



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 10:29 AM BST

PDB ID : 6HMY  
Title : Cholera toxin classical B-pentamer in complex with fucosyl-GM1  
Authors : Krengel, U.; Heim, J.B.  
Deposited on : 2018-09-13  
Resolution : 1.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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

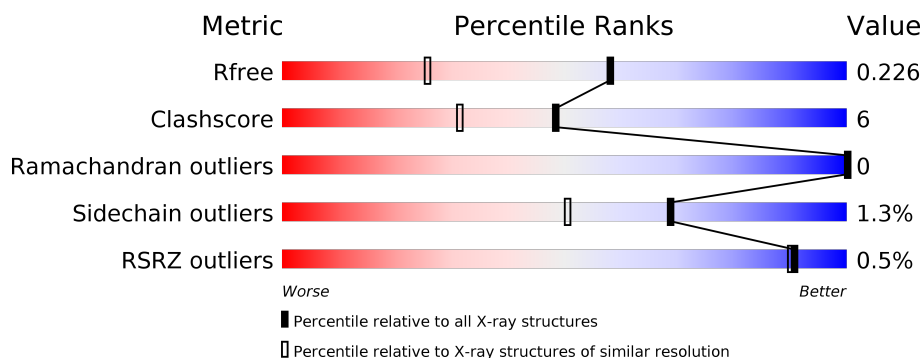
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	103	<div> <div>89%</div> <div>9%</div> <div>•</div> </div>
1	B	103	<div> <div>88%</div> <div>11%</div> <div>•</div> </div>
1	C	103	<div> <div>2%</div> <div>91%</div> <div>9%</div> </div>
1	D	103	<div> <div>90%</div> <div>10%</div> </div>
1	E	103	<div> <div>%</div> <div>91%</div> <div>9%</div> </div>
1	F	103	<div> <div>%</div> <div>91%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	103	 95% . .
1	H	103	 93% 6% .
1	I	103	 85% 14% .
1	J	103	 % 88% 12%
2	K	6	 17% 83%
2	N	6	 50% 50%
2	O	6	 67% 33%
2	P	6	 33% 50% 17%
2	S	6	 50% 17% 33%
2	T	6	 33% 67%
3	L	7	 43% 43% 14%
3	R	7	 57% 43%
4	M	7	 57% 43%
4	Q	7	 86% 14%

## 2 Entry composition [i](#)

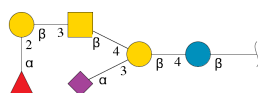
There are 8 unique types of molecules in this entry. The entry contains 10879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cholera enterotoxin B-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	9	0
			866	548	147	165	6			
1	B	103	Total	C	N	O	S	0	11	0
			883	561	152	164	6			
1	C	103	Total	C	N	O	S	0	7	0
			862	547	148	161	6			
1	D	103	Total	C	N	O	S	0	9	0
			866	547	150	163	6			
1	E	103	Total	C	N	O	S	0	7	0
			854	541	146	161	6			
1	F	103	Total	C	N	O	S	0	9	0
			872	550	150	166	6			
1	G	103	Total	C	N	O	S	0	8	0
			867	550	149	162	6			
1	H	103	Total	C	N	O	S	0	10	0
			881	558	151	166	6			
1	I	103	Total	C	N	O	S	0	8	0
			867	550	148	163	6			
1	J	103	Total	C	N	O	S	0	9	0
			874	553	153	162	6			

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



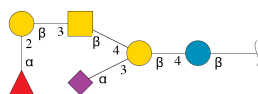
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	6	Total	C	N	O	0	0	0
			78	43	2	33			

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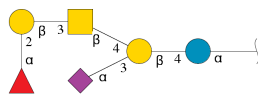
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	N	6	Total	C	N	O	0	6	0
			156	86	4	66			
2	O	6	Total	C	N	O	0	0	0
			78	43	2	33			
2	P	6	Total	C	N	O	0	0	0
			78	43	2	33			
2	S	6	Total	C	N	O	0	0	0
			78	43	2	33			
2	T	6	Total	C	N	O	0	6	0
			156	86	4	66			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	L	6	Total	C	N	O	0	6	0
			156	86	4	66			
3	R	6	Total	C	N	O	0	6	0
			156	86	4	66			

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

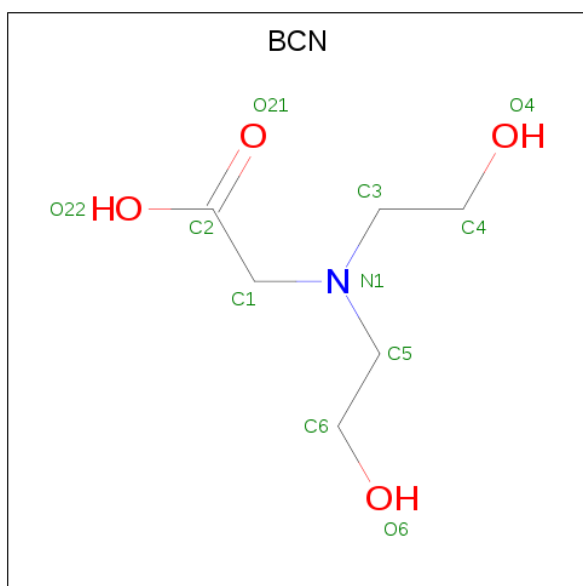


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	6	Total	C	N	O	0	6	0
			156	86	4	66			
4	Q	6	Total	C	N	O	0	6	0
			156	86	4	66			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Ca 2 2	0	0
5	A	2	Total Ca 2 2	0	0
5	D	2	Total Ca 2 2	0	0
5	C	2	Total Ca 2 2	0	0
5	E	2	Total Ca 2 2	0	0

- Molecule 6 is BICINE (three-letter code: BCN) (formula:  $C_6H_{13}NO_4$ ).



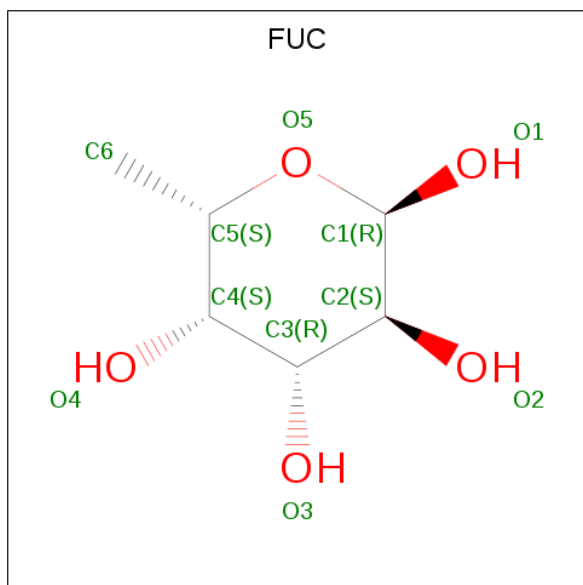
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 11 6 1 4	0	0
6	A	1	Total C N O 11 6 1 4	0	0
6	B	1	Total C N O 11 6 1 4	0	0
6	B	1	Total C N O 11 6 1 4	0	0
6	C	1	Total C N O 11 6 1 4	0	0
6	C	1	Total C N O 11 6 1 4	0	0
6	D	1	Total C N O 11 6 1 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			11	6	1	4		
6	E	1	Total	C	N	O	0	0
			11	6	1	4		
6	E	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 7 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			11	6	5		
7	J	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	81	Total	O	0	0
			81	81		
8	B	79	Total	O	0	0
			79	79		
8	C	76	Total	O	0	0
			76	76		
8	D	75	Total	O	0	0
			75	75		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	81	Total 81	O 81	0	0
8	F	84	Total 84	O 84	0	0
8	G	92	Total 92	O 92	0	0
8	H	79	Total 79	O 79	0	0
8	I	71	Total 71	O 71	0	0
8	J	79	Total 79	O 79	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.

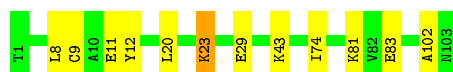
- Molecule 1: Cholera enterotoxin B-subunit

Chain A:  89% 9%

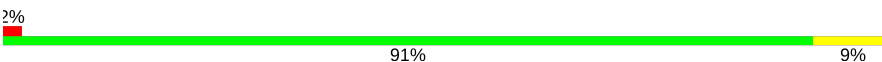


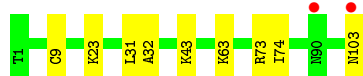
- Molecule 1: Cholera enterotoxin B-subunit

Chain B:  88% 11%




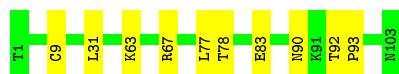
- Molecule 1: Cholera enterotoxin B-subunit

Chain C:  91% 9%

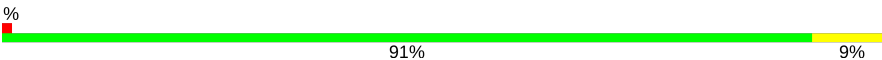


- Molecule 1: Cholera enterotoxin B-subunit

Chain D:  90% 10%




- Molecule 1: Cholera enterotoxin B-subunit

Chain E:  91% 9%



- Molecule 1: Cholera enterotoxin B-subunit

Chain F:  91% 9%



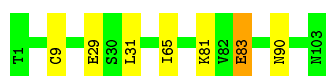
- Molecule 1: Cholera enterotoxin B-subunit

Chain G: 95% ..



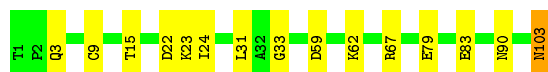
- Molecule 1: Cholera enterotoxin B-subunit

Chain H: 93% 6% .



- Molecule 1: Cholera enterotoxin B-subunit

Chain I: 85% 14% .



- Molecule 1: Cholera enterotoxin B-subunit

Chain J: 88% 12%



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

Chain K: 17% 83%

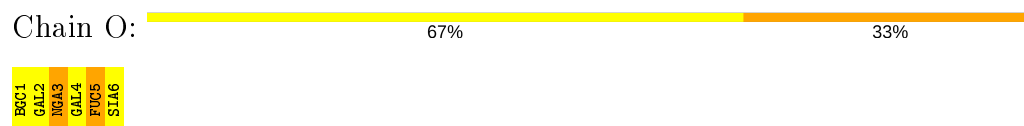


- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain N: 50% 50%



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



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



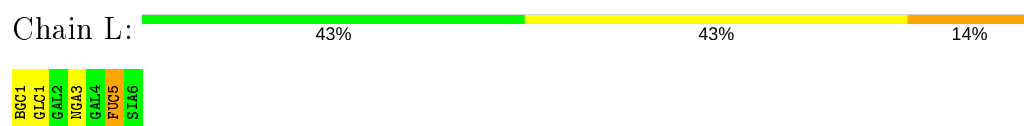
- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



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



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



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




BGC1	GLC1	GAL2	NGA3	GAL4	FUC5	SLA6
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- Molecule 4: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain M:  57% 43%

GLC1	BGC1	GAL2	NGA3	GAL4	FUC5	SLA6
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- Molecule 4: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain Q:  86% 14%

GLC1	BGC1	GAL2	NGA3	GAL4	FUC5	SLA6
------	------	------	------	------	------	------

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.63Å 74.14Å 111.25Å 90.00° 105.59° 90.00°	Depositor
Resolution (Å)	44.32 – 1.60 44.32 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.32-1.60) 98.2 (44.32-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.184 , 0.214 0.197 , 0.226	Depositor DCC
$R_{free}$ test set	7592 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.1	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCN, BGC, NGA, CA, GLC, SIA, GAL, FUC

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	0.84	1/901 (0.1%)	0.86	0/1213
1	B	0.86	3/918 (0.3%)	0.84	0/1235
1	C	0.80	0/889	0.88	1/1197 (0.1%)
1	D	0.82	1/901 (0.1%)	0.88	0/1214
1	E	0.84	0/886	0.84	0/1193
1	F	0.87	1/901 (0.1%)	0.87	0/1214
1	G	0.86	2/902 (0.2%)	0.85	0/1214
1	H	0.93	2/910 (0.2%)	0.85	0/1224
1	I	0.84	2/899 (0.2%)	0.82	0/1211
1	J	0.83	1/903 (0.1%)	0.88	1/1214 (0.1%)
All	All	0.85	13/9010 (0.1%)	0.86	2/12129 (0.0%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	66	GLU	CD-OE2	8.51	1.35	1.25
1	H	83[A]	GLU	C-O	7.22	1.37	1.23
1	H	83[B]	GLU	C-O	7.22	1.37	1.23
1	A	36	GLU	CD-OE1	6.85	1.33	1.25
1	B	29	GLU	CD-OE2	6.46	1.32	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	J	67	ARG	NE-CZ-NH1	-6.85	116.88	120.30

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	866	0	891	10	0
1	B	883	0	922	10	0
1	C	862	0	880	10	0
1	D	866	0	894	9	0
1	E	854	0	881	13	0
1	F	872	0	891	10	0
1	G	867	0	902	4	0
1	H	881	0	908	10	0
1	I	867	0	896	22	0
1	J	874	0	906	17	0
2	K	78	0	67	0	0
2	N	156	0	134	9	0
2	O	78	0	67	1	0
2	P	78	0	67	2	0
2	S	78	0	67	3	0
2	T	156	0	133	7	0
3	L	156	0	134	3	0
3	R	156	0	134	8	0
4	M	156	0	133	5	0
4	Q	156	0	133	3	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
6	A	22	0	20	0	0
6	B	22	0	20	0	0
6	C	22	0	20	0	0
6	D	22	0	20	1	0
6	E	22	0	20	0	0
7	F	11	0	12	0	0
7	J	11	0	12	0	0
8	A	81	0	0	1	0
8	B	79	0	0	2	0
8	C	76	0	0	2	0
8	D	75	0	0	2	0
8	E	81	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	84	0	0	3	0
8	G	92	0	0	1	0
8	H	79	0	0	1	0
8	I	71	0	0	2	0
8	J	79	0	0	3	0
All	All	10879	0	10164	121	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 6.

The worst 5 of 121 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:3[A]:NGA:O7	2:T:5[A]:FUC:H3	1.31	1.27
1:H:90:ASN:ND2	3:R:5[A]:FUC:O2	1.84	1.09
4:M:3[A]:NGA:O7	4:M:5[A]:FUC:H3	1.53	1.07
2:N:3[B]:NGA:C7	2:N:5[B]:FUC:H3	1.85	1.07
1:F:59[B]:ASP:OD1	1:F:62[B]:LYS:NZ	1.88	1.06

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	110/103 (107%)	106 (96%)	4 (4%)	0	100	100
1	B	112/103 (109%)	111 (99%)	1 (1%)	0	100	100
1	C	108/103 (105%)	107 (99%)	1 (1%)	0	100	100
1	D	110/103 (107%)	108 (98%)	2 (2%)	0	100	100
1	E	108/103 (105%)	107 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	110/103 (107%)	110 (100%)	0	0	100	100
1	G	110/103 (107%)	107 (97%)	3 (3%)	0	100	100
1	H	111/103 (108%)	111 (100%)	0	0	100	100
1	I	110/103 (107%)	108 (98%)	2 (2%)	0	100	100
1	J	110/103 (107%)	109 (99%)	1 (1%)	0	100	100
All	All	1099/1030 (107%)	1084 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	98/89 (110%)	91 (93%)	7 (7%)	14	3
1	B	100/89 (112%)	93 (93%)	7 (7%)	15	3
1	C	96/89 (108%)	94 (98%)	2 (2%)	53	29
1	D	98/89 (110%)	96 (98%)	2 (2%)	55	31
1	E	96/89 (108%)	96 (100%)	0	100	100
1	F	98/89 (110%)	98 (100%)	0	100	100
1	G	98/89 (110%)	98 (100%)	0	100	100
1	H	99/89 (111%)	97 (98%)	2 (2%)	55	31
1	I	98/89 (110%)	97 (99%)	1 (1%)	76	61
1	J	98/89 (110%)	98 (100%)	0	100	100
All	All	979/890 (110%)	958 (98%)	21 (2%)	69	29

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	20	LEU
1	B	23[B]	LYS

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Mol	Chain	Res	Type
1	D	9[B]	CYS
1	B	9[B]	CYS
1	H	9[A]	CYS

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

Mol	Chain	Res	Type
1	F	14	ASN
1	I	103	ASN
1	H	90	ASN
1	D	103	ASN
1	F	103	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 ⓘ

96 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	BGC	K	1	2	12,12,12	0.52	0	17,17,17	1.70	2 (11%)
2	GAL	K	2	2	11,11,12	0.85	0	15,15,17	0.94	1 (6%)
2	NGA	K	3	2	14,14,15	0.96	1 (7%)	17,19,21	0.95	0
2	GAL	K	4	2	11,11,12	0.65	0	15,15,17	0.84	0
2	FUC	K	5	2	10,10,11	0.47	0	14,14,16	1.13	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SIA	K	6	2	17,20,21	0.46	0	21,28,31	0.92	1 (4%)
3	BGC	L	1[A]	3	12,12,12	0.95	1 (8%)	17,17,17	0.77	1 (5%)
3	GLC	L	1[B]	3	12,12,12	0.79	1 (8%)	17,17,17	1.19	1 (5%)
3	GAL	L	2[A]	3	11,11,12	0.64	0	15,15,17	0.90	0
3	GAL	L	2[B]	3	11,11,12	0.72	0	15,15,17	0.61	0
3	NGA	L	3[A]	3	14,14,15	0.46	0	17,19,21	0.84	0
3	NGA	L	3[B]	3	14,14,15	0.36	0	17,19,21	0.59	0
3	GAL	L	4[A]	3	11,11,12	0.62	0	15,15,17	0.91	0
3	GAL	L	4[B]	3	11,11,12	0.73	0	15,15,17	0.77	0
3	FUC	L	5[A]	3	10,10,11	0.62	0	14,14,16	1.19	2 (14%)
3	FUC	L	5[B]	3	10,10,11	0.67	0	14,14,16	0.89	1 (7%)
3	SIA	L	6[A]	3	17,20,21	0.52	0	21,28,31	0.76	0
3	SIA	L	6[B]	3	17,20,21	0.61	0	21,28,31	0.58	0
4	BGC	M	1[B]	4	12,12,12	0.46	0	17,17,17	1.29	2 (11%)
4	GLC	M	1[A]	4	12,12,12	0.29	0	17,17,17	0.77	1 (5%)
4	GAL	M	2[A]	4	11,11,12	0.62	0	15,15,17	1.47	2 (13%)
4	GAL	M	2[B]	4	11,11,12	0.81	1 (9%)	15,15,17	1.24	2 (13%)
4	NGA	M	3[A]	4	14,14,15	0.40	0	17,19,21	1.08	1 (5%)
4	NGA	M	3[B]	4	14,14,15	0.44	0	17,19,21	0.62	0
4	GAL	M	4[A]	4	11,11,12	1.04	2 (18%)	15,15,17	0.97	0
4	GAL	M	4[B]	4	11,11,12	0.88	0	15,15,17	1.26	2 (13%)
4	FUC	M	5[A]	4	10,10,11	0.45	0	14,14,16	1.23	2 (14%)
4	FUC	M	5[B]	1,4	10,10,11	1.07	1 (10%)	14,14,16	1.64	1 (7%)
4	SIA	M	6[A]	4	17,20,21	0.85	1 (5%)	21,28,31	0.84	1 (4%)
4	SIA	M	6[B]	4	17,20,21	0.75	1 (5%)	21,28,31	1.31	3 (14%)
2	BGC	N	1[A]	2	12,12,12	0.39	0	17,17,17	0.70	0
2	BGC	N	1[B]	2	12,12,12	0.38	0	17,17,17	1.44	4 (23%)
2	GAL	N	2[A]	2	11,11,12	0.34	0	15,15,17	1.60	3 (20%)
2	GAL	N	2[B]	2	11,11,12	0.49	0	15,15,17	0.65	0
2	NGA	N	3[A]	2	14,14,15	0.41	0	17,19,21	0.87	0
2	NGA	N	3[B]	2	14,14,15	0.58	0	17,19,21	1.02	2 (11%)
2	GAL	N	4[A]	2	11,11,12	0.44	0	15,15,17	0.90	1 (6%)
2	GAL	N	4[B]	2	11,11,12	1.19	1 (9%)	15,15,17	1.27	1 (6%)
2	FUC	N	5[A]	2	10,10,11	0.69	0	14,14,16	0.91	0
2	FUC	N	5[B]	2	10,10,11	1.12	1 (10%)	14,14,16	2.17	3 (21%)
2	SIA	N	6[A]	2	17,20,21	0.48	0	21,28,31	0.65	0
2	SIA	N	6[B]	2	17,20,21	0.55	0	21,28,31	1.06	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BGC	O	1	2	12,12,12	0.44	0	17,17,17	1.05	1 (5%)
2	GAL	O	2	2	11,11,12	1.07	1 (9%)	15,15,17	0.91	1 (6%)
2	NGA	O	3	2	14,14,15	0.69	0	17,19,21	0.94	1 (5%)
2	GAL	O	4	2	11,11,12	0.70	0	15,15,17	1.13	1 (6%)
2	FUC	O	5	2	10,10,11	0.87	0	14,14,16	1.30	1 (7%)
2	SIA	O	6	2	17,20,21	0.75	1 (5%)	21,28,31	0.91	0
2	BGC	P	1	2	12,12,12	0.83	0	17,17,17	0.77	1 (5%)
2	GAL	P	2	2	11,11,12	0.74	0	15,15,17	0.86	1 (6%)
2	NGA	P	3	2	14,14,15	0.67	0	17,19,21	0.87	0
2	GAL	P	4	2	11,11,12	1.00	0	15,15,17	0.85	0
2	FUC	P	5	2	10,10,11	0.59	0	14,14,16	1.01	1 (7%)
2	SIA	P	6	2	17,20,21	0.53	0	21,28,31	0.78	0
4	BGC	Q	1[B]	4	12,12,12	0.50	0	17,17,17	0.75	0
4	GLC	Q	1[A]	4	12,12,12	0.66	0	17,17,17	1.28	2 (11%)
4	GAL	Q	2[A]	4	11,11,12	1.00	1 (9%)	15,15,17	0.94	1 (6%)
4	GAL	Q	2[B]	4	11,11,12	0.67	0	15,15,17	1.04	1 (6%)
4	NGA	Q	3[A]	4	14,14,15	0.62	0	17,19,21	1.02	0
4	NGA	Q	3[B]	4	14,14,15	0.41	0	17,19,21	0.65	0
4	GAL	Q	4[A]	4	11,11,12	0.36	0	15,15,17	0.97	1 (6%)
4	GAL	Q	4[B]	4	11,11,12	0.67	0	15,15,17	1.20	1 (6%)
4	FUC	Q	5[A]	4	10,10,11	1.03	2 (20%)	14,14,16	1.07	0
4	FUC	Q	5[B]	4	10,10,11	0.72	0	14,14,16	1.74	5 (35%)
4	SIA	Q	6[A]	4	17,20,21	0.39	0	21,28,31	0.72	0
4	SIA	Q	6[B]	4	17,20,21	0.34	0	21,28,31	0.71	0
3	BGC	R	1[A]	3	12,12,12	0.72	0	17,17,17	1.18	1 (5%)
3	GLC	R	1[B]	3	12,12,12	0.77	0	17,17,17	1.27	2 (11%)
3	GAL	R	2[A]	3	11,11,12	0.52	0	15,15,17	1.20	1 (6%)
3	GAL	R	2[B]	3	11,11,12	0.61	0	15,15,17	1.18	1 (6%)
3	NGA	R	3[A]	3	14,14,15	0.40	0	17,19,21	0.94	1 (5%)
3	NGA	R	3[B]	3	14,14,15	0.47	0	17,19,21	0.87	1 (5%)
3	GAL	R	4[A]	3	11,11,12	0.61	0	15,15,17	1.23	2 (13%)
3	GAL	R	4[B]	3	11,11,12	0.72	0	15,15,17	0.82	0
3	FUC	R	5[A]	3	10,10,11	1.34	1 (10%)	14,14,16	1.56	3 (21%)
3	FUC	R	5[B]	3	10,10,11	0.56	0	14,14,16	1.50	3 (21%)
3	SIA	R	6[A]	3	17,20,21	0.42	0	21,28,31	0.80	2 (9%)
3	SIA	R	6[B]	3	17,20,21	0.39	0	21,28,31	0.96	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BGC	S	1	2	12,12,12	0.54	0	17,17,17	1.14	1 (5%)
2	GAL	S	2	2	11,11,12	0.46	0	15,15,17	0.89	0
2	NGA	S	3	2	14,14,15	0.55	0	17,19,21	0.79	1 (5%)
2	GAL	S	4	2	11,11,12	0.79	0	15,15,17	0.55	0
2	FUC	S	5	2	10,10,11	0.34	0	14,14,16	1.53	2 (14%)
2	SIA	S	6	2	17,20,21	0.68	0	21,28,31	0.75	0
2	BGC	T	1[A]	2	12,12,12	0.32	0	17,17,17	0.71	0
2	BGC	T	1[B]	2	12,12,12	0.32	0	17,17,17	1.23	2 (11%)
2	GAL	T	2[A]	2	11,11,12	0.46	0	15,15,17	0.90	1 (6%)
2	GAL	T	2[B]	2	11,11,12	0.66	0	15,15,17	1.21	1 (6%)
2	NGA	T	3[A]	2	14,14,15	0.36	0	17,19,21	0.82	1 (5%)
2	NGA	T	3[B]	2	14,14,15	0.46	0	17,19,21	0.78	1 (5%)
2	GAL	T	4[A]	2	11,11,12	0.91	0	15,15,17	1.43	3 (20%)
2	GAL	T	4[B]	2	11,11,12	0.97	1 (9%)	15,15,17	1.17	2 (13%)
2	FUC	T	5[A]	2	10,10,11	1.42	1 (10%)	14,14,16	2.33	5 (35%)
2	FUC	T	5[B]	2	10,10,11	0.54	0	14,14,16	1.30	2 (14%)
2	SIA	T	6[A]	2	17,20,21	0.70	0	21,28,31	1.20	1 (4%)
2	SIA	T	6[B]	2	17,20,21	0.76	0	21,28,31	0.92	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
2	BGC	K	1	2	-	2/2/22/22	0/1/1/1
2	GAL	K	2	2	-	0/2/19/22	0/1/1/1
2	NGA	K	3	2	-	0/6/23/26	0/1/1/1
2	GAL	K	4	2	-	0/2/19/22	0/1/1/1
2	FUC	K	5	2	-	-	0/1/1/1
2	SIA	K	6	2	-	0/14/34/38	0/1/1/1
3	BGC	L	1[A]	3	-	2/2/22/22	0/1/1/1
3	GLC	L	1[B]	3	-	2/2/22/22	0/1/1/1
3	GAL	L	2[A]	3	-	1/2/19/22	0/1/1/1
3	GAL	L	2[B]	3	-	2/2/19/22	0/1/1/1
3	NGA	L	3[A]	3	-	0/6/23/26	0/1/1/1
3	NGA	L	3[B]	3	-	0/6/23/26	0/1/1/1
3	GAL	L	4[A]	3	-	0/2/19/22	0/1/1/1
3	GAL	L	4[B]	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	L	5[A]	3	-	-	0/1/1/1
3	FUC	L	5[B]	3	-	-	0/1/1/1
3	SIA	L	6[A]	3	-	2/14/34/38	0/1/1/1
3	SIA	L	6[B]	3	-	0/14/34/38	0/1/1/1
4	BGC	M	1[B]	4	-	2/2/22/22	0/1/1/1
4	GLC	M	1[A]	4	-	0/2/22/22	0/1/1/1
4	GAL	M	2[A]	4	-	2/2/19/22	0/1/1/1
4	GAL	M	2[B]	4	-	2/2/19/22	0/1/1/1
4	NGA	M	3[A]	4	-	2/6/23/26	0/1/1/1
4	NGA	M	3[B]	4	-	1/6/23/26	0/1/1/1
4	GAL	M	4[A]	4	-	1/2/19/22	0/1/1/1
4	GAL	M	4[B]	4	-	0/2/19/22	0/1/1/1
4	FUC	M	5[A]	4	-	-	0/1/1/1
4	FUC	M	5[B]	1,4	-	-	0/1/1/1
4	SIA	M	6[A]	4	-	0/14/34/38	0/1/1/1
4	SIA	M	6[B]	4	-	6/14/34/38	0/1/1/1
2	BGC	N	1[A]	2	-	0/2/22/22	0/1/1/1
2	BGC	N	1[B]	2	-	0/2/22/22	0/1/1/1
2	GAL	N	2[A]	2	-	1/2/19/22	0/1/1/1
2	GAL	N	2[B]	2	-	0/2/19/22	0/1/1/1
2	NGA	N	3[A]	2	-	0/6/23/26	0/1/1/1
2	NGA	N	3[B]	2	-	0/6/23/26	0/1/1/1
2	GAL	N	4[A]	2	-	0/2/19/22	0/1/1/1
2	GAL	N	4[B]	2	-	0/2/19/22	0/1/1/1
2	FUC	N	5[A]	2	-	-	0/1/1/1
2	FUC	N	5[B]	2	-	-	0/1/1/1
2	SIA	N	6[A]	2	-	0/14/34/38	0/1/1/1
2	SIA	N	6[B]	2	-	0/14/34/38	0/1/1/1
2	BGC	O	1	2	-	0/2/22/22	0/1/1/1
2	GAL	O	2	2	-	0/2/19/22	0/1/1/1
2	NGA	O	3	2	-	0/6/23/26	0/1/1/1
2	GAL	O	4	2	-	0/2/19/22	0/1/1/1
2	FUC	O	5	2	-	-	0/1/1/1
2	SIA	O	6	2	-	0/14/34/38	0/1/1/1
2	BGC	P	1	2	-	0/2/22/22	0/1/1/1
2	GAL	P	2	2	-	1/2/19/22	0/1/1/1
2	NGA	P	3	2	-	0/6/23/26	0/1/1/1
2	GAL	P	4	2	-	0/2/19/22	0/1/1/1
2	FUC	P	5	2	-	-	0/1/1/1
2	SIA	P	6	2	-	0/14/34/38	0/1/1/1
4	BGC	Q	1[B]	4	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLC	Q	1[A]	4	-	0/2/22/22	0/1/1/1
4	GAL	Q	2[A]	4	-	1/2/19/22	0/1/1/1
4	GAL	Q	2[B]	4	-	1/2/19/22	0/1/1/1
4	NGA	Q	3[A]	4	-	0/6/23/26	0/1/1/1
4	NGA	Q	3[B]	4	-	1/6/23/26	0/1/1/1
4	GAL	Q	4[A]	4	-	0/2/19/22	0/1/1/1
4	GAL	Q	4[B]	4	-	2/2/19/22	0/1/1/1
4	FUC	Q	5[A]	4	-	-	0/1/1/1
4	FUC	Q	5[B]	4	-	-	0/1/1/1
4	SIA	Q	6[A]	4	-	1/14/34/38	0/1/1/1
4	SIA	Q	6[B]	4	-	2/14/34/38	0/1/1/1
3	BGC	R	1[A]	3	-	0/2/22/22	0/1/1/1
3	GLC	R	1[B]	3	-	0/2/22/22	0/1/1/1
3	GAL	R	2[A]	3	-	0/2/19/22	0/1/1/1
3	GAL	R	2[B]	3	-	1/2/19/22	0/1/1/1
3	NGA	R	3[A]	3	-	0/6/23/26	0/1/1/1
3	NGA	R	3[B]	3	-	2/6/23/26	0/1/1/1
3	GAL	R	4[A]	3	-	0/2/19/22	0/1/1/1
3	GAL	R	4[B]	3	-	0/2/19/22	0/1/1/1
3	FUC	R	5[A]	3	-	-	0/1/1/1
3	FUC	R	5[B]	3	-	-	0/1/1/1
3	SIA	R	6[A]	3	-	2/14/34/38	0/1/1/1
3	SIA	R	6[B]	3	-	2/14/34/38	0/1/1/1
2	BGC	S	1	2	-	0/2/22/22	0/1/1/1
2	GAL	S	2	2	-	0/2/19/22	0/1/1/1
2	NGA	S	3	2	-	0/6/23/26	0/1/1/1
2	GAL	S	4	2	-	0/2/19/22	0/1/1/1
2	FUC	S	5	2	-	-	0/1/1/1
2	SIA	S	6	2	-	0/14/34/38	0/1/1/1
2	BGC	T	1[A]	2	-	2/2/22/22	0/1/1/1
2	BGC	T	1[B]	2	-	0/2/22/22	0/1/1/1
2	GAL	T	2[A]	2	-	0/2/19/22	0/1/1/1
2	GAL	T	2[B]	2	-	0/2/19/22	0/1/1/1
2	NGA	T	3[A]	2	-	1/6/23/26	0/1/1/1
2	NGA	T	3[B]	2	-	0/6/23/26	0/1/1/1
2	GAL	T	4[A]	2	-	0/2/19/22	0/1/1/1
2	GAL	T	4[B]	2	-	0/2/19/22	0/1/1/1
2	FUC	T	5[A]	2	-	-	0/1/1/1
2	FUC	T	5[B]	2	-	-	0/1/1/1
2	SIA	T	6[A]	2	-	6/14/34/38	0/1/1/1
2	SIA	T	6[B]	2	-	1/14/34/38	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	5[A]	FUC	C2-C3	3.77	1.58	1.52
2	T	5[A]	FUC	C2-C3	3.63	1.57	1.52
4	M	5[B]	FUC	C2-C3	3.27	1.57	1.52
3	L	1[A]	BGC	O6-C6	3.18	1.55	1.42
2	K	3	NGA	O5-C1	-2.93	1.39	1.43

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	5[B]	FUC	C1-C2-C3	6.54	117.71	109.67
2	T	5[A]	FUC	O3-C3-C2	5.73	120.96	109.99
4	M	5[B]	FUC	C1-C2-C3	5.45	116.36	109.67
2	K	1	BGC	O4-C4-C3	-4.96	98.89	110.35
4	M	2[A]	GAL	O3-C3-C2	-4.54	101.31	109.99

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Q	6[B]	SIA	C7-C8-C9-O9
4	Q	6[B]	SIA	O8-C8-C9-O9
4	M	6[B]	SIA	C7-C8-C9-O9
4	M	6[B]	SIA	O8-C8-C9-O9
3	L	6[A]	SIA	C7-C8-C9-O9

There are no ring outliers.

33 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	6[B]	SIA	1	0
3	L	3[B]	NGA	1	0
2	T	3[B]	NGA	1	0
2	N	3[B]	NGA	4	0
2	N	3[A]	NGA	1	0
3	L	5[A]	FUC	1	0
2	N	5[A]	FUC	2	0
4	M	3[A]	NGA	5	0
2	N	5[B]	FUC	5	0
4	Q	5[B]	FUC	1	0
2	S	5	FUC	3	0

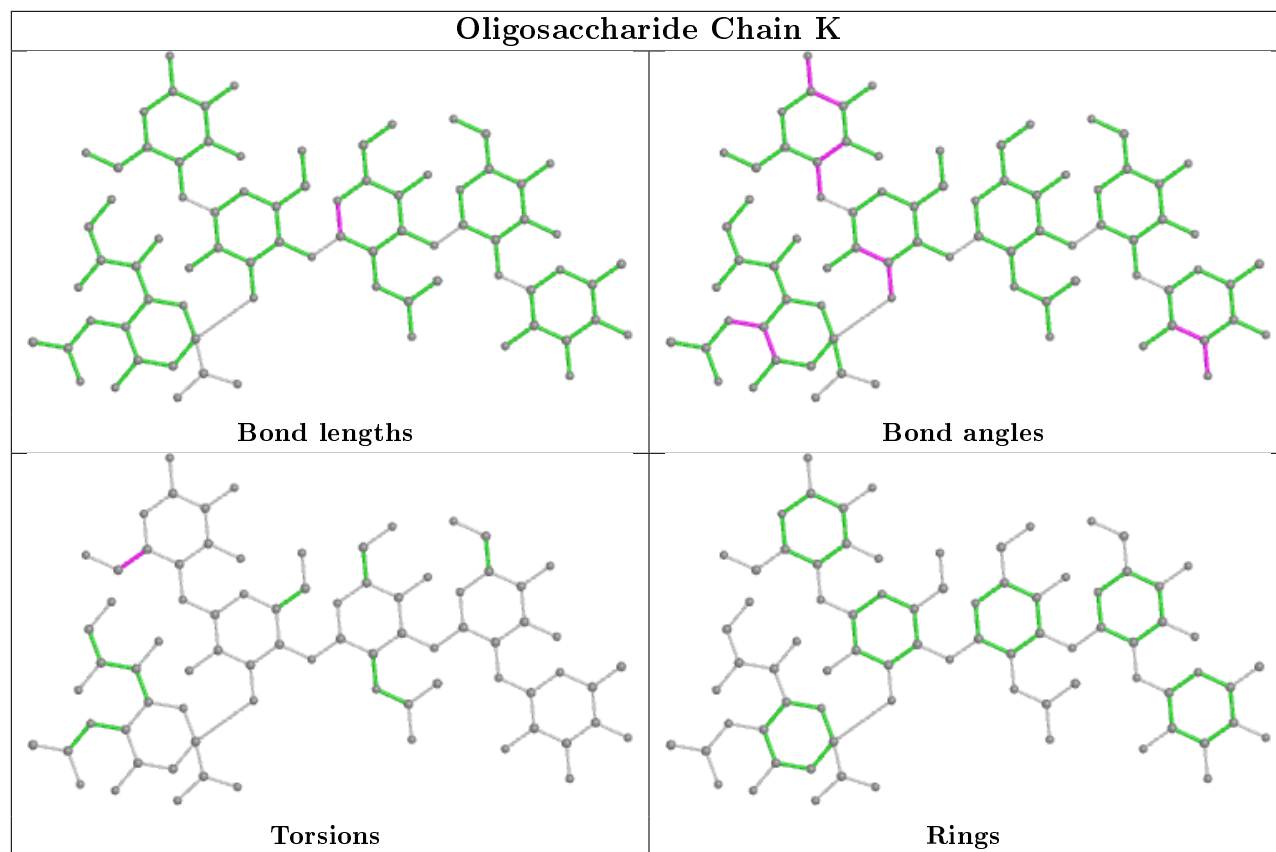
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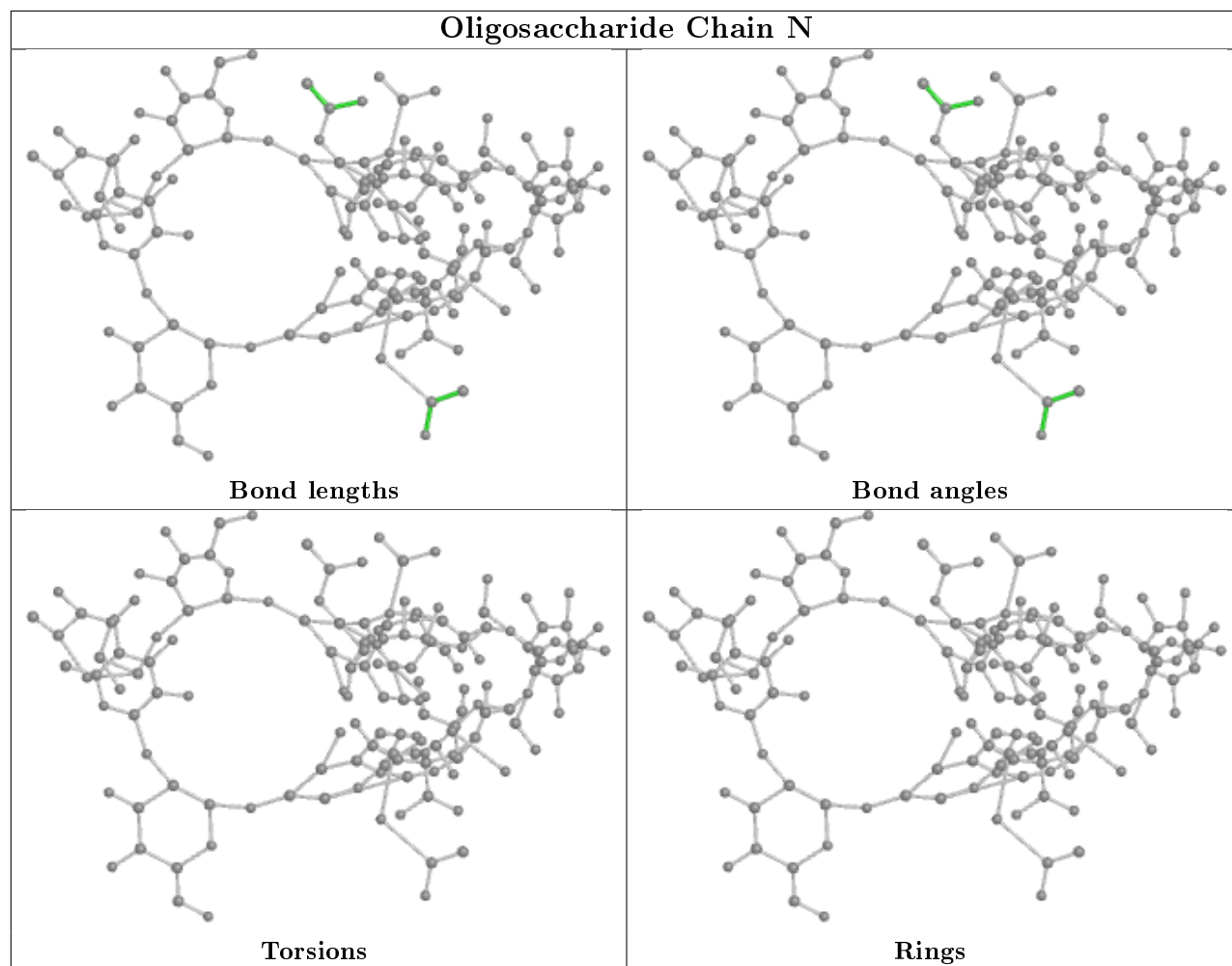


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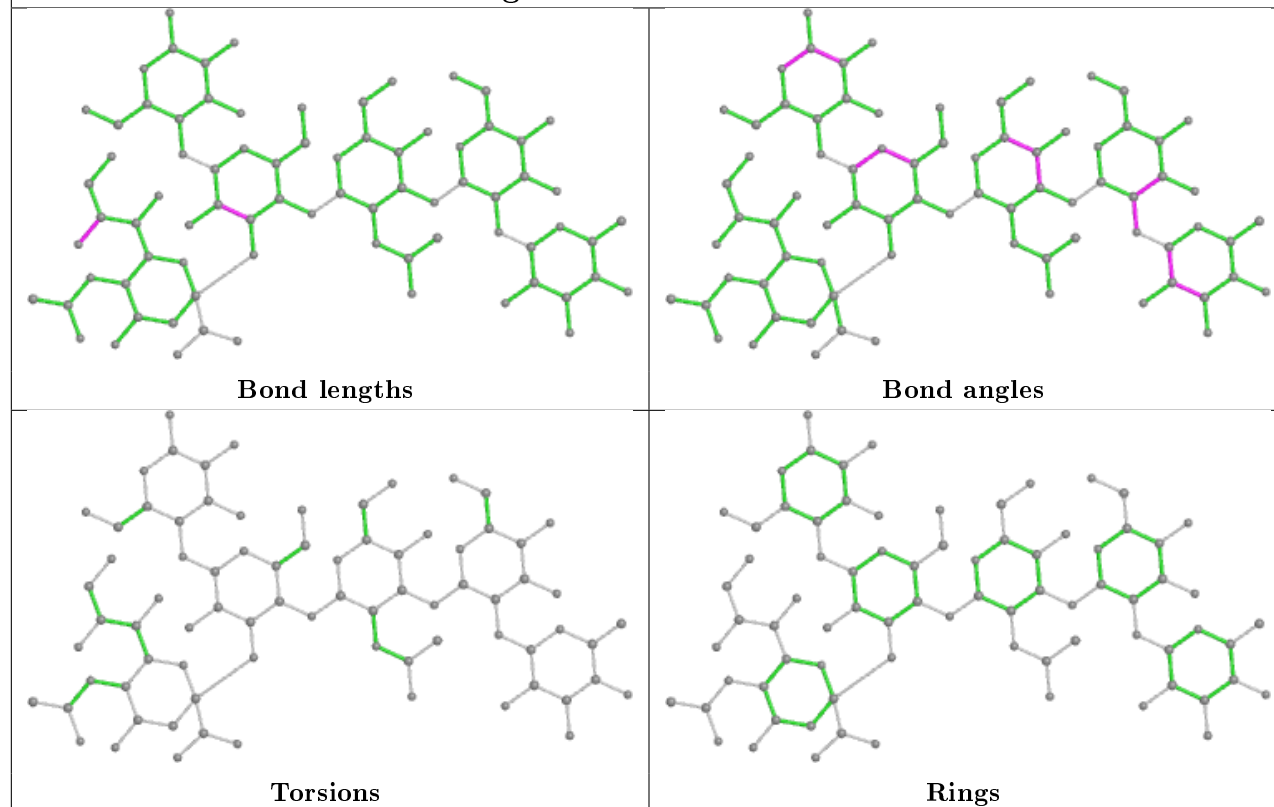
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	5	FUC	1	0
2	T	4[A]	GAL	1	0
4	M	5[A]	FUC	4	0
3	R	6[B]	SIA	1	0
3	R	5[A]	FUC	4	0
3	R	5[B]	FUC	2	0
3	R	6[A]	SIA	1	0
2	P	3	NGA	1	0
3	L	3[A]	NGA	1	0
2	T	3[A]	NGA	3	0
3	L	5[B]	FUC	2	0
4	M	6[A]	SIA	1	0
2	P	5	FUC	2	0
3	R	3[B]	NGA	2	0
2	T	6[B]	SIA	2	0
4	Q	3[B]	NGA	2	0
3	R	3[A]	NGA	1	0
2	N	6[B]	SIA	1	0
2	N	6[A]	SIA	1	0
2	S	3	NGA	1	0
2	T	5[A]	FUC	4	0
2	O	3	NGA	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.

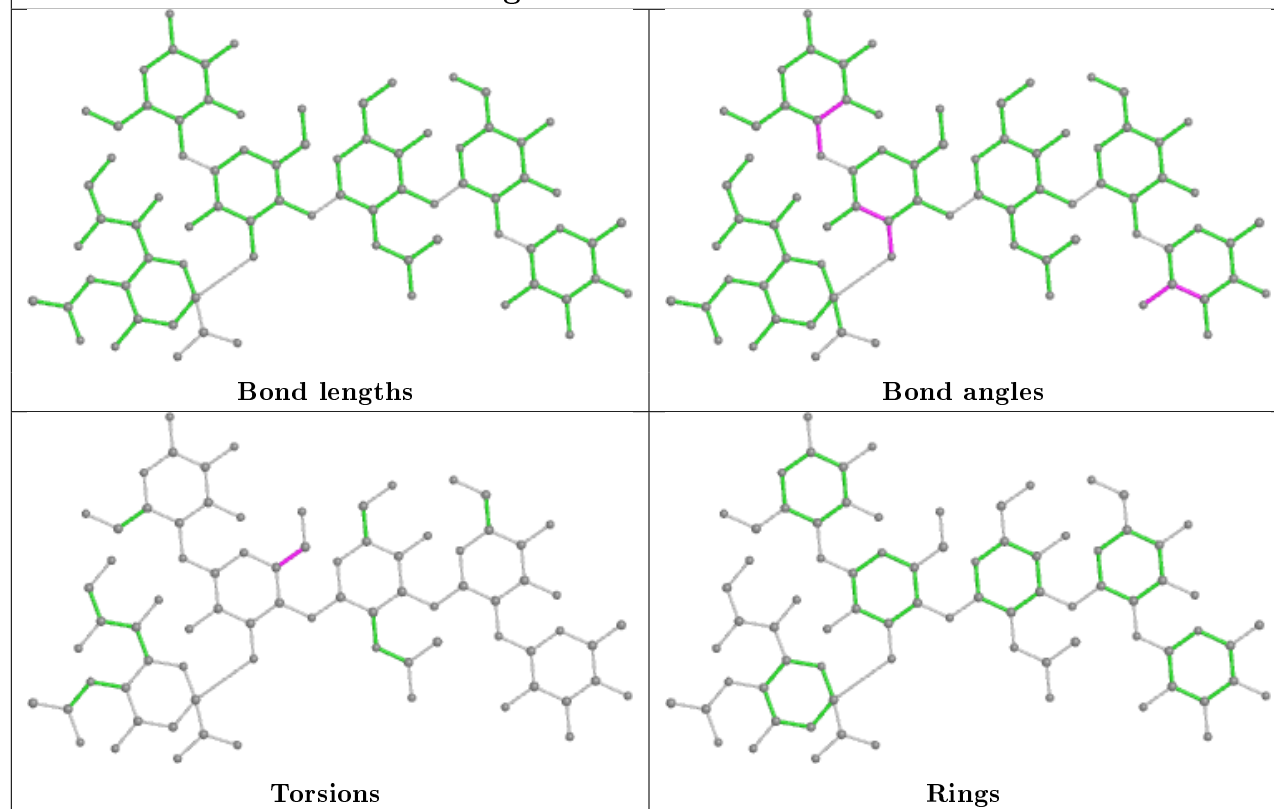


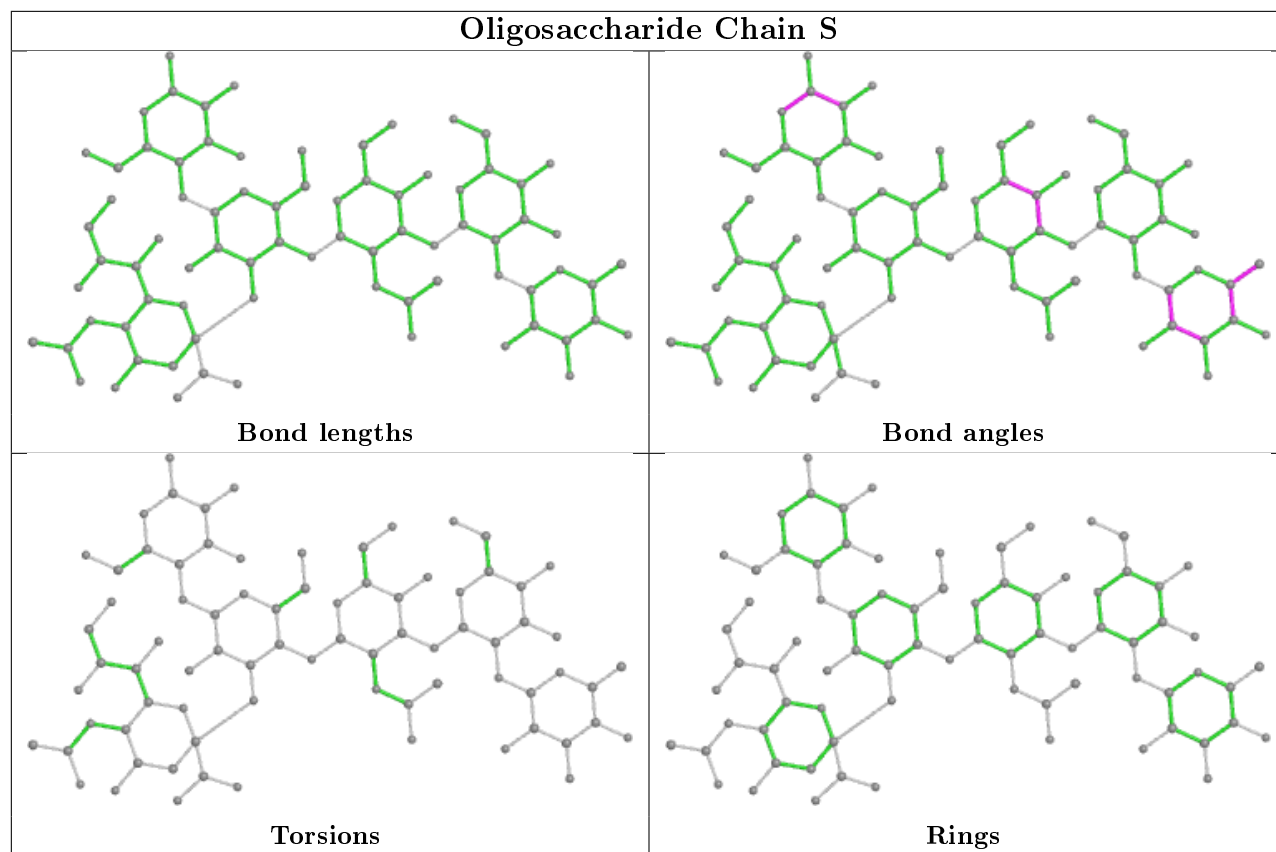


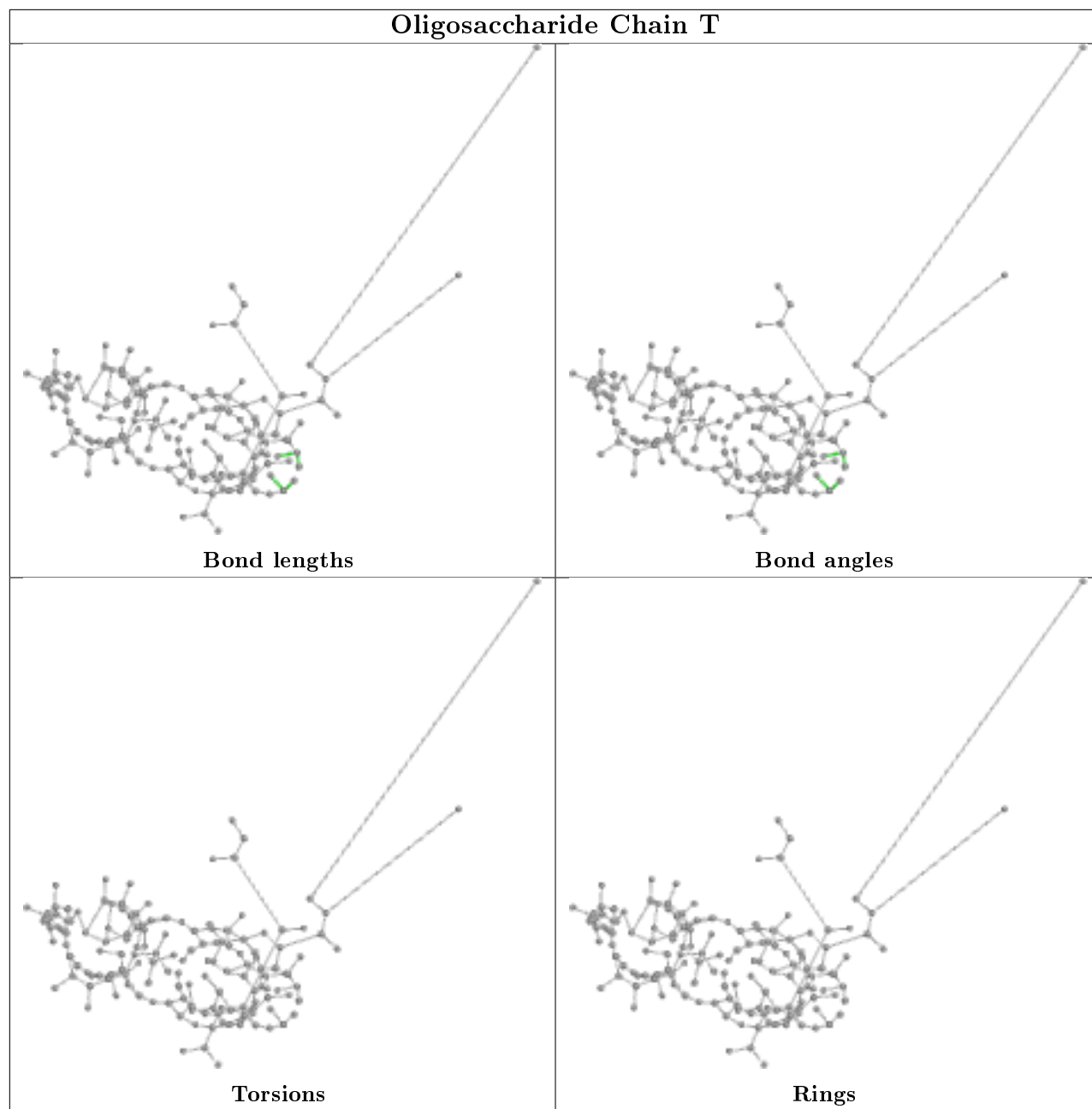
## Oligosaccharide Chain O

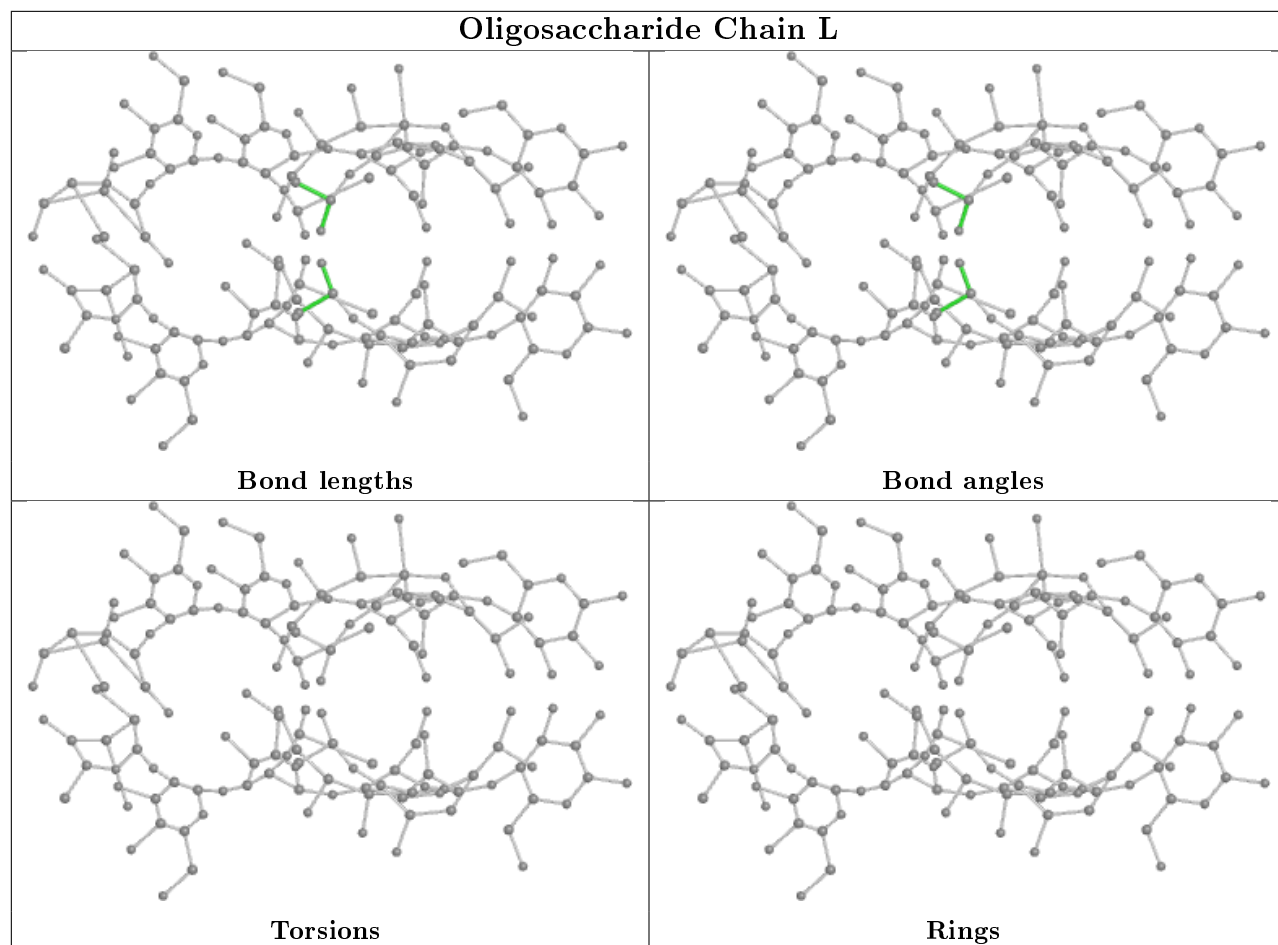


## Oligosaccharide Chain P

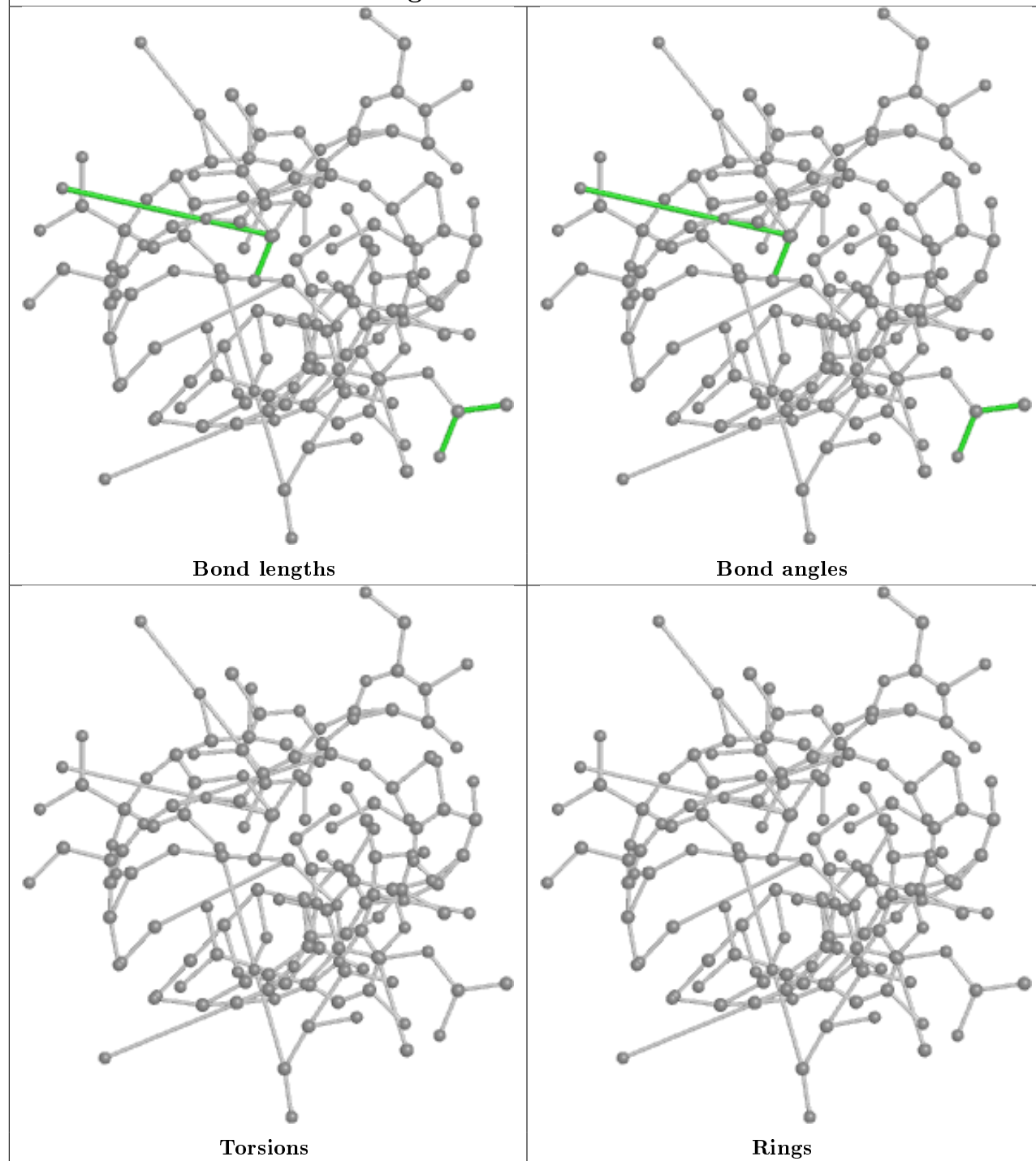




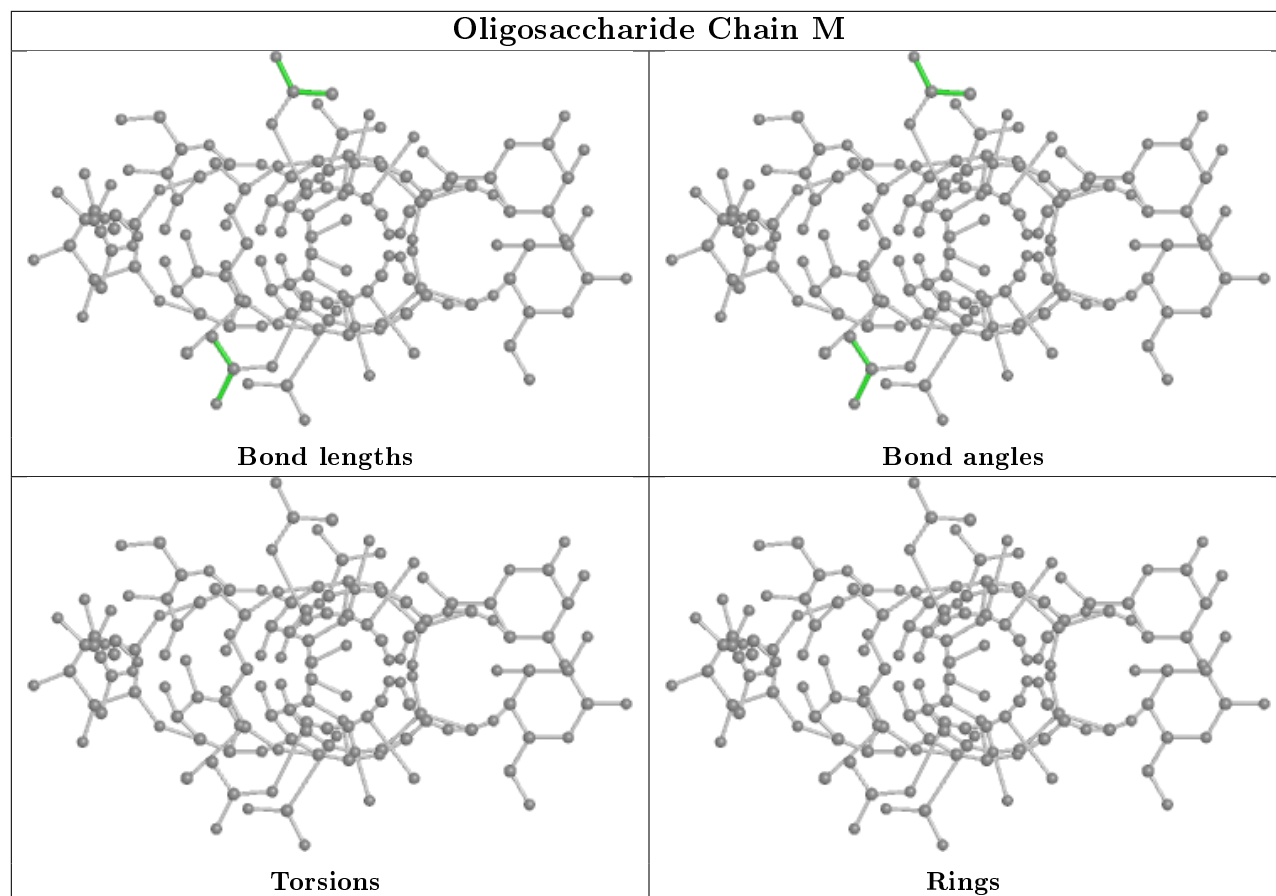


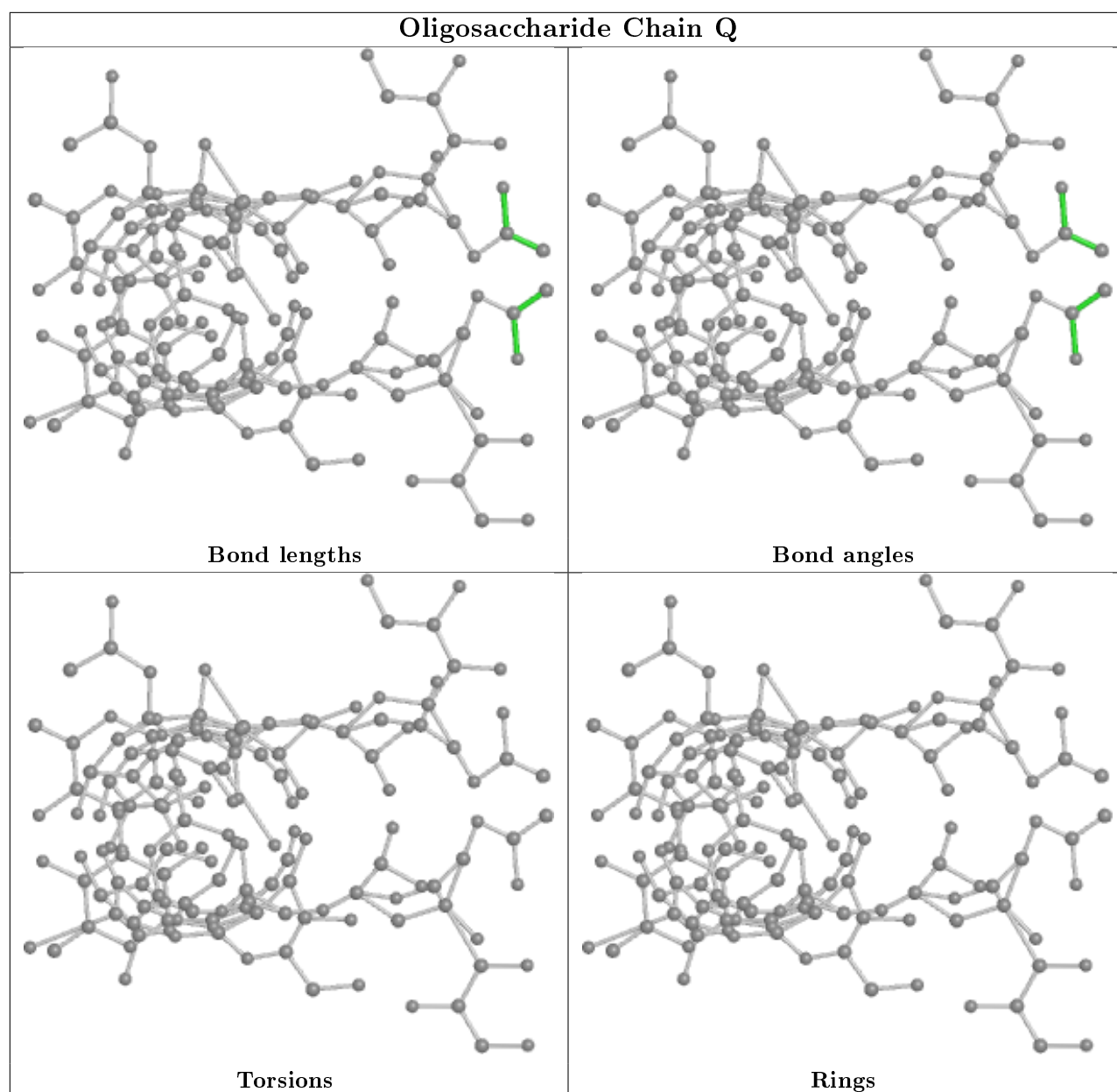


## Oligosaccharide Chain R









## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 for Mogul analysis.

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
6	BCN	C	201	5	7,10,10	0.56	0	8,11,11	0.78	0
7	FUC	F	201	-	11,11,11	1.02	0	15,16,16	2.40	7 (46%)
6	BCN	C	210	5	7,10,10	0.29	0	8,11,11	0.79	0
6	BCN	D	201	5	7,10,10	0.43	0	8,11,11	1.08	0
6	BCN	B	201	5	7,10,10	0.92	0	8,11,11	1.17	1 (12%)
6	BCN	E	209	5	7,10,10	0.18	0	8,11,11	1.06	0
6	BCN	A	209	5	7,10,10	0.43	0	8,11,11	1.08	1 (12%)
6	BCN	B	211	5	7,10,10	0.72	0	8,11,11	0.88	0
6	BCN	E	201	5	7,10,10	0.92	1 (14%)	8,11,11	1.00	0
7	FUC	J	201	-	11,11,11	0.72	0	15,16,16	1.24	0
6	BCN	D	210	5	7,10,10	0.40	0	8,11,11	0.75	0
6	BCN	A	208	5	7,10,10	0.32	0	8,11,11	1.15	1 (12%)

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	BCN	C	201	5	-	3/8/10/10	-
7	FUC	F	201	-	-	-	0/1/1/1
6	BCN	C	210	5	-	1/8/10/10	-
6	BCN	D	201	5	-	3/8/10/10	-
6	BCN	B	201	5	-	2/8/10/10	-
6	BCN	E	209	5	-	2/8/10/10	-
6	BCN	A	209	5	-	2/8/10/10	-
6	BCN	B	211	5	-	2/8/10/10	-
6	BCN	E	201	5	-	1/8/10/10	-
7	FUC	J	201	-	-	-	0/1/1/1
6	BCN	D	210	5	-	2/8/10/10	-
6	BCN	A	208	5	-	3/8/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	201	BCN	C1-N1	2.14	1.51	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	201	FUC	O4-C4-C3	-4.85	99.15	110.35
7	F	201	FUC	O4-C4-C5	4.65	119.97	109.67
7	F	201	FUC	O3-C3-C4	-2.91	103.62	110.35
7	F	201	FUC	C4-C3-C2	-2.60	106.28	110.82
7	F	201	FUC	O5-C5-C4	2.40	113.83	109.52

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	210	BCN	C2-C1-N1-C5
6	D	201	BCN	C2-C1-N1-C5
6	B	201	BCN	C2-C1-N1-C5
6	B	211	BCN	C2-C1-N1-C5
6	A	208	BCN	C2-C1-N1-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	201	BCN	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	103/103 (100%)	-0.14	0 100 100	8, 13, 20, 34	0
1	B	103/103 (100%)	-0.15	0 100 100	7, 13, 19, 24	0
1	C	103/103 (100%)	-0.14	2 (1%) 66 65	8, 14, 20, 40	0
1	D	103/103 (100%)	-0.07	0 100 100	7, 12, 17, 21	0
1	E	103/103 (100%)	-0.11	1 (0%) 82 82	7, 12, 19, 33	0
1	F	103/103 (100%)	-0.20	1 (0%) 82 82	7, 11, 17, 34	0
1	G	103/103 (100%)	-0.25	0 100 100	7, 11, 18, 22	0
1	H	103/103 (100%)	-0.15	0 100 100	8, 13, 20, 27	0
1	I	103/103 (100%)	-0.13	0 100 100	8, 14, 22, 28	0
1	J	103/103 (100%)	-0.18	1 (0%) 82 82	8, 13, 18, 31	0
All	All	1030/1030 (100%)	-0.15	5 (0%) 91 90	7, 13, 20, 40	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	103	ASN	2.7
1	F	103	ASN	2.7
1	C	103	ASN	2.7
1	J	103	ASN	2.2
1	C	90	ASN	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FUC	S	5	10/11	0.63	0.29	30,36,39,40	0
2	FUC	T	5[B]	10/11	0.69	0.38	13,14,15,15	10
2	FUC	T	5[A]	10/11	0.69	0.38	18,20,20,21	10
2	FUC	N	5[A]	10/11	0.70	0.40	15,17,18,18	10
2	FUC	N	5[B]	10/11	0.70	0.40	18,20,22,22	10
4	FUC	Q	5[A]	10/11	0.70	0.33	16,18,19,20	10
4	FUC	Q	5[B]	10/11	0.70	0.33	16,18,20,21	10
2	FUC	O	5	10/11	0.72	0.29	27,32,34,35	0
2	BGC	K	1	12/12	0.77	0.19	29,35,37,41	0
2	BGC	O	1	12/12	0.78	0.25	28,36,40,43	0
2	BGC	S	1	12/12	0.79	0.26	30,37,41,43	0
4	FUC	M	5[A]	10/11	0.80	0.37	23,25,27,27	10
4	FUC	M	5[B]	10/11	0.80	0.37	21,23,24,25	10
3	FUC	R	5[A]	10/11	0.81	0.27	19,20,22,22	10
3	FUC	R	5[B]	10/11	0.81	0.27	18,19,21,21	10
2	FUC	P	5	10/11	0.83	0.15	19,22,25,28	0
4	GAL	M	2[B]	11/12	0.84	0.13	21,23,25,25	11
4	GAL	M	2[A]	11/12	0.84	0.13	20,22,23,24	11
4	GAL	M	4[A]	11/12	0.84	0.18	15,16,18,21	11
4	GAL	M	4[B]	11/12	0.84	0.18	15,16,18,19	11
4	SIA	M	6[B]	20/21	0.85	0.14	16,18,20,20	20
3	GLC	L	1[B]	12/12	0.85	0.16	22,24,26,26	12
2	BGC	N	1[B]	12/12	0.85	0.27	20,23,25,26	12
2	BGC	N	1[A]	12/12	0.85	0.27	20,24,25,27	12
2	FUC	K	5	10/11	0.85	0.20	25,29,31,31	0
3	FUC	L	5[A]	10/11	0.85	0.24	20,21,23,23	10
3	FUC	L	5[B]	10/11	0.85	0.24	19,21,22,22	10
4	SIA	M	6[A]	20/21	0.85	0.14	16,17,18,19	20
3	BGC	L	1[A]	12/12	0.86	0.18	21,23,25,26	12
2	GAL	S	2	11/12	0.86	0.10	22,25,27,27	0
4	GLC	M	1[A]	12/12	0.86	0.25	25,28,31,32	12
3	BGC	R	1[A]	12/12	0.87	0.17	23,26,28,30	12
4	BGC	M	1[B]	12/12	0.87	0.23	27,30,34,35	12
3	GLC	R	1[B]	12/12	0.88	0.18	22,25,28,28	12
2	GAL	O	2	11/12	0.88	0.12	20,23,25,26	0
2	GAL	K	2	11/12	0.88	0.10	21,24,26,27	0
2	SIA	T	6[A]	20/21	0.91	0.12	12,13,14,15	20

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GAL	L	4[B]	11/12	0.91	0.10	14,15,16,17	11
2	SIA	T	6[B]	20/21	0.91	0.12	10,11,12,12	20
3	GAL	L	4[A]	11/12	0.91	0.10	14,15,16,18	11
4	BGC	Q	1[B]	12/12	0.92	0.11	13,15,16,17	12
2	BGC	T	1[B]	12/12	0.92	0.14	13,14,16,16	12
2	BGC	T	1[A]	12/12	0.92	0.14	16,18,20,20	12
3	NGA	R	3[B]	14/15	0.92	0.11	15,16,17,17	14
2	SIA	S	6	20/21	0.92	0.09	18,20,22,22	0
2	SIA	K	6	20/21	0.92	0.08	16,18,19,20	0
3	NGA	R	3[A]	14/15	0.92	0.11	16,17,18,18	14
4	NGA	Q	3[B]	14/15	0.93	0.11	11,11,12,12	14
4	GLC	Q	1[A]	12/12	0.93	0.09	14,16,17,17	12
2	GAL	S	4	11/12	0.93	0.09	16,17,20,24	0
4	NGA	M	3[B]	14/15	0.93	0.12	18,20,21,22	14
3	GAL	L	2[B]	11/12	0.93	0.10	17,19,20,21	11
3	GAL	L	2[A]	11/12	0.93	0.10	17,19,20,21	11
2	NGA	S	3	14/15	0.93	0.10	19,21,23,23	0
2	GAL	N	2[A]	11/12	0.93	0.09	16,18,19,19	11
4	NGA	M	3[A]	14/15	0.93	0.12	18,19,20,21	14
4	NGA	Q	3[A]	14/15	0.93	0.11	11,11,12,12	14
3	NGA	L	3[A]	14/15	0.93	0.10	16,17,17,18	14
2	GAL	N	2[B]	11/12	0.93	0.09	15,17,18,18	11
2	NGA	O	3	14/15	0.93	0.10	17,18,20,22	0
3	NGA	L	3[B]	14/15	0.93	0.10	16,17,18,18	14
2	SIA	O	6	20/21	0.94	0.09	17,17,19,20	0
2	GAL	T	4[A]	11/12	0.94	0.10	11,12,14,16	11
2	GAL	T	4[B]	11/12	0.94	0.10	9,10,11,12	11
2	NGA	K	3	14/15	0.94	0.08	19,20,22,23	0
4	GAL	Q	4[A]	11/12	0.94	0.11	9,10,12,14	11
4	GAL	Q	4[B]	11/12	0.94	0.11	10,11,12,14	11
3	SIA	L	6[B]	20/21	0.94	0.10	14,15,17,17	20
3	SIA	R	6[B]	20/21	0.94	0.10	14,15,17,17	20
2	GAL	O	4	11/12	0.94	0.07	14,15,18,22	0
3	SIA	L	6[A]	20/21	0.94	0.10	14,15,17,17	20
3	GAL	R	4[B]	11/12	0.94	0.10	13,14,15,17	11
3	SIA	R	6[A]	20/21	0.94	0.10	14,15,17,17	20
2	GAL	K	4	11/12	0.94	0.07	14,15,18,22	0
3	GAL	R	4[A]	11/12	0.94	0.10	13,14,15,17	11
2	BGC	P	1	12/12	0.94	0.09	14,17,19,20	0
2	GAL	N	4[B]	11/12	0.94	0.09	11,12,14,16	11
2	GAL	N	4[A]	11/12	0.94	0.09	11,11,13,14	11
2	NGA	T	3[A]	14/15	0.95	0.09	13,13,14,14	14

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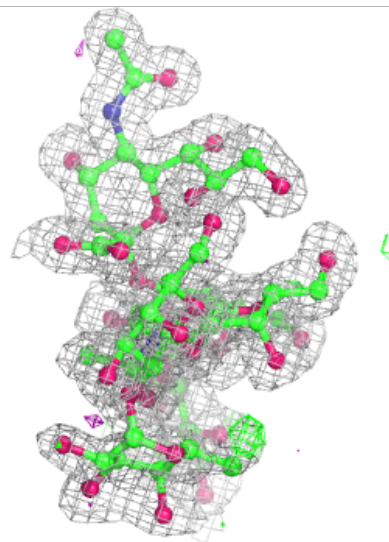
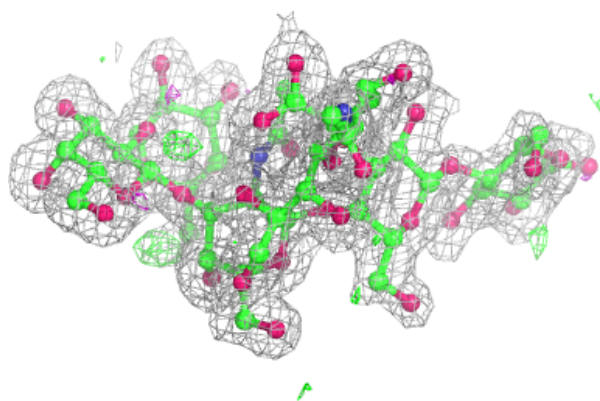
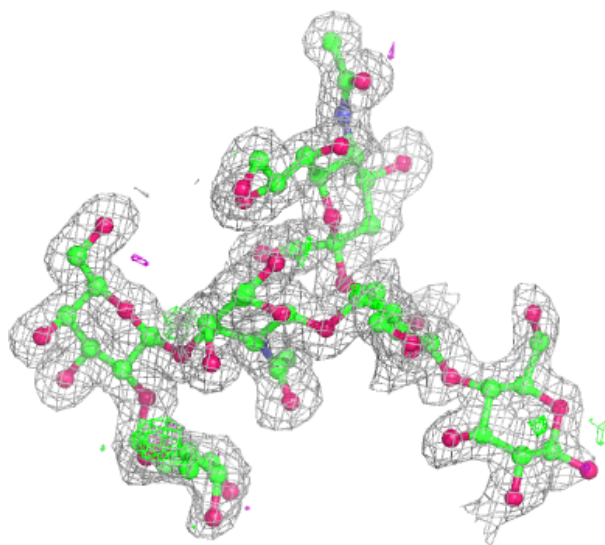
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GAL	R	2[A]	11/12	0.95	0.10	17,20,21,21	11
4	SIA	Q	6[B]	20/21	0.95	0.11	9,10,11,11	20
2	SIA	N	6[B]	20/21	0.95	0.10	12,13,15,15	20
2	GAL	T	2[B]	11/12	0.95	0.09	11,12,13,13	11
2	GAL	T	2[A]	11/12	0.95	0.09	14,15,15,16	11
2	SIA	N	6[A]	20/21	0.95	0.10	13,14,16,16	20
2	NGA	N	3[B]	14/15	0.95	0.11	14,15,15,15	14
4	GAL	Q	2[B]	11/12	0.95	0.11	11,12,13,13	11
3	GAL	R	2[B]	11/12	0.95	0.10	17,19,21,21	11
4	GAL	Q	2[A]	11/12	0.95	0.11	12,12,13,14	11
4	SIA	Q	6[A]	20/21	0.95	0.11	10,11,12,12	20
2	GAL	P	2	11/12	0.95	0.08	11,12,13,14	0
2	NGA	N	3[A]	14/15	0.95	0.11	13,15,16,16	14
2	NGA	T	3[B]	14/15	0.95	0.09	11,11,12,12	14
2	SIA	P	6	20/21	0.96	0.07	10,11,12,12	0
2	NGA	P	3	14/15	0.96	0.08	10,10,11,11	0
2	GAL	P	4	11/12	0.97	0.09	9,9,11,14	0

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



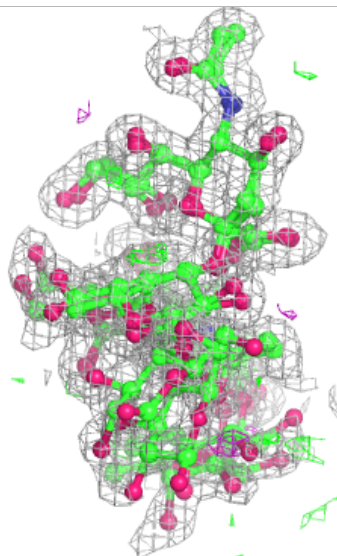
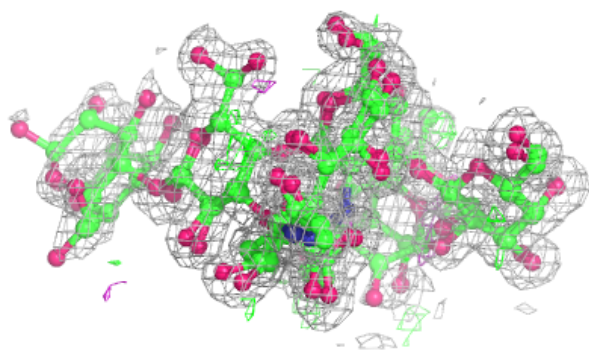
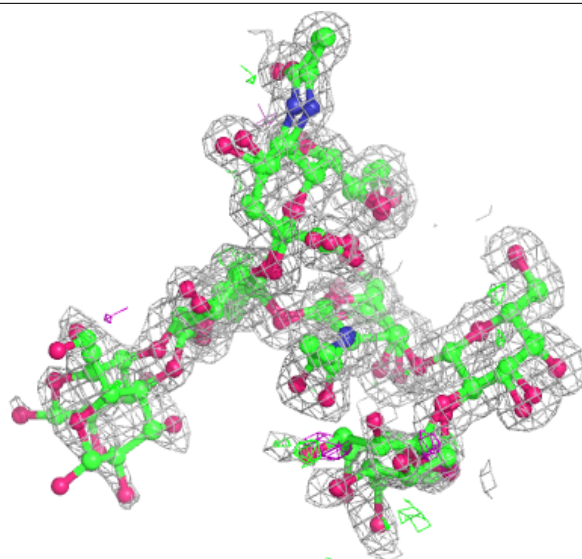
**Electron density around Chain K:**

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



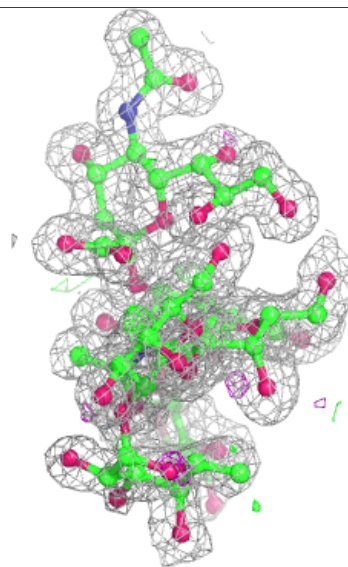
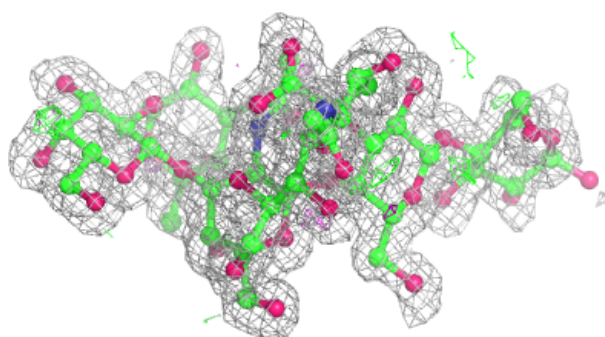
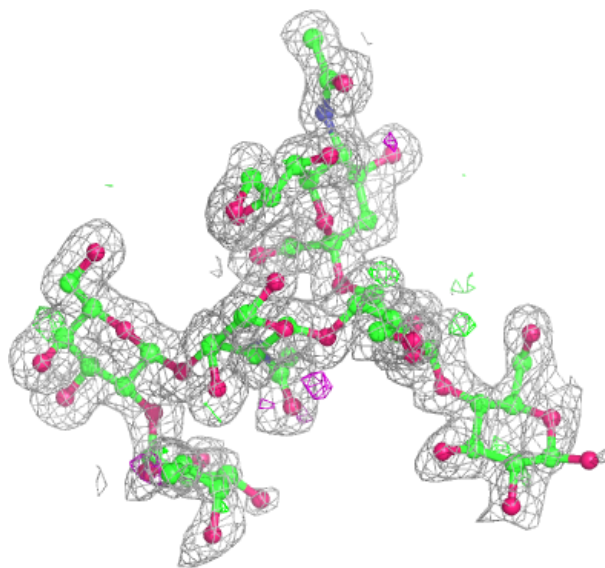
**Electron density around Chain N:**

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



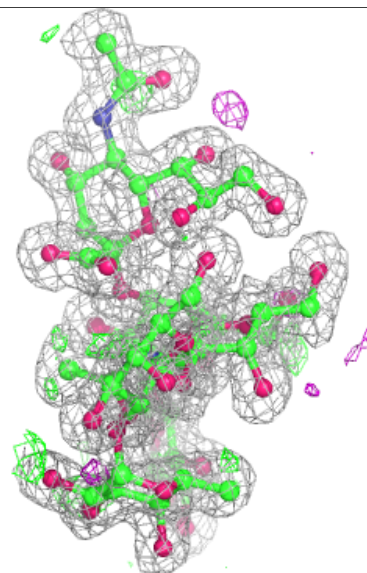
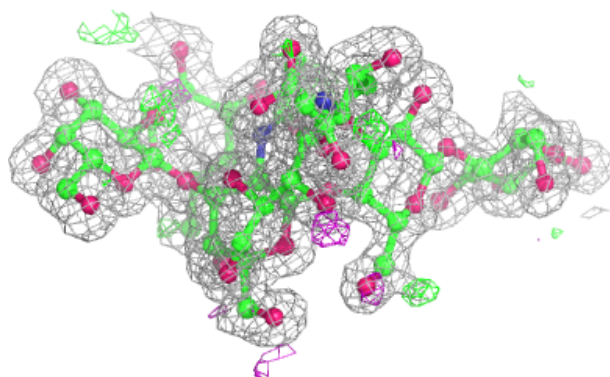
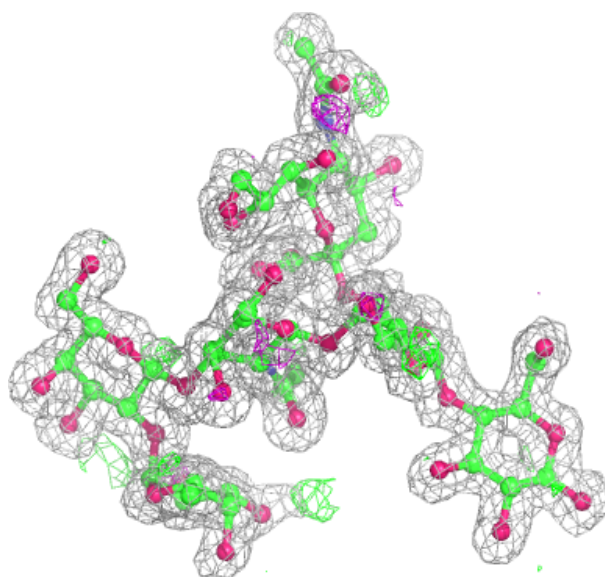
**Electron density around Chain O:**

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



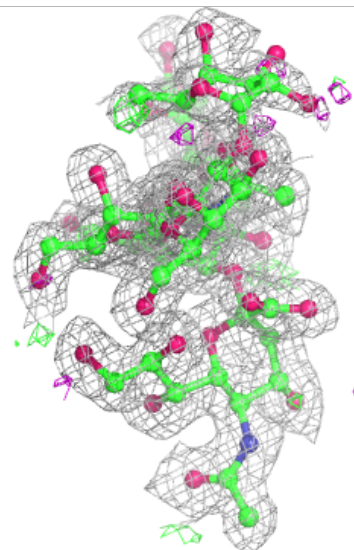
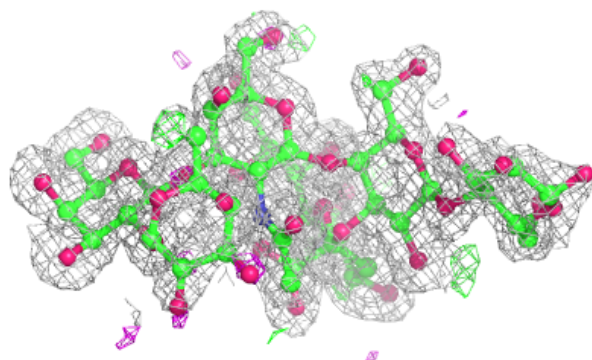
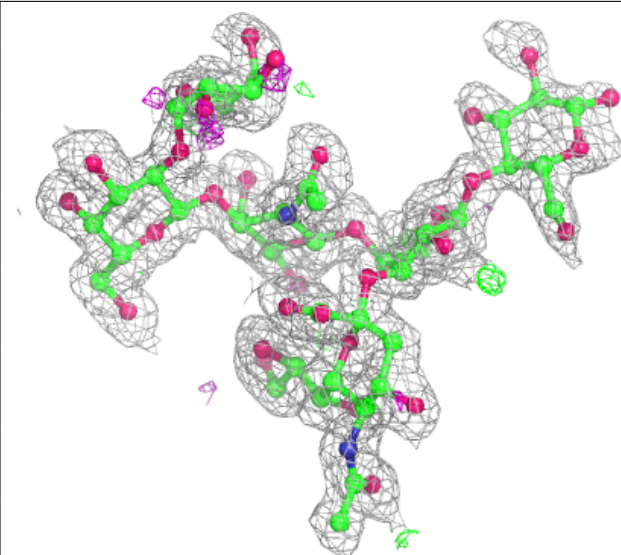
**Electron density around Chain P:**

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



**Electron density around Chain S:**

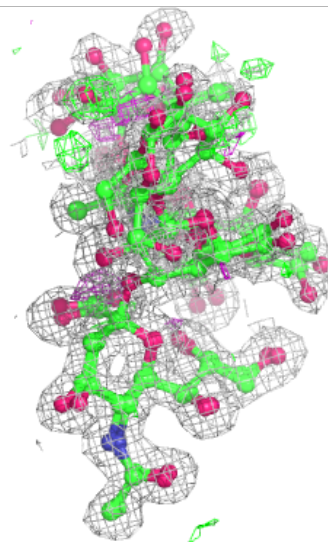
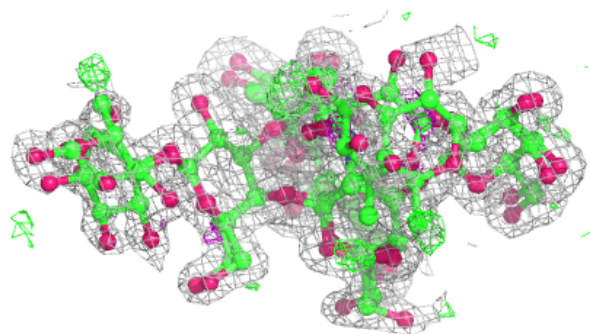
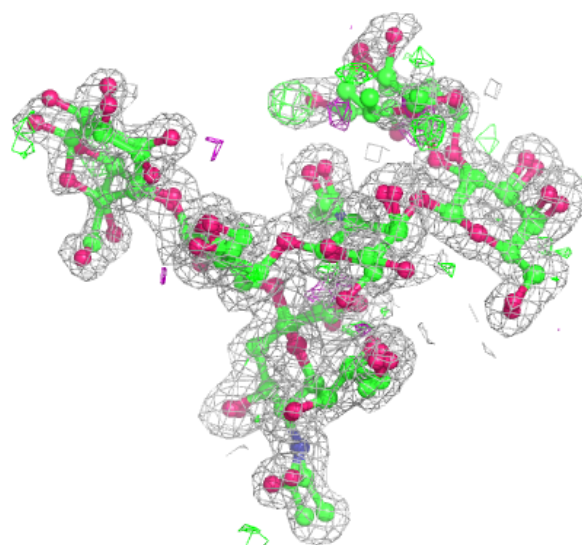
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





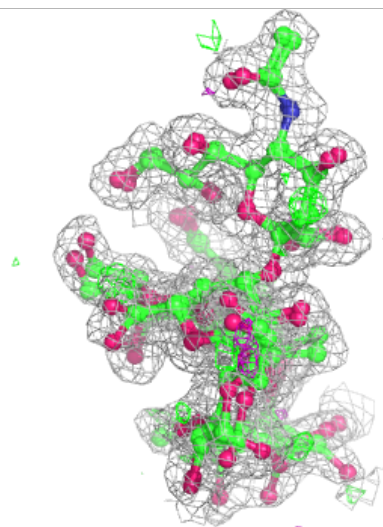
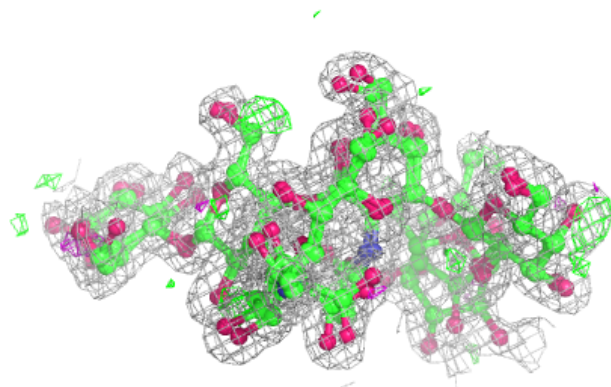
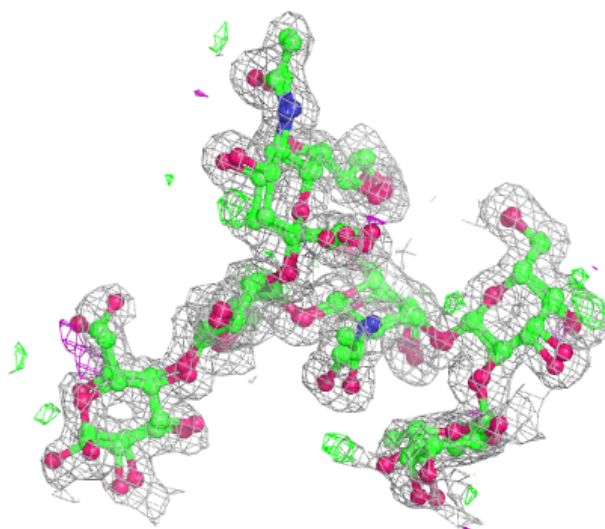
**Electron density around Chain T:**

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



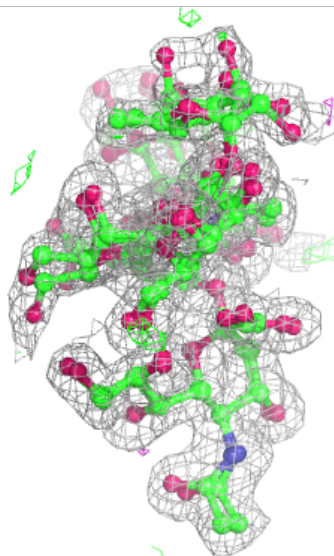
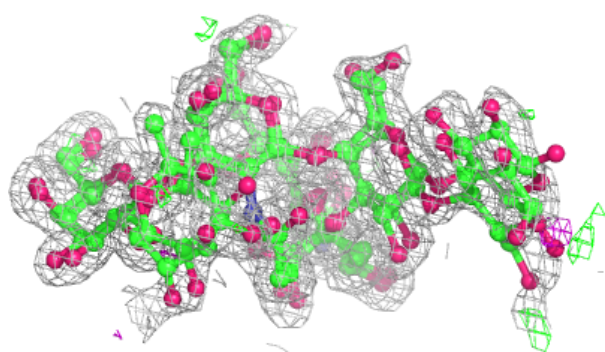
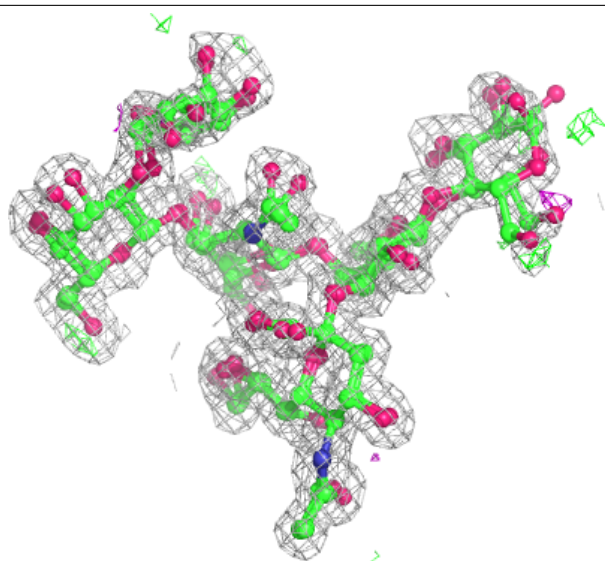
**Electron density around Chain L:**

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



**Electron density around Chain R:**

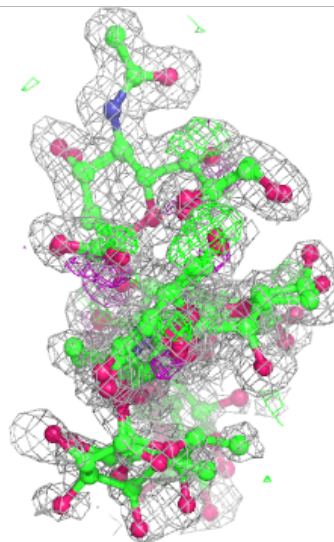
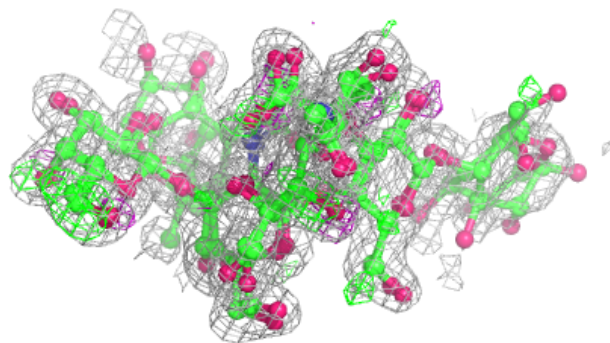
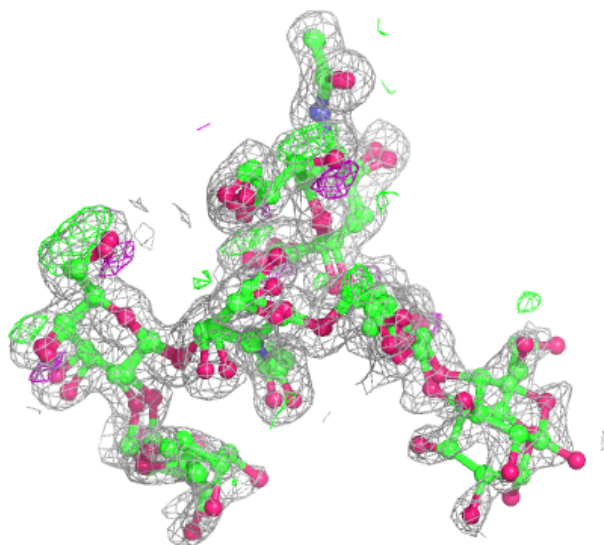
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

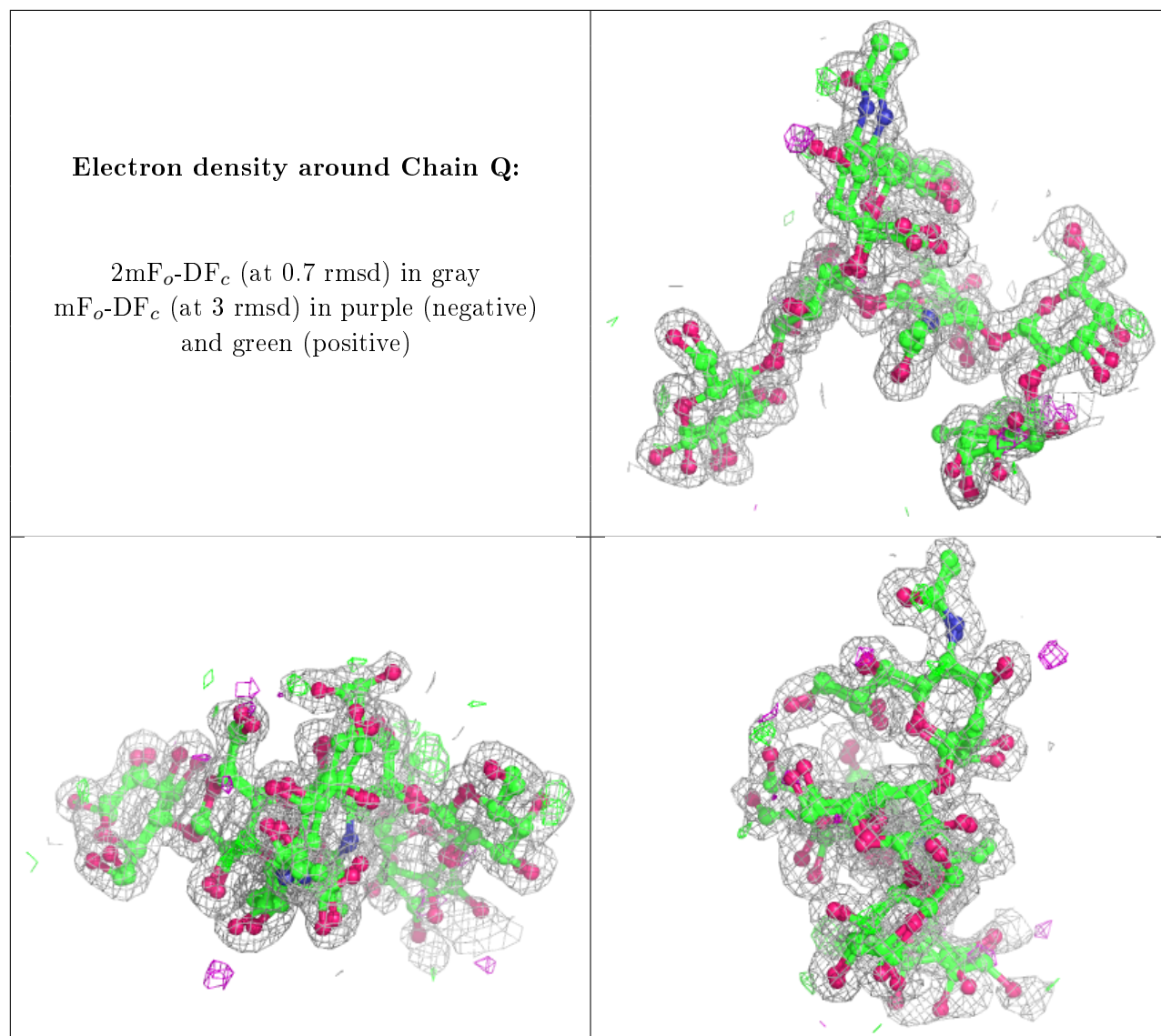




**Electron density around Chain M:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	FUC	F	201	11/11	0.73	0.21	17,19,22,23	11
7	FUC	J	201	11/11	0.74	0.19	23,25,26,26	11
6	BCN	B	201	11/11	0.90	0.12	13,17,21,23	0
6	BCN	D	210	11/11	0.92	0.11	15,20,22,22	0
6	BCN	A	209	11/11	0.94	0.09	13,17,20,21	0
6	BCN	E	201	11/11	0.94	0.11	13,15,22,25	0
6	BCN	A	208	11/11	0.94	0.10	13,17,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	BCN	B	211	11/11	0.94	0.10	12,17,22,23	0
6	BCN	C	210	11/11	0.94	0.10	14,18,20,20	0
6	BCN	C	201	11/11	0.95	0.09	13,18,21,22	0
6	BCN	E	209	11/11	0.95	0.08	12,15,23,25	0
6	BCN	D	201	11/11	0.95	0.09	13,18,20,21	0
5	CA	B	210	1/1	0.98	0.08	10,10,10,10	0
5	CA	D	202	1/1	0.99	0.05	11,11,11,11	0
5	CA	C	202	1/1	0.99	0.06	11,11,11,11	0
5	CA	E	202	1/1	0.99	0.05	11,11,11,11	0
5	CA	D	209	1/1	0.99	0.07	10,10,10,10	0
5	CA	E	210	1/1	0.99	0.06	11,11,11,11	0
5	CA	B	202	1/1	0.99	0.05	11,11,11,11	0
5	CA	C	211	1/1	1.00	0.06	10,10,10,10	0
5	CA	A	201	1/1	1.00	0.05	10,10,10,10	0
5	CA	A	210	1/1	1.00	0.06	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.