



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 05:05 AM BST

PDB ID : 6P95
Title : Structure of Lassa virus glycoprotein in complex with Fab 25.6A
Authors : Sapphire, E.O.; Hastie, K.M.
Deposited on : 2019-06-09
Resolution : 3.50 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 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
buster-report : 1.1.7 (2018)
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

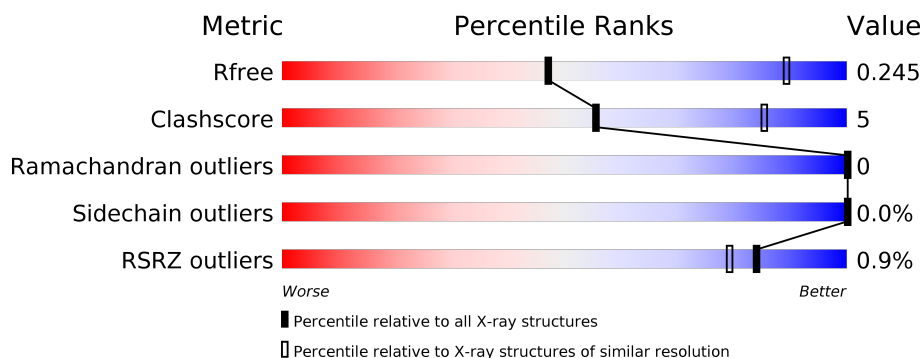
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.









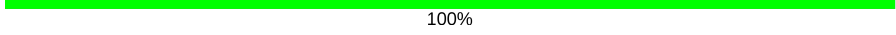
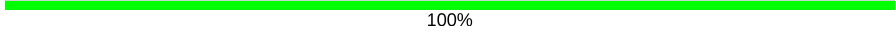





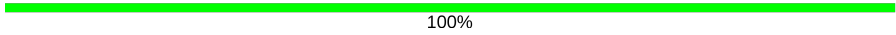

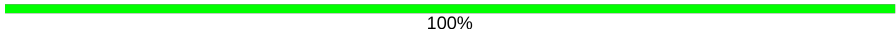
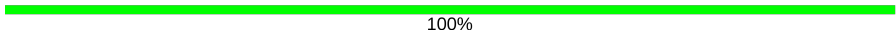





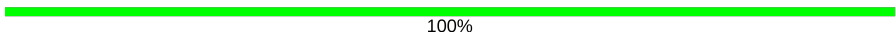


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 ≥ 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	259	<div> <div></div> <div>62%10%27%</div> </div>
1	B	259	<div> <div>%</div> <div>61%9%30%</div> </div>
1	C	259	<div> <div>3%</div> <div>66%7%27%</div> </div>
2	D	231	<div> <div></div> <div>79%15%6%</div> </div>
2	F	231	<div> <div></div> <div>80%14%6%</div> </div>
2	H	231	<div> <div></div> <div>77%17%5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	217	
3	G	217	
3	L	217	
4	a	180	
4	b	180	
4	c	180	
5	I	3	
5	M	3	
5	P	3	
5	R	3	
6	J	2	
6	K	2	
6	N	2	
6	Q	2	
6	S	2	
6	X	2	
6	d	2	
7	O	4	
7	W	4	
7	Z	4	
8	T	5	
9	U	5	
10	V	3	
10	Y	3	
10	e	3	

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	V	2	-	-	-	X
10	NAG	Y	2	-	-	-	X
11	NAG	B	306	-	-	-	X
11	NAG	C	306	-	-	-	X
5	NAG	R	2	-	-	-	X
5	BMA	R	3	-	-	-	X
6	NAG	J	2	-	-	-	X
6	NAG	Q	2	-	-	-	X
7	NAG	O	2	-	-	-	X
7	BMA	O	3	-	-	-	X
7	MAN	O	4	-	-	-	X
8	MAN	T	5	-	-	-	X
9	MAN	U	4	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18593 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 Pre-glycoprotein polyprotein GP complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1488	938	249	285	16			
1	B	181	Total	C	N	O	S	0	0	0
			1428	901	239	272	16			
1	C	189	Total	C	N	O	S	0	0	0
			1499	944	253	286	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	CYS	ARG	engineered mutation	UNP P08669
A	258	ARG	LEU	engineered mutation	UNP P08669
A	259	ARG	LEU	engineered mutation	UNP P08669
B	207	CYS	ARG	engineered mutation	UNP P08669
B	258	ARG	LEU	engineered mutation	UNP P08669
B	259	ARG	LEU	engineered mutation	UNP P08669
C	207	CYS	ARG	engineered mutation	UNP P08669
C	258	ARG	LEU	engineered mutation	UNP P08669
C	259	ARG	LEU	engineered mutation	UNP P08669

- Molecule 2 is a protein called FAB Antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	218	Total	C	N	O	S	0	0	0
			1628	1018	286	318	6			
2	F	218	Total	C	N	O	S	0	0	0
			1628	1018	286	318	6			
2	H	219	Total	C	N	O	S	0	0	0
			1632	1020	287	319	6			

- Molecule 3 is a protein called FAB Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	212	Total 1585	C 997	N 264	O 320	S 4	0	0	0
3	G	212	Total 1584	C 995	N 264	O 321	S 4	0	0	0
3	L	212	Total 1584	C 995	N 264	O 321	S 4	0	0	0

- Molecule 4 is a protein called Pre-glycoprotein polypeptide GP complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	a	153	Total 1242	C 784	N 209	O 236	S 13	0	0	0
4	b	145	Total 1185	C 753	N 200	O 219	S 13	0	0	0
4	c	152	Total 1246	C 791	N 209	O 232	S 14	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

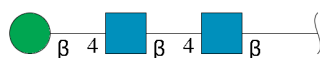
Chain	Residue	Modelled	Actual	Comment	Reference
a	329	PRO	GLU	engineered mutation	UNP P08669
a	332	THR	MET	engineered mutation	UNP P08669
a	360	CYS	GLY	engineered mutation	UNP P08669
a	434	GLU	-	expression tag	UNP P08669
a	435	VAL	-	expression tag	UNP P08669
a	436	ASP	-	expression tag	UNP P08669
a	437	ASP	-	expression tag	UNP P08669
a	438	ASP	-	expression tag	UNP P08669
a	439	ASP	-	expression tag	UNP P08669
b	329	PRO	GLU	engineered mutation	UNP P08669
b	332	THR	MET	engineered mutation	UNP P08669
b	360	CYS	GLY	engineered mutation	UNP P08669
b	434	GLU	-	expression tag	UNP P08669
b	435	VAL	-	expression tag	UNP P08669
b	436	ASP	-	expression tag	UNP P08669
b	437	ASP	-	expression tag	UNP P08669
b	438	ASP	-	expression tag	UNP P08669
b	439	ASP	-	expression tag	UNP P08669
c	329	PRO	GLU	engineered mutation	UNP P08669
c	332	THR	MET	engineered mutation	UNP P08669
c	360	CYS	GLY	engineered mutation	UNP P08669
c	434	GLU	-	expression tag	UNP P08669
c	435	VAL	-	expression tag	UNP P08669

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
c	436	ASP	-	expression tag	UNP P08669
c	437	ASP	-	expression tag	UNP P08669
c	438	ASP	-	expression tag	UNP P08669
c	439	ASP	-	expression tag	UNP P08669

- 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	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	R	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



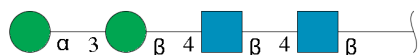
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	X	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	d	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



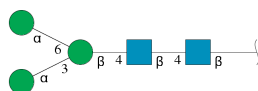
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
7	W	4	Total	C	N	O	0	0	0
			50	28	2	20			
7	Z	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



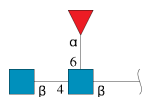
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	T	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



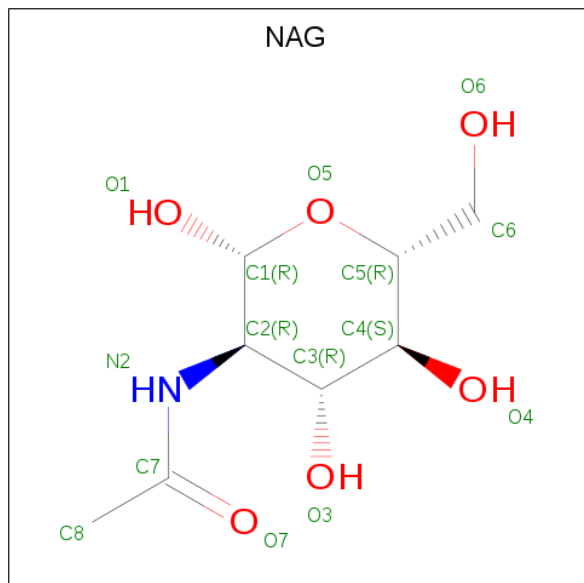
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	U	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 10 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
10	V	3	Total	C	N	O	0	0	0
			38	22	2	14			
10	Y	3	Total	C	N	O	0	0	0
			38	22	2	14			
10	e	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by author).



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

Continued on next page...

Continued from previous page...

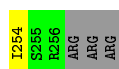
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	C	1	Total	C	N	O	0	0
			14	8	1	5		
11	C	1	Total	C	N	O	0	0
			14	8	1	5		
11	a	1	Total	C	N	O	0	0
			14	8	1	5		

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.

- Chain A:
-
- 62% 10% 27%
- MET GLY GLN ILE VAL THR PHE PHE GLN GLY VAL PRO HIS VAL ILE ILE GLY GLU GLU VAL MET ASN ASN ILE VAL VAL LEU LEU ILE ALA SER SER VAL LEU ALA LEU VAL LEU LYS GLY LEU THR ASN PHE ALA THR CYS GLY LEU VAL GLY LEU VAL THR PHE LEU LEU CYS LEU CYS GLY ARG CYS THR T59
- L84 K88 I95 M96 G102 L103 E104 L105 T106 L107 F117 G118 N119 L120 L133 I137 S138 T139 M148 K161 I162 S163 V164 H170 SER TYR ALA ASP ALA ALA ASN HIS C180 S216 L220 E228 D229 H230 G231 Q232 P236 S237 P238 L242
- R248 T249 R250 S255 ARG ARG ARG ARG

- Chain B:
-
- 61% 9% 30%
- 0.00 0.05 0.10 0.15 0.20 0.25
- MET GLY ILE THR PHE GLN VAL HIS PRO VAL ILE GLU MET ASN ILE VAL LEU ILE ALA SER VAL LEU LYS GLY LEU THR ASN PHE ALA THR CYS GLY LEU VAL GLY LEU THR PHE LEU CYS GLY ARG SER CYS THR T59

- Chain C:
-
- 3% 66% 7% 27%
- Met GLY GLN ILE VAL THR PHE PHE GLN VAL VAL PRO PHE HIS ILE ILE GLU VAL MET ASN ILE VAL LEU ILE LEU LEU VAL VAL LEU ALA VAL LEU LYS GLY LEU LEU THR ASP PHE ALA THR CYS GLY LEU VAL GLY LEU VAL THR PHE LEU LEU CYS GLY ARG SER CYS THR T59
- L84 K88 R83 Y94 I95 E100 L105 T106 L107 I113 N114 H115 N119 K125 L128 T139 G159 G160 K161 H170 T170 T171 T172 T173 T174 T175 T176 T177 T178 T179 T180 T181 T182 T183 T184 T185 T186 T187 T188 T189 T190 T191 T192 T193 T194 T195 T196 T197 T198 T199 T200 T201 T202 T203 T204 T205 T206 T207 T208 T209 T210 T211 T212 T213 T214 T215 T216 T217 T218 T219 T220 T221 T222 T223 T224 T225 T226 T227 T228 T229 T230 T231 T232 T233 T234 T235 T236 T237 T238 T239 T240 T241 T242 T243 T244 T245 T246 T247 T248 T249 T250



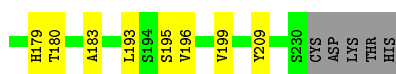
- Molecule 2: FAB Antibody heavy chain

Chain D: 79% 15% 6%



- Molecule 2: FAB Antibody heavy chain

Chain F: 80% 14% 6%



- Molecule 2: FAB Antibody heavy chain

Chain H: 77% 17% 5%



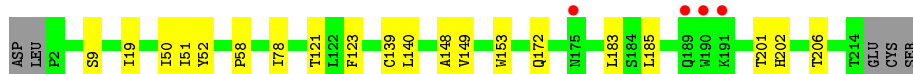
- Molecule 3: FAB Antibody light chain

Chain E: 88% 10% 2%



- Molecule 3: FAB Antibody light chain

Chain G: 88% 9% 2%




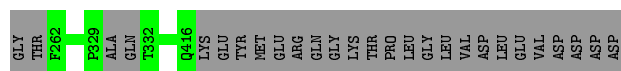
- Molecule 3: FAB Antibody light chain

Chain L:  90% 7%




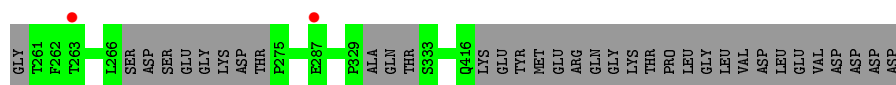
- Molecule 4: Pre-glycoprotein polyprotein GP complex

Chain a:  85% 15%




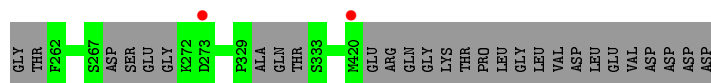
- Molecule 4: Pre-glycoprotein polyprotein GP complex

Chain b:  81% 19%



- Molecule 4: Pre-glycoprotein polyprotein GP complex

Chain c:  84% 16%



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

Chain I:  100%



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

Chain M:  100%



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

Chain P:  67% 33%



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

Chain R:  67% 33%



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

Chain J:  50% 50%



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

Chain K:  50% 50%



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

Chain N:  50% 50%



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

Chain Q:  100%



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

Chain S:  50% 50%



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

Chain X:  100%



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

Chain d:



- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%

HA01
HA02
FUC3

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%

HA01
HA02
FUC3

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%

HA01
HA02
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	152.24Å 152.24Å 453.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.66 – 3.50 29.66 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.66-3.50) 100.0 (29.66-3.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.47Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.205 , 0.247 0.203 , 0.245	Depositor DCC
R_{free} test set	2000 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	119.4	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 89.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18593	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, NAG, 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	0.24	0/1521	0.42	0/2061
1	B	0.24	0/1458	0.41	0/1974
1	C	0.23	0/1532	0.41	0/2075
2	D	0.24	0/1663	0.45	0/2260
2	F	0.24	0/1663	0.45	0/2260
2	H	0.25	0/1667	0.46	0/2265
3	E	0.24	0/1626	0.43	0/2222
3	G	0.24	0/1625	0.44	0/2220
3	L	0.24	0/1625	0.43	0/2220
4	a	0.25	0/1268	0.42	0/1714
4	b	0.24	0/1210	0.40	0/1634
4	c	0.24	0/1272	0.41	0/1716
All	All	0.24	0/18130	0.43	0/24621

There are no bond length outliers.

There are no bond angle outliers.

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	1488	0	1418	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1428	0	1366	14	0
1	C	1499	0	1431	12	0
2	D	1628	0	1612	19	0
2	F	1628	0	1612	21	0
2	H	1632	0	1615	22	0
3	E	1585	0	1547	12	0
3	G	1584	0	1541	15	0
3	L	1584	0	1541	10	0
4	a	1242	0	1192	0	0
4	b	1185	0	1146	0	0
4	c	1246	0	1204	0	0
5	I	39	0	34	0	0
5	M	39	0	34	0	0
5	P	39	0	34	0	0
5	R	39	0	34	1	0
6	J	28	0	25	0	0
6	K	28	0	25	1	0
6	N	28	0	25	0	0
6	Q	28	0	25	0	0
6	S	28	0	25	1	0
6	X	28	0	25	0	0
6	d	28	0	25	0	0
7	O	50	0	43	1	0
7	W	50	0	43	0	0
7	Z	50	0	43	0	0
8	T	61	0	52	0	0
9	U	61	0	52	0	0
10	V	38	0	34	0	0
10	Y	38	0	34	0	0
10	e	38	0	34	0	0
11	A	42	0	39	1	0
11	B	42	0	39	1	0
11	C	28	0	26	1	0
11	a	14	0	13	0	0
All	All	18593	0	17988	133	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 5.

The worst 5 of 133 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:C:139:THR:HG22	1:C:248:ARG:HH21	1.49	0.74
2:F:196:VAL:HG11	3:G:140:LEU:HD13	1.72	0.70
2:H:23:CYS:HB3	2:H:87:LEU:HB3	1.74	0.69
1:A:250:ARG:O	1:B:248:ARG:NH1	2.29	0.66
2:D:46:PRO:HD3	2:D:100:ALA:HA	1.83	0.61

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/259 (71%)	171 (93%)	13 (7%)	0	100	100
1	B	175/259 (68%)	163 (93%)	12 (7%)	0	100	100
1	C	185/259 (71%)	173 (94%)	12 (6%)	0	100	100
2	D	214/231 (93%)	204 (95%)	10 (5%)	0	100	100
2	F	214/231 (93%)	205 (96%)	9 (4%)	0	100	100
2	H	215/231 (93%)	204 (95%)	11 (5%)	0	100	100
3	E	210/217 (97%)	202 (96%)	8 (4%)	0	100	100
3	G	210/217 (97%)	203 (97%)	7 (3%)	0	100	100
3	L	210/217 (97%)	202 (96%)	8 (4%)	0	100	100
4	a	149/180 (83%)	145 (97%)	4 (3%)	0	100	100
4	b	139/180 (77%)	138 (99%)	1 (1%)	0	100	100
4	c	146/180 (81%)	144 (99%)	2 (1%)	0	100	100
All	All	2251/2661 (85%)	2154 (96%)	97 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	169/228 (74%)	169 (100%)	0	100	100
1	B	162/228 (71%)	162 (100%)	0	100	100
1	C	170/228 (75%)	170 (100%)	0	100	100
2	D	185/197 (94%)	185 (100%)	0	100	100
2	F	185/197 (94%)	185 (100%)	0	100	100
2	H	185/197 (94%)	185 (100%)	0	100	100
3	E	180/185 (97%)	179 (99%)	1 (1%)	86	94
3	G	180/185 (97%)	180 (100%)	0	100	100
3	L	180/185 (97%)	180 (100%)	0	100	100
4	a	139/162 (86%)	139 (100%)	0	100	100
4	b	132/162 (82%)	132 (100%)	0	100	100
4	c	139/162 (86%)	139 (100%)	0	100	100
All	All	2006/2316 (87%)	2005 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	33	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

57 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	$\# Z > 2$
5	NAG	I	1	1,5	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	I	2	5	14,14,15	0.18	0	17,19,21	0.47	0
5	BMA	I	3	5	11,11,12	0.63	0	15,15,17	0.87	0
6	NAG	J	1	1,6	14,14,15	0.33	0	17,19,21	0.49	0
6	NAG	J	2	6	14,14,15	0.18	0	17,19,21	0.70	1 (5%)
6	NAG	K	1	1,6	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	K	2	6	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	M	1	1,5	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	M	2	5	14,14,15	0.19	0	17,19,21	0.48	0
5	BMA	M	3	5	11,11,12	0.64	0	15,15,17	0.87	0
6	NAG	N	1	1,6	14,14,15	0.27	0	17,19,21	0.46	0
6	NAG	N	2	6	14,14,15	0.21	0	17,19,21	0.69	1 (5%)
7	NAG	O	1	1,7	14,14,15	0.23	0	17,19,21	0.43	0
7	NAG	O	2	7	14,14,15	0.20	0	17,19,21	0.43	0
7	BMA	O	3	7	11,11,12	0.61	0	15,15,17	0.78	0
7	MAN	O	4	7	11,11,12	0.73	0	15,15,17	1.06	2 (13%)
5	NAG	P	1	1,5	14,14,15	0.25	0	17,19,21	0.48	0
5	NAG	P	2	5	14,14,15	0.22	0	17,19,21	0.68	1 (5%)
5	BMA	P	3	5	11,11,12	0.75	0	15,15,17	1.03	0
6	NAG	Q	1	1,6	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	Q	2	6	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	R	1	1,5	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	R	2	5	14,14,15	0.20	0	17,19,21	0.43	0
5	BMA	R	3	5	11,11,12	0.61	0	15,15,17	0.77	0
6	NAG	S	1	1,6	14,14,15	0.31	0	17,19,21	0.47	0
6	NAG	S	2	6	14,14,15	0.20	0	17,19,21	0.44	0
8	NAG	T	1	8,4	14,14,15	0.22	0	17,19,21	0.47	0
8	NAG	T	2	8	14,14,15	0.20	0	17,19,21	0.42	0
8	BMA	T	3	8	11,11,12	0.60	0	15,15,17	0.77	0
8	MAN	T	4	8	11,11,12	0.76	0	15,15,17	1.10	2 (13%)
8	MAN	T	5	8	11,11,12	0.73	0	15,15,17	1.02	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	U	1	9,4	14,14,15	0.22	0	17,19,21	0.44	0
9	NAG	U	2	9	14,14,15	0.19	0	17,19,21	0.42	0
9	BMA	U	3	9	11,11,12	0.66	0	15,15,17	0.79	0
9	MAN	U	4	9	11,11,12	0.73	0	15,15,17	1.10	2 (13%)
9	MAN	U	5	9	11,11,12	0.68	0	15,15,17	1.04	2 (13%)
10	NAG	V	1	10,4	14,14,15	0.34	0	17,19,21	0.42	0
10	NAG	V	2	10	14,14,15	0.26	0	17,19,21	0.39	0
10	FUC	V	3	10	10,10,11	0.76	0	14,14,16	0.86	0
7	NAG	W	1	4,7	14,14,15	0.19	0	17,19,21	0.50	0
7	NAG	W	2	7	14,14,15	0.20	0	17,19,21	0.41	0
7	BMA	W	3	7	11,11,12	0.60	0	15,15,17	0.78	0
7	MAN	W	4	7	11,11,12	0.68	0	15,15,17	1.06	2 (13%)
6	NAG	X	1	4,6	14,14,15	0.20	0	17,19,21	0.45	0
6	NAG	X	2	6	14,14,15	0.22	0	17,19,21	0.41	0
10	NAG	Y	1	10,4	14,14,15	0.35	0	17,19,21	0.40	0
10	NAG	Y	2	10	14,14,15	0.26	0	17,19,21	0.38	0
10	FUC	Y	3	10	10,10,11	0.78	0	14,14,16	0.85	0
7	NAG	Z	1	4,7	14,14,15	0.16	0	17,19,21	0.52	0
7	NAG	Z	2	7	14,14,15	0.20	0	17,19,21	0.42	0
7	BMA	Z	3	7	11,11,12	0.61	0	15,15,17	0.79	0
7	MAN	Z	4	7	11,11,12	0.68	0	15,15,17	1.10	2 (13%)
6	NAG	d	1	4,6	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	d	2	6	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	e	1	10,4	14,14,15	0.34	0	17,19,21	0.39	0
10	NAG	e	2	10	14,14,15	0.25	0	17,19,21	0.39	0
10	FUC	e	3	10	10,10,11	0.75	0	14,14,16	0.83	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
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
7	NAG	O	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	0/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1
7	MAN	O	4	7	-	0/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	BMA	P	3	5	-	0/2/19/22	0/1/1/1
6	NAG	Q	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	0/1/1/1
5	NAG	R	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
5	BMA	R	3	5	-	0/2/19/22	0/1/1/1
6	NAG	S	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
8	NAG	T	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	T	2	8	-	0/6/23/26	0/1/1/1
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
8	MAN	T	4	8	-	0/2/19/22	0/1/1/1
8	MAN	T	5	8	-	0/2/19/22	0/1/1/1
9	NAG	U	1	9,4	-	2/6/23/26	0/1/1/1
9	NAG	U	2	9	-	0/6/23/26	0/1/1/1
9	BMA	U	3	9	-	0/2/19/22	0/1/1/1
9	MAN	U	4	9	-	0/2/19/22	0/1/1/1
9	MAN	U	5	9	-	1/2/19/22	0/1/1/1
10	NAG	V	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	V	2	10	-	2/6/23/26	0/1/1/1
10	FUC	V	3	10	-	-	0/1/1/1
7	NAG	W	1	4,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
7	BMA	W	3	7	-	0/2/19/22	0/1/1/1
7	MAN	W	4	7	-	0/2/19/22	0/1/1/1
6	NAG	X	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
10	NAG	Y	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	Y	2	10	-	2/6/23/26	0/1/1/1
10	FUC	Y	3	10	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	Z	1	4,7	-	0/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	0/6/23/26	0/1/1/1
7	BMA	Z	3	7	-	0/2/19/22	0/1/1/1
7	MAN	Z	4	7	-	0/2/19/22	0/1/1/1
6	NAG	d	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	d	2	6	-	2/6/23/26	0/1/1/1
10	NAG	e	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	e	2	10	-	2/6/23/26	0/1/1/1
10	FUC	e	3	10	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	2	NAG	C1-O5-C5	2.47	115.54	112.19
6	N	2	NAG	C1-O5-C5	2.45	115.51	112.19
5	P	2	NAG	C1-O5-C5	2.41	115.46	112.19
7	O	4	MAN	C1-O5-C5	2.39	115.43	112.19
8	T	5	MAN	C1-O5-C5	2.38	115.41	112.19

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	Y	2	NAG	O5-C5-C6-O6
10	Y	2	NAG	C4-C5-C6-O6
10	Y	1	NAG	O5-C5-C6-O6
10	V	1	NAG	O5-C5-C6-O6
10	Y	1	NAG	C4-C5-C6-O6

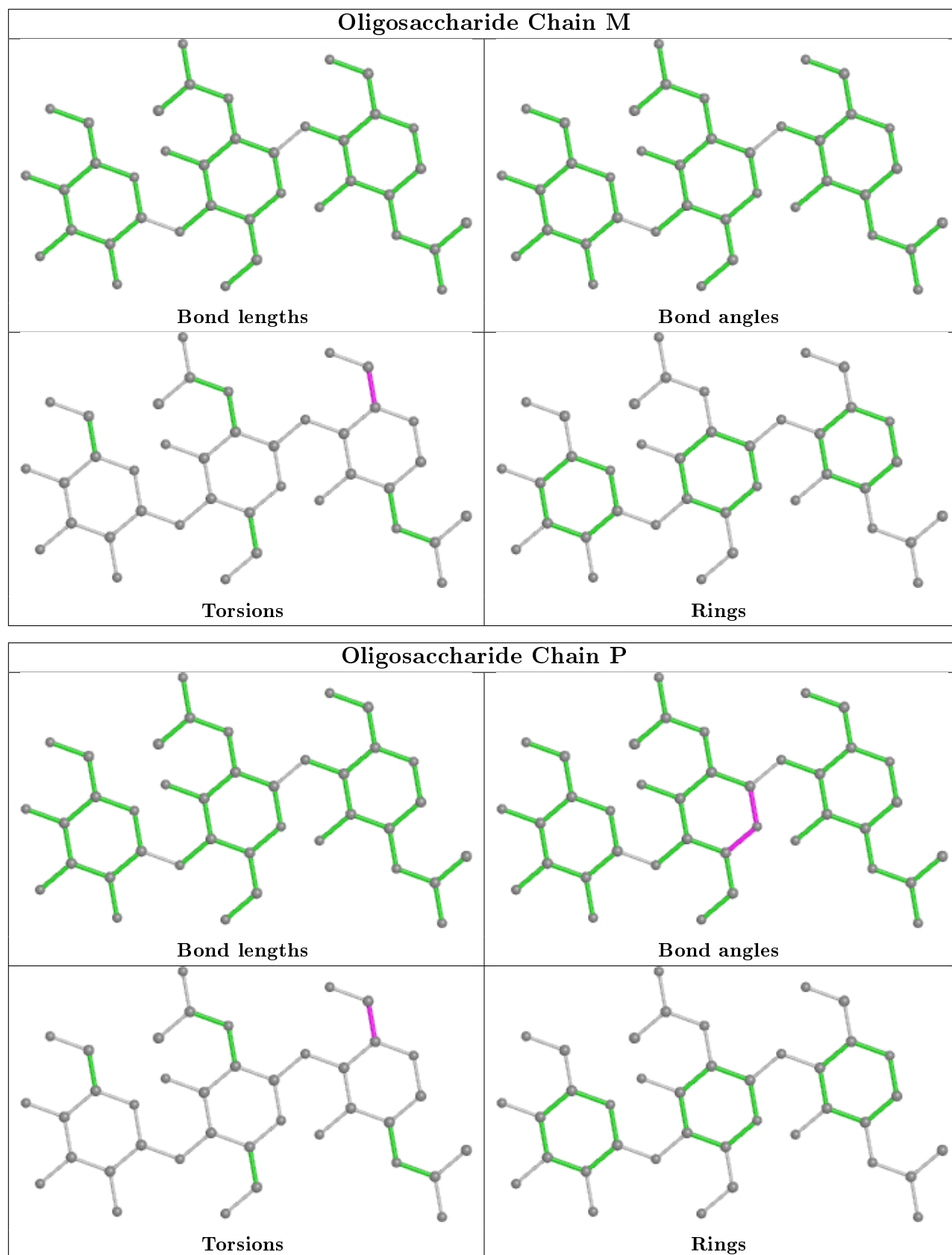
There are no ring outliers.

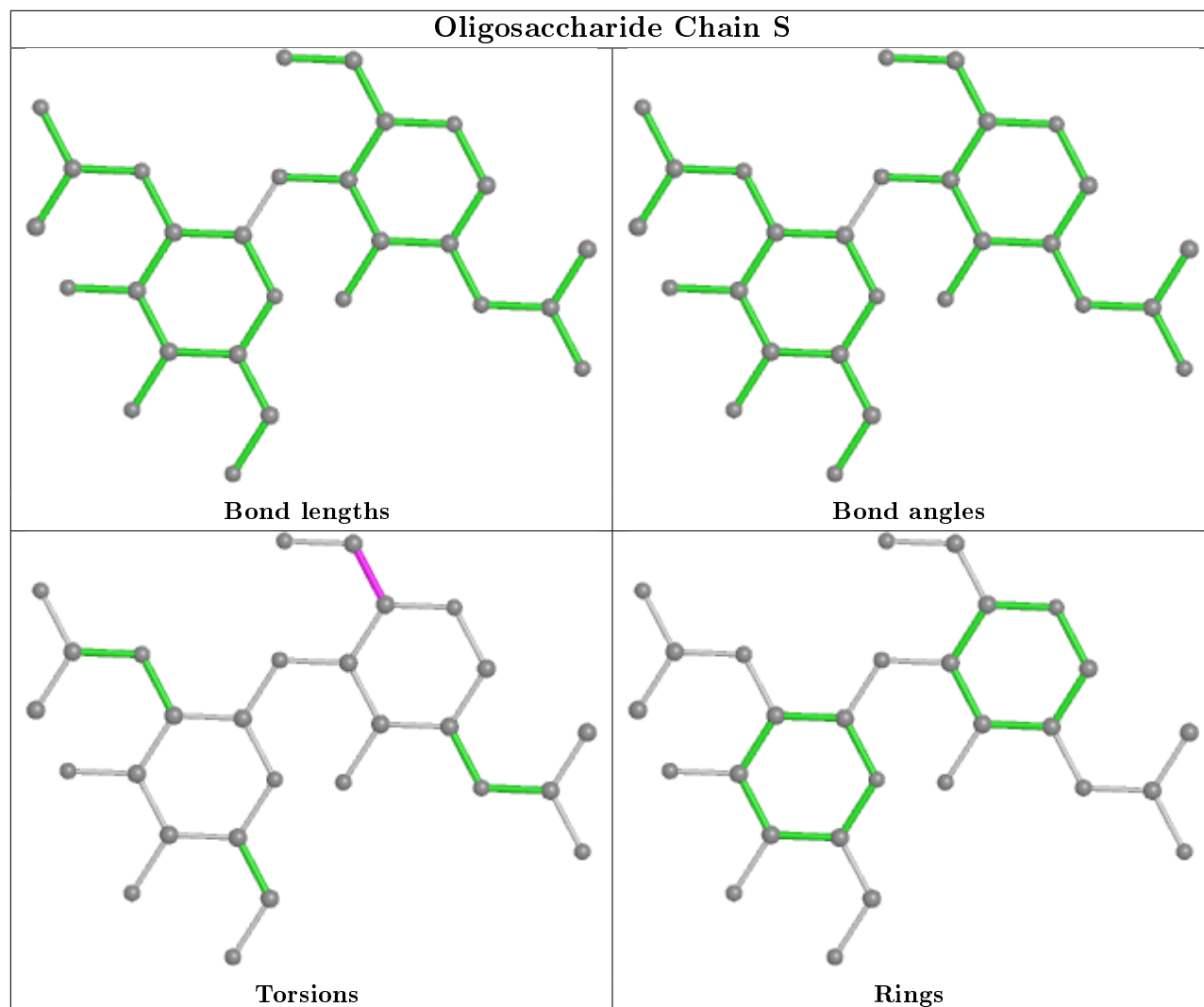
4 monomers are involved in 4 short contacts:

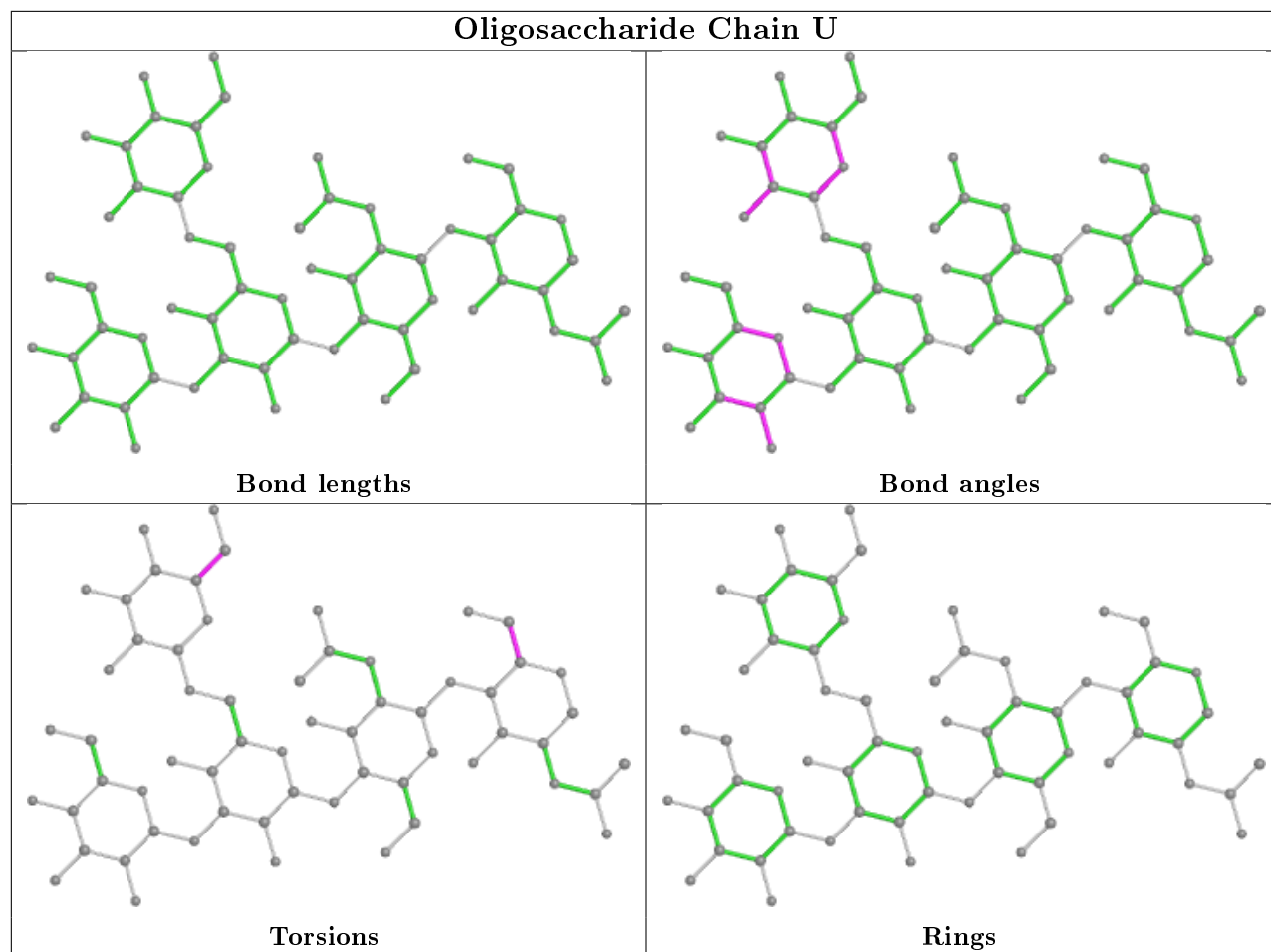
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	1	NAG	1	0
6	K	1	NAG	1	0
5	R	1	NAG	1	0
7	O	1	NAG	1	0

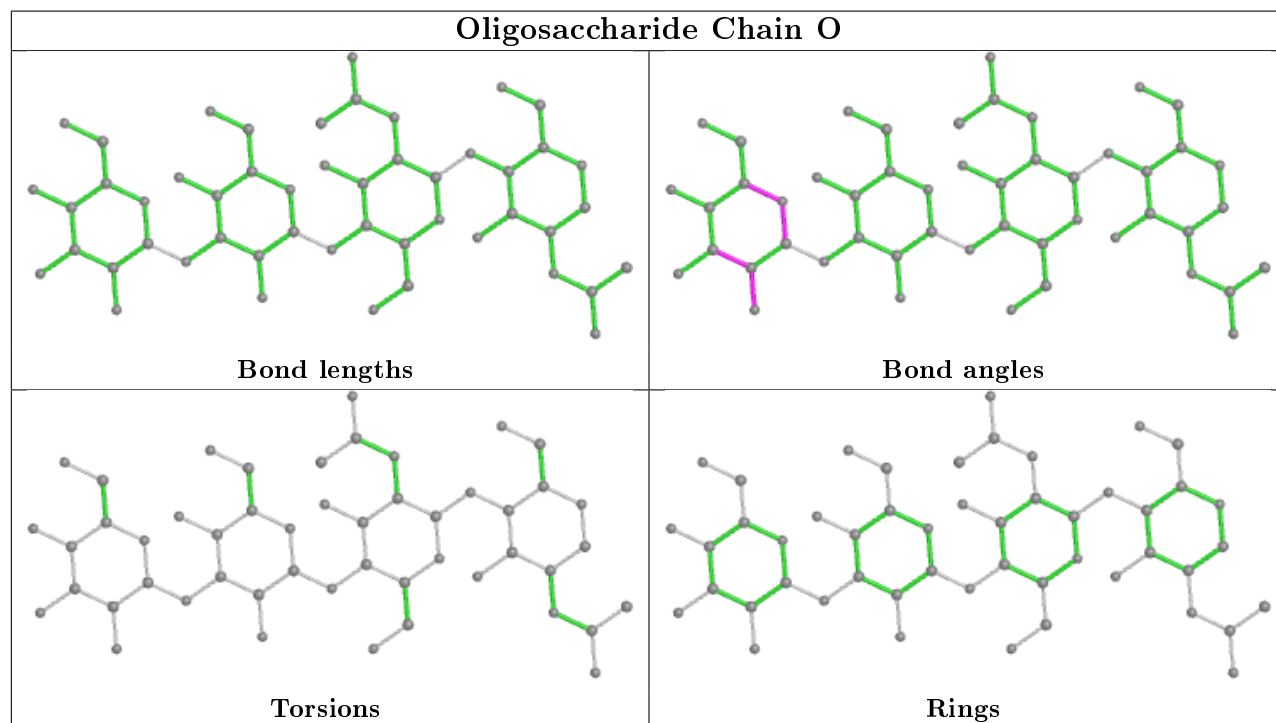
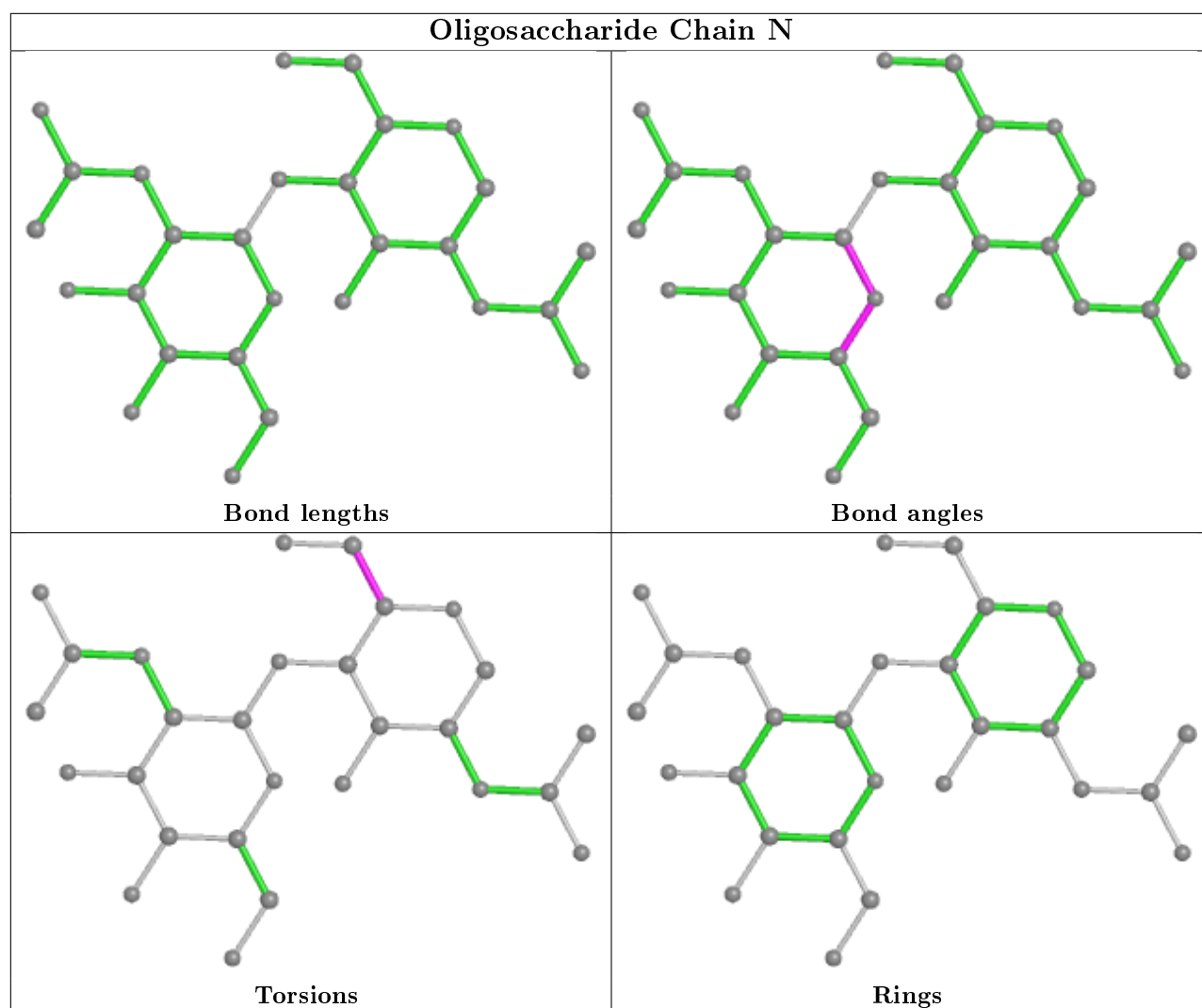
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

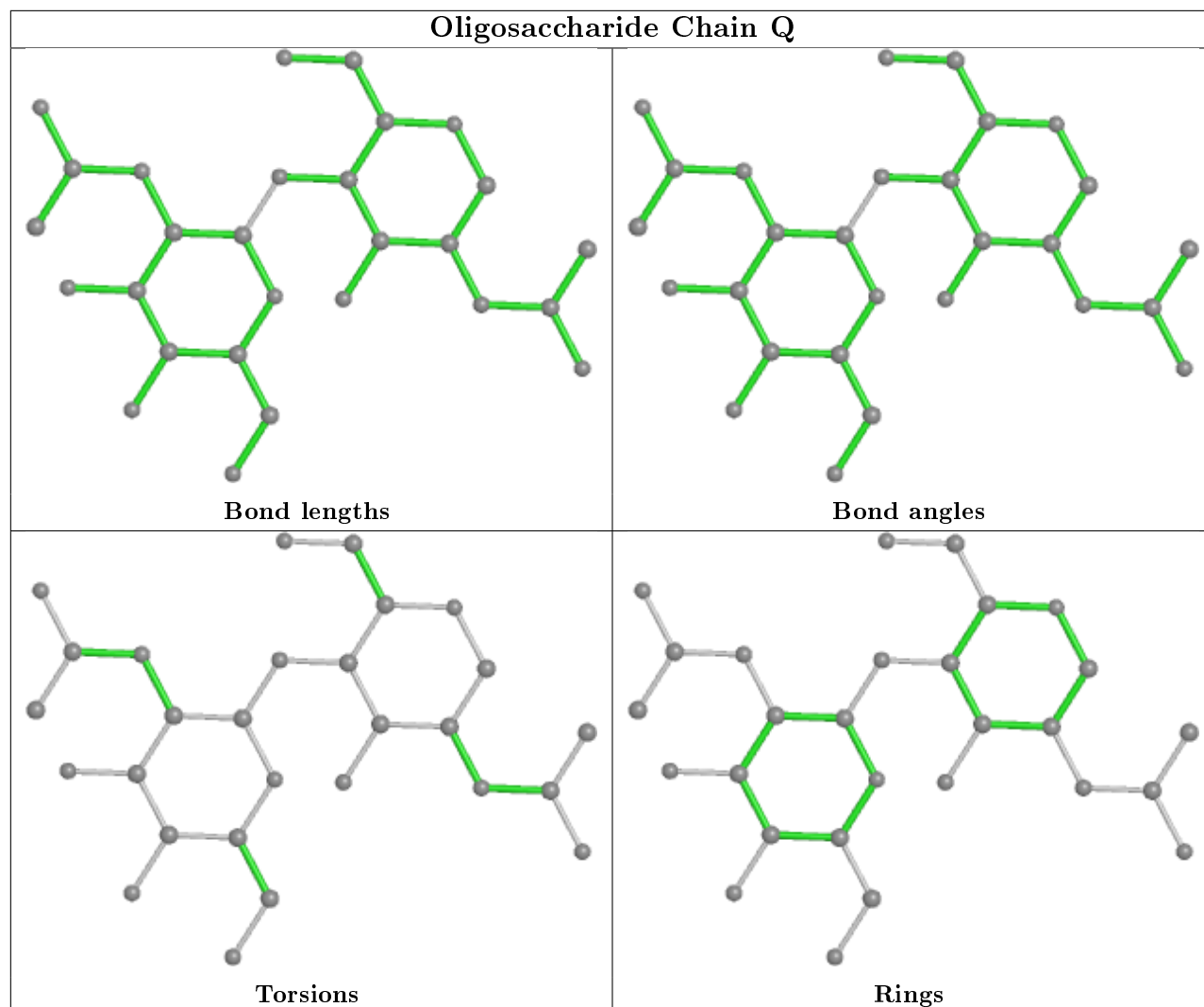
bond angles, torsion angles, and ring geometry for oligosaccharide.

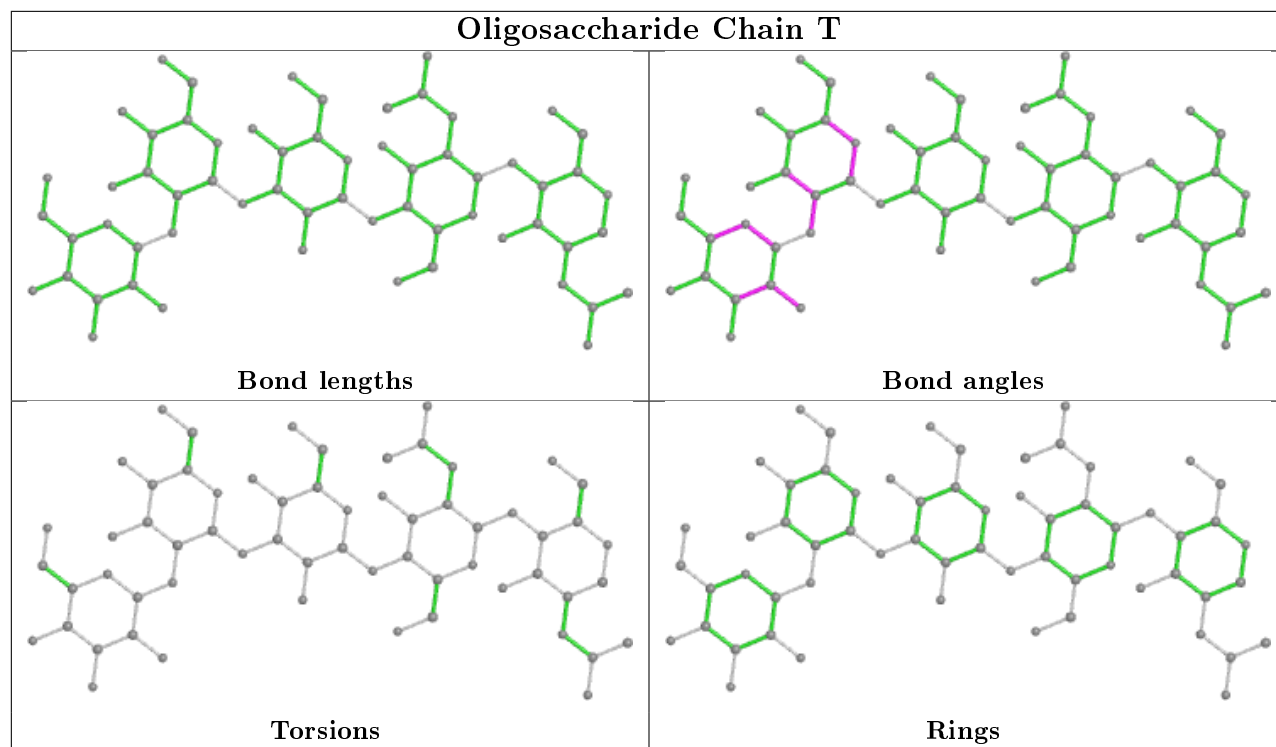


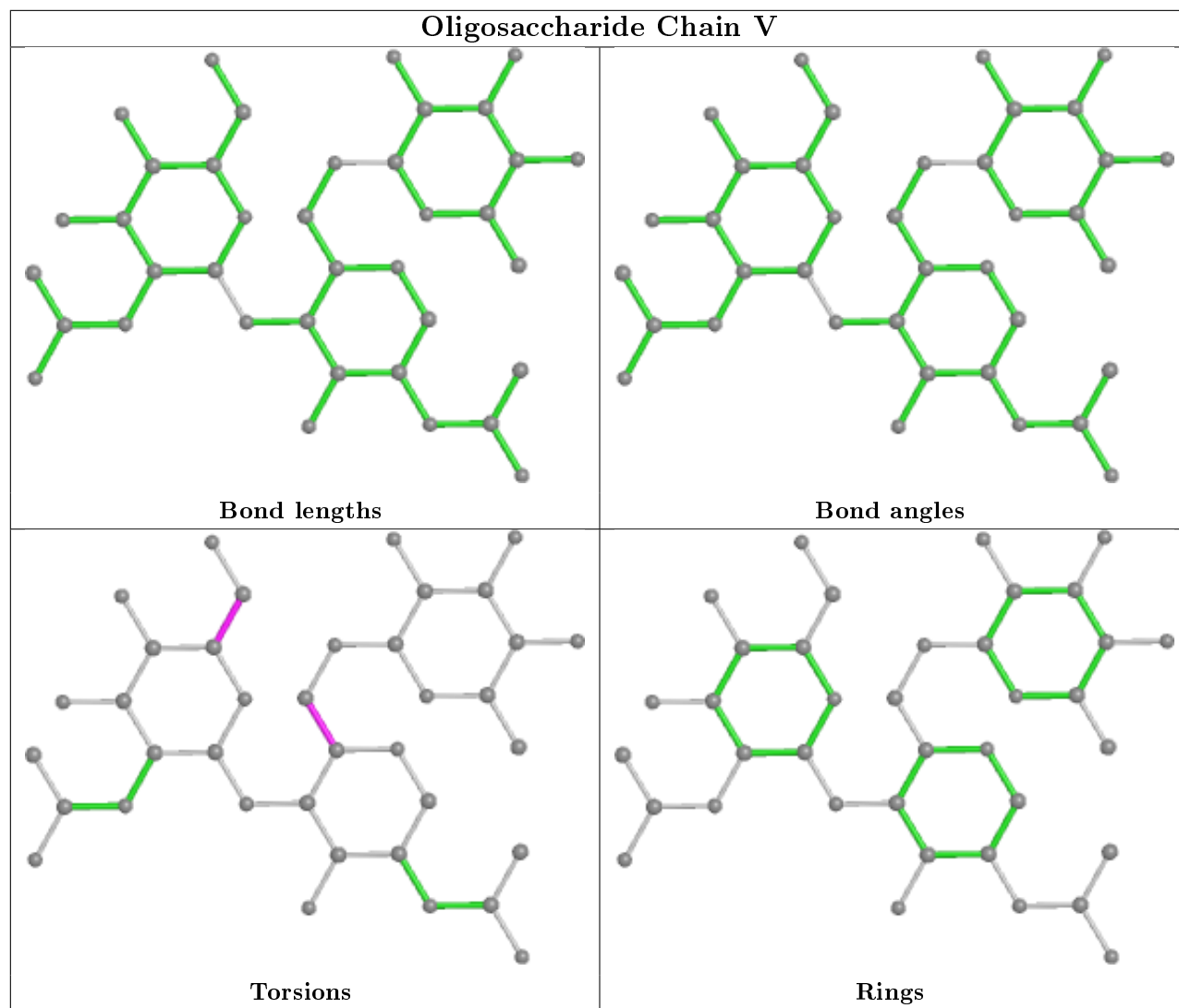


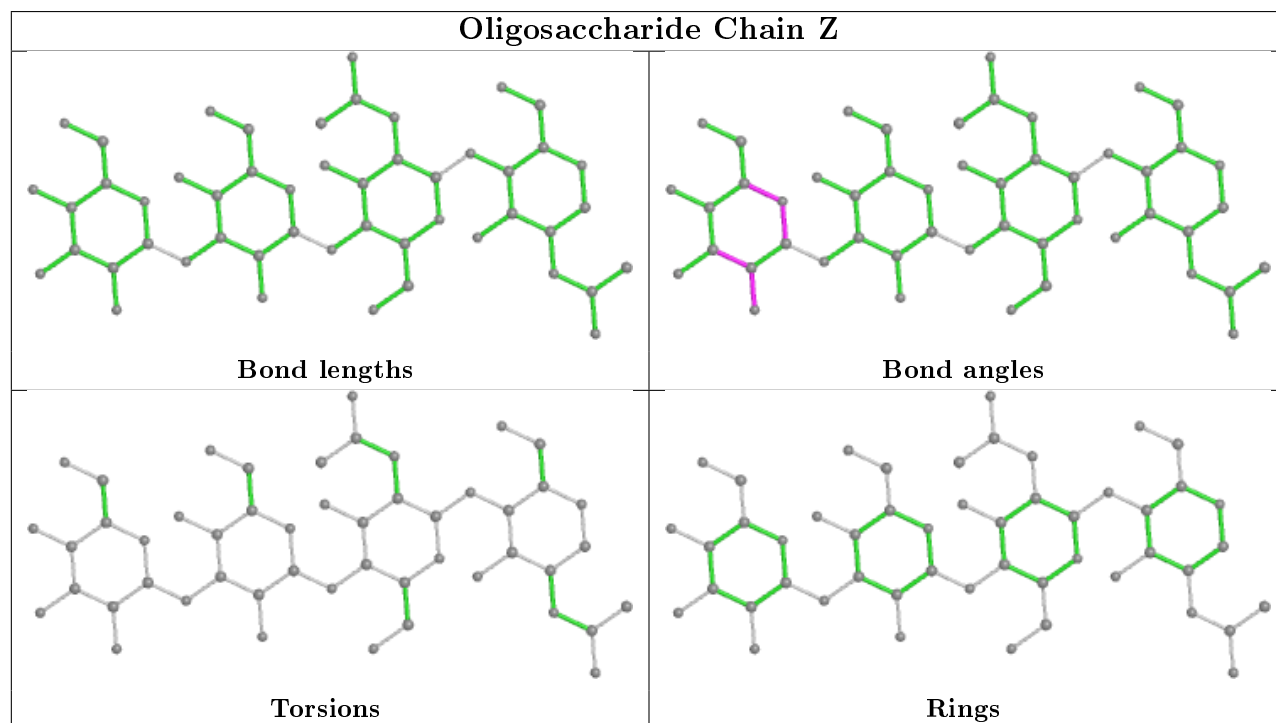
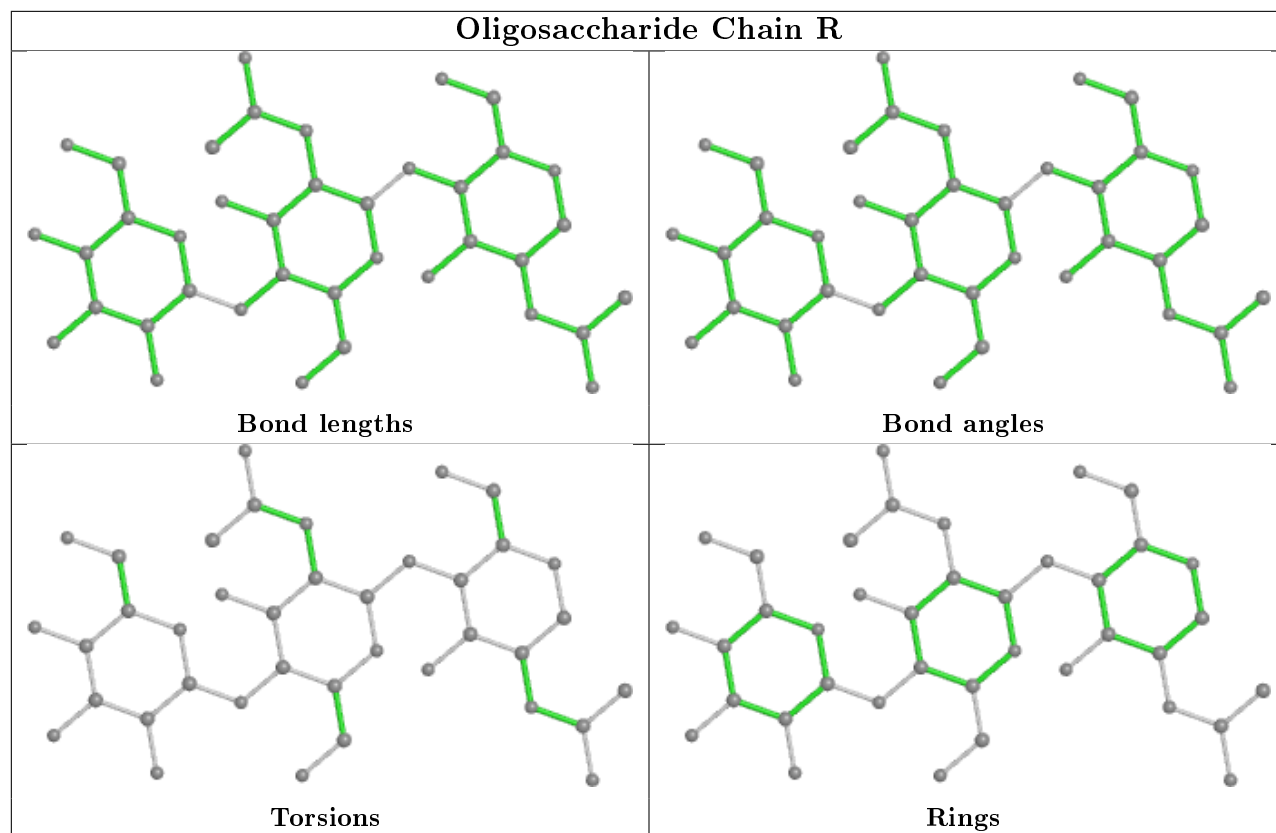




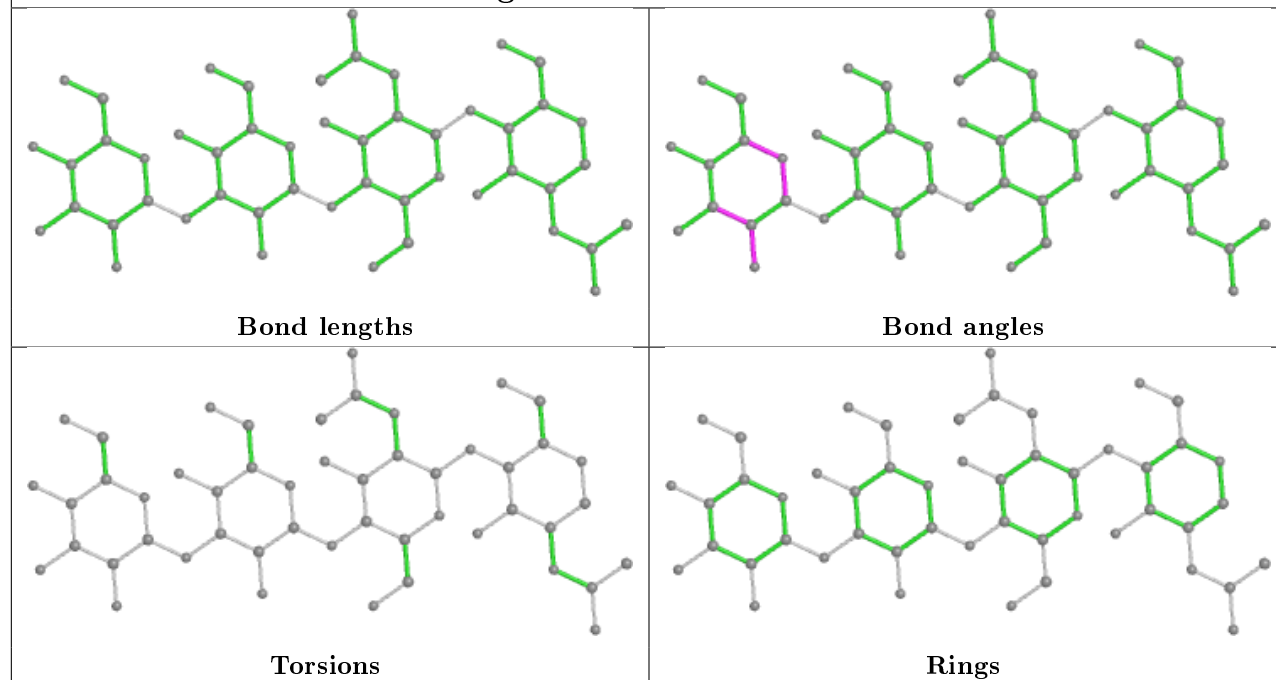




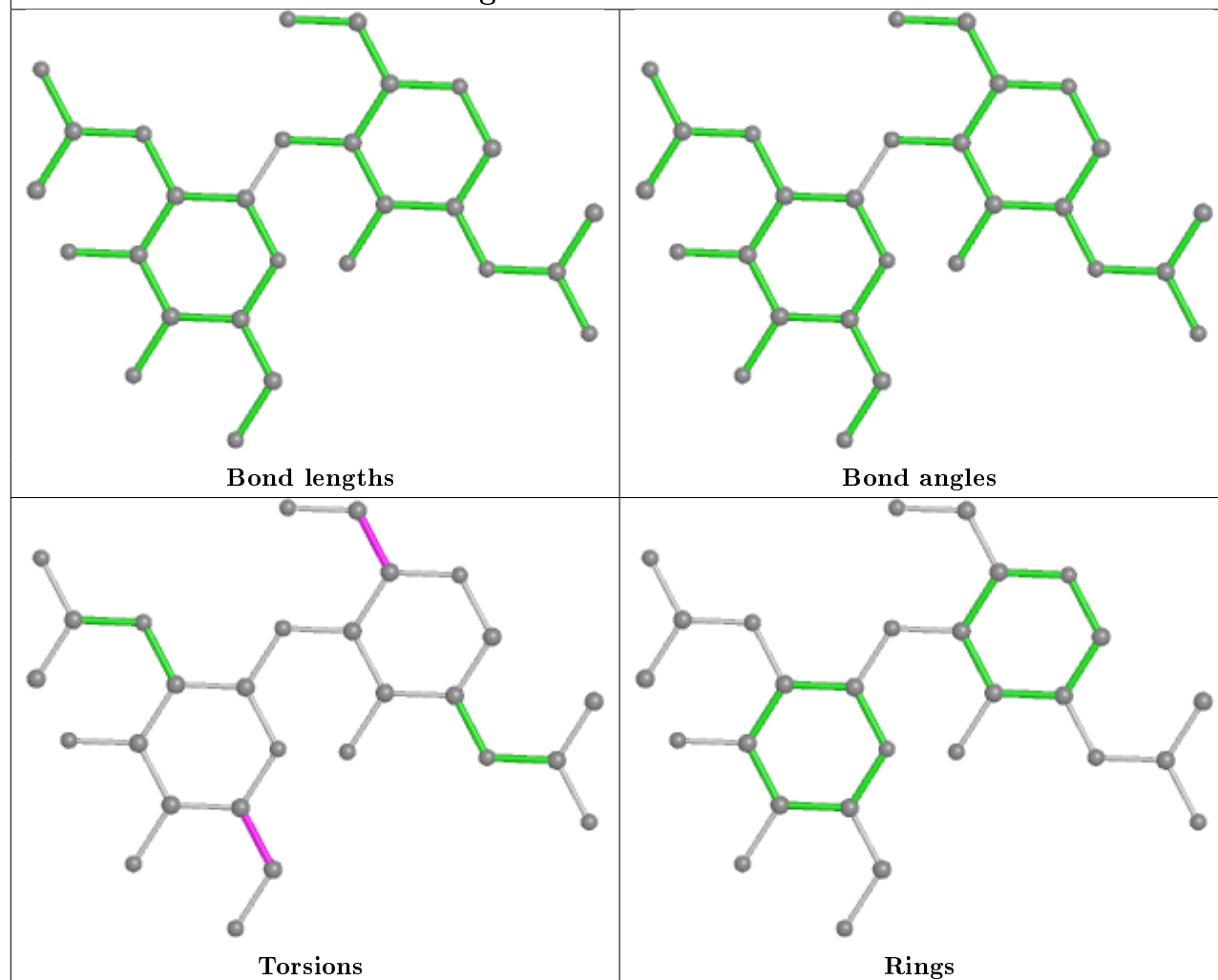


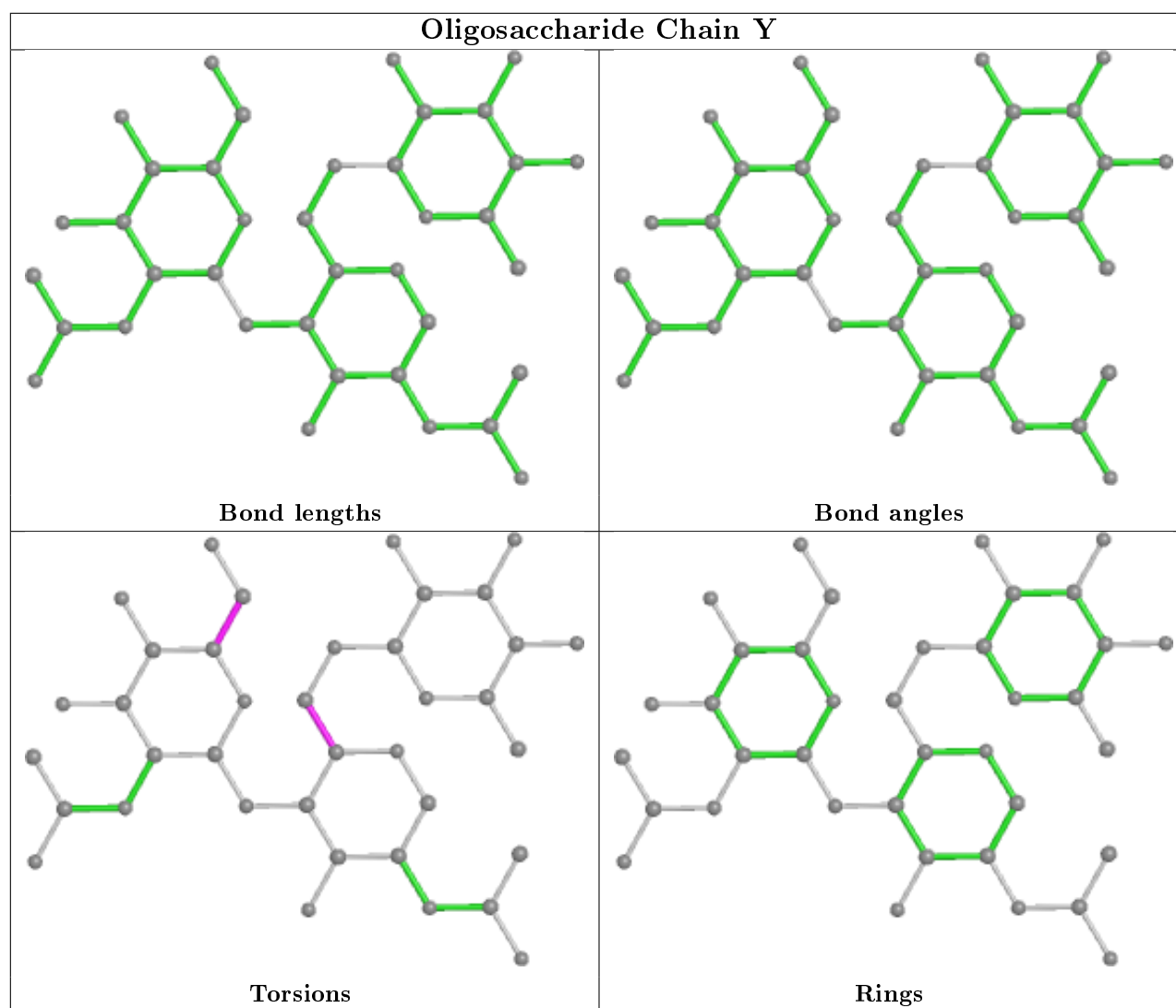


Oligosaccharide Chain W



Oligosaccharide Chain X





5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
11	NAG	B	306	1	14,14,15	0.26	0	17,19,21	0.47	0
11	NAG	B	312	1	14,14,15	0.30	0	17,19,21	0.47	0
11	NAG	C	310	1	14,14,15	0.22	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	A	310	1	14,14,15	0.29	0	17,19,21	0.46	0
11	NAG	A	309	1	14,14,15	0.21	0	17,19,21	0.43	0
11	NAG	A	306	1	14,14,15	0.24	0	17,19,21	0.46	0
11	NAG	a	511	4	14,14,15	0.48	0	17,19,21	0.70	0
11	NAG	C	306	1	14,14,15	0.23	0	17,19,21	0.48	0
11	NAG	B	311	1	14,14,15	0.20	0	17,19,21	0.44	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
11	NAG	B	306	1	-	2/6/23/26	0/1/1/1
11	NAG	B	312	1	-	2/6/23/26	0/1/1/1
11	NAG	C	310	1	-	0/6/23/26	0/1/1/1
11	NAG	A	310	1	-	2/6/23/26	0/1/1/1
11	NAG	A	309	1	-	0/6/23/26	0/1/1/1
11	NAG	A	306	1	-	2/6/23/26	0/1/1/1
11	NAG	a	511	4	-	3/6/23/26	0/1/1/1
11	NAG	C	306	1	-	2/6/23/26	0/1/1/1
11	NAG	B	311	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

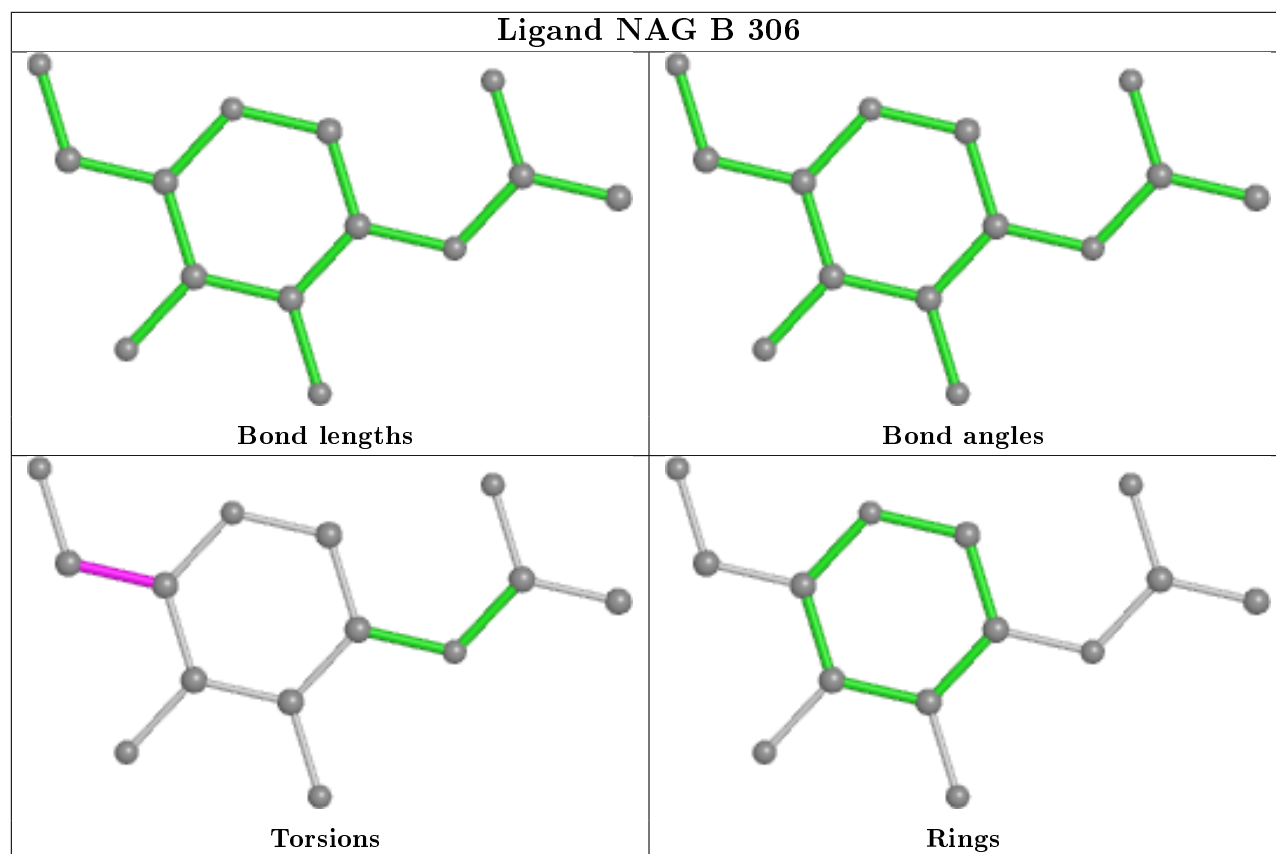
Mol	Chain	Res	Type	Atoms
11	a	511	NAG	O5-C5-C6-O6
11	a	511	NAG	C4-C5-C6-O6
11	C	306	NAG	O5-C5-C6-O6
11	C	306	NAG	C4-C5-C6-O6
11	A	306	NAG	C4-C5-C6-O6

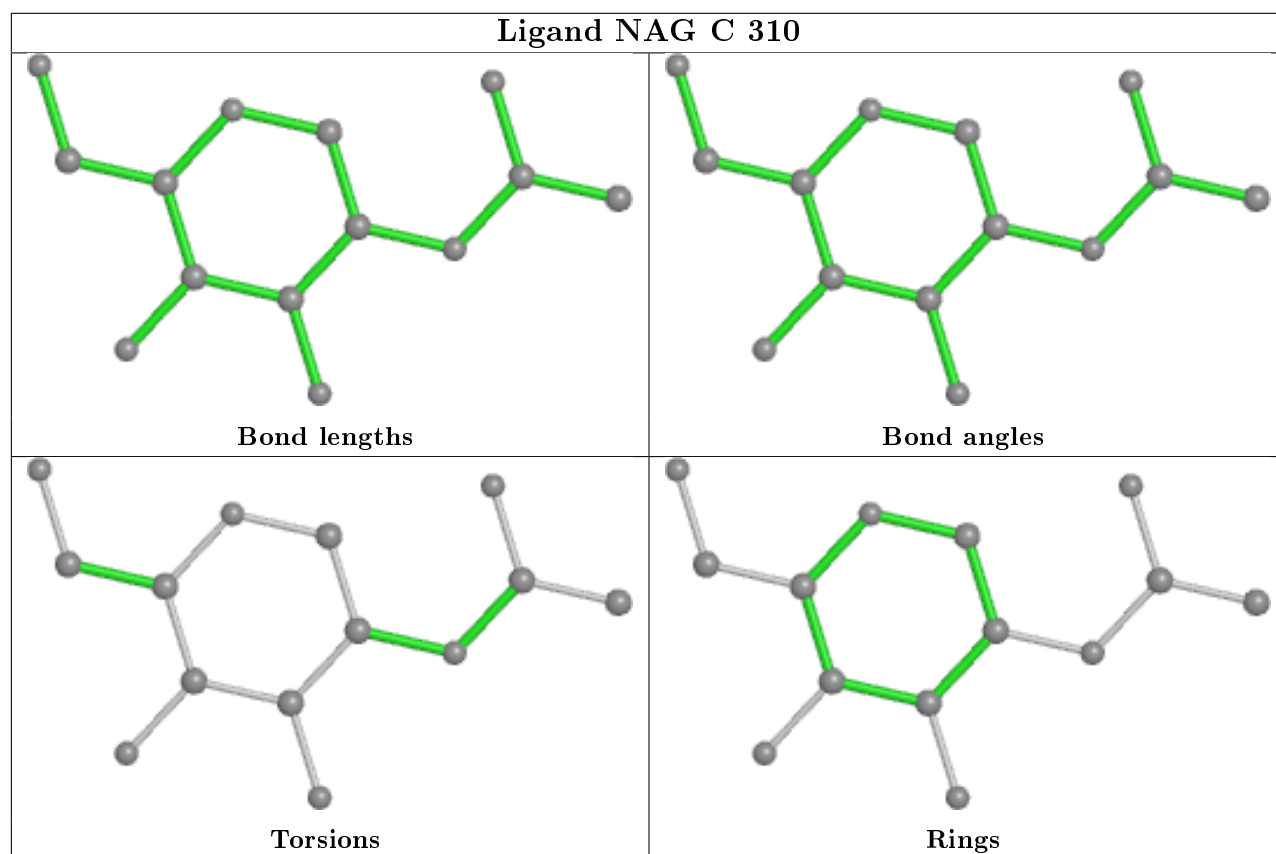
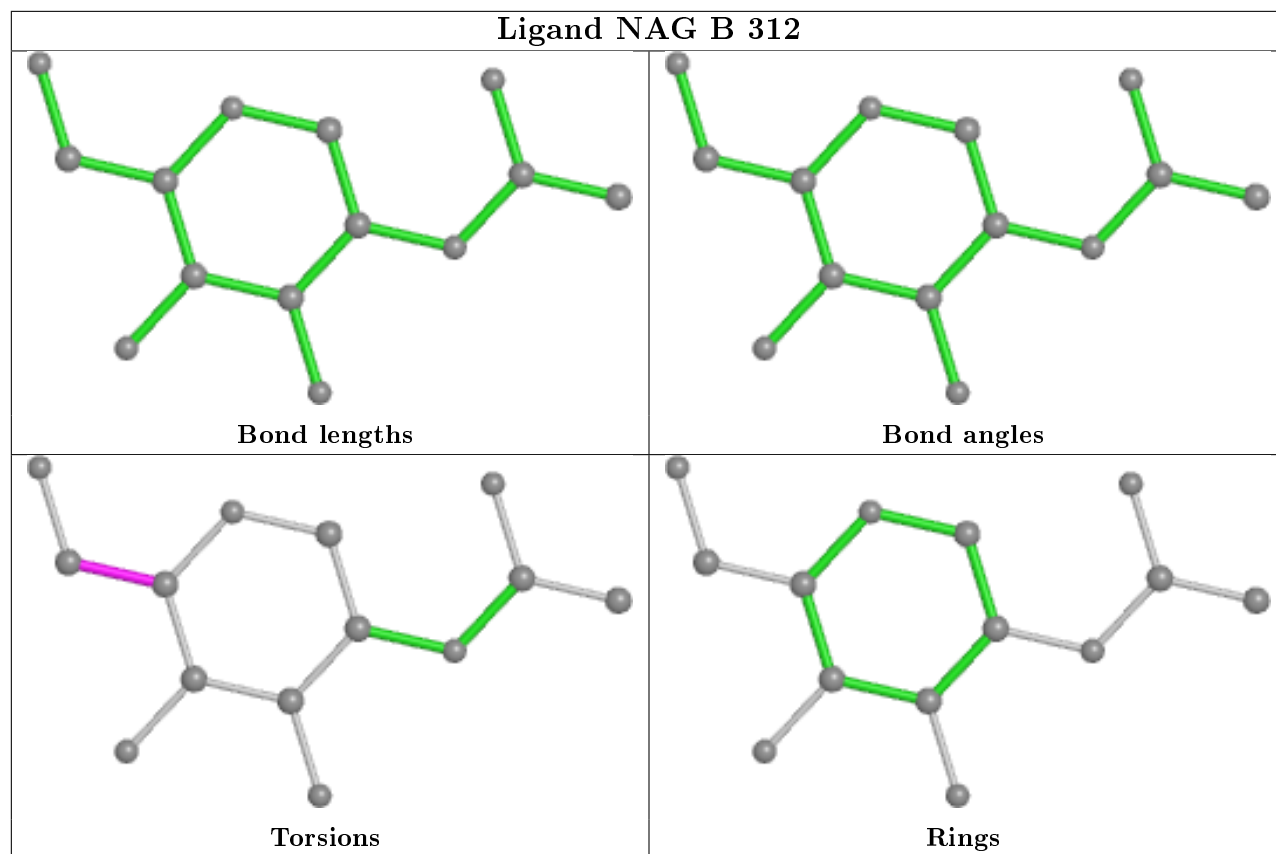
There are no ring outliers.

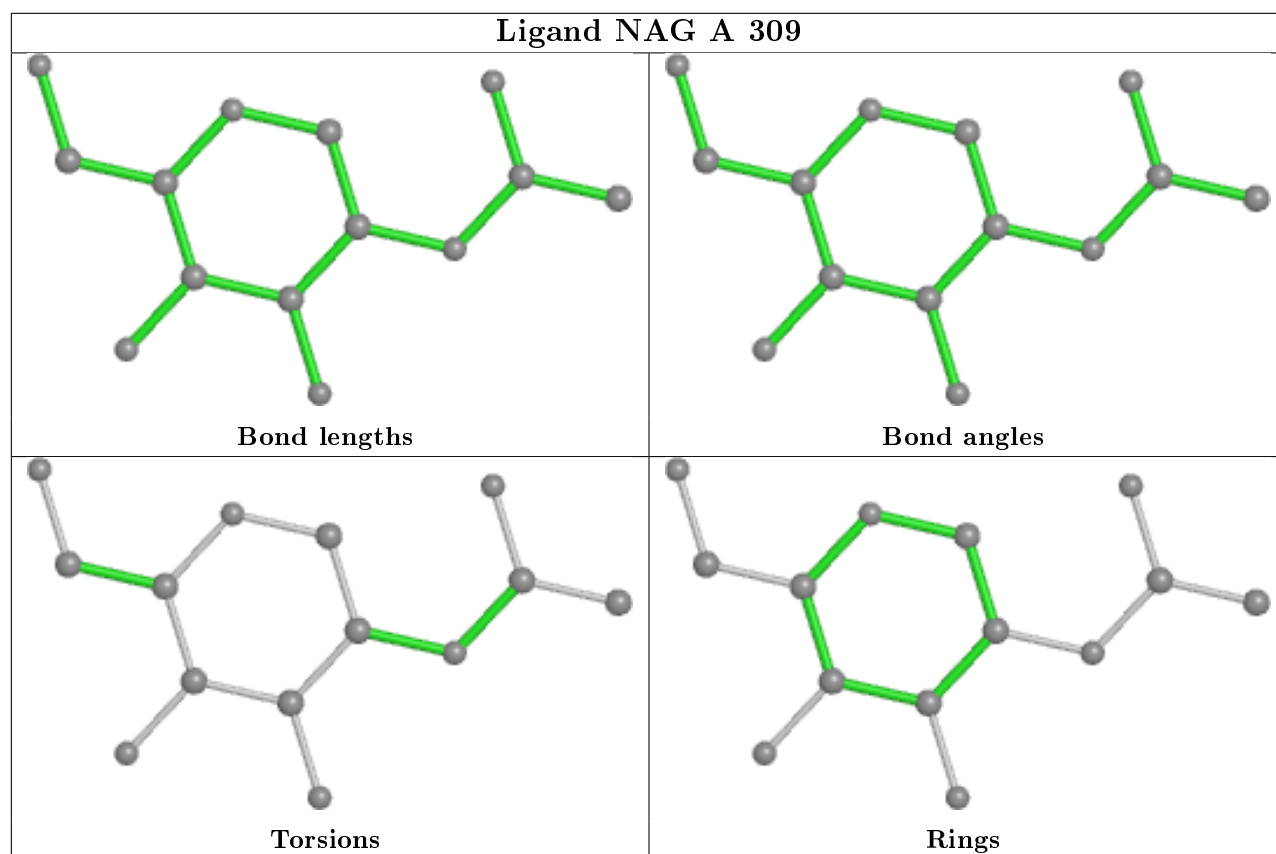
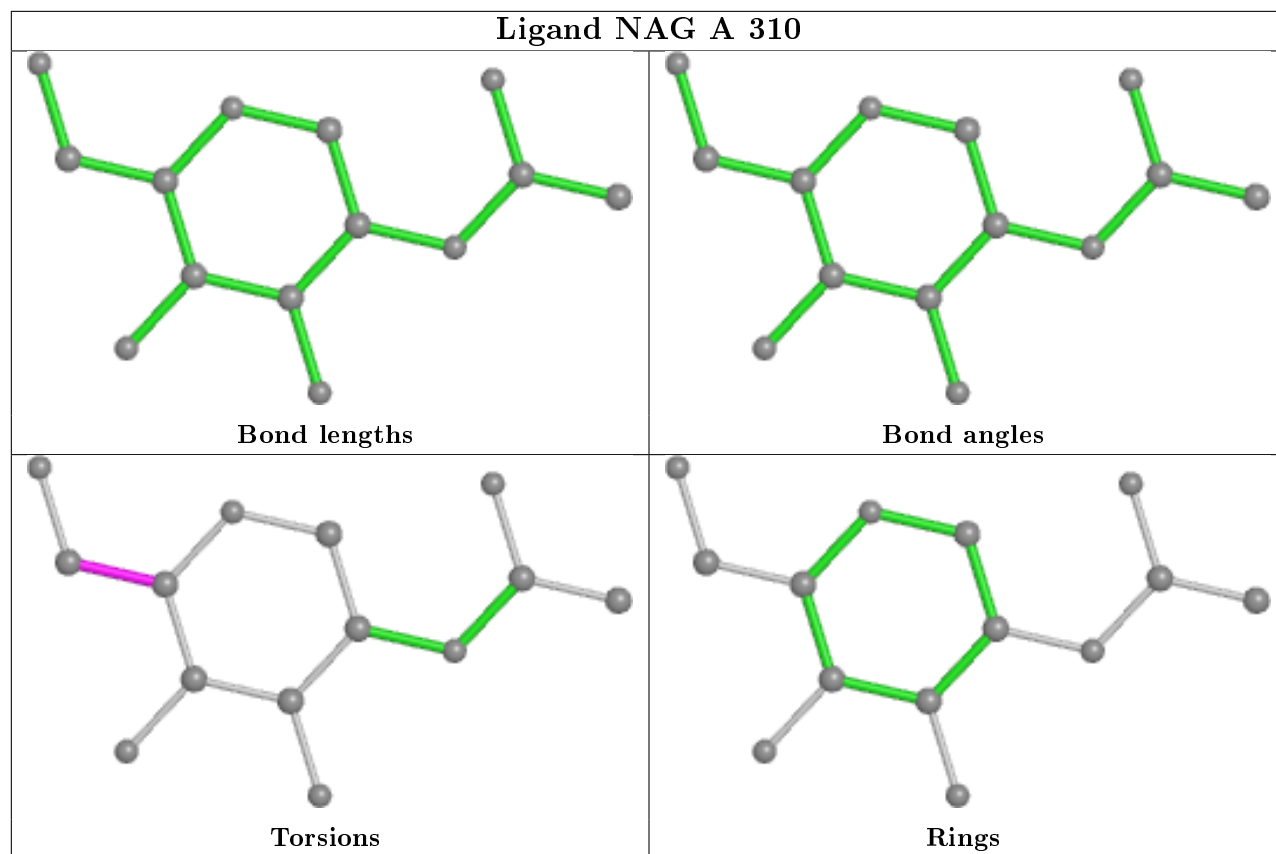
3 monomers are involved in 3 short contacts:

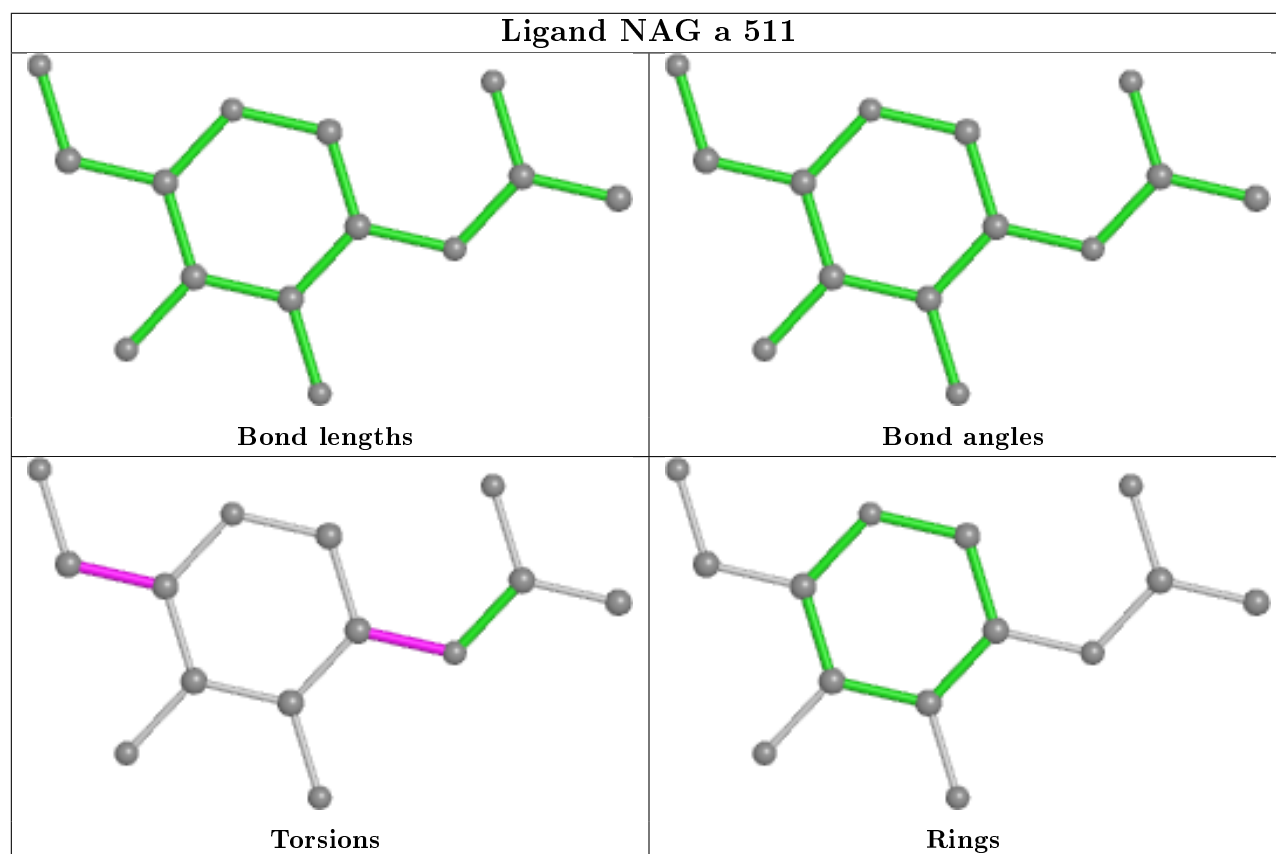
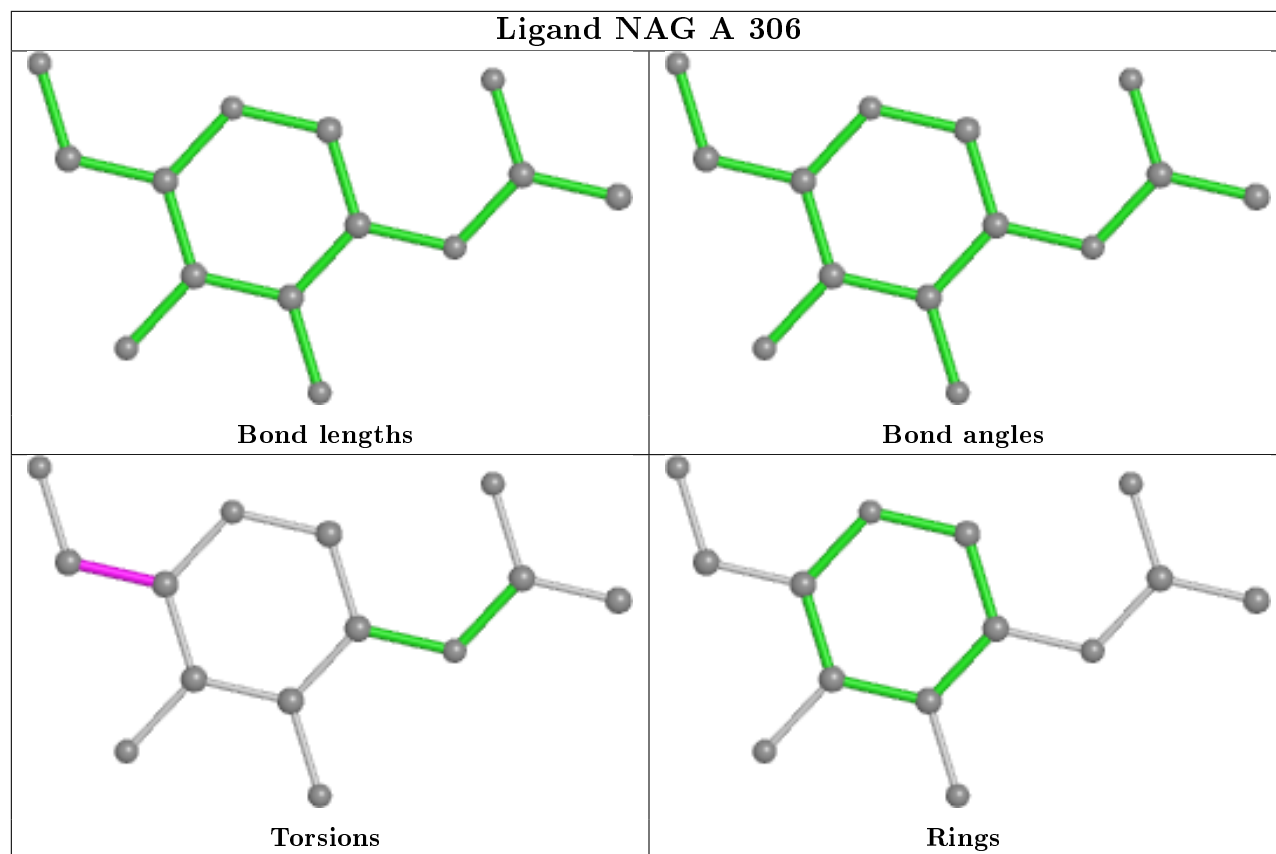
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	312	NAG	1	0
11	A	310	NAG	1	0
11	C	306	NAG	1	0

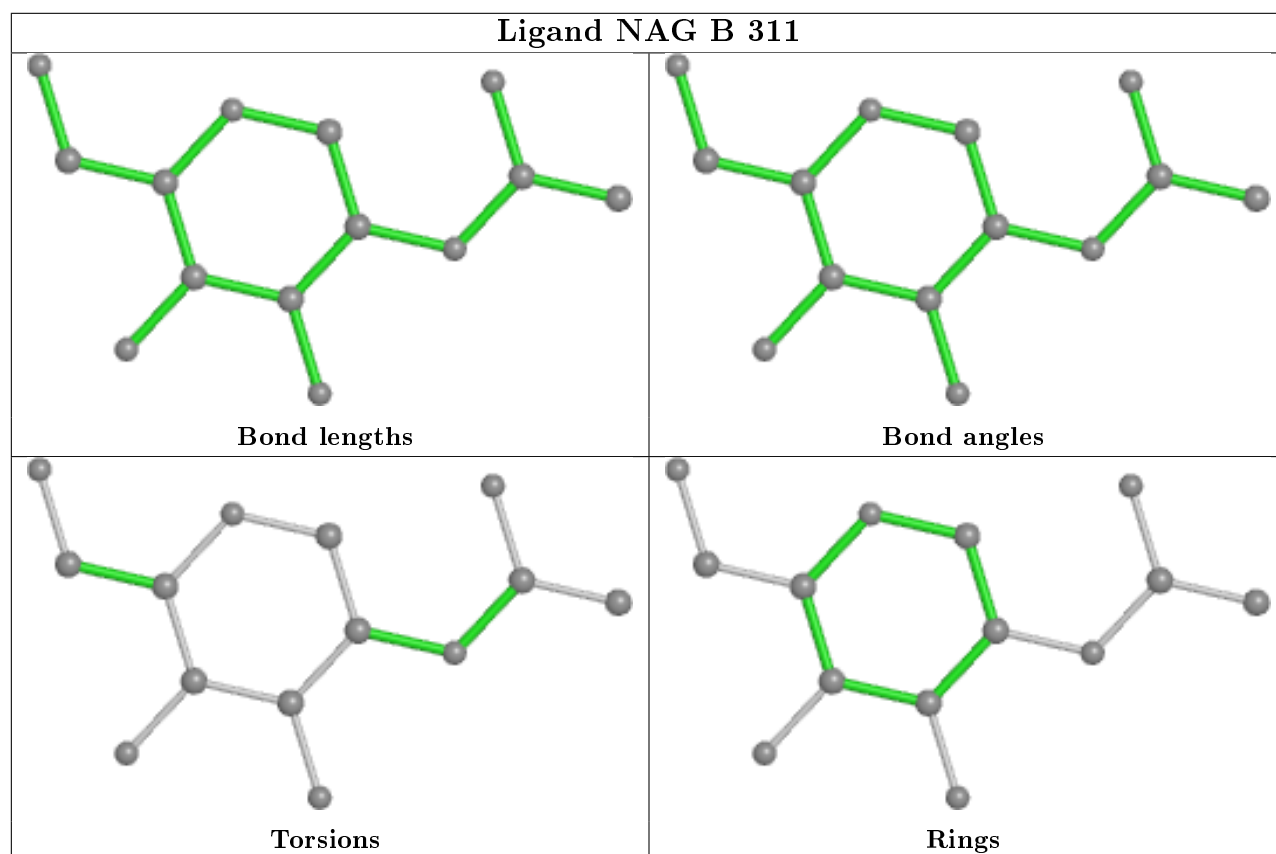
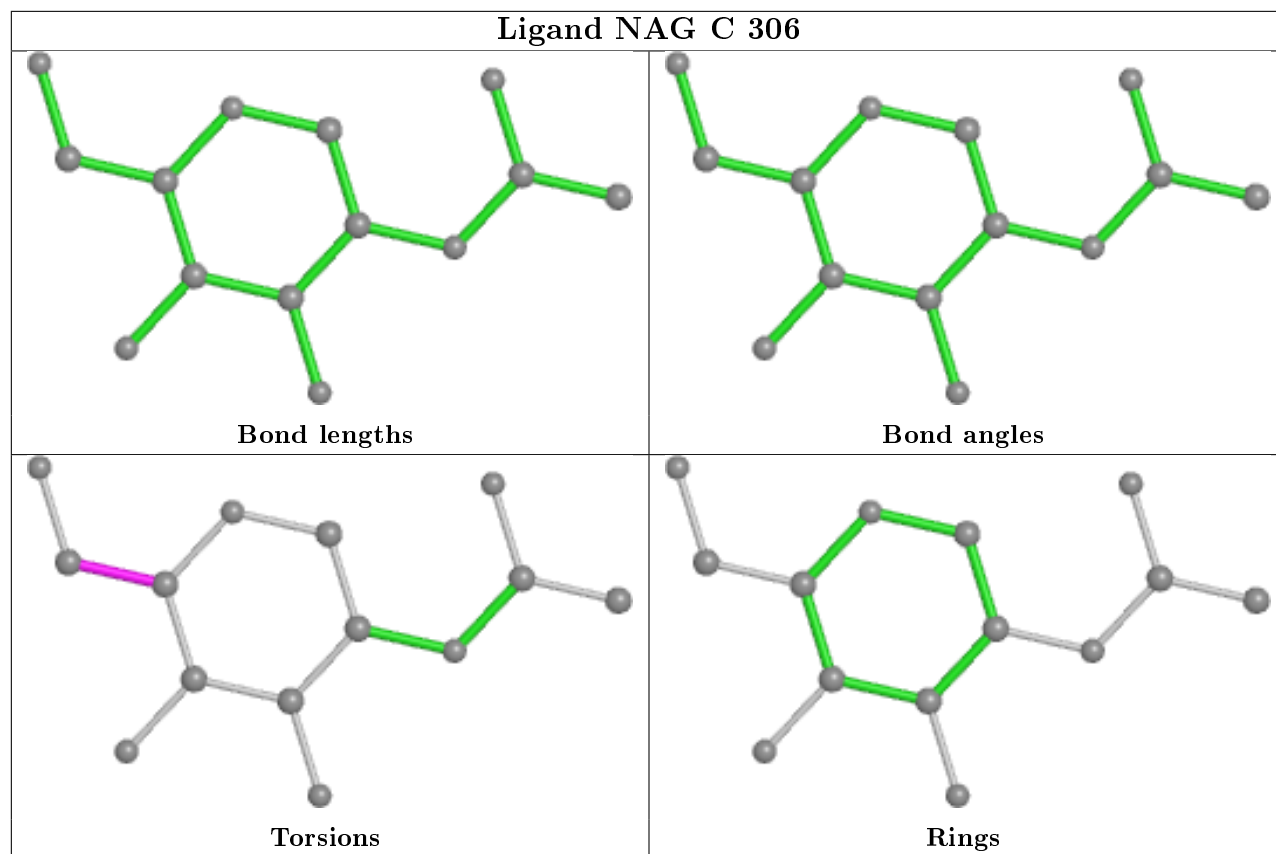
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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	188/259 (72%)	-0.07	1 (0%) 91 88	80, 136, 193, 230	0
1	B	181/259 (69%)	-0.08	2 (1%) 80 75	89, 146, 205, 246	0
1	C	189/259 (72%)	0.12	9 (4%) 30 27	97, 147, 213, 256	0
2	D	218/231 (94%)	-0.31	0 100 100	71, 104, 144, 180	0
2	F	218/231 (94%)	-0.21	0 100 100	86, 115, 153, 186	0
2	H	219/231 (94%)	-0.37	0 100 100	65, 103, 148, 181	0
3	E	212/217 (97%)	-0.34	0 100 100	71, 101, 153, 219	0
3	G	212/217 (97%)	-0.24	4 (1%) 66 61	80, 115, 155, 201	0
3	L	212/217 (97%)	-0.44	0 100 100	66, 93, 134, 175	0
4	a	153/180 (85%)	-0.29	0 100 100	78, 104, 175, 232	0
4	b	145/180 (80%)	-0.26	2 (1%) 75 69	85, 115, 180, 198	0
4	c	152/180 (84%)	-0.17	2 (1%) 77 71	82, 121, 205, 250	0
All	All	2299/2661 (86%)	-0.23	20 (0%) 84 79	65, 115, 185, 256	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	GLY	3.6
1	C	119	ASN	3.5
4	b	287	GLU	3.4
1	C	125	LYS	3.2
3	G	191	LYS	2.9

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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MAN	O	4	11/12	0.46	0.82	233,240,247,248	0
7	BMA	O	3	11/12	0.54	0.64	240,245,248,249	0
5	BMA	R	3	11/12	0.55	0.65	221,232,234,235	0
5	BMA	I	3	11/12	0.63	0.37	171,181,187,195	0
10	NAG	Y	2	14/15	0.65	0.56	159,174,184,186	0
9	MAN	U	4	11/12	0.67	0.48	159,176,186,187	0
10	NAG	V	2	14/15	0.70	0.59	168,194,201,201	0
9	BMA	U	3	11/12	0.70	0.27	162,173,176,178	0
10	FUC	Y	3	10/11	0.73	0.34	158,166,169,169	0
5	BMA	M	3	11/12	0.74	0.35	191,196,197,197	0
6	NAG	Q	2	14/15	0.75	0.40	166,190,201,203	0
5	BMA	P	3	11/12	0.76	0.30	151,173,178,188	0
8	MAN	T	5	11/12	0.77	0.42	195,199,205,206	0
6	NAG	J	2	14/15	0.77	0.47	162,173,184,191	0
5	NAG	M	2	14/15	0.77	0.30	169,182,192,194	0
6	NAG	S	2	14/15	0.77	0.37	180,195,201,204	0
7	MAN	W	4	11/12	0.78	0.33	167,178,183,186	0
9	MAN	U	5	11/12	0.78	0.24	147,170,178,188	0
5	NAG	R	2	14/15	0.79	0.56	217,226,235,236	0
7	BMA	W	3	11/12	0.79	0.39	167,177,183,184	0
7	NAG	O	2	14/15	0.80	0.45	211,221,226,239	0
10	FUC	e	3	10/11	0.81	0.36	123,147,152,158	0
6	NAG	K	2	14/15	0.81	0.47	196,207,218,220	0
6	NAG	S	1	14/15	0.81	0.28	154,169,197,200	0
5	NAG	I	2	14/15	0.81	0.24	137,151,177,177	0
6	NAG	N	2	14/15	0.83	0.42	175,185,195,203	0
10	NAG	Y	1	14/15	0.83	0.35	127,157,171,175	0
10	NAG	e	1	14/15	0.83	0.19	114,132,156,160	0
10	NAG	e	2	14/15	0.83	0.46	148,178,184,185	0
6	NAG	Q	1	14/15	0.84	0.32	137,169,181,185	0
10	NAG	V	1	14/15	0.84	0.20	99,136,160,183	0
6	NAG	X	2	14/15	0.85	0.39	154,168,172,174	0
7	BMA	Z	3	11/12	0.86	0.55	173,175,178,178	0
6	NAG	d	2	14/15	0.86	0.25	169,187,195,196	0
7	NAG	Z	2	14/15	0.86	0.33	136,153,166,167	0
7	NAG	Z	1	14/15	0.87	0.25	108,129,138,145	0

Continued on next page...

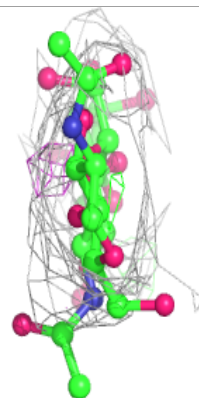
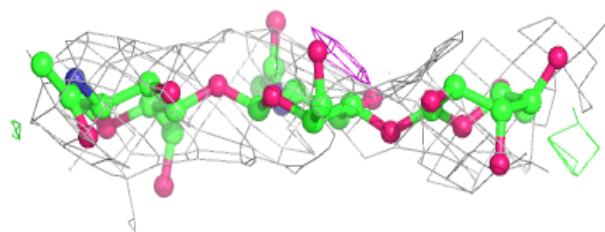
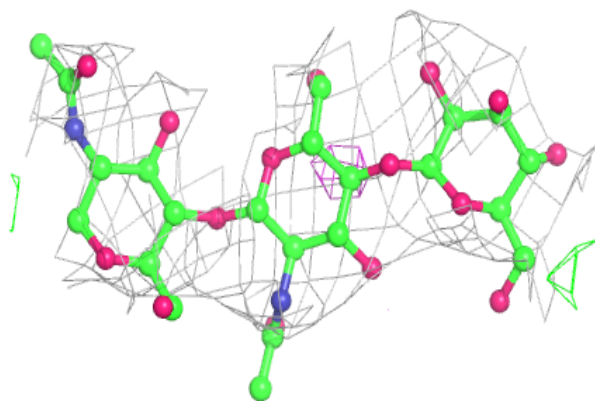
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MAN	T	4	11/12	0.88	0.33	149,171,186,193	0
6	NAG	X	1	14/15	0.88	0.30	116,136,163,163	0
10	FUC	V	3	10/11	0.88	0.21	137,150,156,160	0
7	NAG	O	1	14/15	0.89	0.26	187,192,203,203	0
9	NAG	U	2	14/15	0.89	0.27	134,163,173,176	0
8	BMA	T	3	11/12	0.89	0.33	155,173,178,181	0
5	NAG	R	1	14/15	0.89	0.25	191,193,201,211	0
8	NAG	T	2	14/15	0.90	0.22	138,147,154,155	0
8	NAG	T	1	14/15	0.90	0.24	89,114,125,132	0
6	NAG	N	1	14/15	0.90	0.29	130,140,151,166	0
7	MAN	Z	4	11/12	0.90	0.32	144,160,168,168	0
5	NAG	P	2	14/15	0.90	0.24	160,167,173,174	0
6	NAG	K	1	14/15	0.91	0.24	147,163,182,188	0
9	NAG	U	1	14/15	0.91	0.18	92,112,146,148	0
7	NAG	W	1	14/15	0.91	0.21	104,126,142,151	0
5	NAG	M	1	14/15	0.91	0.24	106,124,156,157	0
6	NAG	d	1	14/15	0.92	0.20	132,152,173,175	0
7	NAG	W	2	14/15	0.92	0.28	166,177,180,183	0
6	NAG	J	1	14/15	0.93	0.32	115,137,151,160	0
5	NAG	I	1	14/15	0.93	0.18	79,107,137,138	0
5	NAG	P	1	14/15	0.95	0.27	105,123,146,148	0

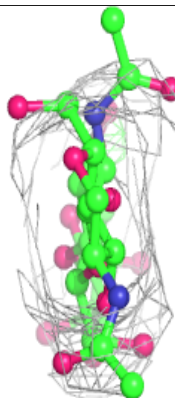
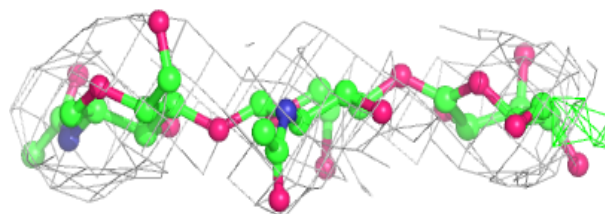
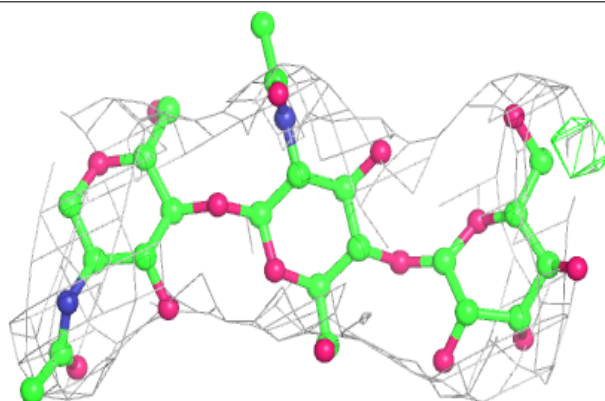
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

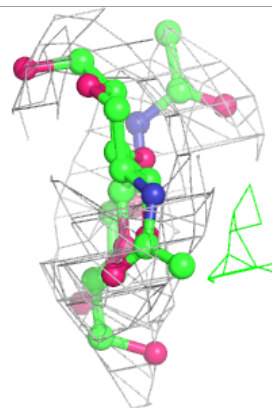
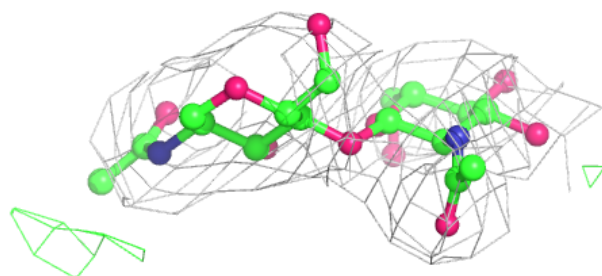
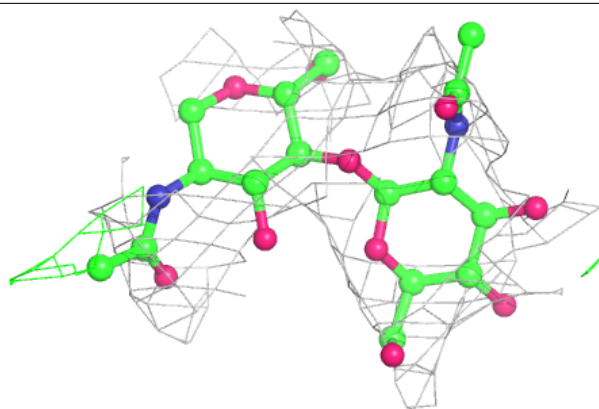
**Electron density around Chain P:**

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

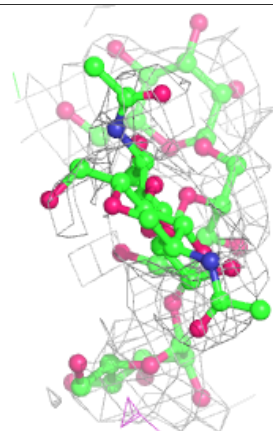
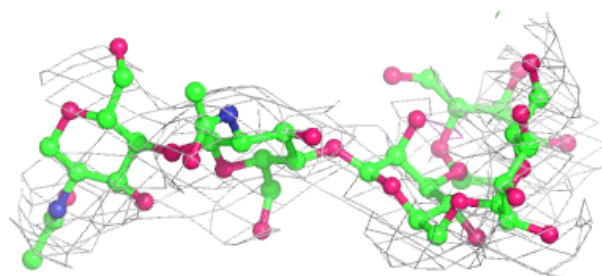
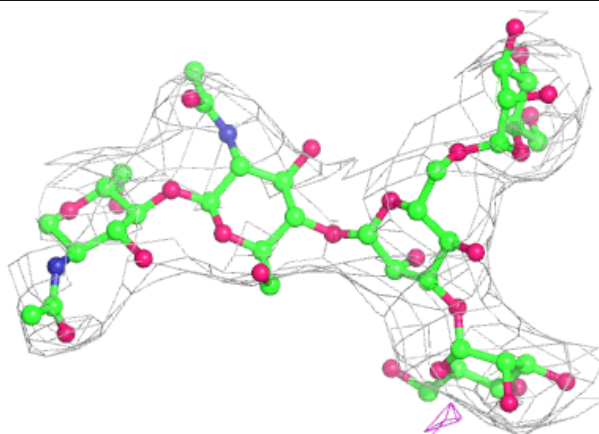


Electron density around Chain S:

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

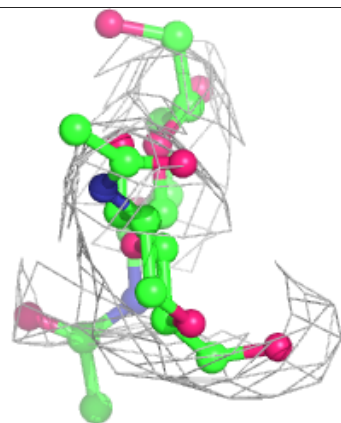
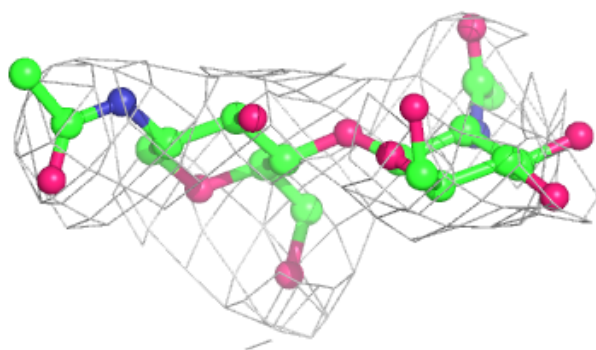
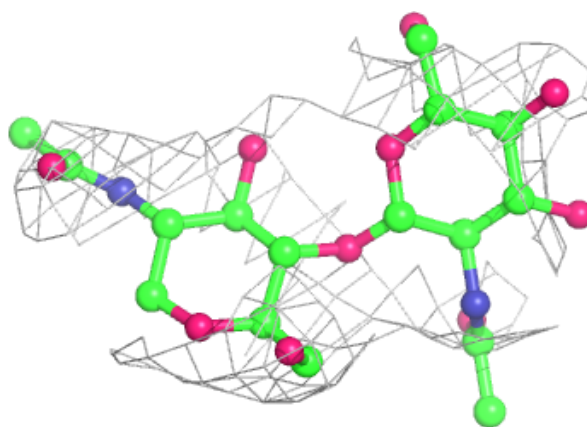
**Electron density around Chain U:**

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

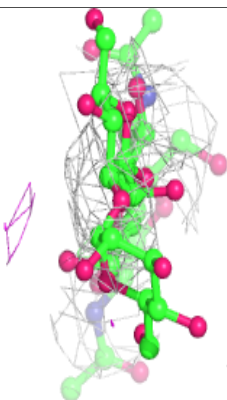
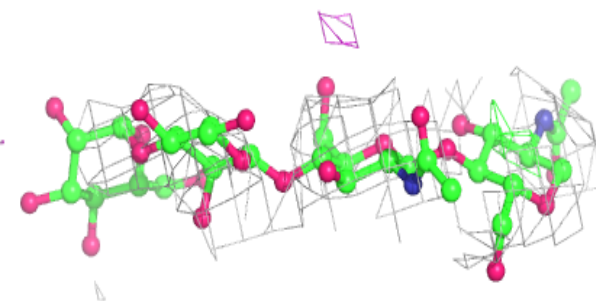
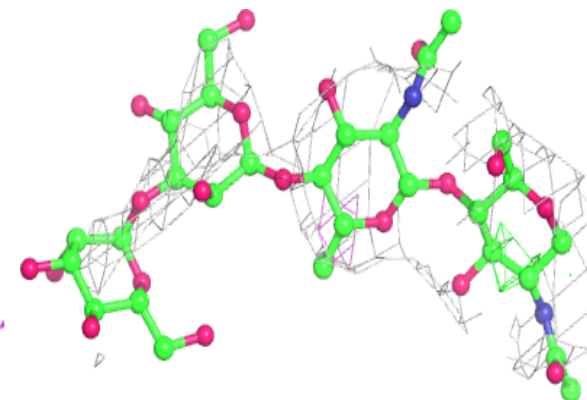


Electron density around Chain N:

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

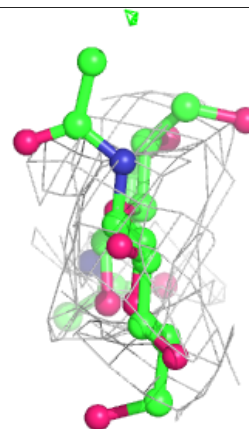
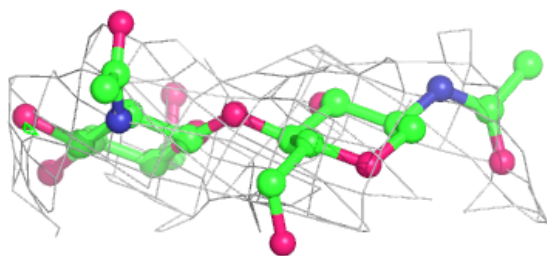
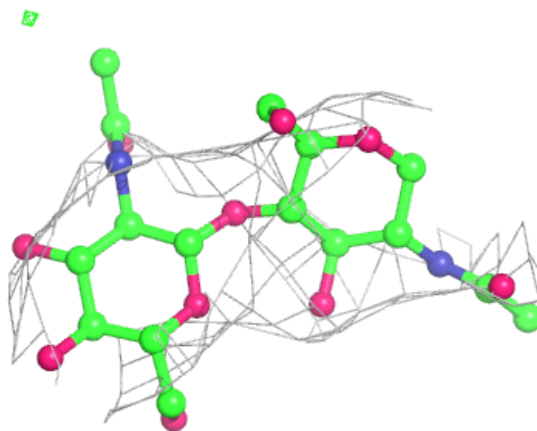
**Electron density around Chain O:**

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

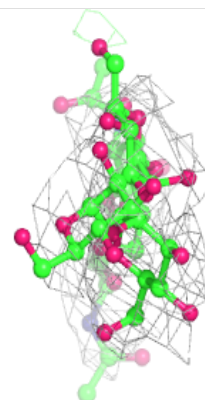
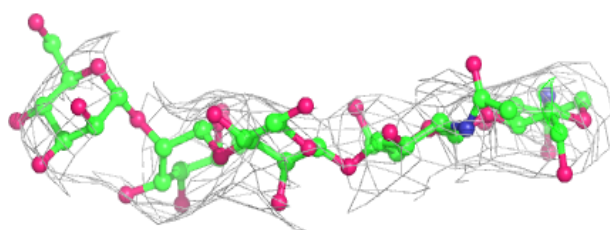
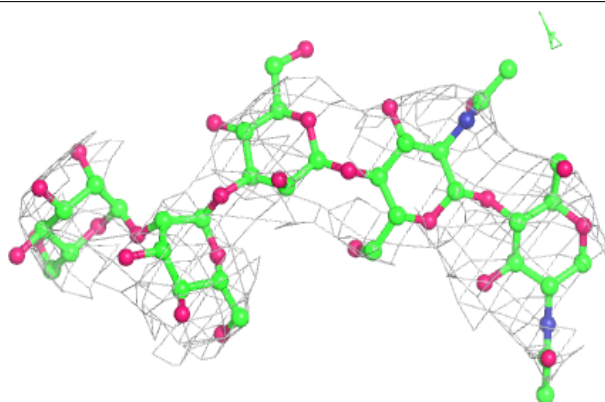


Electron density around Chain Q:

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

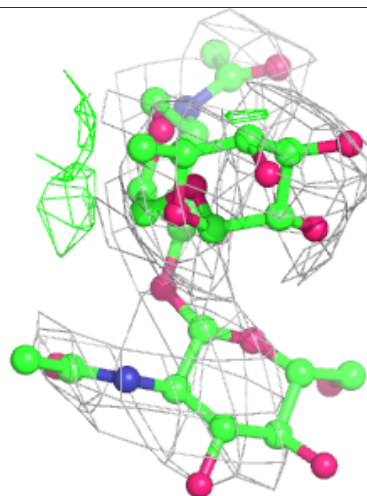
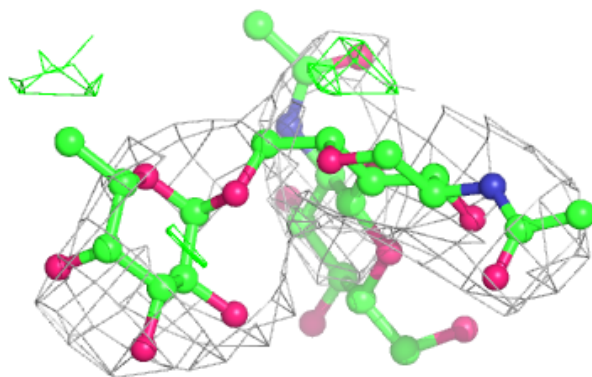
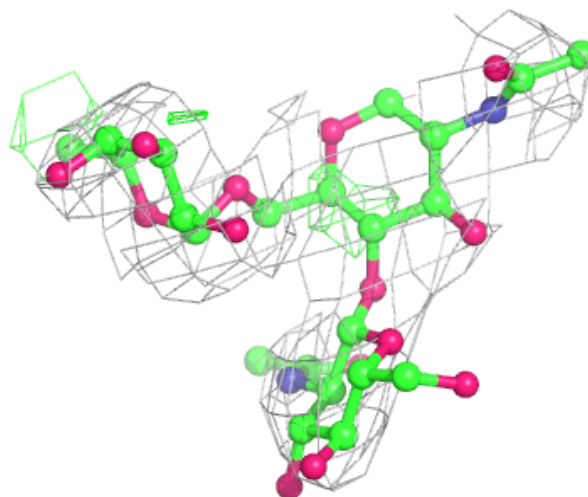
**Electron density around Chain T:**

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



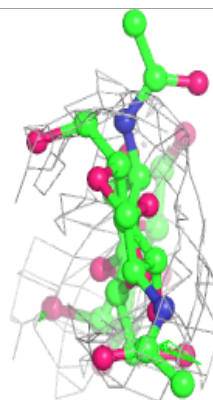
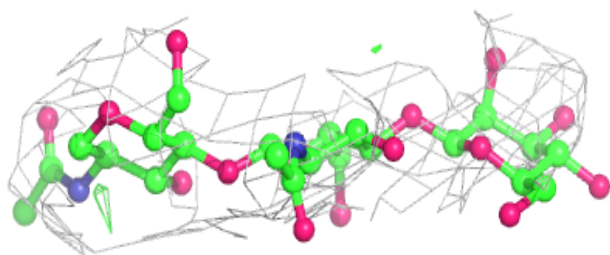
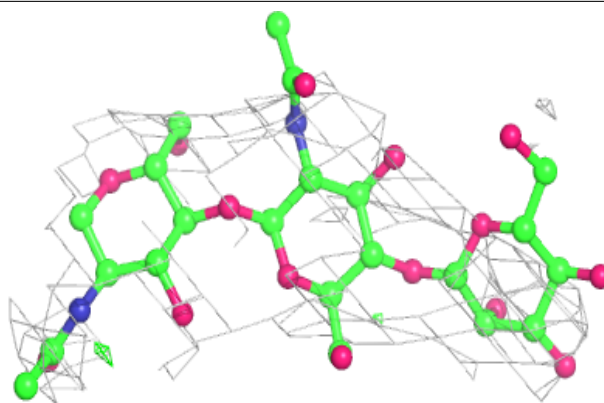
Electron density around Chain V:

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

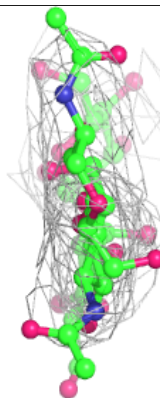
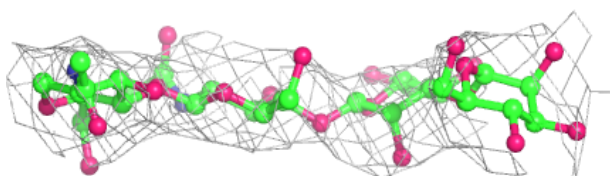
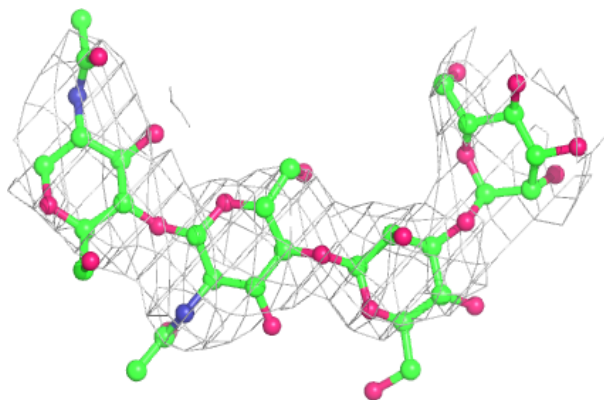


Electron density around Chain R:

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

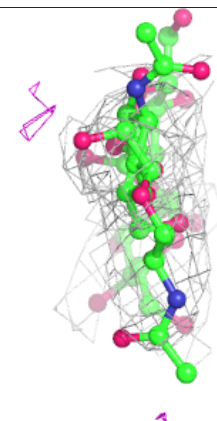
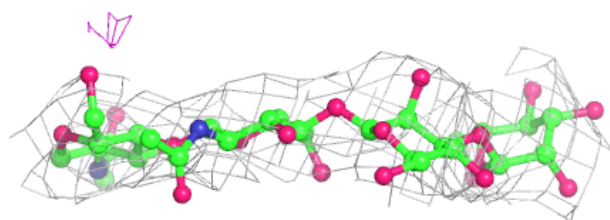
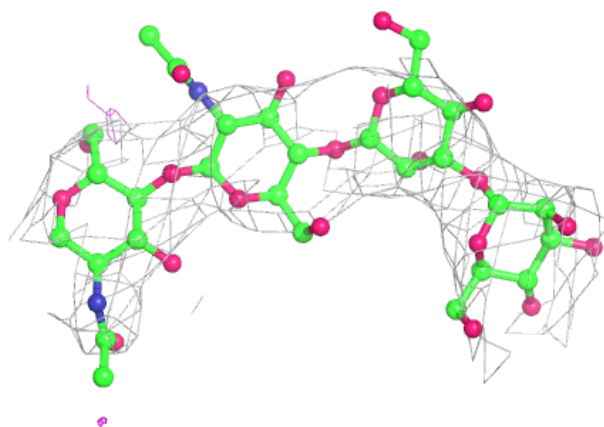
**Electron density around Chain Z:**

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

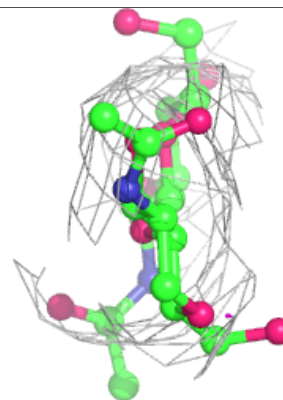
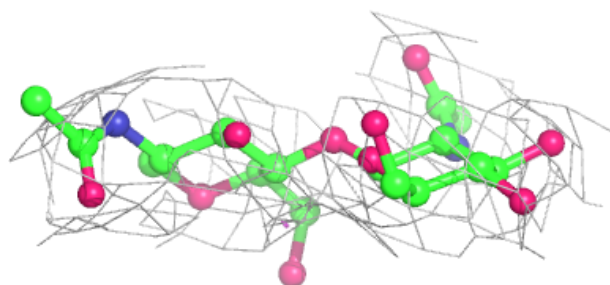
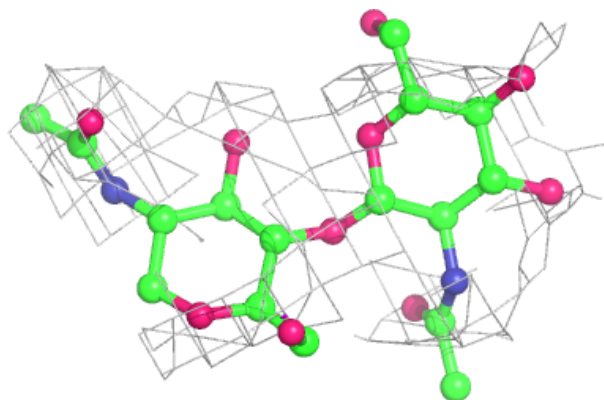


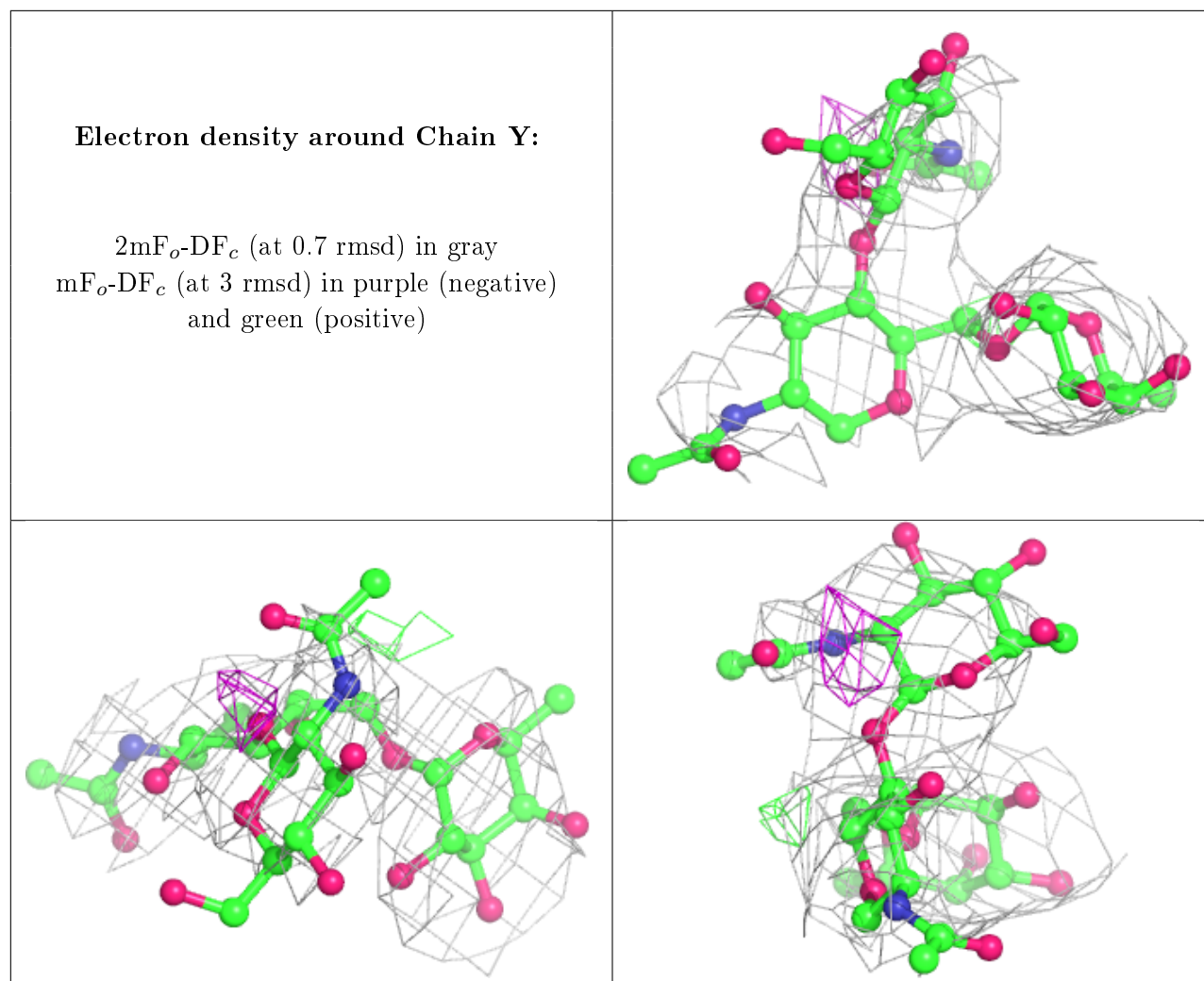
Electron density around Chain W:

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

**Electron density around Chain X:**

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





6.4 Ligands ⓘ

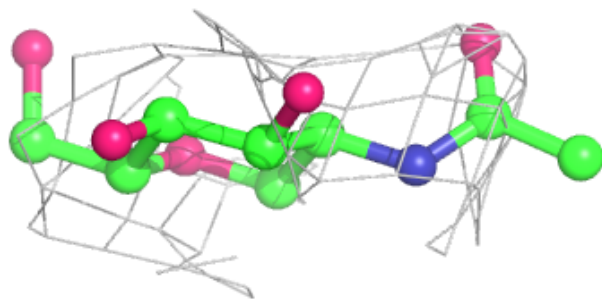
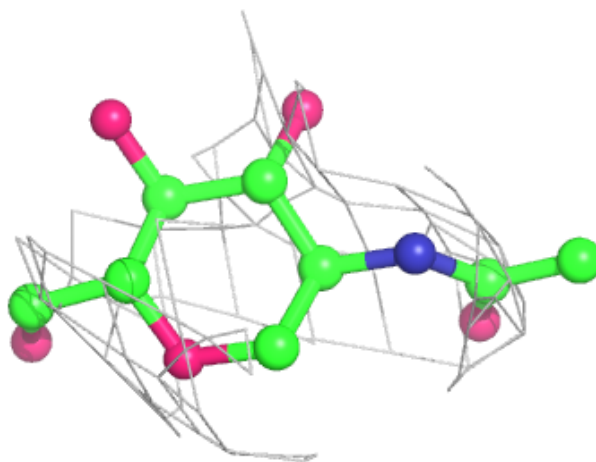
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	NAG	C	310	14/15	0.71	0.34	184,196,210,213	0
11	NAG	C	306	14/15	0.74	0.58	145,167,178,184	0
11	NAG	B	306	14/15	0.77	0.40	141,167,175,178	0
11	NAG	A	306	14/15	0.79	0.35	125,150,156,158	0
11	NAG	A	309	14/15	0.79	0.38	138,157,171,177	0
11	NAG	a	511	14/15	0.80	0.44	142,161,179,189	0
11	NAG	B	311	14/15	0.81	0.22	184,193,198,202	0
11	NAG	B	312	14/15	0.82	0.24	134,154,183,187	0
11	NAG	A	310	14/15	0.87	0.24	122,140,158,158	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

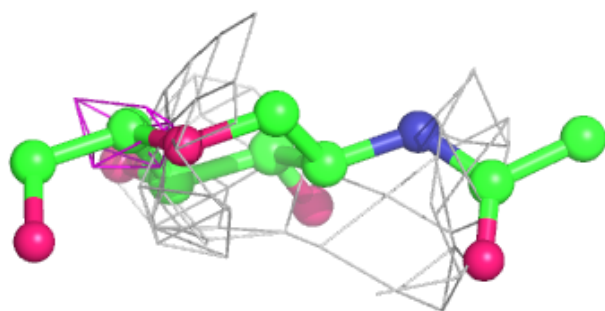
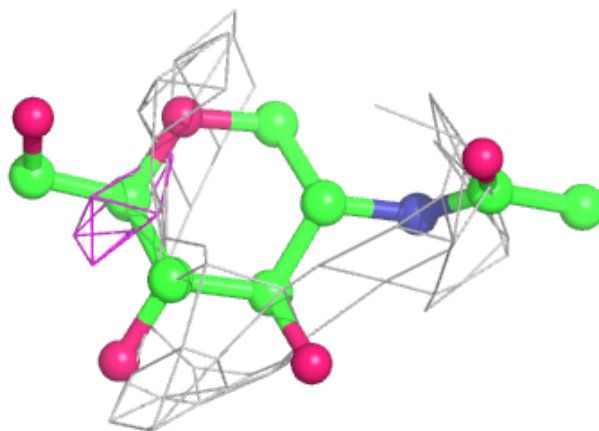
Electron density around NAG C 310:

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



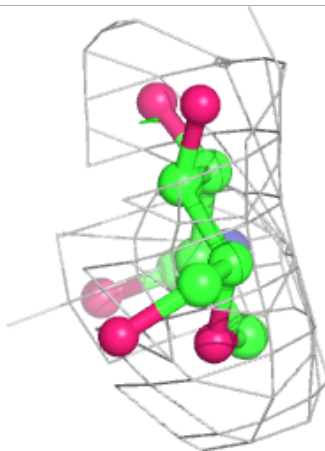
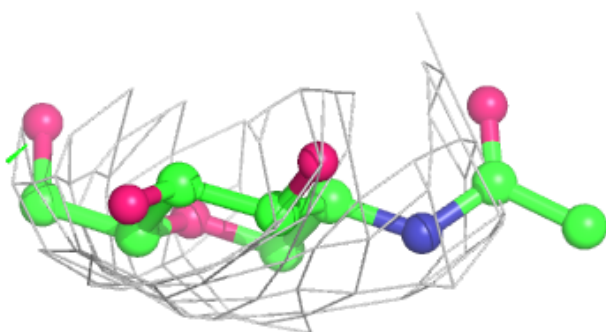
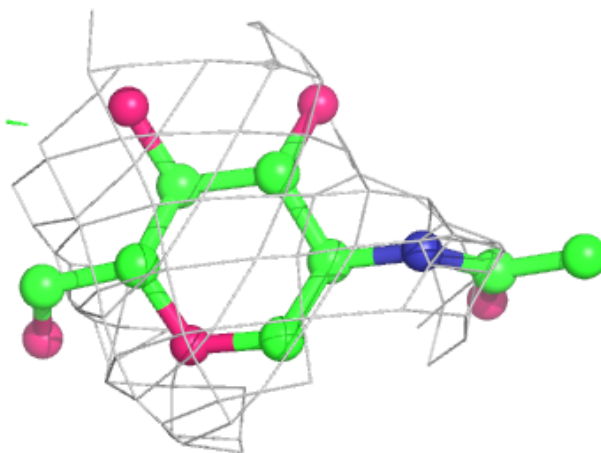
Electron density around NAG C 306:

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



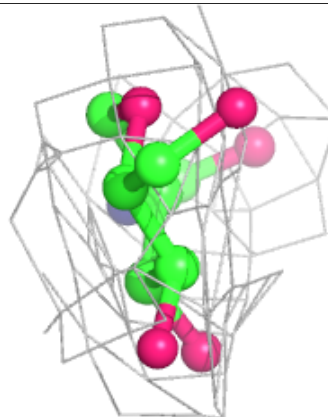
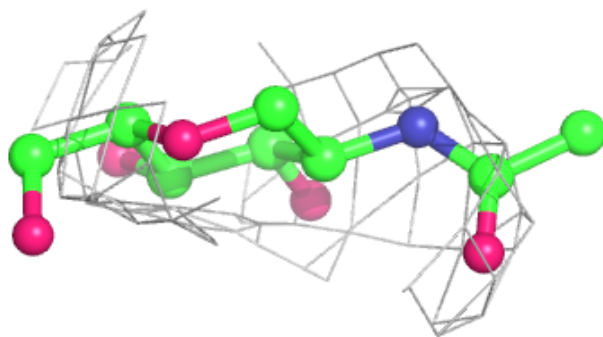
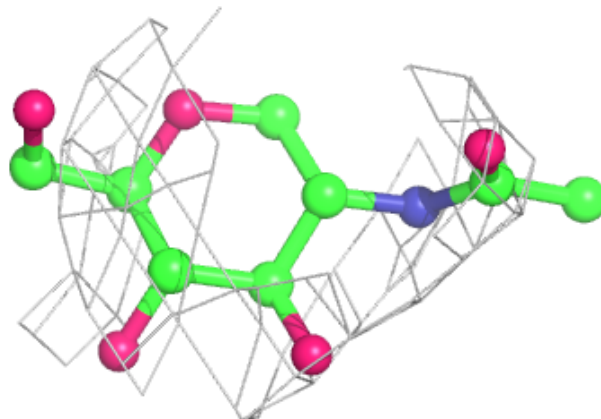
Electron density around NAG B 306:

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

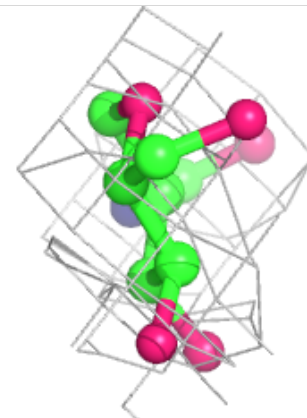
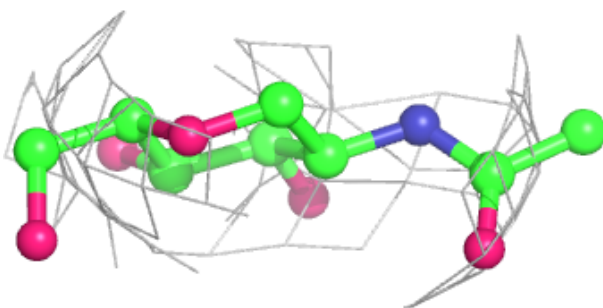
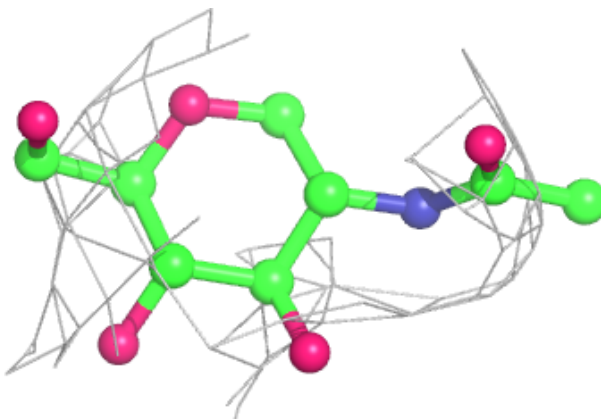


Electron density around NAG A 306:

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

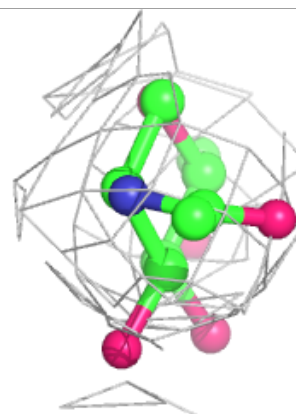
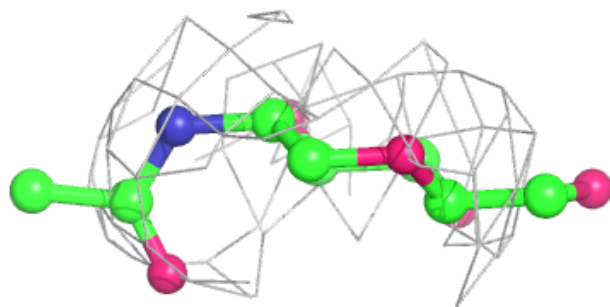
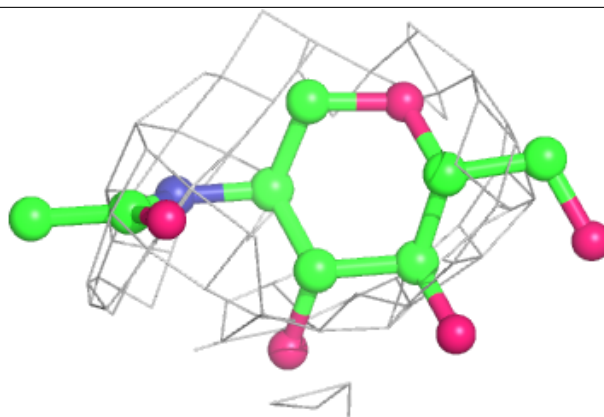
**Electron density around NAG A 309:**

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

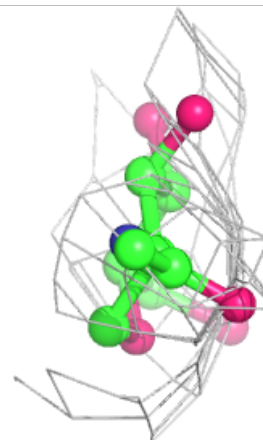
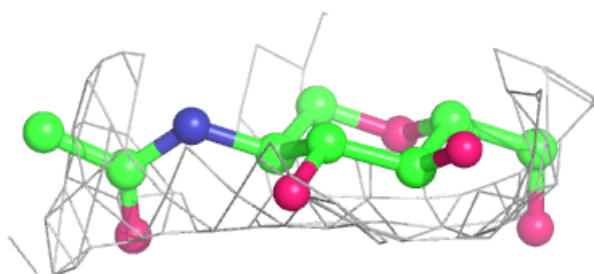
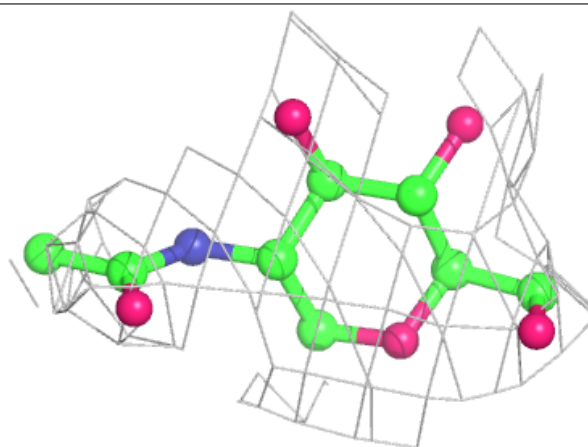


Electron density around NAG a 511:

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

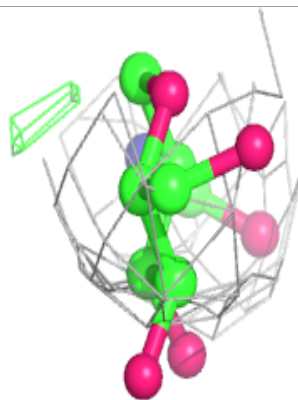
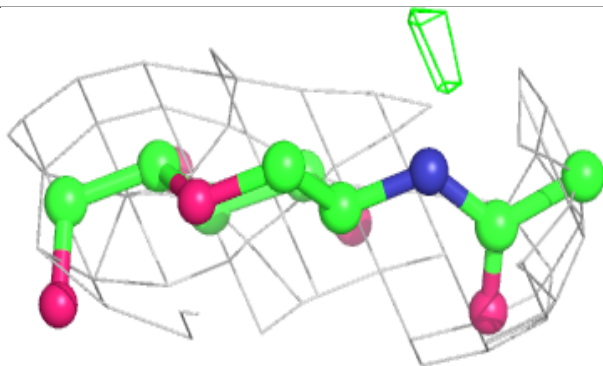
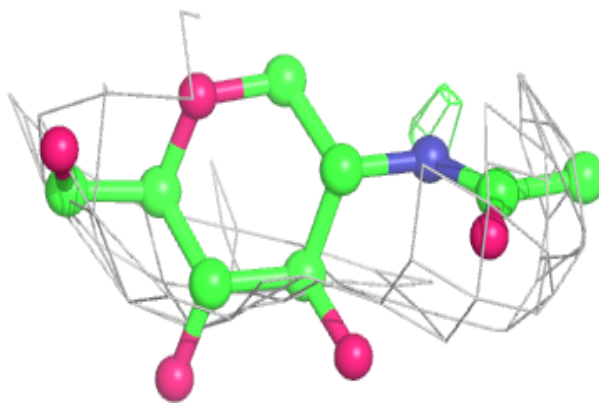
**Electron density around NAG B 311:**

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

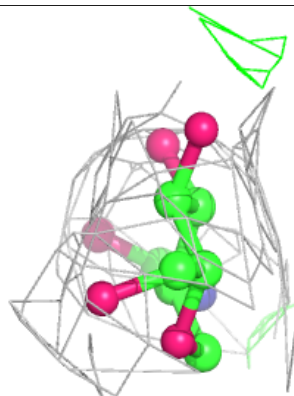
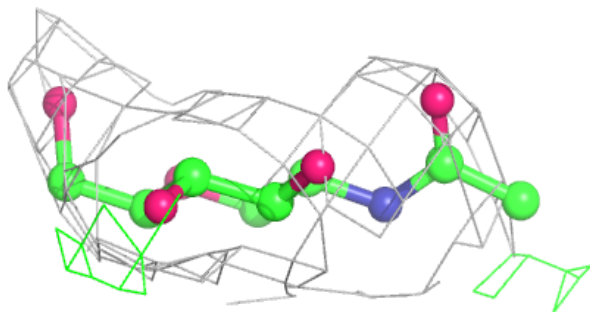
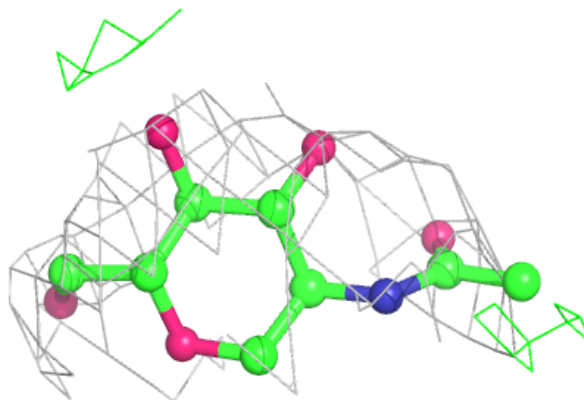


Electron density around NAG B 312:

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

**Electron density around NAG A 310:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.