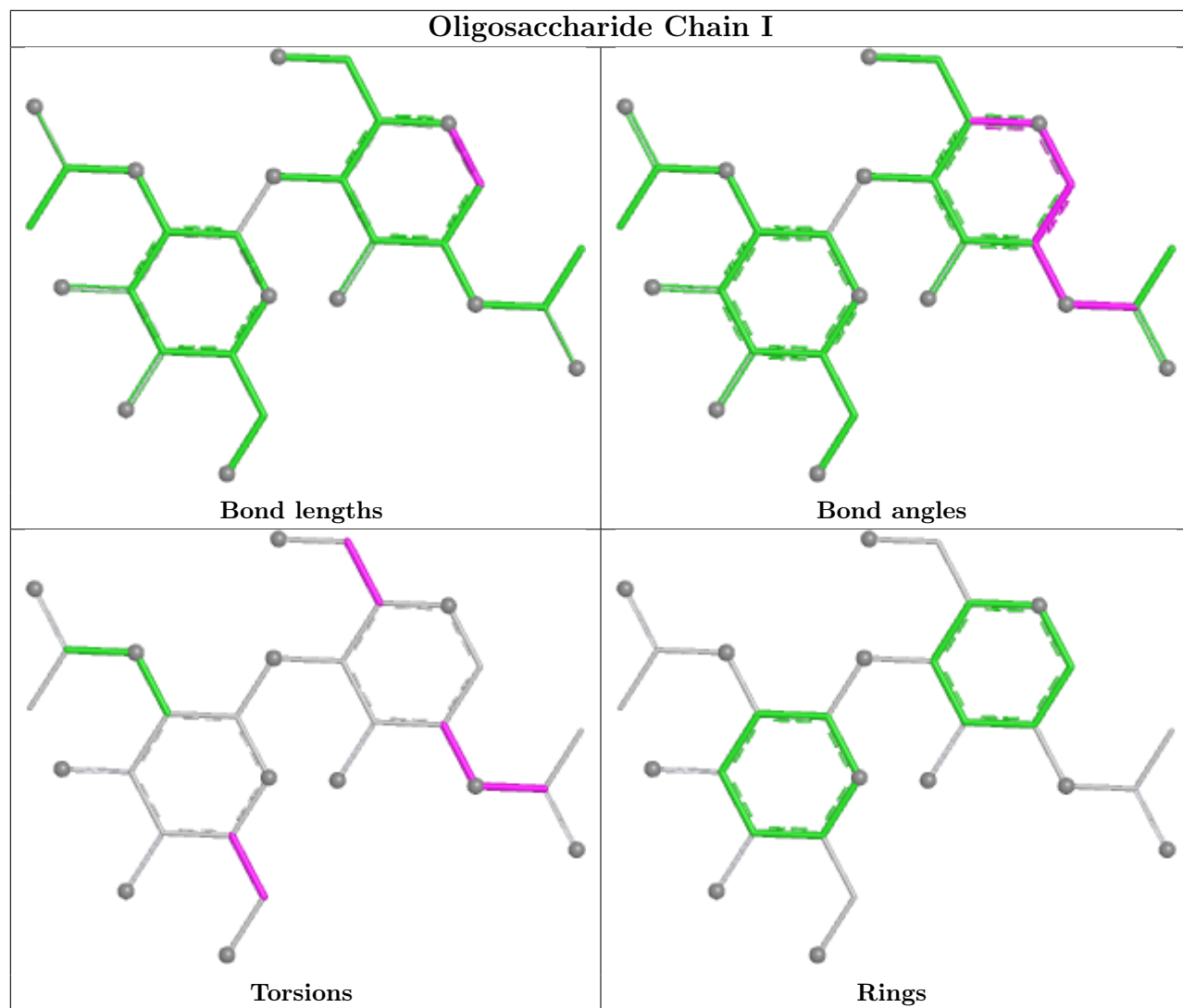
Oligosaccharide Chain L

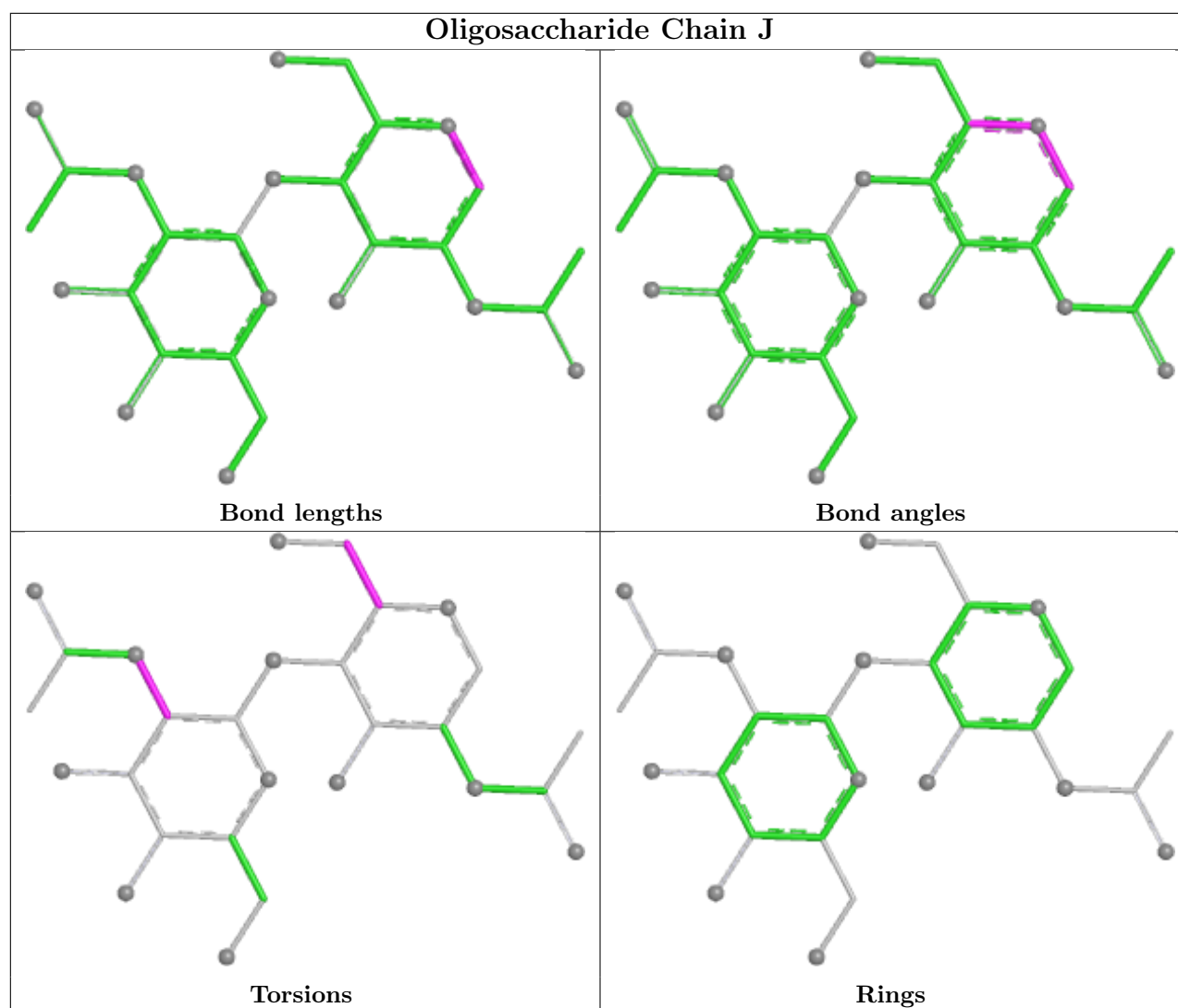


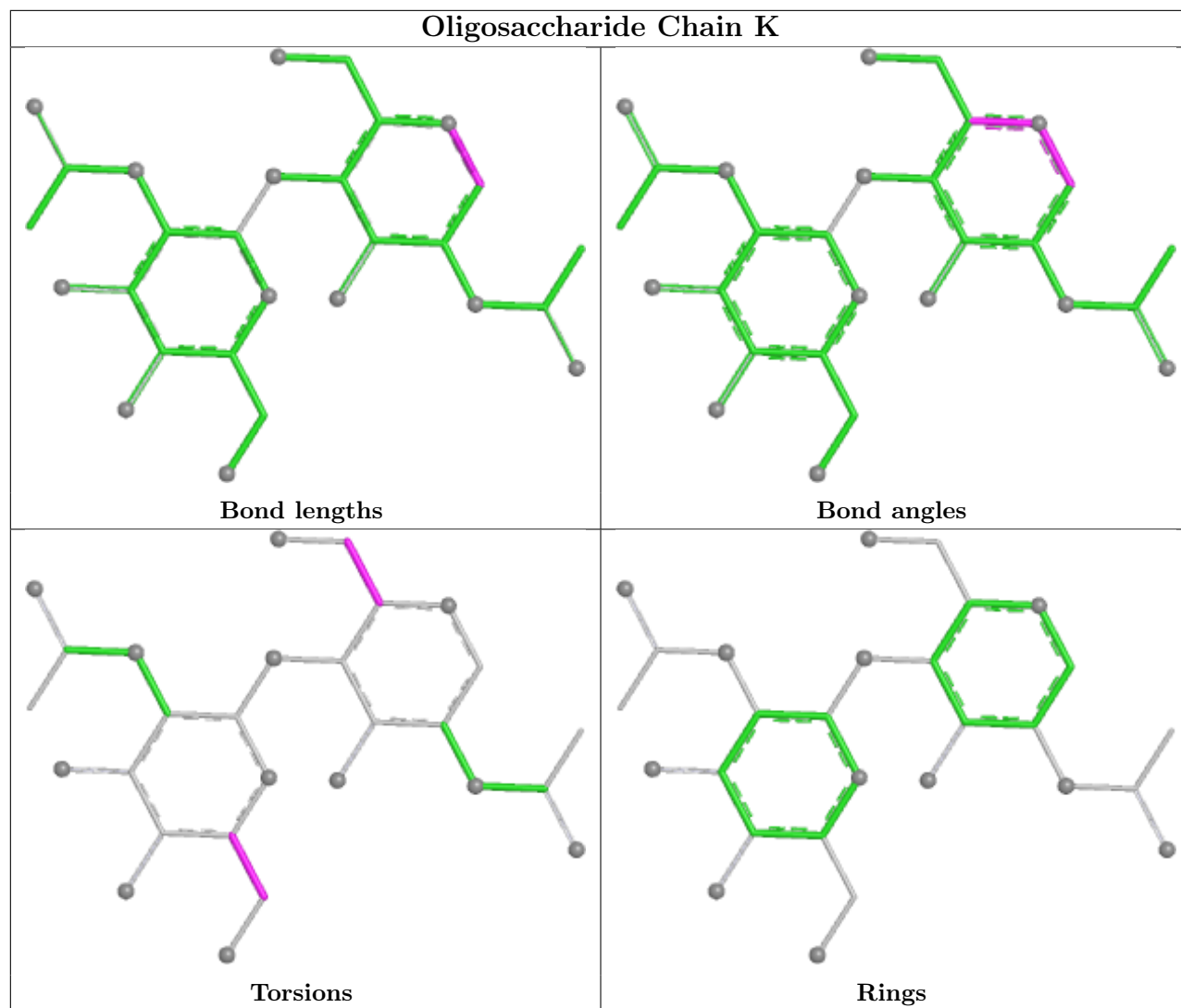
Oligosaccharide Chain Q

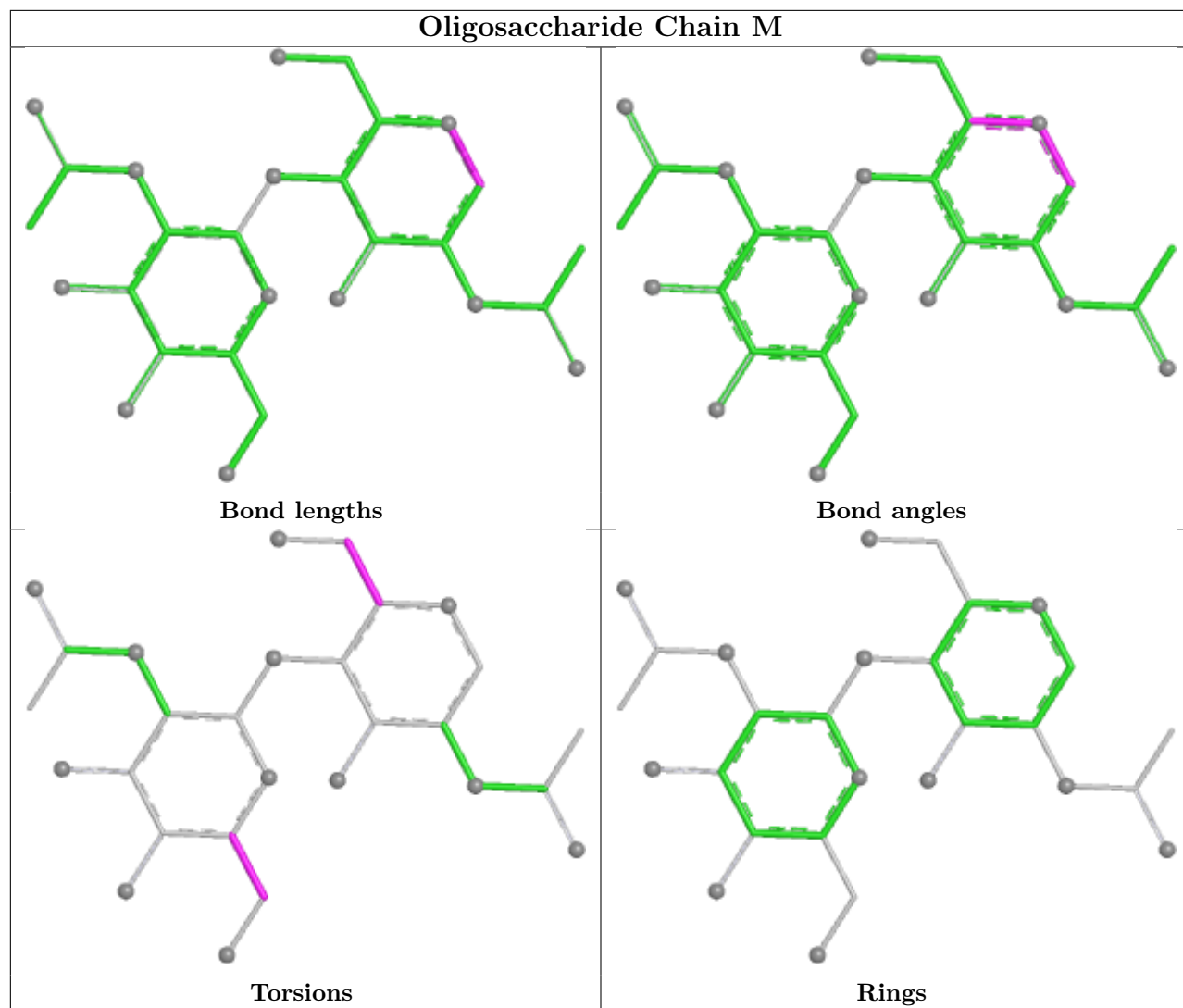


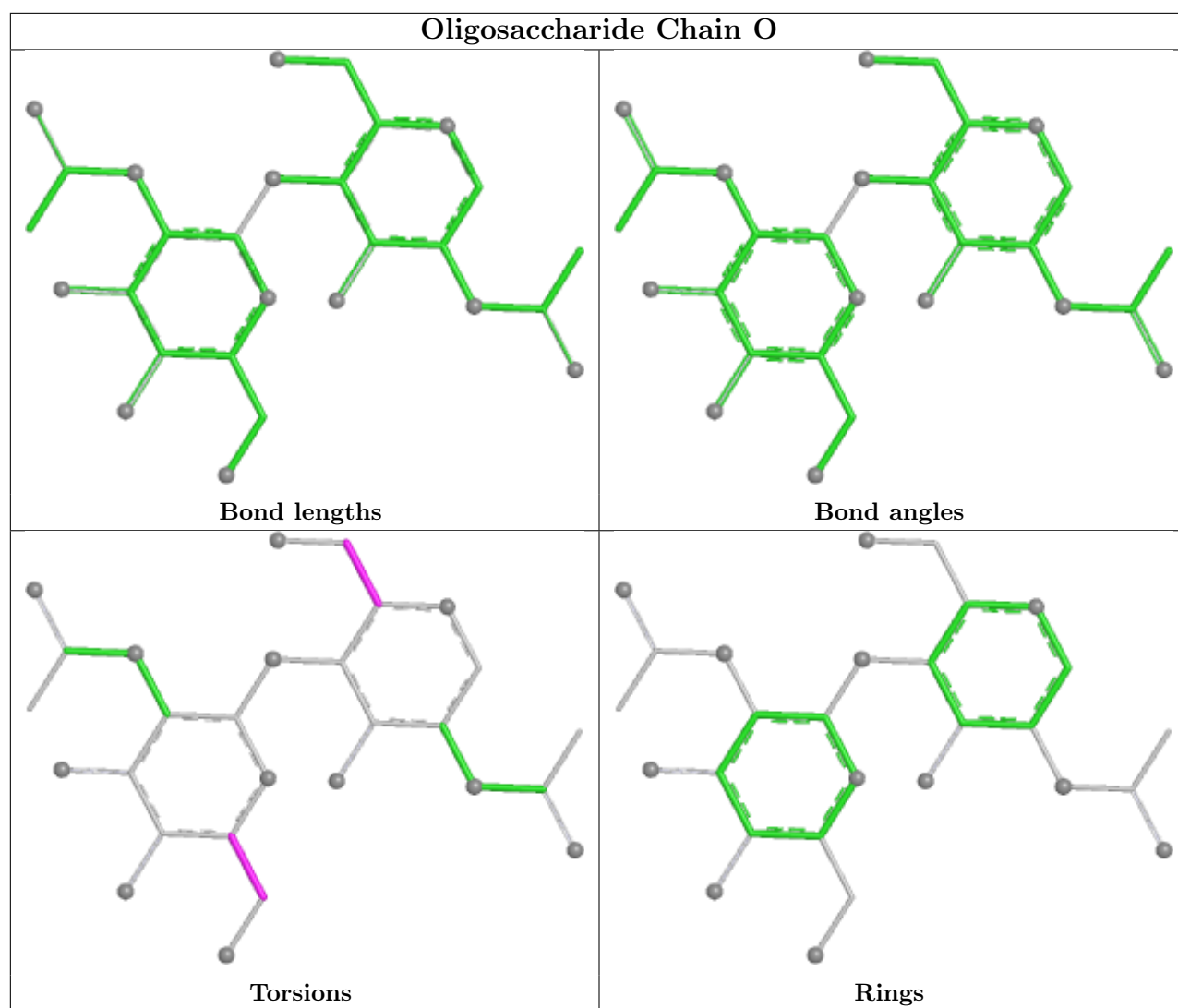


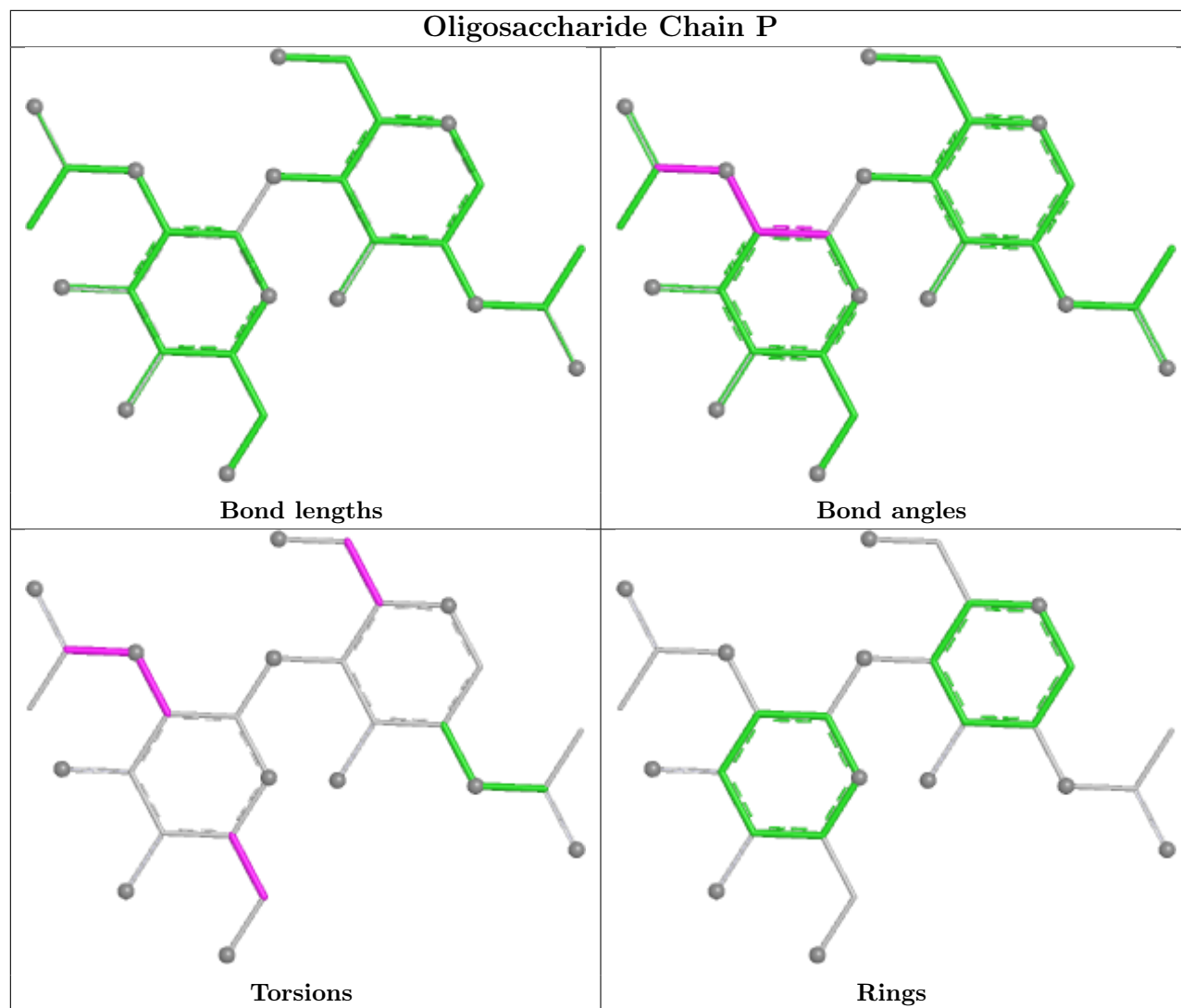


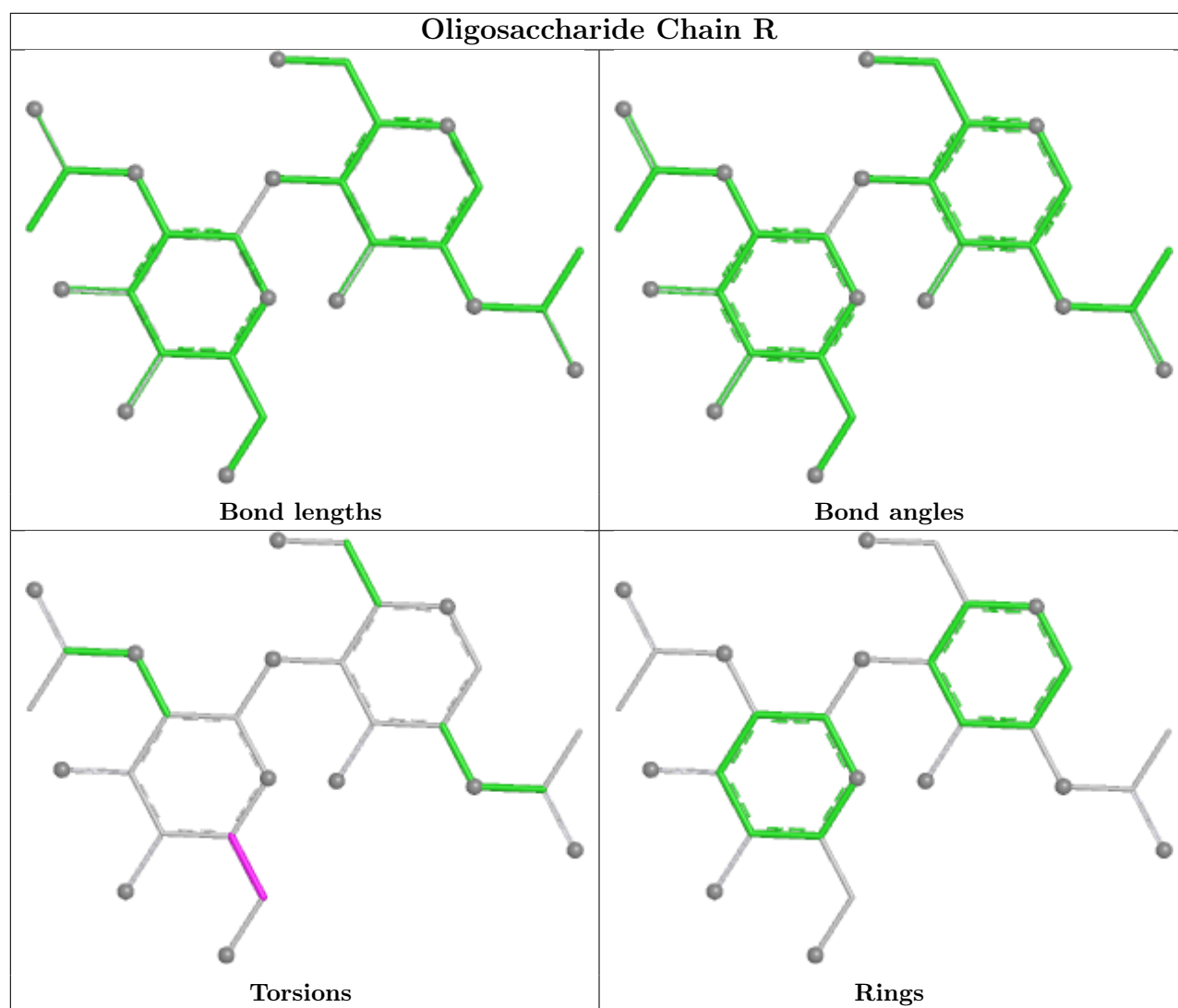


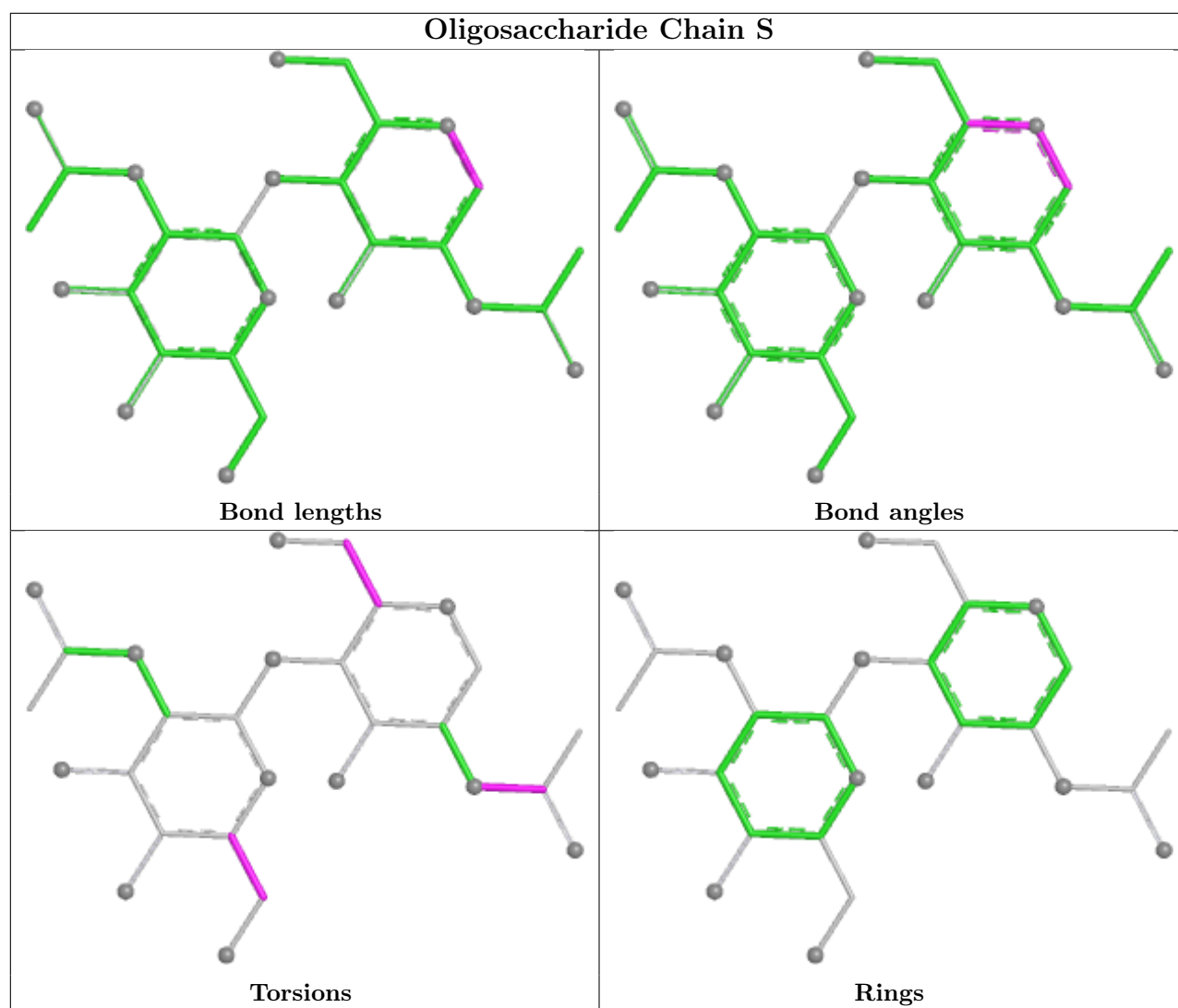


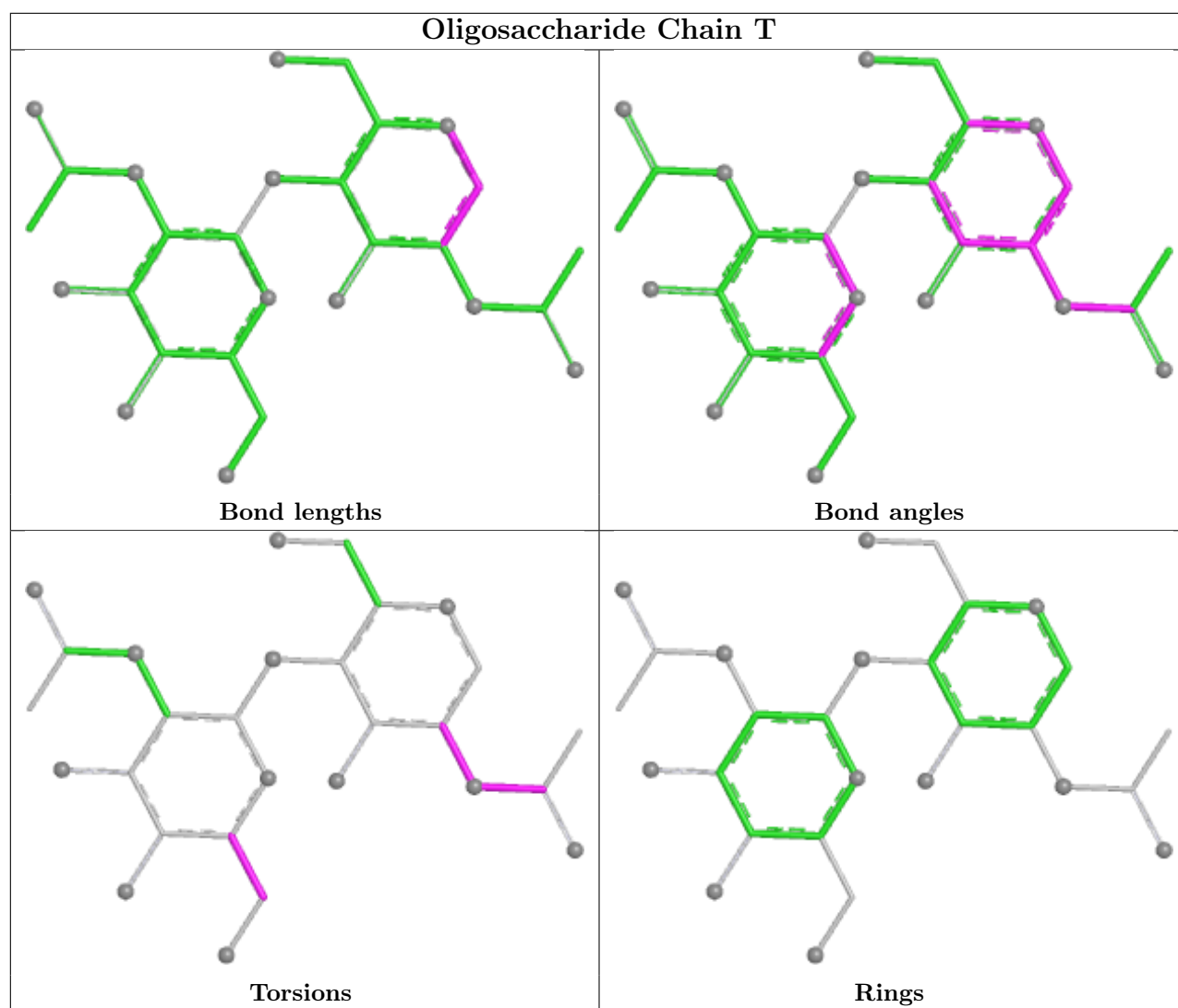


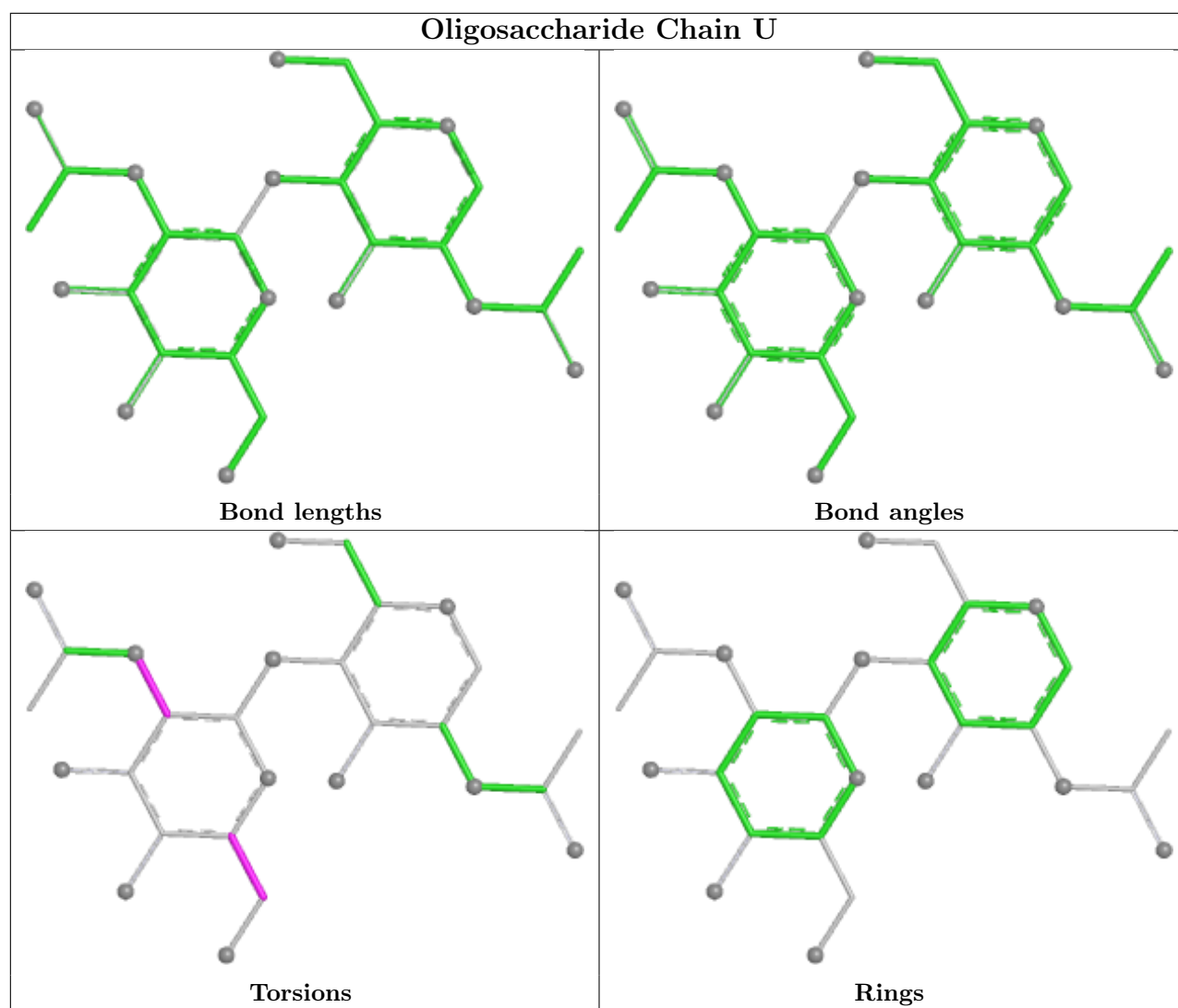


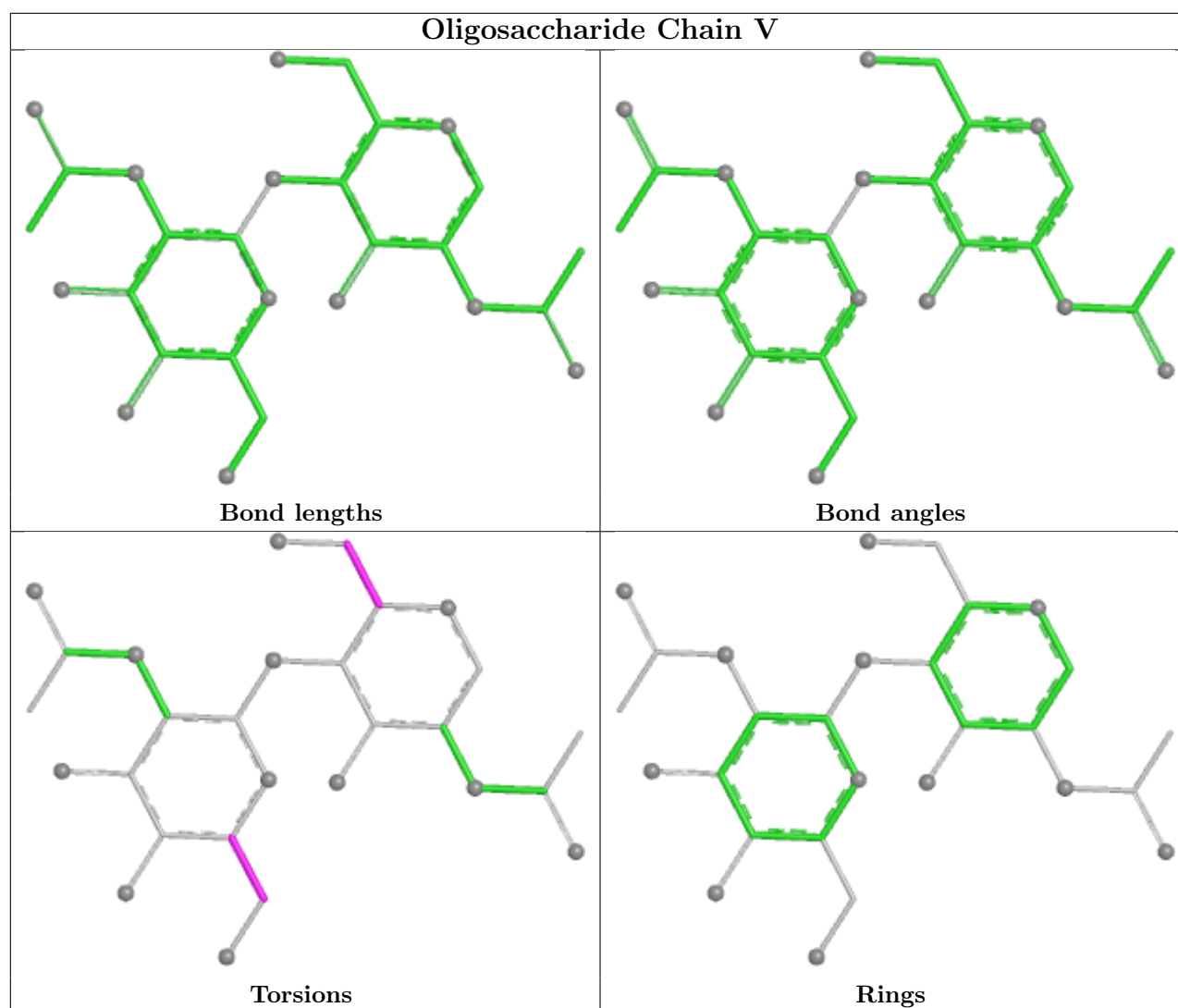


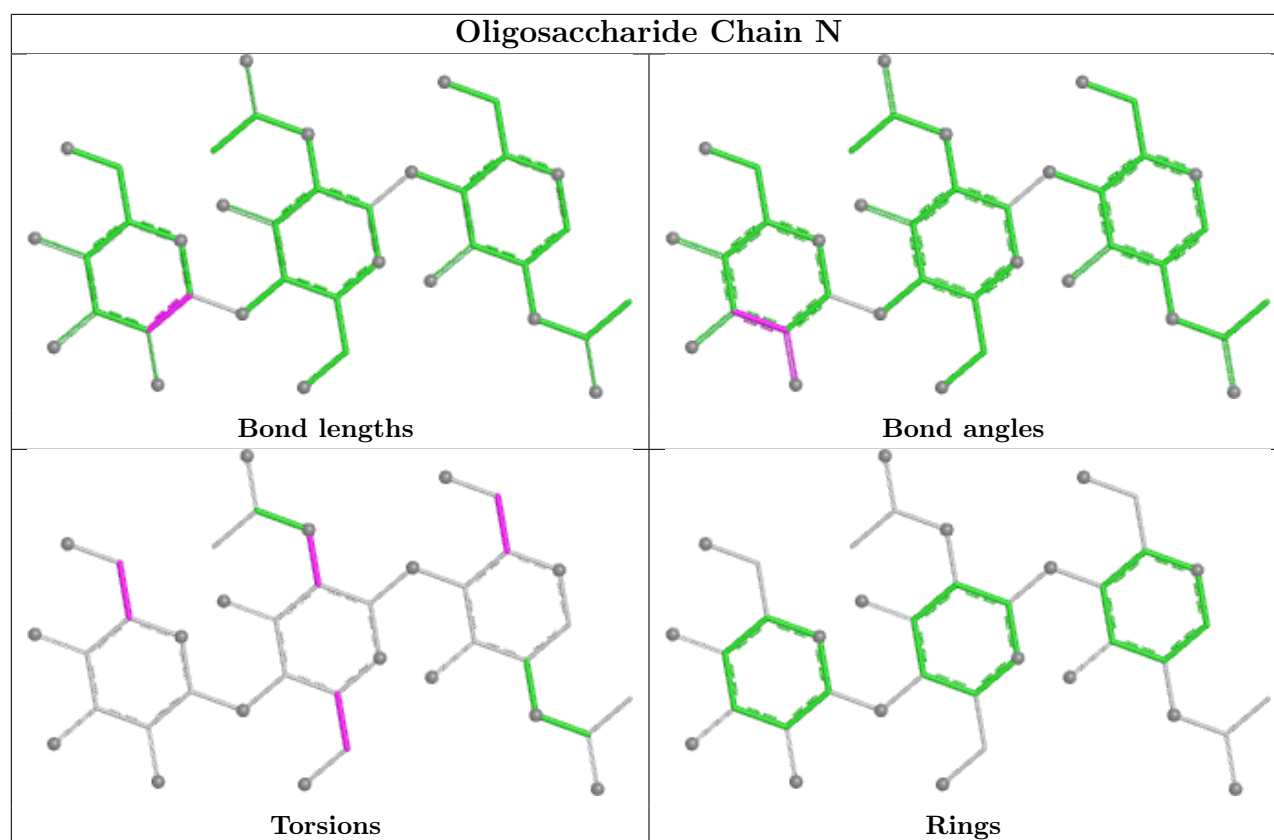












5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	201	2	14,14,15	1.97	2 (14%)	17,19,21	2.36	1 (5%)
6	NAG	B	201	2	14,14,15	1.55	1 (7%)	17,19,21	1.18	1 (5%)
6	NAG	E	408	1	14,14,15	0.78	1 (7%)	17,19,21	0.69	0
6	NAG	A	410	1	14,14,15	0.55	0	17,19,21	0.90	1 (5%)
6	NAG	C	411	1	14,14,15	0.78	1 (7%)	17,19,21	0.63	0
6	NAG	F	201	2	14,14,15	0.34	0	17,19,21	0.89	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
6	NAG	D	201	2	-	0/6/23/26	0/1/1/1
6	NAG	B	201	2	-	3/6/23/26	0/1/1/1
6	NAG	E	408	1	-	2/6/23/26	0/1/1/1
6	NAG	A	410	1	-	2/6/23/26	0/1/1/1
6	NAG	C	411	1	-	1/6/23/26	0/1/1/1
6	NAG	F	201	2	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	201	NAG	O5-C1	6.42	1.54	1.43
6	B	201	NAG	O5-C1	-5.65	1.34	1.43
6	D	201	NAG	C1-C2	3.51	1.57	1.52
6	E	408	NAG	O5-C1	-2.74	1.39	1.43
6	C	411	NAG	O5-C1	-2.67	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	201	NAG	C1-O5-C5	9.40	124.79	112.19
6	B	201	NAG	C1-O5-C5	-4.03	106.79	112.19
6	A	410	NAG	C1-O5-C5	3.24	116.53	112.19
6	F	201	NAG	C1-O5-C5	2.22	115.16	112.19

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	201	NAG	C4-C5-C6-O6
6	B	201	NAG	O5-C5-C6-O6
6	F	201	NAG	O5-C5-C6-O6
6	A	410	NAG	C4-C5-C6-O6
6	C	411	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	201	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	341/346 (98%)	-0.38	2 (0%) 85 85	14, 27, 46, 77	0
1	C	341/346 (98%)	-0.11	8 (2%) 61 60	18, 32, 50, 69	0
1	E	341/346 (98%)	-0.42	2 (0%) 85 85	15, 27, 44, 78	0
2	B	170/182 (93%)	-0.00	3 (1%) 67 67	15, 41, 70, 85	0
2	D	169/182 (92%)	-0.38	0 100 100	15, 33, 45, 77	0
2	F	169/182 (92%)	-0.16	3 (1%) 67 67	13, 37, 57, 83	0
All	All	1531/1584 (96%)	-0.26	18 (1%) 76 76	13, 31, 53, 85	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	170	LEU	3.8
1	A	341	LYS	3.7
2	F	169	SER	3.2
1	C	341	LYS	3.2
1	C	148	ASN	3.0

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

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

6.3 Carbohydrates [i](#)

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

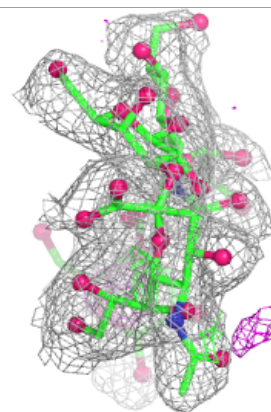
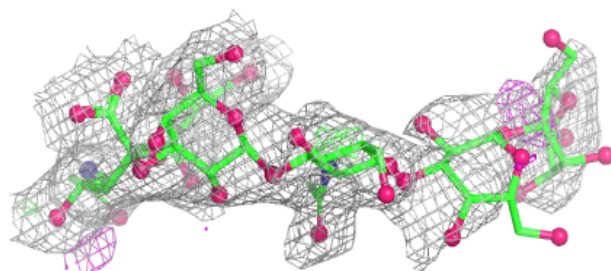
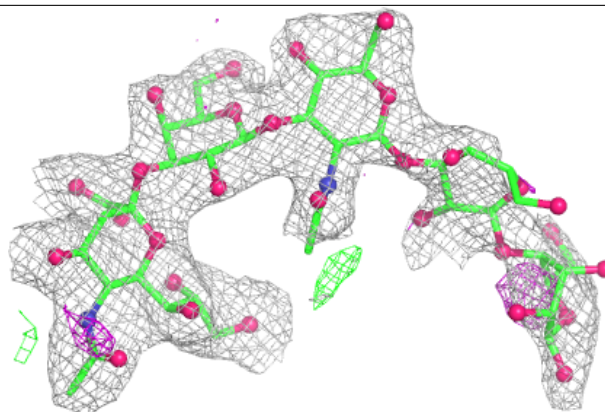
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GAL	L	2	11/12	0.45	0.17	87,97,104,105	0
4	NAG	V	2	14/15	0.50	0.19	67,75,81,81	0
4	NAG	T	1	14/15	0.52	0.22	57,67,78,80	0
4	NAG	J	2	14/15	0.53	0.20	74,83,93,99	0
3	GAL	G	2	11/12	0.60	0.18	76,86,96,99	0
4	NAG	M	2	14/15	0.60	0.17	68,76,83,85	0
4	NAG	K	2	14/15	0.63	0.19	60,83,87,87	0
4	NAG	T	2	14/15	0.64	0.20	74,84,89,91	0
3	BGC	Q	1	12/12	0.65	0.20	63,91,101,101	0
3	BGC	G	1	12/12	0.65	0.17	71,85,93,96	0
4	NAG	P	2	14/15	0.65	0.17	55,70,85,86	0
3	BGC	L	1	12/12	0.66	0.17	83,98,102,102	0
4	NAG	R	2	14/15	0.68	0.15	70,77,88,89	0
3	NAG	L	3	14/15	0.68	0.17	69,89,97,100	0
3	NAG	G	3	14/15	0.71	0.15	61,72,78,79	0
4	NAG	H	2	14/15	0.73	0.13	63,80,86,87	0
4	NAG	S	2	14/15	0.74	0.14	44,58,66,73	0
3	GAL	Q	2	11/12	0.74	0.15	83,99,104,106	0
4	NAG	U	2	14/15	0.76	0.13	64,80,83,86	0
5	BMA	N	3	11/12	0.76	0.16	39,53,60,63	0
4	NAG	I	2	14/15	0.78	0.15	65,75,81,85	0
5	NAG	N	2	14/15	0.80	0.20	33,46,59,60	0
4	NAG	K	1	14/15	0.81	0.14	48,59,72,81	0
3	NAG	Q	3	14/15	0.82	0.13	57,74,80,81	0
4	NAG	I	1	14/15	0.82	0.17	40,59,67,67	0
5	NAG	N	1	14/15	0.83	0.16	38,45,54,63	0
4	NAG	O	2	14/15	0.83	0.13	60,76,90,93	0
4	NAG	M	1	14/15	0.83	0.15	41,54,65,69	0
4	NAG	R	1	14/15	0.85	0.12	44,57,65,71	0
3	SIA	L	5	20/21	0.86	0.12	35,46,52,53	0
4	NAG	H	1	14/15	0.86	0.10	42,51,63,70	0
4	NAG	O	1	14/15	0.87	0.11	45,53,62,73	0
4	NAG	U	1	14/15	0.88	0.10	34,45,68,70	0
4	NAG	V	1	14/15	0.88	0.11	43,49,57,63	0
4	NAG	P	1	14/15	0.90	0.10	34,45,59,64	0
4	NAG	S	1	14/15	0.90	0.11	33,41,46,51	0
4	NAG	J	1	14/15	0.90	0.10	41,53,64,66	0
3	GAL	L	4	11/12	0.90	0.11	52,55,63,65	0
3	GAL	G	4	11/12	0.93	0.08	36,40,49,51	0
3	SIA	Q	5	20/21	0.94	0.08	24,27,31,32	0
3	GAL	Q	4	11/12	0.94	0.08	31,34,42,42	0
3	SIA	G	5	20/21	0.95	0.07	20,28,36,38	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.

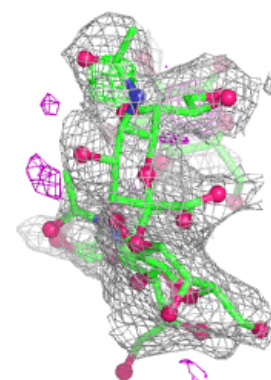
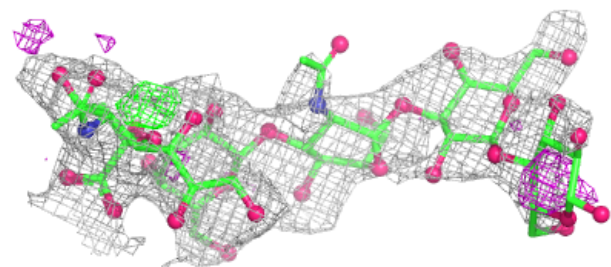
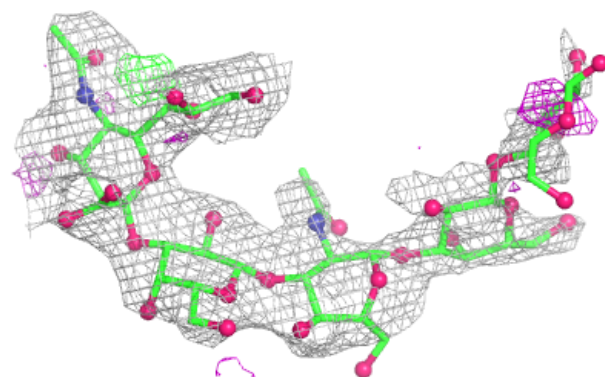
Electron density around Chain G:

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



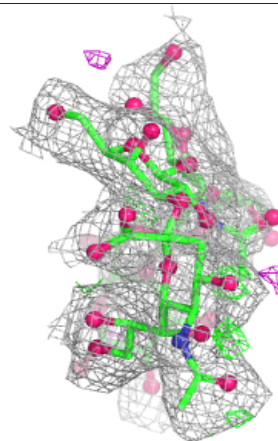
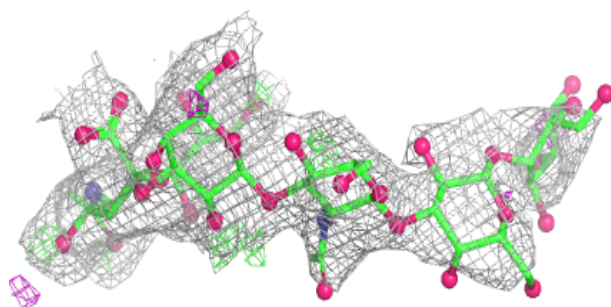
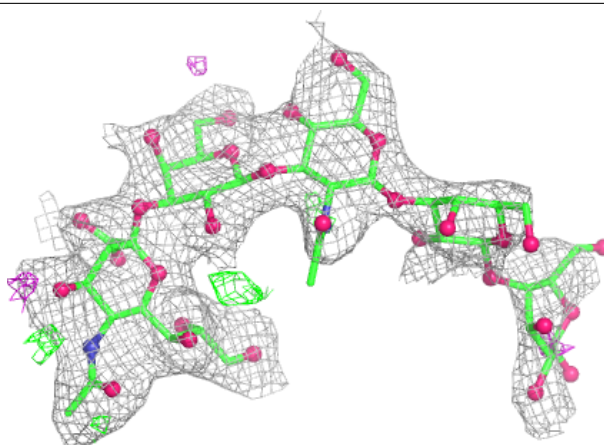
Electron density around Chain L:

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



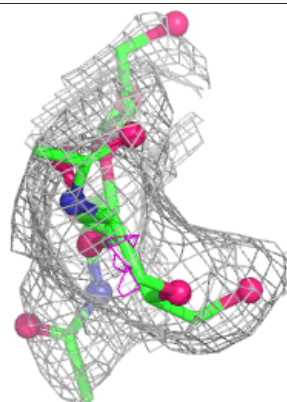
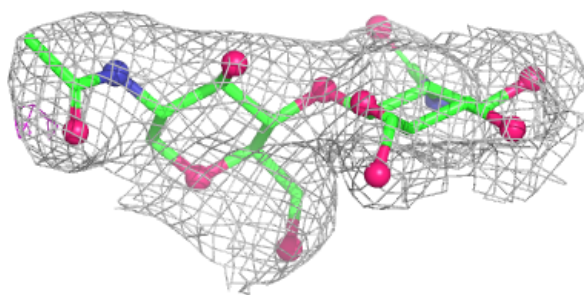
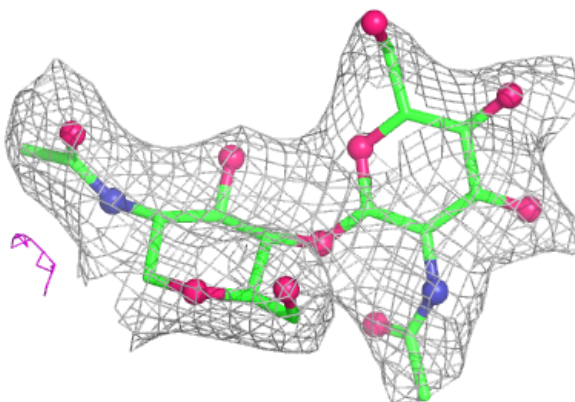
Electron density around Chain Q:

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

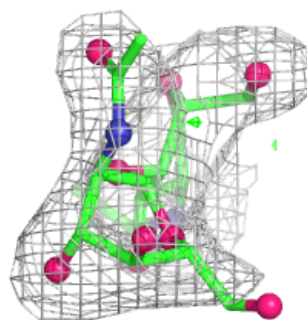
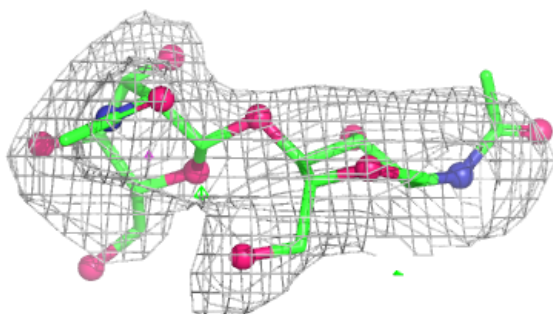
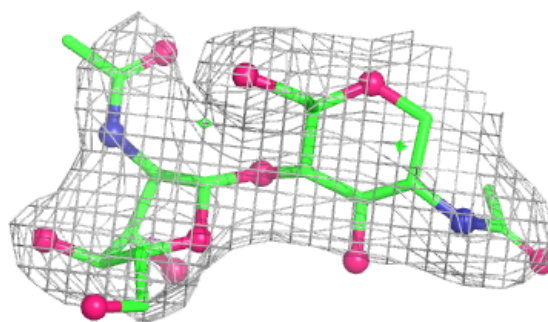


Electron density around Chain H:

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

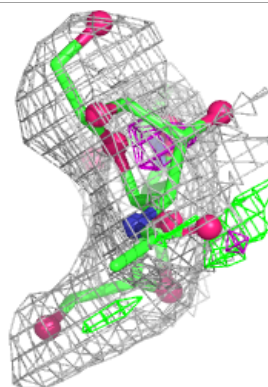
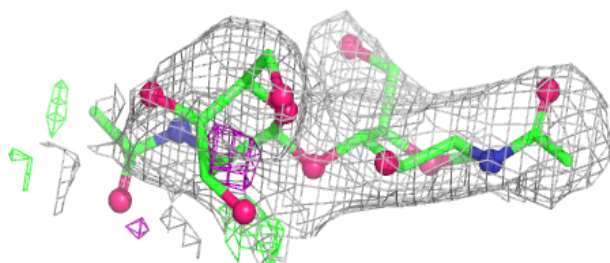
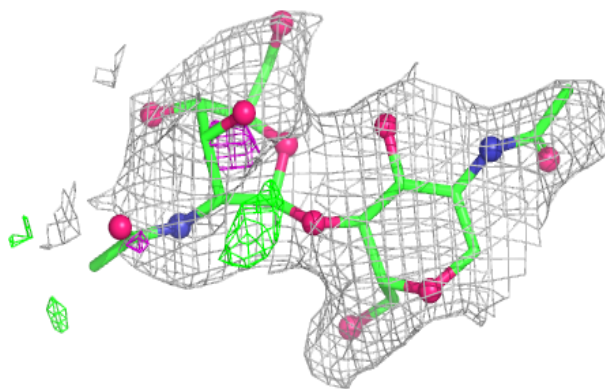
**Electron density around Chain I:**

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



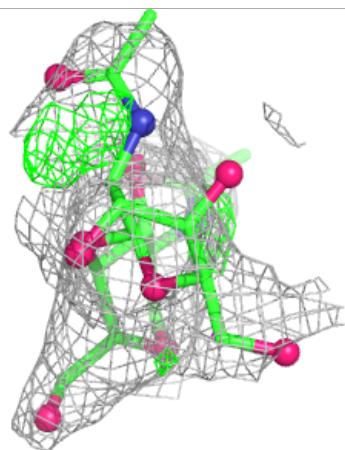
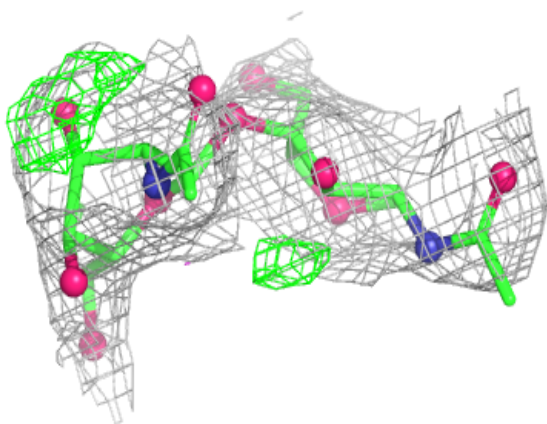
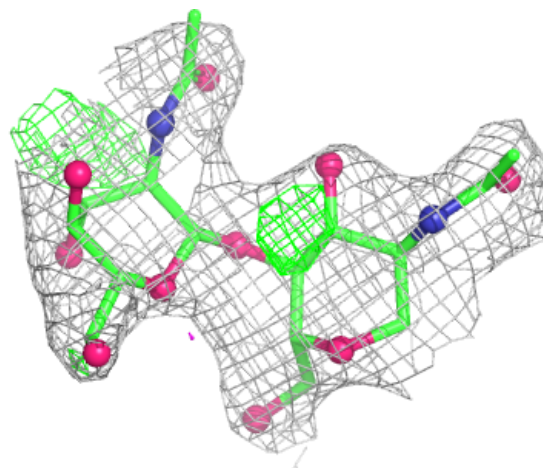
Electron density around Chain J:

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



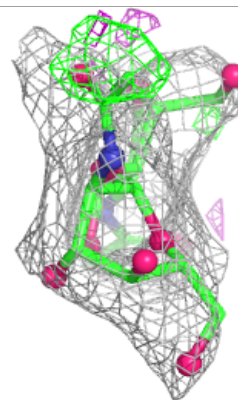
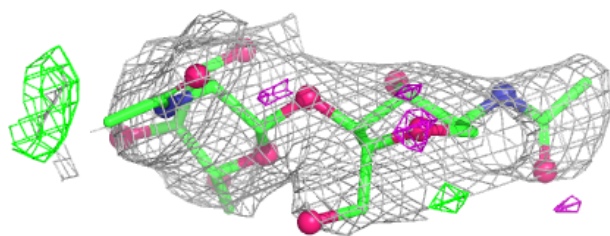
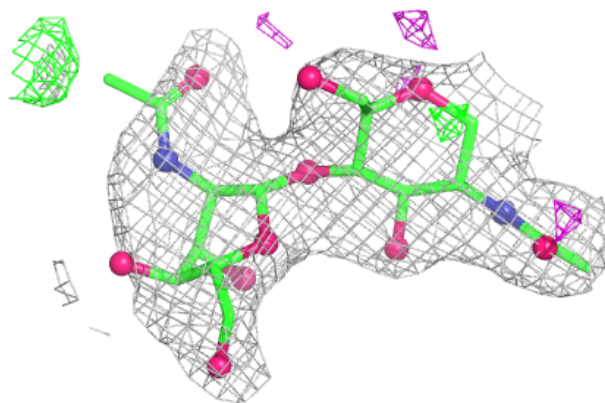
Electron density around Chain K:

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

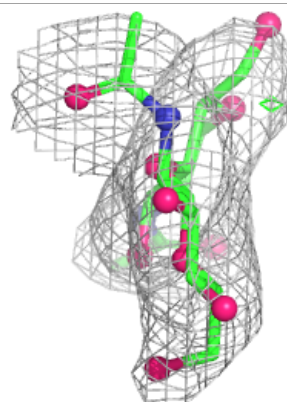
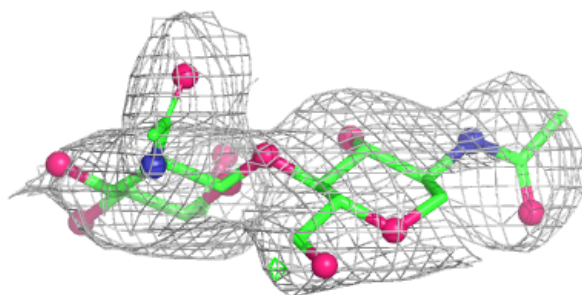
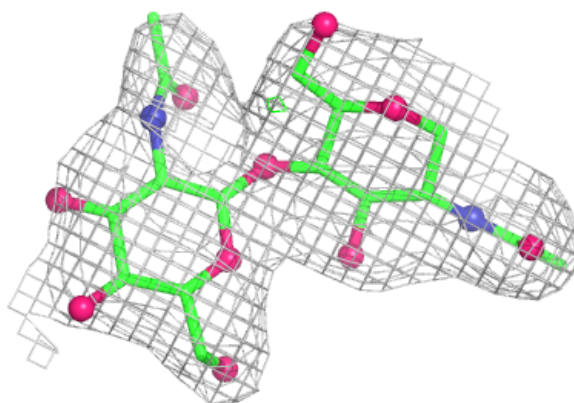


Electron density around Chain M:

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

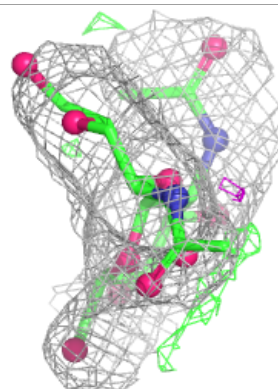
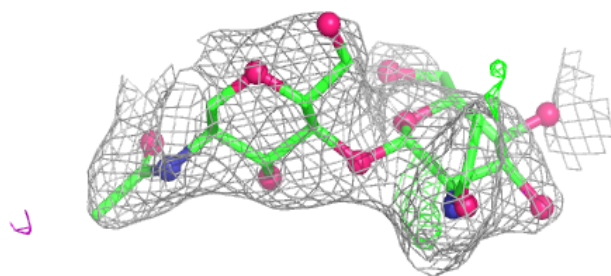
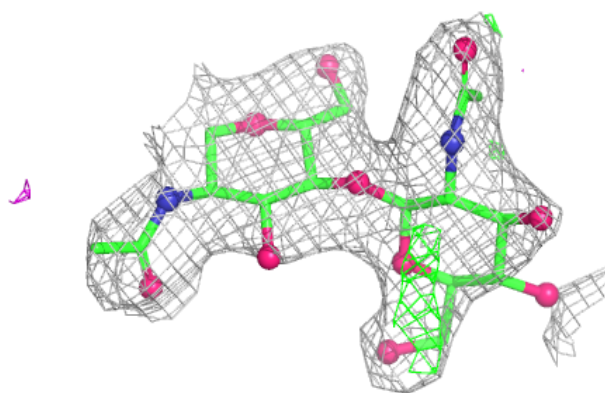
**Electron density around Chain O:**

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

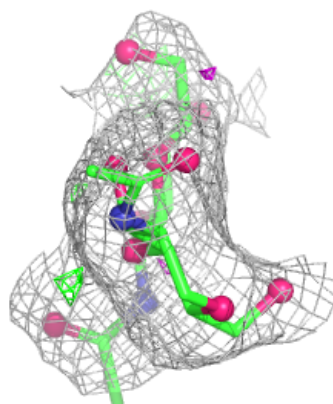
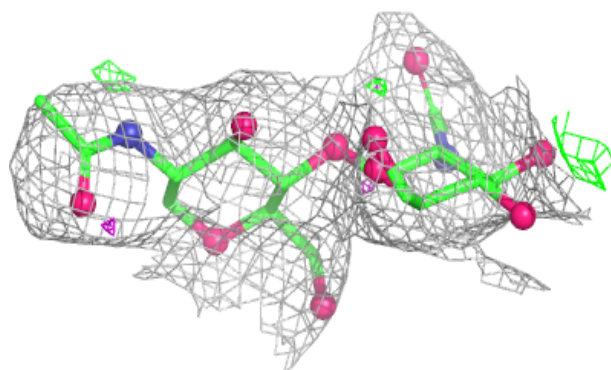
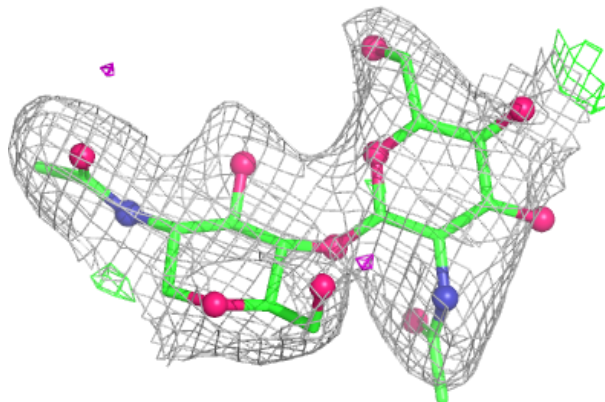


Electron density around Chain P:

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

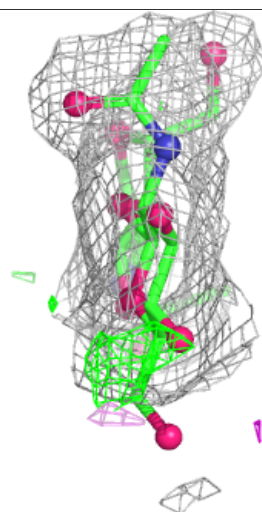
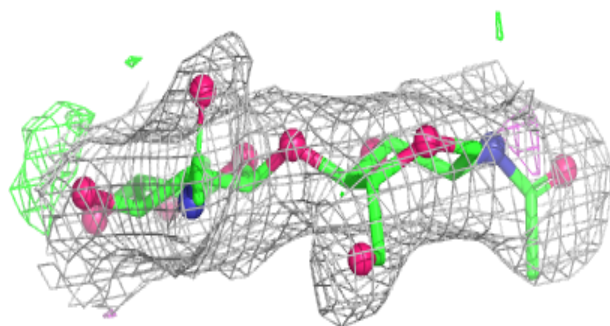
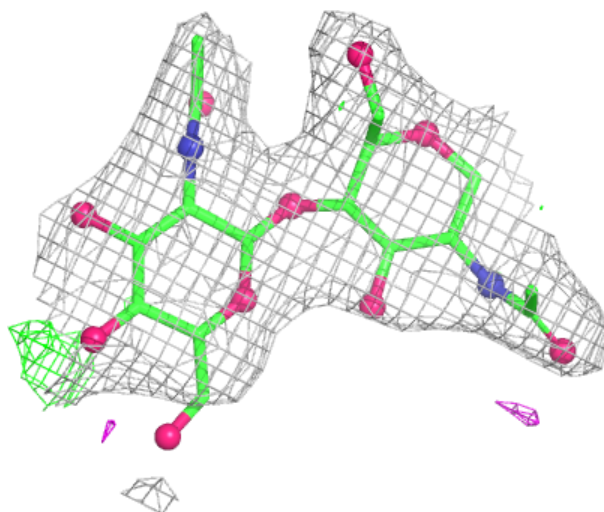
**Electron density around Chain R:**

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



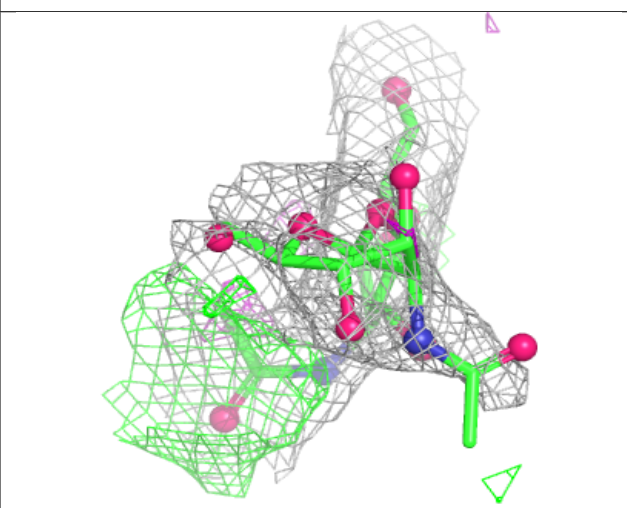
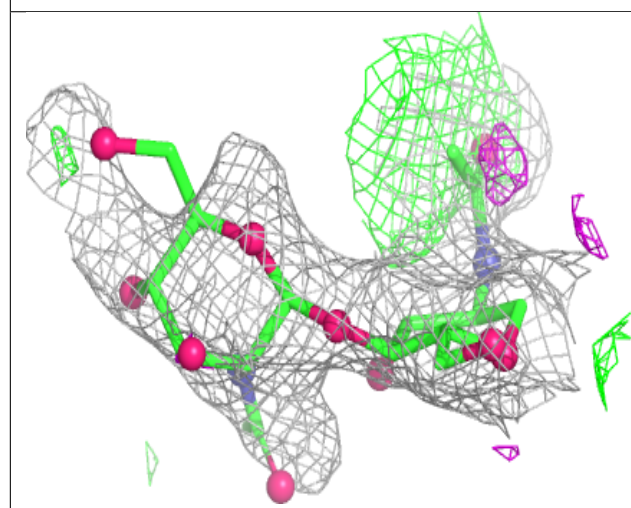
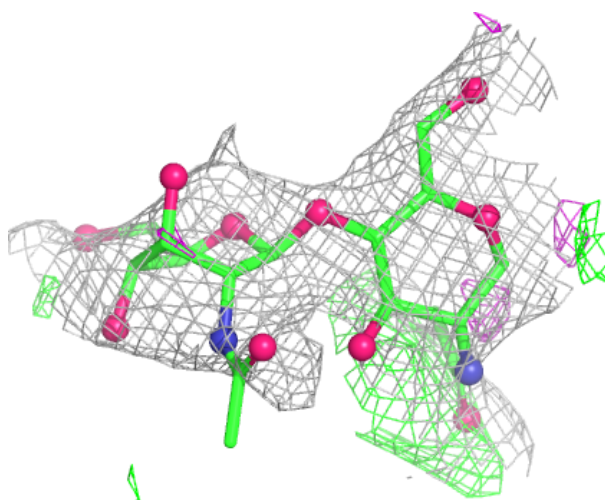
Electron density around Chain S:

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



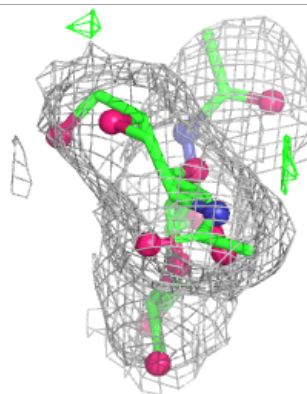
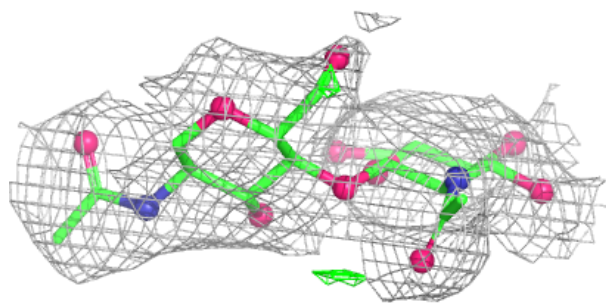
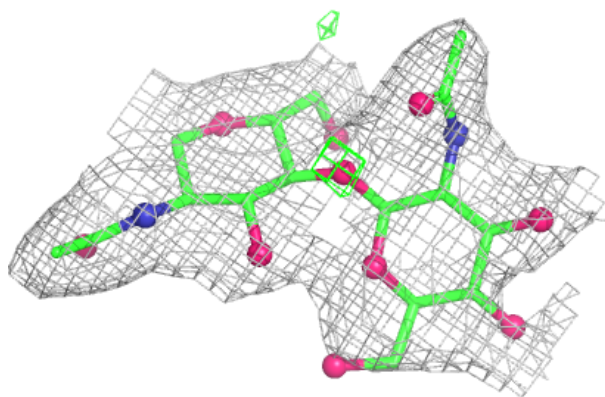
Electron density around Chain T:

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



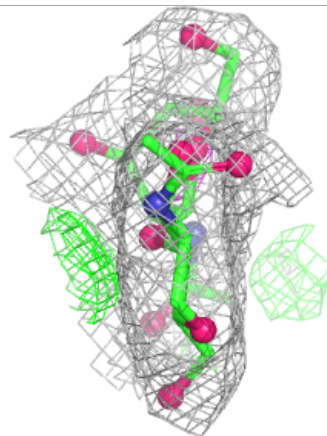
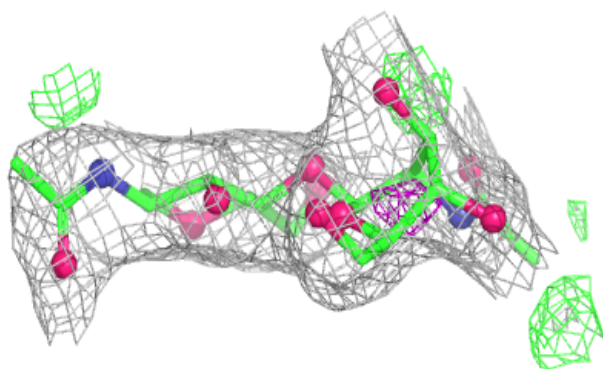
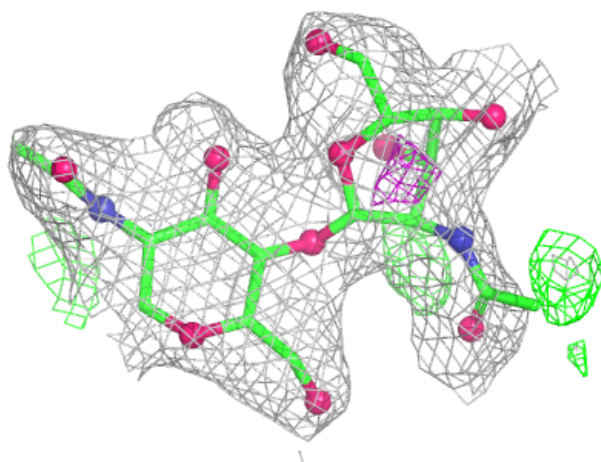
Electron density around Chain U:

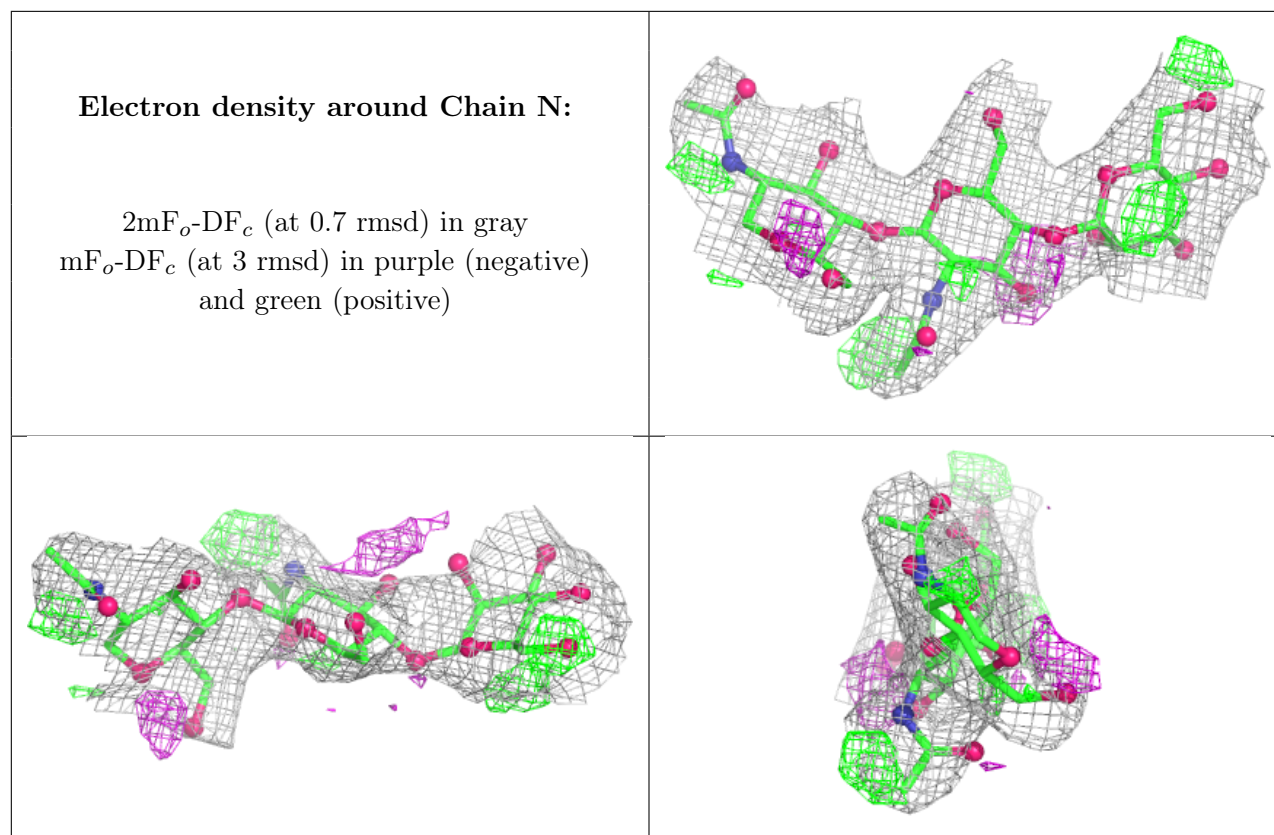
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain V:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	C	411	14/15	0.43	0.22	77,89,106,108	0
6	NAG	E	408	14/15	0.47	0.22	51,82,88,92	0
6	NAG	B	201	14/15	0.50	0.22	91,104,114,115	0
6	NAG	F	201	14/15	0.65	0.15	61,68,74,76	0
6	NAG	D	201	14/15	0.67	0.18	55,67,74,74	0
6	NAG	A	410	14/15	0.76	0.16	65,72,82,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.