



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 01:25 AM UTC

PDB ID : 4WA1 / pdb_00004wa1
Title : The crystal structure of hemagglutinin from a H3N8 influenza virus isolated from New England harbor seals
Authors : Yang, H.; Villanueva, J.M.; Gubareva, L.V.; Stevens, J.
Deposited on : 2014-08-28
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

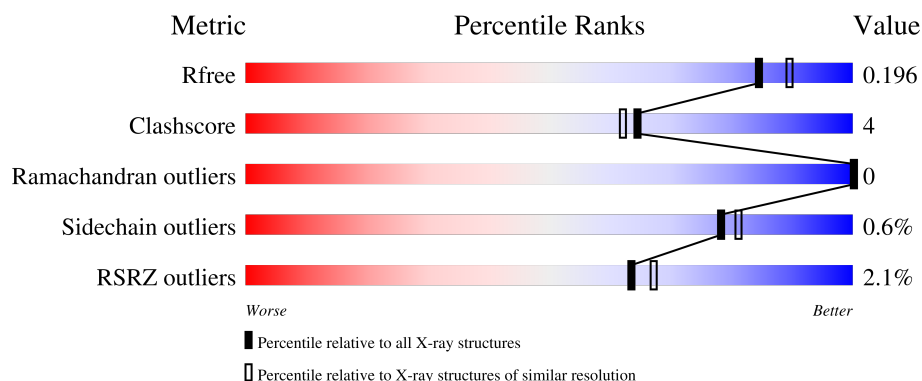
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



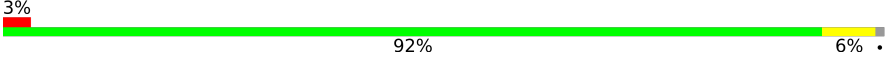
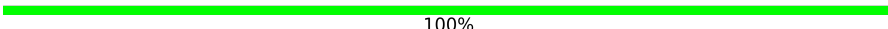
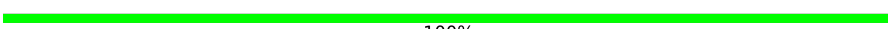
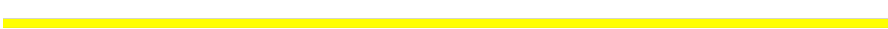
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	496	2% 92% 7% .
1	B	496	% 91% 8% .
1	C	496	2% 90% 9% ..
1	D	496	3% 91% 7% ..
1	E	496	2% 91% 8% .

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Mol	Chain	Length	Quality of chain
1	F	496	
2	G	2	
2	H	2	
2	I	2	
2	J	2	
2	L	2	
2	M	2	
2	N	2	
2	P	2	
3	K	3	
3	O	3	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26664 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	B	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	C	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	D	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	E	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			
1	F	491	Total	C	N	O	S	0	0	0
			3860	2404	683	752	21			

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



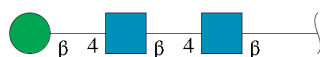
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

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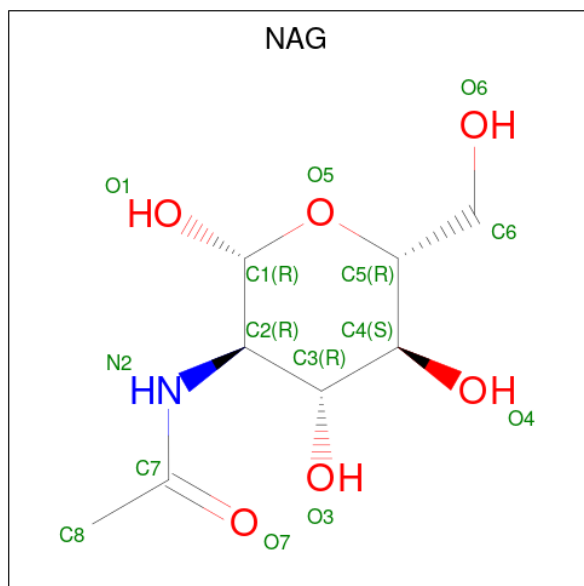
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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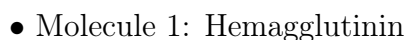
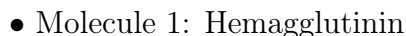
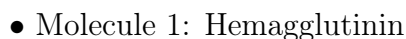
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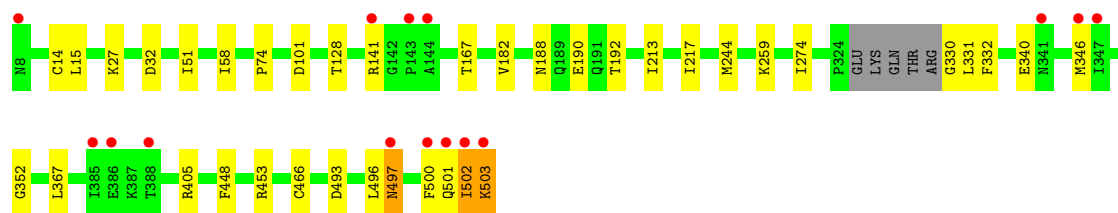
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

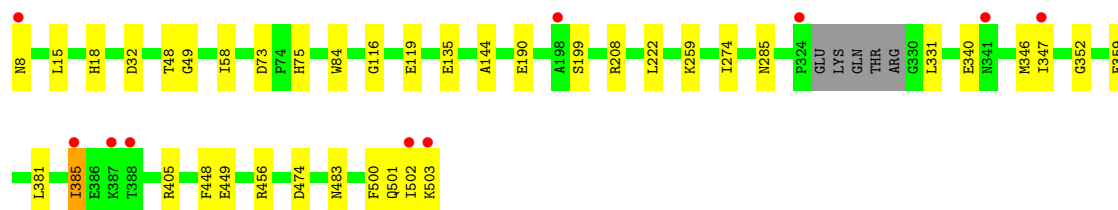
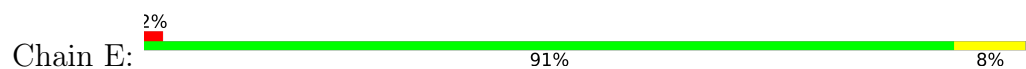
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	527	Total	O	0	0
			527	527		
5	B	543	Total	O	0	0
			543	543		
5	C	499	Total	O	0	0
			499	499		
5	D	517	Total	O	0	0
			517	517		
5	E	501	Total	O	0	0
			501	501		
5	F	503	Total	O	0	0
			503	503		

- Molecule 1: Hemagglutinin

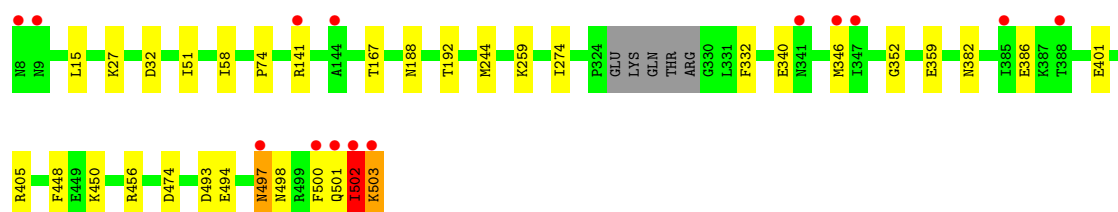
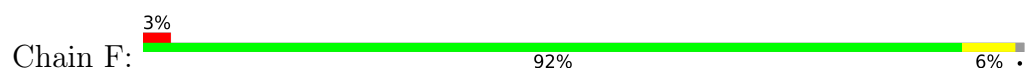




• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin



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



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



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





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

Chain J:  50% 50%



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

Chain L:  50% 50%



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

Chain M:  100%



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

Chain N:  100%



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

Chain P:  100%



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

Chain K:  67% 33%



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

Chain O:  67% 33%

MOL
MAG2
BM13

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.06Å 103.16Å 110.86Å 89.95° 90.00° 90.28°	Depositor
Resolution (Å)	46.78 – 1.90 46.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (46.78-1.90) 91.1 (46.78-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.170 , 0.195 0.171 , 0.196	Depositor DCC
R_{free} test set	13742 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l 0.019 for -h,k,-l 0.440 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26664	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG

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	0.42	0/3937	0.75	2/5333 (0.0%)
1	B	0.43	0/3937	0.75	2/5333 (0.0%)
1	C	0.43	1/3937 (0.0%)	0.77	4/5333 (0.1%)
1	D	0.45	0/3937	0.79	3/5333 (0.1%)
1	E	0.43	0/3937	0.78	3/5333 (0.1%)
1	F	0.45	0/3937	0.79	6/5333 (0.1%)
All	All	0.44	1/23622 (0.0%)	0.77	20/31998 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	198	ALA	CA-CB	-5.11	1.45	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	502	ILE	N-CA-C	11.28	121.14	110.53
1	F	497	ASN	CB-CA-C	-8.79	97.08	110.88
1	D	502	ILE	N-CA-C	7.80	118.60	110.72
1	F	502	ILE	N-CA-C	6.60	118.20	111.00
1	D	497	ASN	CB-CA-C	-6.59	100.54	110.88

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	GLU	Peptide
1	B	340	GLU	Peptide
1	C	340	GLU	Peptide
1	D	340	GLU	Peptide
1	E	340	GLU	Peptide

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	3860	0	3739	26	0
1	B	3860	0	3739	39	0
1	C	3860	0	3739	33	0
1	D	3860	0	3739	40	0
1	E	3860	0	3739	27	0
1	F	3860	0	3739	29	0
2	G	28	0	25	1	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0
2	L	28	0	25	3	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	P	28	0	25	2	0
3	K	39	0	34	1	0
3	O	39	0	34	0	0
4	A	28	0	26	1	0
4	B	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0
5	A	527	0	0	18	1
5	B	543	0	0	18	1
5	C	499	0	0	12	0
5	D	517	0	0	7	0
5	E	501	0	0	11	0
5	F	503	0	0	3	2
All	All	26664	0	22806	179	2

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 179 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:B:411:LYS:NZ	5:B:988:HOH:O	1.87	1.08
1:B:8:ASN:ND2	5:B:1136:HOH:O	1.92	1.02
1:B:201:ARG:NE	5:B:868:HOH:O	1.96	0.97
1:D:500:PHE:HB2	1:D:502:ILE:HG13	1.52	0.91
1:C:141:ARG:NH2	5:C:1084:HOH:O	2.02	0.91

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:711:HOH:O	5:F:772:HOH:O[1_565]	1.99	0.21
5:A:849:HOH:O	5:F:785:HOH:O[1_556]	2.16	0.04

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	487/496 (98%)	472 (97%)	15 (3%)	0	100	100
1	B	487/496 (98%)	472 (97%)	15 (3%)	0	100	100
1	C	487/496 (98%)	470 (96%)	17 (4%)	0	100	100
1	D	487/496 (98%)	472 (97%)	15 (3%)	0	100	100
1	E	487/496 (98%)	471 (97%)	16 (3%)	0	100	100
1	F	487/496 (98%)	472 (97%)	15 (3%)	0	100	100
All	All	2922/2976 (98%)	2829 (97%)	93 (3%)	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	427/432 (99%)	426 (100%)	1 (0%)	87	90
1	B	427/432 (99%)	427 (100%)	0	100	100
1	C	427/432 (99%)	421 (99%)	6 (1%)	59	59
1	D	427/432 (99%)	425 (100%)	2 (0%)	81	84
1	E	427/432 (99%)	423 (99%)	4 (1%)	70	73
1	F	427/432 (99%)	425 (100%)	2 (0%)	81	84
All	All	2562/2592 (99%)	2547 (99%)	15 (1%)	78	81

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	367	LEU
1	F	502	ILE
1	D	503	LYS
1	F	503	LYS
1	E	222	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	189	GLN
1	E	394	GLN
1	F	188	ASN
1	C	96	ASN
1	B	389	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

22 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	$\# Z > 2$
2	NAG	G	1	1,2	14,14,15	0.45	0	17,19,21	0.59	0
2	NAG	G	2	2	14,14,15	0.44	0	17,19,21	0.44	0
2	NAG	H	1	1,2	14,14,15	0.47	0	17,19,21	0.50	0
2	NAG	H	2	2	14,14,15	0.35	0	17,19,21	0.44	0
2	NAG	I	1	1,2	14,14,15	0.22	0	17,19,21	0.49	0
2	NAG	I	2	2	14,14,15	0.42	0	17,19,21	0.40	0
2	NAG	J	1	1,2	14,14,15	0.53	0	17,19,21	0.42	0
2	NAG	J	2	2	14,14,15	0.42	0	17,19,21	0.53	0
3	NAG	K	1	1,3	14,14,15	0.27	0	17,19,21	0.56	0
3	NAG	K	2	3	14,14,15	0.22	0	17,19,21	0.50	0
3	BMA	K	3	3	11,11,12	0.60	0	15,15,17	1.10	2 (13%)
2	NAG	L	1	1,2	14,14,15	0.51	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	L	2	2	14,14,15	0.31	0	17,19,21	0.61	0
2	NAG	M	1	1,2	14,14,15	0.28	0	17,19,21	0.57	0
2	NAG	M	2	2	14,14,15	0.51	0	17,19,21	0.38	0
2	NAG	N	1	1,2	14,14,15	0.39	0	17,19,21	0.44	0
2	NAG	N	2	2	14,14,15	0.39	0	17,19,21	0.59	0
3	NAG	O	1	1,3	14,14,15	0.21	0	17,19,21	0.63	0
3	NAG	O	2	3	14,14,15	0.42	0	17,19,21	0.46	0
3	BMA	O	3	3	11,11,12	0.64	0	15,15,17	1.12	2 (13%)
2	NAG	P	1	1,2	14,14,15	0.32	0	17,19,21	0.55	0
2	NAG	P	2	2	14,14,15	0.43	0	17,19,21	0.70	1 (5%)

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	3	BMA	C1-O5-C5	3.36	116.69	112.19
3	O	3	BMA	C1-O5-C5	2.87	116.03	112.19
3	O	3	BMA	O2-C2-C3	-2.35	105.29	110.15
2	P	2	NAG	C1-O5-C5	2.14	115.05	112.19
3	K	3	BMA	O2-C2-C3	-2.02	105.97	110.15

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

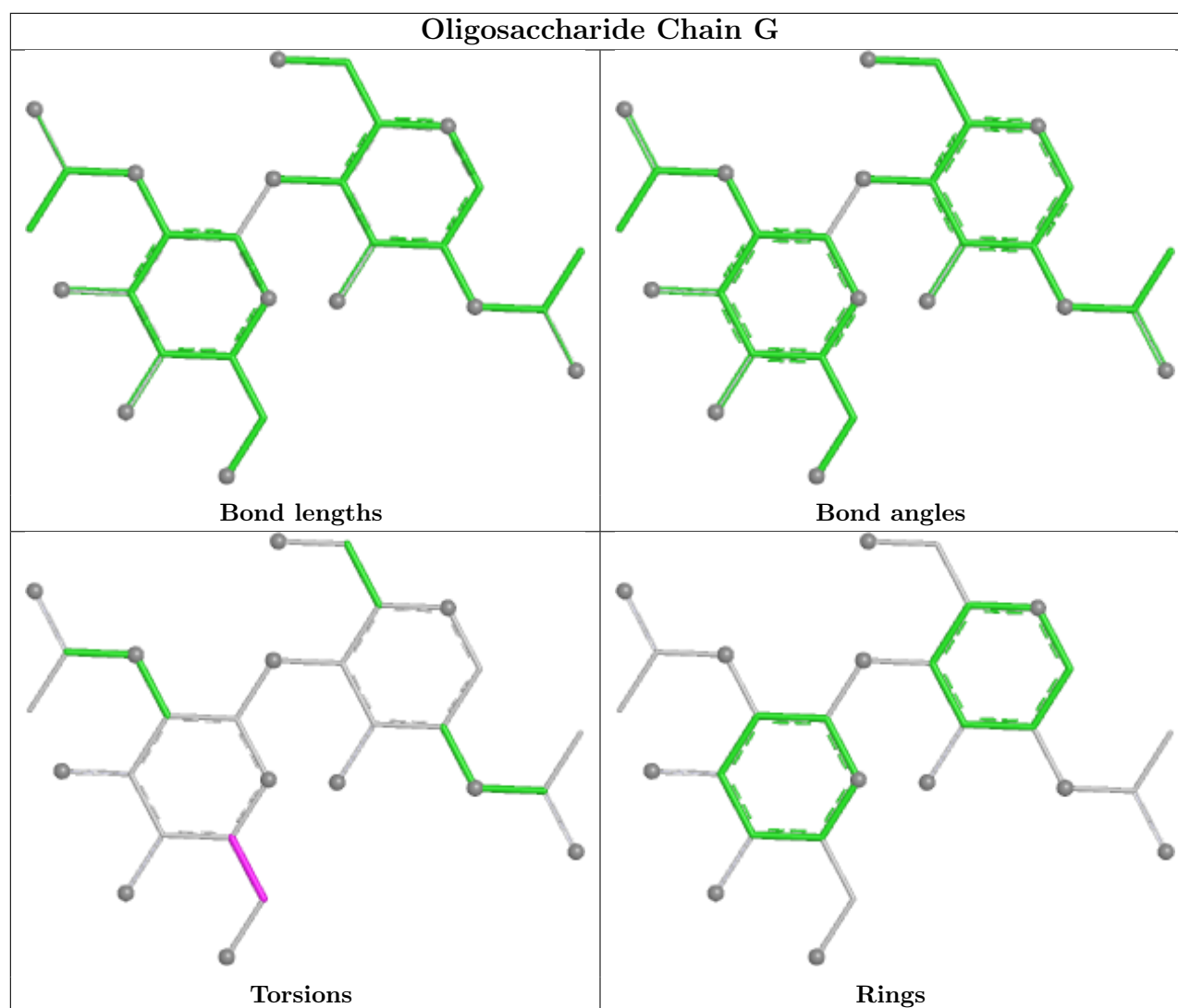
Mol	Chain	Res	Type	Atoms
2	P	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6

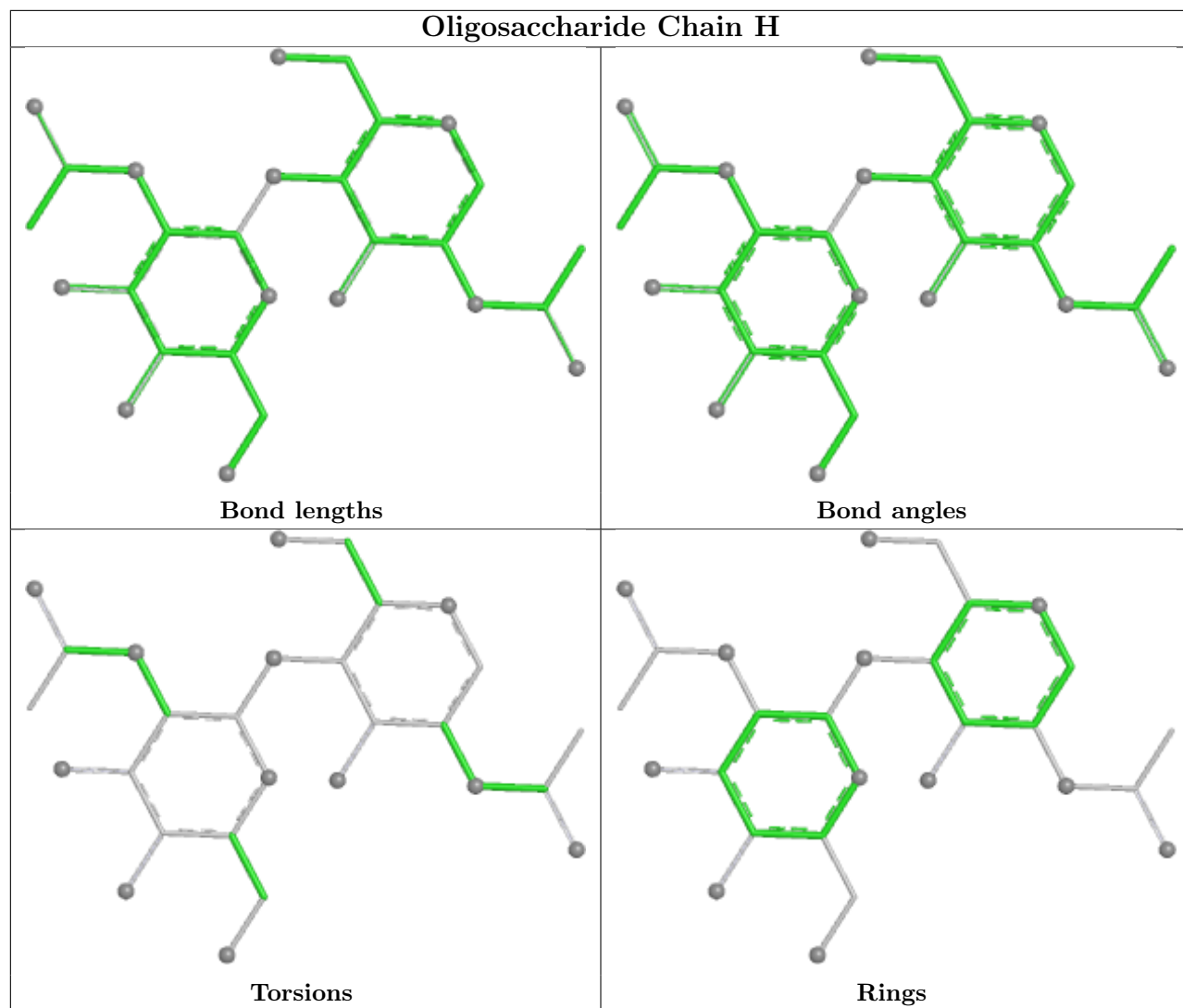
There are no ring outliers.

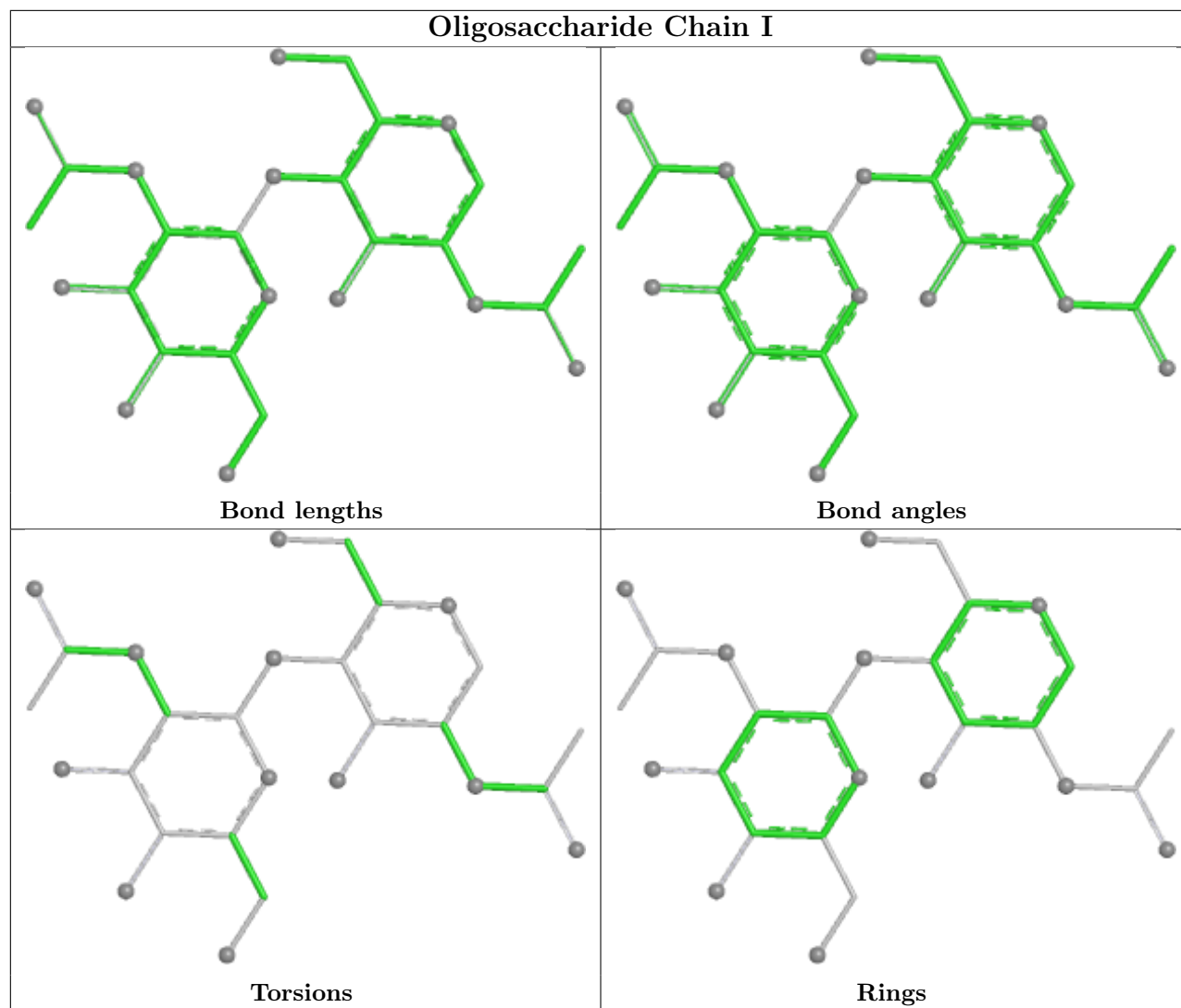
5 monomers are involved in 8 short contacts:

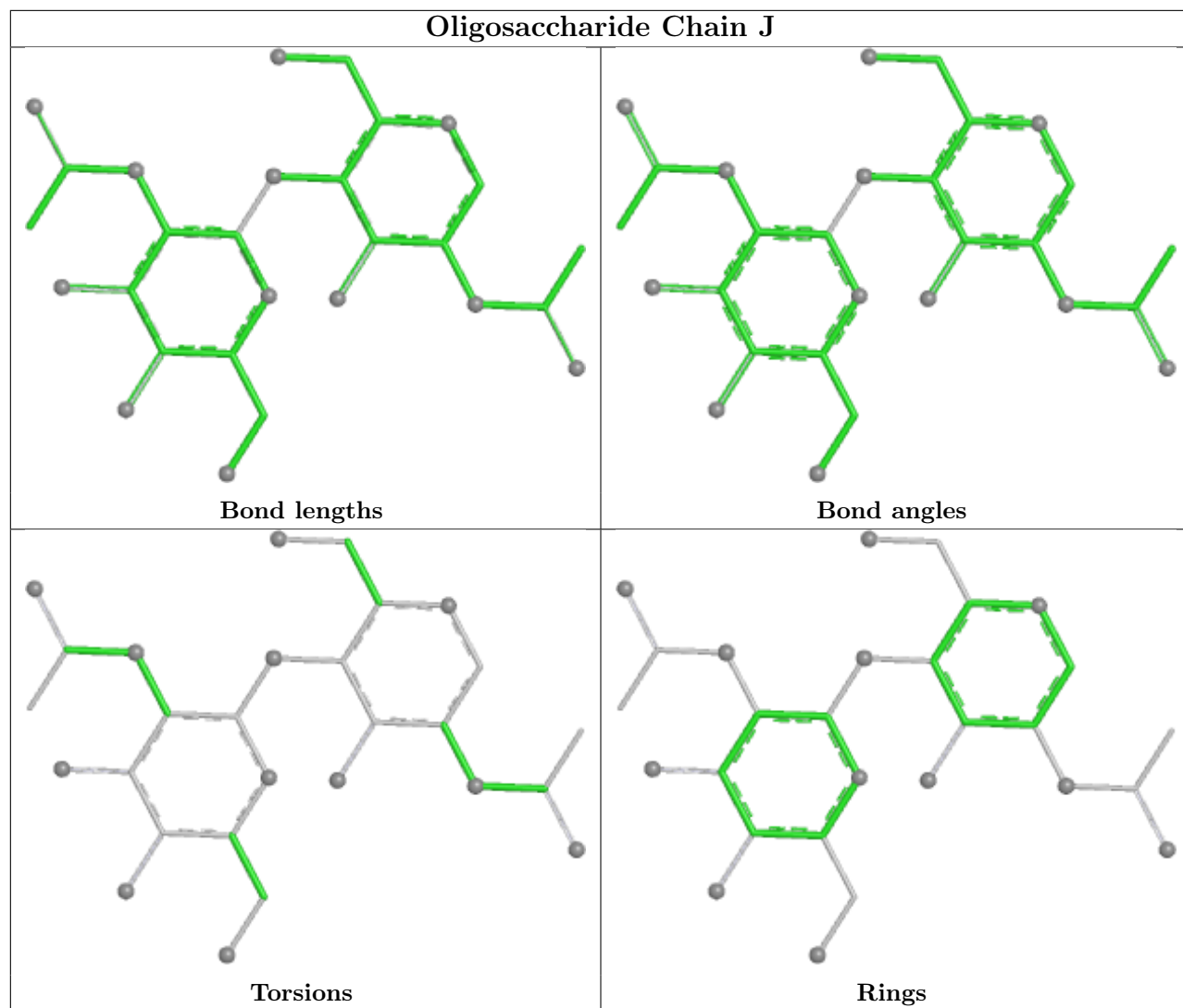
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	NAG	3	0
2	J	2	NAG	1	0
2	G	2	NAG	1	0
2	P	1	NAG	2	0
3	K	3	BMA	1	0

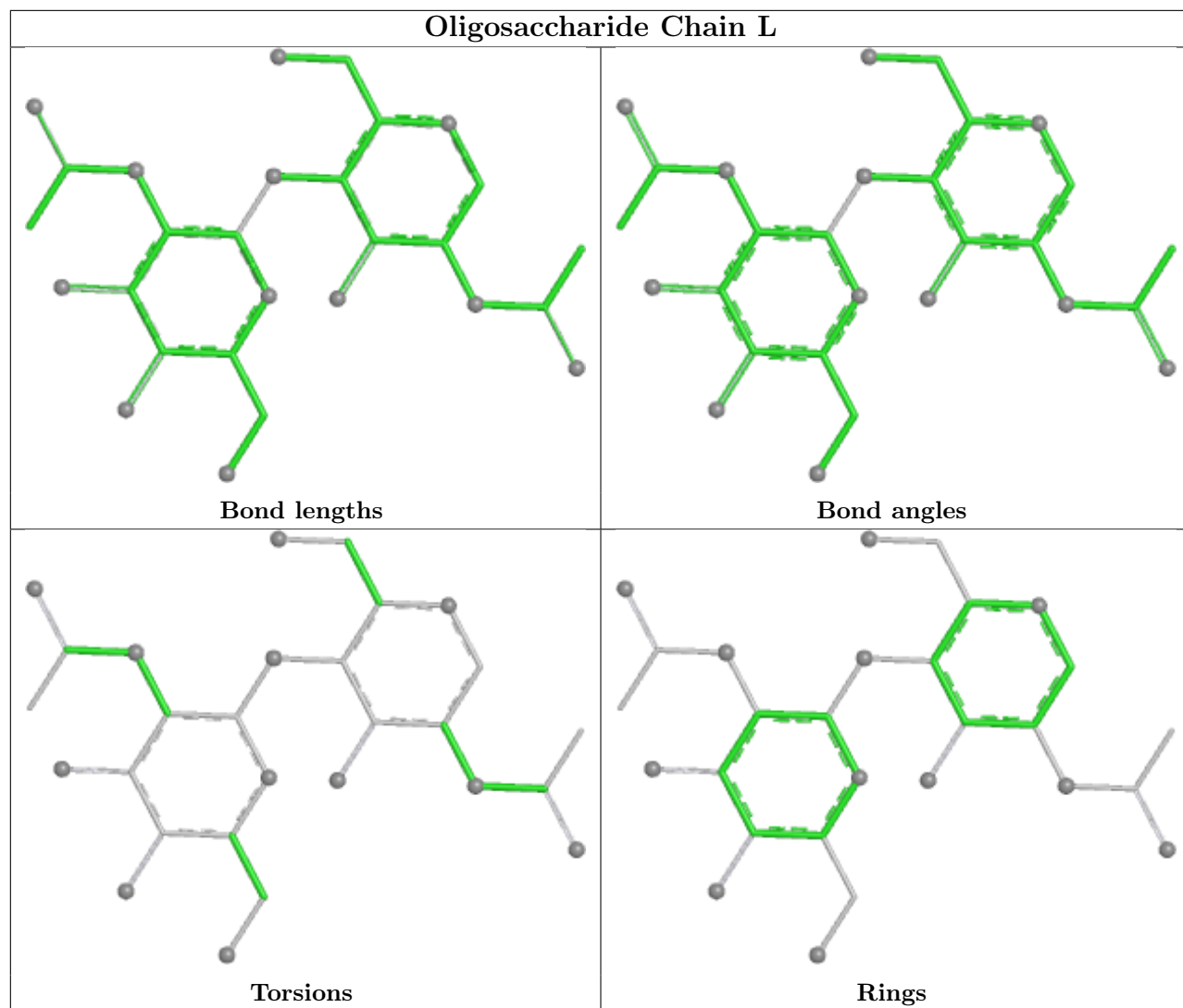
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

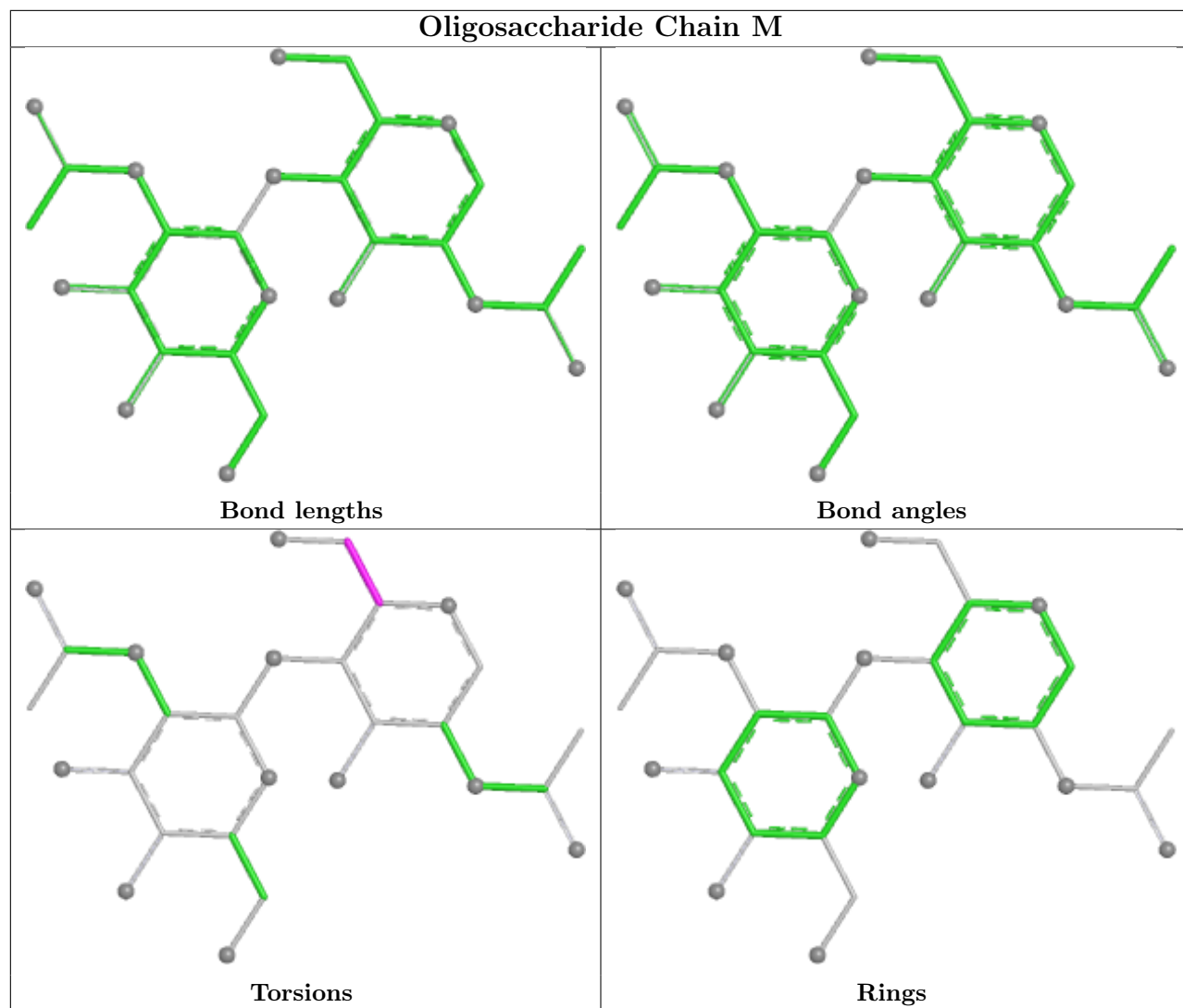


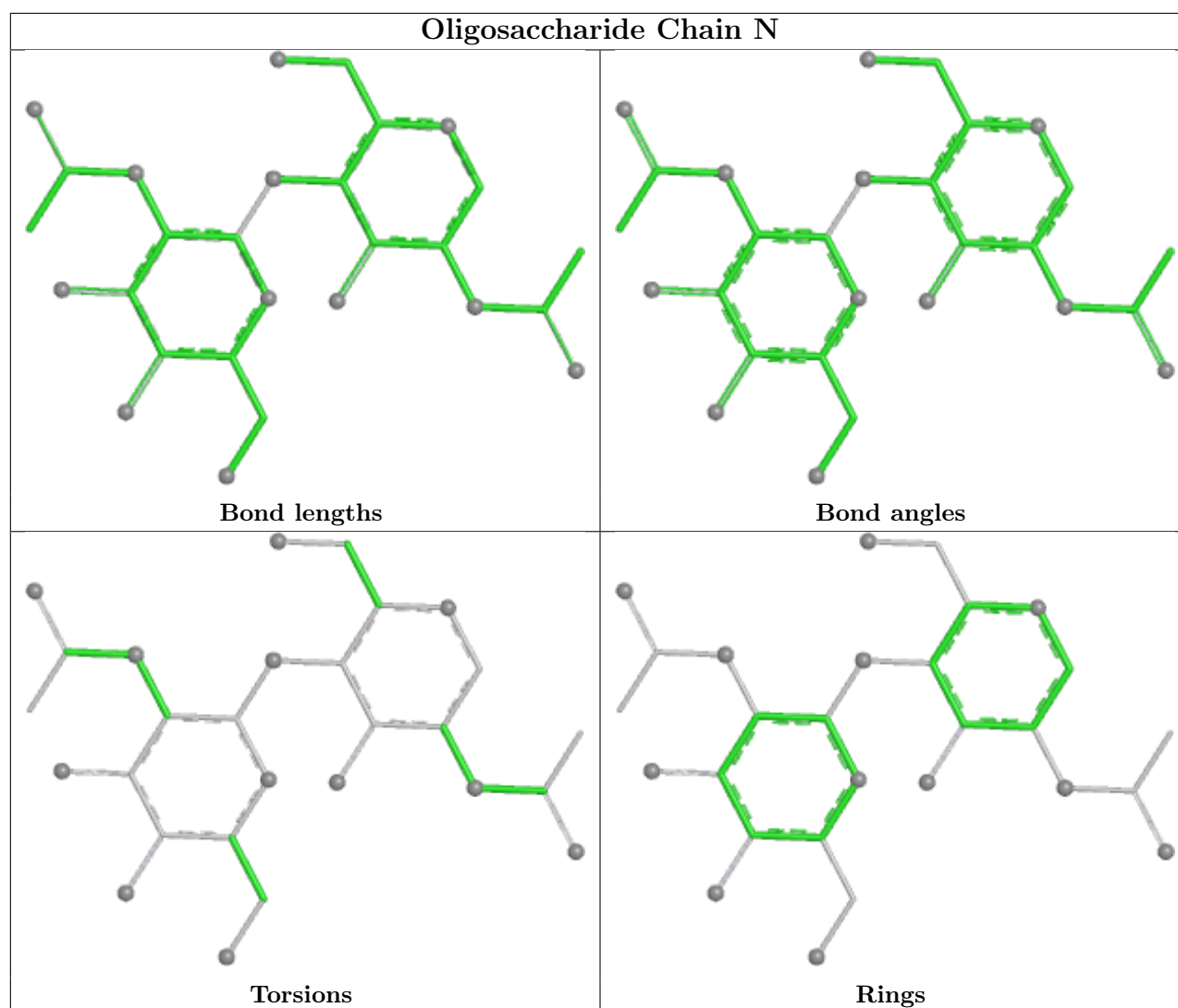


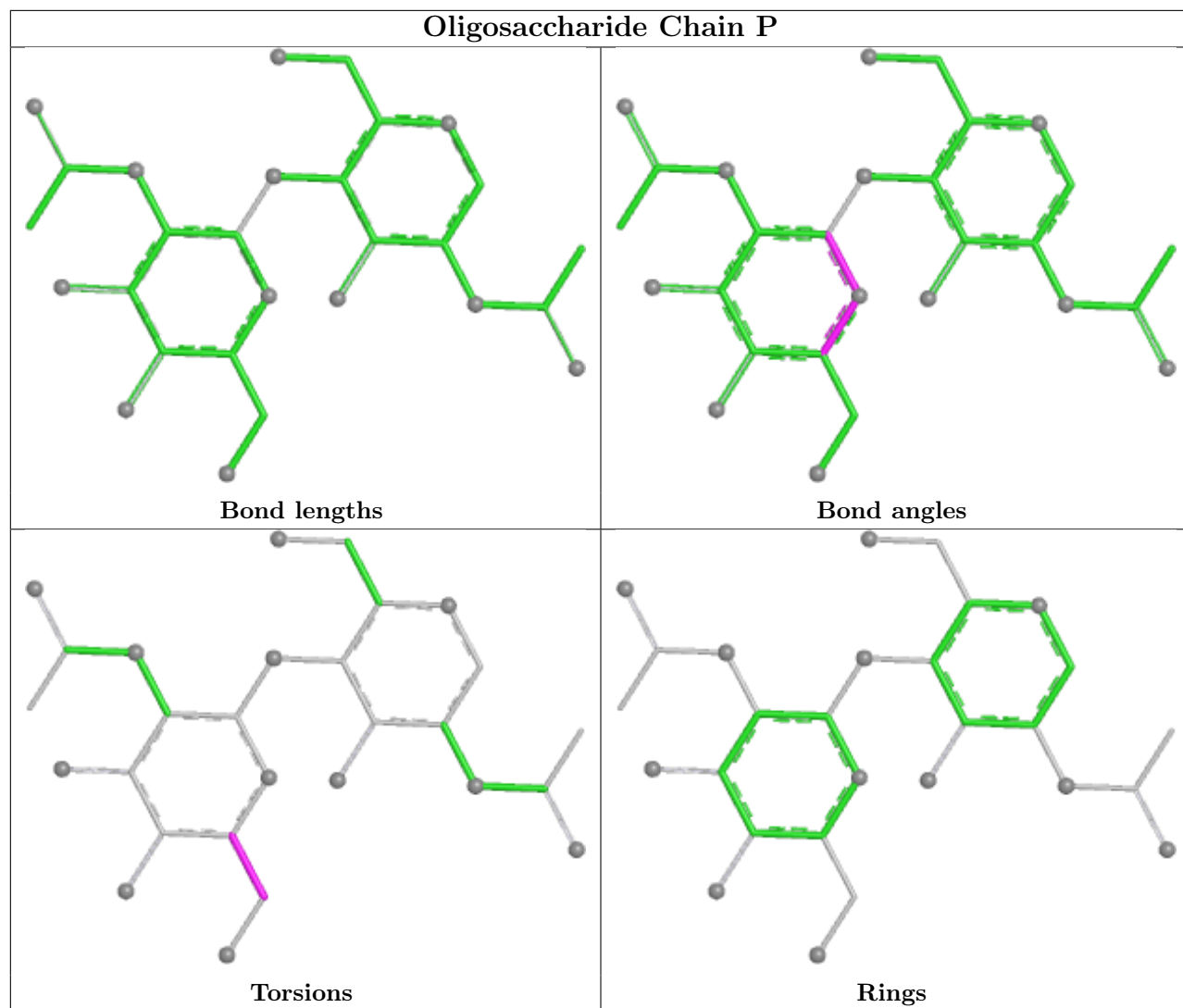


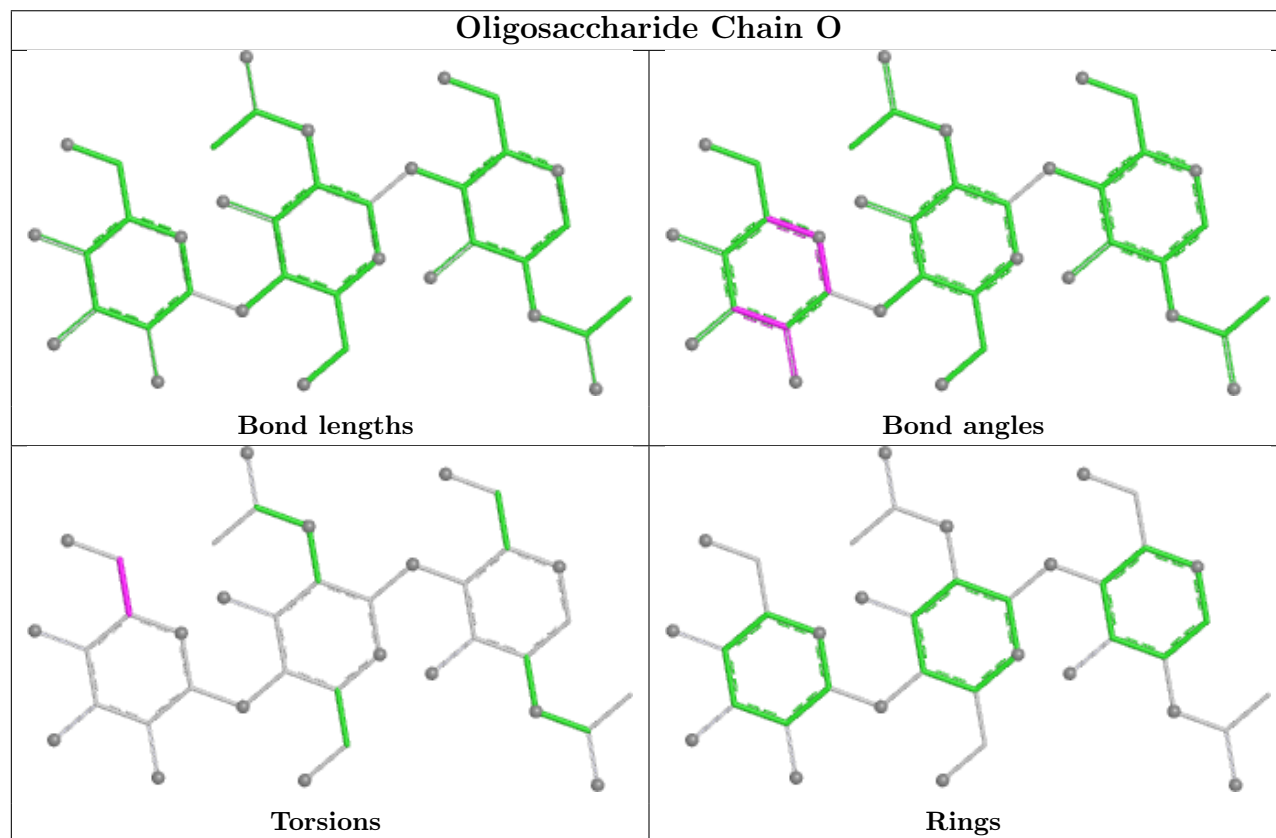
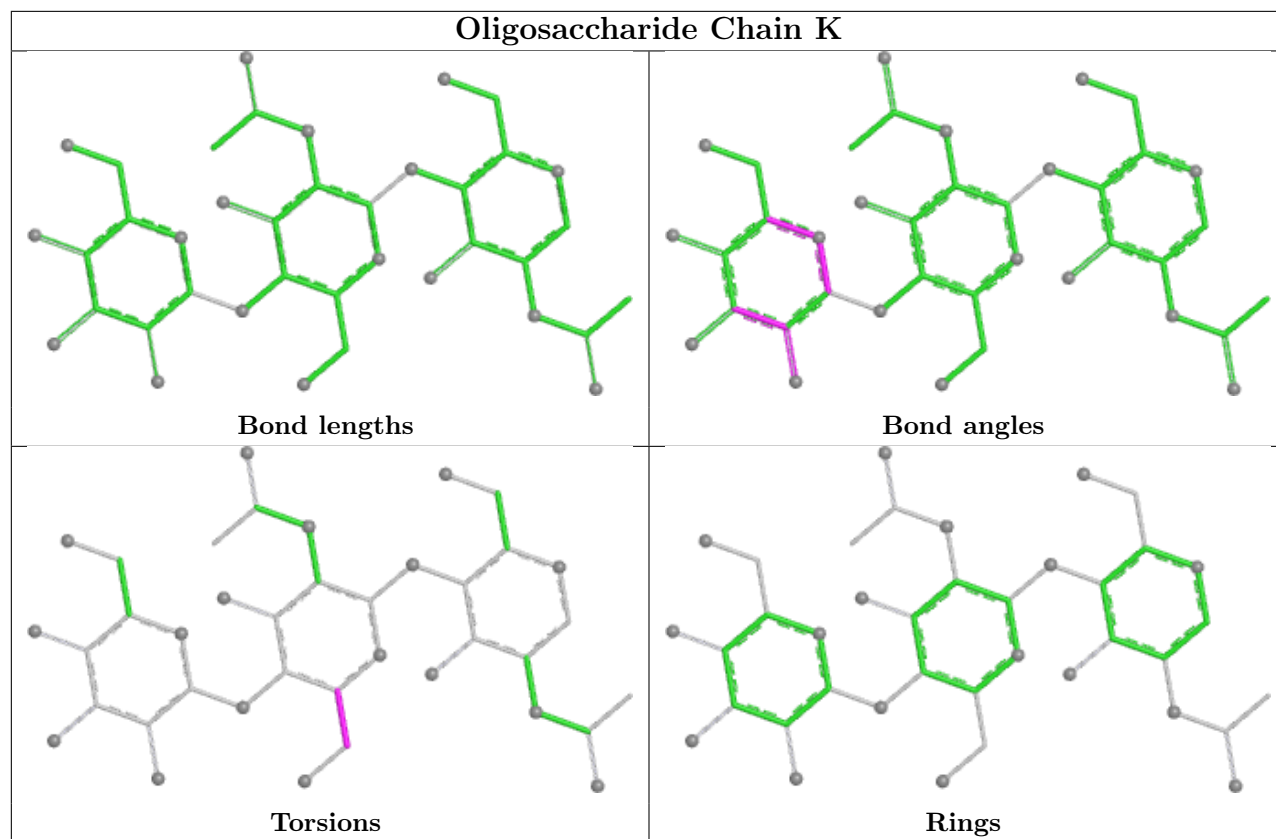












5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	F	606	1	14,14,15	0.50	0	17,19,21	0.45	0
4	NAG	E	605	1	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	A	604	1	14,14,15	0.32	0	17,19,21	0.64	0
4	NAG	A	601	1	14,14,15	0.31	0	17,19,21	0.73	0
4	NAG	C	605	1	14,14,15	0.44	0	17,19,21	0.72	1 (5%)
4	NAG	B	601	1	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
4	NAG	B	604	1	14,14,15	0.25	0	17,19,21	0.65	0
4	NAG	D	606	1	14,14,15	0.66	1 (7%)	17,19,21	0.54	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
4	NAG	F	606	1	-	2/6/23/26	0/1/1/1
4	NAG	E	605	1	-	1/6/23/26	0/1/1/1
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
4	NAG	C	605	1	-	2/6/23/26	0/1/1/1
4	NAG	B	601	1	-	0/6/23/26	0/1/1/1
4	NAG	B	604	1	-	2/6/23/26	0/1/1/1
4	NAG	D	606	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	606	NAG	C1-C2	2.23	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	605	NAG	C1-O5-C5	2.14	115.05	112.19
4	B	601	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	605	NAG	O5-C5-C6-O6
4	A	604	NAG	C4-C5-C6-O6
4	B	604	NAG	C4-C5-C6-O6
4	C	605	NAG	C4-C5-C6-O6
4	A	604	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	491/496 (98%)	-0.06	8 (1%) 70 74	15, 24, 40, 66	0
1	B	491/496 (98%)	-0.07	6 (1%) 76 79	14, 23, 39, 66	0
1	C	491/496 (98%)	0.08	9 (1%) 67 71	13, 26, 43, 82	0
1	D	491/496 (98%)	0.06	15 (3%) 51 55	14, 25, 47, 128	0
1	E	491/496 (98%)	0.09	10 (2%) 65 69	15, 26, 45, 77	0
1	F	491/496 (98%)	0.10	14 (2%) 53 57	15, 26, 47, 136	0
All	All	2946/2976 (98%)	0.03	62 (2%) 63 67	13, 25, 43, 136	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	502	ILE	10.3
1	F	502	ILE	10.0
1	D	503	LYS	7.1
1	F	503	LYS	6.5
1	C	503	LYS	5.1

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

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

6.3 Carbohydrates [i](#)

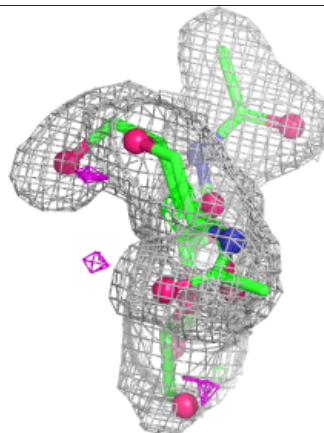
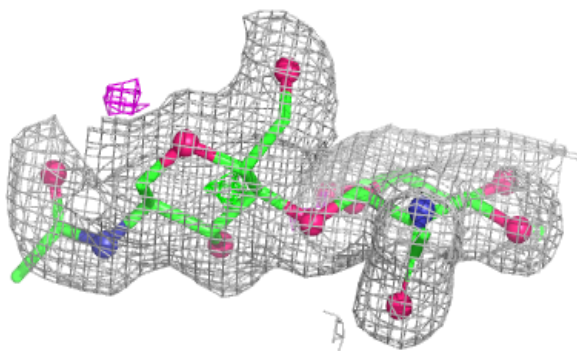
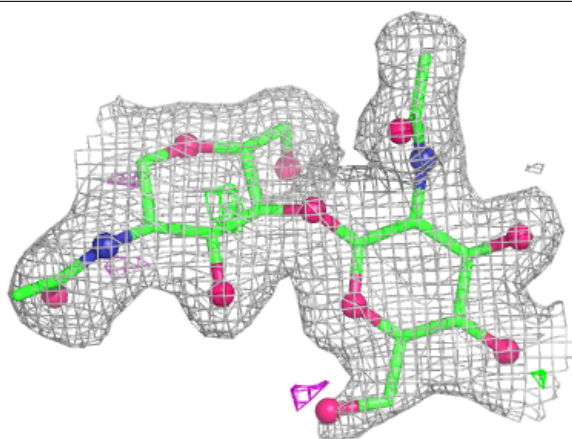
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	K	3	11/12	0.66	0.12	58,65,67,67	0
3	BMA	O	3	11/12	0.69	0.12	60,64,67,67	0
2	NAG	P	2	14/15	0.83	0.13	22,37,43,45	0
2	NAG	M	2	14/15	0.86	0.10	43,46,51,51	0
2	NAG	I	2	14/15	0.86	0.11	45,48,50,51	0
3	NAG	O	2	14/15	0.87	0.10	41,45,53,53	0
3	NAG	K	2	14/15	0.88	0.10	41,43,49,50	0
2	NAG	N	2	14/15	0.89	0.10	32,40,48,51	0
3	NAG	O	1	14/15	0.89	0.10	29,36,40,44	0
2	NAG	L	2	14/15	0.89	0.10	22,34,42,46	0
2	NAG	H	2	14/15	0.89	0.10	27,36,46,50	0
2	NAG	G	2	14/15	0.90	0.10	26,34,45,49	0
2	NAG	M	1	14/15	0.90	0.10	31,39,50,50	0
2	NAG	J	2	14/15	0.91	0.09	26,41,46,48	0
2	NAG	N	1	14/15	0.91	0.10	22,35,45,49	0
2	NAG	I	1	14/15	0.91	0.10	29,38,45,46	0
2	NAG	H	1	14/15	0.91	0.10	23,29,36,37	0
3	NAG	K	1	14/15	0.91	0.09	29,35,39,44	0
2	NAG	J	1	14/15	0.92	0.09	22,34,42,45	0
2	NAG	G	1	14/15	0.94	0.09	23,31,39,41	0
2	NAG	P	1	14/15	0.95	0.07	23,32,39,41	0
2	NAG	L	1	14/15	0.95	0.08	21,28,36,39	0

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

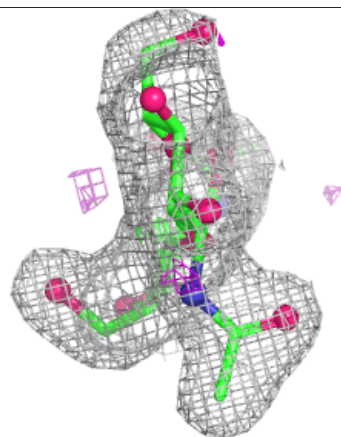
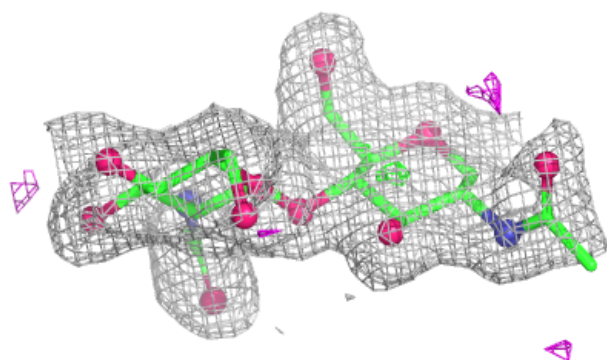
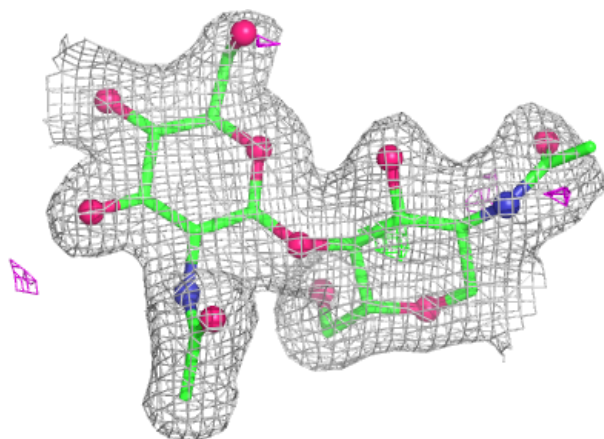
Electron density around Chain G:

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



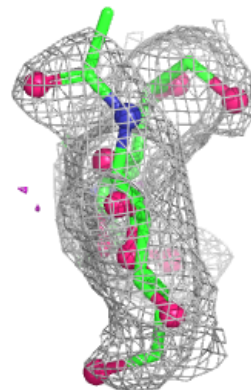
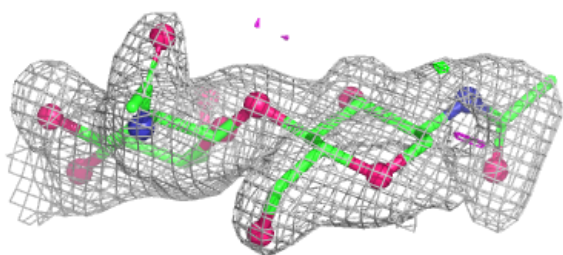
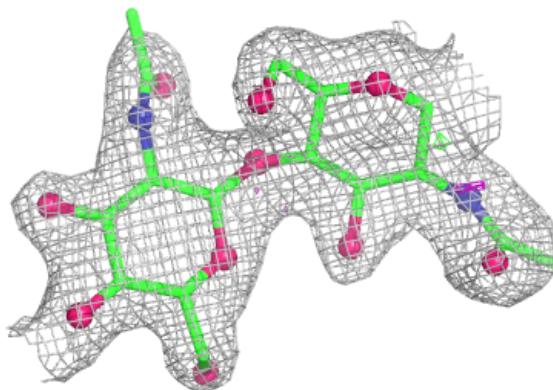
Electron density around Chain H:

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



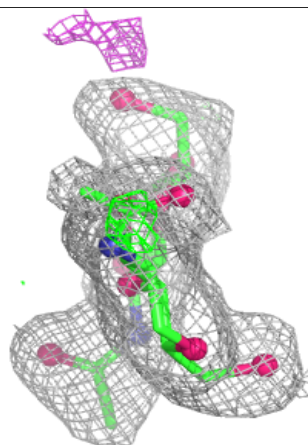
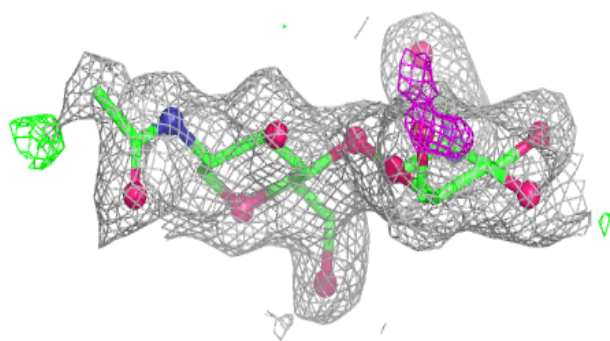
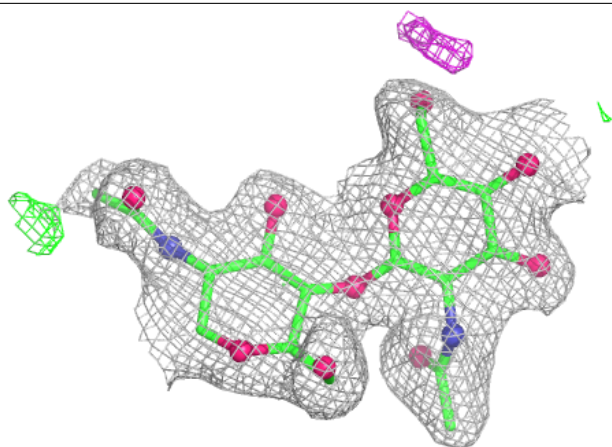
Electron density around Chain I:

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



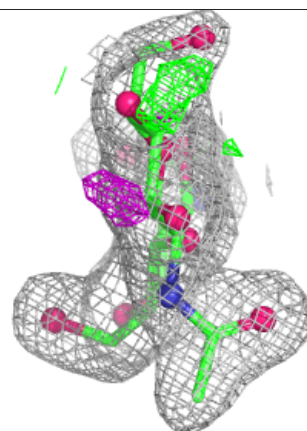
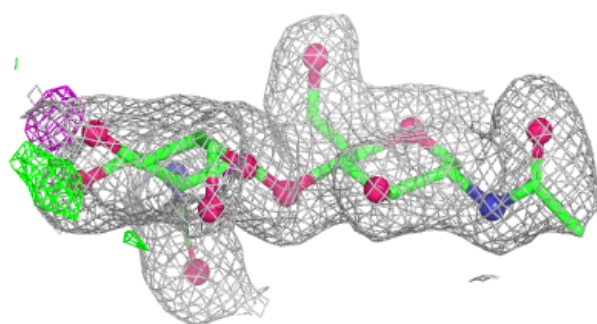
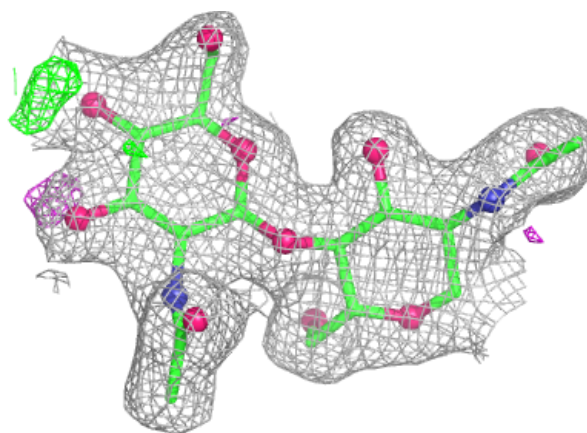
Electron density around Chain J:

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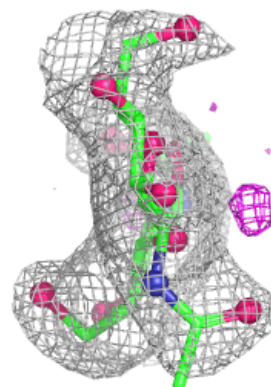
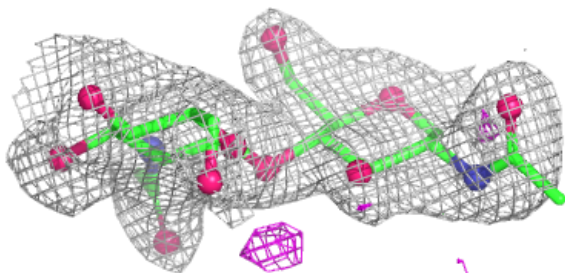
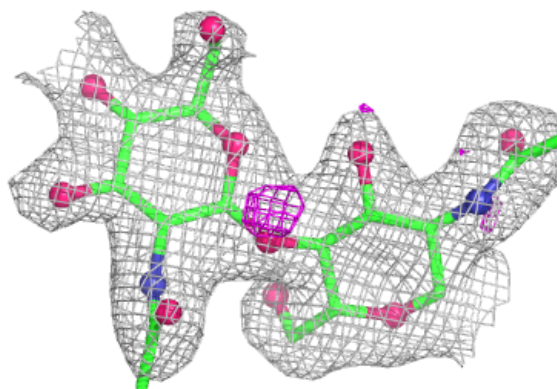


Electron density around Chain L:

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

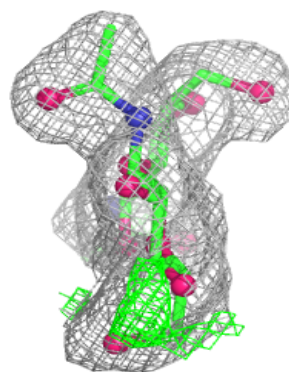
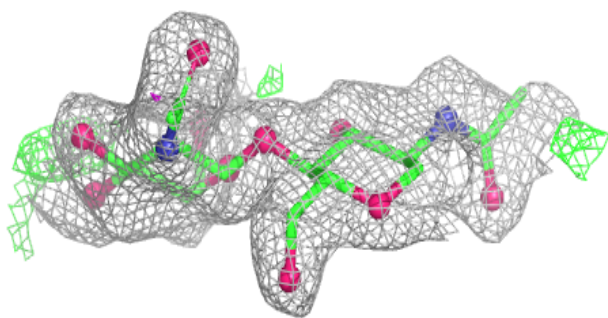
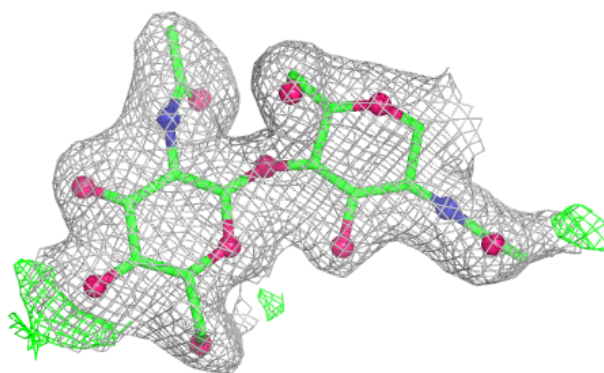
**Electron density around Chain M:**

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



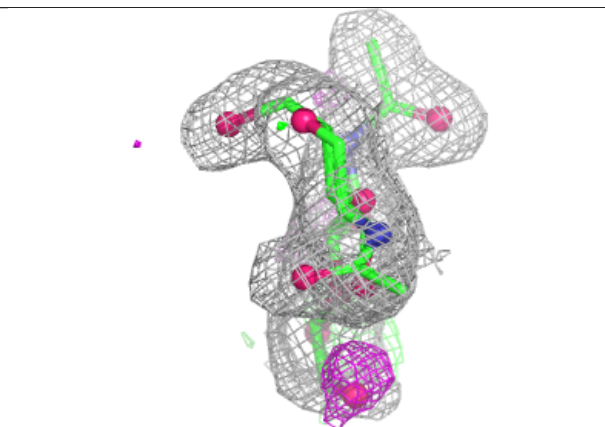
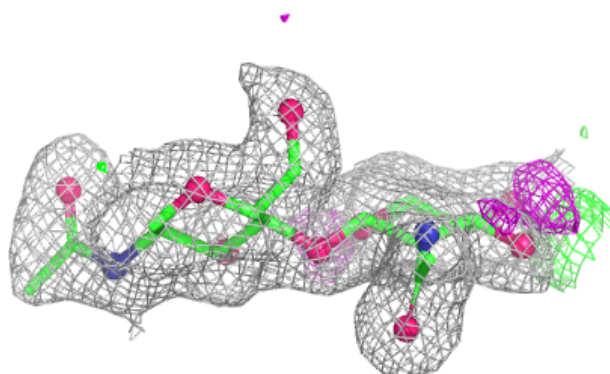
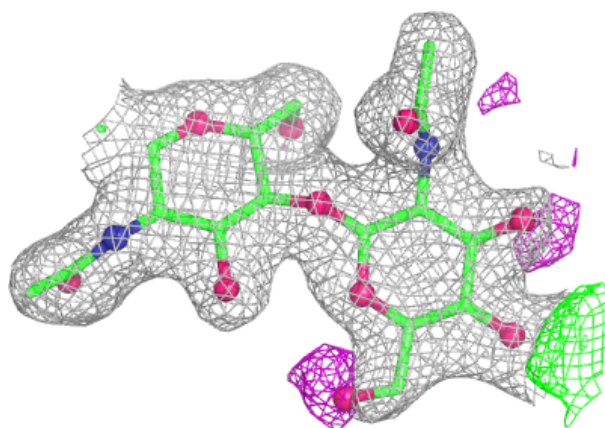
Electron density around Chain N:

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and green (positive)

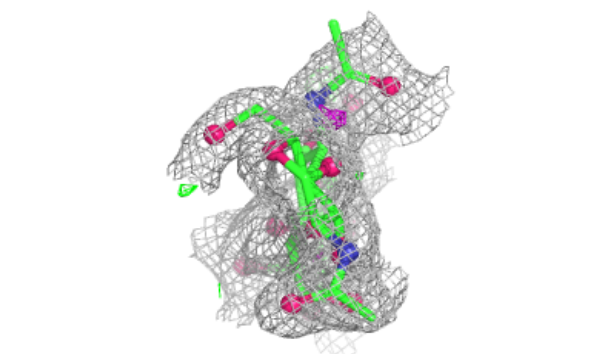
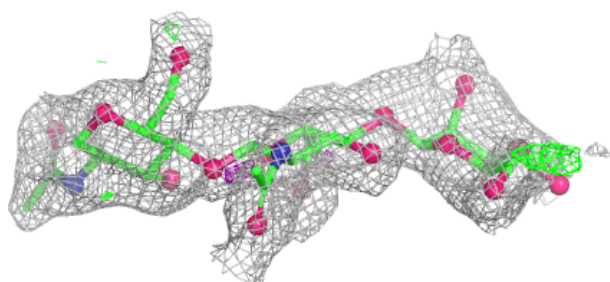
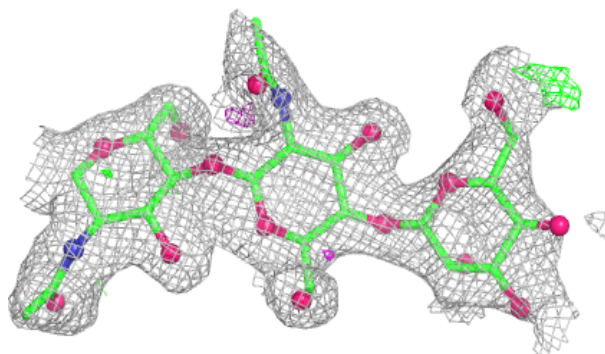


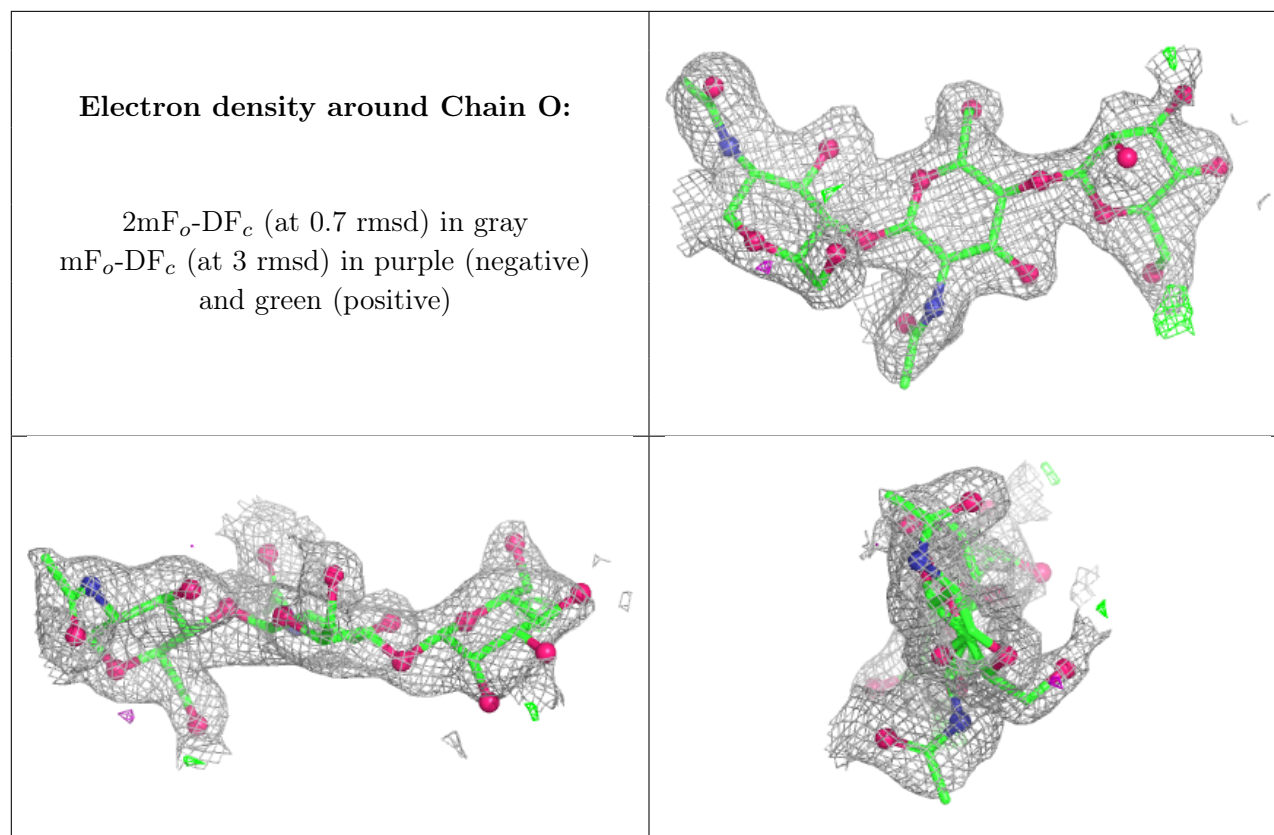
Electron density around Chain P:

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

**Electron density around Chain K:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	601	14/15	0.80	0.13	35,43,50,54	0
4	NAG	C	605	14/15	0.80	0.13	36,44,52,56	0
4	NAG	B	601	14/15	0.81	0.13	31,41,48,49	0
4	NAG	B	604	14/15	0.85	0.12	33,37,46,47	0
4	NAG	D	606	14/15	0.85	0.11	30,37,44,46	0
4	NAG	F	606	14/15	0.85	0.10	30,38,43,44	0
4	NAG	E	605	14/15	0.86	0.10	37,44,48,51	0
4	NAG	A	604	14/15	0.87	0.10	34,38,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.