



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:23 AM UTC

PDB ID : 6CEX / pdb_00006cex
Title : Crystal structure of the A/Hong Kong/1/1968 (H3N2) influenza virus hemagglutinin in complex with small molecule N-Cyclohexyltaurine
Authors : wilson, I.A.; Kadam, R.U.
Deposited on : 2018-02-12
Resolution : 2.57 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

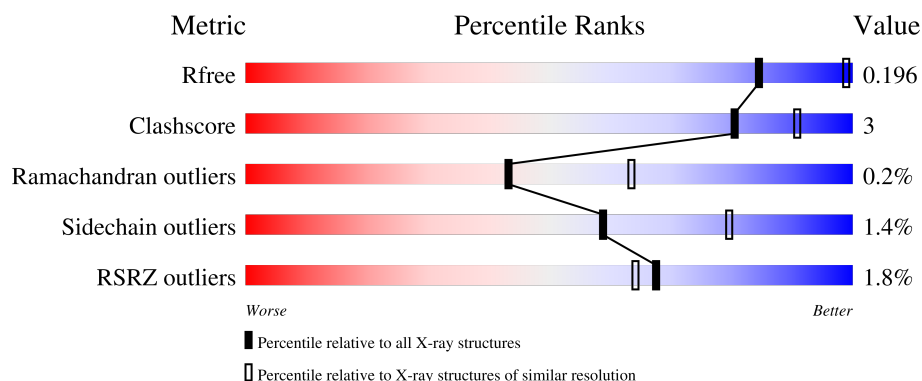
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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.



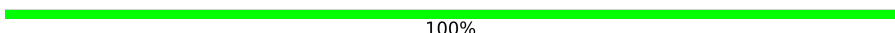
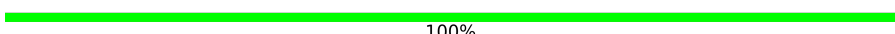
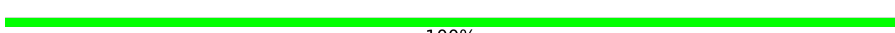
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	323	% 91% 7% .
1	C	323	% 91% 7% .
1	E	323	% 92% 6% .
2	B	174	3% 91% 7% ..
2	D	174	3% 86% 10% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	174	 3% 86% 12% **
3	G	3	 67% 33%
3	K	3	 67% 33%
4	H	2	 100%
4	I	2	 100%
4	J	2	 50% 50%
4	L	2	 100%
4	M	2	 100%
4	O	2	 100%
5	N	5	 20% 80%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12978 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	317	Total	C	N	O	S	0	4	0
			2476	1549	437	476	14			
1	C	316	Total	C	N	O	S	0	8	0
			2493	1560	441	478	14			
1	E	318	Total	C	N	O	S	0	3	0
			2476	1551	437	475	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q91MA7
A	8	ASP	-	expression tag	UNP Q91MA7
A	9	PRO	-	expression tag	UNP Q91MA7
A	10	GLY	-	expression tag	UNP Q91MA7
C	7	ALA	-	expression tag	UNP Q91MA7
C	8	ASP	-	expression tag	UNP Q91MA7
C	9	PRO	-	expression tag	UNP Q91MA7
C	10	GLY	-	expression tag	UNP Q91MA7
E	7	ALA	-	expression tag	UNP Q91MA7
E	8	ASP	-	expression tag	UNP Q91MA7
E	9	PRO	-	expression tag	UNP Q91MA7
E	10	GLY	-	expression tag	UNP Q91MA7

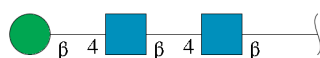
- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	3	0
			1404	872	244	281	7			
2	D	171	Total	C	N	O	S	0	3	0
			1404	870	245	282	7			
2	F	172	Total	C	N	O	S	0	4	0
			1422	883	248	284	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	conflict	UNP P03436
D	123	GLY	ARG	conflict	UNP P03436
F	123	GLY	ARG	conflict	UNP P03436

- 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.



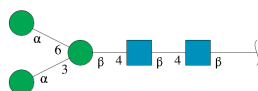
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



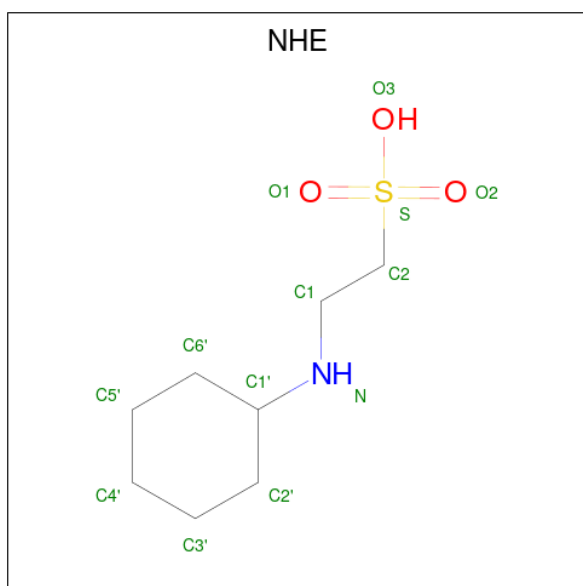
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
6	B	1	Total	C	N	O	S	0	1
			26	16	2	6	2		
6	C	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
6	C	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
6	E	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
6	F	1	Total	C	N	O	S	0	1
			26	16	2	6	2		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		
8	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	143	Total	O	0	0
			143	143		
10	B	100	Total	O	0	0
			100	100		
10	C	125	Total	O	0	0
			125	125		
10	D	110	Total	O	0	0
			110	110		
10	E	147	Total	O	0	0
			147	147		
10	F	119	Total	O	0	0
			119	119		

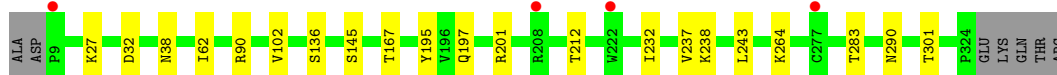
3 Residue-property plots [i](#)

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.

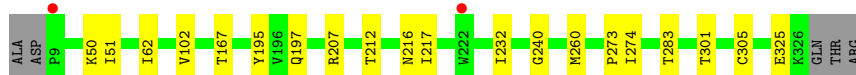
- Molecule 1: Hemagglutinin



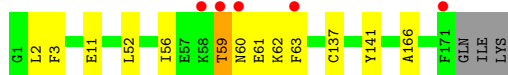
- Molecule 1: Hemagglutinin



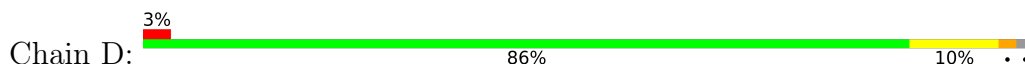
- Molecule 1: Hemagglutinin



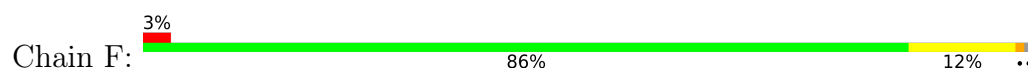
- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



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



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



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



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



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



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



MAG1
MAG2

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

Chain M:  100%MAG1
MAG2

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

Chain O:  100%MAG1
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  20% 80%MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.85Å 151.67Å 346.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.74 – 2.57 47.74 – 2.57	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.74-2.57) 98.3 (47.74-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.95 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.170 , 0.204 (Not available) , 0.196	Depositor DCC
R_{free} test set	4354 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12978	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NHE, BMA, SO4, GOL, 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	0.21	0/2532	0.40	0/3447
1	C	0.23	1/2553 (0.0%)	0.40	0/3477
1	E	0.18	0/2533	0.41	0/3450
2	B	0.20	0/1428	0.44	0/1919
2	D	0.58	5/1428 (0.4%)	0.51	0/1919
2	F	0.36	1/1446 (0.1%)	0.49	1/1942 (0.1%)
All	All	0.30	7/11920 (0.1%)	0.43	1/16154 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	109	ASP	C-O	-6.72	1.15	1.24
2	F	111	THR	C-O	-6.65	1.16	1.24
2	D	111	THR	C-O	-6.48	1.16	1.24
1	C	38	ASN	C-O	-6.43	1.16	1.23
2	D	72	GLU	C-O	-5.85	1.16	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	111	THR	N-CA-C	-5.21	105.05	111.40

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	2476	0	2423	17	0
1	C	2493	0	2443	13	0
1	E	2476	0	2426	11	0
2	B	1404	0	1320	14	0
2	D	1404	0	1315	13	0
2	F	1422	0	1340	13	0
3	G	39	0	34	0	0
3	K	39	0	34	1	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	O	28	0	25	0	0
5	N	61	0	52	1	0
6	A	13	0	17	0	0
6	B	26	0	34	0	0
6	C	26	0	34	1	0
6	E	13	0	16	0	0
6	F	26	0	34	1	0
7	A	42	0	39	0	0
7	B	14	0	13	0	0
7	E	42	0	39	0	0
7	F	14	0	13	1	0
8	A	10	0	0	0	0
8	B	5	0	0	0	0
8	D	10	0	0	0	0
8	F	5	0	0	0	0
9	C	6	0	8	1	0
10	A	143	0	0	1	0
10	B	100	0	0	0	0
10	C	125	0	0	0	0
10	D	110	0	0	0	0
10	E	147	0	0	0	0
10	F	119	0	0	0	0
All	All	12978	0	11784	63	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 3.

The worst 5 of 63 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ASN:HB2	2:D:59:THR:HG21	1.64	0.78
2:B:62:LYS:NZ	2:D:86:ASP:OD2	2.27	0.67
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.36	0.60
1:A:207:ARG:NH1	1:A:240:GLY:O	2.36	0.59
1:C:90:ARG:HD2	9:C:412:GOL:H11	1.85	0.58

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	319/323 (99%)	307 (96%)	11 (3%)	1 (0%)	36	56
1	C	322/323 (100%)	311 (97%)	10 (3%)	1 (0%)	36	56
1	E	319/323 (99%)	309 (97%)	9 (3%)	1 (0%)	36	56
2	B	172/174 (99%)	165 (96%)	7 (4%)	0	100	100
2	D	172/174 (99%)	163 (95%)	9 (5%)	0	100	100
2	F	174/174 (100%)	166 (95%)	8 (5%)	0	100	100
All	All	1478/1491 (99%)	1421 (96%)	54 (4%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE

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	282/283 (100%)	280 (99%)	2 (1%)	76	88
1	C	285/283 (101%)	285 (100%)	0	100	100
1	E	282/283 (100%)	280 (99%)	2 (1%)	76	88
2	B	148/148 (100%)	147 (99%)	1 (1%)	76	88
2	D	148/148 (100%)	142 (96%)	6 (4%)	27	51
2	F	150/148 (101%)	143 (95%)	7 (5%)	23	46
All	All	1295/1293 (100%)	1277 (99%)	18 (1%)	59	79

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	86	ASP
2	F	168	ASN
2	F	110	LEU
2	D	120	GLU
2	F	59	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	216	ASN
1	E	188	ASN
1	C	197	GLN
1	E	80	GLN
1	C	188	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 [i](#)

23 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	3,1	14,14,15	0.38	0	17,19,21	0.46	0
3	NAG	G	2	3	14,14,15	0.32	0	17,19,21	0.43	0
3	BMA	G	3	3	11,11,12	0.92	1 (9%)	15,15,17	1.12	1 (6%)
4	NAG	H	1	4,1	14,14,15	0.34	0	17,19,21	0.35	0
4	NAG	H	2	4	14,14,15	0.19	0	17,19,21	0.48	0
4	NAG	I	1	4,1	14,14,15	0.34	0	17,19,21	0.47	0
4	NAG	I	2	4	14,14,15	0.42	0	17,19,21	0.41	0
4	NAG	J	1	4,1	14,14,15	0.47	0	17,19,21	0.87	1 (5%)
4	NAG	J	2	4	14,14,15	0.27	0	17,19,21	0.43	0
3	NAG	K	1	3,1	14,14,15	0.28	0	17,19,21	0.41	0
3	NAG	K	2	3	14,14,15	0.36	0	17,19,21	0.46	0
3	BMA	K	3	3	11,11,12	0.80	0	15,15,17	0.82	0
4	NAG	L	1	4,1	14,14,15	0.44	0	17,19,21	0.48	0
4	NAG	L	2	4	14,14,15	0.21	0	17,19,21	0.38	0
4	NAG	M	1	2,4	14,14,15	0.39	0	17,19,21	0.48	0
4	NAG	M	2	4	14,14,15	0.34	0	17,19,21	0.36	0
5	NAG	N	1	5,1	14,14,15	0.46	0	17,19,21	0.52	0
5	NAG	N	2	5	14,14,15	0.29	0	17,19,21	0.49	0
5	BMA	N	3	5	11,11,12	1.06	1 (9%)	15,15,17	1.45	2 (13%)
5	MAN	N	4	5	11,11,12	0.81	0	15,15,17	1.07	1 (6%)
5	MAN	N	5	5	11,11,12	0.81	0	15,15,17	0.86	1 (6%)
4	NAG	O	1	4,1	14,14,15	0.40	0	17,19,21	0.41	0
4	NAG	O	2	4	14,14,15	0.26	0	17,19,21	0.48	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
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
4	NAG	H	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	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	-	2/2/19/22	0/1/1/1
4	NAG	L	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	NAG	M	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	BMA	N	3	5	-	0/2/19/22	0/1/1/1
5	MAN	N	4	5	-	2/2/19/22	0/1/1/1
5	MAN	N	5	5	-	2/2/19/22	0/1/1/1
4	NAG	O	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	3	BMA	O5-C5	-2.33	1.38	1.43
3	G	3	BMA	C2-C3	2.06	1.55	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	3	BMA	O5-C1-C2	-3.21	103.14	110.79
4	J	1	NAG	C1-O5-C5	2.99	116.19	112.19
5	N	3	BMA	O5-C5-C4	-2.78	104.07	110.83
5	N	4	MAN	C1-O5-C5	2.67	115.77	112.19
3	G	3	BMA	C1-O5-C5	2.21	115.14	112.19

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

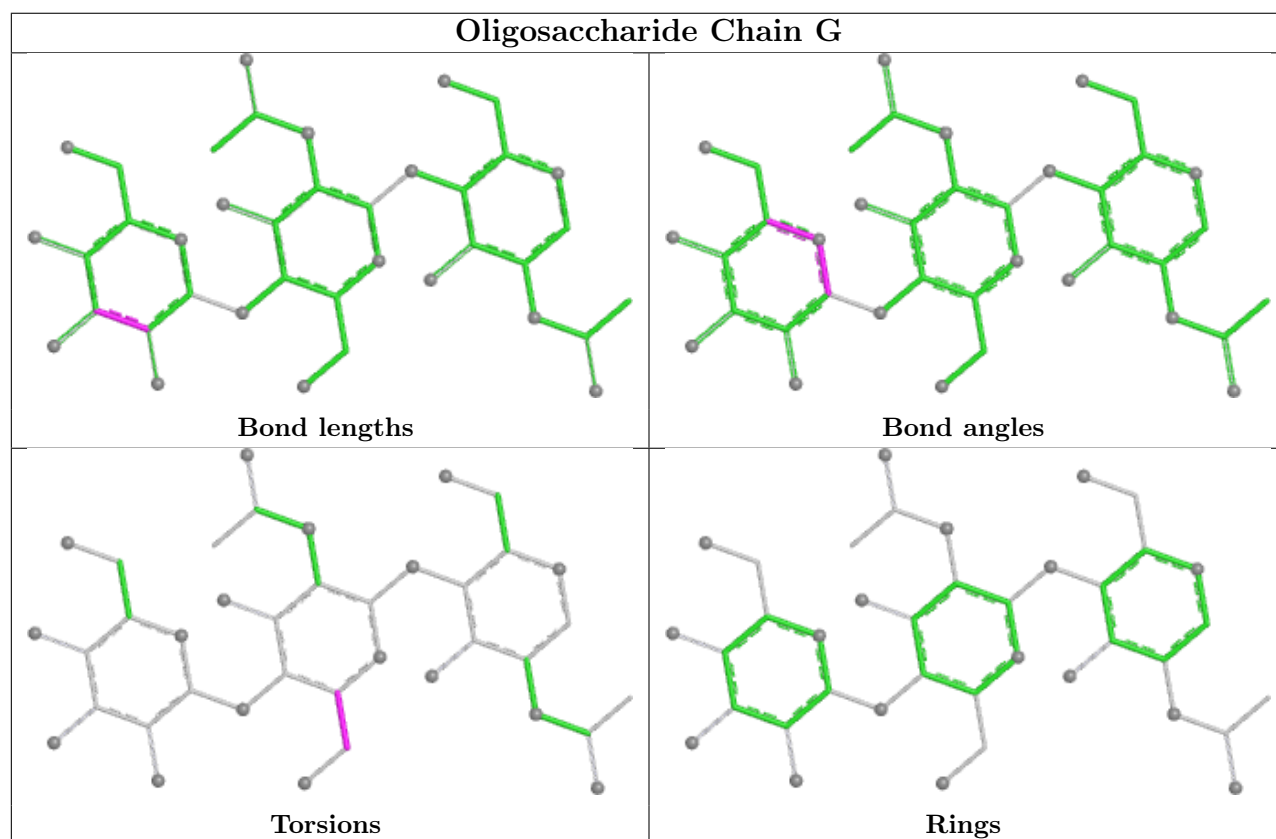
Mol	Chain	Res	Type	Atoms
3	K	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6

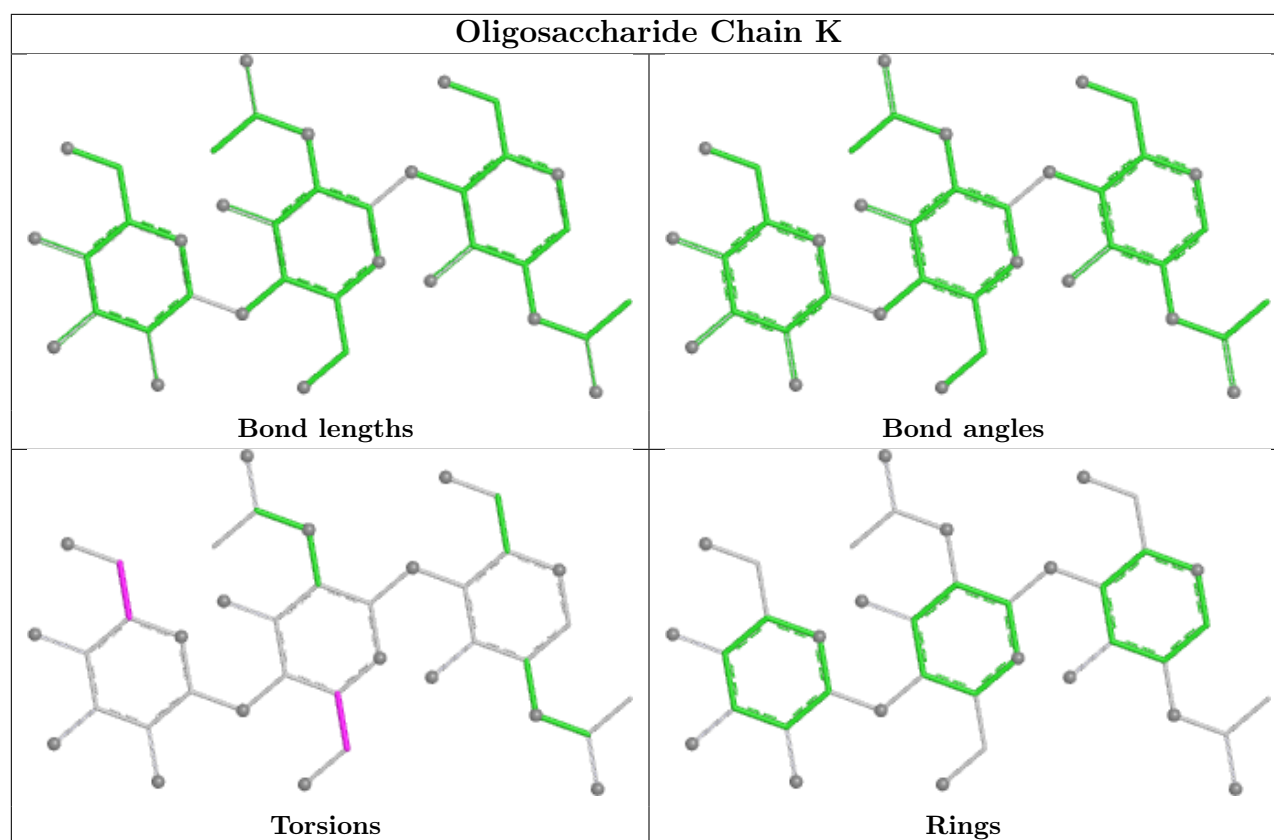
There are no ring outliers.

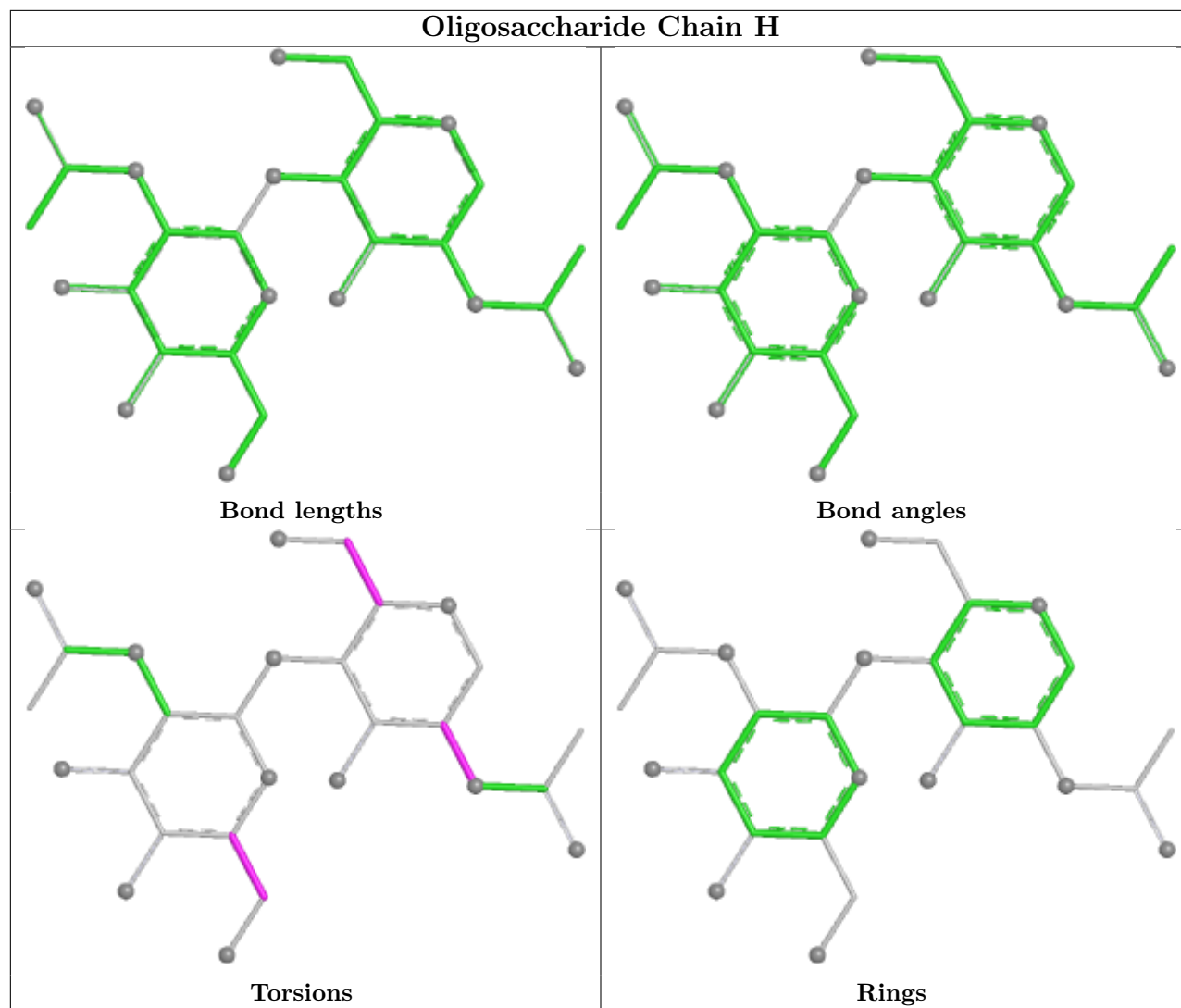
2 monomers are involved in 2 short contacts:

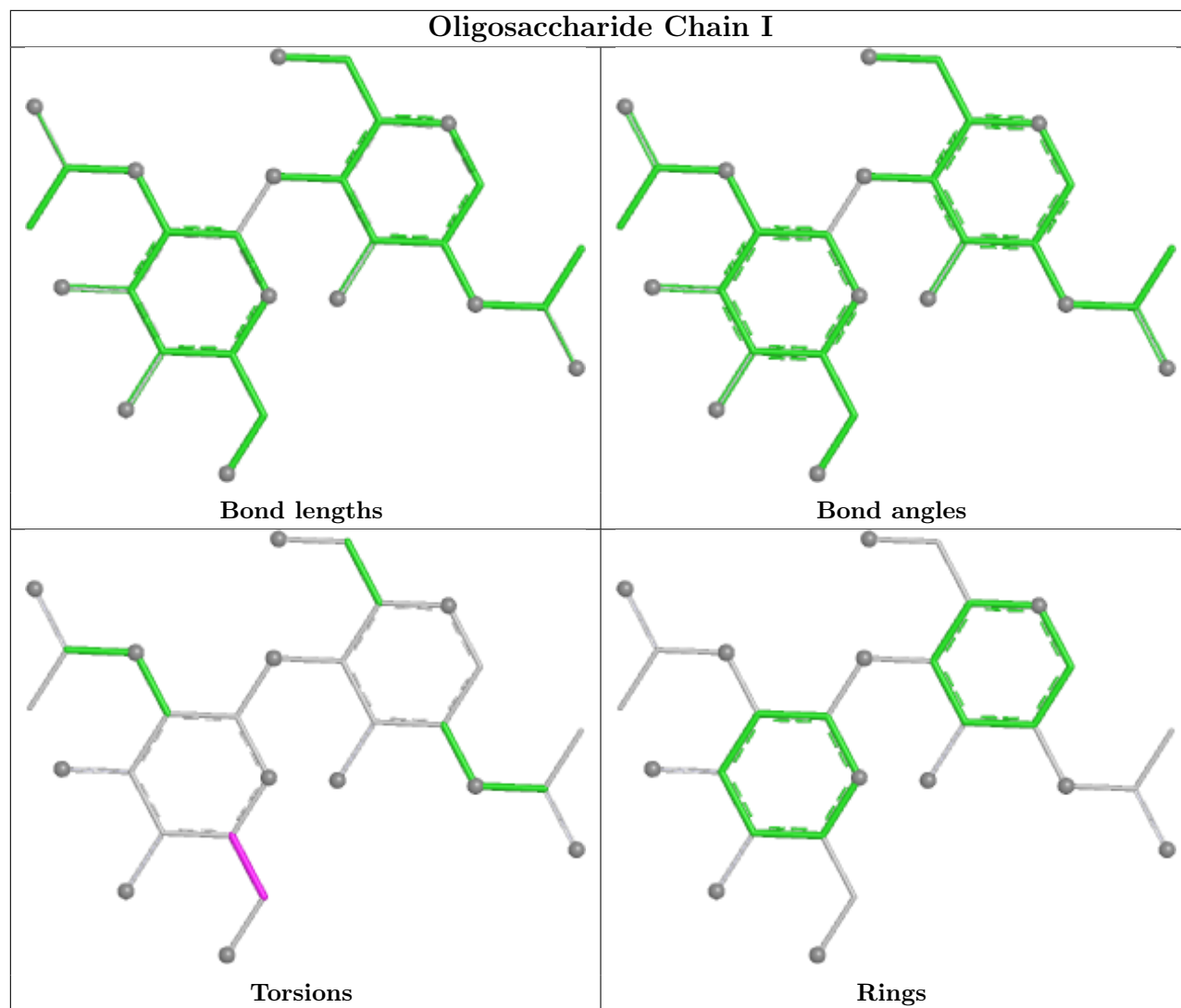
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1	NAG	1	0
5	N	1	NAG	1	0

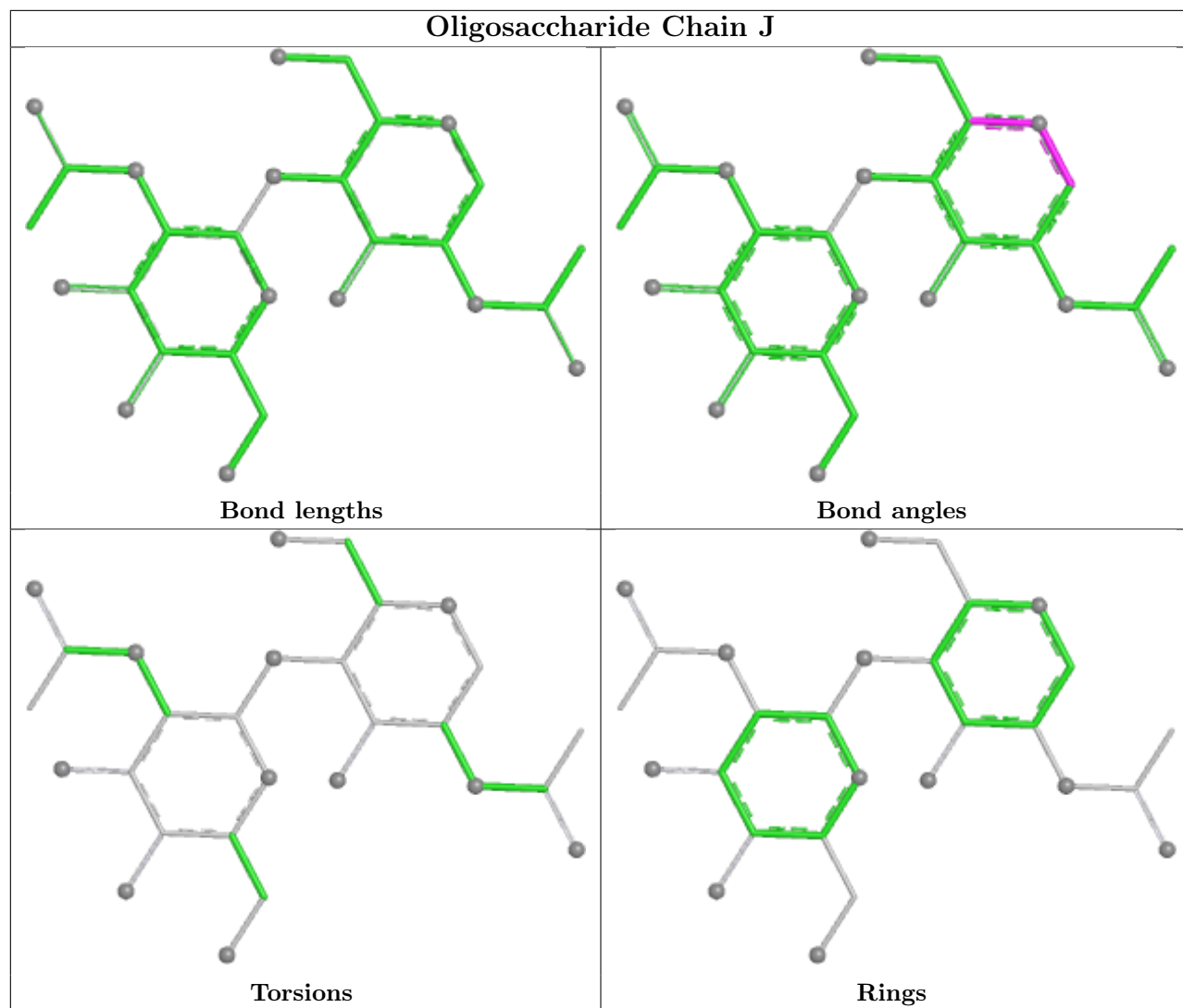
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

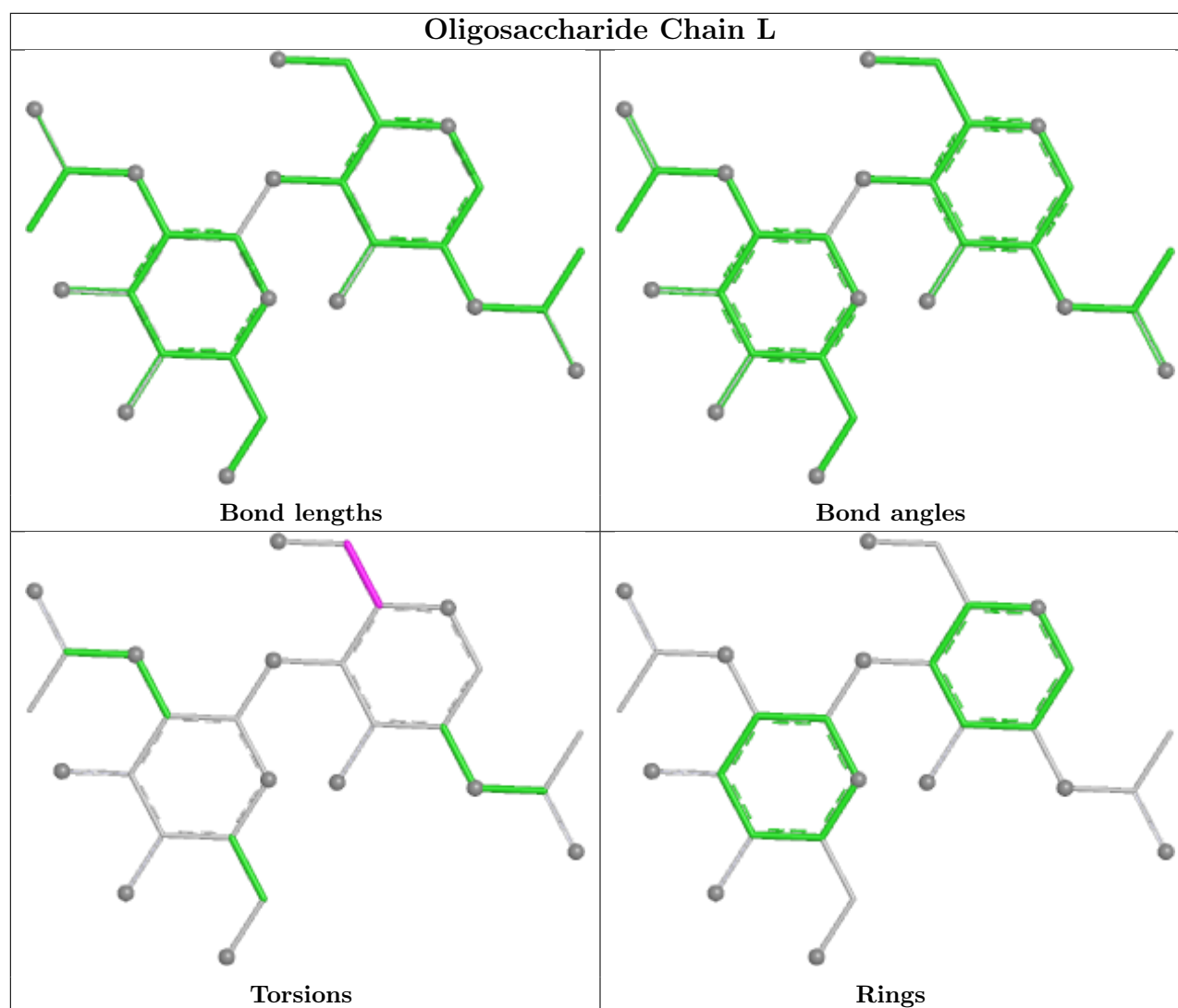


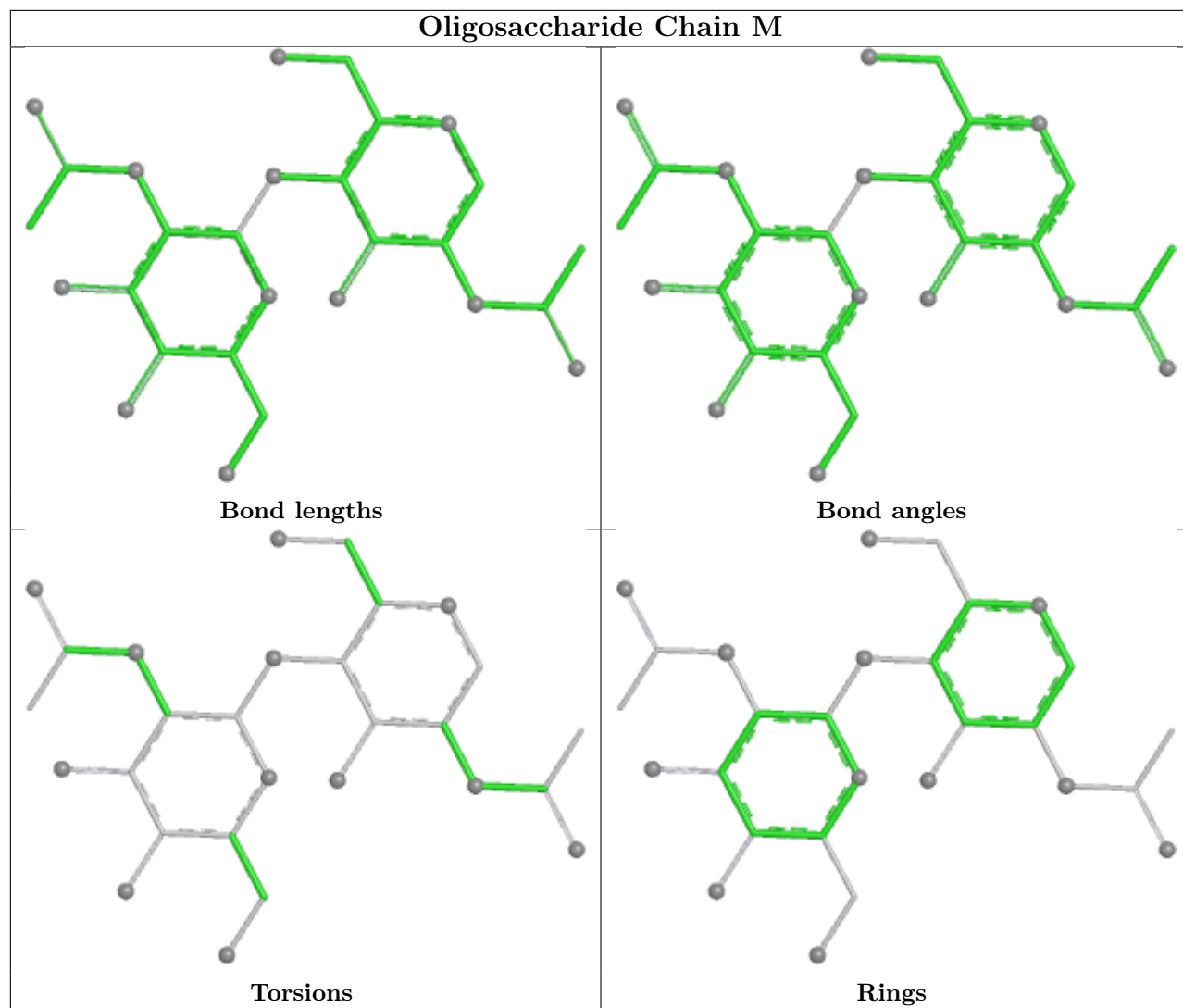


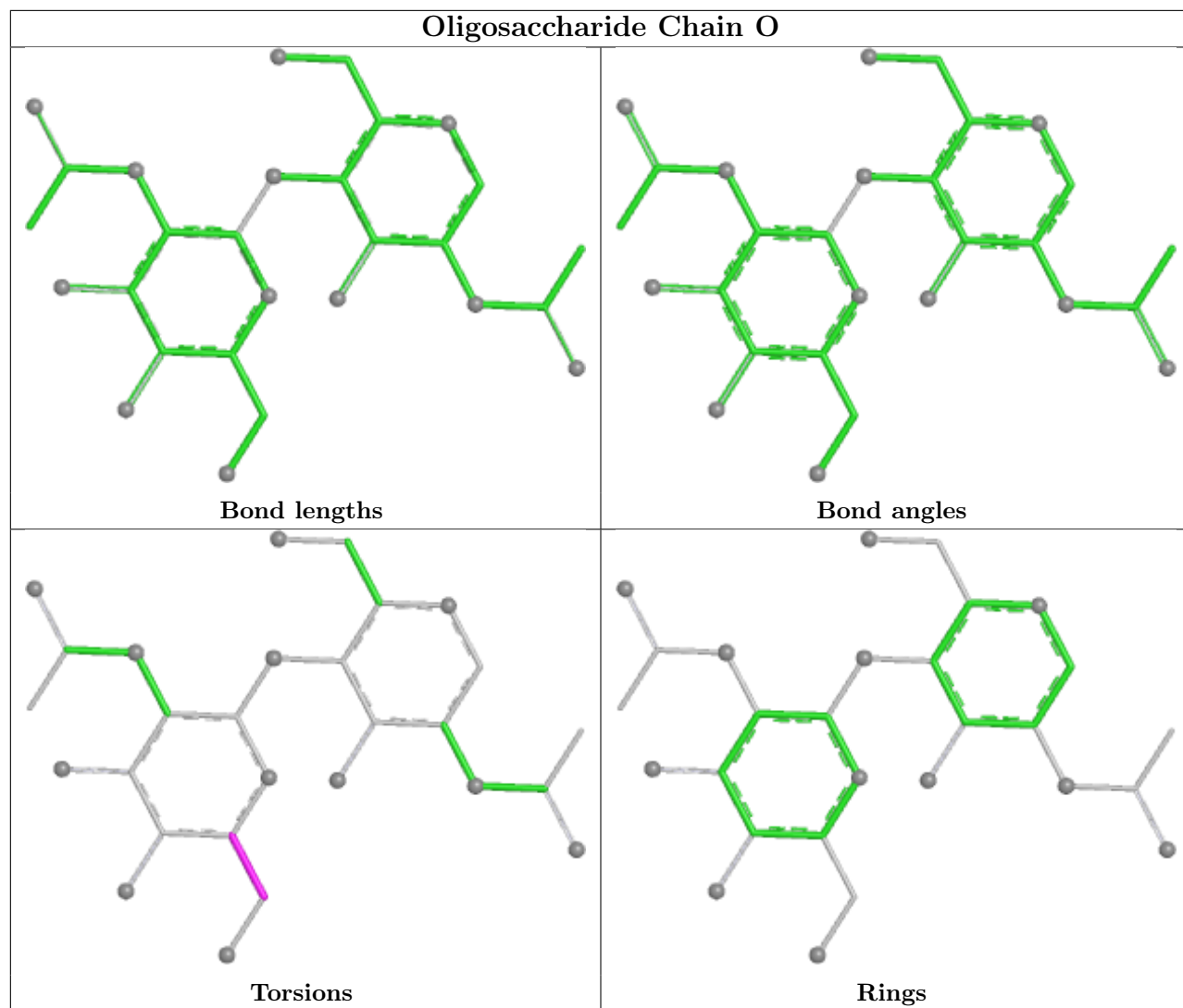


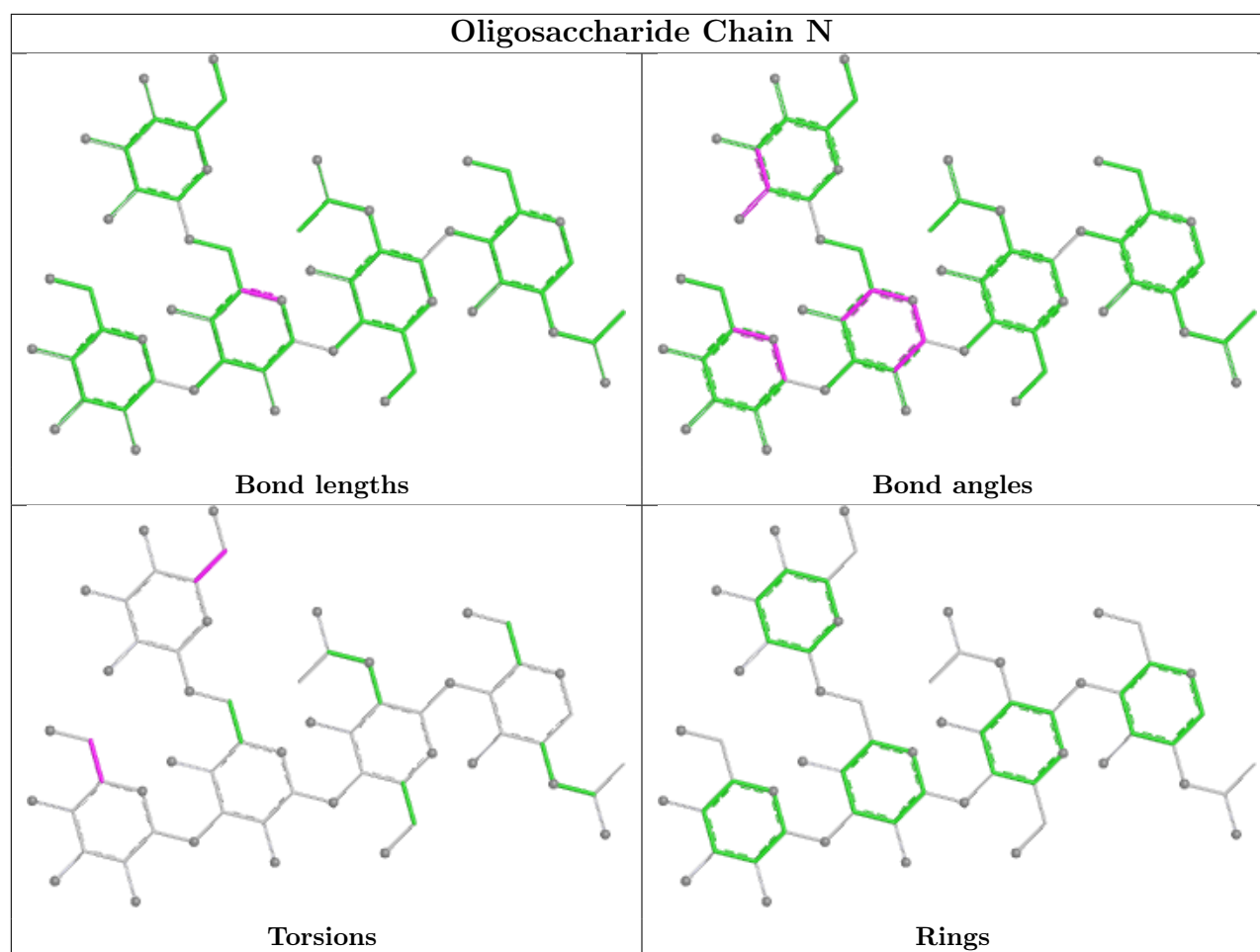












5.6 Ligand geometry [i](#)

23 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	$\# Z > 2$
8	SO4	D	204	-	4,4,4	0.23	0	6,6,6	0.10	0
6	NHE	C	401	-	13,13,13	1.76	3 (23%)	16,17,17	1.17	1 (6%)
7	NAG	B	202	2	14,14,15	0.37	0	17,19,21	0.44	0
7	NAG	A	403	1	14,14,15	0.16	0	17,19,21	0.51	0
7	NAG	E	403	1	14,14,15	0.27	0	17,19,21	0.71	1 (5%)
8	SO4	A	410	-	4,4,4	0.25	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	D	203	-	4,4,4	0.23	0	6,6,6	0.07	0
6	NHE	B	201[A]	-	13,13,13	1.74	3 (23%)	16,17,17	1.06	0
7	NAG	F	202	2	14,14,15	0.32	0	17,19,21	0.65	1 (5%)
6	NHE	E	401	-	13,13,13	2.35	6 (46%)	16,17,17	2.23	5 (31%)
6	NHE	B	201[B]	-	13,13,13	1.78	3 (23%)	16,17,17	1.16	2 (12%)
6	NHE	C	402	-	13,13,13	2.65	8 (61%)	16,17,17	2.56	8 (50%)
8	SO4	F	203	-	4,4,4	0.25	0	6,6,6	0.12	0
7	NAG	E	402	1	14,14,15	0.19	0	17,19,21	0.55	0
7	NAG	E	411	1	14,14,15	0.26	0	17,19,21	0.43	0
6	NHE	F	201[A]	-	13,13,13	1.82	3 (23%)	16,17,17	1.07	1 (6%)
8	SO4	B	203	-	4,4,4	0.23	0	6,6,6	0.08	0
7	NAG	A	402	1	14,14,15	0.47	0	17,19,21	0.48	0
6	NHE	F	201[B]	-	13,13,13	1.75	3 (23%)	16,17,17	1.05	1 (6%)
6	NHE	A	401	-	13,13,13	2.72	5 (38%)	16,17,17	2.57	6 (37%)
8	SO4	A	411	-	4,4,4	0.27	0	6,6,6	0.13	0
9	GOL	C	412	-	5,5,5	0.89	0	5,5,5	1.10	1 (20%)
7	NAG	A	404	1	14,14,15	0.30	0	17,19,21	0.78	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
6	NHE	B	201[A]	-	-	5/7/15/15	0/1/1/1
6	NHE	F	201[B]	-	-	5/7/15/15	0/1/1/1
7	NAG	A	404	1	-	2/6/23/26	0/1/1/1
6	NHE	C	401	-	-	3/7/15/15	0/1/1/1
7	NAG	B	202	2	-	0/6/23/26	0/1/1/1
7	NAG	A	403	1	-	0/6/23/26	0/1/1/1
6	NHE	A	401	-	-	0/7/15/15	0/1/1/1
7	NAG	E	403	1	-	2/6/23/26	0/1/1/1
7	NAG	F	202	2	-	1/6/23/26	0/1/1/1
6	NHE	E	401	-	-	1/7/15/15	0/1/1/1
7	NAG	E	402	1	-	2/6/23/26	0/1/1/1
7	NAG	E	411	1	-	0/6/23/26	0/1/1/1
9	GOL	C	412	-	-	1/4/4/4	-
6	NHE	B	201[B]	-	-	2/7/15/15	0/1/1/1
6	NHE	F	201[A]	-	-	5/7/15/15	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NHE	C	402	-	-	1/7/15/15	0/1/1/1
7	NAG	A	402	1	-	0/6/23/26	0/1/1/1

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	401	NHE	C6'-C1'	-6.86	1.36	1.52
6	C	402	NHE	C6'-C1'	-5.36	1.39	1.52
6	A	401	NHE	C5'-C6'	-5.08	1.40	1.53
6	F	201[A]	NHE	C2-S	4.67	1.84	1.77
6	B	201[B]	NHE	C2-S	4.53	1.83	1.77

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	401	NHE	O2-S-C2	6.62	116.73	106.73
6	E	401	NHE	O2-S-O1	-5.22	96.86	113.82
6	C	402	NHE	O1-S-C2	5.11	114.45	106.73
6	A	401	NHE	O2-S-O1	-4.84	98.07	113.82
6	E	401	NHE	O1-S-C2	4.28	113.20	106.73

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	201[A]	NHE	C2'-C1'-N-C1
6	B	201[A]	NHE	C1-C2-S-O2
6	C	401	NHE	C2'-C1'-N-C1
6	C	401	NHE	N-C1-C2-S
6	F	201[A]	NHE	N-C1-C2-S

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	401	NHE	1	0
7	F	202	NAG	1	0
6	F	201[B]	NHE	1	0
9	C	412	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	317/323 (98%)	-0.33	3 (0%) 81 79	10, 30, 52, 80	4 (1%)
1	C	316/323 (97%)	-0.29	4 (1%) 75 72	10, 29, 51, 86	8 (2%)
1	E	318/323 (98%)	-0.31	2 (0%) 85 84	11, 29, 50, 76	3 (0%)
2	B	171/174 (98%)	-0.30	5 (2%) 53 49	9, 27, 56, 103	3 (1%)
2	D	171/174 (98%)	-0.37	6 (3%) 47 42	11, 25, 52, 93	3 (1%)
2	F	172/174 (98%)	-0.29	6 (3%) 47 42	10, 26, 58, 85	4 (2%)
All	All	1465/1491 (98%)	-0.31	26 (1%) 67 64	9, 28, 52, 103	25 (1%)

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	60	ASN	6.1
1	E	9	PRO	6.0
1	C	9	PRO	5.9
2	F	60	ASN	5.3
2	B	60	ASN	5.3

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](#)

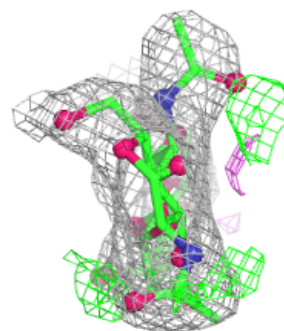
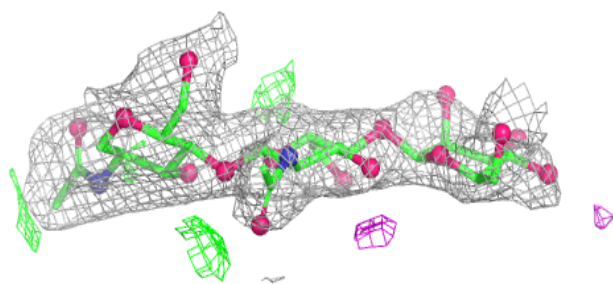
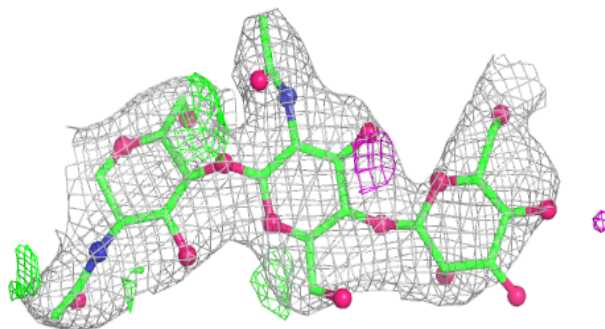
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
5	MAN	N	4	11/12	0.44	0.21	92,102,115,119	0
5	MAN	N	5	11/12	0.49	0.19	94,106,117,118	0
4	NAG	M	2	14/15	0.57	0.21	85,105,122,124	0
3	BMA	G	3	11/12	0.61	0.17	77,86,107,110	0
4	NAG	I	2	14/15	0.66	0.22	66,85,97,98	0
4	NAG	H	2	14/15	0.72	0.19	75,90,107,108	0
4	NAG	J	2	14/15	0.73	0.20	55,87,107,112	0
4	NAG	I	1	14/15	0.74	0.18	34,68,92,97	0
4	NAG	L	2	14/15	0.76	0.16	62,81,95,100	0
4	NAG	O	2	14/15	0.77	0.15	54,72,88,89	0
3	BMA	K	3	11/12	0.79	0.13	63,74,80,82	0
5	BMA	N	3	11/12	0.83	0.13	71,82,93,100	0
4	NAG	J	1	14/15	0.87	0.12	41,63,72,89	0
3	NAG	G	2	14/15	0.87	0.14	47,67,80,88	0
4	NAG	L	1	14/15	0.87	0.13	39,58,70,74	0
3	NAG	K	2	14/15	0.88	0.13	31,52,75,75	0
4	NAG	M	1	14/15	0.89	0.14	54,70,83,103	0
3	NAG	G	1	14/15	0.89	0.11	42,55,63,64	0
4	NAG	H	1	14/15	0.90	0.11	44,60,68,86	0
5	NAG	N	2	14/15	0.92	0.10	33,52,72,78	0
5	NAG	N	1	14/15	0.92	0.10	25,41,57,63	0
3	NAG	K	1	14/15	0.95	0.09	36,46,67,67	0
4	NAG	O	1	14/15	0.95	0.08	39,47,60,73	0

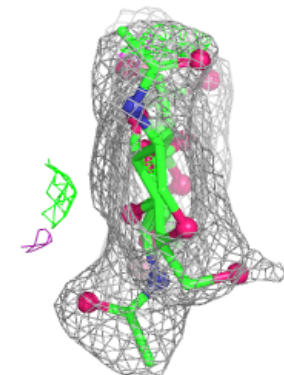
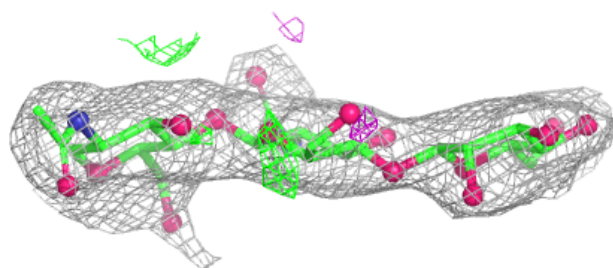
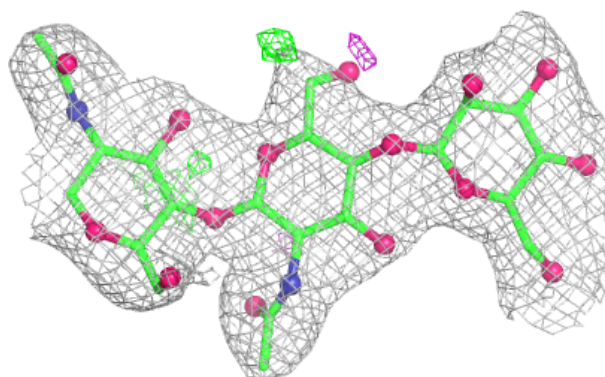
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

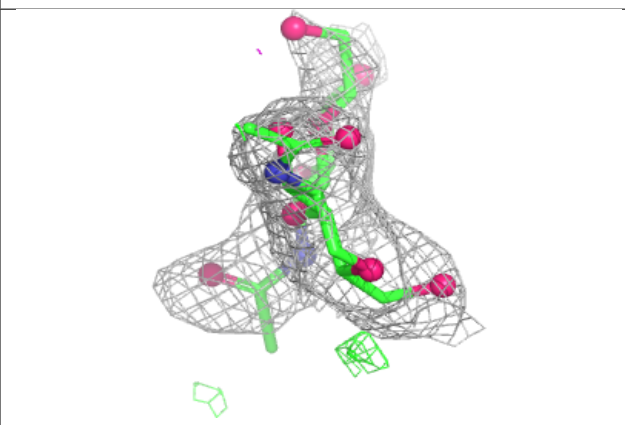
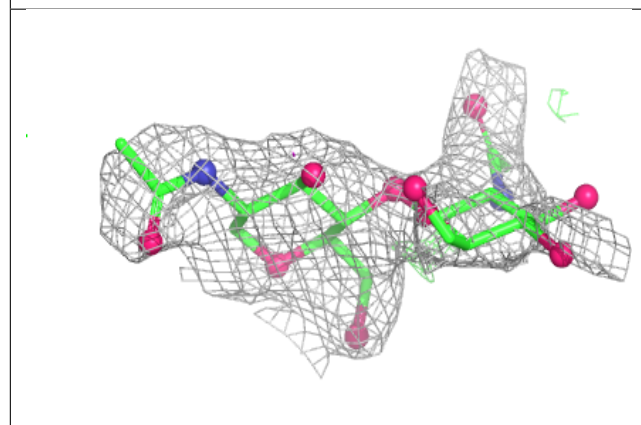
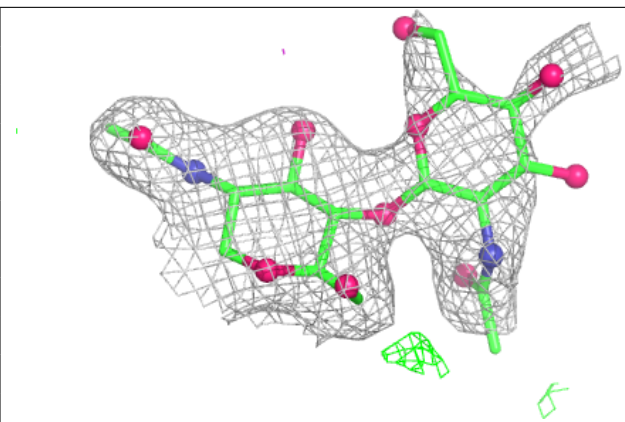
**Electron density around Chain K:**

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

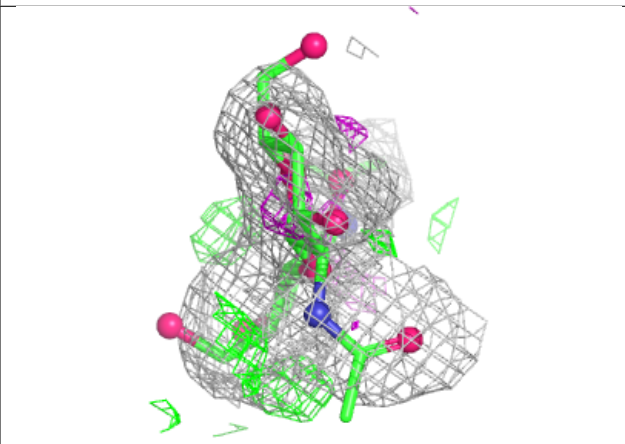
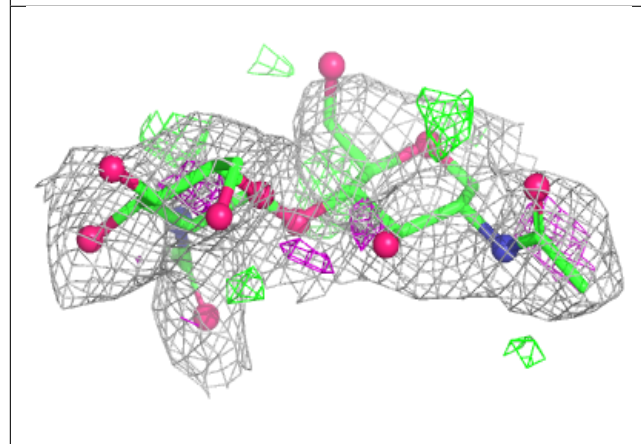
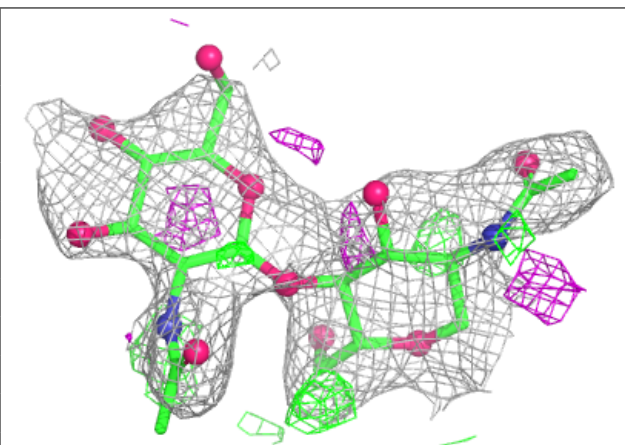


Electron density around Chain H:

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

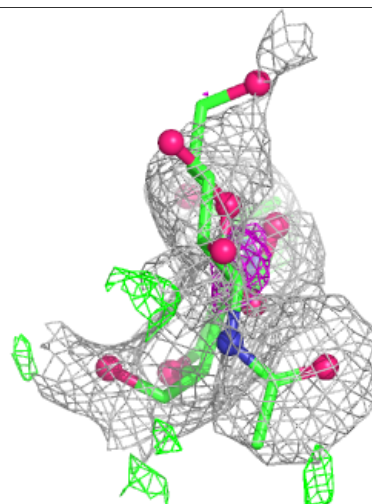
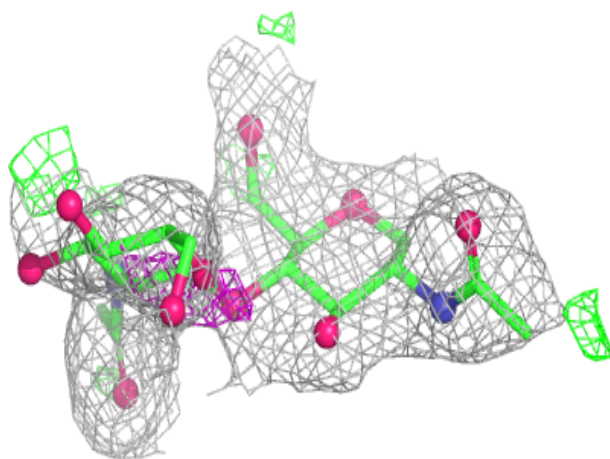
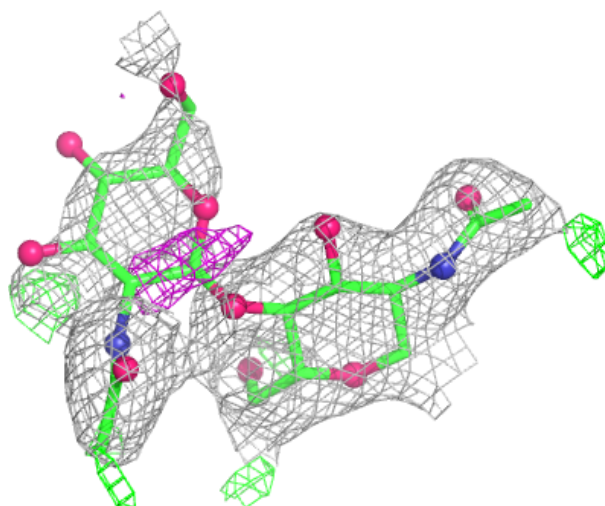
**Electron density around Chain I:**

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



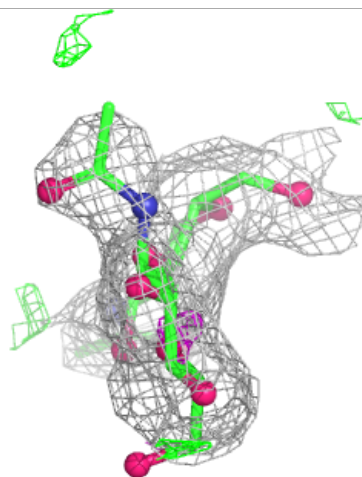
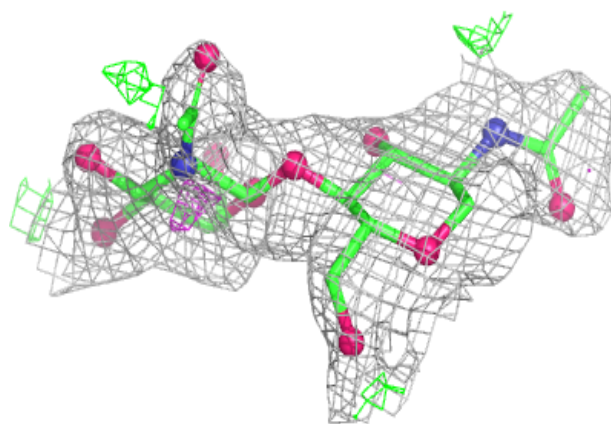
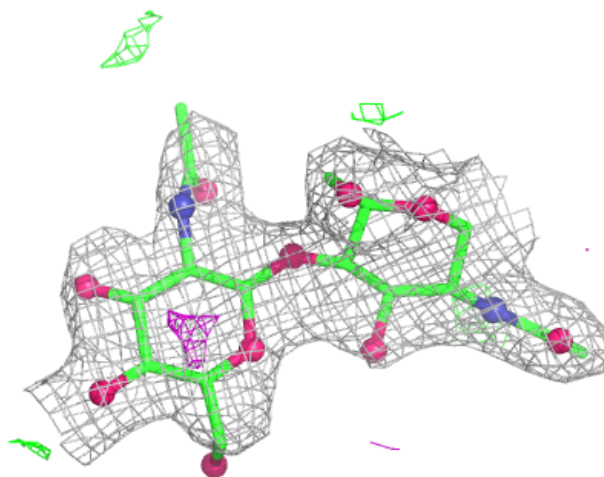
Electron density around Chain J:

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



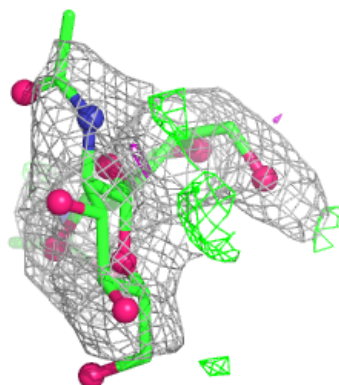
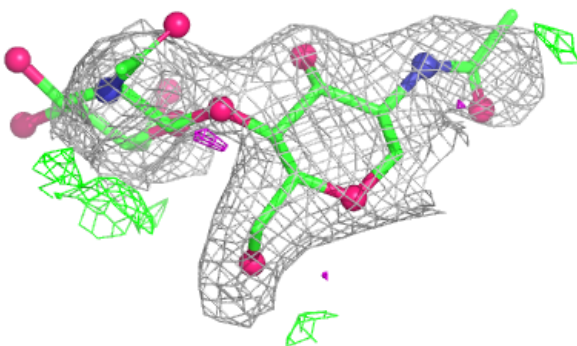
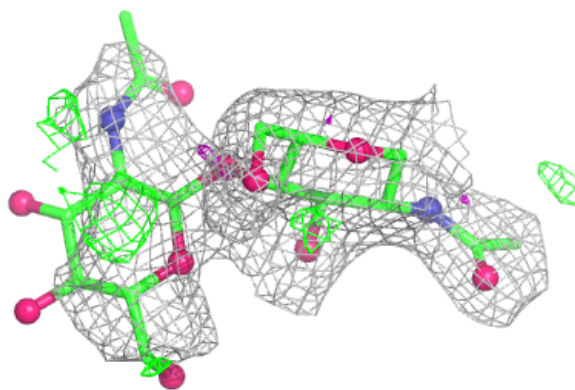
Electron density around Chain L:

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

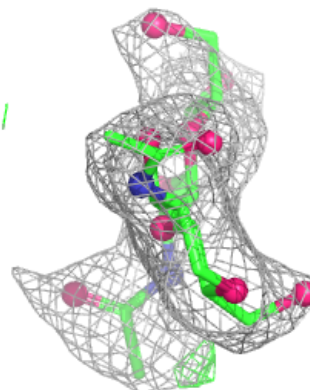
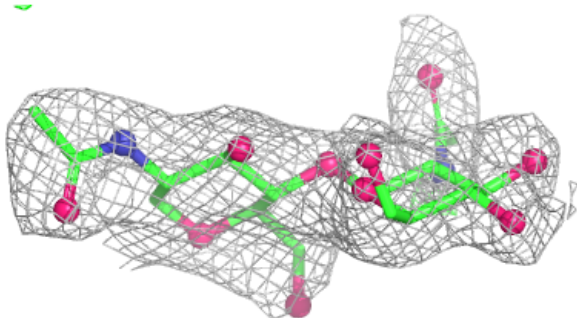
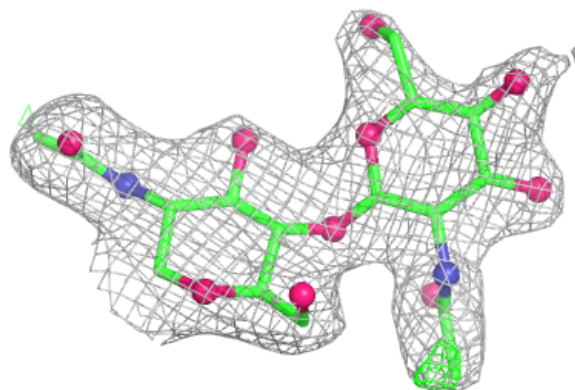


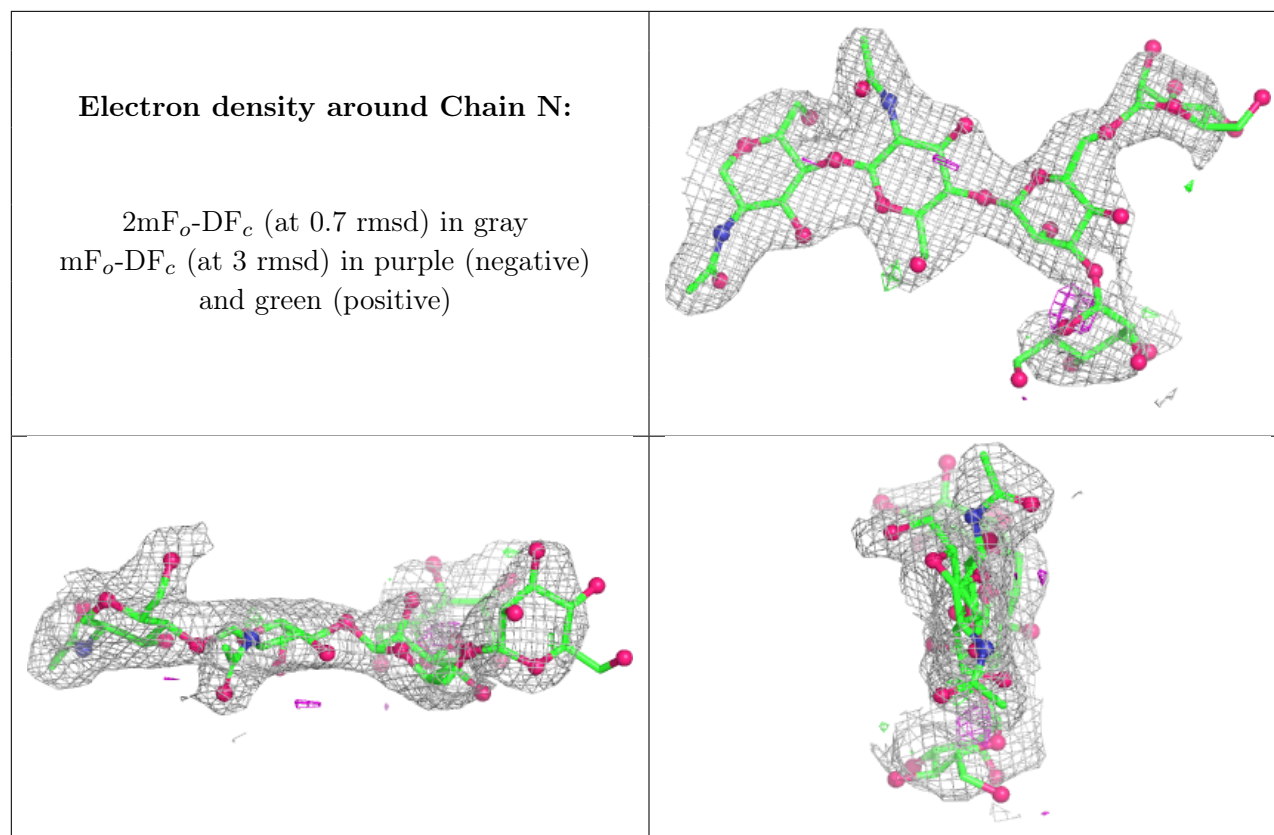
Electron density around Chain M:

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

**Electron density around Chain O:**

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





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($\text{\AA}^2$)	Q<0.9
7	NAG	A	402	14/15	0.78	0.15	41,58,66,67	0
8	SO4	A	411	5/5	0.80	0.20	34,40,68,94	5
7	NAG	E	411	14/15	0.81	0.17	64,71,83,90	0
7	NAG	F	202	14/15	0.82	0.15	60,68,77,77	0
7	NAG	B	202	14/15	0.82	0.14	51,64,74,74	0
7	NAG	A	403	14/15	0.84	0.16	49,64,92,93	0
6	NHE	A	401	13/13	0.86	0.16	33,51,80,82	0
7	NAG	E	403	14/15	0.87	0.12	38,53,63,64	0
7	NAG	E	402	14/15	0.87	0.15	39,61,82,85	0
7	NAG	A	404	14/15	0.88	0.12	33,48,65,80	0
6	NHE	C	402	13/13	0.90	0.13	24,32,86,100	0
8	SO4	B	203	5/5	0.91	0.11	64,73,80,88	0
8	SO4	D	204	5/5	0.91	0.14	53,65,74,78	0
8	SO4	F	203	5/5	0.91	0.12	50,52,77,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NHE	B	201[A]	13/13	0.92	0.15	29,32,75,85	13
6	NHE	B	201[B]	13/13	0.92	0.15	26,32,72,82	13
6	NHE	C	401	13/13	0.92	0.12	36,41,77,78	0
8	SO4	A	410	5/5	0.92	0.13	39,42,78,80	5
6	NHE	E	401	13/13	0.93	0.11	29,37,58,63	0
9	GOL	C	412	6/6	0.93	0.11	38,41,56,60	0
6	NHE	F	201[A]	13/13	0.94	0.12	24,31,56,60	13
6	NHE	F	201[B]	13/13	0.94	0.12	22,29,39,58	13
8	SO4	D	203	5/5	0.97	0.12	25,25,27,30	5

6.5 Other polymers [i](#)

There are no such residues in this entry.