



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:22 PM UTC

PDB ID : 9NRT / pdb\_00009nrt  
Title : Crystal structure of the H5 influenza virus hemagglutinin from A/duck/France/161108h/2016 (H5N8) clade 2.3.4.4b in complex with O-linked glycan 25  
Authors : Zhu, X.; Wilson, I.A.  
Deposited on : 2025-03-14  
Resolution : 1.98 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](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.

The types of validation reports are described at

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

---

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

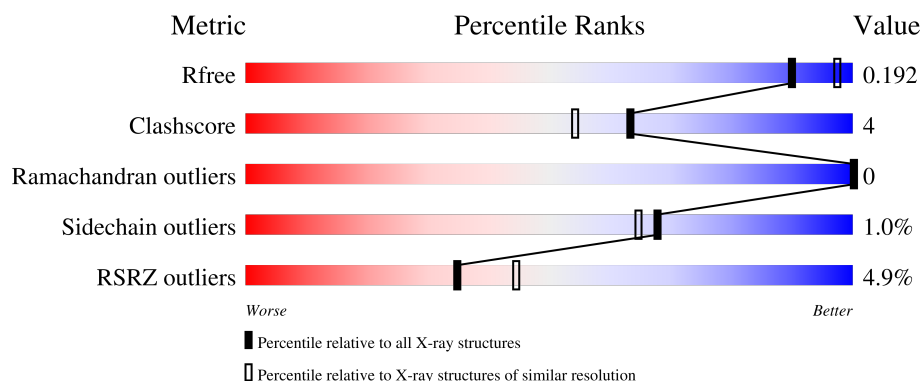
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	329	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>..</div> </div> </div>
1	C	329	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>..</div> </div> </div>
1	E	329	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>.</div> </div> </div>
2	B	181	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>7%</div> </div> </div>
2	D	181	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>• 7%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	181	
3	G	5	
3	H	5	
3	I	5	
3	J	5	
4	K	5	
5	L	3	
6	M	3	
6	O	3	
7	N	4	
8	P	3	
9	Q	4	
10	I	4	
11	R	2	
11	S	2	
11	T	2	
11	U	2	

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 14468 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2537	1605	442	476	14			
1	C	323	Total	C	N	O	S	0	0	0
			2555	1619	444	478	14			
1	E	321	Total	C	N	O	S	0	0	0
			2536	1604	442	476	14			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	-	expression tag	UNP A0A6M2RJB8
A	9	PRO	-	expression tag	UNP A0A6M2RJB8
A	10	GLY	-	expression tag	UNP A0A6M2RJB8
C	8	ASP	-	expression tag	UNP A0A6M2RJB8
C	9	PRO	-	expression tag	UNP A0A6M2RJB8
C	10	GLY	-	expression tag	UNP A0A6M2RJB8
E	8	ASP	-	expression tag	UNP A0A6M2RJB8
E	9	PRO	-	expression tag	UNP A0A6M2RJB8
E	10	GLY	-	expression tag	UNP A0A6M2RJB8

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1378	855	240	275	8			
2	D	169	Total	C	N	O	S	0	0	0
			1378	855	240	275	8			
2	F	172	Total	C	N	O	S	0	0	0
			1399	866	246	279	8			

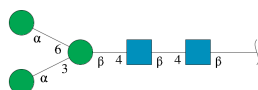
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A6M2RJB8
B	176	GLY	-	expression tag	UNP A0A6M2RJB8
B	177	ARG	-	expression tag	UNP A0A6M2RJB8
B	178	LEU	-	expression tag	UNP A0A6M2RJB8
B	179	VAL	-	expression tag	UNP A0A6M2RJB8
B	180	PRO	-	expression tag	UNP A0A6M2RJB8
B	181	ARG	-	expression tag	UNP A0A6M2RJB8
D	175	SER	-	expression tag	UNP A0A6M2RJB8
D	176	GLY	-	expression tag	UNP A0A6M2RJB8
D	177	ARG	-	expression tag	UNP A0A6M2RJB8
D	178	LEU	-	expression tag	UNP A0A6M2RJB8
D	179	VAL	-	expression tag	UNP A0A6M2RJB8
D	180	PRO	-	expression tag	UNP A0A6M2RJB8
D	181	ARG	-	expression tag	UNP A0A6M2RJB8
F	175	SER	-	expression tag	UNP A0A6M2RJB8
F	176	GLY	-	expression tag	UNP A0A6M2RJB8
F	177	ARG	-	expression tag	UNP A0A6M2RJB8
F	178	LEU	-	expression tag	UNP A0A6M2RJB8
F	179	VAL	-	expression tag	UNP A0A6M2RJB8
F	180	PRO	-	expression tag	UNP A0A6M2RJB8
F	181	ARG	-	expression tag	UNP A0A6M2RJB8

- Molecule 3 is a protein called Peptide linker.

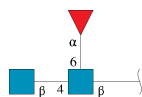
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	5	Total	C	N	O	0	0	0
			37	26	5	6			
3	H	5	Total	C	N	O	0	0	0
			37	26	5	6			
3	I	5	Total	C	N	O	0	0	0
			37	26	5	6			
3	J	5	Total	C	N	O	0	0	0
			37	26	5	6			

- Molecule 4 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.



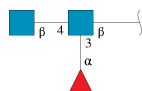
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	K	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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	L	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



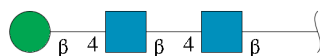
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	O	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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.



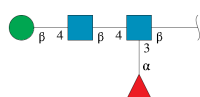
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	N	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



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

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



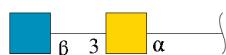
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	Q	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 10 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	4	Total	C	N	O	0	0	0
			59	33	3	23			

- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose.



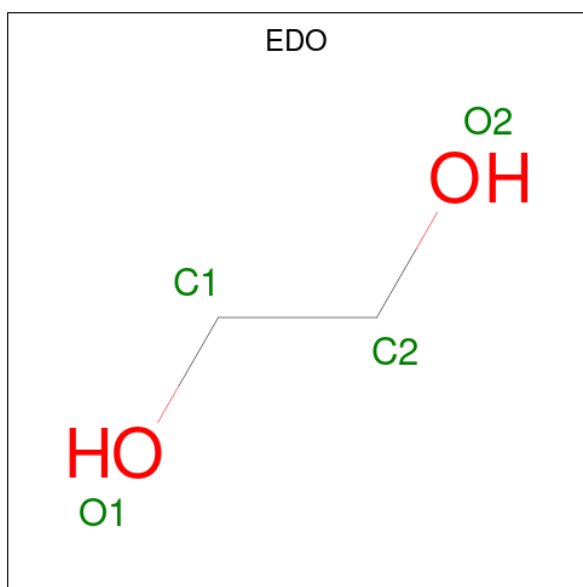
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
11	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
11	U	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 12 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		
12	A	1	Total	C	O	0	0
			4	2	2		
12	B	1	Total	C	O	0	0
			4	2	2		
12	B	1	Total	C	O	0	0
			4	2	2		

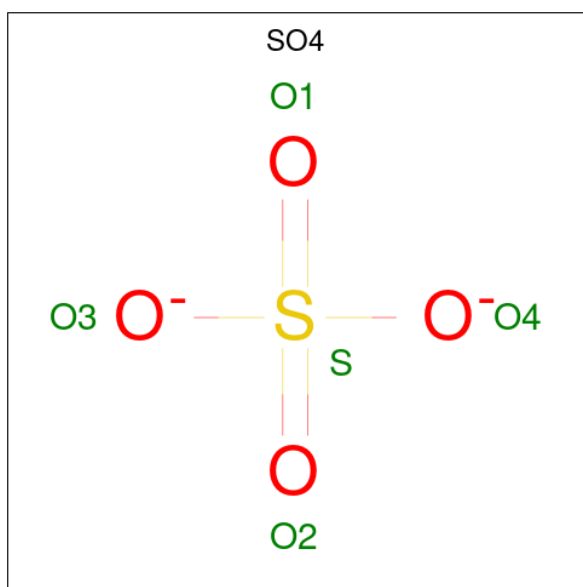
Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			4	2	2		
12	C	1	Total	C	O	0	0
			4	2	2		
12	C	1	Total	C	O	0	0
			4	2	2		
12	C	1	Total	C	O	0	0
			4	2	2		
12	C	1	Total	C	O	0	0
			4	2	2		
12	D	1	Total	C	O	0	0
			4	2	2		
12	E	1	Total	C	O	0	0
			4	2	2		
12	E	1	Total	C	O	0	0
			4	2	2		
12	E	1	Total	C	O	0	0
			4	2	2		
12	E	1	Total	C	O	0	0
			4	2	2		
12	E	1	Total	C	O	0	0
			4	2	2		
12	E	1	Total	C	O	0	0
			4	2	2		
12	E	1	Total	C	O	0	0
			4	2	2		
12	F	1	Total	C	O	0	0
			4	2	2		
12	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 13 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



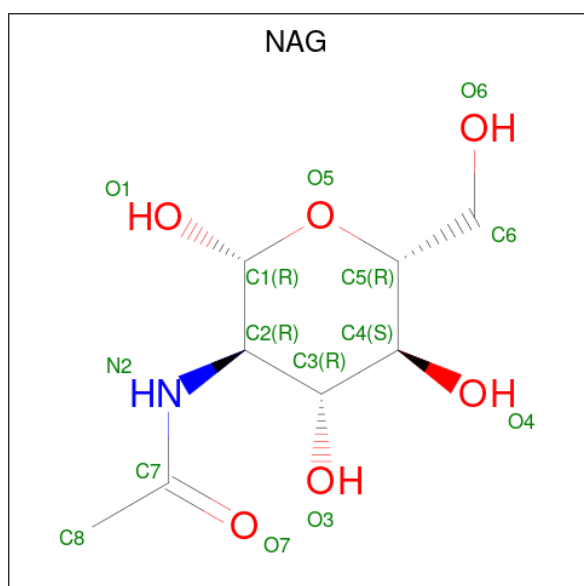
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	O	S	0	0
			5	4	1		
13	A	1	Total	O	S	0	0
			5	4	1		
13	A	1	Total	O	S	0	0
			5	4	1		
13	A	1	Total	O	S	0	0
			5	4	1		
13	A	1	Total	O	S	0	0
			5	4	1		
13	A	1	Total	O	S	0	0
			5	4	1		
13	A	1	Total	O	S	0	0
			5	4	1		
13	C	1	Total	O	S	0	0
			5	4	1		
13	C	1	Total	O	S	0	0
			5	4	1		
13	C	1	Total	O	S	0	0
			5	4	1		
13	C	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	O	S	0	0
			5	4	1		
13	C	1	Total	O	S	0	0
			5	4	1		
13	C	1	Total	O	S	0	0
			5	4	1		
13	C	1	Total	O	S	0	0
			5	4	1		
13	C	1	Total	O	S	0	0
			5	4	1		
13	E	1	Total	O	S	0	0
			5	4	1		
13	E	1	Total	O	S	0	0
			5	4	1		
13	E	1	Total	O	S	0	0
			5	4	1		
13	E	1	Total	O	S	0	0
			5	4	1		
13	E	1	Total	O	S	0	0
			5	4	1		
13	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



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

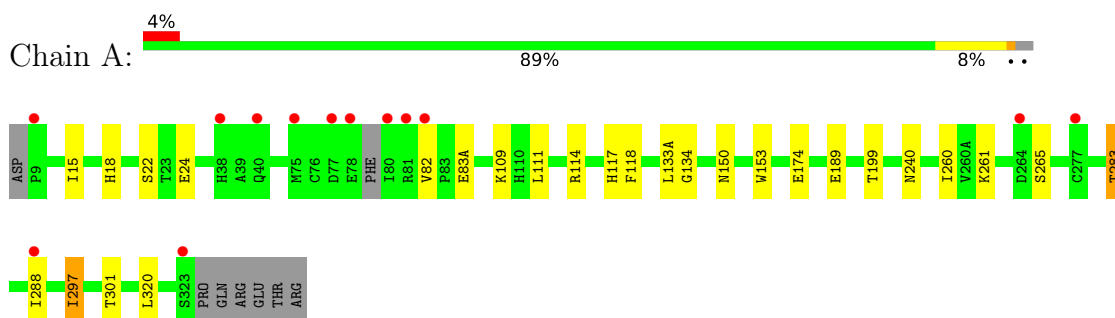
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	386	Total	O	0	0
			386	386		
15	B	176	Total	O	0	0
			176	176		
15	C	401	Total	O	0	0
			401	401		
15	D	158	Total	O	0	0
			158	158		
15	E	420	Total	O	0	0
			420	420		
15	F	231	Total	O	0	0
			231	231		
15	G	5	Total	O	0	0
			5	5		
15	H	7	Total	O	0	0
			7	7		
15	I	4	Total	O	0	0
			4	4		
15	J	3	Total	O	0	0
			3	3		

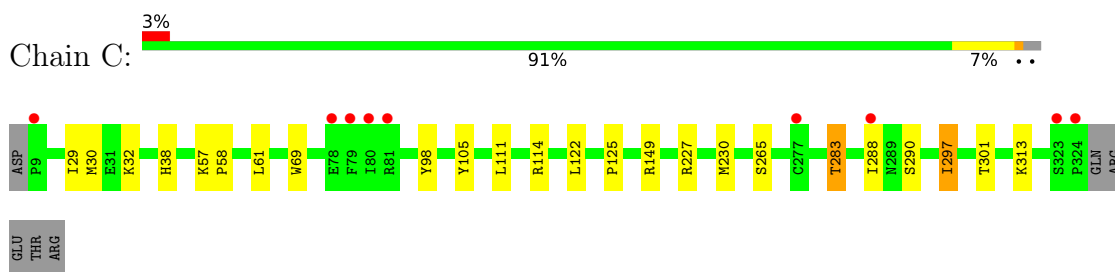
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

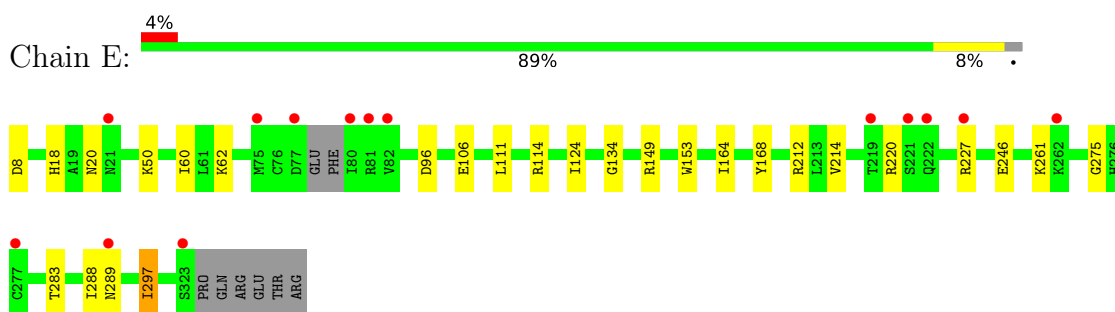
- Molecule 1: Hemagglutinin HA1 chain



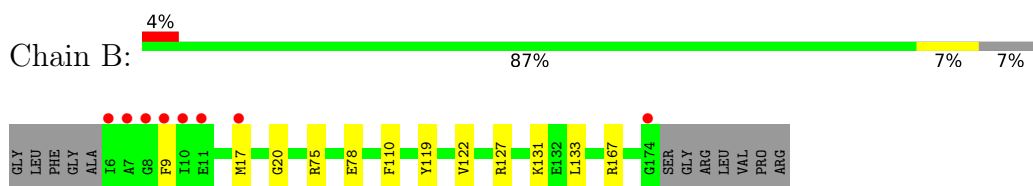
- Molecule 1: Hemagglutinin HA1 chain



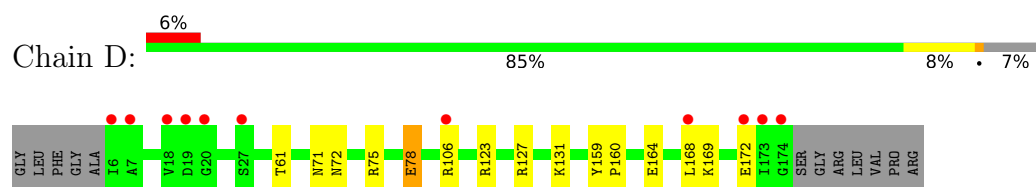
- Molecule 1: Hemagglutinin HA1 chain



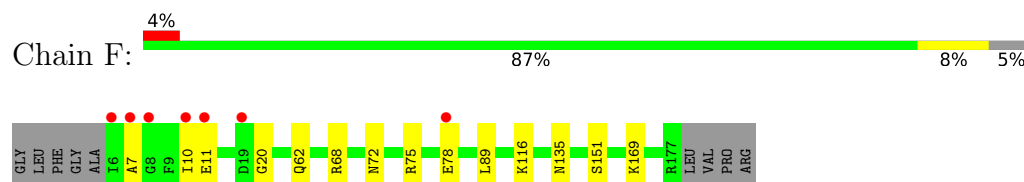
- Molecule 2: Hemagglutinin HA2 chain



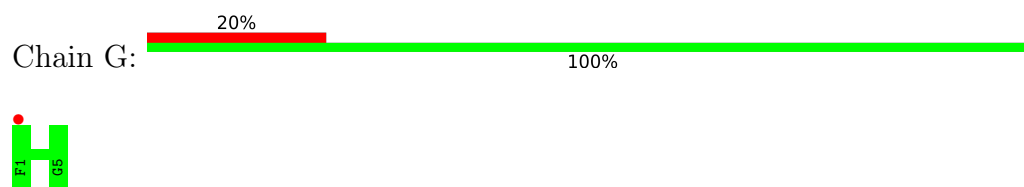
- Molecule 2: Hemagglutinin HA2 chain



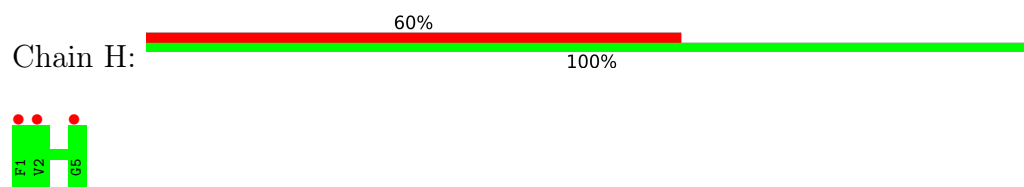
- Molecule 2: Hemagglutinin HA2 chain



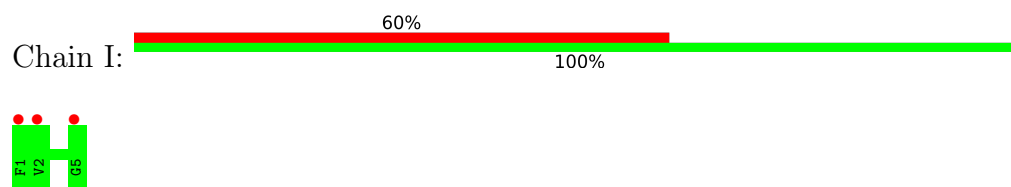
- Molecule 3: Peptide linker



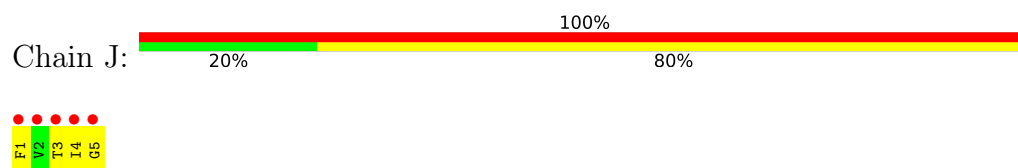
- Molecule 3: Peptide linker



- Molecule 3: Peptide linker



- Molecule 3: Peptide linker



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





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

Chain L:



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

Chain M:



- Molecule 6: alpha-L-fucopyranose-(1-3)-[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 N:



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

Chain P:



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

Chain Q:



- Molecule 10: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain I:  25% 50% 25%

A2G1  
NAG2  
GAL3  
STIA4

- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain R:  100%

A2G1  
NAG2

- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain S:  100%

A2G1  
NAG2

- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain T:  50% 50%

A2G1  
NAG2

- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain U:  100%

A2G1  
NAG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.17Å 171.62Å 226.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.87 – 1.98 43.87 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.5 (43.87-1.98) 99.0 (43.87-1.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.98Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5127: ???)	Depositor
R, $R_{free}$	0.165 , 0.189 0.170 , 0.192	Depositor DCC
$R_{free}$ test set	12588 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.4	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	0.96	EDS
Total number of atoms	14468	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, EDO, SO4, GAL, SIA, NAG, A2G, 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	0.29	0/2599	0.49	0/3533
1	C	0.32	0/2620	0.51	0/3564
1	E	0.31	0/2598	0.50	0/3533
2	B	0.28	0/1404	0.46	0/1887
2	D	0.24	0/1404	0.42	0/1887
2	F	0.28	0/1425	0.47	0/1914
3	G	0.22	0/37	0.46	0/49
3	H	0.20	0/37	0.33	0/49
3	I	0.18	0/37	0.29	0/49
3	J	0.34	0/37	0.60	0/49
All	All	0.29	0/12198	0.48	0/16514

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

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	2537	0	2492	19	0
1	C	2555	0	2509	21	0
1	E	2536	0	2489	24	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1378	0	1282	12	0
2	D	1378	0	1282	13	0
2	F	1399	0	1303	9	0
3	G	37	0	40	0	0
3	H	37	0	40	0	0
3	I	37	0	40	0	0
3	J	37	0	40	2	0
4	K	61	0	52	0	0
5	L	38	0	34	0	0
6	M	38	0	34	0	0
6	O	38	0	34	0	0
7	N	50	0	43	0	0
8	P	39	0	34	0	0
9	Q	49	0	43	2	0
10	I	59	0	49	1	0
11	R	28	0	24	0	0
11	S	28	0	24	0	0
11	T	28	0	24	0	0
11	U	28	0	24	0	0
12	A	24	0	36	2	0
12	B	8	0	12	2	0
12	C	24	0	36	3	0
12	D	4	0	6	2	0
12	E	36	0	54	9	0
12	F	8	0	12	3	0
13	A	50	0	0	0	0
13	C	45	0	0	4	0
13	E	35	0	0	2	0
14	C	14	0	13	1	0
14	E	14	0	13	0	0
15	A	386	0	0	3	0
15	B	176	0	0	3	0
15	C	401	0	0	10	0
15	D	158	0	0	2	0
15	E	420	0	0	6	0
15	F	231	0	0	1	0
15	G	5	0	0	0	0
15	H	7	0	0	0	0
15	I	4	0	0	0	0
15	J	3	0	0	0	0
All	All	14468	0	12118	99	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 99 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:D:75:ARG:HH12	2:D:78:GLU:CD	1.61	1.08
2:F:72:ASN:H	12:F:201:EDO:H11	1.38	0.87
2:D:75:ARG:NH1	2:D:78:GLU:CD	2.37	0.82
12:A:404:EDO:H21	12:A:405:EDO:H22	1.65	0.77
1:C:69:TRP:HD1	12:C:606:EDO:H21	1.50	0.76

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/329 (96%)	310 (98%)	7 (2%)	0	100	100
1	C	321/329 (98%)	311 (97%)	10 (3%)	0	100	100
1	E	317/329 (96%)	307 (97%)	10 (3%)	0	100	100
2	B	167/181 (92%)	164 (98%)	3 (2%)	0	100	100
2	D	167/181 (92%)	165 (99%)	2 (1%)	0	100	100
2	F	170/181 (94%)	169 (99%)	1 (1%)	0	100	100
3	G	3/5 (60%)	3 (100%)	0	0	100	100
3	H	3/5 (60%)	3 (100%)	0	0	100	100
3	I	3/5 (60%)	3 (100%)	0	0	100	100
3	J	3/5 (60%)	3 (100%)	0	0	100	100
All	All	1471/1550 (95%)	1438 (98%)	33 (2%)	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	286/294 (97%)	283 (99%)	3 (1%)	68	65
1	C	288/294 (98%)	286 (99%)	2 (1%)	76	73
1	E	286/294 (97%)	284 (99%)	2 (1%)	76	73
2	B	146/154 (95%)	146 (100%)	0	100	100
2	D	146/154 (95%)	145 (99%)	1 (1%)	76	73
2	F	148/154 (96%)	145 (98%)	3 (2%)	48	42
3	G	4/4 (100%)	4 (100%)	0	100	100
3	H	4/4 (100%)	4 (100%)	0	100	100
3	I	4/4 (100%)	4 (100%)	0	100	100
3	J	4/4 (100%)	2 (50%)	2 (50%)	0	0
All	All	1316/1360 (97%)	1303 (99%)	13 (1%)	68	65

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	297	ILE
2	F	62	GLN
3	J	3	THR
2	F	116	LYS
3	J	1	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	42	GLN
2	D	161	GLN
2	F	117	ASN
1	E	289	ASN
2	D	62	GLN

### 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 ⓘ

37 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	$\# Z  > 2$
4	NAG	K	1	4,1	14,14,15	0.74	0	17,19,21	1.00	2 (11%)
4	NAG	K	2	4	14,14,15	0.72	0	17,19,21	1.27	3 (17%)
4	BMA	K	3	4	11,11,12	0.81	0	15,15,17	1.66	3 (20%)
4	MAN	K	4	4	11,11,12	0.67	0	15,15,17	1.33	1 (6%)
4	MAN	K	5	4	11,11,12	0.69	0	15,15,17	1.59	1 (6%)
5	NAG	L	1	5,1	14,14,15	0.74	0	17,19,21	1.10	1 (5%)
5	NAG	L	2	5	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
5	FUC	L	3	5	10,10,11	0.75	0	14,14,16	0.94	0
6	NAG	M	1	6,2	14,14,15	0.80	0	17,19,21	1.09	1 (5%)
6	FUC	M	2	6	10,10,11	0.74	0	14,14,16	1.18	1 (7%)
6	NAG	M	3	6	14,14,15	0.74	0	17,19,21	0.78	0
7	NAG	N	1	7,1	14,14,15	0.81	0	17,19,21	1.57	1 (5%)
7	NAG	N	2	7	14,14,15	0.76	0	17,19,21	1.24	2 (11%)
7	BMA	N	3	7	11,11,12	0.85	0	15,15,17	1.58	4 (26%)
7	MAN	N	4	7	11,11,12	0.68	0	15,15,17	1.45	1 (6%)
6	NAG	O	1	6,2	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
6	FUC	O	2	6	10,10,11	0.65	0	14,14,16	1.28	1 (7%)
6	NAG	O	3	6	14,14,15	0.74	0	17,19,21	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	P	1	8,1	14,14,15	0.75	0	17,19,21	1.24	1 (5%)
8	NAG	P	2	8	14,14,15	0.74	0	17,19,21	1.06	0
8	BMA	P	3	8	11,11,12	0.84	0	15,15,17	1.71	3 (20%)
9	NAG	Q	1	9,2	14,14,15	0.81	0	17,19,21	0.84	0
9	NAG	Q	2	9	14,14,15	0.72	0	17,19,21	1.05	0
9	BMA	Q	3	9	11,11,12	0.85	0	15,15,17	2.01	3 (20%)
9	FUC	Q	4	9	10,10,11	0.68	0	14,14,16	1.17	1 (7%)
11	A2G	R	1	11,3	14,14,15	0.77	0	17,19,21	0.72	0
11	NAG	R	2	11	14,14,15	0.69	0	17,19,21	0.98	0
11	A2G	S	1	11,3	14,14,15	0.77	0	17,19,21	0.94	0
11	NAG	S	2	11	14,14,15	0.70	0	17,19,21	0.78	0
11	A2G	T	1	11,3	14,14,15	0.77	0	17,19,21	0.84	0
11	NAG	T	2	11	14,14,15	0.76	0	17,19,21	1.01	1 (5%)
11	A2G	U	1	11,3	14,14,15	0.82	0	17,19,21	1.03	1 (5%)
11	NAG	U	2	11	14,14,15	0.67	0	17,19,21	1.15	1 (5%)
10	A2G	l	1	10	14,14,15	0.82	0	17,19,21	0.89	0
10	NAG	l	2	10	14,14,15	0.65	0	17,19,21	1.08	1 (5%)
10	GAL	l	3	10	11,11,12	0.68	0	15,15,17	1.11	1 (6%)
10	SIA	l	4	10	20,20,21	1.85	3 (15%)	21,28,31	1.72	3 (14%)

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
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	BMA	K	3	4	-	1/2/19/22	0/1/1/1
4	MAN	K	4	4	-	2/2/19/22	0/1/1/1
4	MAN	K	5	4	-	0/2/19/22	0/1/1/1
5	NAG	L	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	1/6/23/26	0/1/1/1
5	FUC	L	3	5	-	-	0/1/1/1
6	NAG	M	1	6,2	-	0/6/23/26	0/1/1/1
6	FUC	M	2	6	-	-	0/1/1/1
6	NAG	M	3	6	-	0/6/23/26	0/1/1/1
7	NAG	N	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1
7	BMA	N	3	7	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	N	4	7	-	1/2/19/22	0/1/1/1
6	NAG	O	1	6,2	-	0/6/23/26	0/1/1/1
6	FUC	O	2	6	-	-	0/1/1/1
6	NAG	O	3	6	-	2/6/23/26	0/1/1/1
8	NAG	P	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	P	2	8	-	2/6/23/26	0/1/1/1
8	BMA	P	3	8	-	0/2/19/22	0/1/1/1
9	NAG	Q	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	2/6/23/26	0/1/1/1
9	BMA	Q	3	9	-	2/2/19/22	0/1/1/1
9	FUC	Q	4	9	-	-	0/1/1/1
11	A2G	R	1	11,3	-	0/6/23/26	0/1/1/1
11	NAG	R	2	11	-	0/6/23/26	0/1/1/1
11	A2G	S	1	11,3	-	0/6/23/26	0/1/1/1
11	NAG	S	2	11	-	1/6/23/26	0/1/1/1
11	A2G	T	1	11,3	-	0/6/23/26	0/1/1/1
11	NAG	T	2	11	-	2/6/23/26	0/1/1/1
11	A2G	U	1	11,3	-	1/6/23/26	0/1/1/1
11	NAG	U	2	11	-	2/6/23/26	0/1/1/1
10	A2G	l	1	10	-	2/6/23/26	0/1/1/1
10	NAG	l	2	10	-	0/6/23/26	0/1/1/1
10	GAL	l	3	10	-	0/2/19/22	0/1/1/1
10	SIA	l	4	10	-	0/18/34/38	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	l	4	SIA	C2-C1	6.10	1.59	1.52
10	l	4	SIA	C7-C6	3.17	1.56	1.52
10	l	4	SIA	O6-C2	2.47	1.48	1.43

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	3	BMA	C1-O5-C5	5.92	120.11	112.19
4	K	5	MAN	C1-O5-C5	5.09	119.01	112.19
7	N	1	NAG	C1-O5-C5	4.88	118.73	112.19
7	N	4	MAN	C1-O5-C5	4.50	118.22	112.19
8	P	3	BMA	C1-O5-C5	4.32	117.97	112.19

There are no chirality outliers.



5 of 25 torsion outliers are listed below:

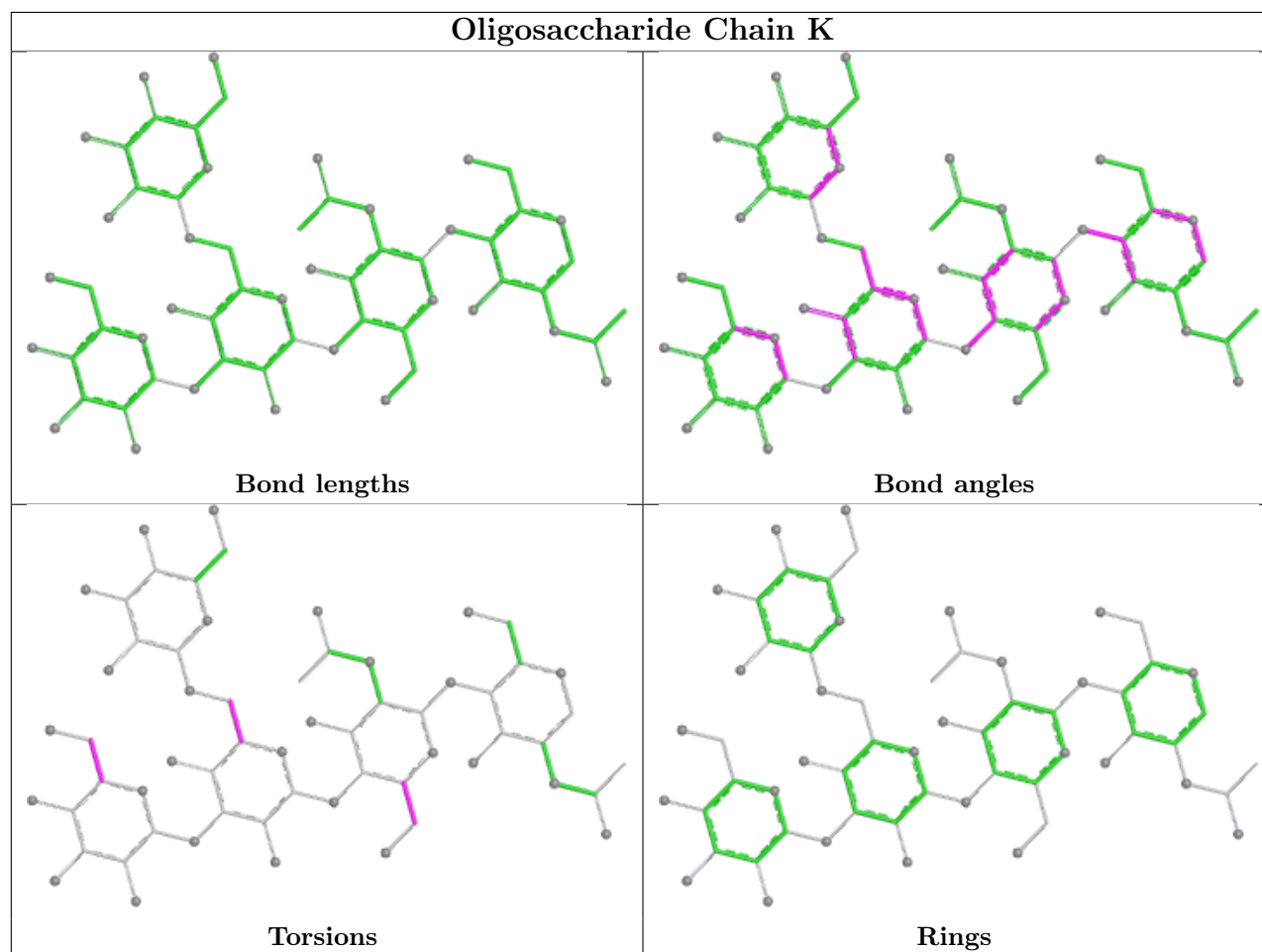
Mol	Chain	Res	Type	Atoms
7	N	3	BMA	O5-C5-C6-O6
6	O	3	NAG	O5-C5-C6-O6
9	Q	3	BMA	O5-C5-C6-O6
9	Q	2	NAG	C4-C5-C6-O6
9	Q	2	NAG	O5-C5-C6-O6

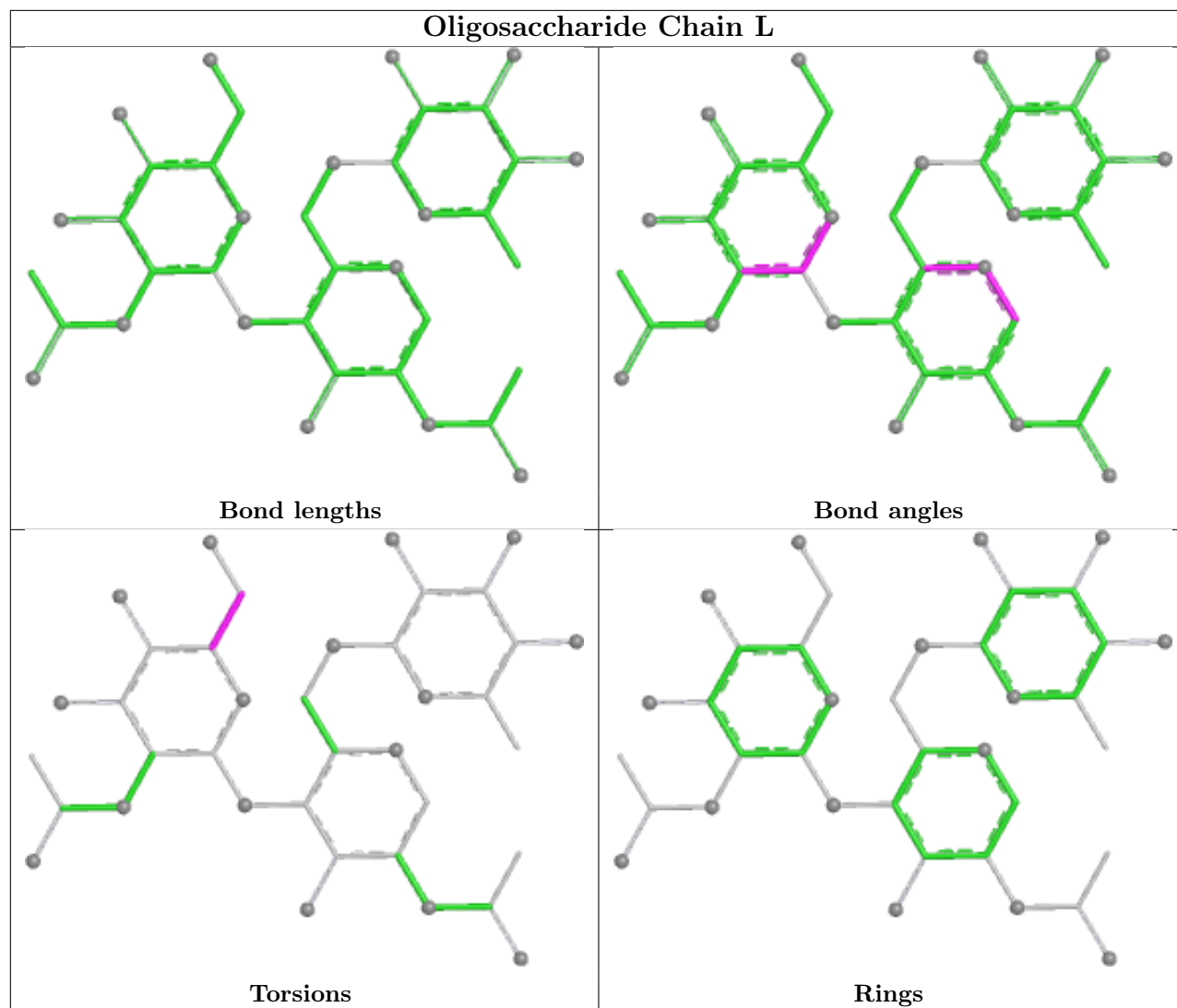
There are no ring outliers.

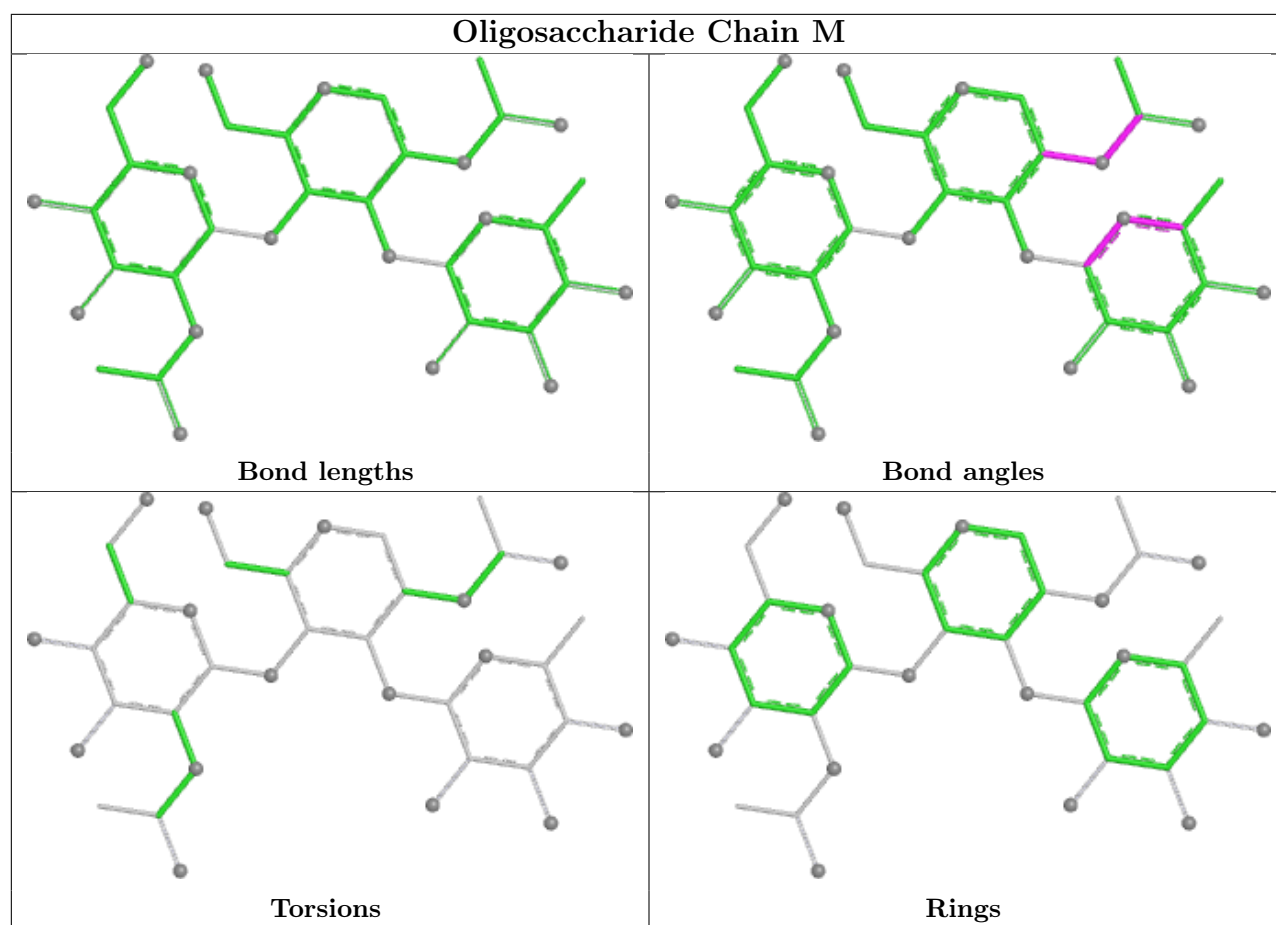
4 monomers are involved in 3 short contacts:

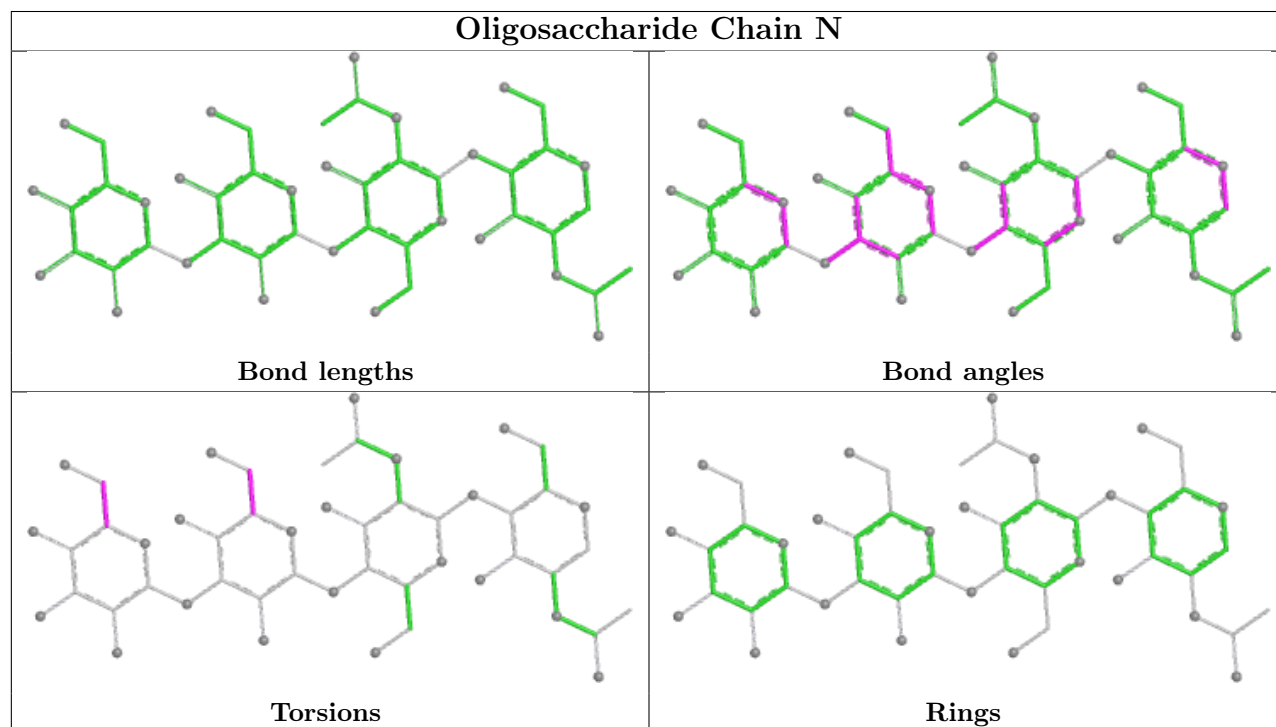
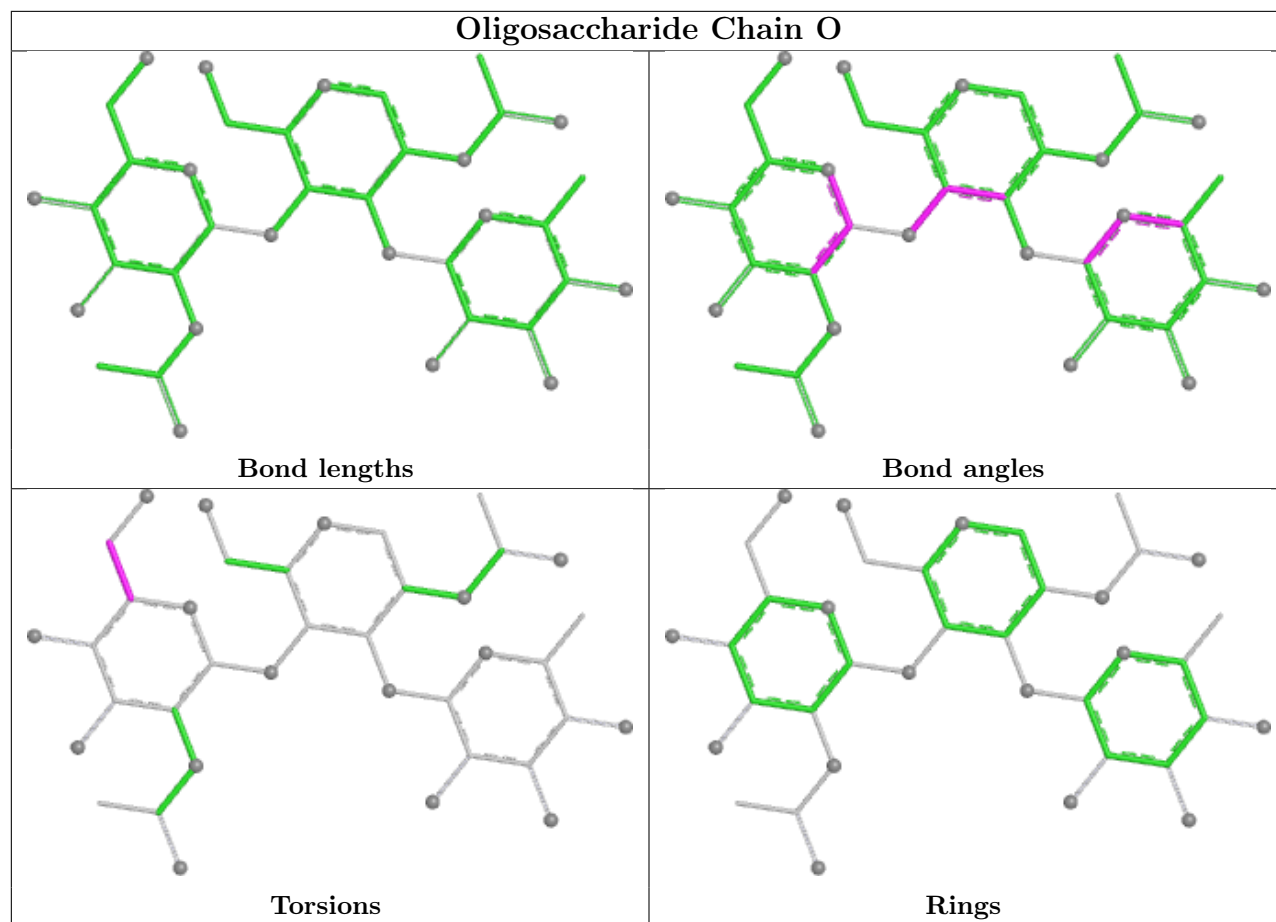
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Q	4	FUC	1	0
9	Q	1	NAG	1	0
10	1	4	SIA	1	0
9	Q	2	NAG	1	0

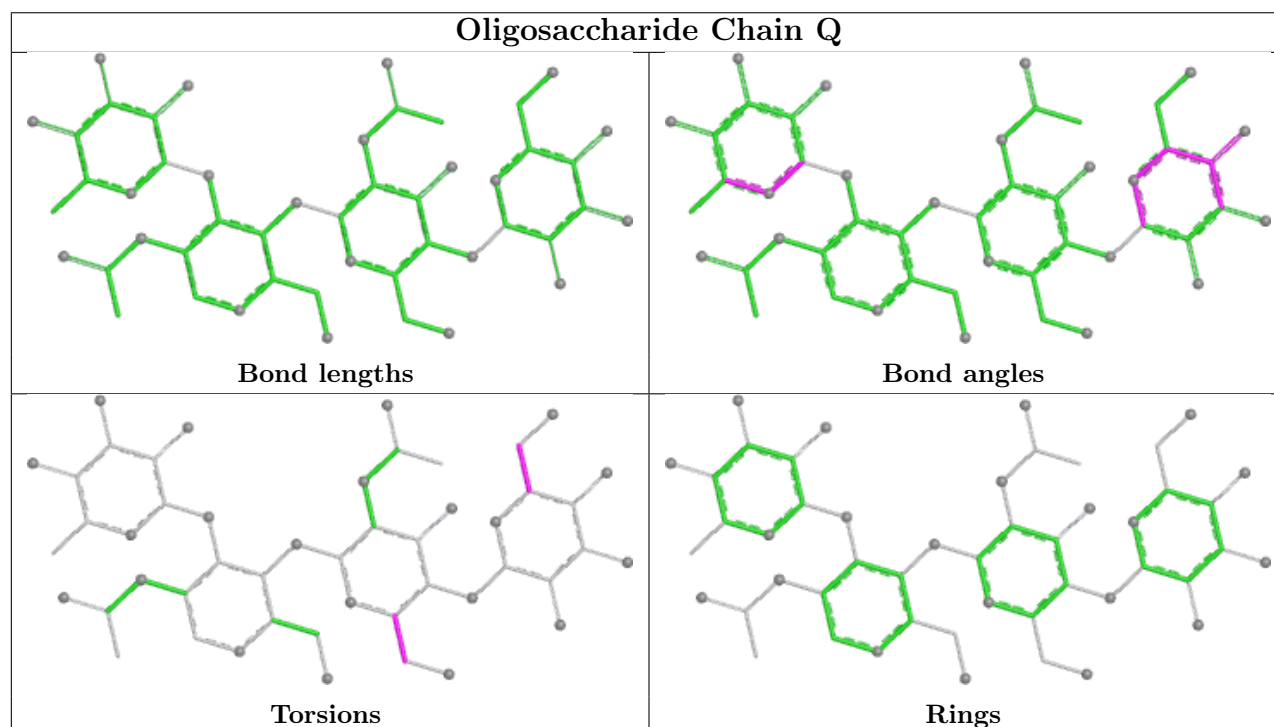
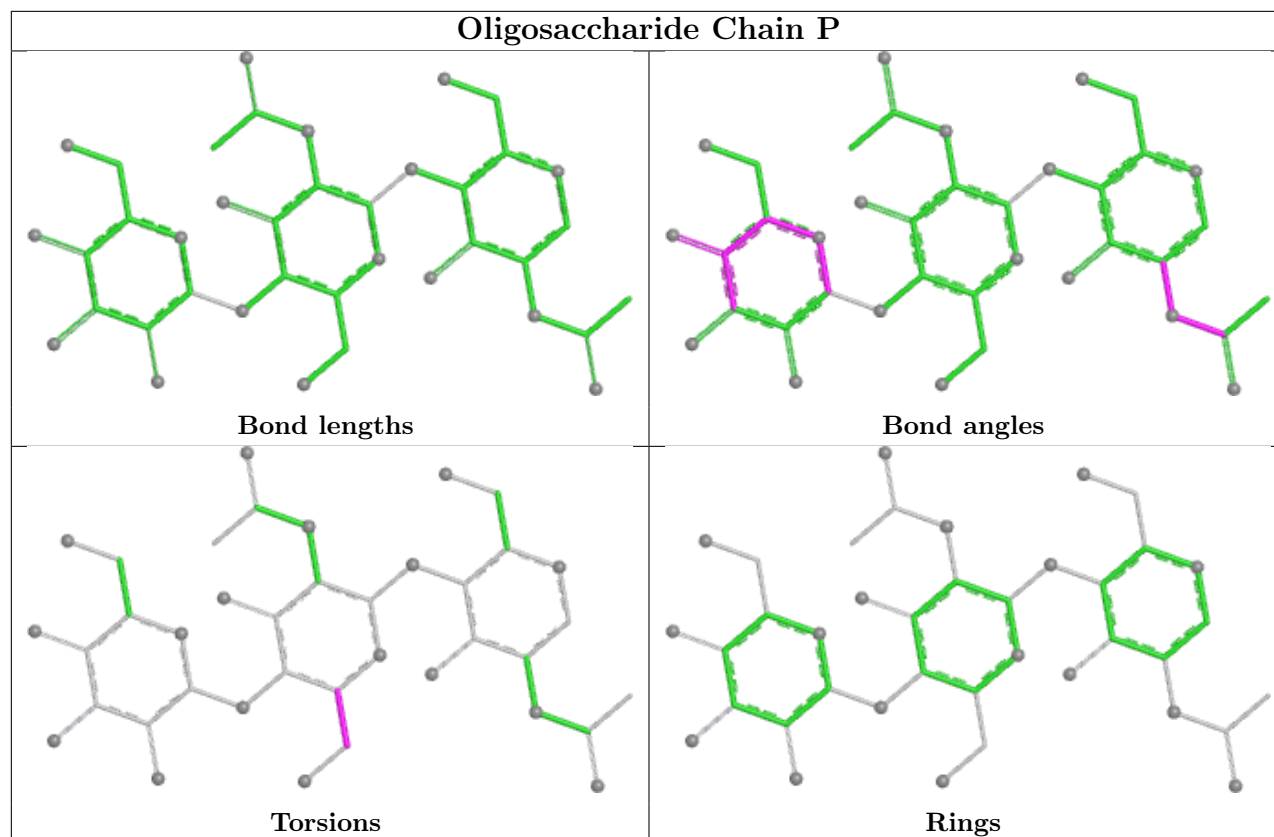
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

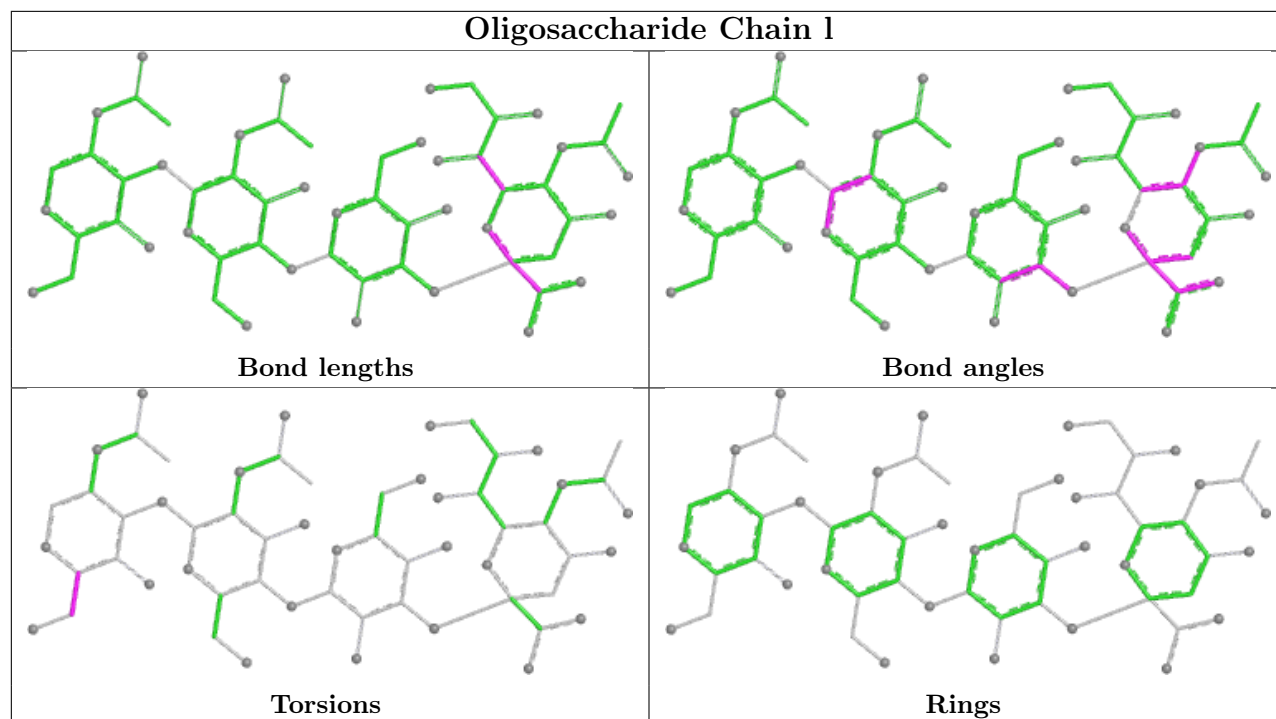


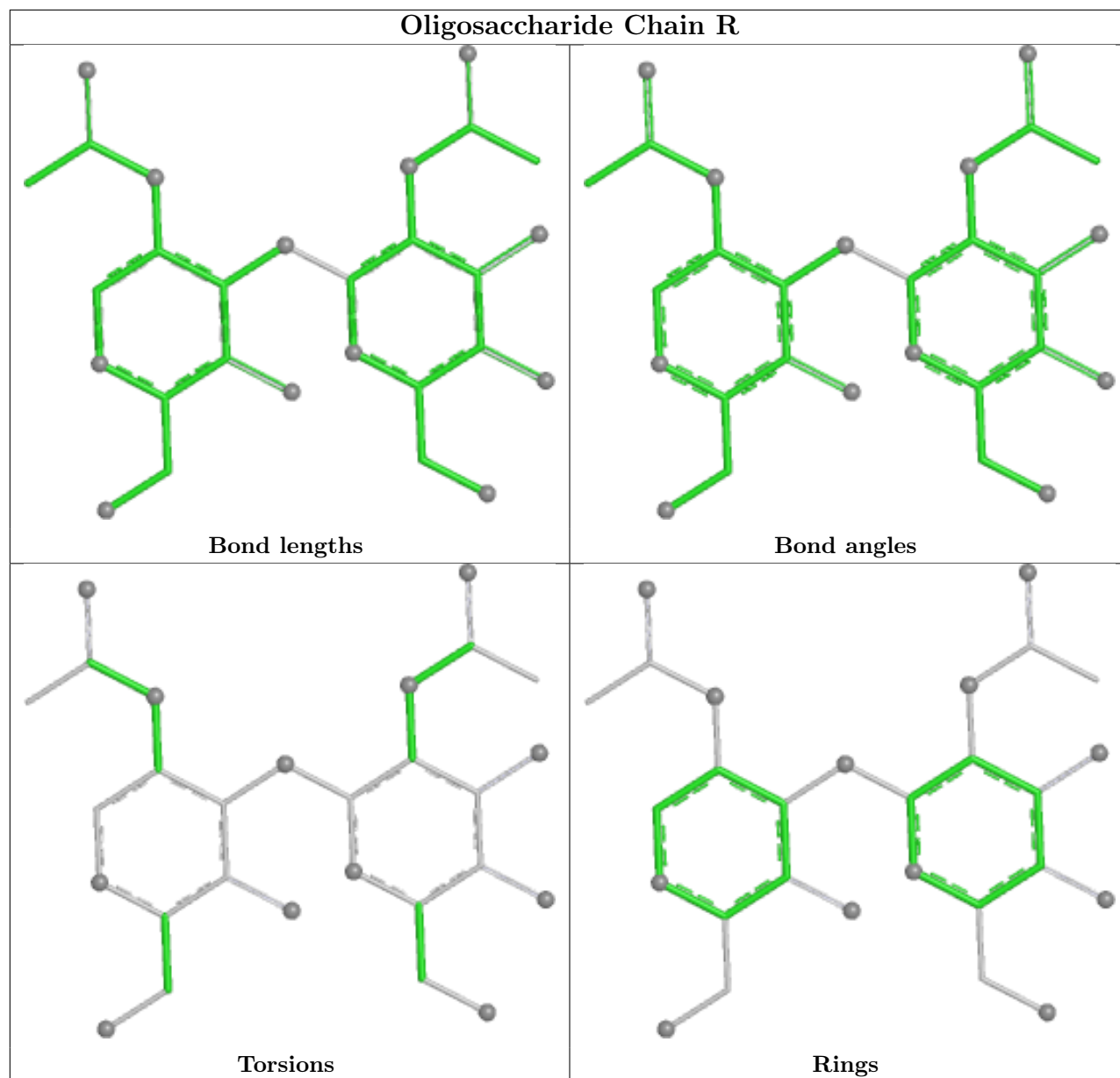


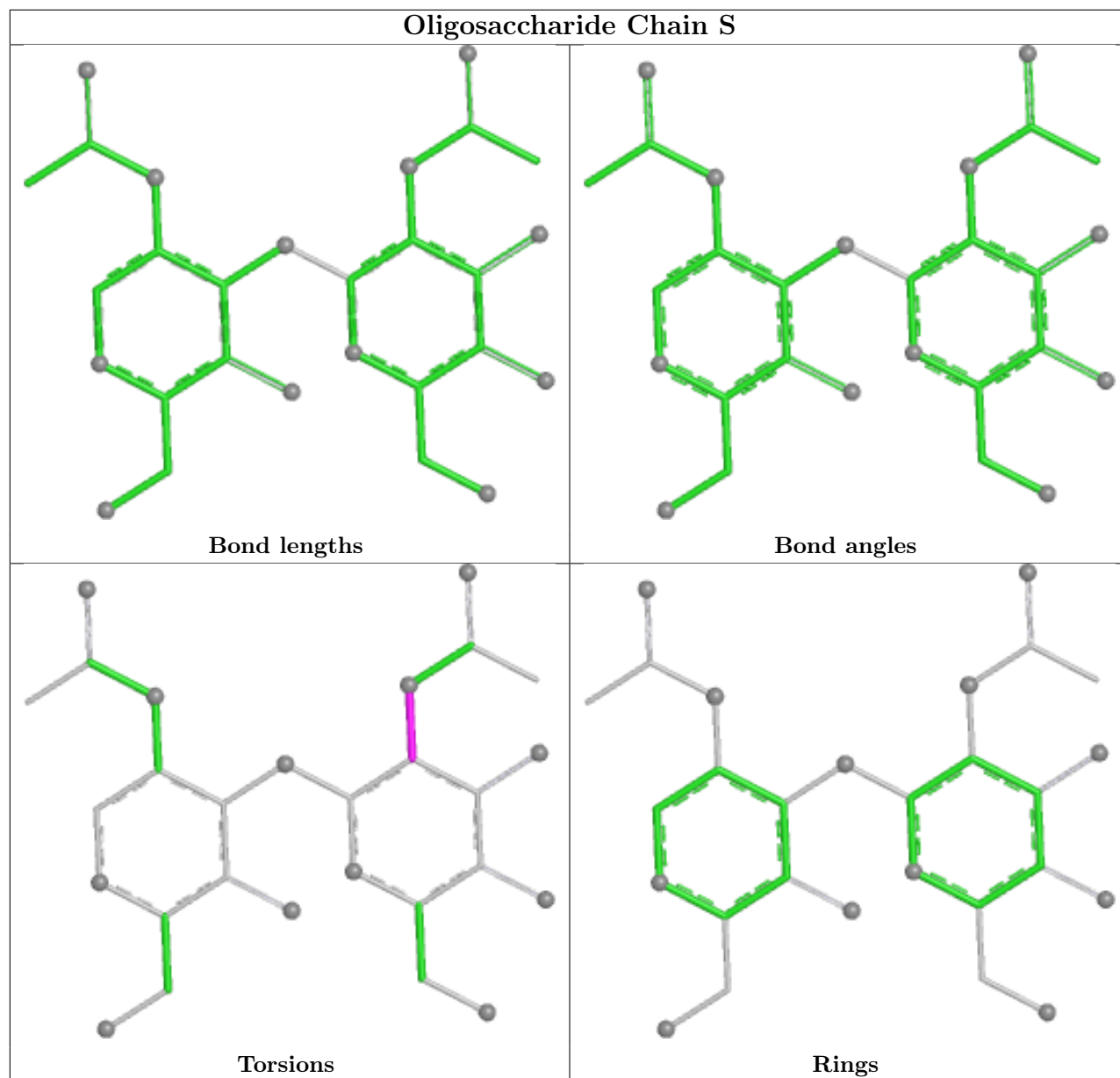




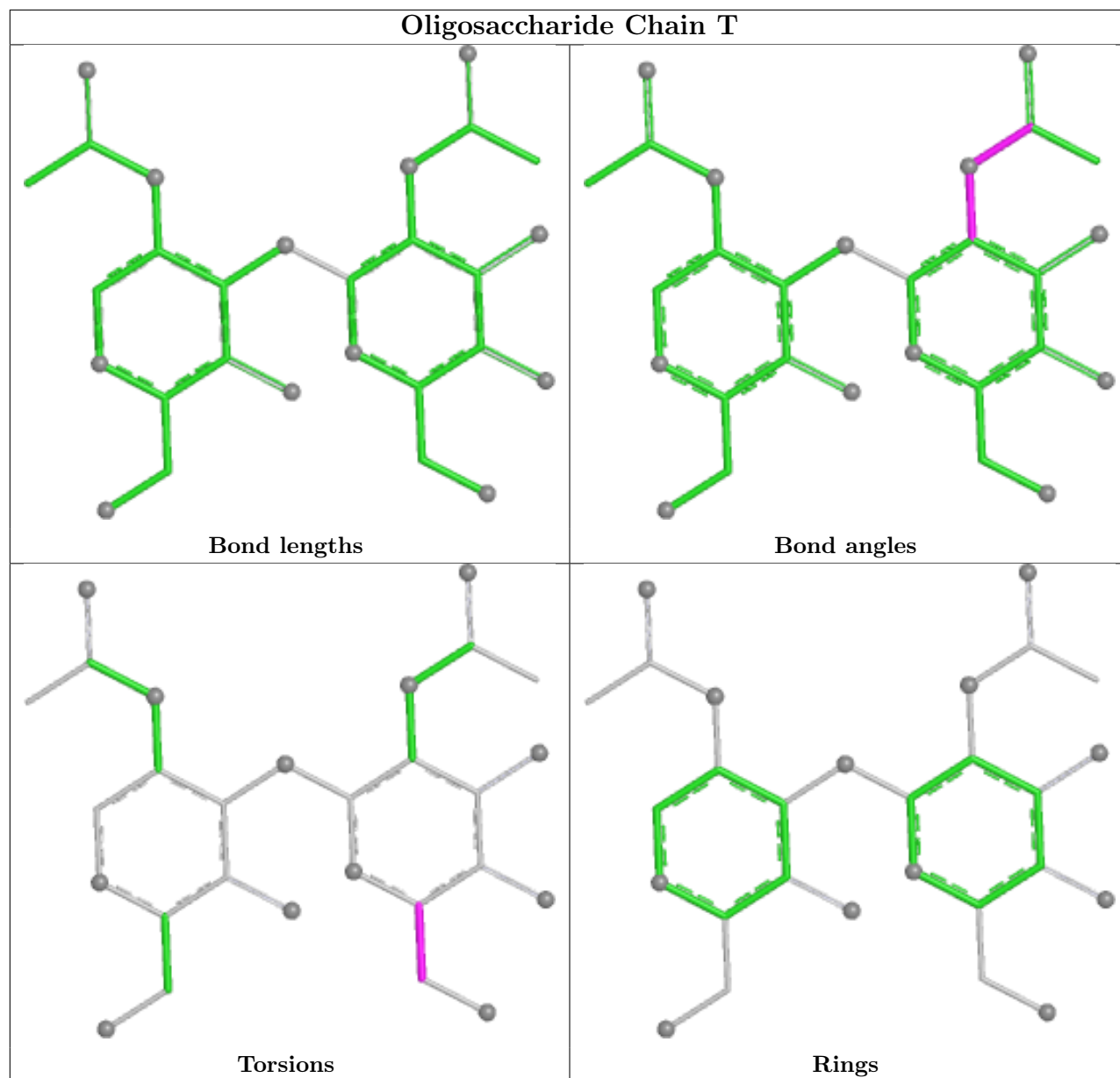


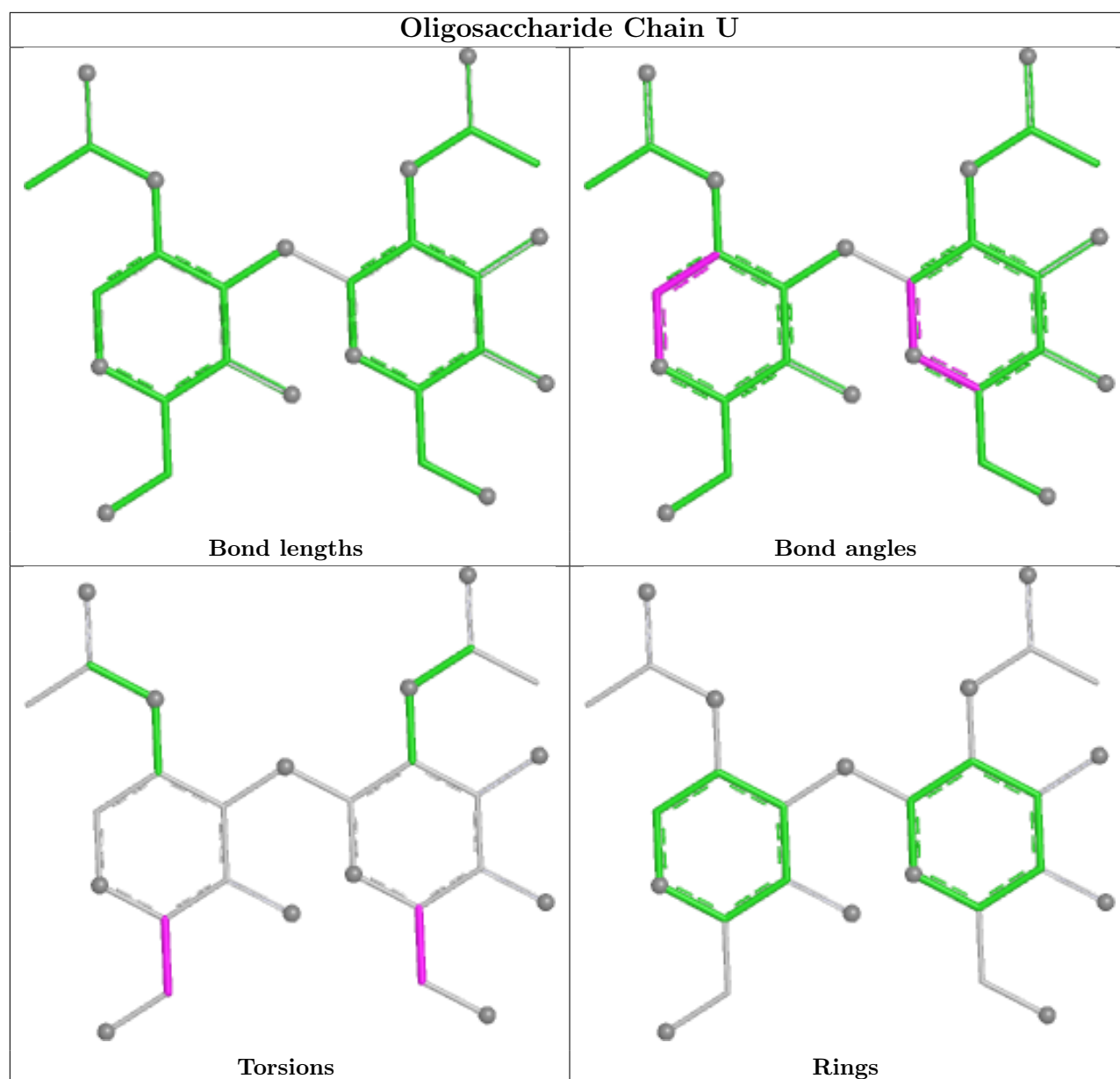












## 5.6 Ligand geometry [i](#)

54 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
12	EDO	A	403	-	3,3,3	0.27	0	2,2,2	0.17	0
12	EDO	A	406	-	3,3,3	0.25	0	2,2,2	0.20	0
12	EDO	E	606	-	3,3,3	0.26	0	2,2,2	0.25	0
13	SO4	E	615	-	4,4,4	0.66	0	6,6,6	0.09	0
13	SO4	A	411	-	4,4,4	0.70	0	6,6,6	0.09	0
13	SO4	E	616	-	4,4,4	0.70	0	6,6,6	0.10	0
12	EDO	D	201	-	3,3,3	0.24	0	2,2,2	0.26	0
13	SO4	E	612	-	4,4,4	0.74	0	6,6,6	0.21	0
12	EDO	C	602	-	3,3,3	0.26	0	2,2,2	0.26	0
13	SO4	A	407	-	4,4,4	0.66	0	6,6,6	0.34	0
12	EDO	C	606	-	3,3,3	0.29	0	2,2,2	0.25	0
12	EDO	C	607	-	3,3,3	0.31	0	2,2,2	0.19	0
12	EDO	C	604	-	3,3,3	0.27	0	2,2,2	0.19	0
12	EDO	E	609	-	3,3,3	0.22	0	2,2,2	0.46	0
13	SO4	A	416	-	4,4,4	0.68	0	6,6,6	0.15	0
13	SO4	C	610	-	4,4,4	0.88	0	6,6,6	0.53	0
13	SO4	C	613	-	4,4,4	0.69	0	6,6,6	0.13	0
13	SO4	A	409	-	4,4,4	0.70	0	6,6,6	0.11	0
13	SO4	E	611	-	4,4,4	0.68	0	6,6,6	0.08	0
14	NAG	C	601	1	14,14,15	0.65	0	17,19,21	1.47	1 (5%)
12	EDO	C	603	-	3,3,3	0.28	0	2,2,2	0.38	0
12	EDO	B	201	-	3,3,3	0.27	0	2,2,2	0.02	0
12	EDO	A	401	-	3,3,3	0.21	0	2,2,2	0.42	0
12	EDO	E	608	-	3,3,3	0.24	0	2,2,2	0.34	0
13	SO4	C	615	-	4,4,4	0.71	0	6,6,6	0.11	0
13	SO4	A	415	-	4,4,4	0.73	0	6,6,6	0.15	0
12	EDO	E	604	-	3,3,3	0.25	0	2,2,2	0.83	0
12	EDO	E	610	-	3,3,3	0.26	0	2,2,2	0.48	0
13	SO4	E	613	-	4,4,4	0.69	0	6,6,6	0.15	0
13	SO4	C	614	-	4,4,4	0.69	0	6,6,6	0.09	0
13	SO4	E	617	-	4,4,4	0.70	0	6,6,6	0.07	0
14	NAG	E	601	1	14,14,15	0.63	0	17,19,21	1.47	1 (5%)
12	EDO	F	201	-	3,3,3	0.25	0	2,2,2	0.24	0
13	SO4	C	608	-	4,4,4	0.69	0	6,6,6	0.14	0
13	SO4	C	612	-	4,4,4	0.81	0	6,6,6	0.40	0
12	EDO	E	603	-	3,3,3	0.34	0	2,2,2	0.14	0
12	EDO	E	602	-	3,3,3	0.22	0	2,2,2	0.34	0
13	SO4	A	414	-	4,4,4	0.70	0	6,6,6	0.06	0
12	EDO	B	202	-	3,3,3	0.25	0	2,2,2	0.36	0
13	SO4	A	412	-	4,4,4	0.68	0	6,6,6	0.10	0
12	EDO	A	405	-	3,3,3	0.29	0	2,2,2	0.25	0
13	SO4	A	410	-	4,4,4	0.73	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	SO4	C	609	-	4,4,4	0.72	0	6,6,6	0.18	0
12	EDO	E	607	-	3,3,3	0.27	0	2,2,2	0.08	0
13	SO4	C	611	-	4,4,4	0.74	0	6,6,6	0.44	0
12	EDO	E	605	-	3,3,3	0.25	0	2,2,2	0.41	0
12	EDO	A	404	-	3,3,3	0.25	0	2,2,2	0.25	0
13	SO4	A	413	-	4,4,4	0.68	0	6,6,6	0.09	0
13	SO4	C	616	-	4,4,4	0.68	0	6,6,6	0.11	0
12	EDO	F	202	-	3,3,3	0.26	0	2,2,2	0.31	0
12	EDO	A	402	-	3,3,3	0.28	0	2,2,2	0.16	0
13	SO4	E	614	-	4,4,4	0.70	0	6,6,6	0.12	0
13	SO4	A	408	-	4,4,4	0.67	0	6,6,6	0.10	0
12	EDO	C	605	-	3,3,3	0.24	0	2,2,2	0.34	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
12	EDO	A	403	-	-	1/1/1/1	-
12	EDO	A	406	-	-	1/1/1/1	-
12	EDO	E	606	-	-	0/1/1/1	-
12	EDO	D	201	-	-	0/1/1/1	-
12	EDO	C	602	-	-	1/1/1/1	-
12	EDO	C	606	-	-	0/1/1/1	-
12	EDO	C	607	-	-	1/1/1/1	-
12	EDO	C	604	-	-	1/1/1/1	-
12	EDO	E	609	-	-	0/1/1/1	-
14	NAG	C	601	1	-	0/6/23/26	0/1/1/1
12	EDO	C	603	-	-	1/1/1/1	-
12	EDO	B	201	-	-	0/1/1/1	-
12	EDO	A	401	-	-	0/1/1/1	-
12	EDO	E	608	-	-	1/1/1/1	-
12	EDO	E	604	-	-	0/1/1/1	-
12	EDO	E	610	-	-	1/1/1/1	-
14	NAG	E	601	1	-	0/6/23/26	0/1/1/1
12	EDO	F	201	-	-	0/1/1/1	-
12	EDO	E	603	-	-	1/1/1/1	-
12	EDO	E	602	-	-	0/1/1/1	-
12	EDO	B	202	-	-	1/1/1/1	-
12	EDO	A	405	-	-	0/1/1/1	-
12	EDO	E	607	-	-	0/1/1/1	-
12	EDO	E	605	-	-	1/1/1/1	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	EDO	A	404	-	-	1/1/1/1	-
12	EDO	F	202	-	-	1/1/1/1	-
12	EDO	A	402	-	-	0/1/1/1	-
12	EDO	C	605	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	E	601	NAG	C1-O5-C5	5.34	119.35	112.19
14	C	601	NAG	C1-O5-C5	5.02	118.91	112.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	202	EDO	O1-C1-C2-O2
12	C	604	EDO	O1-C1-C2-O2
12	C	607	EDO	O1-C1-C2-O2
12	F	202	EDO	O1-C1-C2-O2
12	A	406	EDO	O1-C1-C2-O2

There are no ring outliers.

21 monomers are involved in 28 short contacts:

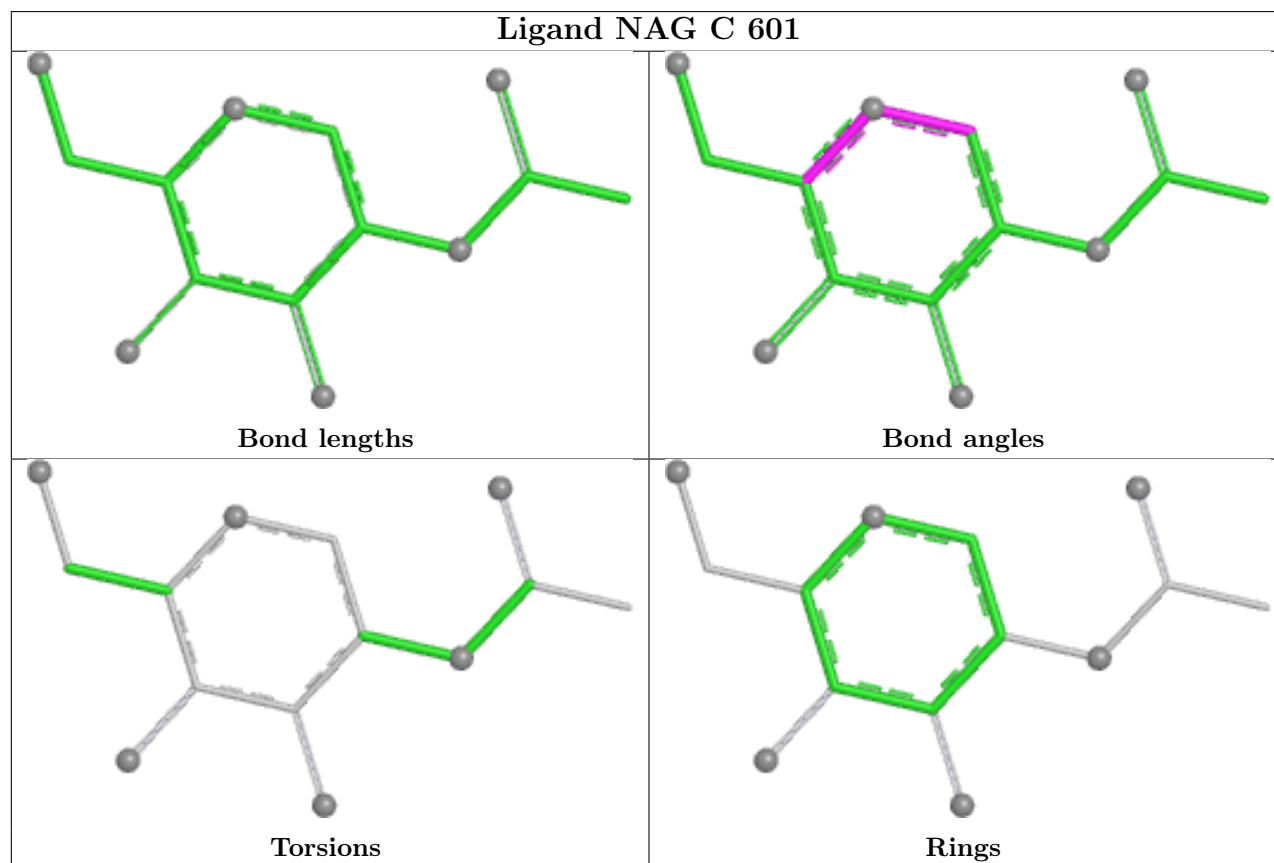
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	606	EDO	2	0
13	E	615	SO4	1	0
12	D	201	EDO	2	0
12	C	606	EDO	2	0
12	C	607	EDO	1	0
12	E	609	EDO	1	0
13	C	610	SO4	1	0
13	E	611	SO4	1	0
14	C	601	NAG	1	0
12	B	201	EDO	2	0
12	E	608	EDO	1	0
12	E	604	EDO	2	0
13	C	614	SO4	1	0
12	F	201	EDO	2	0
13	C	608	SO4	1	0

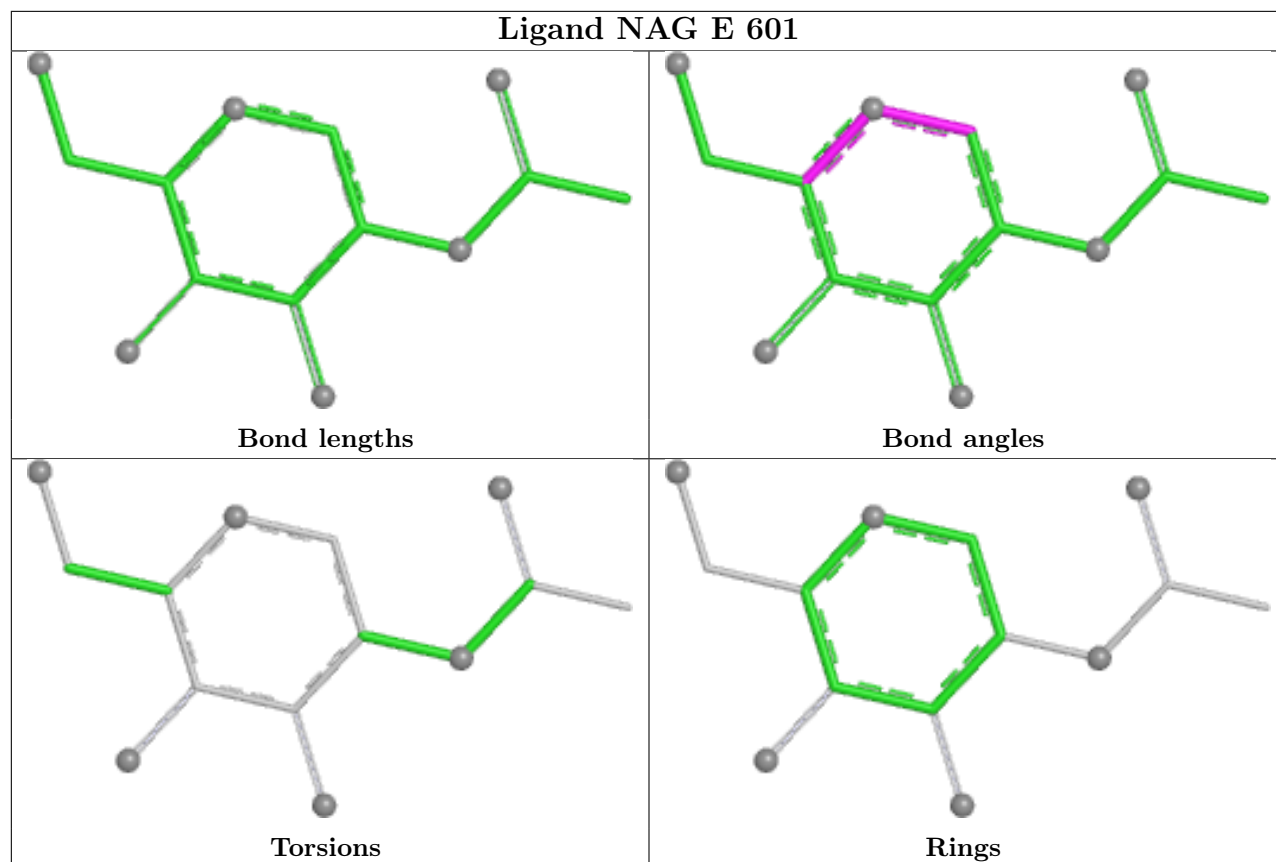
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	602	EDO	3	0
12	A	405	EDO	1	0
12	A	404	EDO	1	0
13	C	616	SO4	1	0
12	F	202	EDO	1	0
12	A	402	EDO	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, 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	321/329 (97%)	-0.07	13 (4%) 42 52	21, 35, 60, 114	0
1	C	323/329 (98%)	-0.10	9 (2%) 55 65	20, 33, 57, 113	0
1	E	321/329 (97%)	-0.15	14 (4%) 39 49	19, 32, 54, 109	0
2	B	169/181 (93%)	0.26	8 (4%) 36 46	23, 39, 78, 126	0
2	D	169/181 (93%)	0.39	11 (6%) 25 33	25, 45, 72, 98	0
2	F	172/181 (95%)	-0.03	7 (4%) 41 51	24, 37, 57, 81	0
3	G	5/5 (100%)	1.56	1 (20%) 3 3	44, 50, 54, 93	0
3	H	5/5 (100%)	2.97	3 (60%) 0 0	60, 63, 74, 105	0
3	I	5/5 (100%)	2.59	3 (60%) 0 0	60, 61, 74, 106	0
3	J	5/5 (100%)	6.99	5 (100%) 0 0	78, 83, 112, 131	0
All	All	1495/1550 (96%)	0.05	74 (4%) 35 44	19, 36, 66, 131	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	6	ILE	10.4
3	J	1	PHE	10.4
2	B	6	ILE	10.3
2	B	174	GLY	9.9
2	D	174	GLY	8.6

### 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 ⓘ

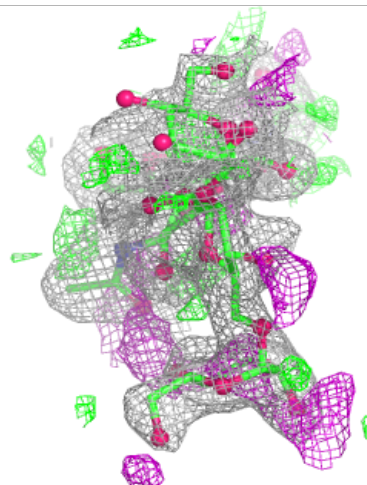
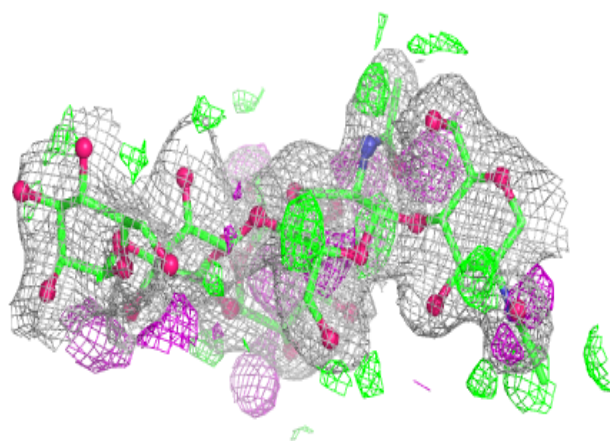
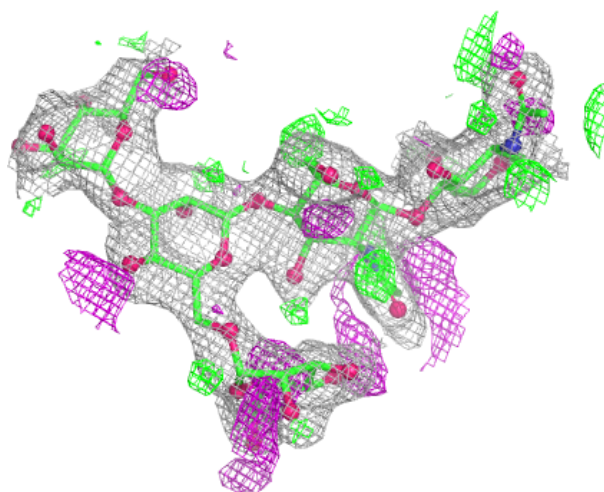
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
6	FUC	O	2	10/11	0.33	0.19	127,142,147,149	0
8	BMA	P	3	11/12	0.34	0.18	115,151,155,156	0
5	NAG	L	2	14/15	0.36	0.18	96,127,136,137	0
5	FUC	L	3	10/11	0.55	0.19	98,118,125,125	0
9	BMA	Q	3	11/12	0.56	0.16	87,106,115,117	0
11	NAG	T	2	14/15	0.66	0.15	94,107,120,120	0
11	NAG	U	2	14/15	0.67	0.15	81,102,112,114	0
6	NAG	M	1	14/15	0.68	0.18	44,86,99,104	0
11	A2G	R	1	14/15	0.68	0.22	45,55,65,70	0
4	MAN	K	4	11/12	0.69	0.19	89,102,115,119	0
6	NAG	O	3	14/15	0.70	0.18	99,115,126,133	0
8	NAG	P	2	14/15	0.71	0.16	65,108,123,141	0
11	NAG	S	2	14/15	0.74	0.15	88,117,135,139	0
6	NAG	M	3	14/15	0.75	0.16	86,96,109,112	0
4	NAG	K	2	14/15	0.77	0.18	48,68,78,83	0
6	FUC	M	2	10/11	0.78	0.22	71,94,103,103	0
9	FUC	Q	4	10/11	0.78	0.14	66,82,92,103	0
6	NAG	O	1	14/15	0.81	0.14	74,108,116,128	0
4	MAN	K	5	11/12	0.82	0.20	48,77,80,85	0
7	BMA	N	3	11/12	0.82	0.15	49,63,79,79	0
11	A2G	U	1	14/15	0.83	0.15	66,84,100,103	0
5	NAG	L	1	14/15	0.83	0.12	68,91,105,121	0
11	A2G	T	1	14/15	0.87	0.12	67,78,95,105	0
4	BMA	K	3	11/12	0.87	0.13	62,72,94,99	0
7	NAG	N	1	14/15	0.90	0.14	43,51,66,68	0
10	A2G	l	1	14/15	-	-	85,95,103,103	0
10	NAG	l	2	14/15	-	-	45,66,87,88	0
10	GAL	l	3	11/12	-	-	29,34,41,43	0
10	SIA	l	4	20/21	-	-	23,28,33,36	0
8	NAG	P	1	14/15	0.91	0.12	36,50,70,76	0
11	NAG	R	2	14/15	0.92	0.12	64,91,105,105	0
7	MAN	N	4	11/12	0.92	0.11	45,52,57,86	0
9	NAG	Q	1	14/15	0.93	0.10	36,56,66,78	0
4	NAG	K	1	14/15	0.93	0.11	36,52,65,69	0
11	A2G	S	1	14/15	0.94	0.08	64,74,85,94	0
7	NAG	N	2	14/15	0.94	0.10	42,49,68,69	0
9	NAG	Q	2	14/15	0.95	0.08	52,63,89,89	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.

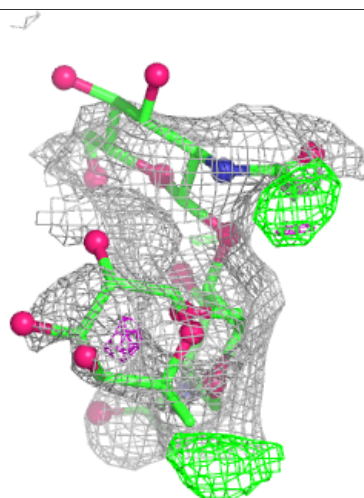
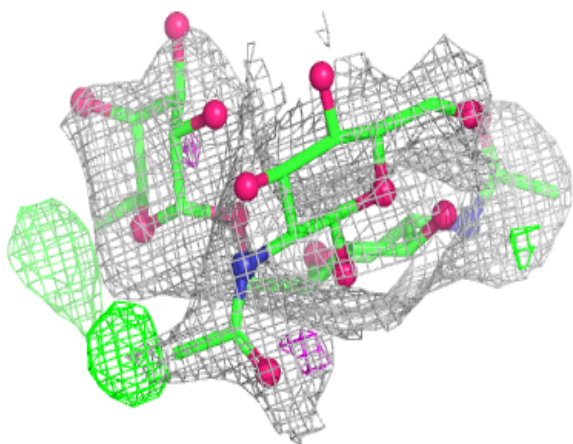
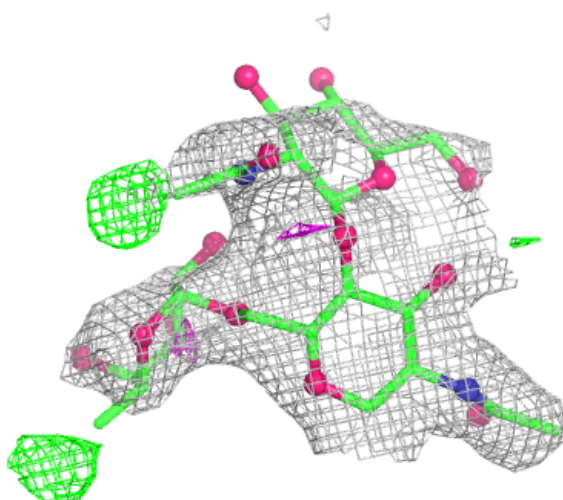
**Electron density around Chain K:**

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



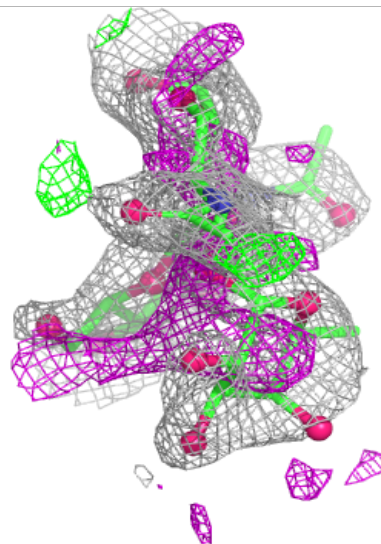
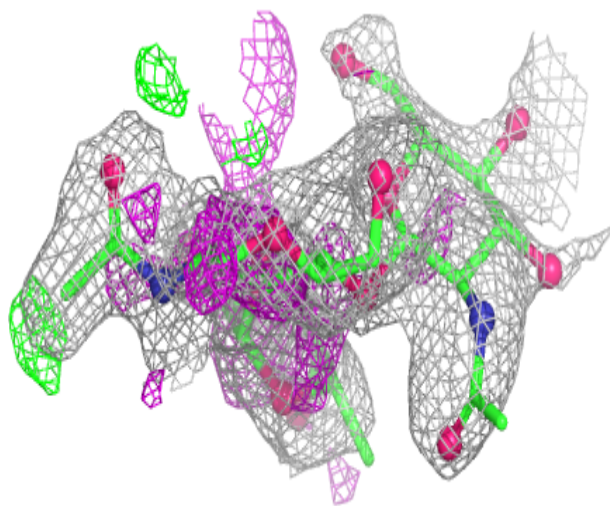
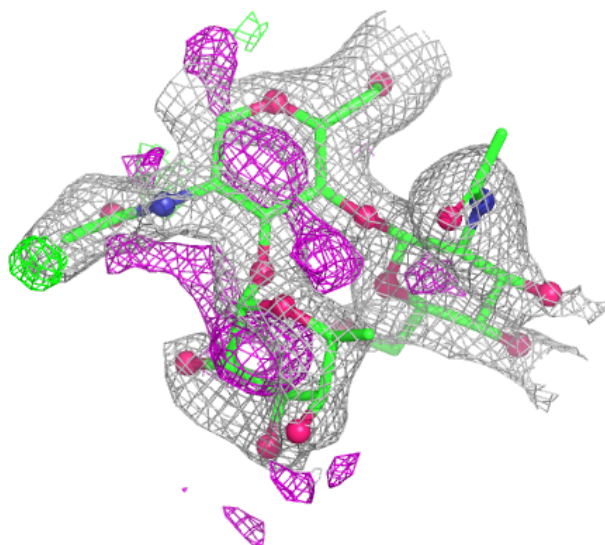
**Electron density around Chain L:**

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



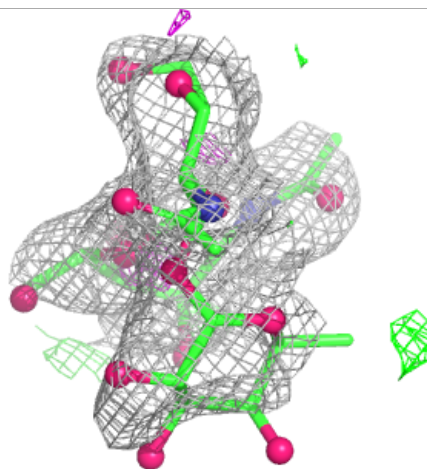
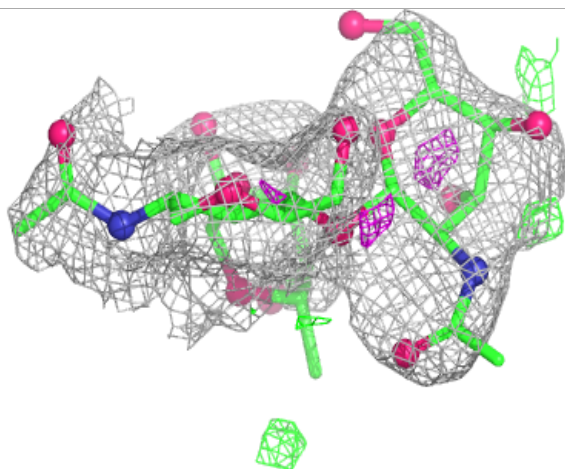
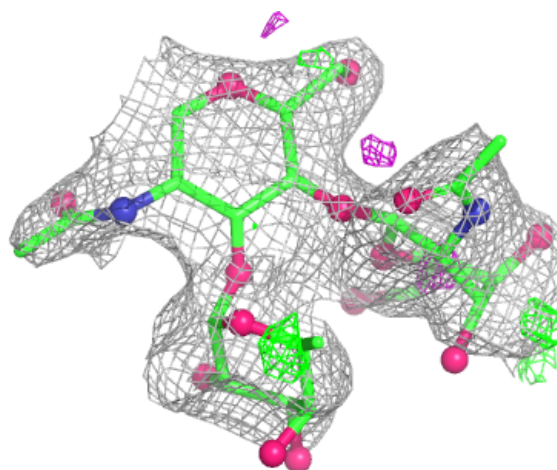
**Electron density around Chain M:**

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



**Electron density around Chain O:**

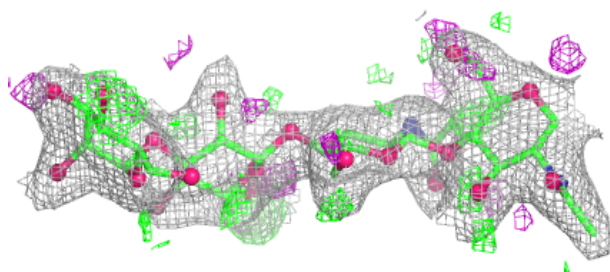
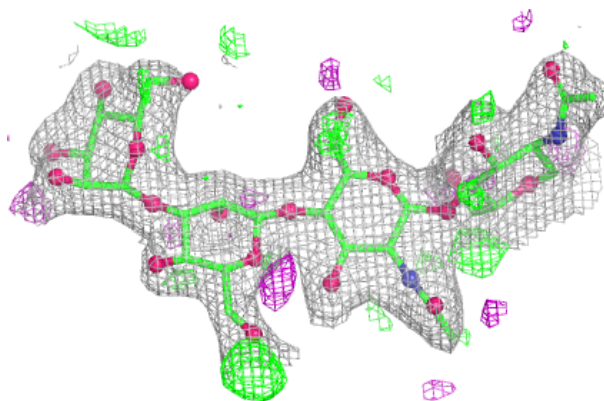
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



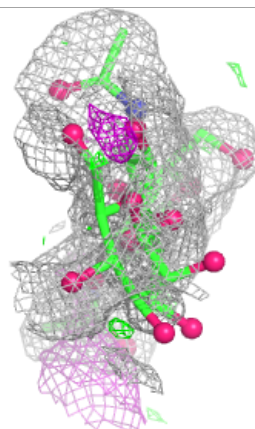
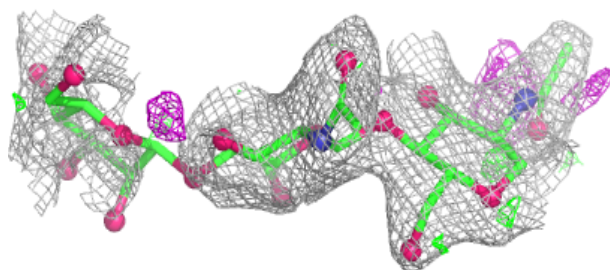
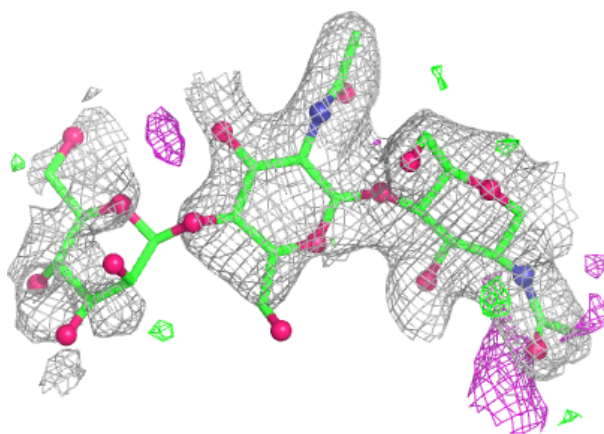


**Electron density around Chain N:**

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

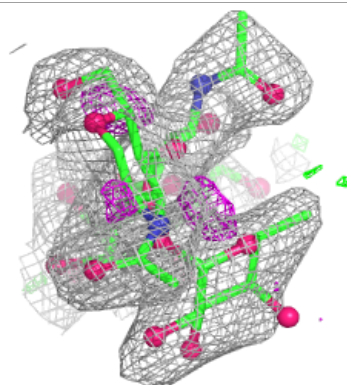
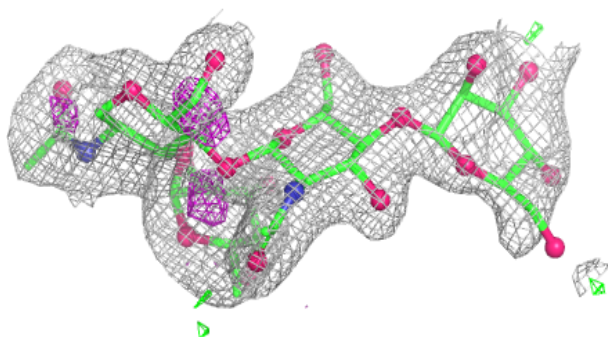
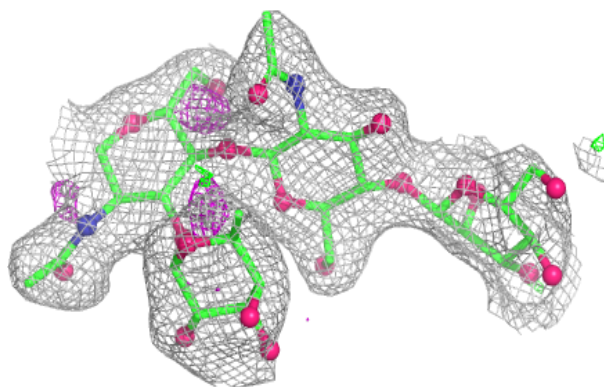
**Electron density around Chain P:**

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

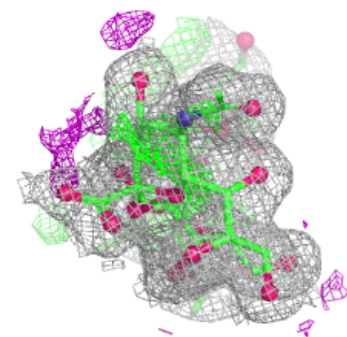
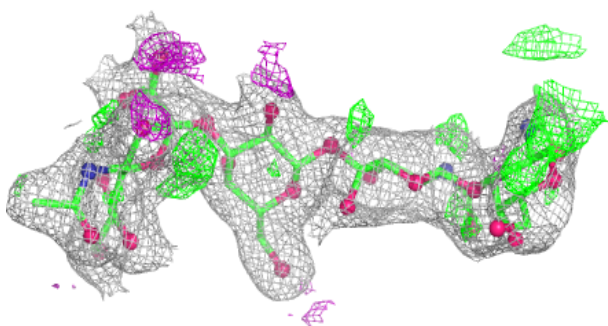
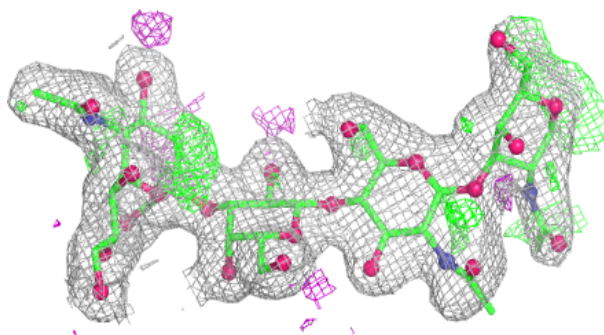


**Electron density around Chain Q:**

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

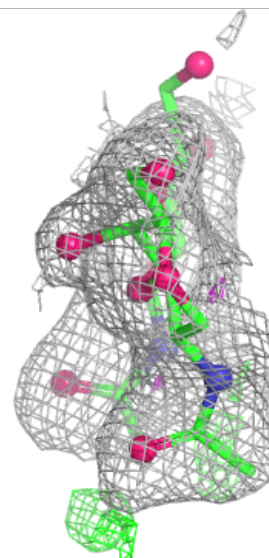
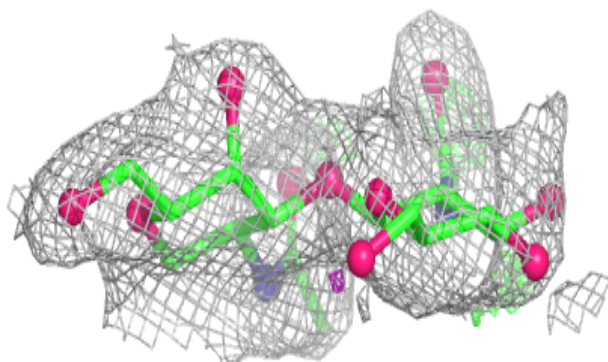
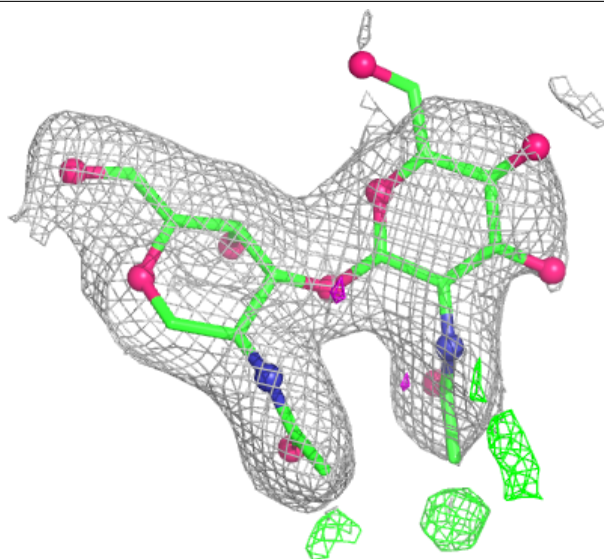
**Electron density around Chain I:**

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



**Electron density around Chain R:**

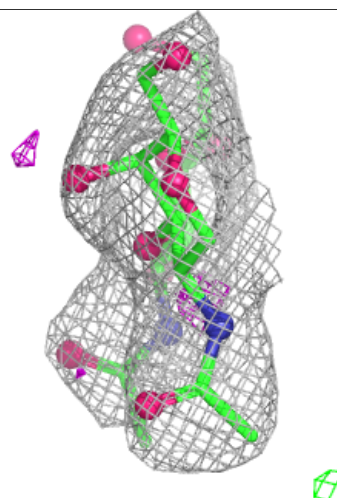
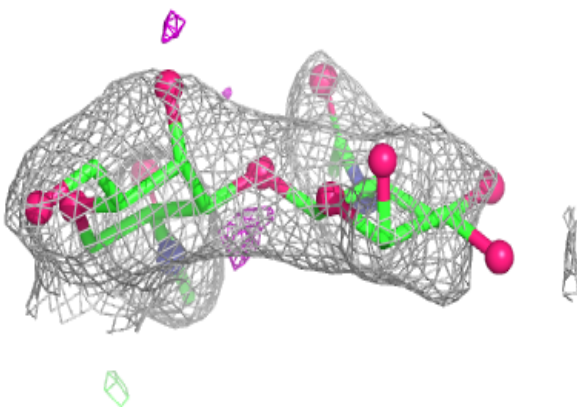
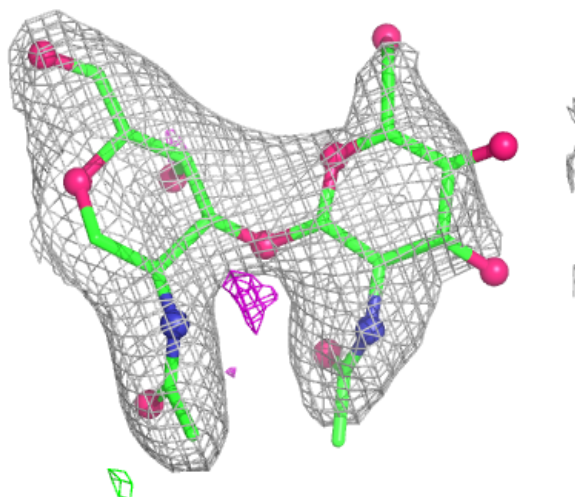
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





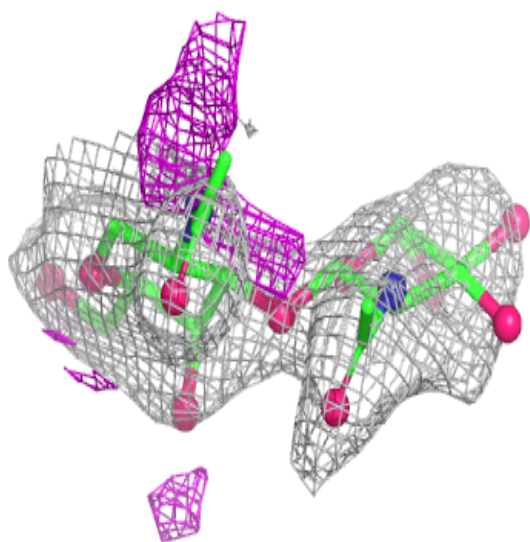
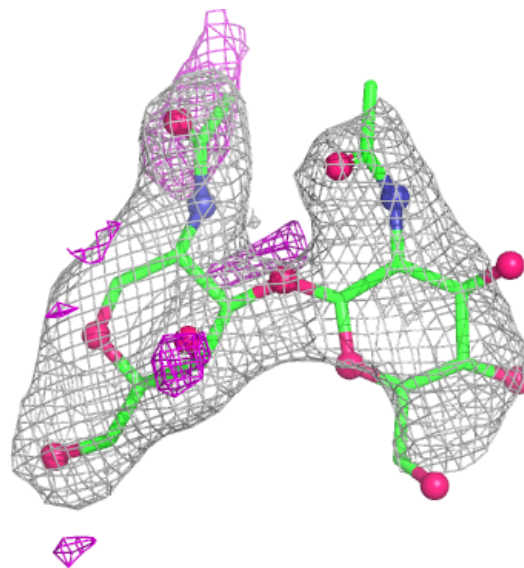
**Electron density around Chain S:**

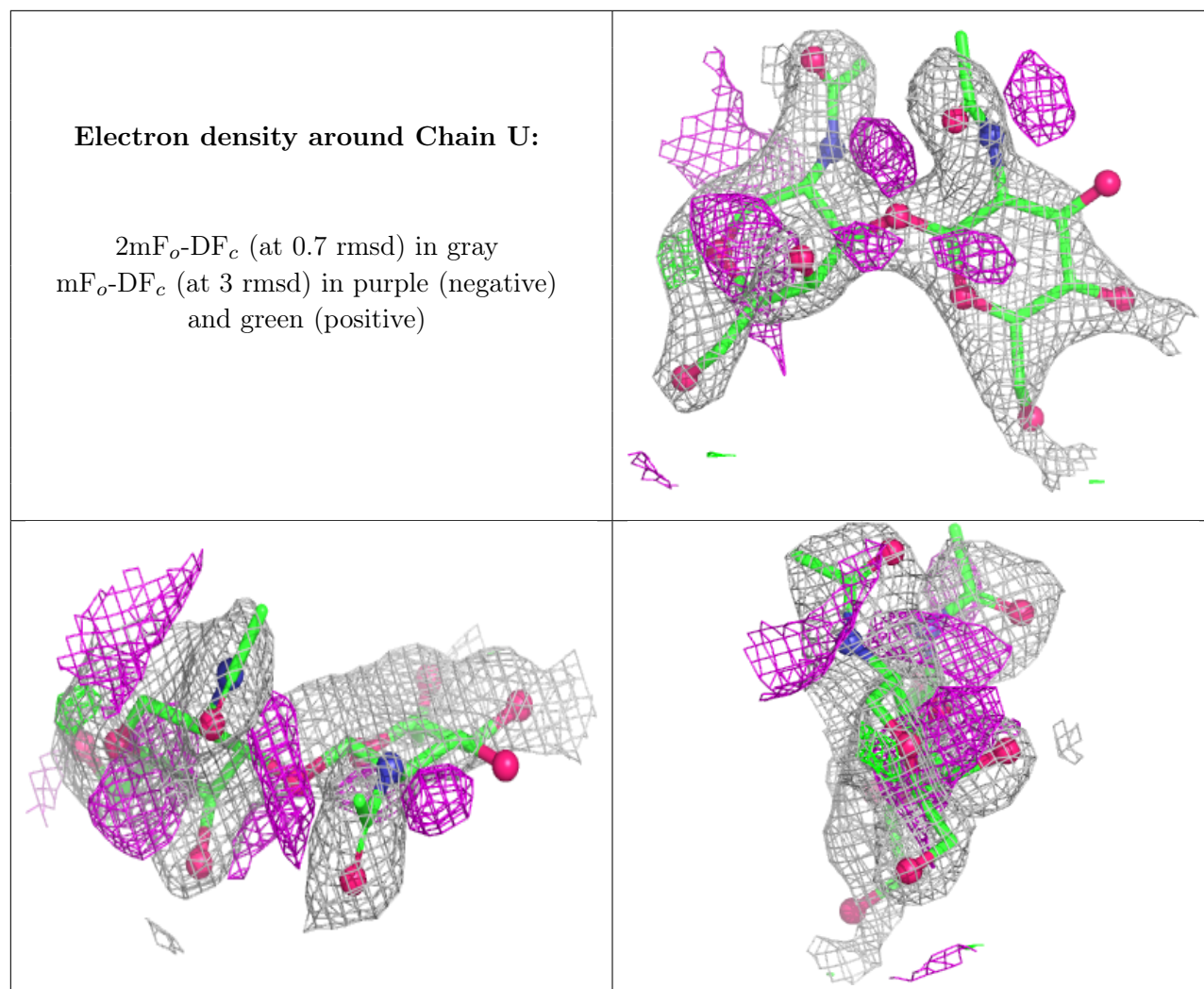
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain T:**

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





## 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(Å <sup>2</sup> )	Q<0.9
13	SO4	C	610	5/5	0.71	0.18	44,46,61,88	0
13	SO4	A	412	5/5	0.72	0.18	106,117,141,143	0
13	SO4	C	615	5/5	0.72	0.16	67,81,115,125	0
13	SO4	A	411	5/5	0.74	0.12	73,94,123,130	0
13	SO4	A	416	5/5	0.74	0.20	72,95,108,127	0
12	EDO	F	202	4/4	0.75	0.18	64,68,73,74	0
13	SO4	E	617	5/5	0.75	0.17	97,97,115,130	0
13	SO4	E	616	5/5	0.76	0.14	83,118,127,138	0
13	SO4	A	409	5/5	0.76	0.13	91,95,122,140	0

*Continued on next page...*

*Continued from previous page...*

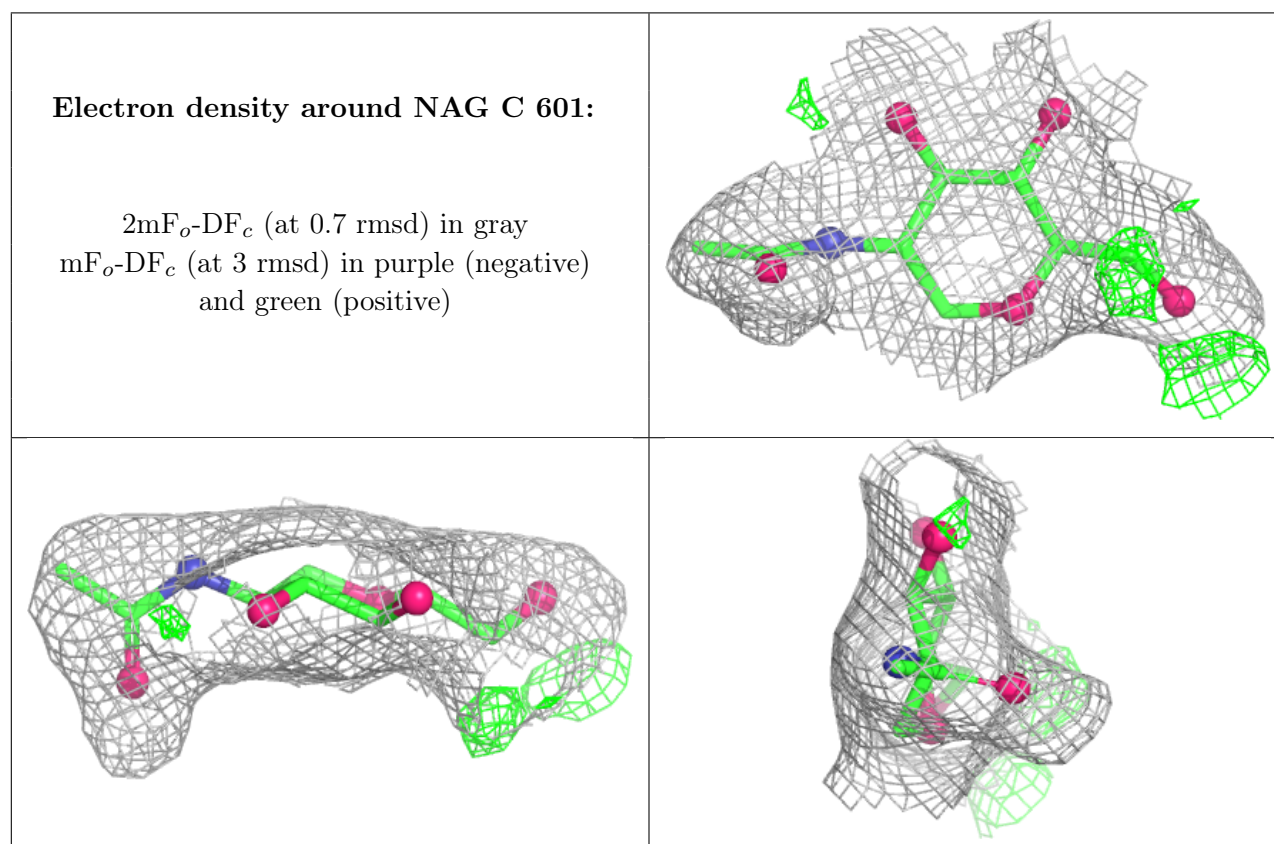
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	SO4	E	614	5/5	0.77	0.11	92,103,115,130	0
13	SO4	A	414	5/5	0.77	0.13	86,101,133,137	0
13	SO4	C	616	5/5	0.77	0.18	63,72,85,88	0
12	EDO	A	405	4/4	0.78	0.20	48,52,64,81	0
13	SO4	A	410	5/5	0.78	0.14	66,76,101,127	0
14	NAG	C	601	14/15	0.78	0.13	66,82,99,100	0
12	EDO	A	402	4/4	0.79	0.31	56,56,57,89	0
13	SO4	C	608	5/5	0.79	0.12	65,87,110,114	0
13	SO4	E	615	5/5	0.79	0.17	96,102,125,136	0
12	EDO	A	406	4/4	0.79	0.28	71,71,75,86	0
13	SO4	C	613	5/5	0.79	0.13	79,90,111,120	0
13	SO4	A	415	5/5	0.79	0.15	54,71,107,130	0
13	SO4	A	408	5/5	0.80	0.13	78,88,109,110	0
14	NAG	E	601	14/15	0.80	0.14	70,86,96,104	0
12	EDO	C	606	4/4	0.81	0.26	47,64,72,77	0
12	EDO	E	606	4/4	0.82	0.21	55,65,74,77	0
12	EDO	E	608	4/4	0.82	0.22	66,71,72,79	0
13	SO4	E	613	5/5	0.82	0.13	43,85,118,133	0
13	SO4	C	609	5/5	0.83	0.16	54,63,76,93	0
12	EDO	C	604	4/4	0.83	0.23	54,56,66,68	0
13	SO4	A	413	5/5	0.83	0.10	82,107,126,137	0
12	EDO	B	201	4/4	0.84	0.25	59,73,79,80	0
13	SO4	A	407	5/5	0.84	0.15	61,73,100,109	0
12	EDO	F	201	4/4	0.85	0.20	33,61,68,69	0
13	SO4	C	612	5/5	0.85	0.14	31,65,79,80	0
12	EDO	B	202	4/4	0.85	0.20	54,56,68,75	0
13	SO4	E	612	5/5	0.86	0.18	52,57,106,132	0
12	EDO	E	604	4/4	0.86	0.16	25,30,37,59	0
12	EDO	C	605	4/4	0.87	0.17	54,66,79,81	0
12	EDO	A	404	4/4	0.88	0.23	34,61,68,73	0
12	EDO	D	201	4/4	0.88	0.17	54,64,64,79	0
13	SO4	C	611	5/5	0.88	0.11	42,43,62,65	0
12	EDO	E	602	4/4	0.89	0.16	37,40,57,57	0
12	EDO	A	401	4/4	0.90	0.17	39,46,48,55	0
13	SO4	E	611	5/5	0.90	0.12	66,67,82,89	0
12	EDO	C	602	4/4	0.90	0.12	46,46,62,63	0
13	SO4	C	614	5/5	0.90	0.13	56,70,81,88	0
12	EDO	C	603	4/4	0.90	0.17	40,47,66,75	0
12	EDO	E	609	4/4	0.91	0.18	39,49,50,59	0
12	EDO	E	605	4/4	0.92	0.13	42,48,55,62	0
12	EDO	E	610	4/4	0.92	0.14	43,49,51,70	0
12	EDO	A	403	4/4	0.94	0.13	36,37,38,41	0

*Continued on next page...*

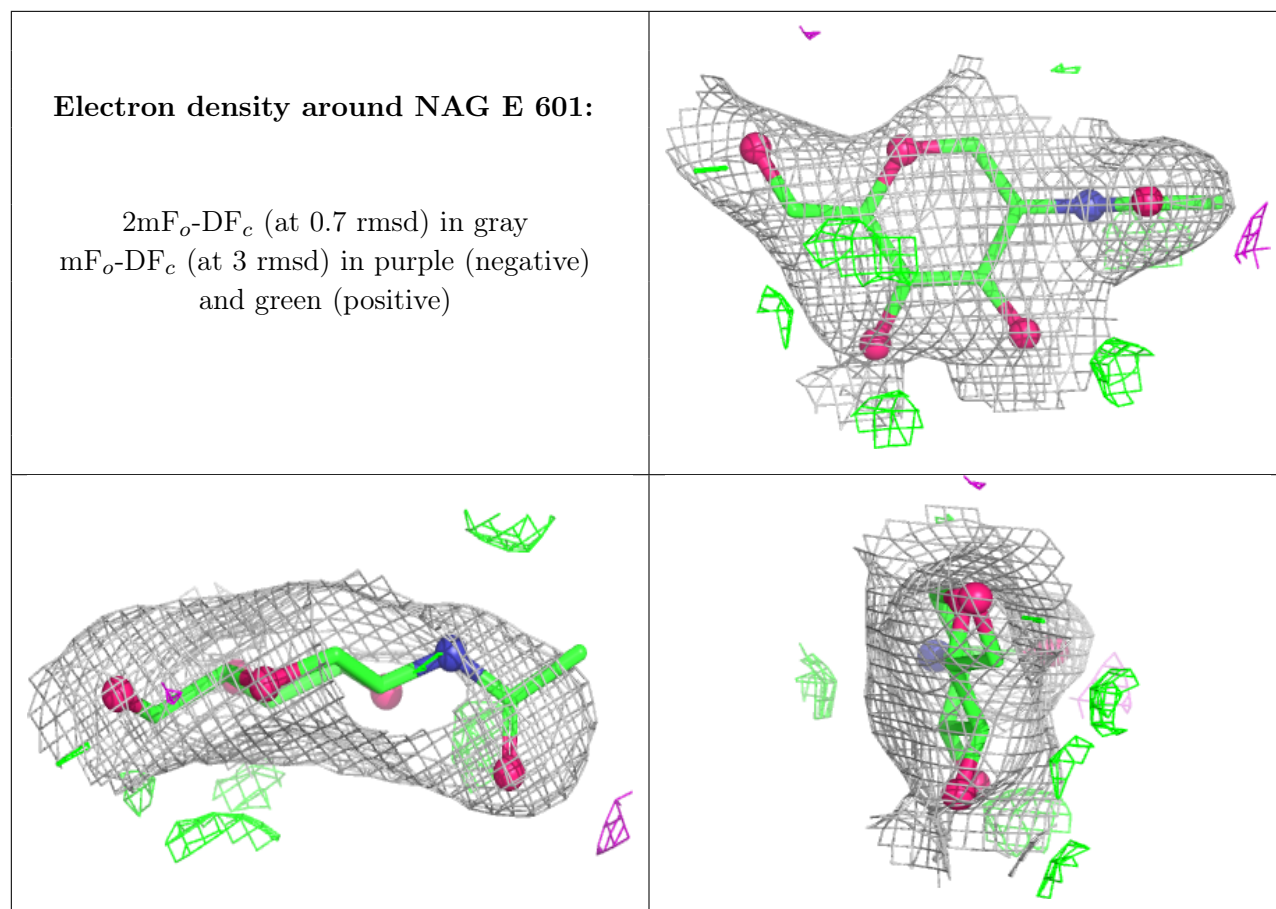
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	EDO	E	607	4/4	0.95	0.10	35,47,48,50	0
12	EDO	E	603	4/4	0.98	0.06	27,30,30,32	0
12	EDO	C	607	4/4	0.98	0.05	27,29,34,35	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.







## 6.5 Other polymers ⓘ

There are no such residues in this entry.