



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:58 PM BST

PDB ID : 4UNZ  
Title : Structure of the A\_Equine\_Newmarket\_2\_93 H3 haemagglutinin in complex with 6SO4-Sialyl Lewis X  
Authors : Vachieri, S.G.; Collins, P.J.; Haire, L.F.; Ogrodowicz, R.W.; Martin, S.R.; Walker, P.A.; Xiong, X.; Gamblin, S.J.; Skehel, J.J.  
Deposited on : 2014-05-31  
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

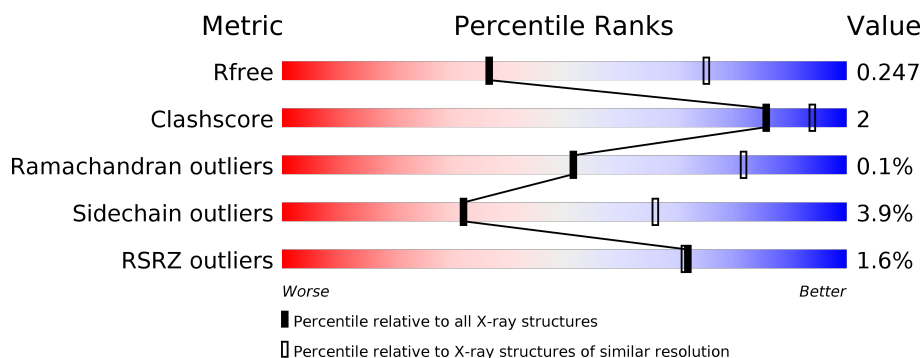
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	330	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>••</div> </div> </div>
1	C	330	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>•</div> </div> </div>
1	E	330	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>•</div> </div> </div>
2	B	173	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>••</div> </div> </div>
2	D	173	<div> <div></div> <div> <div></div> <div>91%</div> <div>8%</div> <div>••</div> </div> </div>
2	F	173	<div> <div></div> <div> <div></div> <div>92%</div> <div>6%</div> <div>•••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	4	 100%
4	H	4	 75% 25%
4	P	4	 50% 50%
4	U	4	 100%
5	I	3	 100%
6	J	2	 50% 50%
6	K	2	 100%
6	L	2	 100%
6	O	2	 100%
6	S	2	 100%
6	T	2	 100%
7	M	3	 67% 33%
7	R	3	 33% 33% 33%
8	N	6	 33% 33% 33%
9	Q	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	C	471	X	-	-	-
10	NAG	E	411	-	-	-	X
3	BMA	G	3	-	-	-	X
3	MAN	G	4	-	-	-	X
4	FUC	H	4	X	-	-	-
4	FUC	P	4	X	-	-	-
4	GAL	U	2	X	-	-	-
4	SIA	U	3	X	-	-	-
4	FUC	U	4	X	-	-	-
5	FUC	I	3	X	-	-	-
6	NAG	J	1	-	-	-	X
6	NAG	J	2	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	L	2	-	-	-	X
6	NAG	O	1	X	-	-	-
8	MAN	N	4	-	-	-	X
8	FUC	N	6	X	-	-	-
9	FUC	Q	2	X	-	-	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 12397 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 HAY SUBUNIT OF HAEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2463	1540	433	476	14			
1	C	330	Total	C	N	O	S	0	0	0
			2564	1599	454	497	14			
1	E	318	Total	C	N	O	S	0	0	0
			2447	1528	431	474	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PRO	-	expression tag	UNP Q82847
A	1	ASP	-	expression tag	UNP Q82847
C	0	PRO	-	expression tag	UNP Q82847
C	1	ASP	-	expression tag	UNP Q82847
E	0	PRO	-	expression tag	UNP Q82847
E	1	ASP	-	expression tag	UNP Q82847

- Molecule 2 is a protein called H3 HAEMAGGLUTININ HA2 CHAIN.

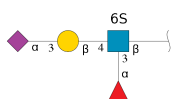
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1404	876	246	276	6			
2	D	172	Total	C	N	O	S	0	0	0
			1396	870	245	275	6			
2	F	172	Total	C	N	O	S	0	0	0
			1388	864	243	275	6			

- Molecule 3 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.



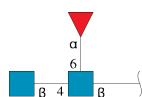
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	S	0	0	0
			60	31	2	26	1			
4	P	4	Total	C	N	O	S	0	0	0
			60	31	2	26	1			
4	U	4	Total	C	N	O	S	0	0	0
			60	31	2	26	1			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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



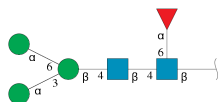
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	R	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



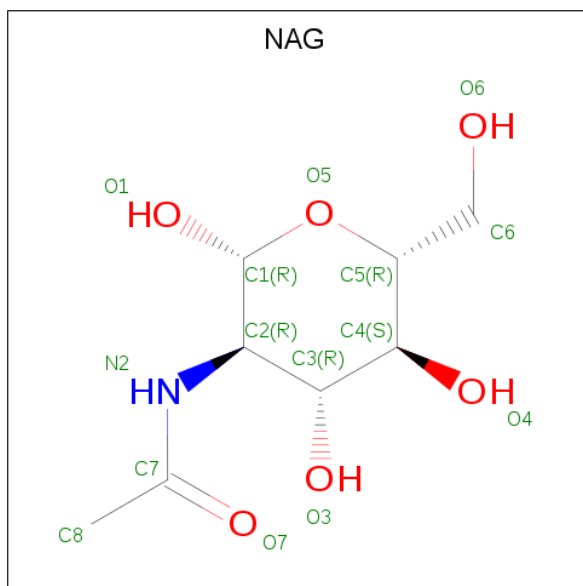
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	N	6	Total	C	N	O	0	0	0
			71	40	2	29			

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



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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 11 is water.

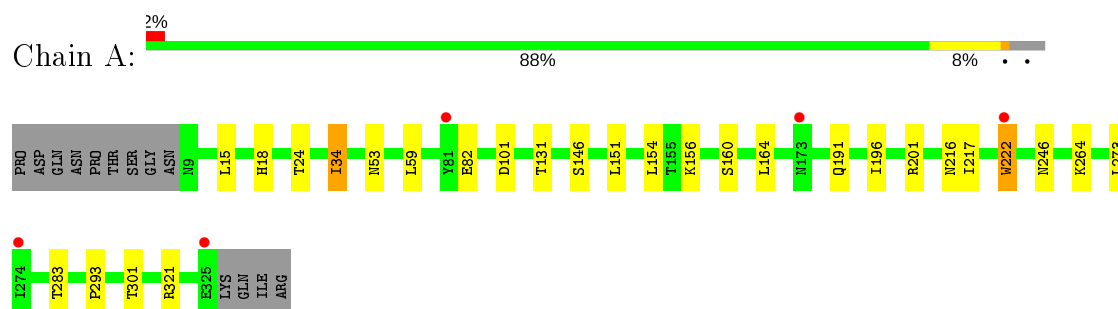


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	12	Total 12	O 12	0	0
11	B	5	Total 5	O 5	0	0
11	C	12	Total 12	O 12	0	0
11	D	8	Total 8	O 8	0	0
11	E	3	Total 3	O 3	0	0
11	F	2	Total 2	O 2	0	0

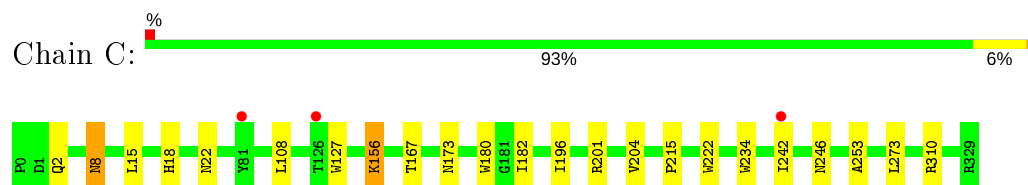
### 3 Residue-property plots [i](#)

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.

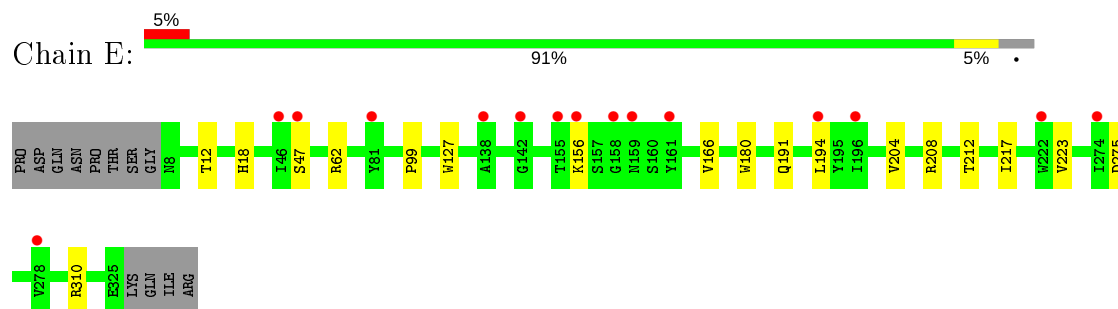
- Molecule 1: HAY SUBUNIT OF HAEMAGGLUTININ



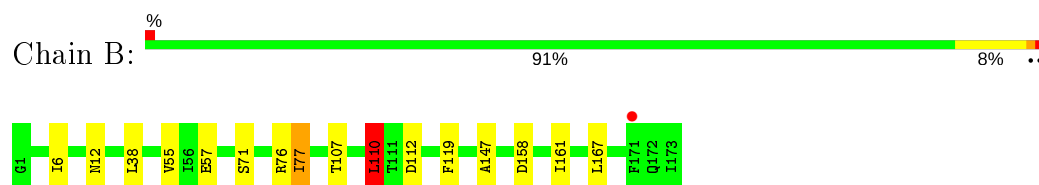
- Molecule 1: HAY SUBUNIT OF HAEMAGGLUTININ




- Molecule 1: HAY SUBUNIT OF HAEMAGGLUTININ

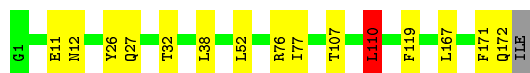


- Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN



- Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN

Chain D:  91% 8% ..



- Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN

Chain F:  92% 6% ...

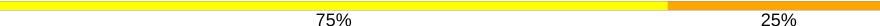


- Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranose

Chain H:  75% 25%



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranose

Chain P:  50% 50%



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranose

Chain U:  100%



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

Chain I:  100%



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

Chain J:  50% 50%

NAG1  
NAG2

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

Chain K:  100%

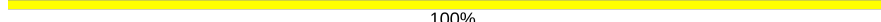
NAG1  
NAG2

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

Chain L:  100%

NAG1  
NAG2

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

Chain O:  100%

NAG1  
NAG2

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

Chain S:  100%

NAG1  
NAG2

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

Chain T:  100%

NAG1  
NAG2

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

Chain M:  67% 33%



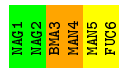
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  33% 33% 33%



- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  33% 33% 33%



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

Chain Q:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.55Å 125.75Å 165.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.04 – 2.90 47.66 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (100.04-2.90) 98.2 (47.66-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.198 , 0.248 0.202 , 0.247	Depositor DCC
$R_{free}$ test set	2333 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.3	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, SIA, GAL, FUC, NGS, MAN

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	0.30	0/2516	0.54	0/3419
1	C	0.30	0/2619	0.55	0/3558
1	E	0.30	0/2500	0.50	0/3404
2	B	0.34	0/1429	0.57	1/1921 (0.1%)
2	D	0.33	0/1421	0.57	1/1910 (0.1%)
2	F	0.31	0/1413	0.51	1/1902 (0.1%)
All	All	0.31	0/11898	0.54	3/16114 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	110	LEU	CA-CB-CG	6.87	131.09	115.30
2	B	110	LEU	CA-CB-CG	6.77	130.87	115.30
2	D	110	LEU	CA-CB-CG	6.34	129.87	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2463	0	2398	13	0
1	C	2564	0	2496	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2447	0	2352	5	0
2	B	1404	0	1328	11	0
2	D	1396	0	1317	6	0
2	F	1388	0	1295	9	0
3	G	50	0	43	0	0
4	H	60	0	44	1	0
4	P	60	0	44	1	0
4	U	60	0	44	0	0
5	I	38	0	34	1	0
6	J	28	0	25	1	0
6	K	28	0	25	0	0
6	L	28	0	25	0	0
6	O	28	0	25	0	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
7	M	39	0	34	0	0
7	R	39	0	34	2	0
8	N	71	0	61	2	0
9	Q	24	0	22	0	0
10	A	42	0	39	2	0
10	C	14	0	13	0	0
10	E	14	0	13	0	0
10	F	14	0	13	0	0
11	A	12	0	0	0	0
11	B	5	0	0	0	0
11	C	12	0	0	0	0
11	D	8	0	0	0	0
11	E	3	0	0	0	0
11	F	2	0	0	0	0
All	All	12397	0	11774	52	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 2.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:THR:HA	2:B:110:LEU:HD13	1.78	0.65
2:F:56:ILE:HG22	2:F:57:GLU:HG2	1.82	0.61
2:B:76:ARG:NE	2:F:77:ILE:HD11	2.17	0.60
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:ILE:HD11	2:D:76:ARG:NE	2.18	0.59
2:F:107:THR:HA	2:F:110:LEU:HD13	1.84	0.59
10:A:421:NAG:H83	10:A:421:NAG:H3	1.84	0.59
1:A:216:ASN:OD1	1:E:212:THR:HG21	2.04	0.57
2:B:77:ILE:HD11	2:D:76:ARG:CZ	2.35	0.56
2:D:27:GLN:HG3	2:D:32:THR:HG22	1.87	0.56
2:B:76:ARG:CZ	2:F:77:ILE:HD11	2.41	0.51
1:A:164:LEU:O	1:A:246:ASN:HA	2.12	0.50
1:C:22:ASN:N	1:C:22:ASN:OD1	2.45	0.50
1:E:127:TRP:CZ3	1:E:166:VAL:HG21	2.47	0.50
2:F:54:ARG:NH2	2:F:103:GLU:OE2	2.45	0.50
1:A:222:TRP:H	7:R:2:NAG:H83	1.77	0.49
1:C:127:TRP:CZ2	1:C:253:ALA:HB1	2.48	0.48
7:R:2:NAG:O3	7:R:2:NAG:H82	2.13	0.48
1:A:34:ILE:HD11	1:A:321:ARG:NE	2.28	0.48
1:C:180:TRP:CE2	1:C:204:VAL:HG21	2.49	0.48
2:B:147:ALA:HB1	5:I:2:NAG:H82	1.95	0.48
1:C:182:ILE:HD11	1:C:215:PRO:HD3	1.96	0.47
1:C:8:ASN:OD1	1:C:8:ASN:C	2.52	0.47
1:C:167:THR:HB	1:C:242:ILE:HD11	1.98	0.47
1:A:160:SER:HA	1:A:196:ILE:HG13	1.97	0.46
1:A:15:LEU:HD12	1:A:15:LEU:N	2.30	0.46
1:C:108:LEU:HD13	1:C:234:TRP:CD2	2.51	0.45
1:A:201:ARG:NH2	1:A:246:ASN:OD1	2.49	0.45
1:C:156:LYS:HD3	1:C:196:ILE:HD11	1.99	0.45
8:N:3:BMA:O4	8:N:4:MAN:H2	2.16	0.45
1:C:15:LEU:HD22	2:D:119:PHE:HA	2.00	0.44
2:D:107:THR:HA	2:D:110:LEU:HD13	2.00	0.44
1:E:99:PRO:HB3	1:E:223:VAL:HG11	2.00	0.44
10:A:421:NAG:C8	10:A:421:NAG:H3	2.47	0.44
2:D:77:ILE:HD11	2:F:77:ILE:HG22	1.98	0.44
2:F:77:ILE:O	2:F:77:ILE:HD12	2.17	0.43
2:F:9:PHE:O	2:F:135:GLY:HA2	2.19	0.43
8:N:3:BMA:C4	8:N:4:MAN:H2	2.49	0.43
4:P:2:GAL:H4	4:P:3:SIA:O6	2.18	0.43
2:F:110:LEU:HD22	2:F:111:THR:N	2.33	0.43
1:A:283:THR:HG22	1:A:301:THR:HG22	2.00	0.43
2:B:158:ASP:HB3	2:B:161:ILE:HD12	2.00	0.43
1:E:180:TRP:CE2	1:E:204:VAL:HG21	2.55	0.42
1:A:293:PRO:HG3	2:B:55:VAL:HG12	2.02	0.41
1:E:191:GLN:HG2	1:E:217:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:ILE:HD12	2:B:112:ASP:HA	2.01	0.41
1:A:15:LEU:CD2	2:B:119:PHE:HA	2.49	0.41
4:H:3:SIA:O7	4:H:3:SIA:H113	2.21	0.41
1:A:59:LEU:HD21	1:A:82:GLU:HG2	2.04	0.40
6:J:1:NAG:H61	6:J:2:NAG:HN2	1.86	0.40
1:C:201:ARG:NH2	1:C:246:ASN:OD1	2.54	0.40
1:A:191:GLN:HG2	1:A:217:ILE:HD11	2.04	0.40

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	315/330 (96%)	296 (94%)	19 (6%)	0	100	100
1	C	328/330 (99%)	309 (94%)	19 (6%)	0	100	100
1	E	316/330 (96%)	288 (91%)	27 (8%)	1 (0%)	41	71
2	B	171/173 (99%)	157 (92%)	13 (8%)	1 (1%)	25	58
2	D	170/173 (98%)	161 (95%)	9 (5%)	0	100	100
2	F	170/173 (98%)	161 (95%)	9 (5%)	0	100	100
All	All	1470/1509 (97%)	1372 (93%)	96 (6%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	57	GLU
1	E	62	ARG

### 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	277/290 (96%)	264 (95%)	13 (5%)	26	59
1	C	289/290 (100%)	281 (97%)	8 (3%)	43	76
1	E	272/290 (94%)	264 (97%)	8 (3%)	42	76
2	B	145/145 (100%)	139 (96%)	6 (4%)	30	64
2	D	144/145 (99%)	135 (94%)	9 (6%)	18	46
2	F	142/145 (98%)	137 (96%)	5 (4%)	36	70
All	All	1269/1305 (97%)	1220 (96%)	49 (4%)	32	66

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	24	THR
1	A	34	ILE
1	A	53	ASN
1	A	101	ASP
1	A	131	THR
1	A	146	SER
1	A	151	LEU
1	A	154	LEU
1	A	156	LYS
1	A	222	TRP
1	A	264	LYS
1	A	273	LEU
2	B	12	ASN
2	B	38	LEU
2	B	71	SER
2	B	77	ILE
2	B	110	LEU
2	B	167	LEU
1	C	2	GLN
1	C	8	ASN
1	C	18	HIS

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Mol	Chain	Res	Type
1	C	156	LYS
1	C	173	ASN
1	C	222	TRP
1	C	273	LEU
1	C	310	ARG
2	D	11	GLU
2	D	12	ASN
2	D	26	TYR
2	D	38	LEU
2	D	52	LEU
2	D	110	LEU
2	D	167	LEU
2	D	171	PHE
2	D	172	GLN
1	E	12	THR
1	E	18	HIS
1	E	47	SER
1	E	156	LYS
1	E	194	LEU
1	E	208	ARG
1	E	275	ASP
1	E	310	ARG
2	F	12	ASN
2	F	53	ASN
2	F	71	SER
2	F	77	ILE
2	F	110	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	22	ASN
1	A	53	ASN
1	A	211	GLN
2	B	60	ASN
1	C	211	GLN
2	F	12	ASN
2	F	53	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 ⓘ

45 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	G	1	1,3	14,14,15	0.52	0	17,19,21	1.24	3 (17%)
3	NAG	G	2	3	14,14,15	0.57	0	17,19,21	0.93	1 (5%)
3	BMA	G	3	3	11,11,12	0.51	0	15,15,17	1.01	1 (6%)
3	MAN	G	4	3	11,11,12	0.57	0	15,15,17	0.97	1 (6%)
4	NGS	H	1	4	19,19,19	0.72	1 (5%)	26,28,28	1.03	2 (7%)
4	GAL	H	2	4	11,11,12	0.74	0	15,15,17	1.44	1 (6%)
4	SIA	H	3	4	17,20,21	0.32	0	21,28,31	1.33	3 (14%)
4	FUC	H	4	4	10,10,11	0.81	0	14,14,16	1.80	3 (21%)
5	NAG	I	1	2,5	14,14,15	0.61	0	17,19,21	0.87	1 (5%)
5	NAG	I	2	5	14,14,15	0.52	0	17,19,21	1.04	0
5	FUC	I	3	5	10,10,11	0.70	0	14,14,16	1.62	1 (7%)
6	NAG	J	1	1,6	14,14,15	0.48	0	17,19,21	1.43	2 (11%)
6	NAG	J	2	6	14,14,15	0.59	0	17,19,21	0.69	0
6	NAG	K	1	1,6	14,14,15	0.47	0	17,19,21	1.69	4 (23%)
6	NAG	K	2	6	14,14,15	0.50	0	17,19,21	1.08	2 (11%)
6	NAG	L	1	1,6	14,14,15	0.56	0	17,19,21	1.05	2 (11%)
6	NAG	L	2	6	14,14,15	0.43	0	17,19,21	1.00	1 (5%)
7	NAG	M	1	1,7	14,14,15	0.60	0	17,19,21	1.37	3 (17%)
7	NAG	M	2	7	14,14,15	0.57	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BMA	M	3	7	11,11,12	0.38	0	15,15,17	0.65	0
8	NAG	N	1	1,8	14,14,15	0.69	0	17,19,21	0.93	0
8	NAG	N	2	8	14,14,15	0.62	0	17,19,21	0.86	0
8	BMA	N	3	8	11,11,12	0.42	0	15,15,17	1.09	1 (6%)
8	MAN	N	4	8	11,11,12	0.58	0	15,15,17	1.67	2 (13%)
8	MAN	N	5	8	11,11,12	0.63	0	15,15,17	0.99	1 (6%)
8	FUC	N	6	8	10,10,11	0.96	0	14,14,16	2.07	5 (35%)
6	NAG	O	1	1,6	14,14,15	0.48	0	17,19,21	1.19	1 (5%)
6	NAG	O	2	6	14,14,15	0.50	0	17,19,21	1.57	4 (23%)
4	NGS	P	1	4	19,19,19	0.79	1 (5%)	26,28,28	1.42	4 (15%)
4	GAL	P	2	4	11,11,12	0.66	0	15,15,17	1.24	1 (6%)
4	SIA	P	3	4	17,20,21	0.41	0	21,28,31	1.27	2 (9%)
4	FUC	P	4	4	10,10,11	0.68	0	14,14,16	1.58	2 (14%)
9	NAG	Q	1	9,2	14,14,15	0.50	0	17,19,21	2.06	2 (11%)
9	FUC	Q	2	9	10,10,11	0.71	0	14,14,16	1.41	3 (21%)
7	NAG	R	1	1,7	14,14,15	0.57	0	17,19,21	1.04	2 (11%)
7	NAG	R	2	7	14,14,15	0.54	0	17,19,21	1.71	4 (23%)
7	BMA	R	3	7	11,11,12	0.34	0	15,15,17	0.74	0
6	NAG	S	1	1,6	14,14,15	0.55	0	17,19,21	1.41	4 (23%)
6	NAG	S	2	6	14,14,15	0.52	0	17,19,21	1.06	1 (5%)
6	NAG	T	1	1,6	14,14,15	0.60	0	17,19,21	1.50	5 (29%)
6	NAG	T	2	6	14,14,15	0.66	0	17,19,21	1.92	5 (29%)
4	NGS	U	1	4	19,19,19	0.73	1 (5%)	26,28,28	1.11	2 (7%)
4	GAL	U	2	4	11,11,12	0.57	0	15,15,17	2.36	3 (20%)
4	SIA	U	3	4	17,20,21	0.43	0	21,28,31	1.37	3 (14%)
4	FUC	U	4	4	10,10,11	0.71	0	14,14,16	1.92	4 (28%)

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	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	MAN	G	4	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NGS	H	1	4	-	0/10/30/30	0/1/1/1
4	GAL	H	2	4	-	2/2/19/22	0/1/1/1
4	SIA	H	3	4	-	2/14/34/38	0/1/1/1
4	FUC	H	4	4	1/1/4/5	-	0/1/1/1
5	NAG	I	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	FUC	I	3	5	1/1/4/5	-	0/1/1/1
6	NAG	J	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
6	NAG	L	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
7	NAG	M	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	M	2	7	-	2/6/23/26	0/1/1/1
7	BMA	M	3	7	-	2/2/19/22	0/1/1/1
8	NAG	N	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	N	2	8	-	0/6/23/26	0/1/1/1
8	BMA	N	3	8	-	0/2/19/22	0/1/1/1
8	MAN	N	4	8	-	2/2/19/22	0/1/1/1
8	MAN	N	5	8	-	0/2/19/22	0/1/1/1
8	FUC	N	6	8	1/1/4/5	-	0/1/1/1
6	NAG	O	1	1,6	1/1/5/7	1/6/23/26	0/1/1/1
6	NAG	O	2	6	-	5/6/23/26	0/1/1/1
4	NGS	P	1	4	-	5/10/30/30	0/1/1/1
4	GAL	P	2	4	-	2/2/19/22	0/1/1/1
4	SIA	P	3	4	-	2/14/34/38	0/1/1/1
4	FUC	P	4	4	1/1/4/5	-	0/1/1/1
9	NAG	Q	1	9,2	-	2/6/23/26	0/1/1/1
9	FUC	Q	2	9	1/1/4/5	-	0/1/1/1
7	NAG	R	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	R	2	7	-	3/6/23/26	0/1/1/1
7	BMA	R	3	7	-	1/2/19/22	0/1/1/1
6	NAG	S	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	S	2	6	-	1/6/23/26	0/1/1/1
6	NAG	T	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	T	2	6	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NGS	U	1	4	-	2/10/30/30	0/1/1/1
4	GAL	U	2	4	1/1/4/5	2/2/19/22	0/1/1/1
4	SIA	U	3	4	1/1/8/9	2/14/34/38	0/1/1/1
4	FUC	U	4	4	1/1/4/5	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	1	NGS	O8-S	2.26	1.64	1.50
4	U	1	NGS	O8-S	2.24	1.64	1.50
4	H	1	NGS	O8-S	2.19	1.63	1.50

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	2	GAL	O5-C1-C2	7.39	122.17	110.77
9	Q	1	NAG	C1-O5-C5	7.28	122.06	112.19
8	N	6	FUC	O5-C1-C2	5.67	119.52	110.77
5	I	3	FUC	O5-C1-C2	5.44	119.17	110.77
6	K	1	NAG	C1-O5-C5	5.24	119.29	112.19
8	N	4	MAN	C1-C2-C3	4.85	115.62	109.67
4	H	2	GAL	C1-C2-C3	4.64	115.37	109.67
4	P	4	FUC	O5-C1-C2	4.59	117.86	110.77
4	U	3	SIA	C6-O6-C2	4.29	120.52	111.34
6	T	2	NAG	C2-N2-C7	4.22	128.91	122.90
4	H	4	FUC	C1-C2-C3	-4.19	104.51	109.67
4	U	4	FUC	C3-C4-C5	4.08	116.12	109.77
6	J	1	NAG	C1-O5-C5	3.96	117.55	112.19
4	H	4	FUC	O5-C5-C4	3.91	116.53	109.52
4	U	2	GAL	C1-O5-C5	3.89	117.46	112.19
4	P	1	NGS	O5-C1-C2	-3.86	105.64	109.52
6	T	2	NAG	C8-C7-N2	3.81	122.55	116.10
4	U	4	FUC	O5-C5-C4	3.78	116.30	109.52
4	P	3	SIA	C6-O6-C2	3.76	119.39	111.34
7	R	2	NAG	C2-N2-C7	3.52	127.91	122.90
7	R	2	NAG	C8-C7-N2	3.44	121.93	116.10
4	U	2	GAL	C1-C2-C3	3.43	113.88	109.67
9	Q	2	FUC	O5-C1-C2	3.38	115.98	110.77
6	S	1	NAG	C8-C7-N2	3.33	121.74	116.10
4	U	4	FUC	C1-C2-C3	-3.32	105.58	109.67
4	P	2	GAL	C1-C2-C3	3.26	113.67	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	2	NAG	O5-C5-C6	3.23	112.26	107.20
4	H	3	SIA	C11-C10-N5	3.22	121.54	116.10
4	P	1	NGS	O5-C5-C4	3.17	115.45	109.69
4	H	3	SIA	C6-O6-C2	3.12	118.01	111.34
7	M	1	NAG	C1-O5-C5	2.99	116.24	112.19
6	K	2	NAG	O5-C1-C2	-2.98	106.59	111.29
3	G	1	NAG	O5-C5-C6	2.97	111.85	107.20
6	T	1	NAG	C8-C7-N2	2.96	121.12	116.10
6	T	1	NAG	C4-C3-C2	2.94	115.33	111.02
6	O	1	NAG	O5-C5-C6	2.93	111.80	107.20
6	O	2	NAG	O5-C1-C2	-2.88	106.74	111.29
8	N	4	MAN	C1-O5-C5	2.88	116.09	112.19
4	U	1	NGS	C1-C2-C3	2.86	114.45	110.54
3	G	4	MAN	C1-O5-C5	2.86	116.06	112.19
8	N	6	FUC	C3-C4-C5	2.84	114.20	109.77
6	O	2	NAG	C8-C7-N2	2.83	120.88	116.10
7	R	1	NAG	C4-C3-C2	2.75	115.04	111.02
3	G	3	BMA	C1-C2-C3	2.71	112.99	109.67
7	R	2	NAG	O7-C7-C8	-2.70	117.04	122.06
4	P	1	NGS	O3-C3-C2	-2.69	104.23	109.66
6	T	2	NAG	C3-C4-C5	2.68	115.03	110.24
6	O	2	NAG	C1-O5-C5	2.67	115.80	112.19
6	K	1	NAG	O4-C4-C3	2.62	116.40	110.35
6	L	1	NAG	C1-O5-C5	2.53	115.62	112.19
6	O	2	NAG	C2-N2-C7	2.45	126.39	122.90
3	G	1	NAG	C1-O5-C5	2.45	115.51	112.19
9	Q	1	NAG	C1-C2-N2	2.43	114.64	110.49
6	S	2	NAG	O5-C1-C2	-2.42	107.47	111.29
9	Q	2	FUC	C3-C4-C5	2.41	113.53	109.77
4	U	3	SIA	C3-C4-C5	-2.40	108.56	111.46
8	N	6	FUC	C1-O5-C5	-2.40	107.34	112.78
4	P	1	NGS	C3-C4-C5	2.38	114.49	110.24
6	T	1	NAG	O5-C5-C6	2.38	110.93	107.20
7	M	1	NAG	O5-C1-C2	-2.37	107.55	111.29
4	H	4	FUC	C3-C4-C5	2.37	113.46	109.77
6	T	2	NAG	O7-C7-C8	-2.36	117.67	122.06
4	P	3	SIA	C11-C10-N5	2.36	120.09	116.10
7	M	1	NAG	C8-C7-N2	2.32	120.02	116.10
8	N	6	FUC	C1-C2-C3	-2.30	106.84	109.67
7	R	1	NAG	C1-O5-C5	2.25	115.25	112.19
8	N	5	MAN	C3-C4-C5	2.24	114.24	110.24
4	H	1	NGS	O6-C6-C5	2.24	111.80	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	1	NAG	O7-C7-C8	-2.24	117.90	122.06
6	L	2	NAG	C1-O5-C5	2.23	115.22	112.19
6	K	2	NAG	C1-C2-N2	2.23	114.30	110.49
6	S	1	NAG	C2-N2-C7	2.21	126.05	122.90
4	P	4	FUC	C1-C2-C3	-2.18	106.98	109.67
6	K	1	NAG	O5-C5-C6	2.18	110.62	107.20
6	K	1	NAG	C4-C3-C2	-2.17	107.83	111.02
6	J	1	NAG	O5-C1-C2	-2.15	107.90	111.29
8	N	6	FUC	O2-C2-C1	2.14	113.54	109.15
4	H	3	SIA	O10-C10-C11	-2.13	118.09	122.06
6	T	2	NAG	C1-O5-C5	2.13	115.08	112.19
4	U	1	NGS	O5-C1-C2	2.13	111.65	109.52
8	N	3	BMA	O5-C5-C6	2.11	110.51	107.20
3	G	1	NAG	C4-C3-C2	2.11	114.11	111.02
6	L	1	NAG	C4-C3-C2	2.08	114.07	111.02
4	H	1	NGS	O5-C1-C2	-2.06	107.44	109.52
6	T	1	NAG	O7-C7-C8	-2.06	118.24	122.06
4	U	4	FUC	O5-C1-C2	2.05	113.93	110.77
5	I	1	NAG	C1-O5-C5	2.04	114.95	112.19
6	S	1	NAG	O5-C1-C2	-2.03	108.08	111.29
3	G	2	NAG	C1-O5-C5	2.02	114.93	112.19
4	U	3	SIA	C11-C10-N5	2.00	119.49	116.10
9	Q	2	FUC	O2-C2-C1	2.00	113.25	109.15
6	T	1	NAG	C3-C4-C5	2.00	113.81	110.24

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	U	4	FUC	C1
4	P	4	FUC	C1
6	O	1	NAG	C1
4	U	3	SIA	C2
4	H	4	FUC	C1
9	Q	2	FUC	C1
5	I	3	FUC	C1
4	U	2	GAL	C1
8	N	6	FUC	C1

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	1	NGS	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	P	1	NGS	O5-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
8	N	1	NAG	C4-C5-C6-O6
4	U	2	GAL	C4-C5-C6-O6
9	Q	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6
7	M	3	BMA	C4-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6
4	U	2	GAL	O5-C5-C6-O6
9	Q	1	NAG	C4-C5-C6-O6
8	N	4	MAN	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
7	R	2	NAG	C8-C7-N2-C2
7	R	2	NAG	O7-C7-N2-C2
6	T	1	NAG	C8-C7-N2-C2
6	T	1	NAG	O7-C7-N2-C2
4	U	3	SIA	C11-C10-N5-C5
4	U	3	SIA	O10-C10-N5-C5
6	O	2	NAG	C8-C7-N2-C2
6	O	2	NAG	O7-C7-N2-C2
6	S	1	NAG	C8-C7-N2-C2
6	S	1	NAG	O7-C7-N2-C2
7	M	1	NAG	C8-C7-N2-C2
7	M	1	NAG	O7-C7-N2-C2
4	P	3	SIA	C11-C10-N5-C5
4	P	3	SIA	O10-C10-N5-C5
4	H	3	SIA	C11-C10-N5-C5
4	H	3	SIA	O10-C10-N5-C5
6	T	2	NAG	C8-C7-N2-C2
6	T	2	NAG	O7-C7-N2-C2
7	M	3	BMA	O5-C5-C6-O6
4	P	2	GAL	C4-C5-C6-O6
8	N	1	NAG	O5-C5-C6-O6
4	P	1	NGS	C6-O6-S-O7A

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Mol	Chain	Res	Type	Atoms
4	P	1	NGS	C6-O6-S-O9
6	K	1	NAG	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	T	2	NAG	C4-C5-C6-O6
4	H	2	GAL	C4-C5-C6-O6
8	N	4	MAN	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
4	P	2	GAL	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
4	U	1	NGS	O5-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
4	H	2	GAL	O5-C5-C6-O6
4	P	1	NGS	C6-O6-S-O8
3	G	4	MAN	O5-C5-C6-O6
7	R	3	BMA	O5-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
7	M	2	NAG	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
6	T	2	NAG	C3-C2-N2-C7
6	J	1	NAG	C1-C2-N2-C7
6	O	2	NAG	C1-C2-N2-C7
4	U	1	NGS	C4-C5-C6-O6
6	J	1	NAG	C3-C2-N2-C7
7	M	2	NAG	O5-C5-C6-O6

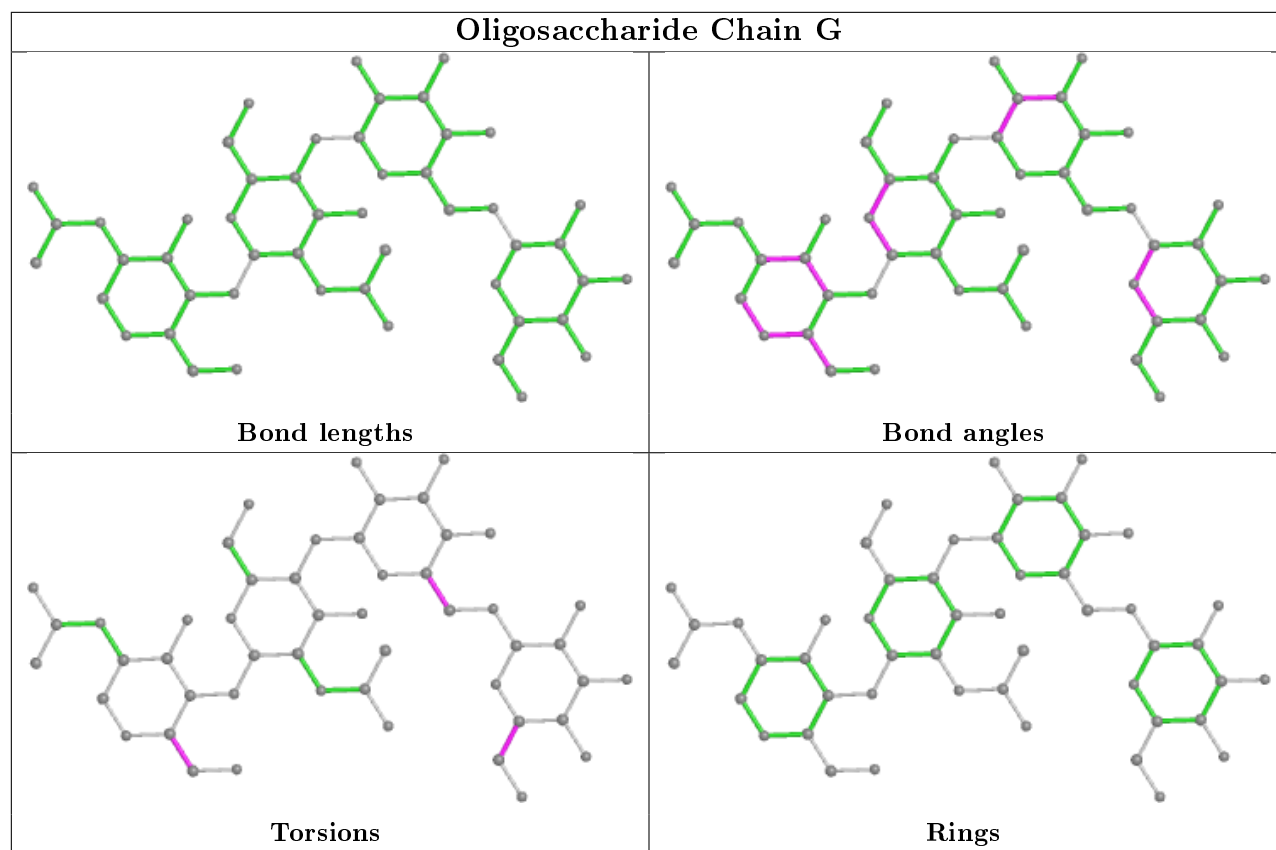
There are no ring outliers.

9 monomers are involved in 8 short contacts:

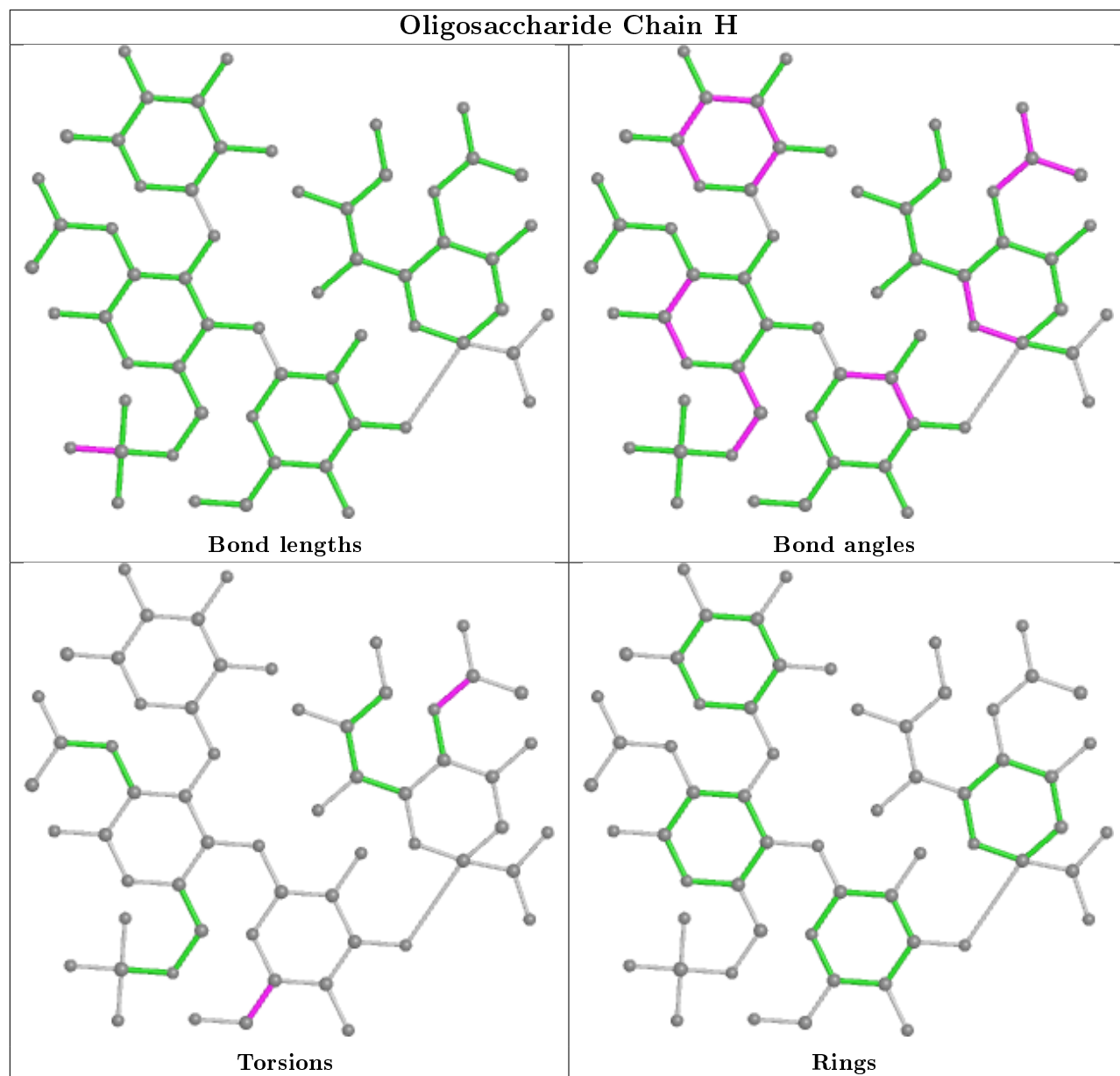
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	NAG	1	0
7	R	2	NAG	2	0
8	N	3	BMA	2	0
5	I	2	NAG	1	0
4	P	3	SIA	1	0
4	H	3	SIA	1	0
8	N	4	MAN	2	0
6	J	2	NAG	1	0
4	P	2	GAL	1	0

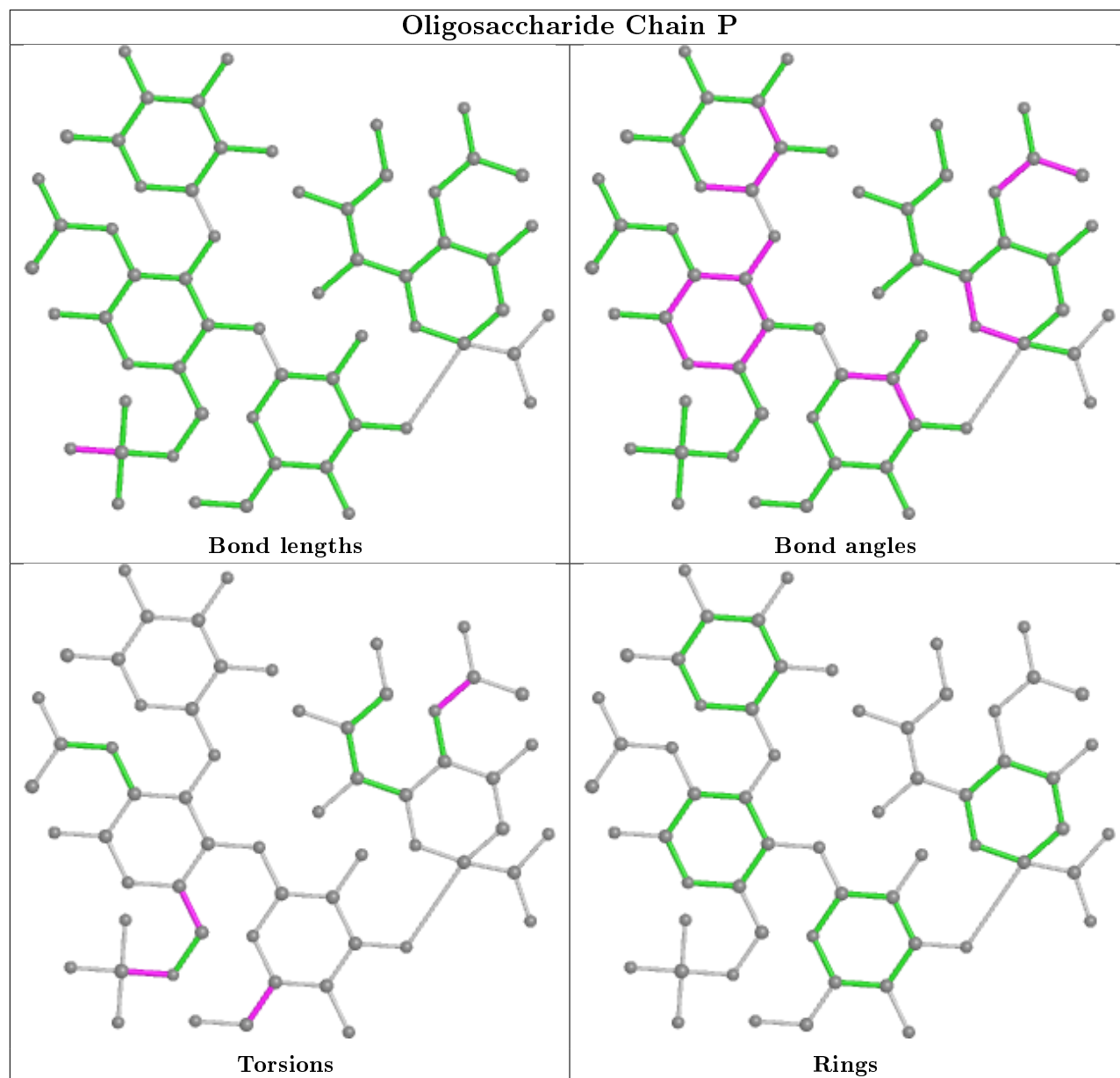
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

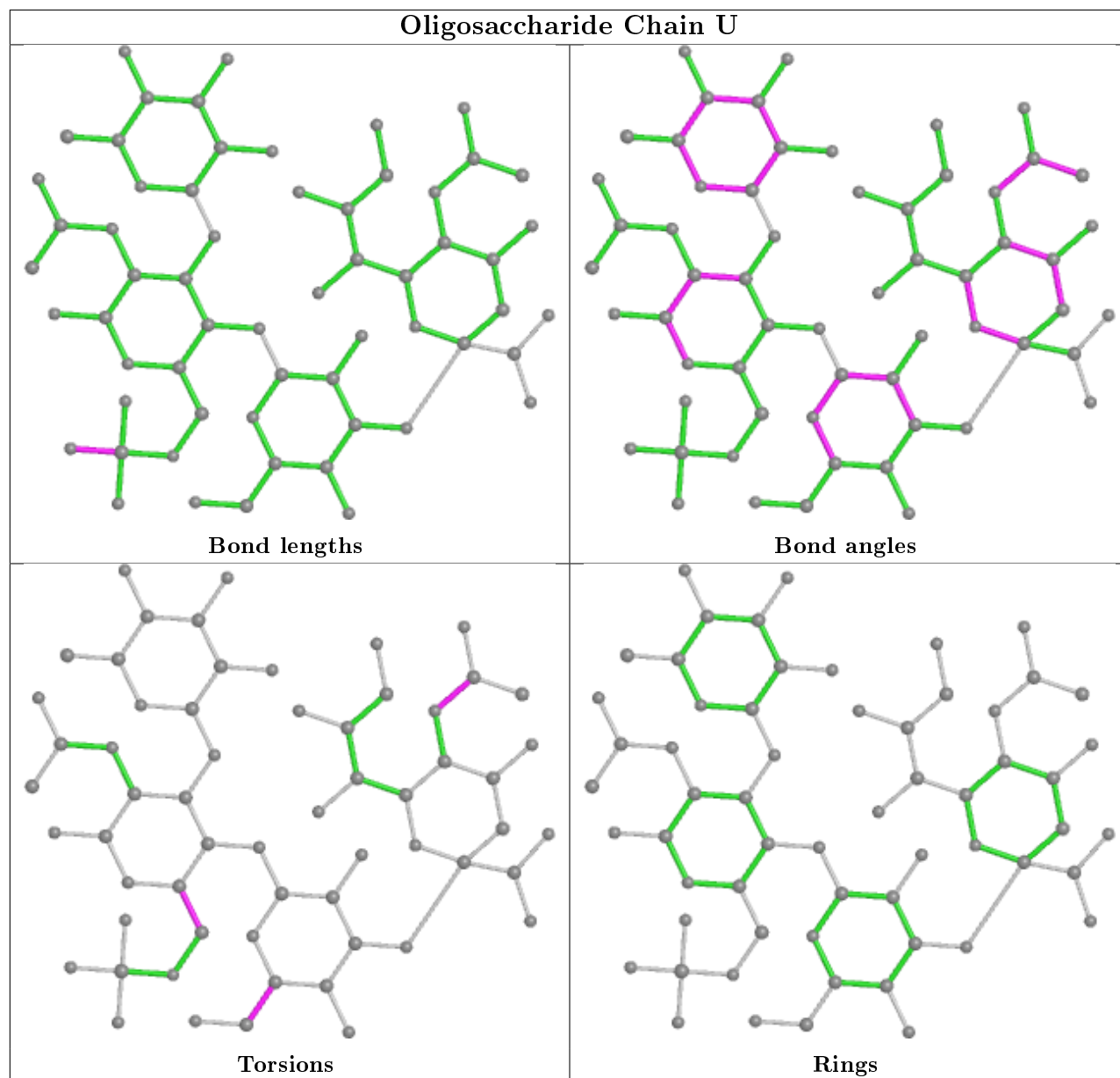
bond angles, torsion angles, and ring geometry for oligosaccharide.



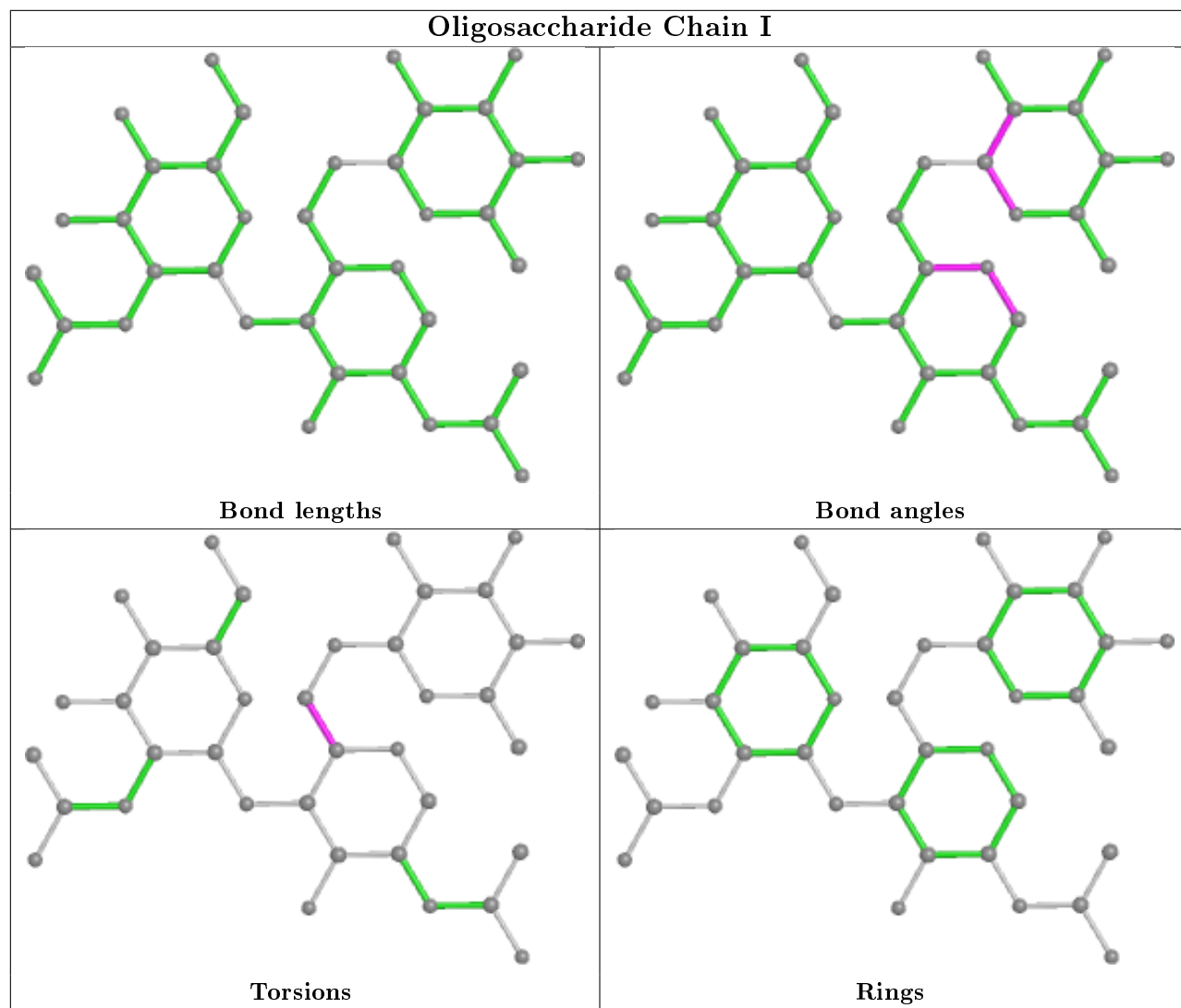
## Oligosaccharide Chain H

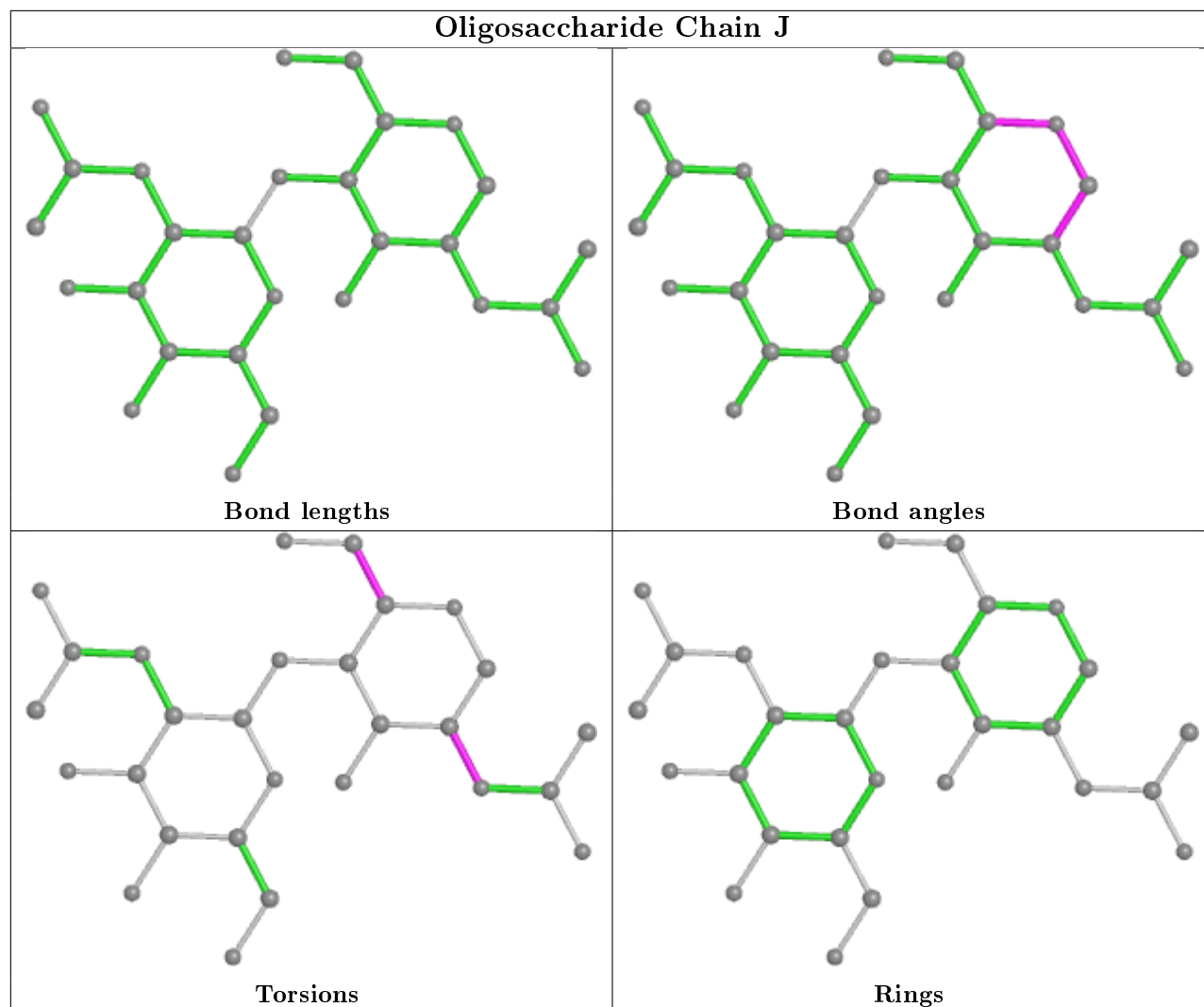


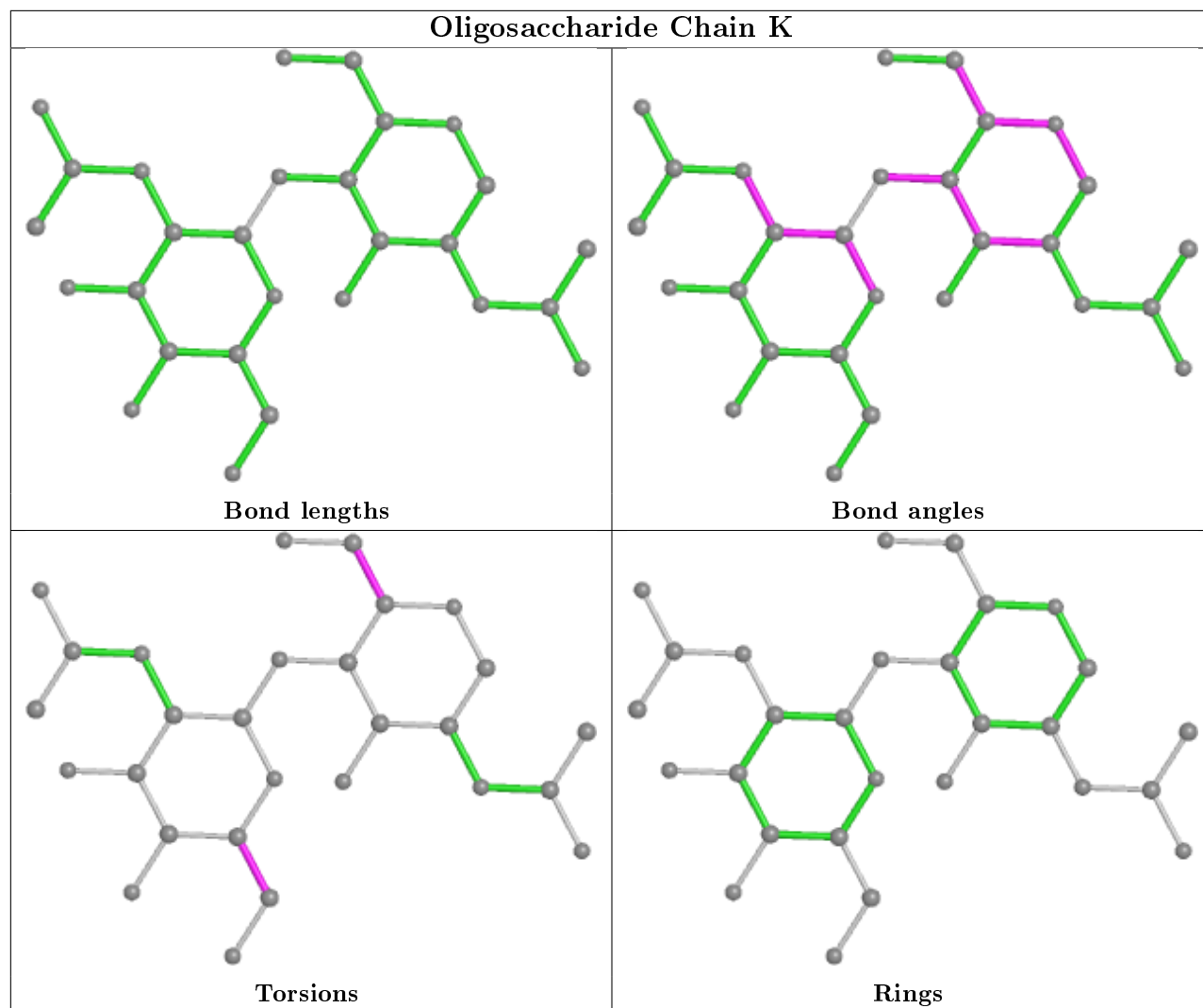


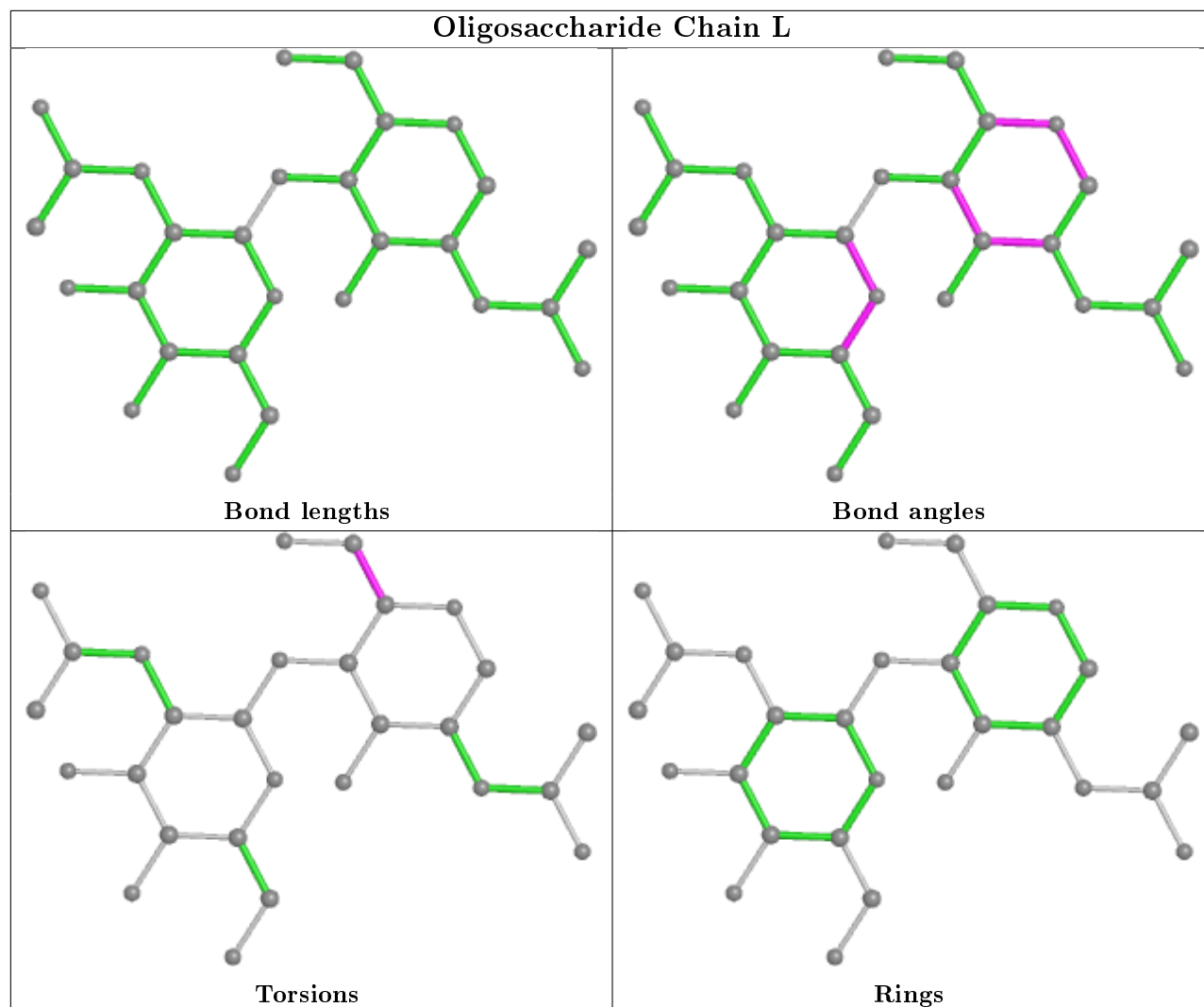


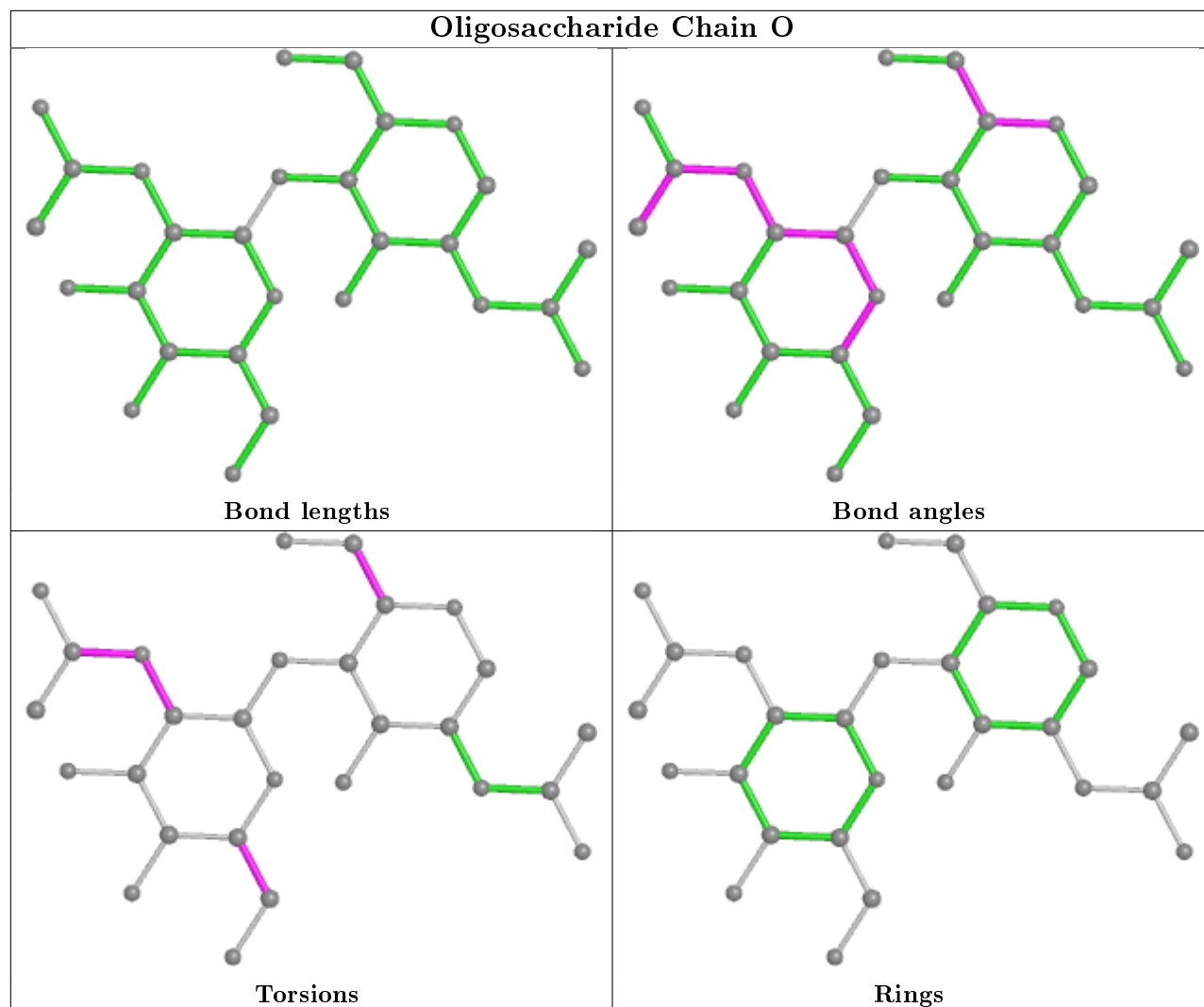


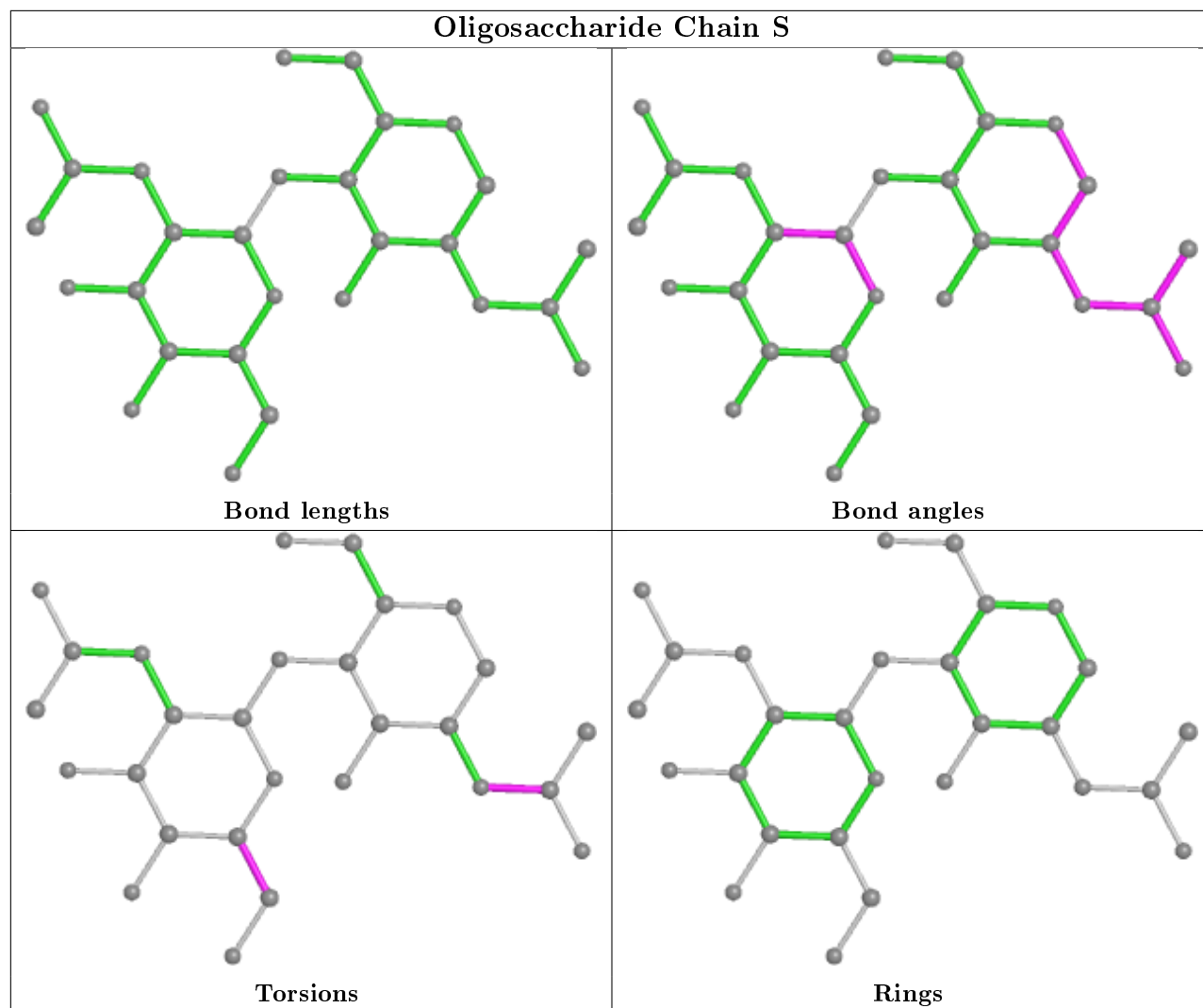


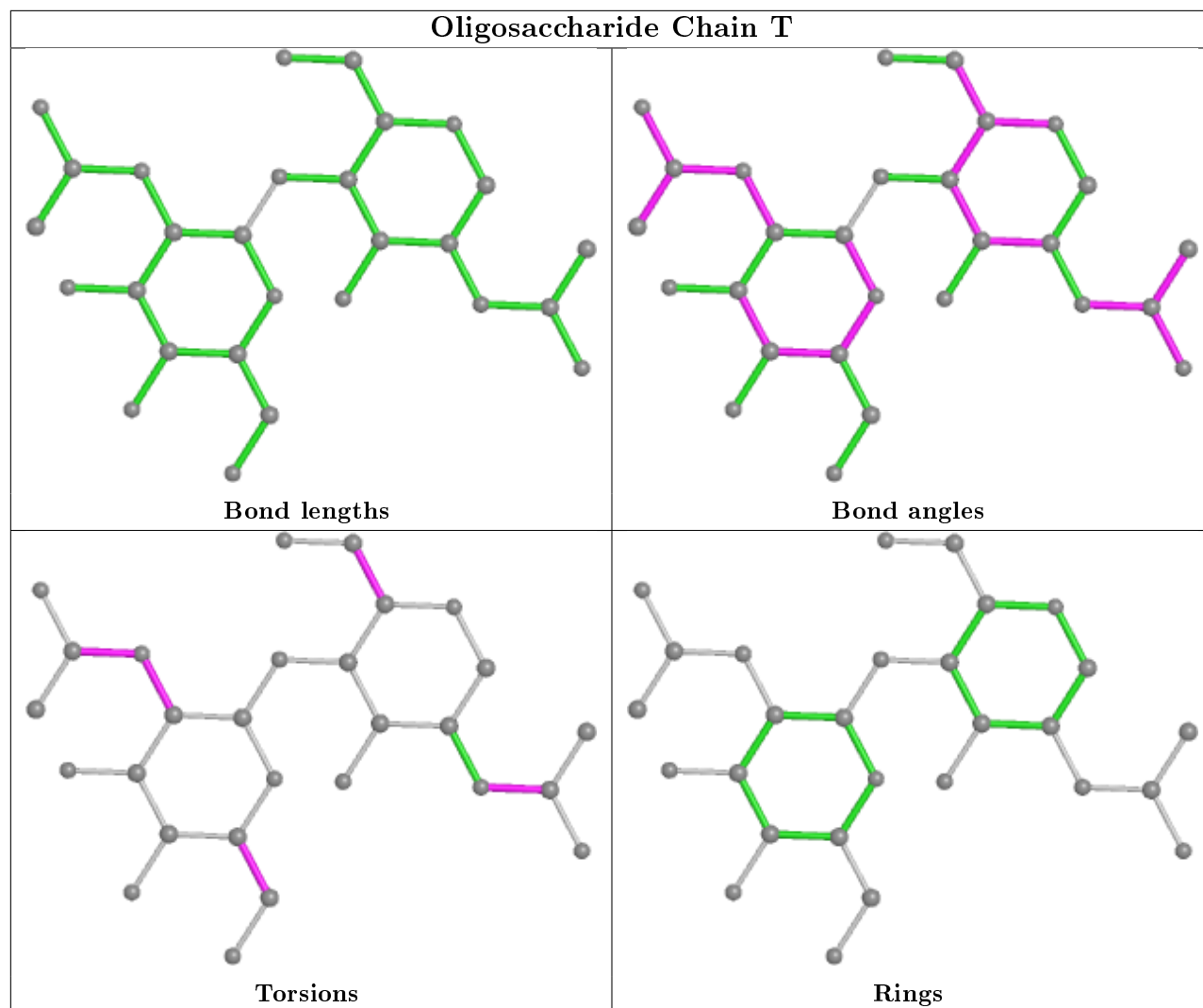


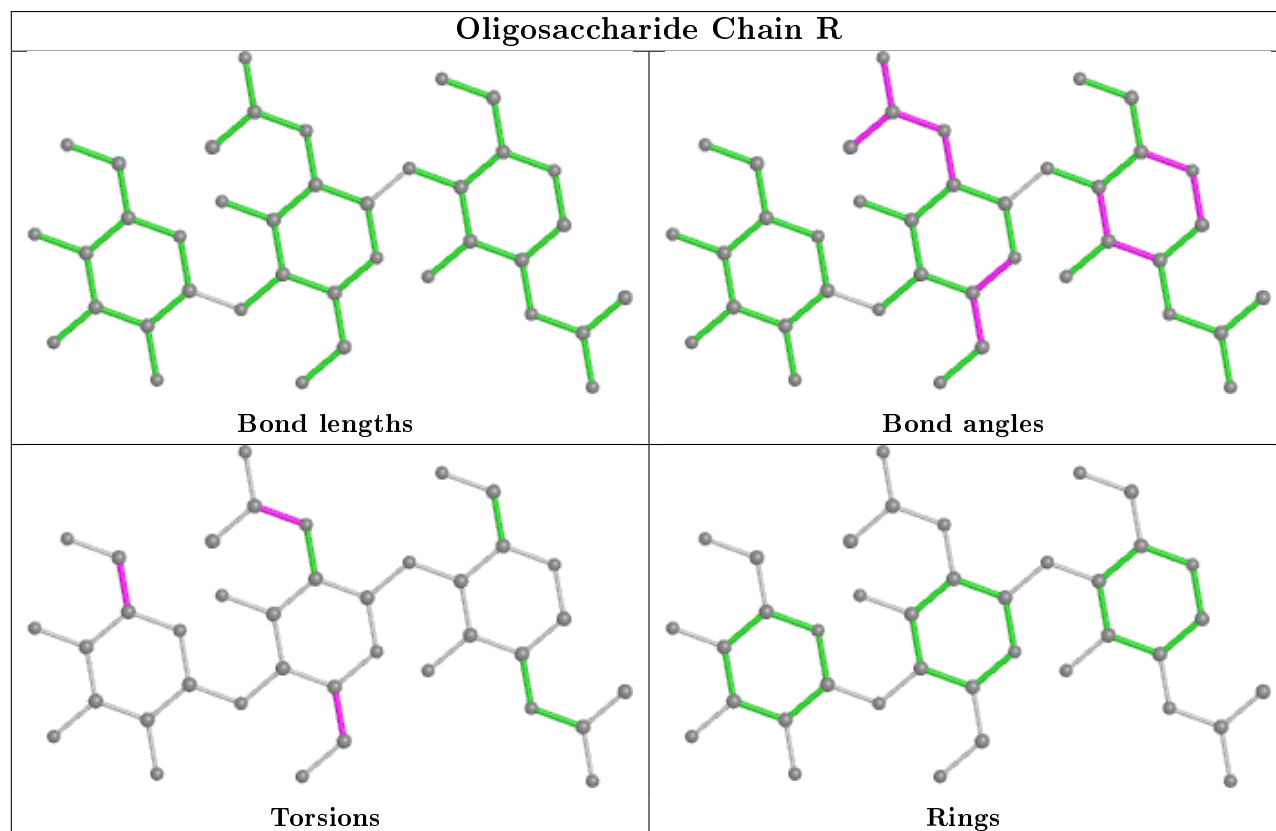
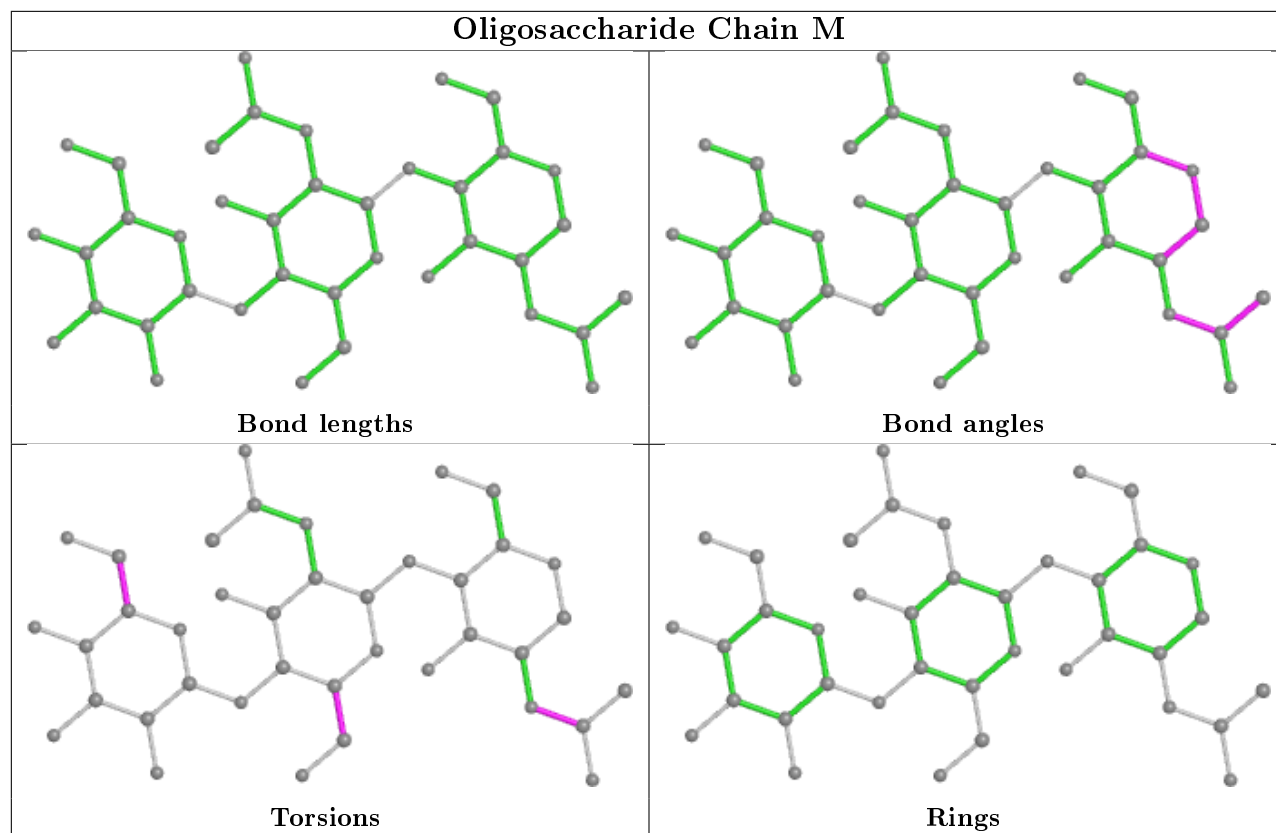




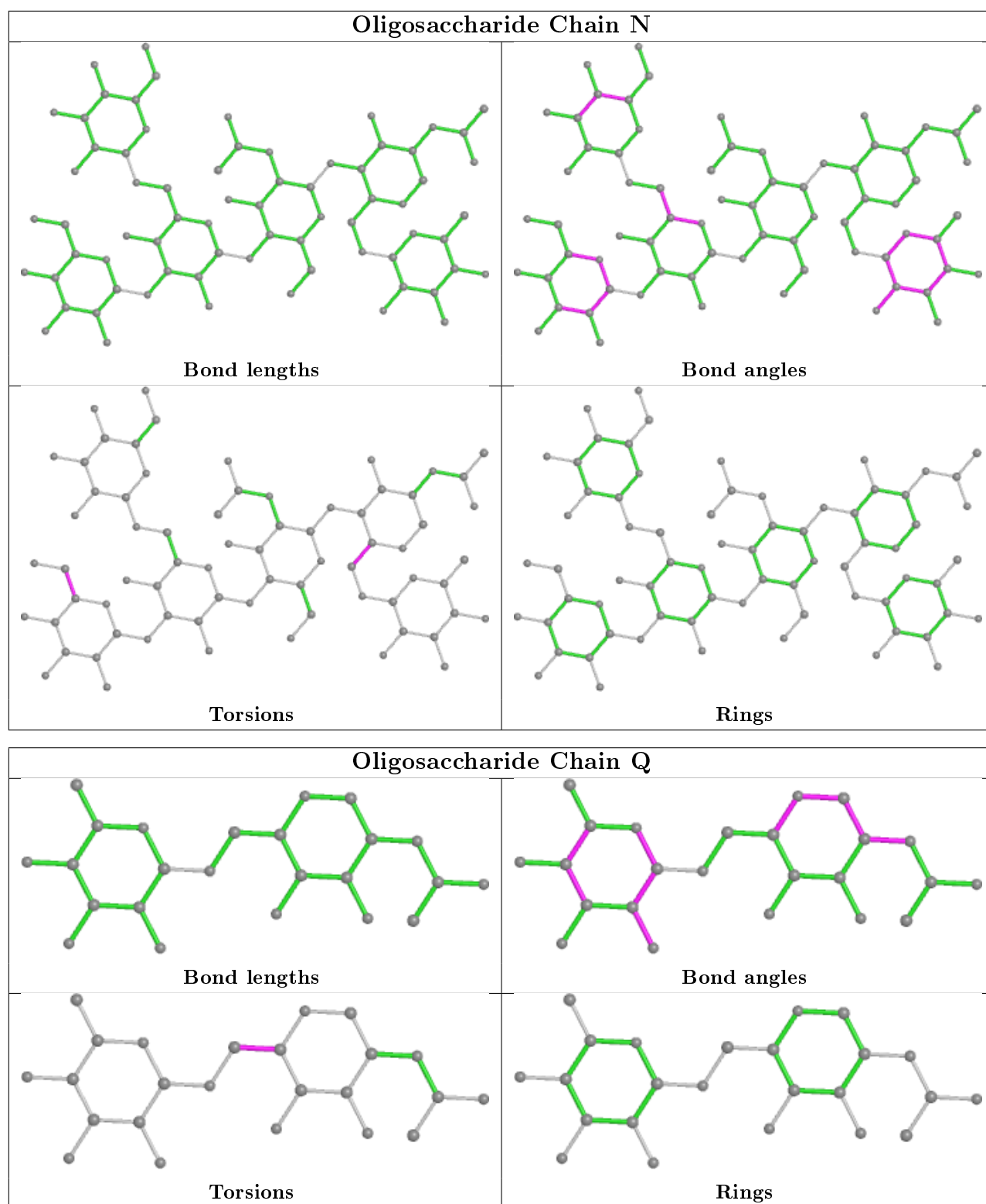












## 5.6 Ligand geometry [i](#)

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$
10	NAG	A	421	1	14,14,15	0.53	0	17,19,21	1.72	4 (23%)
10	NAG	A	441	1	14,14,15	0.53	0	17,19,21	1.91	8 (47%)
10	NAG	E	411	1	14,14,15	0.48	0	17,19,21	1.11	2 (11%)
10	NAG	F	201	2	14,14,15	0.58	0	17,19,21	1.18	1 (5%)
10	NAG	A	601	1	14,14,15	0.44	0	17,19,21	1.00	1 (5%)
10	NAG	C	471	1	14,14,15	0.54	0	17,19,21	1.48	3 (17%)

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
10	NAG	A	421	1	-	5/6/23/26	0/1/1/1
10	NAG	A	441	1	-	4/6/23/26	0/1/1/1
10	NAG	E	411	1	-	1/6/23/26	0/1/1/1
10	NAG	F	201	2	-	2/6/23/26	0/1/1/1
10	NAG	A	601	1	-	2/6/23/26	0/1/1/1
10	NAG	C	471	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	201	NAG	C1-O5-C5	3.82	117.37	112.19
10	A	421	NAG	C8-C7-N2	3.66	122.30	116.10
10	A	441	NAG	O5-C1-C2	3.47	116.77	111.29
10	A	421	NAG	C2-N2-C7	3.44	127.80	122.90
10	C	471	NAG	C1-C2-N2	3.43	116.34	110.49
10	A	421	NAG	C1-O5-C5	3.19	116.51	112.19
10	A	441	NAG	C1-O5-C5	3.11	116.41	112.19
10	E	411	NAG	O5-C1-C2	-3.04	106.49	111.29
10	A	441	NAG	C8-C7-N2	2.92	121.05	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	471	NAG	O5-C1-C2	-2.92	106.68	111.29
10	C	471	NAG	C1-O5-C5	2.63	115.75	112.19
10	A	601	NAG	O5-C5-C6	2.54	111.19	107.20
10	A	441	NAG	C3-C4-C5	-2.52	105.75	110.24
10	A	421	NAG	O7-C7-C8	-2.45	117.51	122.06
10	E	411	NAG	C1-O5-C5	2.35	115.37	112.19
10	A	441	NAG	C4-C3-C2	-2.32	107.62	111.02
10	A	441	NAG	C2-N2-C7	2.31	126.19	122.90
10	A	441	NAG	O7-C7-C8	-2.12	118.12	122.06
10	A	441	NAG	O4-C4-C5	2.05	114.38	109.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	C	471	NAG	C1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	F	201	NAG	O5-C5-C6-O6
10	A	441	NAG	C4-C5-C6-O6
10	F	201	NAG	C4-C5-C6-O6
10	A	421	NAG	C8-C7-N2-C2
10	A	421	NAG	O7-C7-N2-C2
10	A	441	NAG	C8-C7-N2-C2
10	A	441	NAG	O7-C7-N2-C2
10	A	421	NAG	O5-C5-C6-O6
10	A	441	NAG	O5-C5-C6-O6
10	A	601	NAG	C4-C5-C6-O6
10	A	421	NAG	C4-C5-C6-O6
10	E	411	NAG	O5-C5-C6-O6
10	A	601	NAG	O5-C5-C6-O6
10	A	421	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	421	NAG	2	0

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	317/330 (96%)	-0.05	5 (1%) 72 71	52, 65, 88, 112	0
1	C	330/330 (100%)	-0.05	3 (0%) 84 84	49, 69, 104, 122	0
1	E	318/330 (96%)	0.26	15 (4%) 31 28	65, 94, 117, 135	0
2	B	173/173 (100%)	-0.06	1 (0%) 89 89	49, 60, 81, 106	0
2	D	172/173 (99%)	-0.12	0 100 100	48, 61, 81, 91	0
2	F	172/173 (99%)	-0.15	0 100 100	52, 75, 100, 106	0
All	All	1482/1509 (98%)	-0.01	24 (1%) 72 71	48, 70, 108, 135	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	222	TRP	3.7
1	E	196	ILE	3.2
1	C	81	TYR	3.0
1	E	278	VAL	3.0
1	C	242	ILE	2.9
1	A	222	TRP	2.7
1	E	194	LEU	2.6
1	E	155	THR	2.5
1	E	156	LYS	2.5
1	E	46	ILE	2.4
1	E	274	ILE	2.4
1	A	173	ASN	2.4
1	E	81	TYR	2.4
1	E	138	ALA	2.4
1	E	159	ASN	2.3
1	E	158	GLY	2.3
1	E	161	TYR	2.2
2	B	171	PHE	2.2
1	A	325	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	274	ILE	2.2
1	E	47	SER	2.1
1	E	142	GLY	2.1
1	A	81	TYR	2.0
1	C	126	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	G	4	11/12	0.39	0.43	146,151,159,160	0
8	MAN	N	4	11/12	0.54	0.54	117,124,131,136	0
6	NAG	L	2	14/15	0.58	0.66	124,135,142,146	0
3	BMA	G	3	11/12	0.61	0.45	133,140,147,148	0
6	NAG	J	2	14/15	0.66	0.55	131,142,146,149	0
8	MAN	N	5	11/12	0.72	0.35	137,141,146,146	0
6	NAG	S	2	14/15	0.72	0.40	116,120,122,123	0
7	BMA	M	3	11/12	0.73	0.29	120,124,130,132	0
6	NAG	T	2	14/15	0.74	0.38	118,128,131,134	0
7	BMA	R	3	11/12	0.74	0.29	135,138,143,145	0
7	NAG	R	2	14/15	0.76	0.39	123,129,133,134	0
4	NGS	U	1	19/19	0.77	0.24	131,135,141,145	0
6	NAG	T	1	14/15	0.77	0.35	109,116,121,124	0
6	NAG	J	1	14/15	0.78	0.43	121,126,131,135	0
8	BMA	N	3	11/12	0.78	0.36	112,120,130,134	0
6	NAG	K	2	14/15	0.81	0.33	120,127,131,135	0
6	NAG	O	2	14/15	0.81	0.25	94,109,113,117	0
7	NAG	M	2	14/15	0.82	0.26	86,97,106,114	0
5	FUC	I	3	10/11	0.82	0.35	107,110,114,114	0
5	NAG	I	2	14/15	0.83	0.42	99,107,112,114	0
7	NAG	R	1	14/15	0.84	0.38	120,123,125,128	0
6	NAG	K	1	14/15	0.84	0.34	100,109,112,118	0
6	NAG	L	1	14/15	0.85	0.41	117,123,129,130	0

*Continued on next page...*

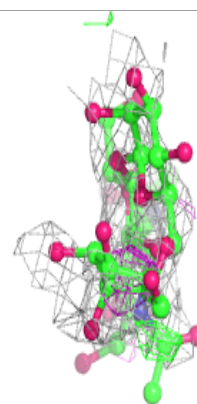
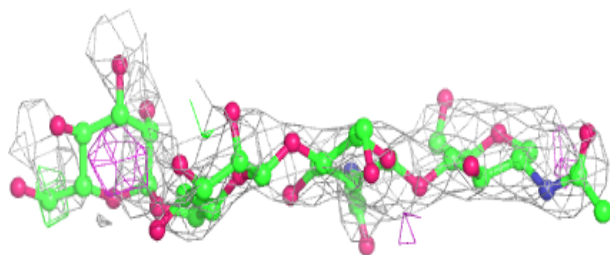
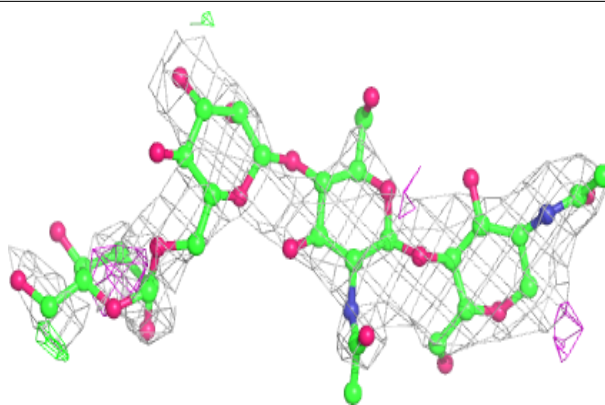
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NAG	Q	1	14/15	0.85	0.30	99,105,109,111	0
9	FUC	Q	2	10/11	0.86	0.29	103,112,114,116	0
6	NAG	O	1	14/15	0.87	0.17	83,91,94,99	0
8	NAG	N	2	14/15	0.87	0.17	84,88,97,102	0
5	NAG	I	1	14/15	0.88	0.33	93,99,104,104	0
3	NAG	G	1	14/15	0.88	0.27	92,98,104,108	0
8	NAG	N	1	14/15	0.89	0.16	62,70,77,80	0
4	FUC	U	4	10/11	0.89	0.29	124,127,131,131	0
4	NGS	H	1	19/19	0.89	0.21	90,96,107,111	0
4	FUC	H	4	10/11	0.90	0.25	96,98,101,102	0
3	NAG	G	2	14/15	0.90	0.44	110,116,123,128	0
4	GAL	U	2	11/12	0.91	0.33	120,122,127,128	0
4	NGS	P	1	19/19	0.91	0.12	93,100,109,113	0
6	NAG	S	1	14/15	0.91	0.17	96,102,106,111	0
4	FUC	P	4	10/11	0.94	0.17	94,95,98,98	0
4	SIA	U	3	20/21	0.95	0.28	107,112,119,120	0
4	SIA	P	3	20/21	0.95	0.17	69,71,77,79	0
4	SIA	H	3	20/21	0.96	0.16	65,69,75,76	0
4	GAL	H	2	11/12	0.96	0.18	79,82,87,87	0
7	NAG	M	1	14/15	0.97	0.11	69,74,77,83	0
8	FUC	N	6	10/11	0.97	0.19	79,80,83,85	0
4	GAL	P	2	11/12	0.97	0.12	81,84,89,89	0

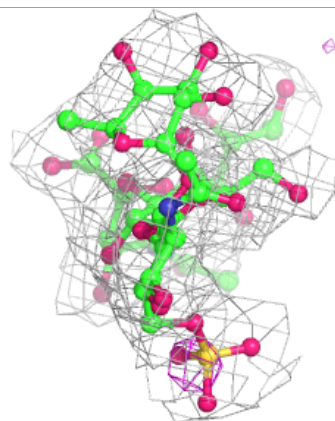
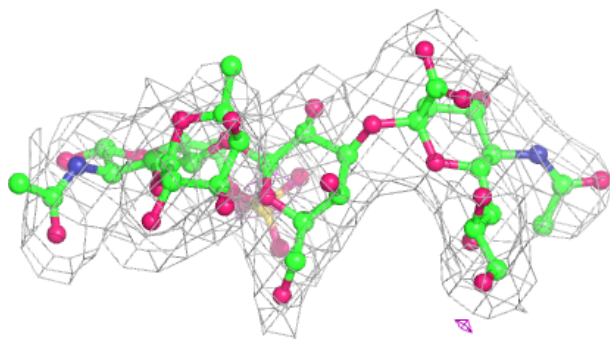
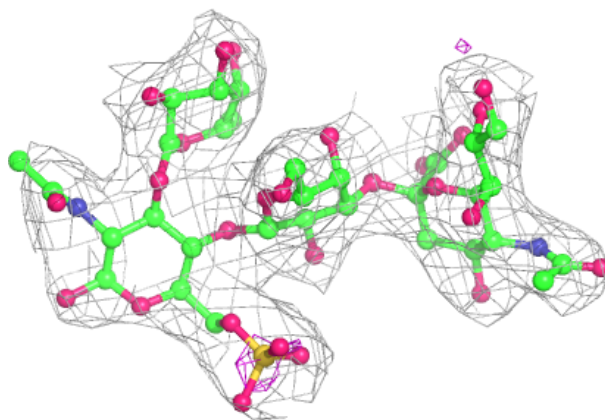
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain 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 H:**

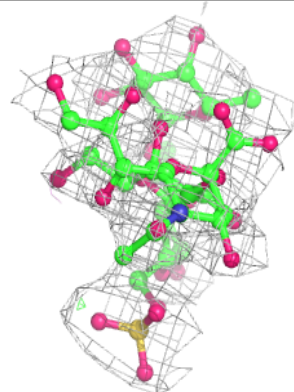
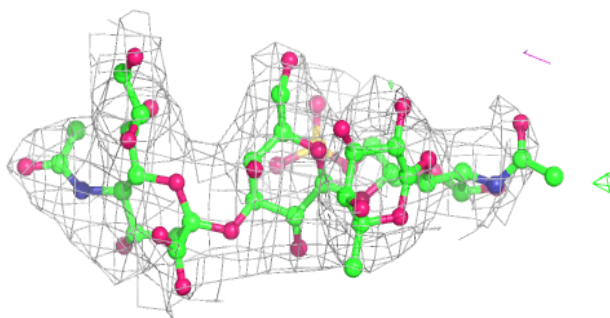
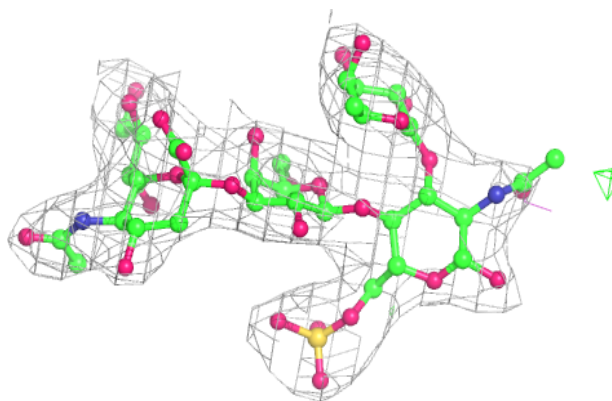
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



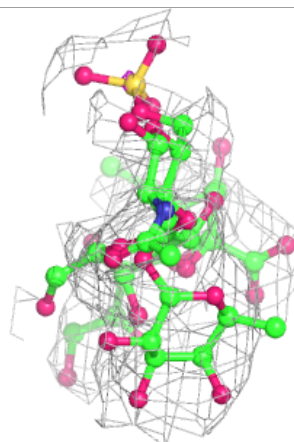
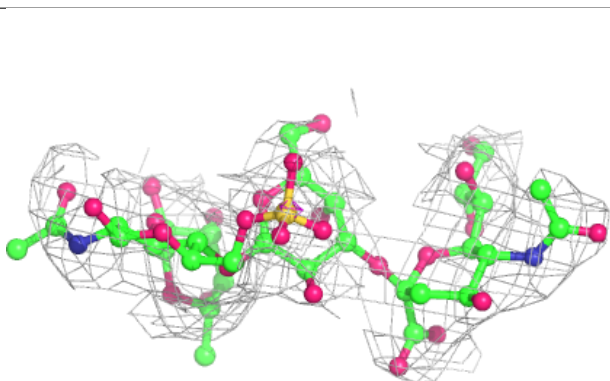
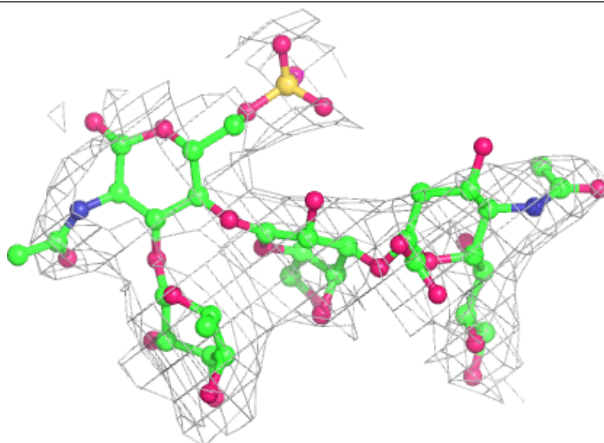


**Electron density around Chain P:**

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

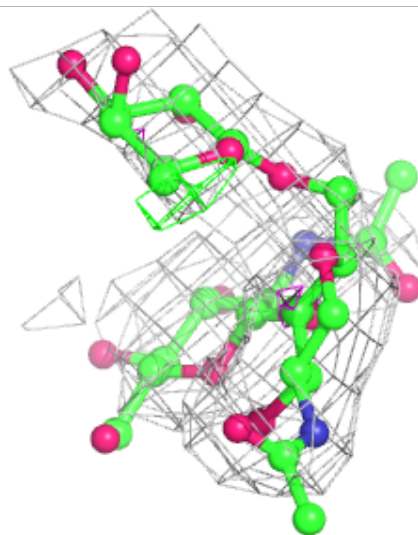
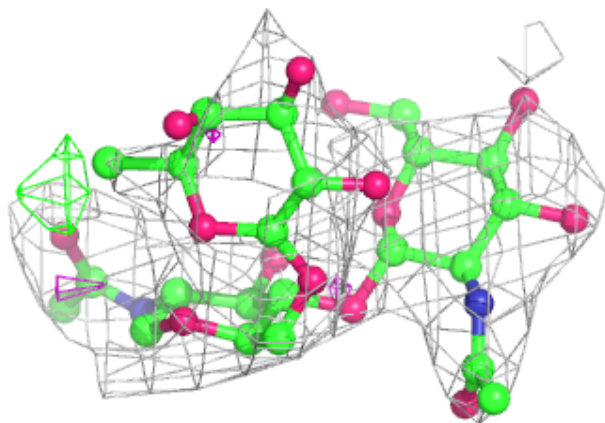
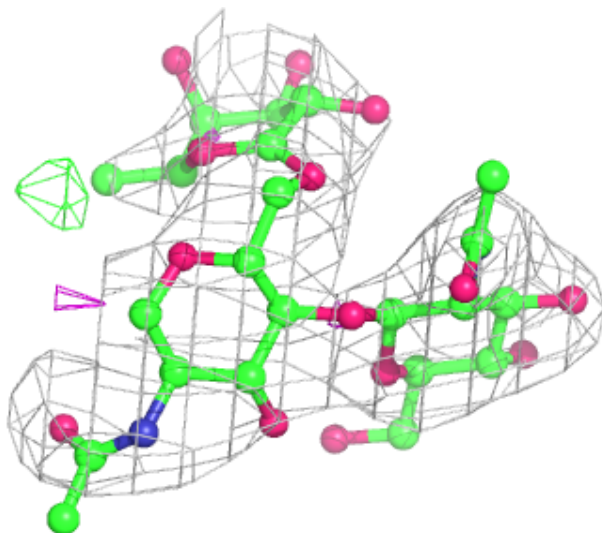
**Electron density around Chain U:**

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



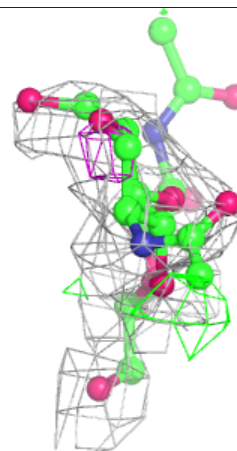
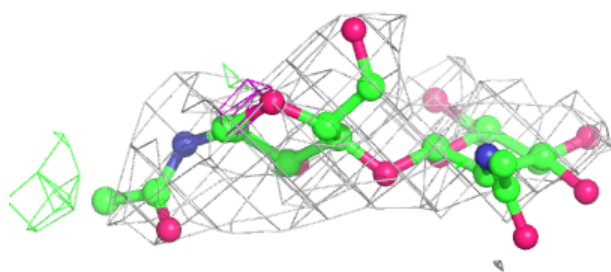
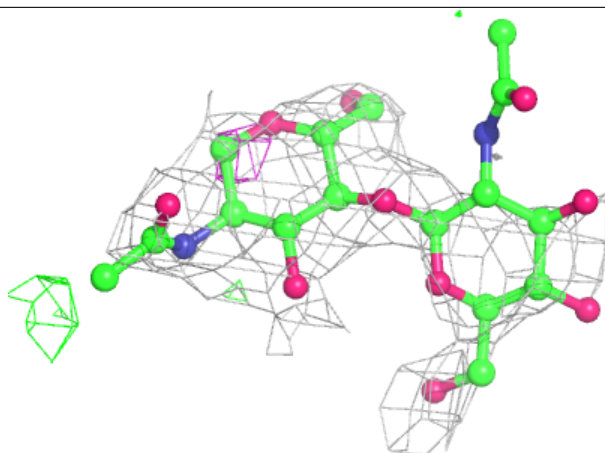
**Electron density around Chain I:**

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



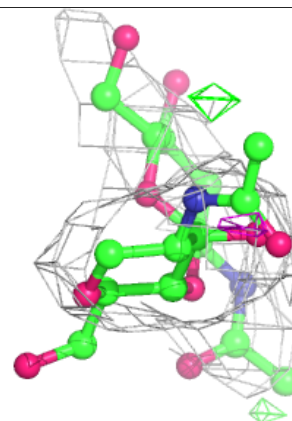
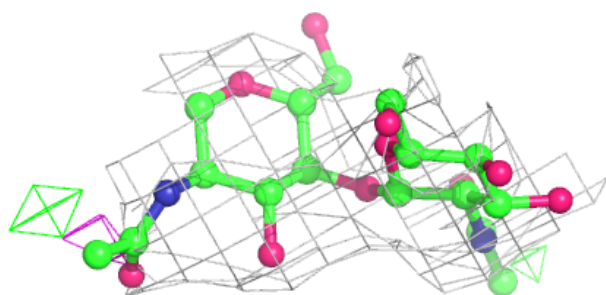
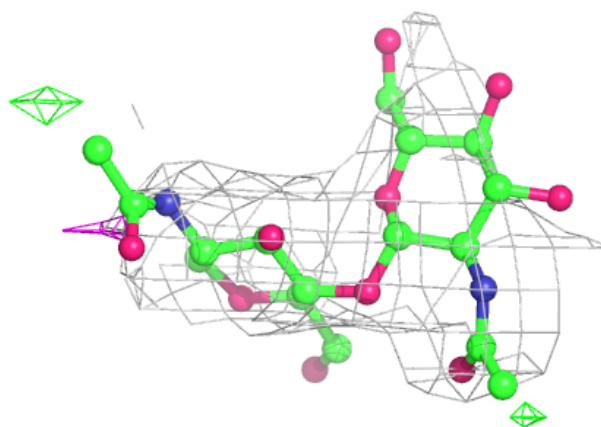
**Electron density around Chain J:**

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



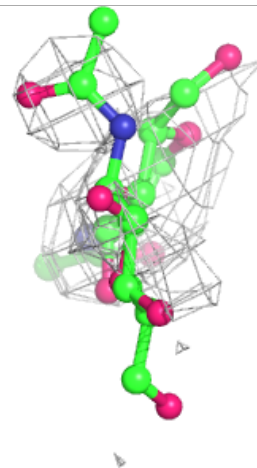
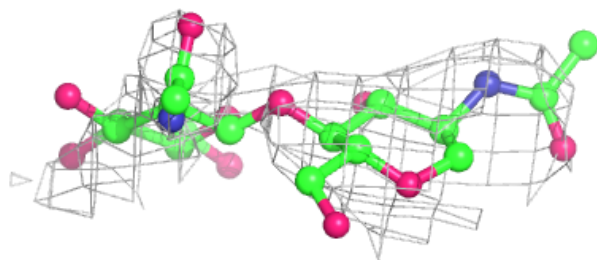
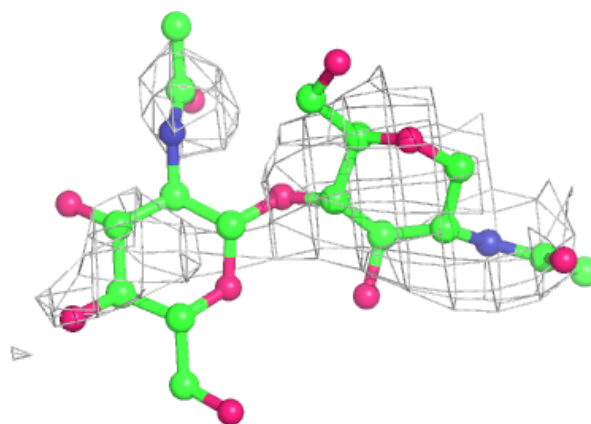
**Electron density around Chain K:**

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



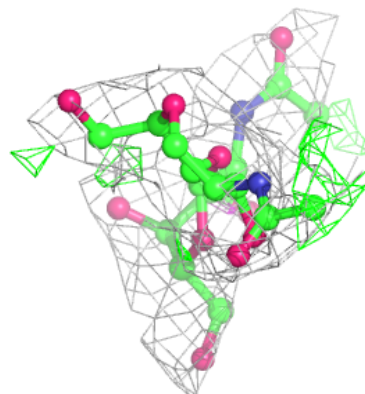
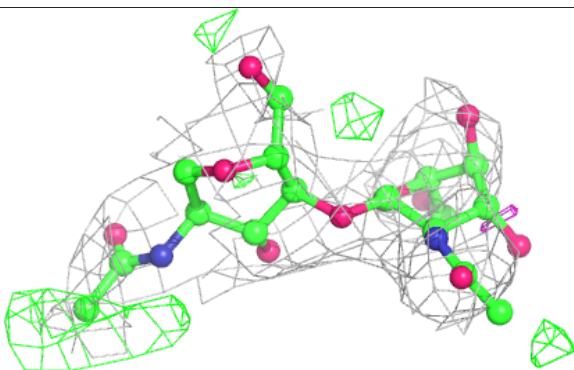
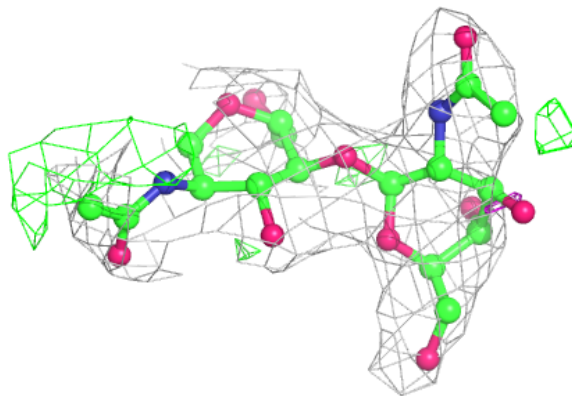
**Electron density around Chain L:**

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



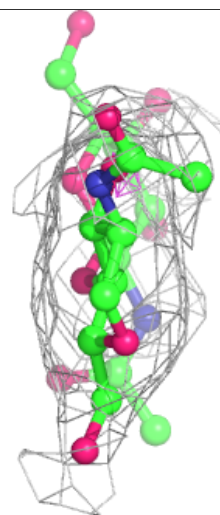
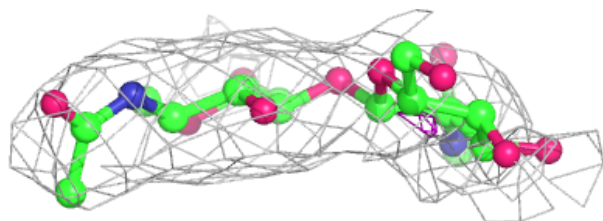
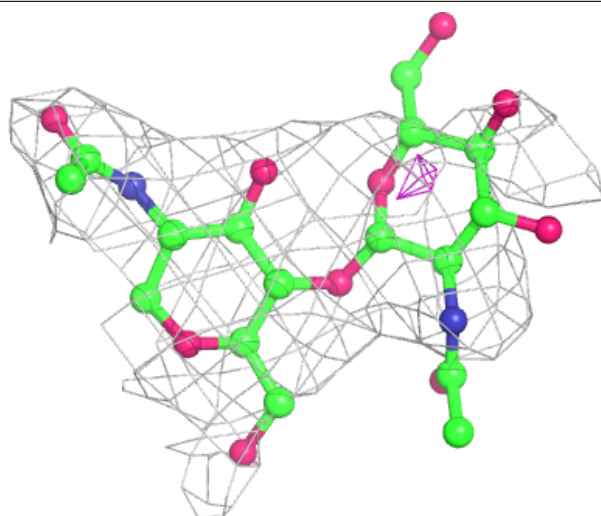
**Electron density around Chain O:**

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



**Electron density around Chain S:**

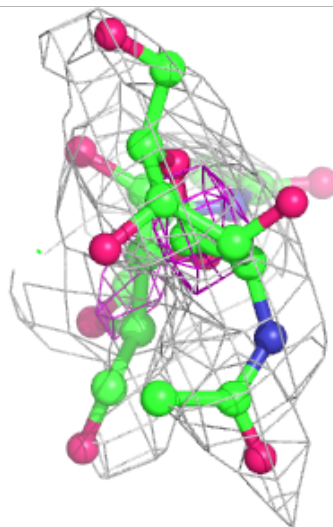
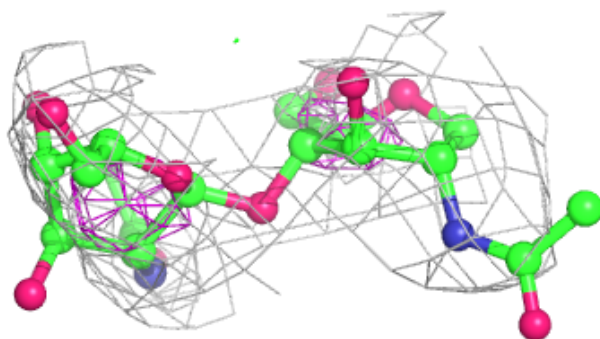
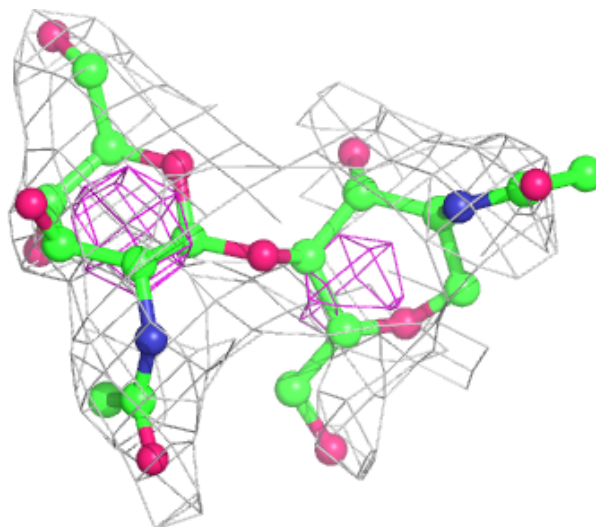
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around Chain T:**

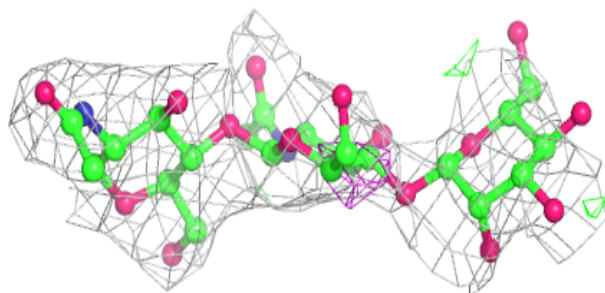
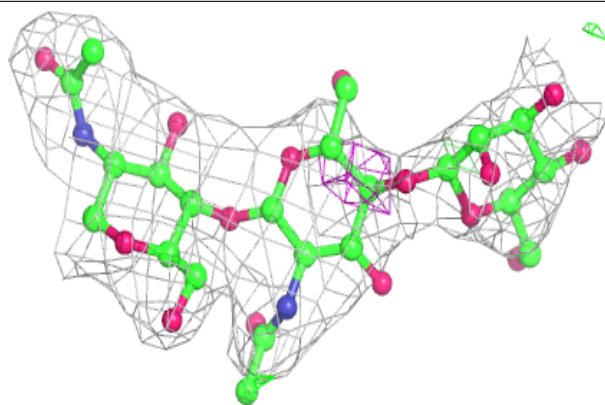
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



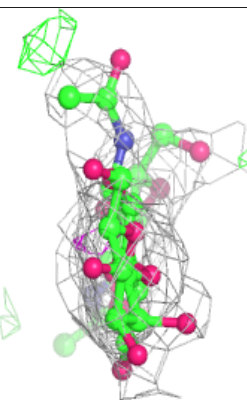
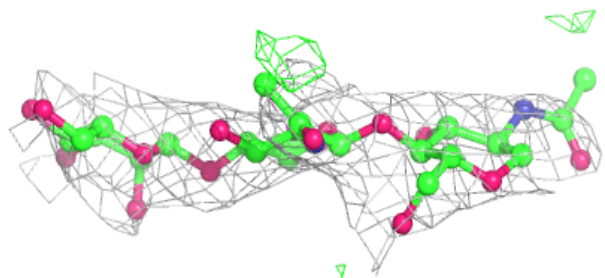
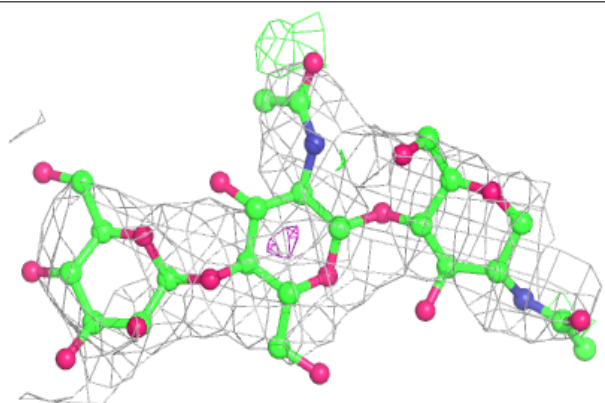


**Electron density around Chain M:**

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

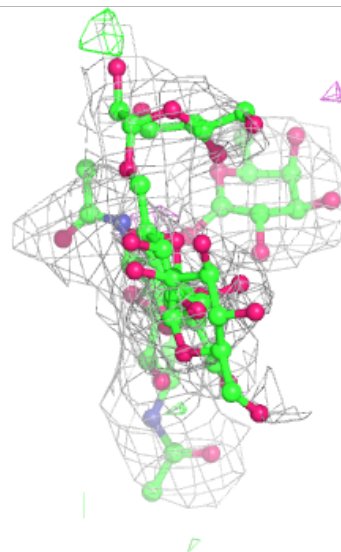
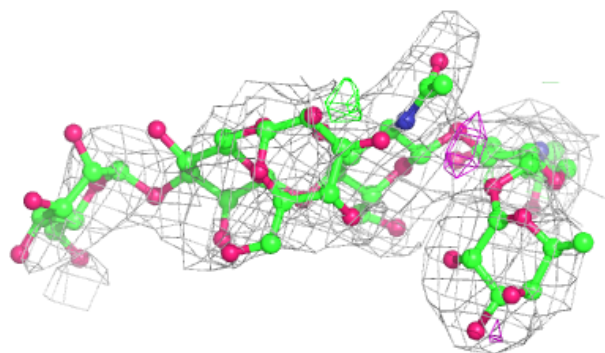
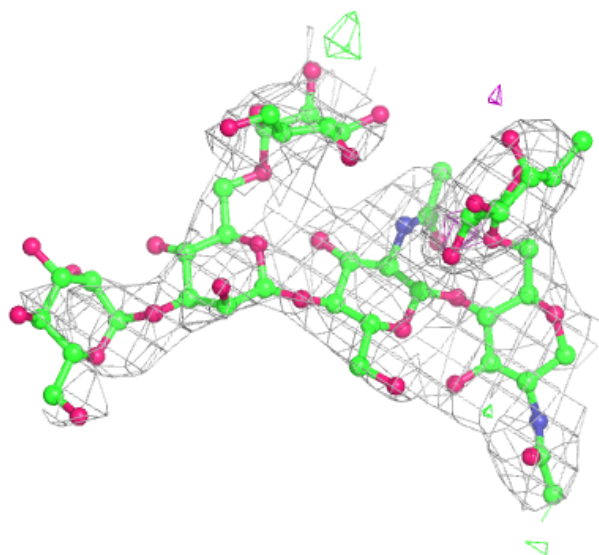
**Electron density around Chain R:**

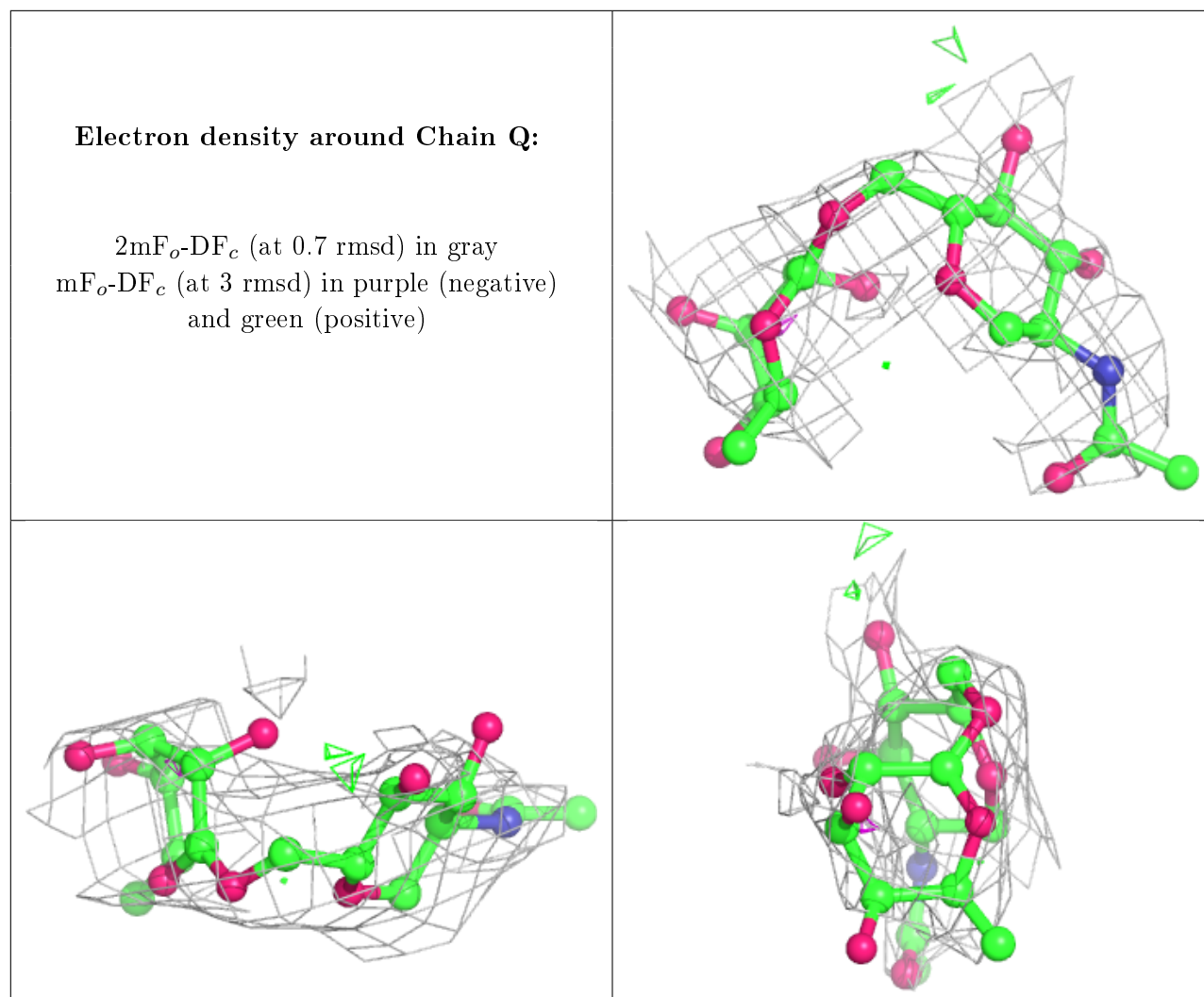
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain N:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	NAG	F	201	14/15	0.69	0.32	107,110,114,116	0
10	NAG	C	471	14/15	0.74	0.31	106,109,110,110	0
10	NAG	E	411	14/15	0.76	0.42	128,133,138,140	0
10	NAG	A	421	14/15	0.78	0.29	96,101,107,109	0
10	NAG	A	601	14/15	0.83	0.31	89,94,100,100	0
10	NAG	A	441	14/15	0.94	0.20	76,79,82,82	0

## 6.5 Other polymers

There are no such residues in this entry.