



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 11:08 AM BST

PDB ID : 4M40
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

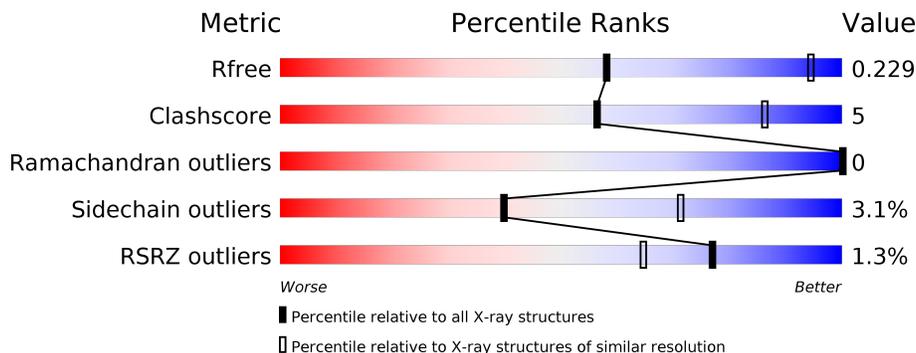
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



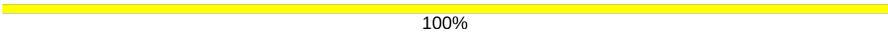
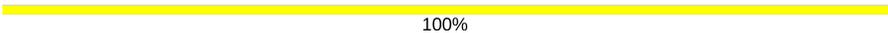
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	346	
1	C	346	
1	E	346	
2	B	182	
2	D	182	
2	F	182	

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Mol	Chain	Length	Quality of chain
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 i

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
			Total	C	N	O	S			
1	A	343	2600	1633	464	487	16	0	0	0
1	C	343	2600	1633	464	487	16	0	0	0
1	E	343	2600	1633	464	487	16	0	0	0

- Molecule 2 is a protein called Hemagglutinin HA2.

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

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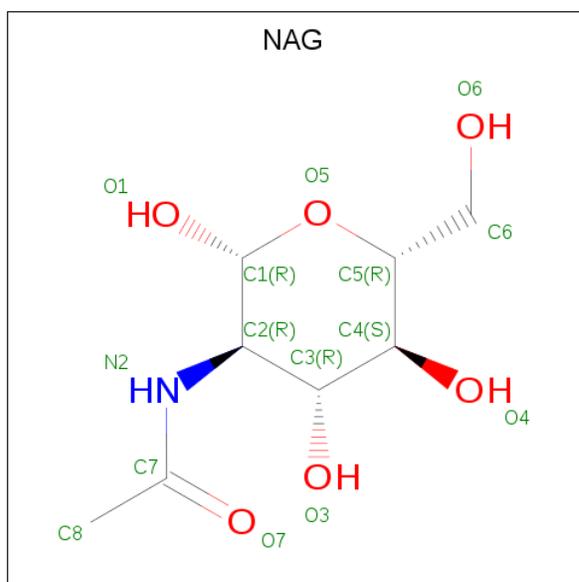
Chain	Residue	Modelled	Actual	Comment	Reference
F	177	GLY	-	expression tag	UNP A3DQM7
F	178	ALA	-	expression tag	UNP A3DQM7
F	179	LEU	-	expression tag	UNP A3DQM7
F	180	VAL	-	expression tag	UNP A3DQM7
F	181	PRO	-	expression tag	UNP A3DQM7
F	182	ARG	-	expression tag	UNP A3DQM7

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

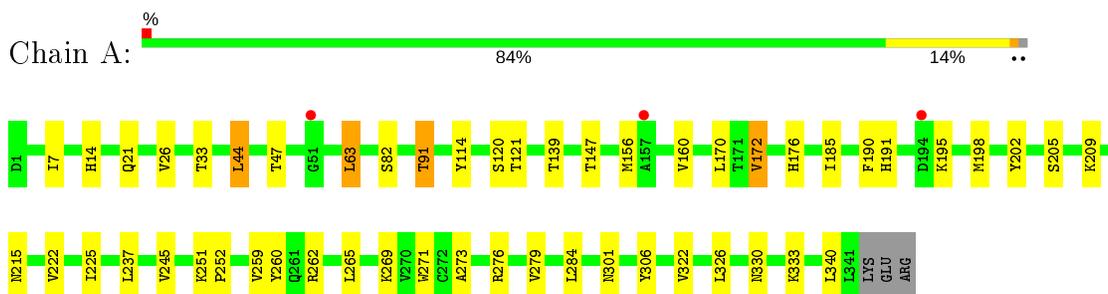


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total 14	8	1	5	0	0
4	A	1	Total 14	8	1	5	0	0
4	A	1	Total 14	8	1	5	0	0
4	B	1	Total 14	8	1	5	0	0
4	C	1	Total 14	8	1	5	0	0
4	C	1	Total 14	8	1	5	0	0
4	C	1	Total 14	8	1	5	0	0
4	D	1	Total 14	8	1	5	0	0
4	E	1	Total 14	8	1	5	0	0
4	E	1	Total 14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

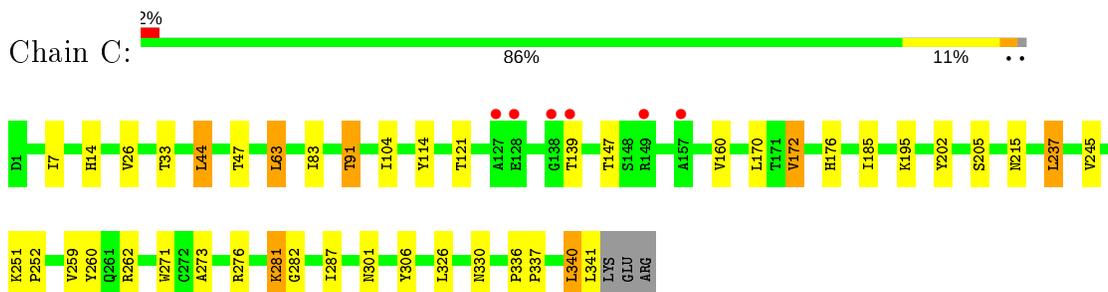
3 Residue-property plots [i](#)

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

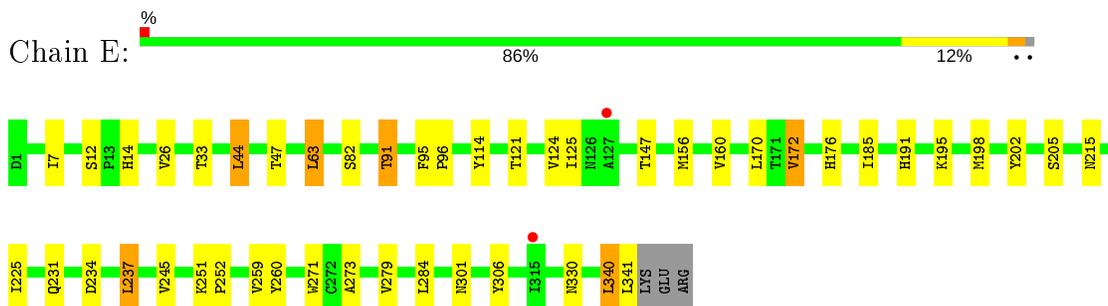
- Molecule 1: Hemagglutinin HA1



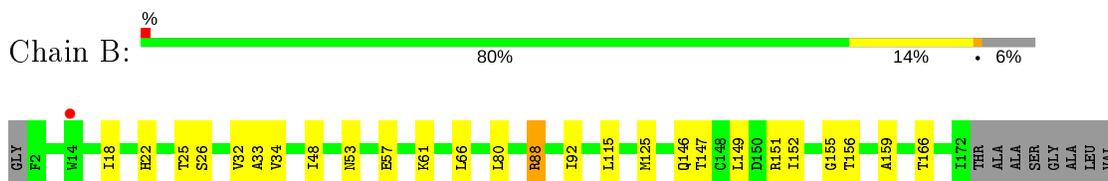
- Molecule 1: Hemagglutinin HA1



- Molecule 1: Hemagglutinin HA1



- Molecule 2: Hemagglutinin HA2



PRO
ARG

- Molecule 2: Hemagglutinin HA2

Chain D:  2% 82% 11% 7%



ARG

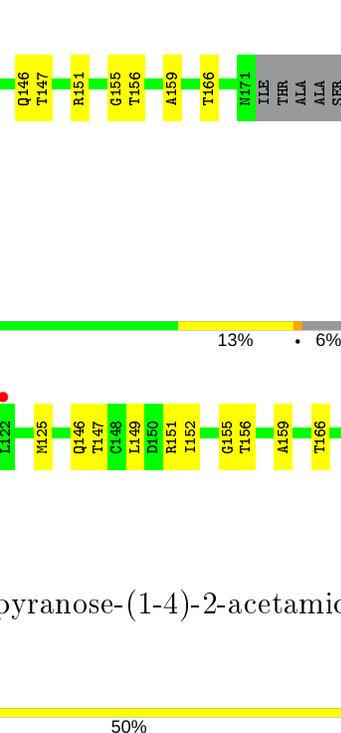
- Molecule 2: Hemagglutinin HA2

Chain F:  2% 81% 13% 6%



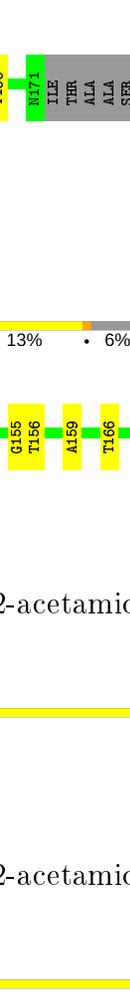
GLY
ALA
LEU
VAL
PRO
ARG

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

Chain G:  50% 50%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

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

Chain I: 50% 50%

MAG1
MAG2

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

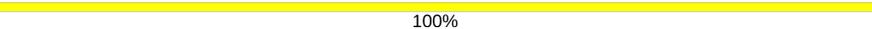
Chain J: 100%

MAG1
MAG2

- 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 i

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 0.214 , 0.229	Depositor DCC
R_{free} test set	1334 reflections (5.03%)	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)	0.33 , 74.0	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	0.93	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.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.26	0/2659	0.51	0/3613
1	C	0.29	1/2659 (0.0%)	0.52	0/3613
1	E	0.26	0/2659	0.52	0/3613
2	B	0.31	0/1320	0.48	0/1780
2	D	0.28	0/1312	0.48	0/1769
2	F	0.28	0/1320	0.47	0/1780
All	All	0.28	1/11929 (0.0%)	0.50	0/16168

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	287	ILE	C-N	5.17	1.42	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2600	0	2622	30	0
1	C	2600	0	2622	24	0
1	E	2600	0	2621	26	0
2	B	1301	0	1273	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1293	0	1262	14	0
2	F	1301	0	1273	16	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	0	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	120	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 120 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%)	281 (97%)	10 (3%)	37	69
1	C	291/294 (99%)	279 (96%)	12 (4%)	30	64
1	E	291/294 (99%)	282 (97%)	9 (3%)	40	71
2	B	139/145 (96%)	136 (98%)	3 (2%)	52	78
2	D	138/145 (95%)	135 (98%)	3 (2%)	52	78
2	F	139/145 (96%)	136 (98%)	3 (2%)	52	78
All	All	1289/1317 (98%)	1249 (97%)	40 (3%)	40	71

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	147	THR
1	C	276	ARG
1	E	340	LEU
1	C	172	VAL
1	C	281	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	42	GLN
1	C	215	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	0.39	0	17,19,21	0.57	0
3	NAG	H	1	1,3	14,14,15	0.41	0	17,19,21	0.72	0
3	NAG	H	2	3	14,14,15	1.13	1 (7%)	17,19,21	1.23	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	0.90	1 (7%)	17,19,21	1.05	1 (5%)
3	NAG	J	1	1,3	14,14,15	0.63	0	17,19,21	1.16	1 (5%)
3	NAG	J	2	3	14,14,15	0.83	1 (7%)	17,19,21	0.99	1 (5%)
3	NAG	K	1	1,3	14,14,15	0.50	0	17,19,21	0.82	1 (5%)
3	NAG	K	2	3	14,14,15	1.04	1 (7%)	17,19,21	1.26	1 (5%)
3	NAG	L	1	1,3	14,14,15	0.27	0	17,19,21	1.24	1 (5%)
3	NAG	L	2	3	14,14,15	0.67	0	17,19,21	0.91	1 (5%)
3	NAG	M	1	1,3	14,14,15	0.55	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	M	2	3	14,14,15	0.40	0	17,19,21	1.32	2 (11%)
3	NAG	N	1	1,3	14,14,15	0.36	0	17,19,21	0.80	1 (5%)
3	NAG	N	2	3	14,14,15	1.08	1 (7%)	17,19,21	1.18	1 (5%)
3	NAG	O	1	1,3	14,14,15	0.26	0	17,19,21	0.63	0
3	NAG	O	2	3	14,14,15	1.01	2 (14%)	17,19,21	0.87	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
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
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	5/6/23/26	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 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	NAG	O5-C1	4.11	1.50	1.43
3	N	2	NAG	O5-C1	3.92	1.50	1.43
3	K	2	NAG	O5-C1	3.77	1.49	1.43
3	I	2	NAG	O5-C1	3.26	1.48	1.43

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2	NAG	O5-C1	2.87	1.48	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	2	NAG	C1-O5-C5	4.95	118.90	112.19
3	H	2	NAG	C1-O5-C5	4.82	118.73	112.19
3	N	2	NAG	C1-O5-C5	4.60	118.42	112.19
3	L	1	NAG	C1-O5-C5	4.33	118.06	112.19
3	M	2	NAG	C2-N2-C7	4.31	129.04	122.90

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

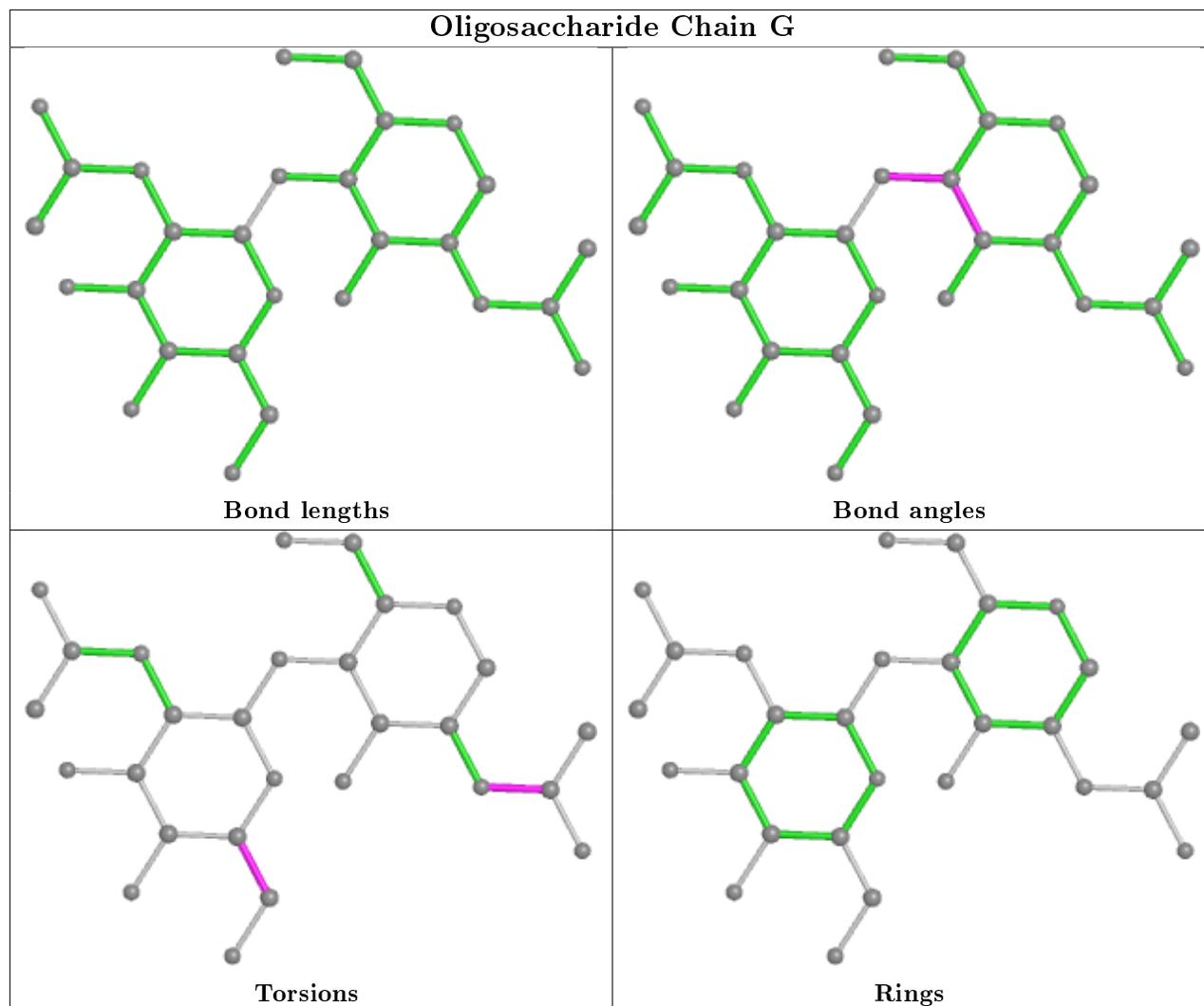
Mol	Chain	Res	Type	Atoms
3	L	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6

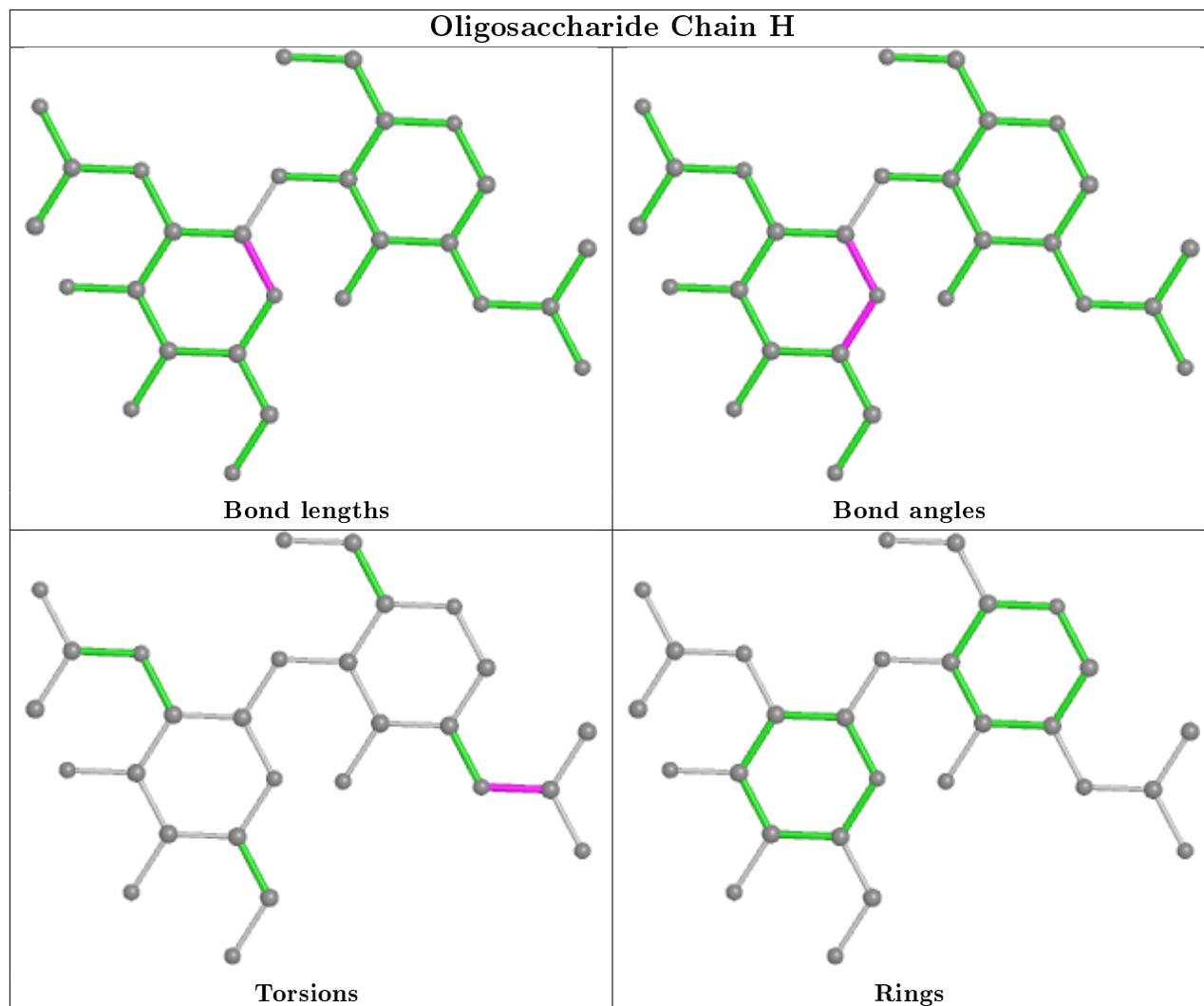
There are no ring outliers.

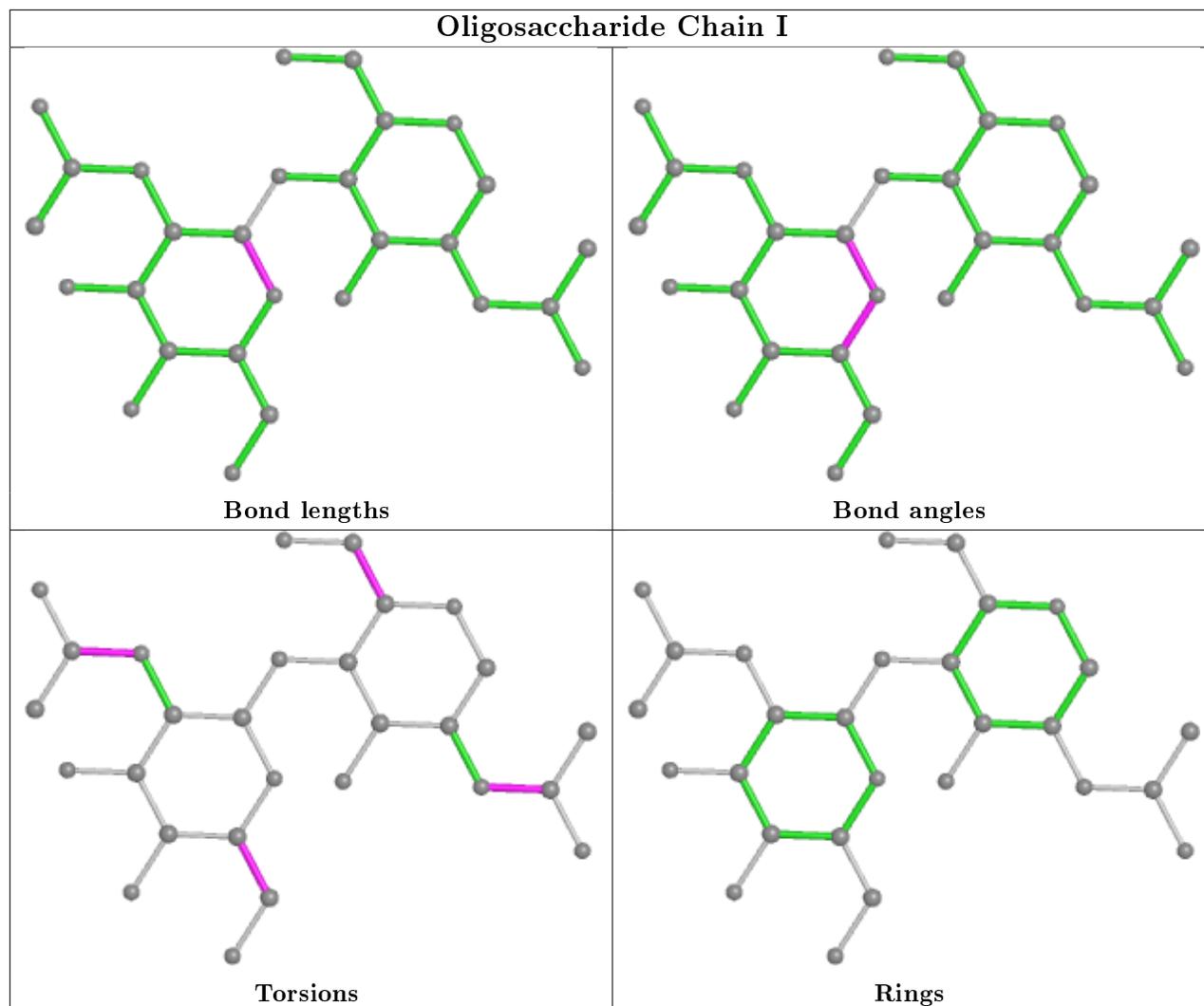
7 monomers are involved in 7 short contacts:

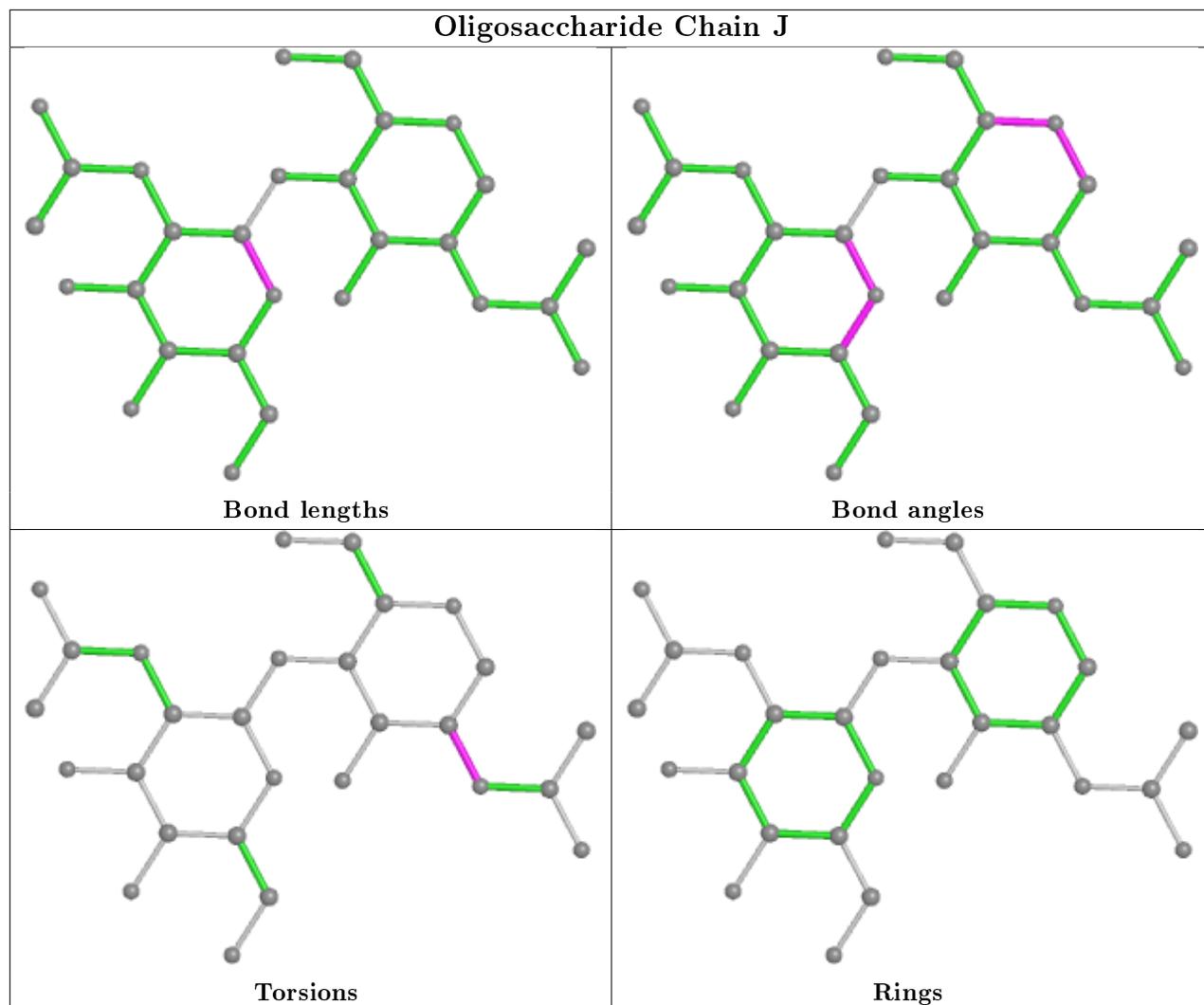
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	NAG	1	0
3	O	2	NAG	2	0
3	N	1	NAG	1	0
3	K	1	NAG	1	0
3	H	1	NAG	1	0
3	M	1	NAG	1	0
3	O	1	NAG	1	0

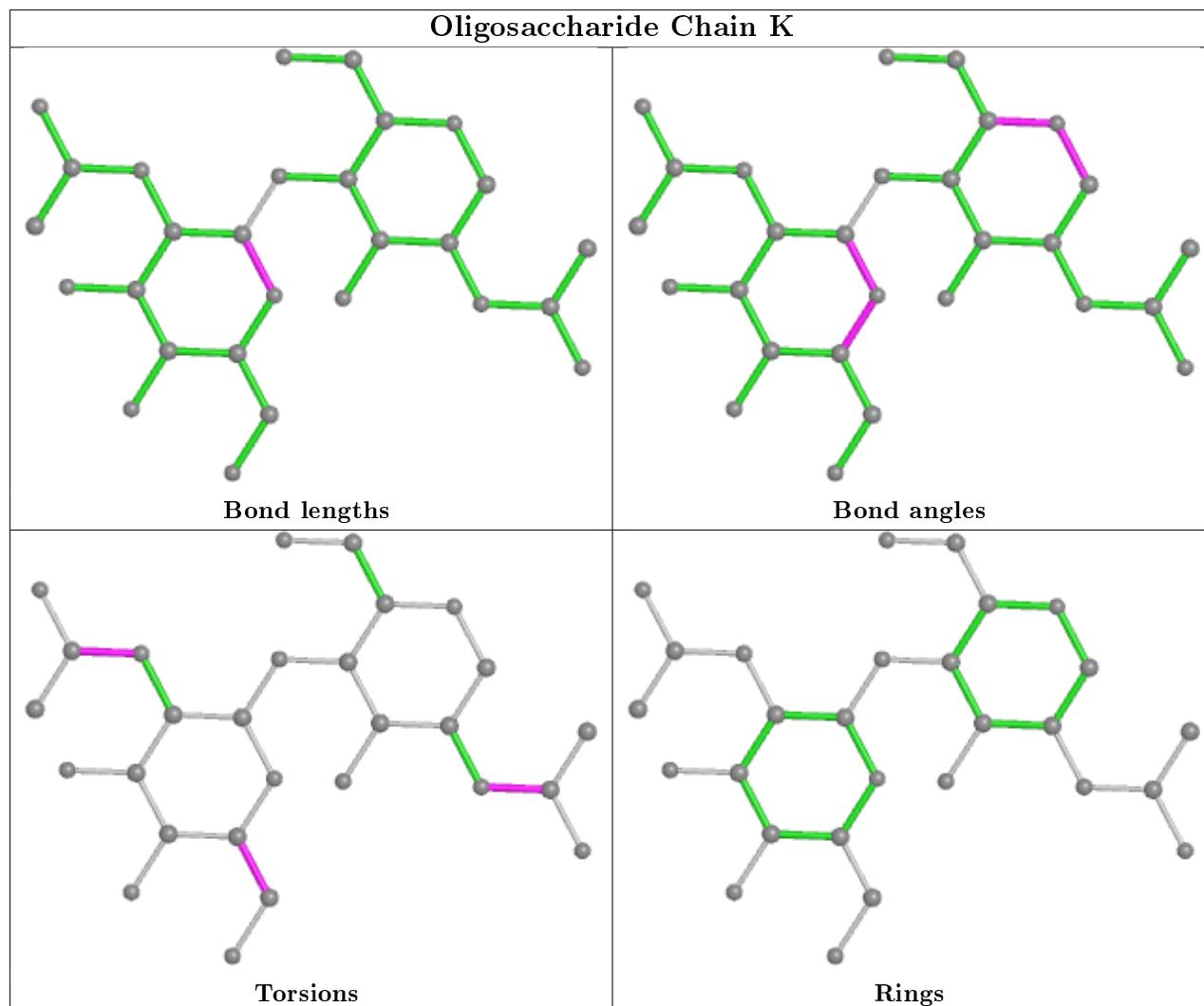
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

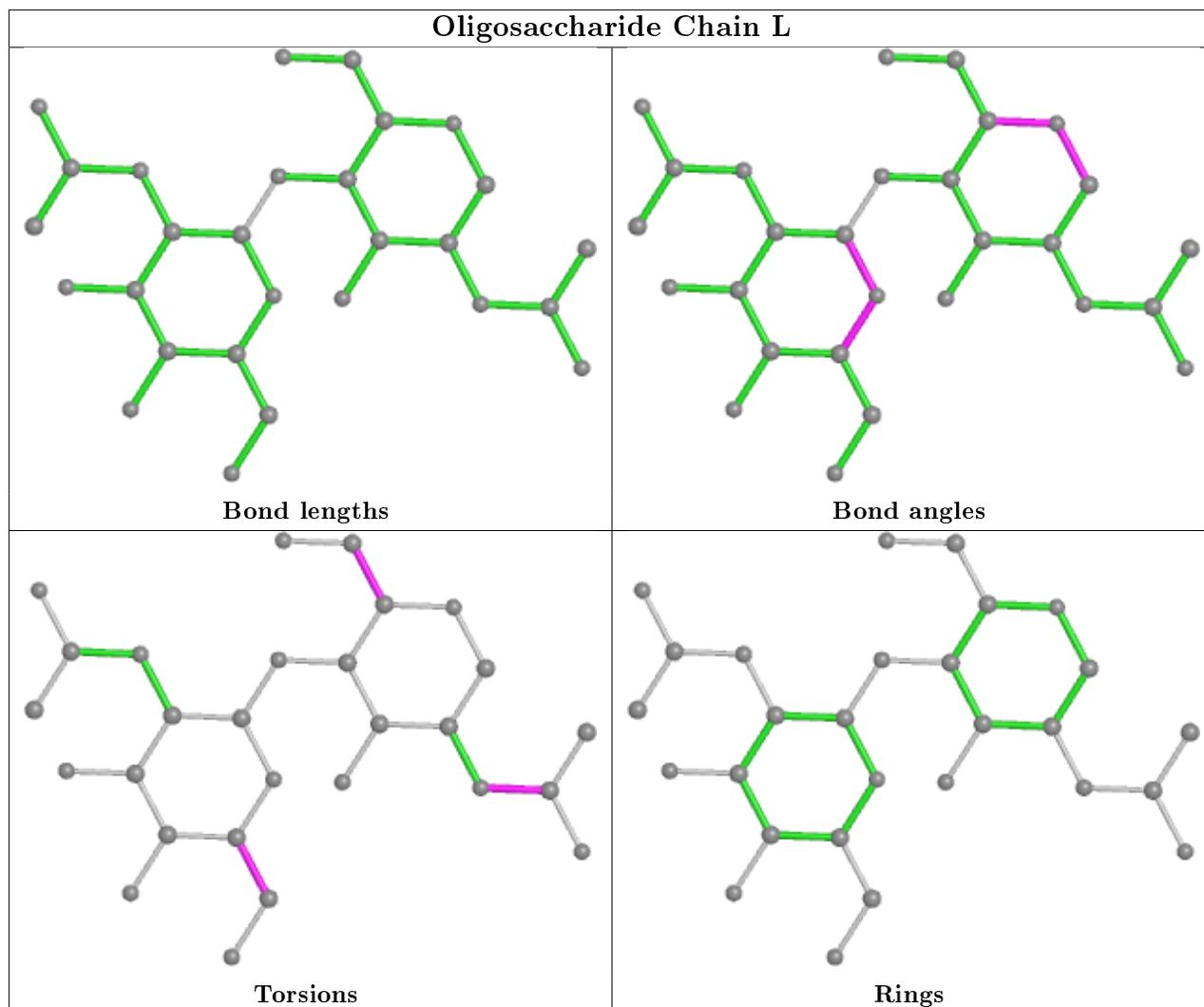


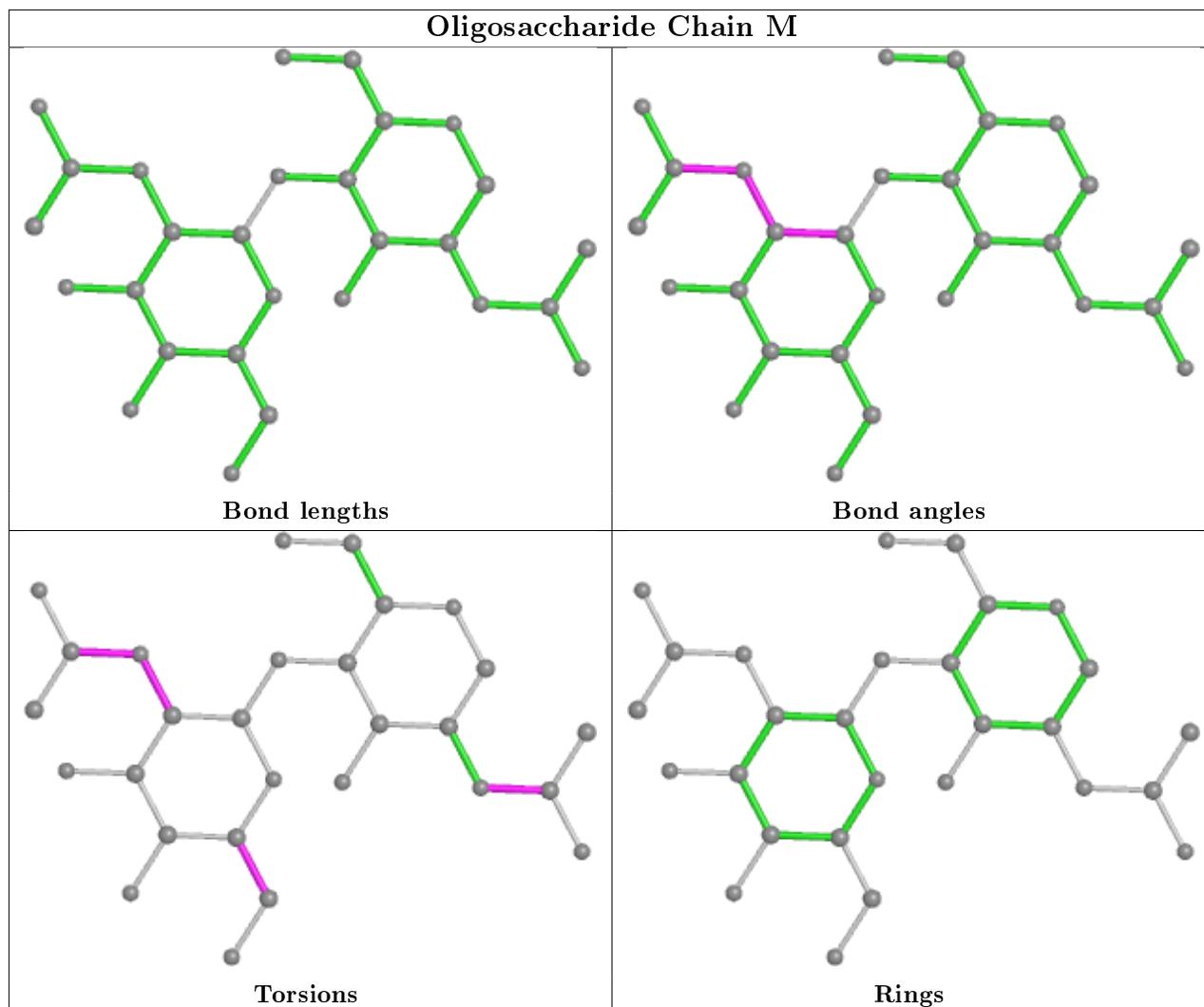


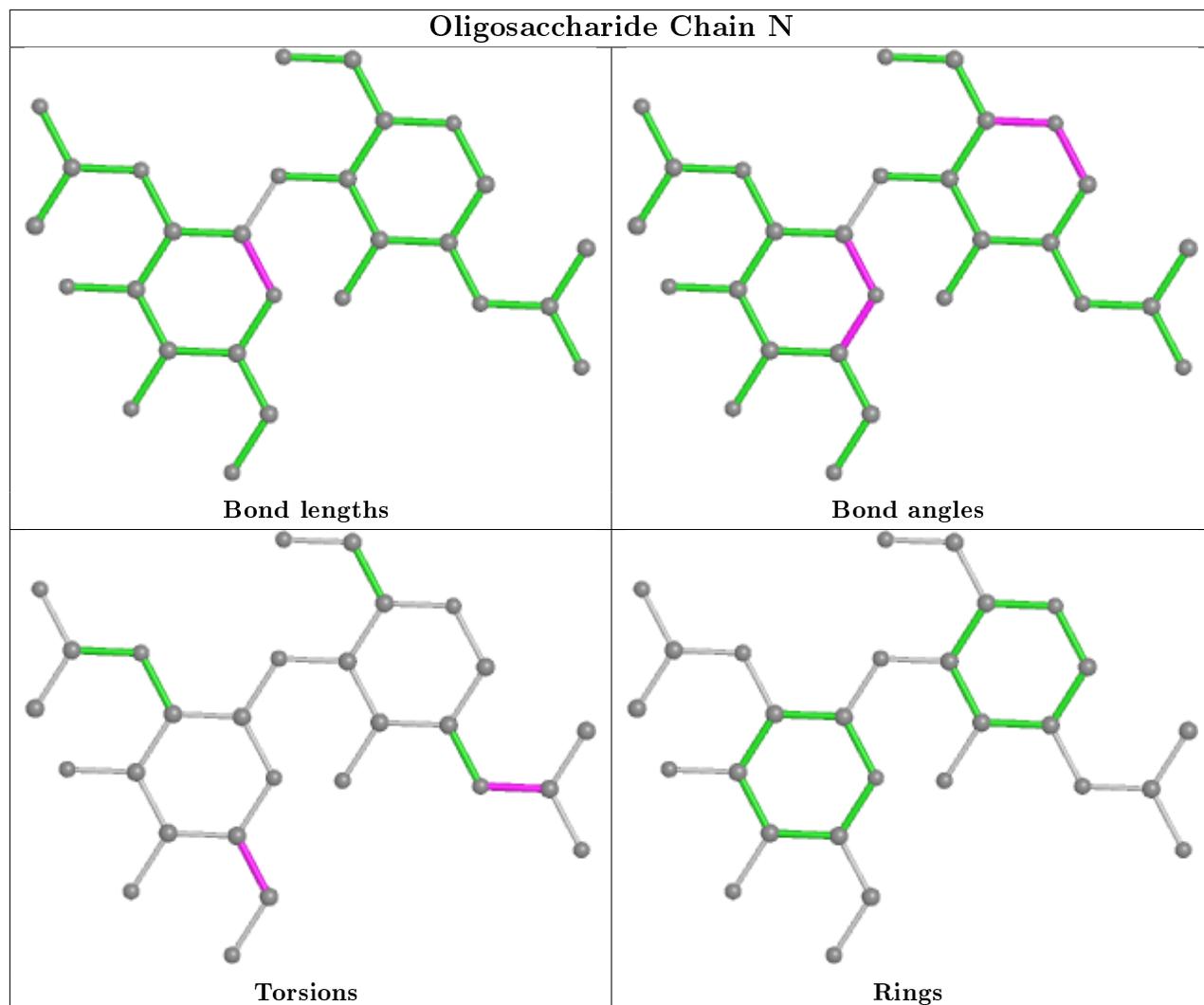


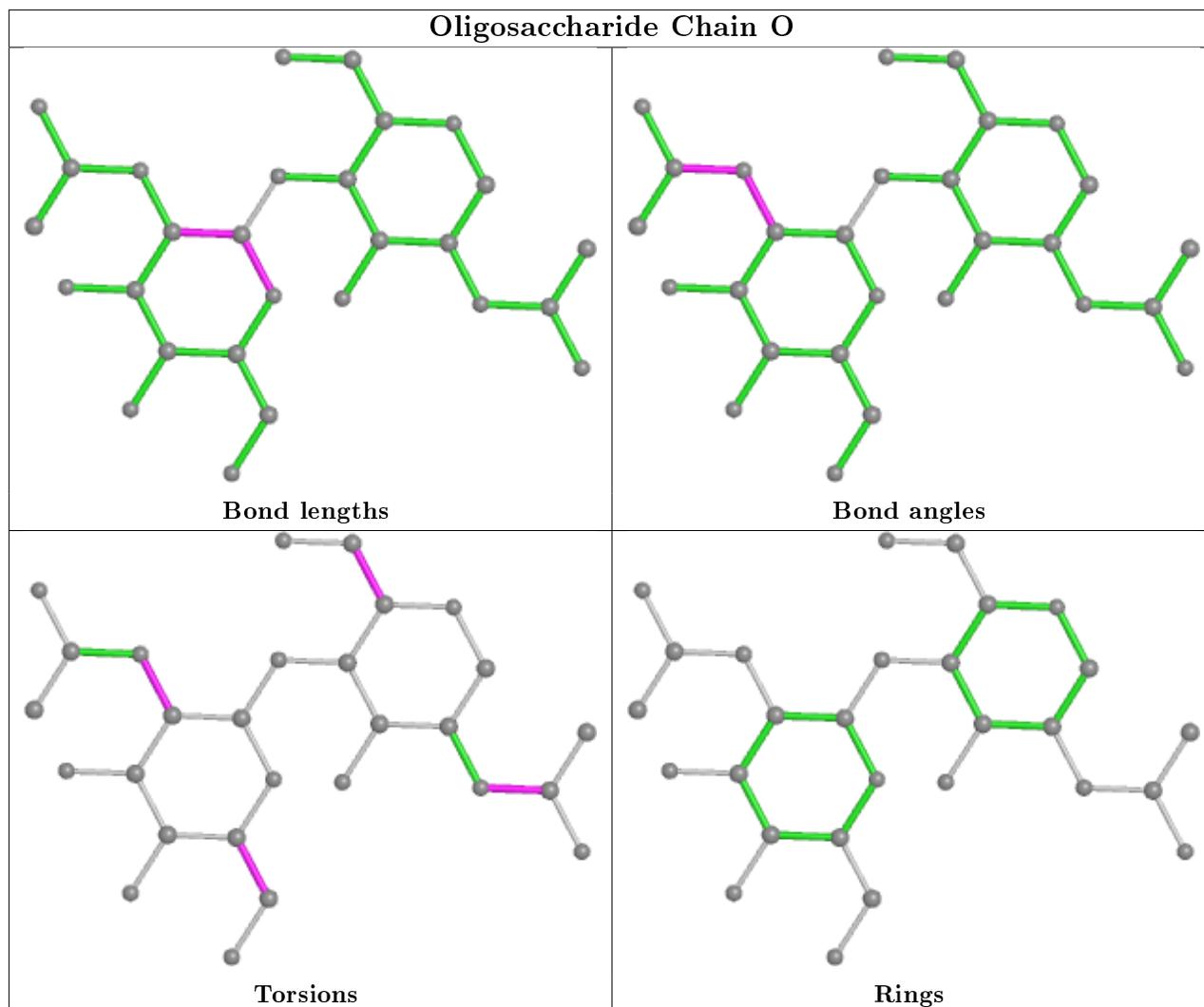












5.6 Ligand geometry [i](#)

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	A	403	1	14,14,15	0.40	0	17,19,21	0.64	0
4	NAG	C	403	1	14,14,15	0.62	1 (7%)	17,19,21	0.59	0
4	NAG	A	406	1	14,14,15	0.26	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	201	2	14,14,15	0.17	0	17,19,21	0.46	0
4	NAG	D	201	2	14,14,15	0.19	0	17,19,21	0.46	0
4	NAG	E	404	1	14,14,15	0.70	1 (7%)	17,19,21	1.03	1 (5%)
4	NAG	E	409	1	14,14,15	0.25	0	17,19,21	0.85	1 (5%)
4	NAG	C	404	1	14,14,15	0.27	0	17,19,21	1.07	1 (5%)
4	NAG	C	409	1	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	B	201	2	14,14,15	0.24	0	17,19,21	0.64	0
4	NAG	A	409	1	14,14,15	0.50	0	17,19,21	0.54	0
4	NAG	E	403	1	14,14,15	1.34	1 (7%)	17,19,21	2.04	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	A	403	1	-	0/6/23/26	0/1/1/1
4	NAG	C	403	1	-	4/6/23/26	0/1/1/1
4	NAG	A	406	1	-	4/6/23/26	0/1/1/1
4	NAG	F	201	2	-	0/6/23/26	0/1/1/1
4	NAG	D	201	2	-	2/6/23/26	0/1/1/1
4	NAG	E	404	1	-	2/6/23/26	0/1/1/1
4	NAG	E	409	1	-	3/6/23/26	0/1/1/1
4	NAG	C	404	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	A	409	1	-	4/6/23/26	0/1/1/1
4	NAG	E	403	1	-	4/6/23/26	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	4.87	1.51	1.43
4	E	404	NAG	O5-C1	2.20	1.47	1.43
4	C	403	NAG	O5-C1	2.12	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	E	403	NAG	C1-O5-C5	7.88	122.87	112.19
4	E	404	NAG	C1-O5-C5	3.79	117.32	112.19
4	C	404	NAG	C1-O5-C5	3.52	116.96	112.19
4	E	409	NAG	C1-O5-C5	2.82	116.02	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	E	403	NAG	O5-C5-C6-O6
4	A	409	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	403	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%)	0.13	3 (0%) 84 73	90, 117, 143, 177	0
1	C	343/346 (99%)	0.16	6 (1%) 70 57	90, 118, 142, 176	0
1	E	343/346 (99%)	0.15	2 (0%) 89 81	92, 118, 144, 174	0
2	B	171/182 (93%)	0.18	1 (0%) 89 81	88, 117, 151, 168	0
2	D	170/182 (93%)	0.21	4 (2%) 59 45	86, 117, 153, 168	0
2	F	171/182 (93%)	0.14	4 (2%) 60 46	86, 117, 151, 171	0
All	All	1541/1584 (97%)	0.16	20 (1%) 77 65	86, 118, 149, 177	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	138	GLY	3.8
1	A	51	GLY	3.6
2	D	34	VAL	3.6
2	D	12	GLY	3.5
2	D	14	TRP	3.4

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

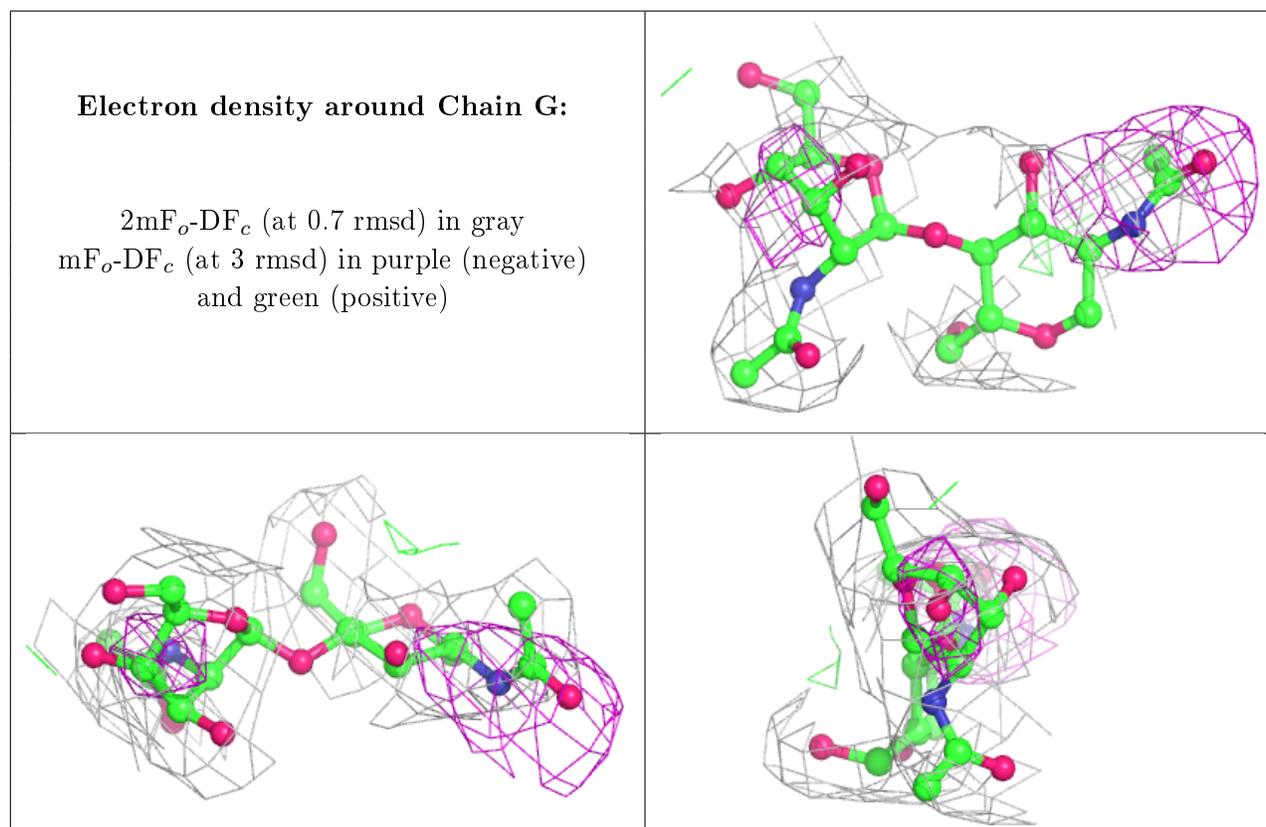
There are no non-standard protein/DNA/RNA residues in this entry.

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.

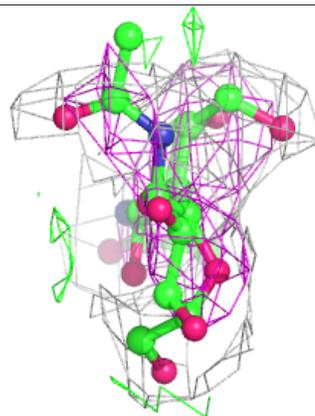
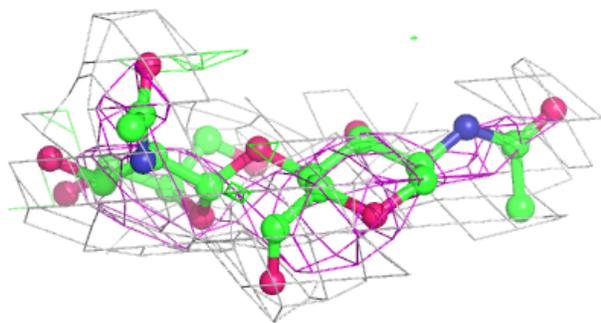
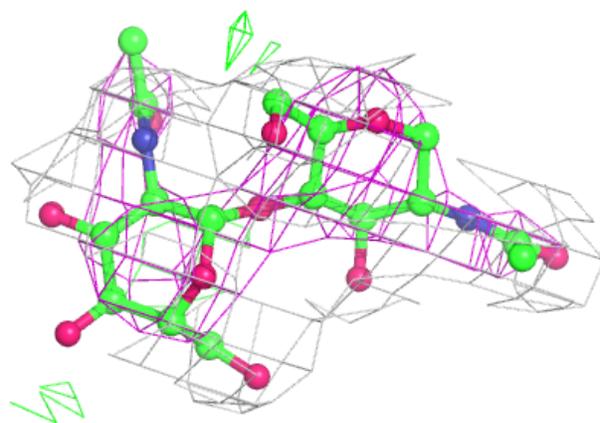
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	N	2	14/15	0.72	0.27	69,85,89,94	0
3	NAG	K	2	14/15	0.73	0.22	69,82,88,89	0
3	NAG	H	2	14/15	0.76	0.23	68,78,86,87	0
3	NAG	G	2	14/15	0.83	0.21	72,89,99,109	0
3	NAG	L	1	14/15	0.84	0.23	47,61,69,71	0
3	NAG	O	1	14/15	0.84	0.18	51,60,71,74	0
3	NAG	O	2	14/15	0.86	0.20	79,94,100,101	0
3	NAG	J	2	14/15	0.86	0.22	72,75,80,80	0
3	NAG	I	1	14/15	0.87	0.20	48,59,70,71	0
3	NAG	G	1	14/15	0.89	0.23	53,59,70,73	0
3	NAG	J	1	14/15	0.90	0.24	48,62,68,72	0
3	NAG	M	2	14/15	0.90	0.15	70,79,84,87	0
3	NAG	L	2	14/15	0.91	0.16	71,89,93,94	0
3	NAG	N	1	14/15	0.92	0.17	57,65,74,75	0
3	NAG	K	1	14/15	0.92	0.14	57,65,72,78	0
3	NAG	H	1	14/15	0.92	0.16	55,63,73,75	0
3	NAG	M	1	14/15	0.93	0.19	48,56,62,67	0
3	NAG	I	2	14/15	0.94	0.13	64,86,92,94	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.



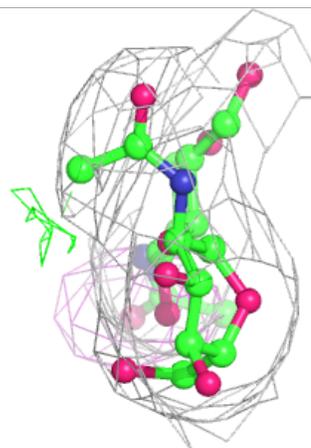
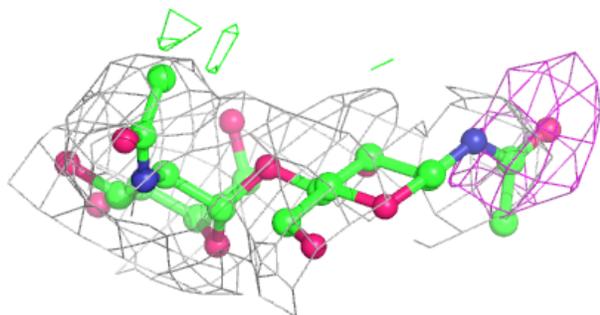
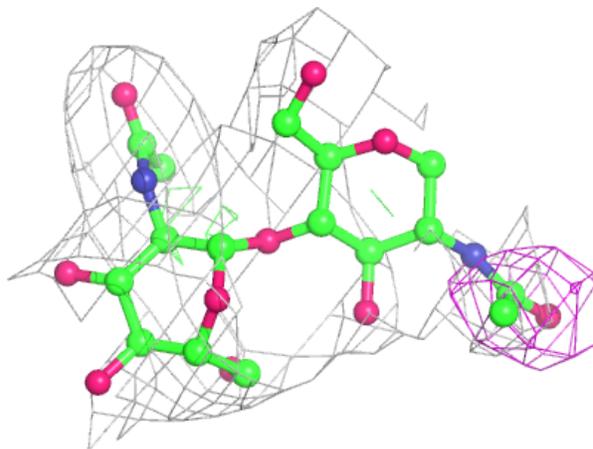
Electron density around Chain H:

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



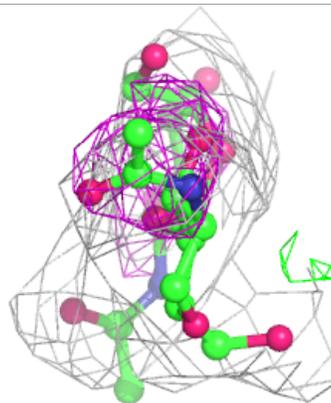
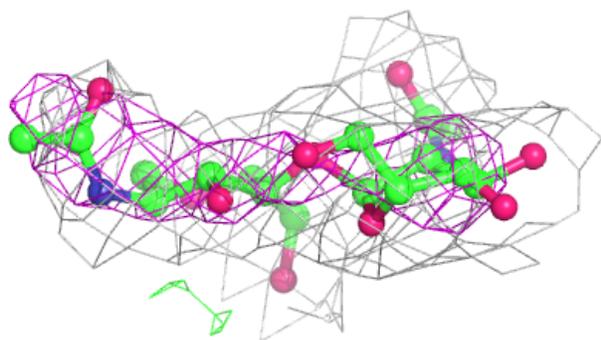
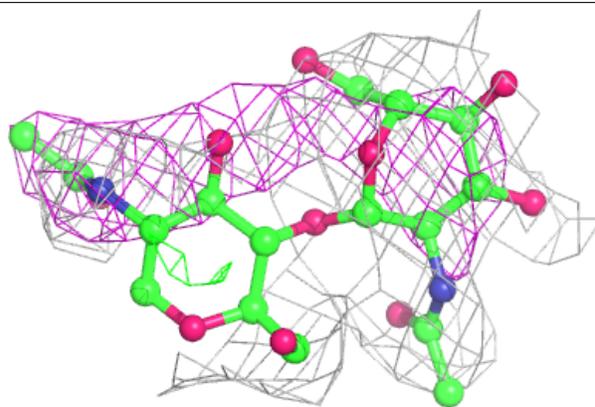
Electron density around Chain I:

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

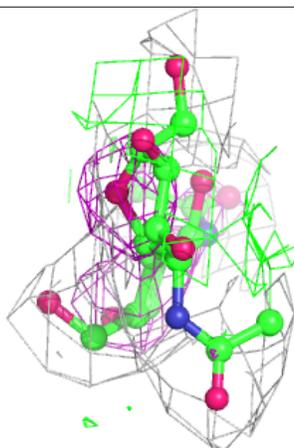
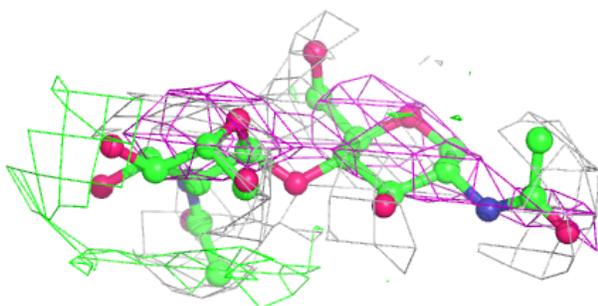
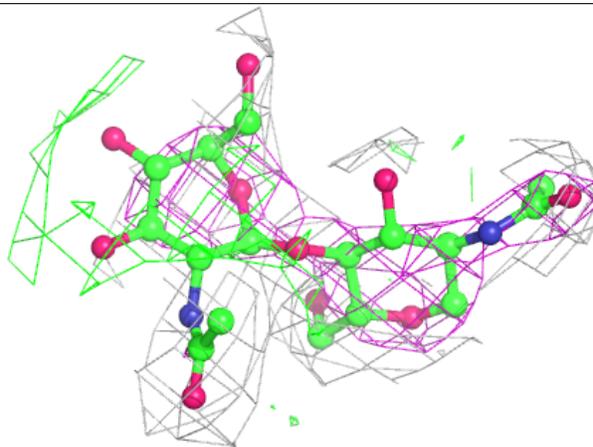


Electron density around Chain J:

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

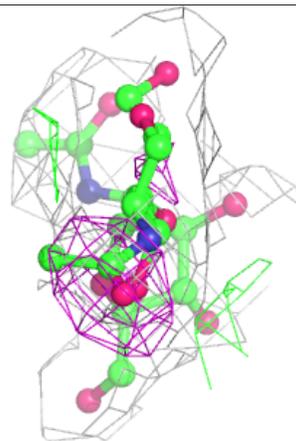
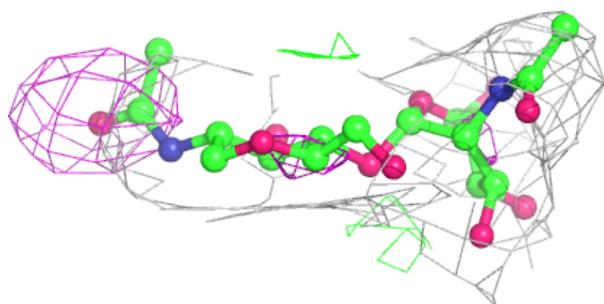
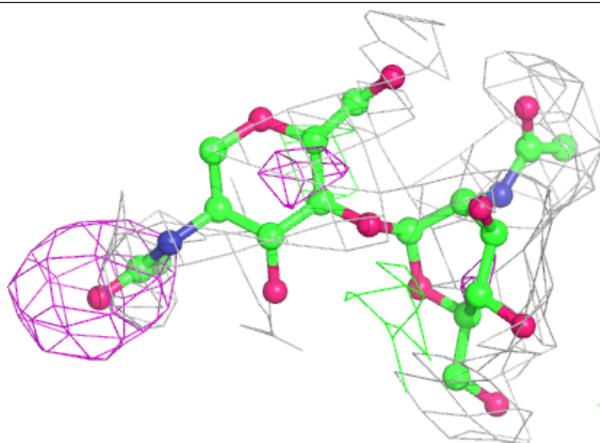
**Electron density around Chain K:**

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



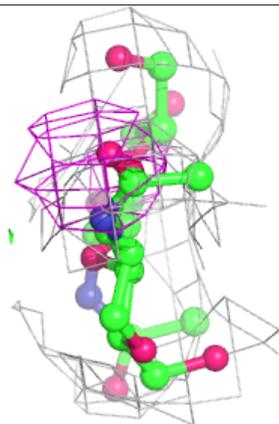
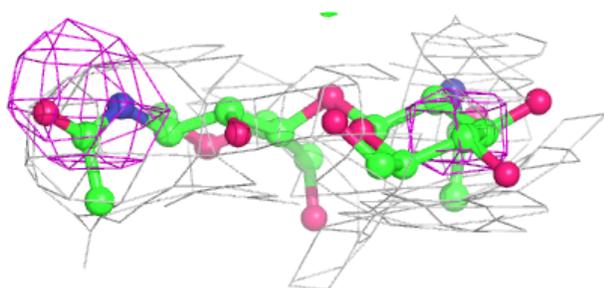
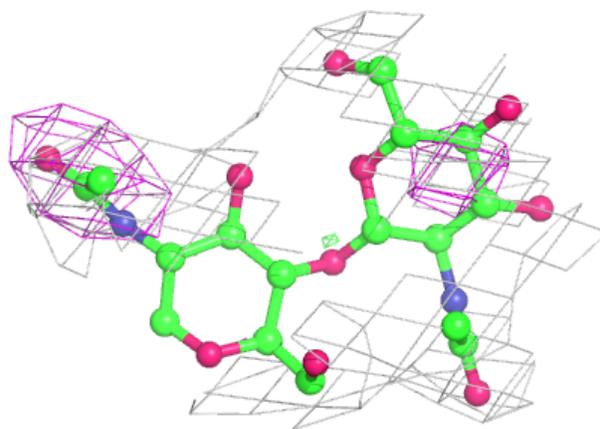
Electron density around Chain L:

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

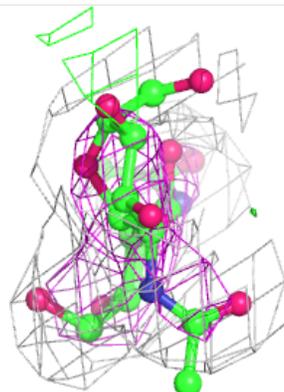
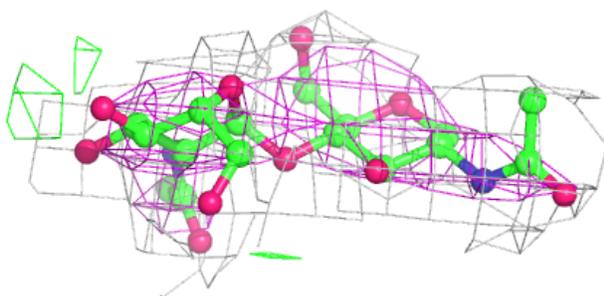
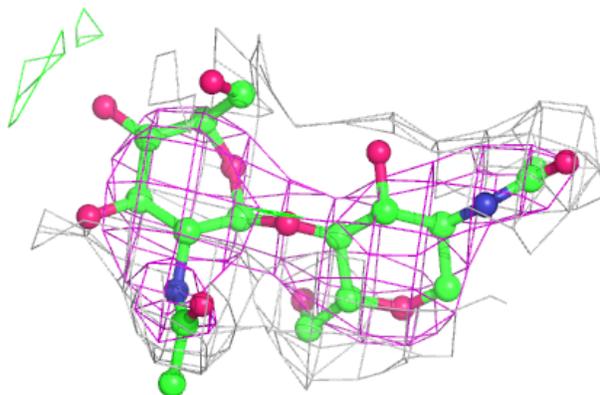


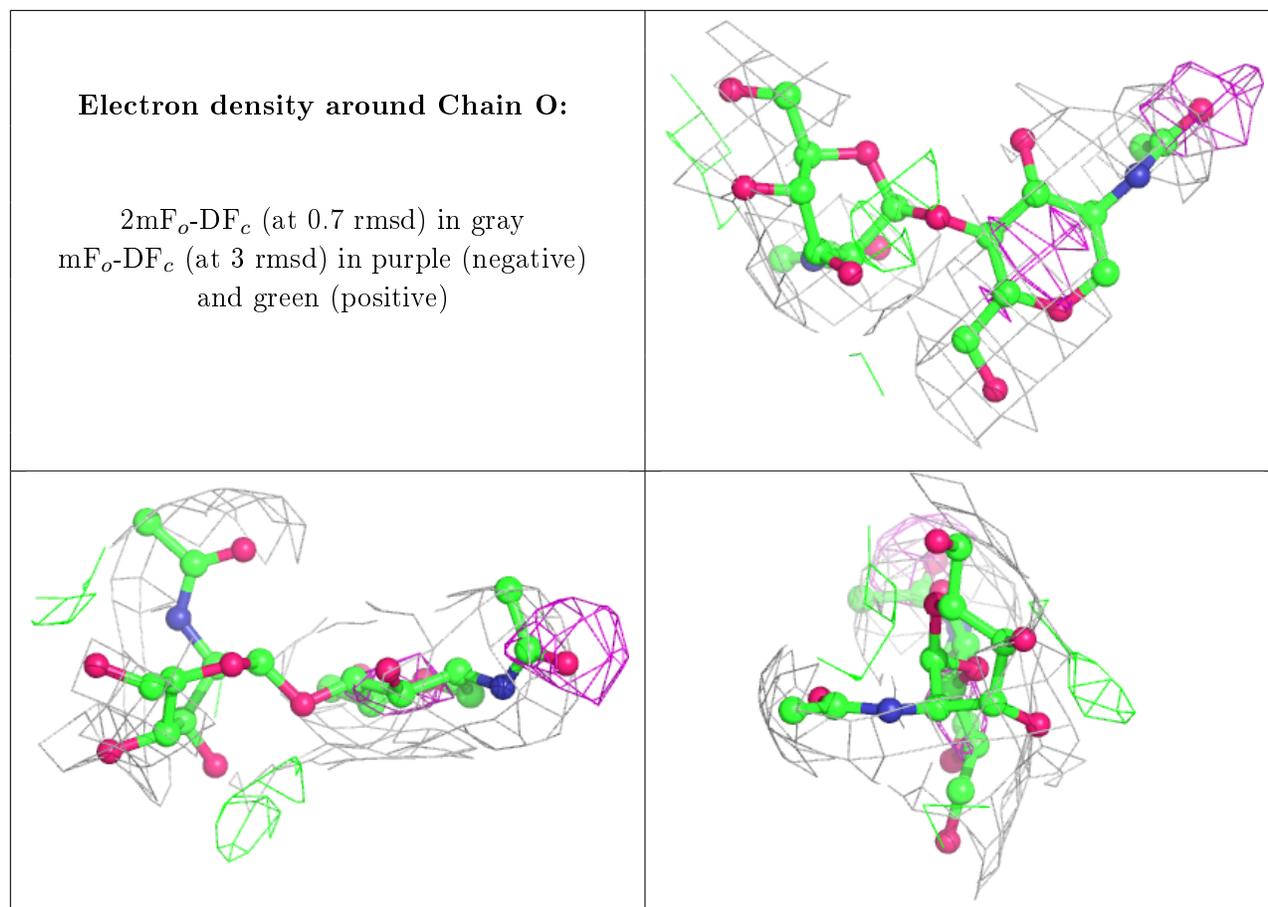
Electron density around Chain M:

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

**Electron density around Chain N:**

$2mF_o-DF_c$ (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	409	14/15	0.53	0.34	105,122,126,127	0
4	NAG	A	406	14/15	0.65	0.31	109,126,133,134	0
4	NAG	B	201	14/15	0.72	0.30	79,92,105,107	0
4	NAG	C	404	14/15	0.73	0.35	106,124,128,134	0
4	NAG	E	409	14/15	0.78	0.19	105,124,129,129	0
4	NAG	A	403	14/15	0.78	0.26	68,73,78,78	0
4	NAG	D	201	14/15	0.80	0.21	81,93,100,105	0
4	NAG	F	201	14/15	0.81	0.23	79,94,102,104	0
4	NAG	C	409	14/15	0.82	0.21	110,124,129,131	0
4	NAG	E	404	14/15	0.83	0.35	106,115,122,124	0
4	NAG	E	403	14/15	0.83	0.23	80,90,97,103	0
4	NAG	C	403	14/15	0.87	0.19	63,71,78,80	0

6.5 Other polymers

There are no such residues in this entry.