



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:33 AM UTC

PDB ID : 4M40 / pdb_00004m40
Title : Crystal structure of hemagglutinin of influenza virus B/Yamanashi/166/1998
Authors : Ni, F.; Kondrashkina, E.; Wang, Q.
Deposited on : 2013-08-06
Resolution : 3.54 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

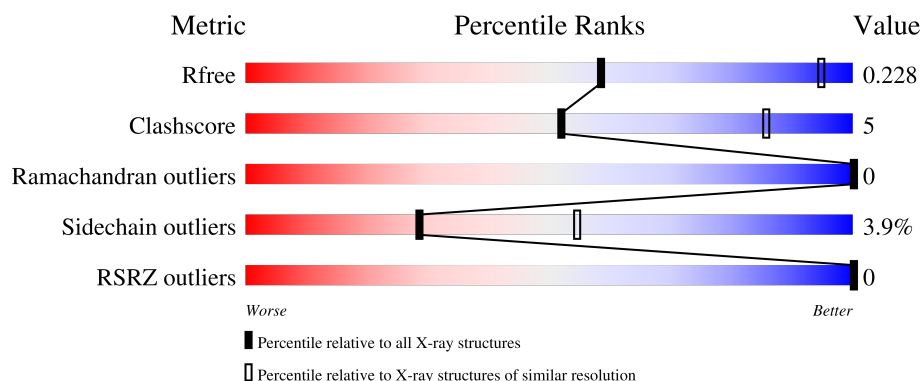
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 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	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	346	 83% 15% ..
1	C	346	 86% 11% ..
1	E	346	 84% 14% ..
2	B	182	 79% 13% • 6%
2	D	182	 81% 12% • 7%

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Mol	Chain	Length	Quality of chain
2	F	182	80%13%6%
3	G	2	50%50%
3	H	2	100%
3	I	2	50%50%
3	J	2	100%
3	K	2	50%50%
3	L	2	100%
3	M	2	50%50%
3	N	2	50%50%
3	O	2	50%50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12115 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2600	1633	464	487	16			
1	C	343	Total	C	N	O	S	0	0	0
			2600	1633	464	487	16			
1	E	343	Total	C	N	O	S	0	0	0
			2600	1633	464	487	16			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1301	814	222	259	6			
2	D	170	Total	C	N	O	S	0	0	0
			1293	808	221	258	6			
2	F	171	Total	C	N	O	S	0	0	0
			1301	814	222	259	6			

There are 18 discrepancies between the modelled and reference sequences:

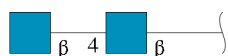
Chain	Residue	Modelled	Actual	Comment	Reference
B	177	GLY	-	expression tag	UNP A3DQM7
B	178	ALA	-	expression tag	UNP A3DQM7
B	179	LEU	-	expression tag	UNP A3DQM7
B	180	VAL	-	expression tag	UNP A3DQM7
B	181	PRO	-	expression tag	UNP A3DQM7
B	182	ARG	-	expression tag	UNP A3DQM7
D	177	GLY	-	expression tag	UNP A3DQM7
D	178	ALA	-	expression tag	UNP A3DQM7
D	179	LEU	-	expression tag	UNP A3DQM7
D	180	VAL	-	expression tag	UNP A3DQM7
D	181	PRO	-	expression tag	UNP A3DQM7
D	182	ARG	-	expression tag	UNP A3DQM7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	177	GLY	-	expression tag	UNP A3DQM7
F	178	ALA	-	expression tag	UNP A3DQM7
F	179	LEU	-	expression tag	UNP A3DQM7
F	180	VAL	-	expression tag	UNP A3DQM7
F	181	PRO	-	expression tag	UNP A3DQM7
F	182	ARG	-	expression tag	UNP A3DQM7

- Molecule 3 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
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

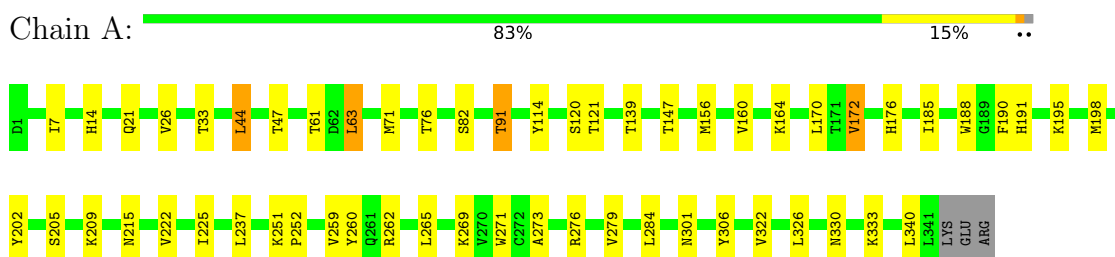


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1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

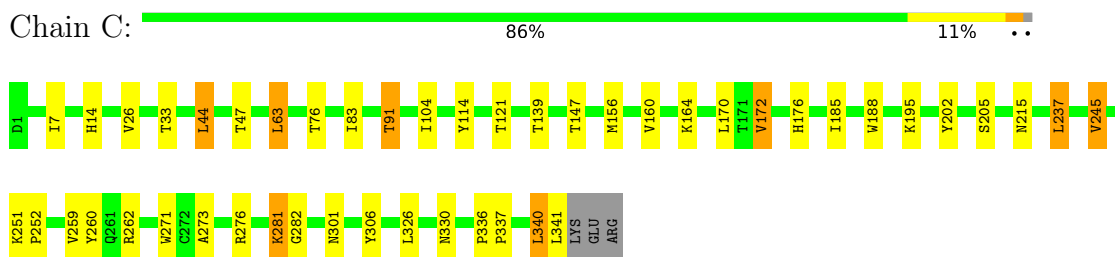
3 Residue-property plots [i](#)

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.

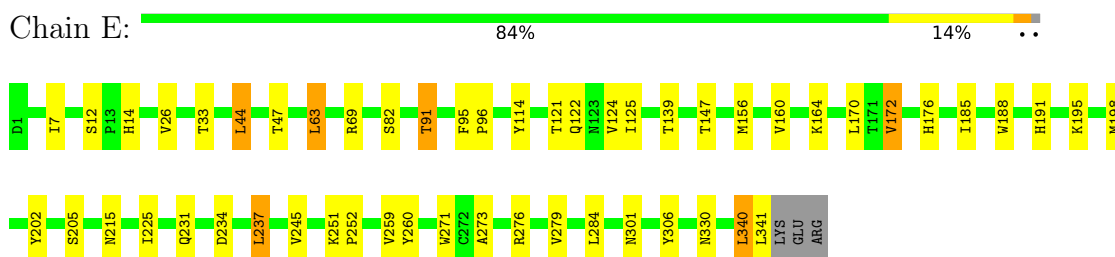
- Molecule 1: Hemagglutinin HA1



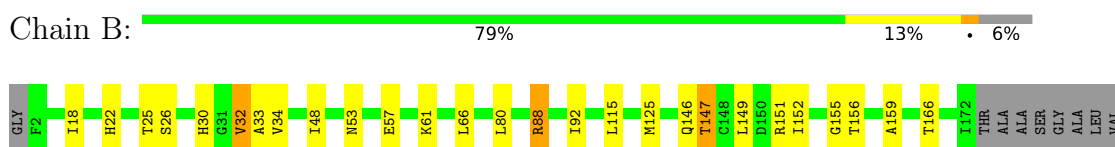
- Molecule 1: Hemagglutinin HA1



- Molecule 1: Hemagglutinin HA1



- Molecule 2: Hemagglutinin HA2



PRO
ARG

• Molecule 2: Hemagglutinin HA2

Chain D:  81% 12% • 7%

GLY F2 I18 H22 S26 H30 G31 V32 A33 I48 K61 L66 I77 R88 I92 E97 L115 M125 L126 Q146 T147 R151 G155 T156 A159 T166 N171 ILE THR ALA ALA SER GLY ALA LEU VAL PRO ARG

• Molecule 2: Hemagglutinin HA2

Chain F:  80% 13% • 6%

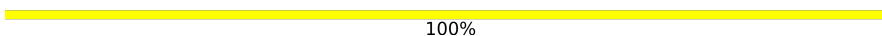
GLY F2 H22 S26 V32 A33 I48 N51 K61 I77 L78 E79 R88 T91 I92 S103 I107 L115 M125 Q146 T147 C148 L149 D150 R151 I152 G155 T156 A159 T166 I172 THR ALA ALA SER GLY ALA LEU VAL PRO ARG

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

Chain G:  50% 50%

NAG1
NAG2

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

Chain H:  100%

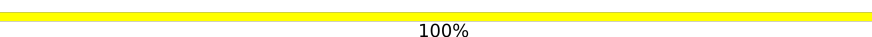
NAG1
NAG2

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

Chain I:  50% 50%

NAG1
NAG2

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

Chain J:  100%

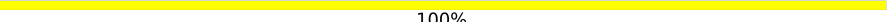
NAG1
NAG2

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

Chain K:  50% 50%

MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2

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

Chain M:  50% 50%

MAG1
MAG2

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

Chain N:  50% 50%

MAG1
MAG2

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

Chain O:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.91Å 101.29Å 136.81Å 90.00° 115.18° 90.00°	Depositor
Resolution (Å)	42.66 – 3.54 42.66 – 3.54	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.66-3.54) 99.1 (42.66-3.54)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1391)	Depositor
R, R_{free}	0.198 , 0.244 0.213 , 0.228	Depositor DCC
R_{free} test set	1334 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	106.9	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 92.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.409 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.409 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12115	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.36	1/2659 (0.0%)	0.83	2/3613 (0.1%)
1	C	0.38	0/2659	0.83	2/3613 (0.1%)
1	E	0.36	0/2659	0.84	2/3613 (0.1%)
2	B	0.41	1/1320 (0.1%)	0.79	1/1780 (0.1%)
2	D	0.36	0/1312	0.79	1/1769 (0.1%)
2	F	0.36	1/1320 (0.1%)	0.78	0/1780
All	All	0.37	3/11929 (0.0%)	0.82	8/16168 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	147	THR	C-N	-7.32	1.24	1.33
2	F	147	THR	C-N	-7.02	1.24	1.33
1	A	61	THR	C-N	-5.78	1.26	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	THR	CA-C-N	5.87	125.83	119.78
1	A	76	THR	C-N-CA	5.87	125.83	119.78
1	C	76	THR	CA-C-N	5.63	125.58	119.78
1	C	76	THR	C-N-CA	5.63	125.58	119.78
1	E	69	ARG	CA-C-N	5.45	125.46	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2600	0	2622	31	0
1	C	2600	0	2622	25	0
1	E	2600	0	2621	27	0
2	B	1301	0	1273	21	0
2	D	1293	0	1262	14	0
2	F	1301	0	1273	17	0
3	G	28	0	25	0	0
3	H	28	0	25	1	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	1	0
3	L	28	0	25	0	0
3	M	28	0	25	2	0
3	N	28	0	25	1	0
3	O	28	0	25	2	0
4	A	42	0	39	1	0
4	B	14	0	13	0	0
4	C	42	0	39	0	0
4	D	14	0	13	0	0
4	E	42	0	39	1	0
4	F	14	0	13	0	0
All	All	12115	0	12054	124	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 124 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:A:340:LEU:HD21	2:B:32:VAL:HG11	1.38	1.03
1:A:209:LYS:HG2	1:A:222:VAL:HG22	1.55	0.88
1:C:83:ILE:HG23	1:C:282:GLY:HA3	1.63	0.79
2:D:61:LYS:O	2:D:88:ARG:NH2	2.19	0.75
2:F:61:LYS:O	2:F:88:ARG:NH2	2.21	0.74

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	341/346 (99%)	327 (96%)	14 (4%)	0	100	100
1	C	341/346 (99%)	327 (96%)	14 (4%)	0	100	100
1	E	341/346 (99%)	328 (96%)	13 (4%)	0	100	100
2	B	169/182 (93%)	163 (96%)	6 (4%)	0	100	100
2	D	168/182 (92%)	163 (97%)	5 (3%)	0	100	100
2	F	169/182 (93%)	164 (97%)	5 (3%)	0	100	100
All	All	1529/1584 (96%)	1472 (96%)	57 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/294 (99%)	280 (96%)	11 (4%)	29	56
1	C	291/294 (99%)	277 (95%)	14 (5%)	23	49
1	E	291/294 (99%)	278 (96%)	13 (4%)	24	51
2	B	139/145 (96%)	135 (97%)	4 (3%)	37	60
2	D	138/145 (95%)	134 (97%)	4 (3%)	37	60
2	F	139/145 (96%)	135 (97%)	4 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1289/1317 (98%)	1239 (96%)	50 (4%)	28 54

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	340	LEU
1	E	91	THR
2	F	88	ARG
2	D	18	ILE
2	D	88	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	42	GLN
1	C	317	ASN
2	B	142	HIS
2	B	95	GLN
1	C	215	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 ⓘ

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	1	1,3	14,14,15	0.28	0	17,19,21	0.76	1 (5%)
3	NAG	G	2	3	14,14,15	0.38	0	17,19,21	0.59	0
3	NAG	H	1	1,3	14,14,15	0.41	0	17,19,21	0.73	0
3	NAG	H	2	3	14,14,15	1.08	1 (7%)	17,19,21	1.25	1 (5%)
3	NAG	I	1	1,3	14,14,15	0.30	0	17,19,21	0.71	0
3	NAG	I	2	3	14,14,15	0.87	1 (7%)	17,19,21	1.07	1 (5%)
3	NAG	J	1	1,3	14,14,15	0.63	0	17,19,21	1.18	2 (11%)
3	NAG	J	2	3	14,14,15	0.81	1 (7%)	17,19,21	1.00	1 (5%)
3	NAG	K	1	1,3	14,14,15	0.49	0	17,19,21	0.83	1 (5%)
3	NAG	K	2	3	14,14,15	1.00	1 (7%)	17,19,21	1.27	1 (5%)
3	NAG	L	1	1,3	14,14,15	0.29	0	17,19,21	1.25	1 (5%)
3	NAG	L	2	3	14,14,15	0.70	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	M	1	1,3	14,14,15	0.53	0	17,19,21	0.58	0
3	NAG	M	2	3	14,14,15	0.43	0	17,19,21	1.40	2 (11%)
3	NAG	N	1	1,3	14,14,15	0.36	0	17,19,21	0.81	1 (5%)
3	NAG	N	2	3	14,14,15	1.04	1 (7%)	17,19,21	1.19	1 (5%)
3	NAG	O	1	1,3	14,14,15	0.26	0	17,19,21	0.64	0
3	NAG	O	2	3	14,14,15	1.03	2 (14%)	17,19,21	0.92	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	4/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	6/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	O	2	3	-	3/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	NAG	O5-C1	3.92	1.50	1.43
3	N	2	NAG	O5-C1	3.74	1.50	1.43
3	K	2	NAG	O5-C1	3.60	1.49	1.43
3	I	2	NAG	O5-C1	3.11	1.48	1.43
3	J	2	NAG	O5-C1	2.74	1.48	1.43

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	2	NAG	C1-O5-C5	5.01	118.90	112.19
3	H	2	NAG	C1-O5-C5	4.88	118.73	112.19
3	N	2	NAG	C1-O5-C5	4.65	118.42	112.19
3	M	2	NAG	C2-N2-C7	4.58	129.04	122.90
3	L	1	NAG	C1-O5-C5	4.38	118.06	112.19

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	2	NAG	C1-C2-N2-C7
3	L	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 7 short contacts:

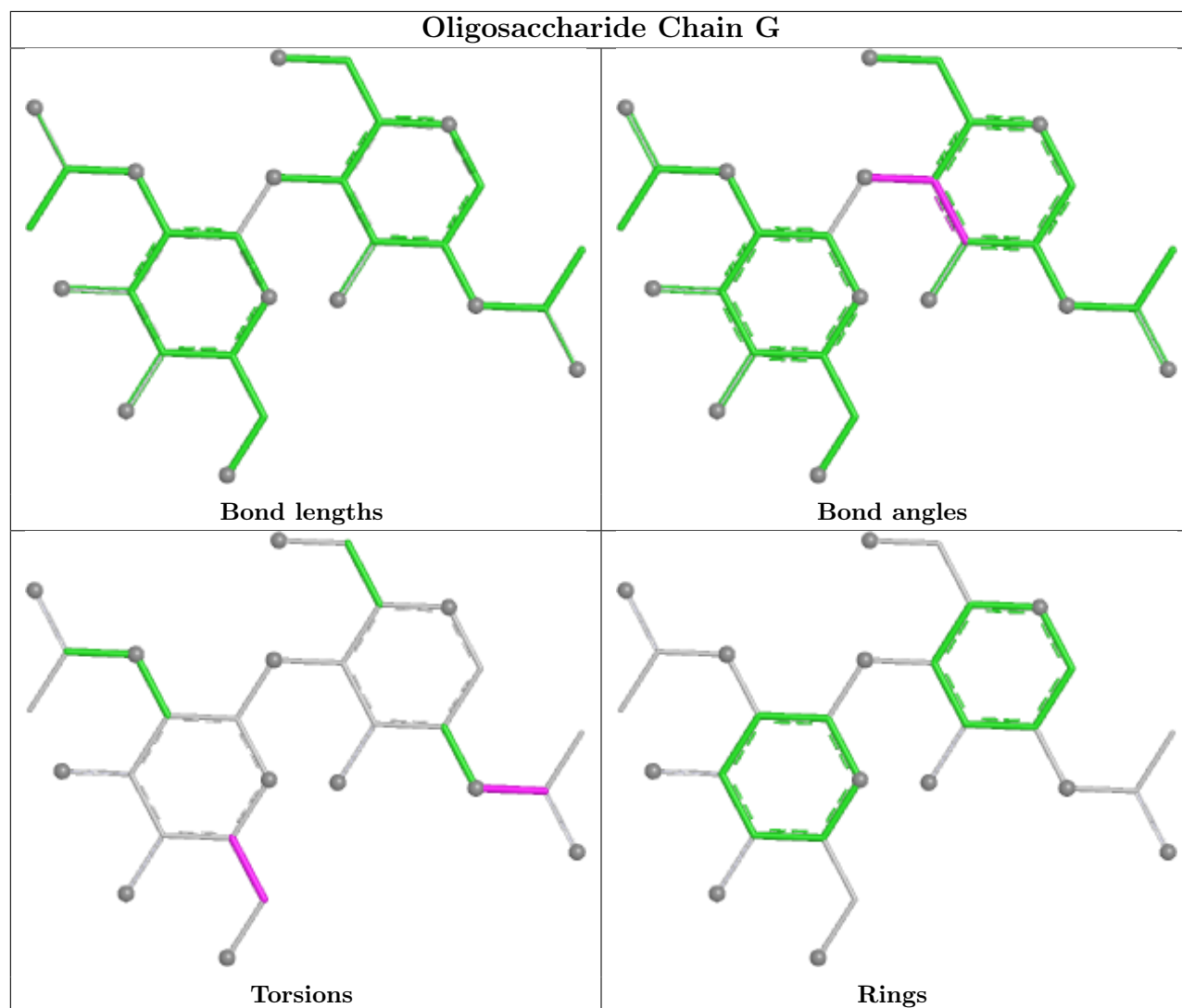
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	1	0

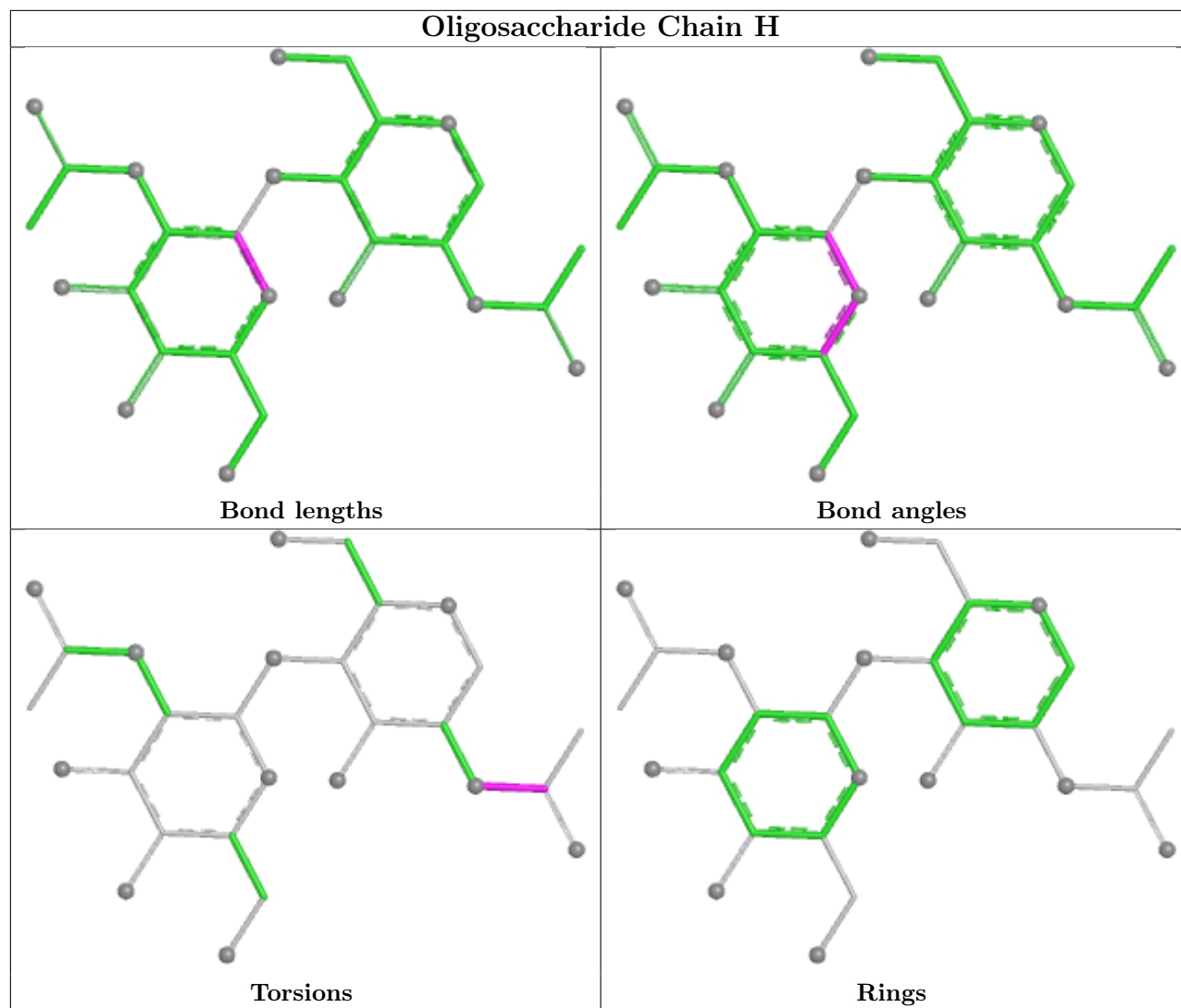
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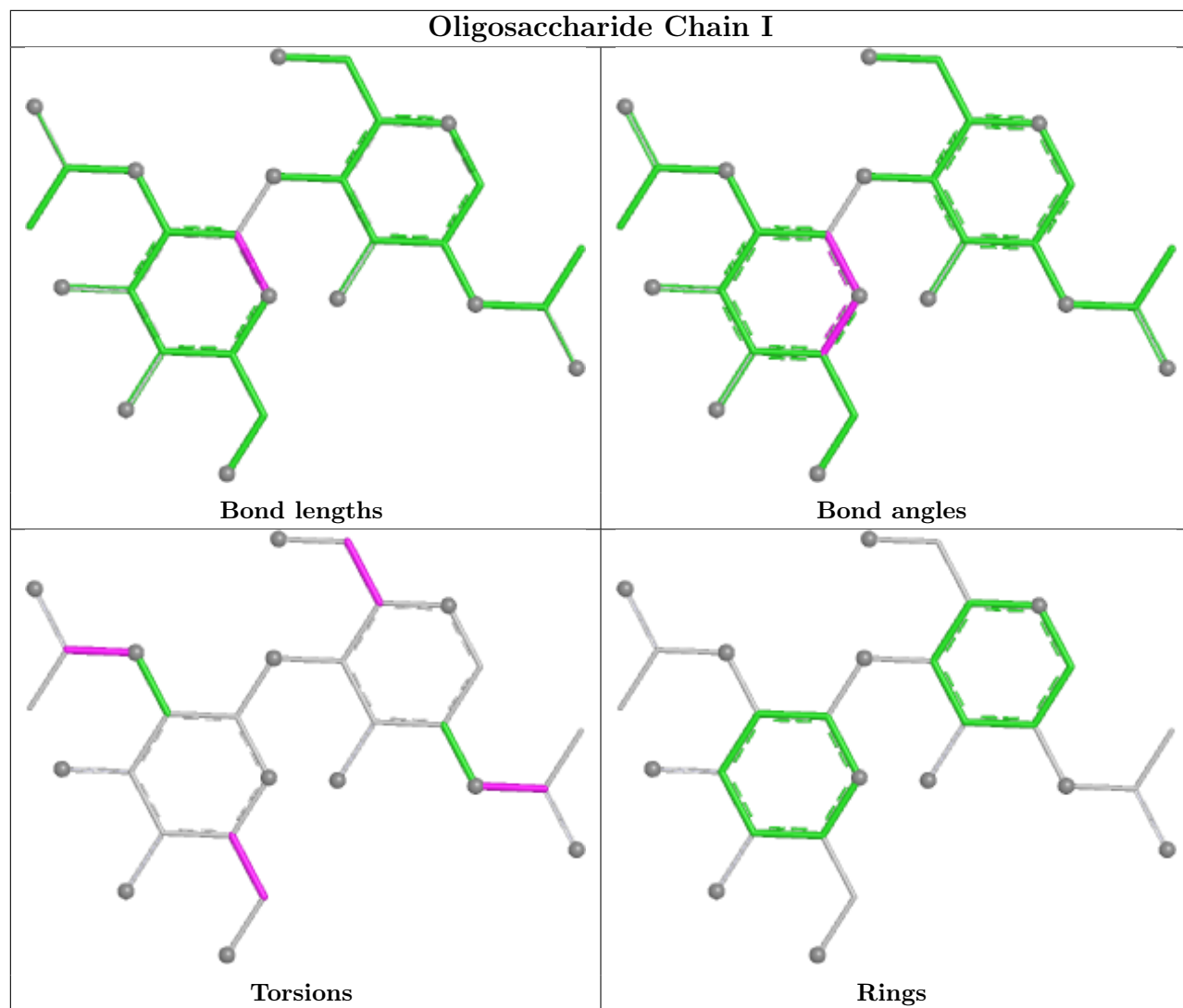
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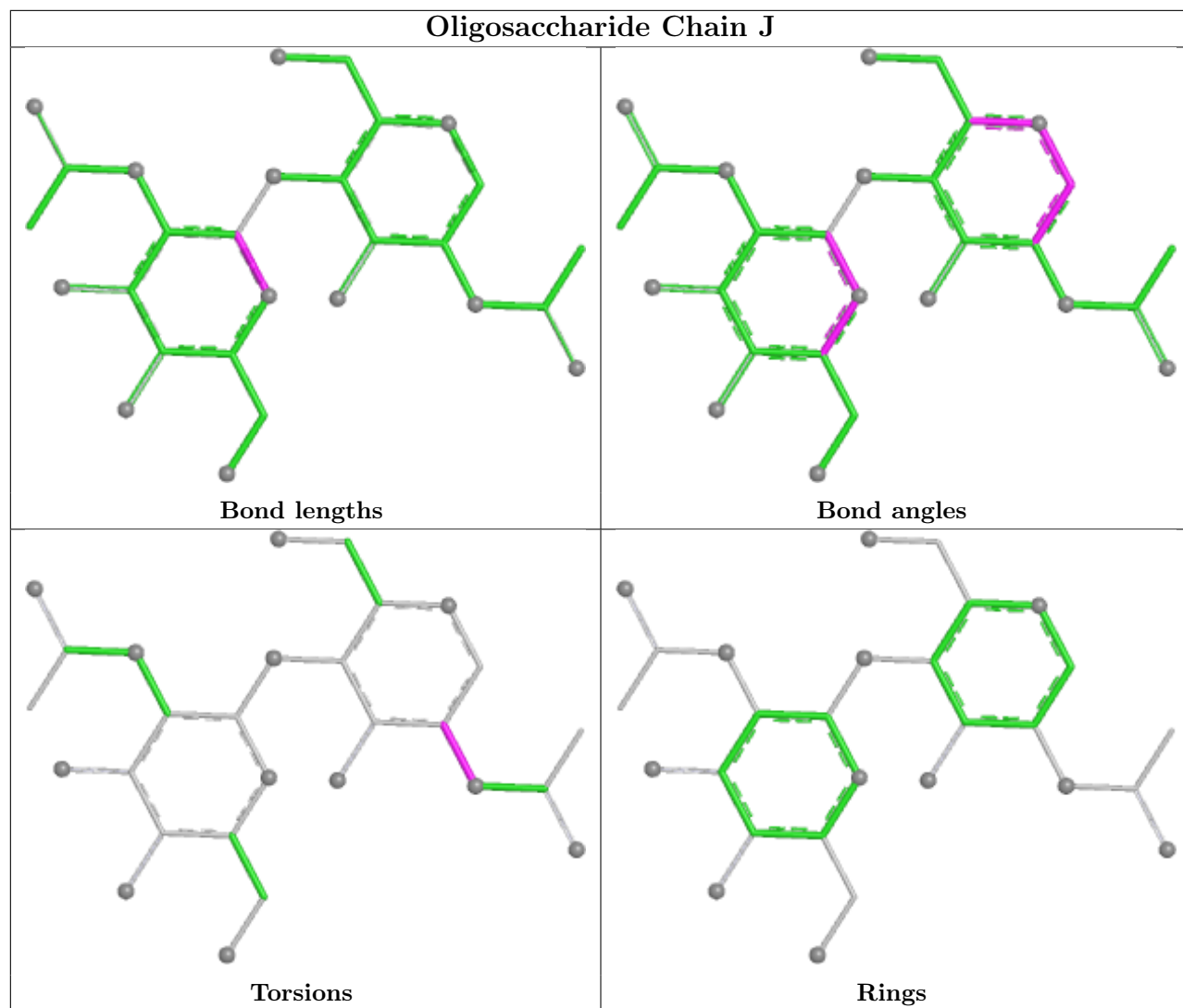
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1	NAG	1	0
3	O	2	NAG	2	0
3	M	2	NAG	1	0
3	H	1	NAG	1	0
3	K	1	NAG	1	0
3	O	1	NAG	1	0

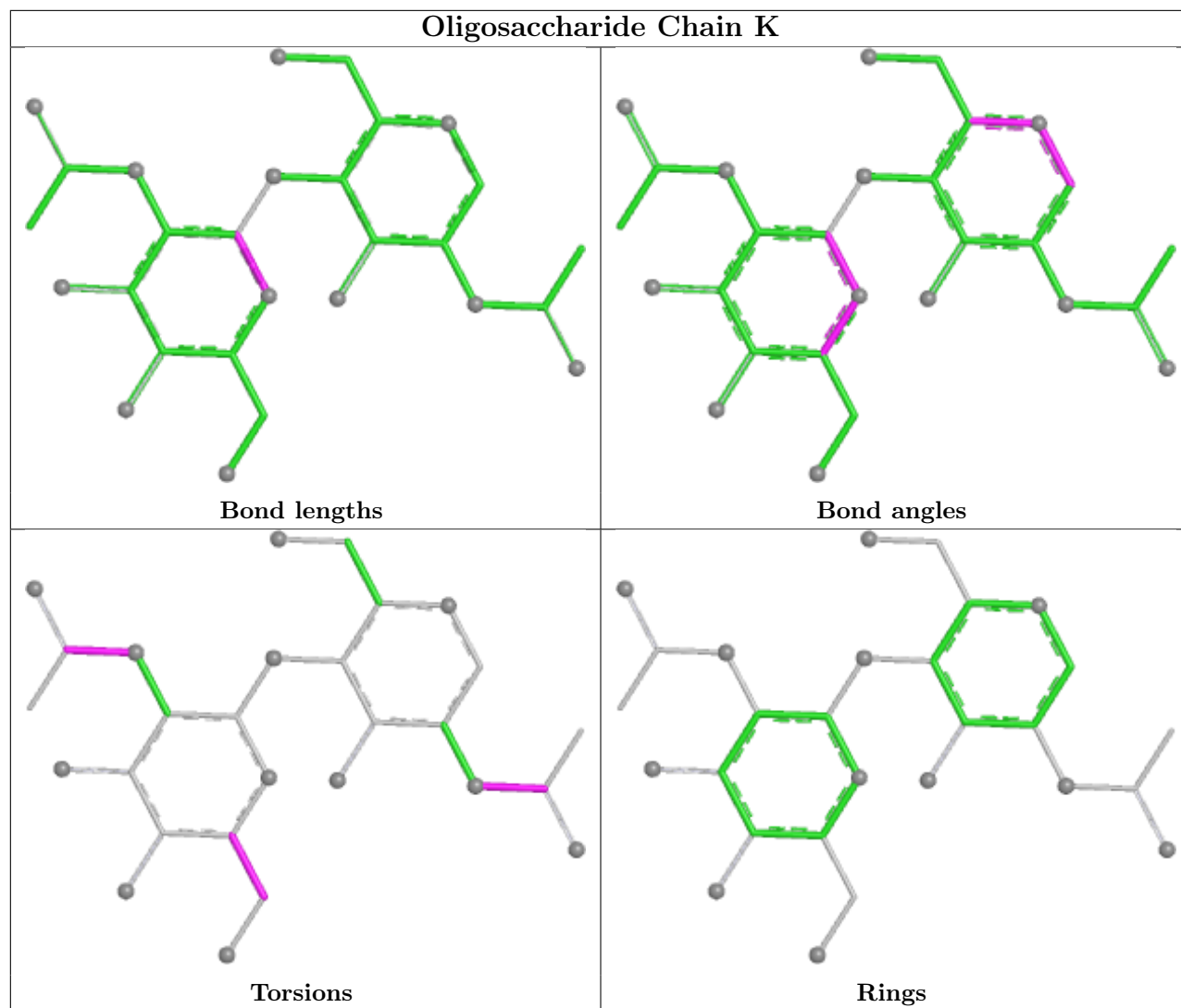
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

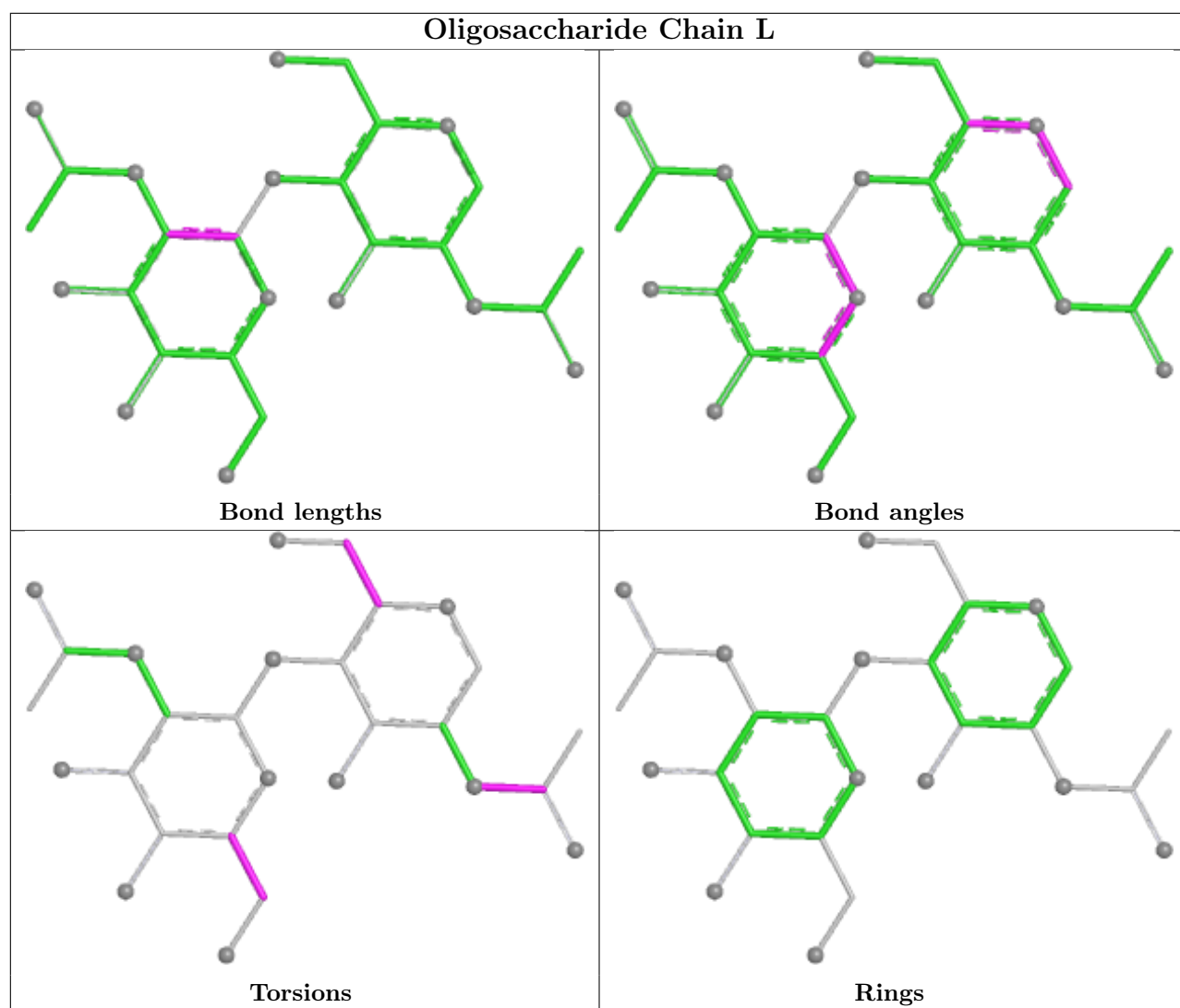


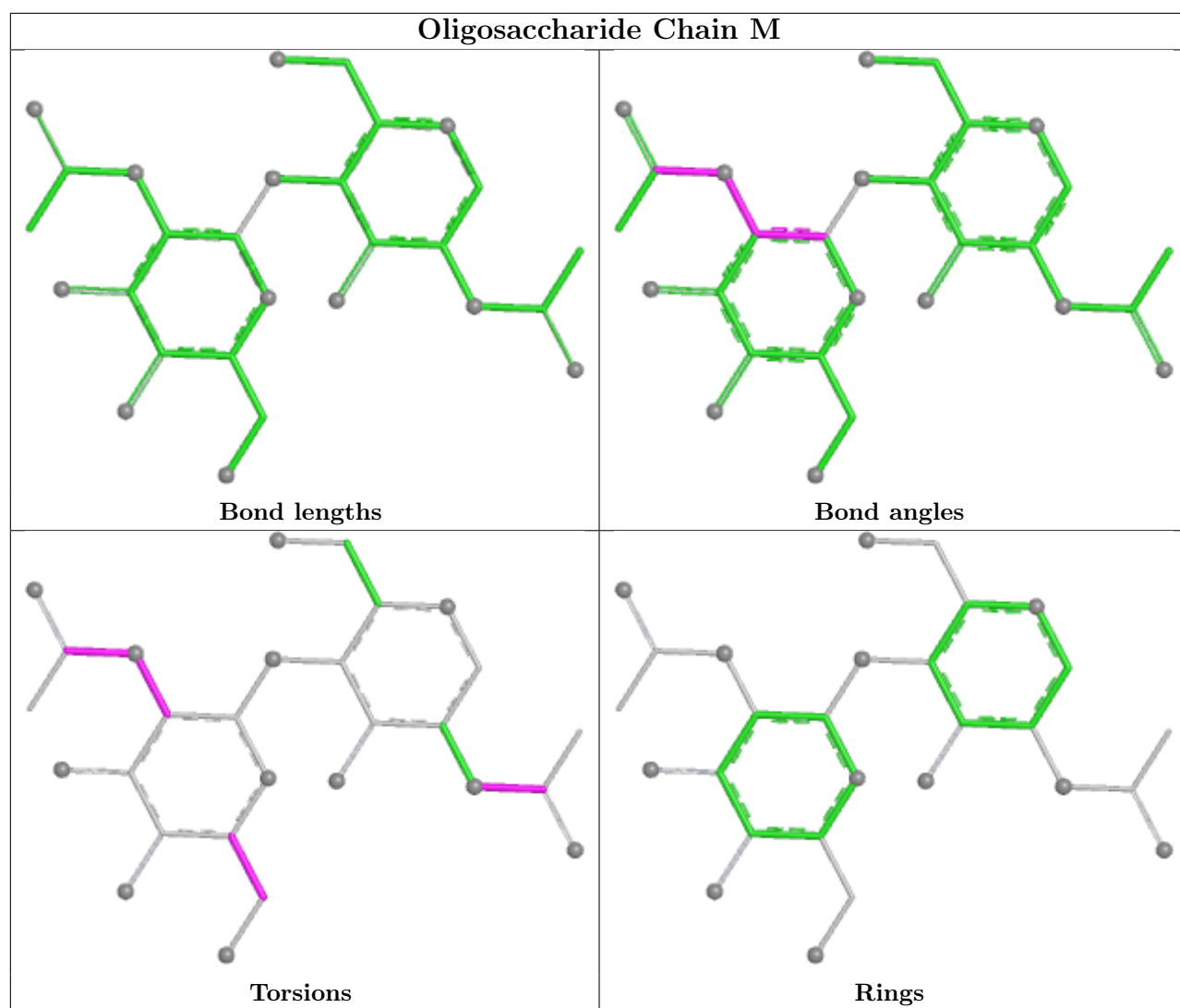


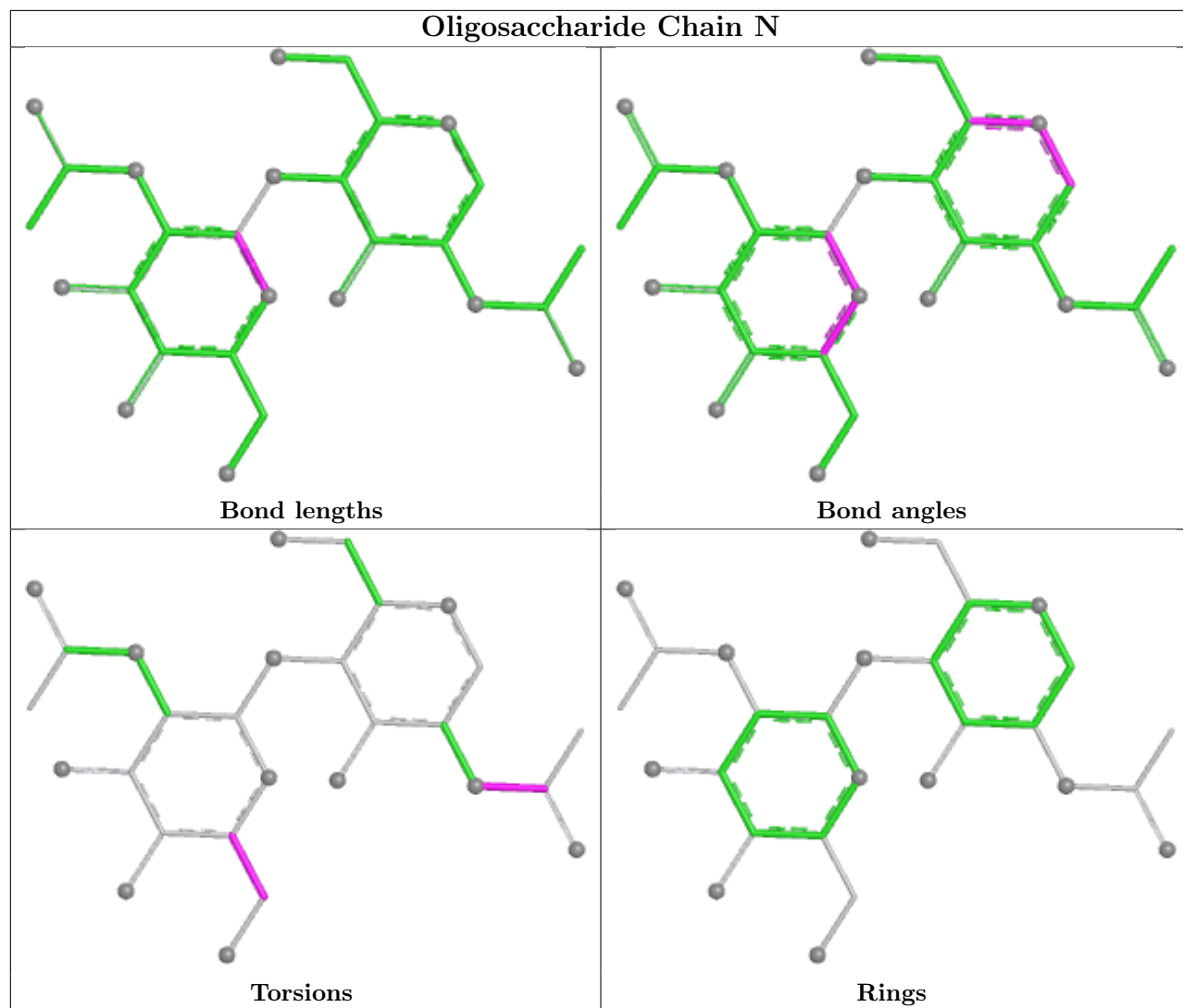


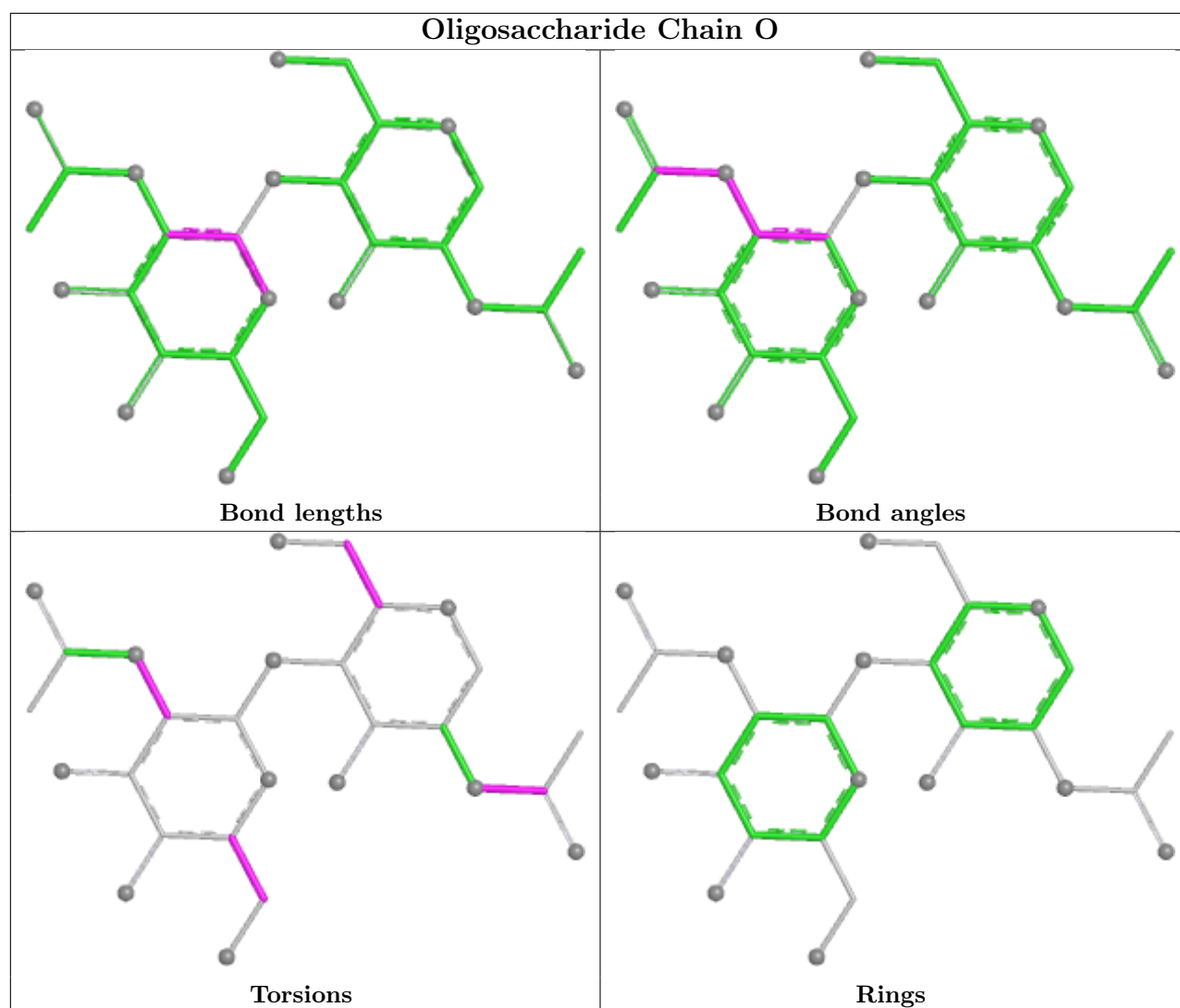












5.6 Ligand geometry [i](#)

12 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	C	403	1	14,14,15	0.60	1 (7%)	17,19,21	0.59	0
4	NAG	A	403	1	14,14,15	0.40	0	17,19,21	0.66	1 (5%)
4	NAG	A	406	1	14,14,15	0.28	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	404	1	14,14,15	0.69	1 (7%)	17,19,21	1.06	1 (5%)
4	NAG	E	403	1	14,14,15	1.29	1 (7%)	17,19,21	2.06	1 (5%)
4	NAG	F	201	2	14,14,15	0.17	0	17,19,21	0.48	0
4	NAG	A	409	1	14,14,15	0.50	0	17,19,21	0.56	0
4	NAG	C	409	1	14,14,15	0.27	0	17,19,21	0.48	0
4	NAG	B	201	2	14,14,15	0.25	0	17,19,21	0.66	0
4	NAG	C	404	1	14,14,15	0.27	0	17,19,21	1.07	1 (5%)
4	NAG	D	201	2	14,14,15	0.19	0	17,19,21	0.48	0
4	NAG	E	409	1	14,14,15	0.25	0	17,19,21	0.88	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
4	NAG	C	403	1	-	4/6/23/26	0/1/1/1
4	NAG	A	403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	406	1	-	4/6/23/26	0/1/1/1
4	NAG	E	404	1	-	2/6/23/26	0/1/1/1
4	NAG	E	403	1	-	4/6/23/26	0/1/1/1
4	NAG	F	201	2	-	0/6/23/26	0/1/1/1
4	NAG	A	409	1	-	4/6/23/26	0/1/1/1
4	NAG	C	409	1	-	4/6/23/26	0/1/1/1
4	NAG	B	201	2	-	1/6/23/26	0/1/1/1
4	NAG	C	404	1	-	4/6/23/26	0/1/1/1
4	NAG	D	201	2	-	2/6/23/26	0/1/1/1
4	NAG	E	409	1	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	403	NAG	O5-C1	4.65	1.51	1.43
4	E	404	NAG	O5-C1	2.10	1.47	1.43
4	C	403	NAG	O5-C1	2.03	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	E	403	NAG	C1-O5-C5	7.97	122.87	112.19
4	E	404	NAG	C1-O5-C5	3.83	117.32	112.19
4	C	404	NAG	C1-O5-C5	3.56	116.96	112.19
4	E	409	NAG	C1-O5-C5	2.86	116.02	112.19
4	A	403	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	409	NAG	O5-C5-C6-O6
4	E	404	NAG	C4-C5-C6-O6
4	E	404	NAG	O5-C5-C6-O6
4	A	409	NAG	C4-C5-C6-O6
4	E	403	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	403	NAG	1	0
4	A	409	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	343/346 (99%)	-1.25	0 100 100	90, 117, 143, 177	0
1	C	343/346 (99%)	-1.25	0 100 100	90, 118, 142, 176	0
1	E	343/346 (99%)	-1.25	0 100 100	92, 118, 144, 174	0
2	B	171/182 (93%)	-1.17	0 100 100	88, 117, 151, 168	0
2	D	170/182 (93%)	-1.25	0 100 100	86, 117, 153, 168	0
2	F	171/182 (93%)	-1.21	0 100 100	86, 117, 151, 171	0
All	All	1541/1584 (97%)	-1.24	0 100 100	86, 118, 149, 177	0

There are no RSRZ outliers to report.

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.

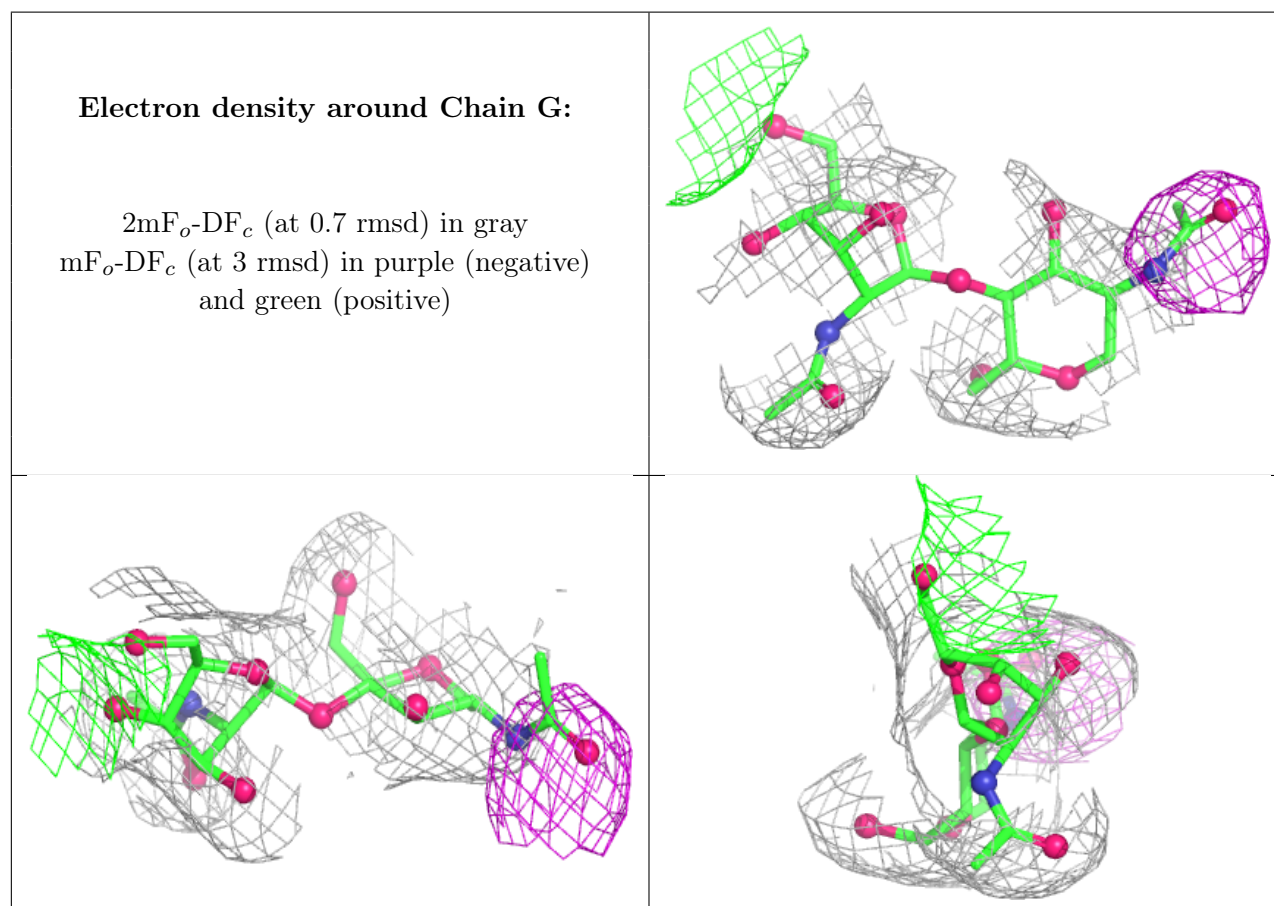
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	G	2	14/15	0.95	0.05	72,89,99,109	0
3	NAG	K	2	14/15	0.95	0.06	69,82,88,89	0
3	NAG	L	2	14/15	0.95	0.04	71,89,93,94	0
3	NAG	N	2	14/15	0.95	0.04	69,85,89,94	0
3	NAG	H	2	14/15	0.96	0.05	68,78,86,87	0
3	NAG	L	1	14/15	0.96	0.05	47,61,69,71	0

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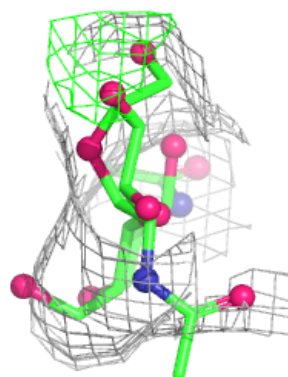
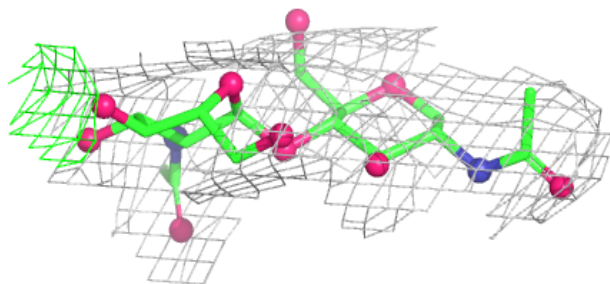
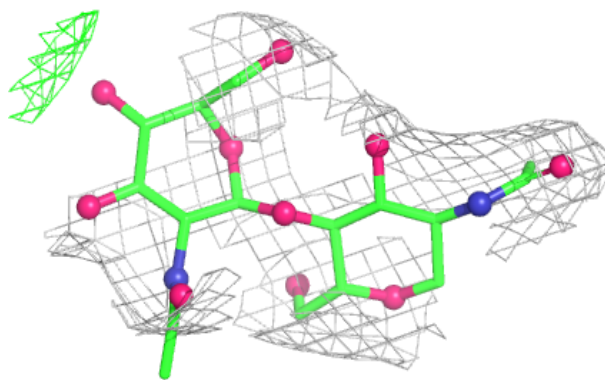
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	J	2	14/15	0.96	0.05	72,75,80,80	0
3	NAG	K	1	14/15	0.96	0.04	57,65,72,78	0
3	NAG	G	1	14/15	0.97	0.07	53,59,70,73	0
3	NAG	N	1	14/15	0.97	0.04	57,65,74,75	0
3	NAG	I	2	14/15	0.97	0.03	64,86,92,94	0
3	NAG	O	1	14/15	0.97	0.06	51,60,71,74	0
3	NAG	I	1	14/15	0.98	0.06	48,59,70,71	0
3	NAG	M	1	14/15	0.98	0.04	48,56,62,67	0
3	NAG	M	2	14/15	0.98	0.03	70,79,84,87	0
3	NAG	O	2	14/15	0.98	0.04	79,94,100,101	0
3	NAG	J	1	14/15	0.99	0.04	48,62,68,72	0
3	NAG	H	1	14/15	0.99	0.02	55,63,73,75	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.



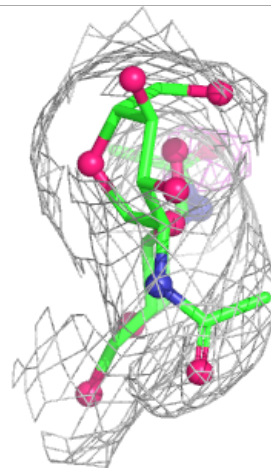
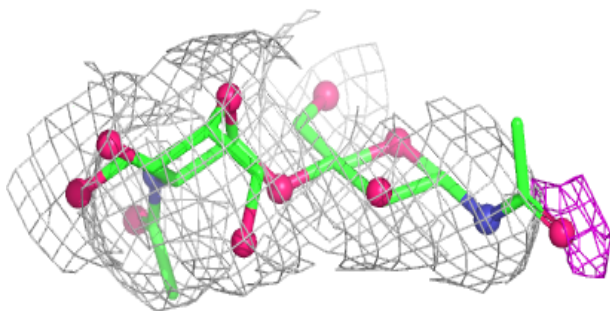
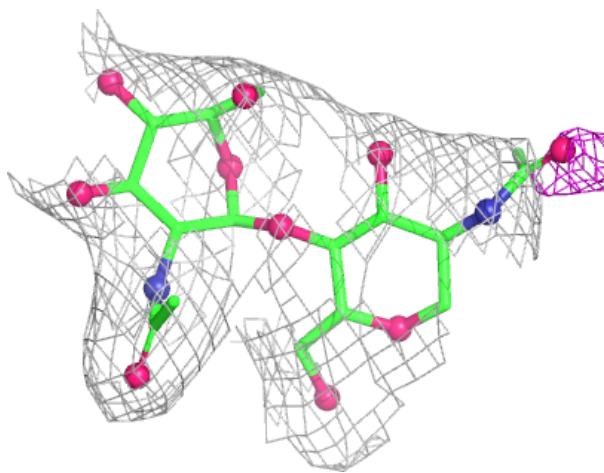
Electron density around Chain H:

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



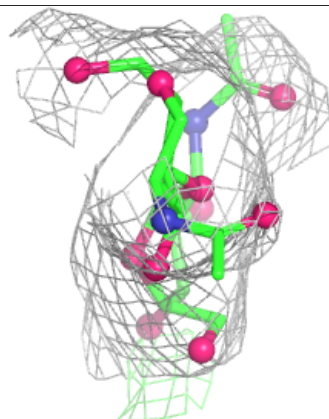
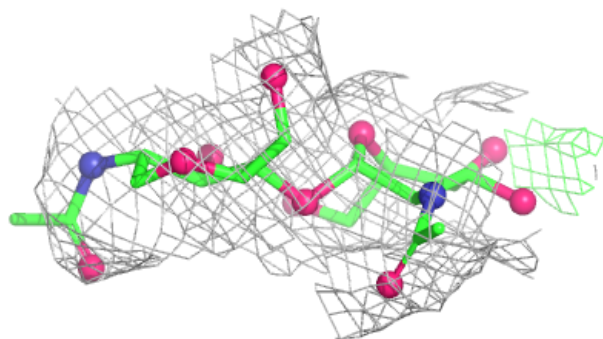
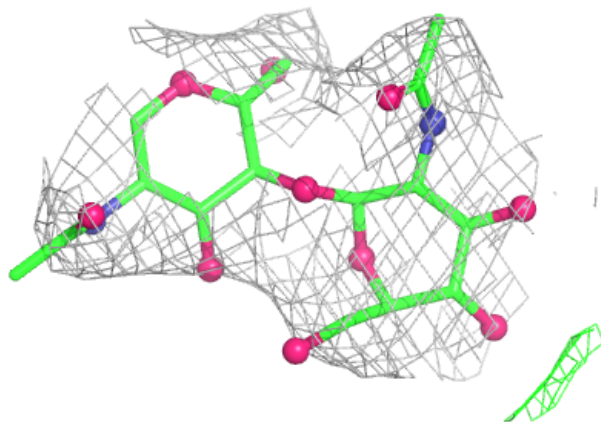
Electron density around Chain I:

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



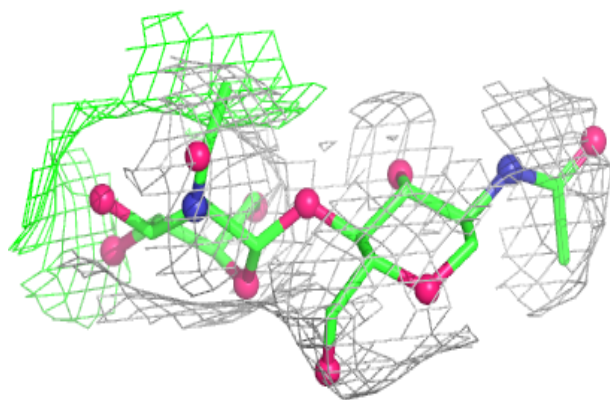
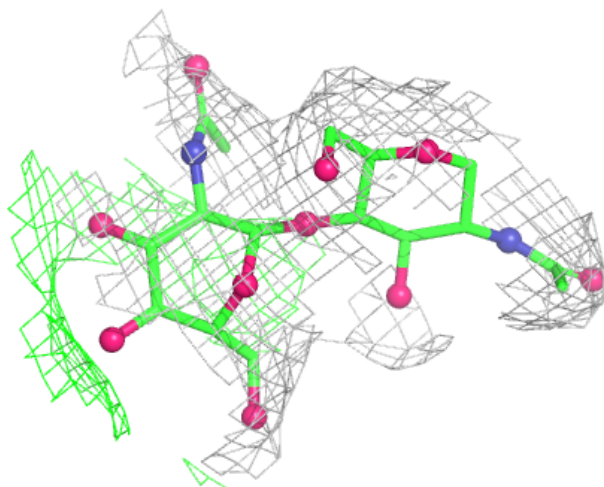
Electron density around Chain J:

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



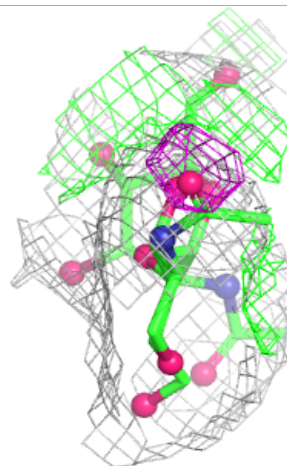
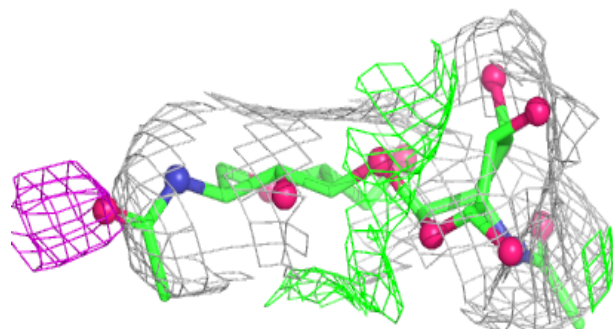
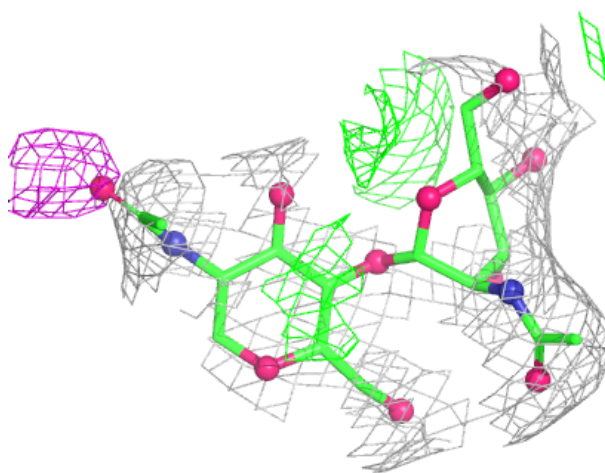
Electron density around Chain K:

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



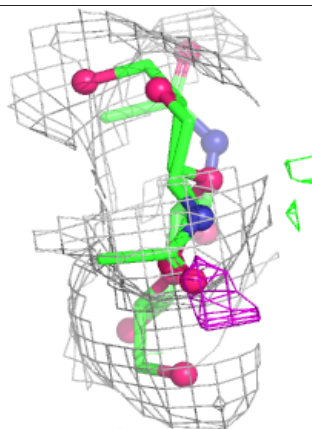
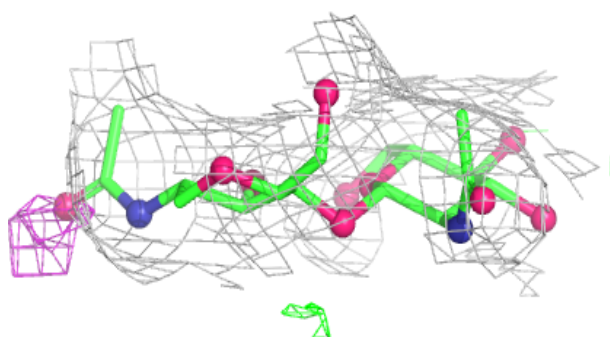
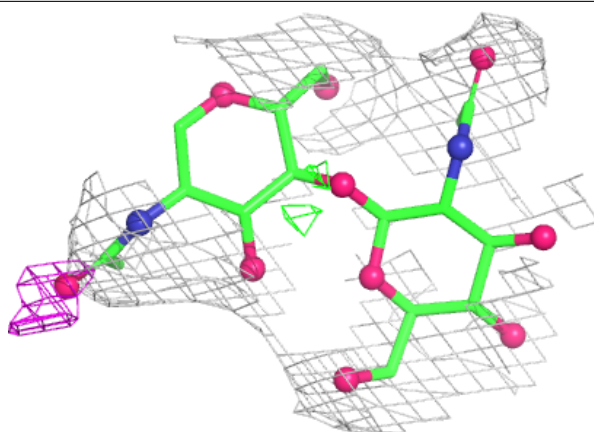
Electron density around Chain L:

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

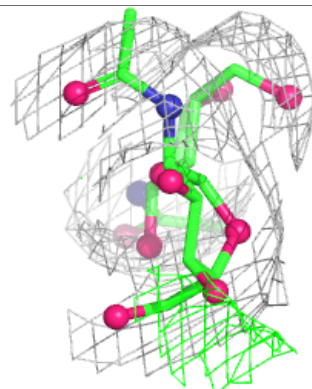
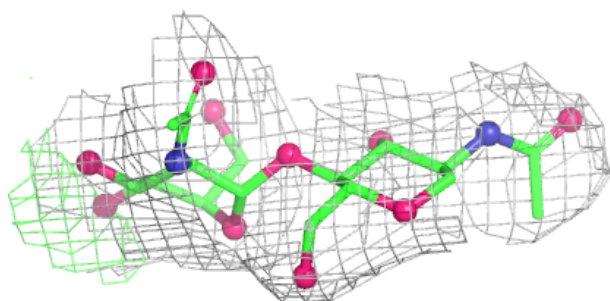
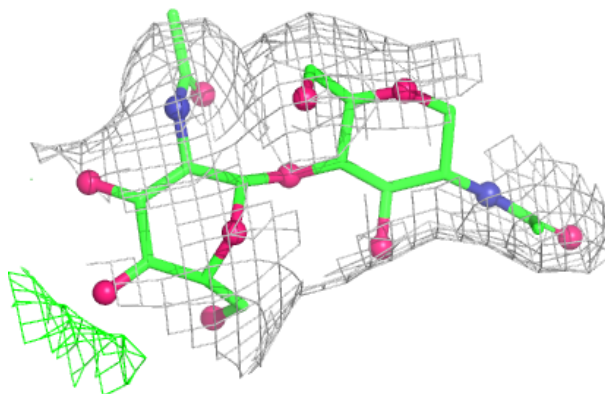


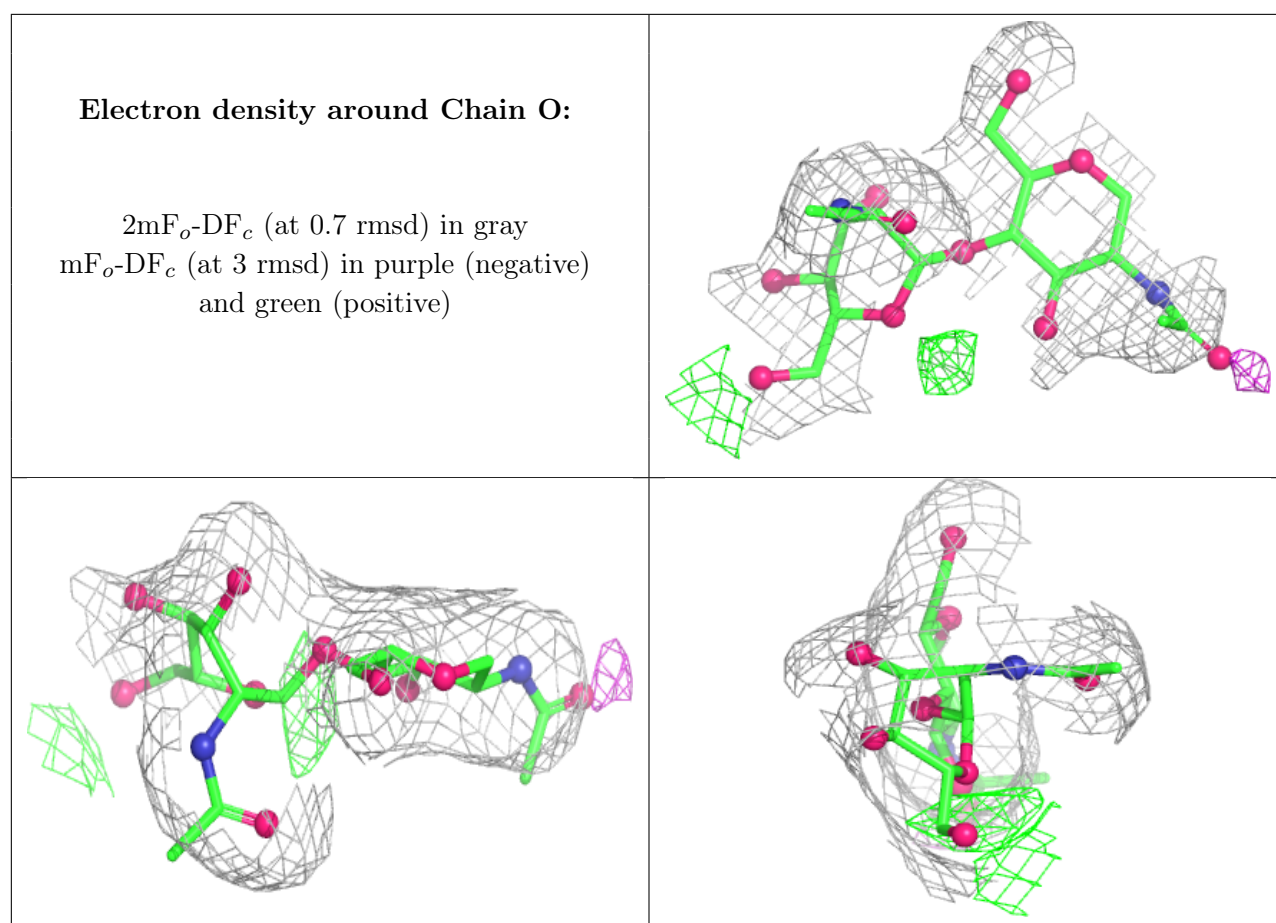
Electron density around Chain M:

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

**Electron density around Chain N:**

$2mF_o - DF_c$ (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	E	409	14/15	0.85	0.07	105,124,129,129	0
4	NAG	B	201	14/15	0.89	0.07	79,92,105,107	0
4	NAG	C	404	14/15	0.93	0.04	106,124,128,134	0
4	NAG	E	404	14/15	0.95	0.05	106,115,122,124	0
4	NAG	A	406	14/15	0.95	0.04	109,126,133,134	0
4	NAG	E	403	14/15	0.96	0.04	80,90,97,103	0
4	NAG	A	409	14/15	0.96	0.04	105,122,126,127	0
4	NAG	C	409	14/15	0.96	0.04	110,124,129,131	0
4	NAG	D	201	14/15	0.97	0.04	81,93,100,105	0
4	NAG	C	403	14/15	0.97	0.03	63,71,78,80	0
4	NAG	F	201	14/15	0.97	0.04	79,94,102,104	0
4	NAG	A	403	14/15	0.98	0.03	68,73,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.