



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:42 PM UTC

PDB ID : 6HMY / pdb_00006hmy
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

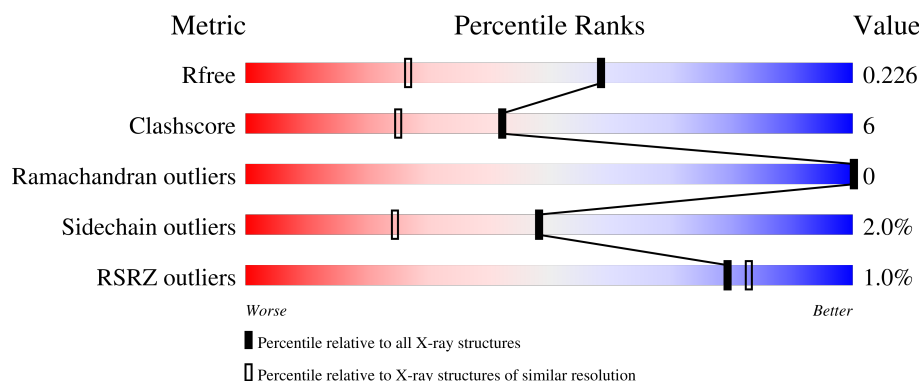
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 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	103	% 88% 11% .
1	B	103	% 86% 12% .
1	C	103	% 89% 11%
1	D	103	% 87% 12% .
1	E	103	% 87% 12% .

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Mol	Chain	Length	Quality of chain
1	F	103	
1	G	103	
1	H	103	
1	I	103	
1	J	103	
2	K	6	
2	N	6	
2	O	6	
2	P	6	
2	S	6	
2	T	6	
3	L	7	
3	R	7	
4	M	7	
4	Q	7	

2 Entry composition [i](#)

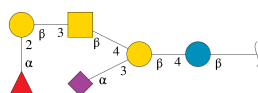
There are 8 unique types of molecules in this entry. The entry contains 10879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.



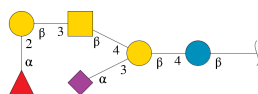
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	6	Total	C	N	O	0	0	0
			78	43	2	33			

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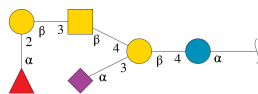
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	N	6	Total	C	N	O	0	6	0
			156	86	4	66			
2	O	6	Total	C	N	O	0	0	0
			78	43	2	33			
2	P	6	Total	C	N	O	0	0	0
			78	43	2	33			
2	S	6	Total	C	N	O	0	0	0
			78	43	2	33			
2	T	6	Total	C	N	O	0	6	0
			156	86	4	66			

- 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.

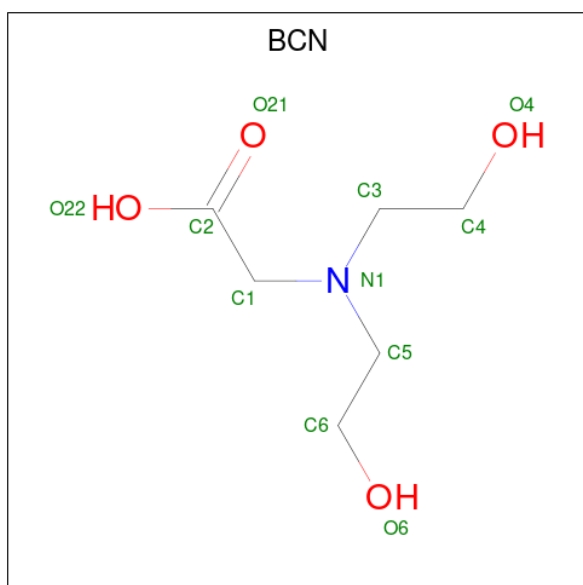


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	6	Total	C	N	O	0	6	0
			156	86	4	66			
4	Q	6	Total	C	N	O	0	6	0
			156	86	4	66			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0
5	E	1	Total Ca 1 1	0	0
5	F	1	Total Ca 1 1	0	0
5	G	1	Total Ca 1 1	0	0
5	H	1	Total Ca 1 1	0	0
5	I	1	Total Ca 1 1	0	0
5	J	1	Total Ca 1 1	0	0

- Molecule 6 is BICINE (CCD ID: BCN) (formula: $C_6H_{13}NO_4$).



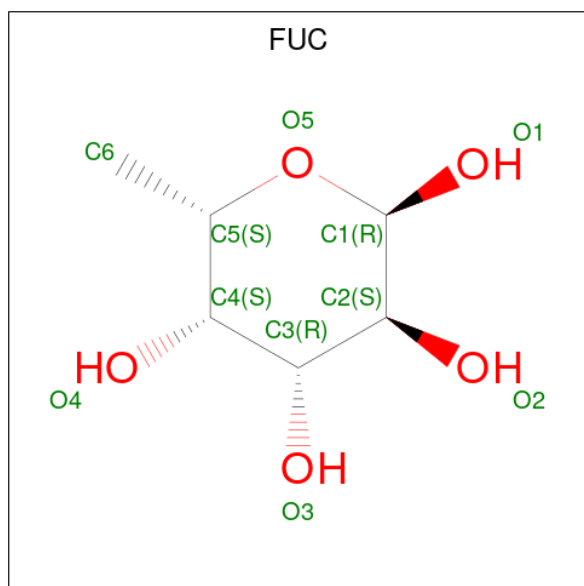
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 11 6 1 4	0	0
6	B	1	Total C N O 11 6 1 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			11	6	1	4		
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	F	1	Total	C	N	O	0	0
			11	6	1	4		
6	G	1	Total	C	N	O	0	0
			11	6	1	4		
6	I	1	Total	C	N	O	0	0
			11	6	1	4		
6	I	1	Total	C	N	O	0	0
			11	6	1	4		
6	J	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 7 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).



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		

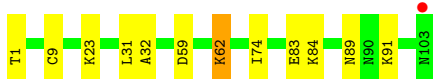
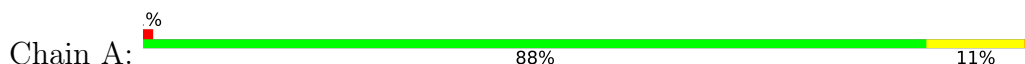
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	79	Total 79	O 79	0	0
8	B	78	Total 78	O 78	0	0
8	C	79	Total 79	O 79	0	0
8	D	83	Total 83	O 83	0	0
8	E	79	Total 79	O 79	0	0
8	F	78	Total 78	O 78	0	0
8	G	88	Total 88	O 88	0	0
8	H	82	Total 82	O 82	0	0
8	I	73	Total 73	O 73	0	0
8	J	78	Total 78	O 78	0	0

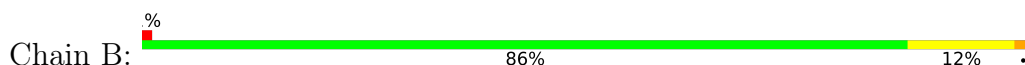
3 Residue-property plots [i](#)

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.

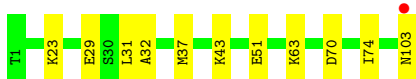
- Molecule 1: Cholera enterotoxin B-subunit



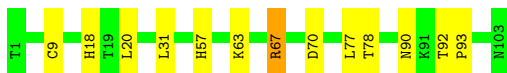
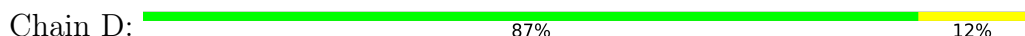
- Molecule 1: Cholera enterotoxin B-subunit



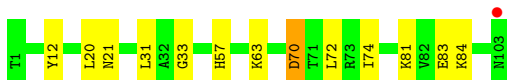
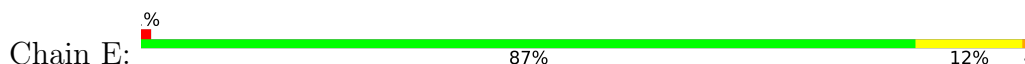
- Molecule 1: Cholera enterotoxin B-subunit



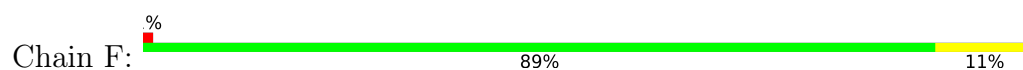
- Molecule 1: Cholera enterotoxin B-subunit



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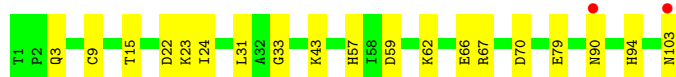
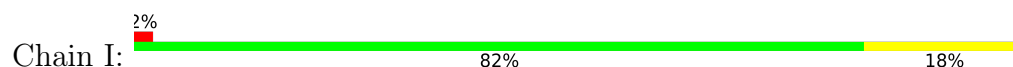
- Molecule 1: Cholera enterotoxin B-subunit



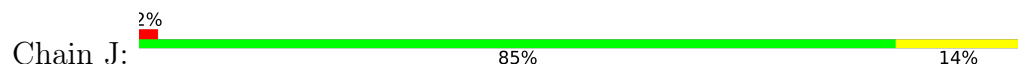
- Molecule 1: Cholera enterotoxin B-subunit



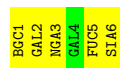
- Molecule 1: Cholera enterotoxin B-subunit



- Molecule 1: Cholera enterotoxin B-subunit



- 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

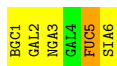




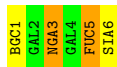
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- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



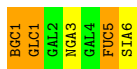
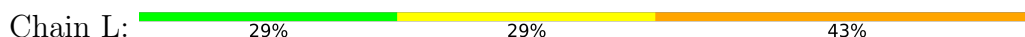
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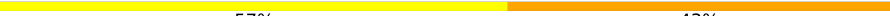
- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- 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

Chain R:  57% 43%

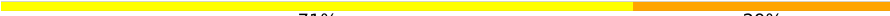


- Molecule 4: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain M:  57% 43%



- 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:  71% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.08	1/901 (0.1%)	1.00	0/1213
1	B	1.11	1/918 (0.1%)	1.02	1/1235 (0.1%)
1	C	1.07	1/889 (0.1%)	1.03	1/1197 (0.1%)
1	D	1.12	2/901 (0.2%)	1.05	1/1214 (0.1%)
1	E	1.11	3/886 (0.3%)	1.02	1/1193 (0.1%)
1	F	1.13	2/901 (0.2%)	0.99	0/1214
1	G	1.06	0/902	1.01	1/1214 (0.1%)
1	H	1.20	7/910 (0.8%)	1.01	1/1224 (0.1%)
1	I	1.14	3/899 (0.3%)	1.02	1/1211 (0.1%)
1	J	1.12	4/903 (0.4%)	1.04	1/1214 (0.1%)
All	All	1.11	24/9010 (0.3%)	1.02	8/12129 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	57	HIS	CE1-NE2	8.26	1.40	1.32
1	I	57	HIS	CE1-NE2	7.18	1.39	1.32
1	H	83[A]	GLU	C-O	6.35	1.31	1.23
1	H	83[B]	GLU	C-O	6.35	1.31	1.23
1	H	99	ILE	C-O	-6.16	1.17	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	70	ASP	CA-CB-CG	8.20	120.80	112.60
1	B	70	ASP	CA-CB-CG	7.76	120.36	112.60
1	D	70	ASP	CA-CB-CG	6.82	119.42	112.60
1	J	70	ASP	CA-CB-CG	6.46	119.06	112.60
1	H	70	ASP	CA-CB-CG	5.88	118.48	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	67[A]	ARG	Sidechain
1	D	67[B]	ARG	Sidechain

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	866	0	891	11	0
1	B	883	0	922	15	0
1	C	862	0	880	11	0
1	D	866	0	894	9	0
1	E	854	0	881	12	0
1	F	872	0	891	11	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	19	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	1
3	R	156	0	134	8	0
4	M	156	0	133	5	0
4	Q	156	0	133	3	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
6	A	11	0	10	0	0
6	B	11	0	10	0	0
6	C	11	0	10	1	0
6	D	11	0	10	0	0
6	E	11	0	10	0	0
6	F	11	0	10	0	0
6	G	11	0	10	0	0
6	I	22	0	20	0	0
6	J	11	0	10	0	0
7	F	11	0	12	0	0
7	J	11	0	12	0	0
8	A	79	0	0	1	0
8	B	78	0	0	2	0
8	C	79	0	0	2	0
8	D	83	0	0	2	0
8	E	79	0	0	0	0
8	F	78	0	0	3	1
8	G	88	0	0	1	0
8	H	82	0	0	1	0
8	I	73	0	0	2	0
8	J	78	0	0	3	0
All	All	10879	0	10164	127	1

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 127 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1[B]:GLC:O2	8:F:562:HOH:O[4_446]	2.18	0.02

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
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%)	93 (95%)	5 (5%)	21	5
1	B	100/89 (112%)	91 (91%)	9 (9%)	9	1
1	C	96/89 (108%)	95 (99%)	1 (1%)	68	50
1	D	98/89 (110%)	95 (97%)	3 (3%)	35	13
1	E	96/89 (108%)	95 (99%)	1 (1%)	68	50
1	F	98/89 (110%)	98 (100%)	0	100	100
1	G	98/89 (110%)	97 (99%)	1 (1%)	68	50
1	H	99/89 (111%)	93 (94%)	6 (6%)	17	3
1	I	98/89 (110%)	97 (99%)	1 (1%)	68	50
1	J	98/89 (110%)	97 (99%)	1 (1%)	68	50
All	All	979/890 (110%)	951 (97%)	28 (3%)	48	14

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29	GLU
1	J	29	GLU
1	D	20	LEU
1	H	81[A]	LYS
1	D	9[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	90	ASN
1	I	103	ASN
1	J	49	GLN
1	D	90	ASN
1	D	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	0.51	0	17,17,17	1.67	2 (11%)
2	GAL	K	2	2	11,11,12	0.85	0	15,15,17	0.85	1 (6%)
2	NGA	K	3	2	14,14,15	0.93	1 (7%)	17,19,21	0.97	0
2	GAL	K	4	2	11,11,12	0.66	0	15,15,17	0.72	0
2	FUC	K	5	2	10,10,11	0.46	0	14,14,16	1.04	1 (7%)
2	SIA	K	6	2	20,20,21	0.78	0	21,28,31	1.27	3 (14%)
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	1.18	1 (5%)
3	GAL	L	2[A]	3	11,11,12	0.64	0	15,15,17	0.86	0
3	GAL	L	2[B]	3	11,11,12	0.72	0	15,15,17	0.56	0
3	NGA	L	3[A]	3	14,14,15	0.47	0	17,19,21	0.83	0
3	NGA	L	3[B]	3	14,14,15	0.37	0	17,19,21	0.56	0
3	GAL	L	4[A]	3	11,11,12	0.61	0	15,15,17	0.85	0
3	GAL	L	4[B]	3	11,11,12	0.72	0	15,15,17	0.74	0
3	FUC	L	5[A]	3	10,10,11	0.60	0	14,14,16	1.15	2 (14%)
3	FUC	L	5[B]	3	10,10,11	0.65	0	14,14,16	0.81	0
3	SIA	L	6[A]	3	20,20,21	1.04	3 (15%)	21,28,31	0.88	2 (9%)
3	SIA	L	6[B]	3	20,20,21	1.04	1 (5%)	21,28,31	0.85	1 (4%)
4	BGC	M	1[B]	4	12,12,12	0.45	0	17,17,17	1.27	2 (11%)
4	GLC	M	1[A]	4	12,12,12	0.29	0	17,17,17	0.77	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GAL	M	2[A]	4	11,11,12	0.61	0	15,15,17	1.40	2 (13%)
4	GAL	M	2[B]	4	11,11,12	0.81	1 (9%)	15,15,17	1.17	2 (13%)
4	NGA	M	3[A]	4	14,14,15	0.40	0	17,19,21	1.09	1 (5%)
4	NGA	M	3[B]	4	14,14,15	0.44	0	17,19,21	0.63	0
4	GAL	M	4[A]	4	11,11,12	1.02	2 (18%)	15,15,17	0.93	0
4	GAL	M	4[B]	4	11,11,12	0.86	0	15,15,17	1.14	2 (13%)
4	FUC	M	5[A]	4	10,10,11	0.44	0	14,14,16	1.15	2 (14%)
4	FUC	M	5[B]	4	10,10,11	1.03	1 (10%)	14,14,16	1.44	1 (7%)
4	SIA	M	6[A]	4	20,20,21	1.59	3 (15%)	21,28,31	1.39	2 (9%)
4	SIA	M	6[B]	4	20,20,21	1.43	2 (10%)	21,28,31	1.27	2 (9%)
2	BGC	N	1[A]	2	12,12,12	0.39	0	17,17,17	0.69	0
2	BGC	N	1[B]	2	12,12,12	0.38	0	17,17,17	1.43	4 (23%)
2	GAL	N	2[A]	2	11,11,12	0.33	0	15,15,17	1.43	2 (13%)
2	GAL	N	2[B]	2	11,11,12	0.47	0	15,15,17	0.61	0
2	NGA	N	3[A]	2	14,14,15	0.42	0	17,19,21	0.88	0
2	NGA	N	3[B]	2	14,14,15	0.61	0	17,19,21	1.02	2 (11%)
2	GAL	N	4[A]	2	11,11,12	0.44	0	15,15,17	0.80	0
2	GAL	N	4[B]	2	11,11,12	1.15	1 (9%)	15,15,17	1.16	1 (6%)
2	FUC	N	5[A]	2	10,10,11	0.67	0	14,14,16	0.78	0
2	FUC	N	5[B]	2	10,10,11	1.07	1 (10%)	14,14,16	1.86	2 (14%)
2	SIA	N	6[A]	2	20,20,21	0.73	1 (5%)	21,28,31	1.07	2 (9%)
2	SIA	N	6[B]	2	20,20,21	0.95	2 (10%)	21,28,31	1.07	2 (9%)
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	1.06	1 (9%)	15,15,17	0.89	1 (6%)
2	NGA	O	3	2	14,14,15	0.68	0	17,19,21	0.94	1 (5%)
2	GAL	O	4	2	11,11,12	0.71	0	15,15,17	1.06	1 (6%)
2	FUC	O	5	2	10,10,11	0.85	0	14,14,16	1.18	2 (14%)
2	SIA	O	6	2	20,20,21	0.82	1 (5%)	21,28,31	1.09	1 (4%)
2	BGC	P	1	2	12,12,12	0.82	0	17,17,17	0.77	1 (5%)
2	GAL	P	2	2	11,11,12	0.71	0	15,15,17	0.81	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	0.97	0	15,15,17	0.74	0
2	FUC	P	5	2	10,10,11	0.58	0	14,14,16	0.97	1 (7%)
2	SIA	P	6	2	20,20,21	0.79	1 (5%)	21,28,31	1.01	1 (4%)
4	BGC	Q	1[B]	4	12,12,12	0.50	0	17,17,17	0.73	0
4	GLC	Q	1[A]	4	12,12,12	0.66	0	17,17,17	1.28	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GAL	Q	2[A]	4	11,11,12	0.98	1 (9%)	15,15,17	0.82	0
4	GAL	Q	2[B]	4	11,11,12	0.64	0	15,15,17	0.90	0
4	NGA	Q	3[A]	4	14,14,15	0.62	0	17,19,21	1.01	0
4	NGA	Q	3[B]	4	14,14,15	0.41	0	17,19,21	0.64	0
4	GAL	Q	4[A]	4	11,11,12	0.36	0	15,15,17	0.92	1 (6%)
4	GAL	Q	4[B]	4	11,11,12	0.67	0	15,15,17	1.13	1 (6%)
4	FUC	Q	5[A]	4	10,10,11	0.99	1 (10%)	14,14,16	1.02	0
4	FUC	Q	5[B]	4	10,10,11	0.70	0	14,14,16	1.59	3 (21%)
4	SIA	Q	6[A]	4	20,20,21	0.64	0	21,28,31	1.33	3 (14%)
4	SIA	Q	6[B]	4	20,20,21	0.79	1 (5%)	21,28,31	1.47	3 (14%)
3	BGC	R	1[A]	3	12,12,12	0.72	0	17,17,17	1.17	1 (5%)
3	GLC	R	1[B]	3	12,12,12	0.77	0	17,17,17	1.25	2 (11%)
3	GAL	R	2[A]	3	11,11,12	0.52	0	15,15,17	1.13	1 (6%)
3	GAL	R	2[B]	3	11,11,12	0.58	0	15,15,17	1.11	1 (6%)
3	NGA	R	3[A]	3	14,14,15	0.41	0	17,19,21	0.92	0
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	0.60	0	15,15,17	1.11	2 (13%)
3	GAL	R	4[B]	3	11,11,12	0.69	0	15,15,17	0.75	0
3	FUC	R	5[A]	3	10,10,11	1.29	1 (10%)	14,14,16	1.38	2 (14%)
3	FUC	R	5[B]	3	10,10,11	0.54	0	14,14,16	1.39	2 (14%)
3	SIA	R	6[A]	3	20,20,21	0.70	0	21,28,31	0.95	2 (9%)
3	SIA	R	6[B]	3	20,20,21	0.54	0	21,28,31	1.06	3 (14%)
2	BGC	S	1	2	12,12,12	0.53	0	17,17,17	1.14	1 (5%)
2	GAL	S	2	2	11,11,12	0.45	0	15,15,17	0.87	0
2	NGA	S	3	2	14,14,15	0.57	0	17,19,21	0.79	1 (5%)
2	GAL	S	4	2	11,11,12	0.78	0	15,15,17	0.53	0
2	FUC	S	5	2	10,10,11	0.33	0	14,14,16	1.42	2 (14%)
2	SIA	S	6	2	20,20,21	0.83	0	21,28,31	1.06	2 (9%)
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	1.22	2 (11%)
2	GAL	T	2[A]	2	11,11,12	0.44	0	15,15,17	0.84	0
2	GAL	T	2[B]	2	11,11,12	0.63	0	15,15,17	1.16	1 (6%)
2	NGA	T	3[A]	2	14,14,15	0.36	0	17,19,21	0.84	1 (5%)
2	NGA	T	3[B]	2	14,14,15	0.45	0	17,19,21	0.78	1 (5%)
2	GAL	T	4[A]	2	11,11,12	0.89	0	15,15,17	1.33	3 (20%)
2	GAL	T	4[B]	2	11,11,12	0.97	1 (9%)	15,15,17	1.00	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FUC	T	5[A]	2	10,10,11	1.37	1 (10%)	14,14,16	2.16	5 (35%)
2	FUC	T	5[B]	2	10,10,11	0.53	0	14,14,16	1.13	1 (7%)
2	SIA	T	6[A]	2	20,20,21	1.46	1 (5%)	21,28,31	1.05	0
2	SIA	T	6[B]	2	20,20,21	1.22	2 (10%)	21,28,31	1.28	2 (9%)

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	-	3/18/34/38	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
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	-	6/18/34/38	0/1/1/1
3	SIA	L	6[B]	3	-	1/18/34/38	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	-	2/6/23/26	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]	4	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SIA	M	6[A]	4	-	1/18/34/38	0/1/1/1
4	SIA	M	6[B]	4	-	7/18/34/38	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	-	0/18/34/38	0/1/1/1
2	SIA	N	6[B]	2	-	2/18/34/38	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	-	1/18/34/38	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	-	3/18/34/38	0/1/1/1
4	BGC	Q	1[B]	4	-	0/2/22/22	0/1/1/1
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	-	1/18/34/38	0/1/1/1
4	SIA	Q	6[B]	4	-	3/18/34/38	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	3/18/34/38	0/1/1/1
3	SIA	R	6[B]	3	-	3/18/34/38	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	-	1/18/34/38	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	-	1/6/23/26	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	-	9/18/34/38	0/1/1/1
2	SIA	T	6[B]	2	-	3/18/34/38	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	6[A]	SIA	C2-C1	5.55	1.59	1.52
4	M	6[B]	SIA	C2-C1	5.18	1.58	1.52
4	M	6[A]	SIA	C2-C1	5.03	1.58	1.52
3	R	5[A]	FUC	C2-C3	3.64	1.58	1.52
4	M	6[A]	SIA	O1B-C1	-3.57	1.19	1.30

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	5[B]	FUC	C1-C2-C3	5.54	117.71	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	5[A]	FUC	O3-C3-C2	5.34	120.96	110.05
2	K	1	BGC	O4-C4-C3	-4.87	98.89	110.38
4	M	5[B]	FUC	C1-C2-C3	4.61	116.36	109.64
4	M	6[A]	SIA	O1A-C1-C2	-4.29	113.58	122.85

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	6[A]	SIA	O1B-C1-C2-C3
2	T	6[A]	SIA	C7-C8-C9-O9
2	T	6[A]	SIA	O8-C8-C9-O9
3	L	6[A]	SIA	C7-C8-C9-O9
3	L	6[A]	SIA	O8-C8-C9-O9

There are no ring outliers.

34 monomers are involved in 42 short contacts:

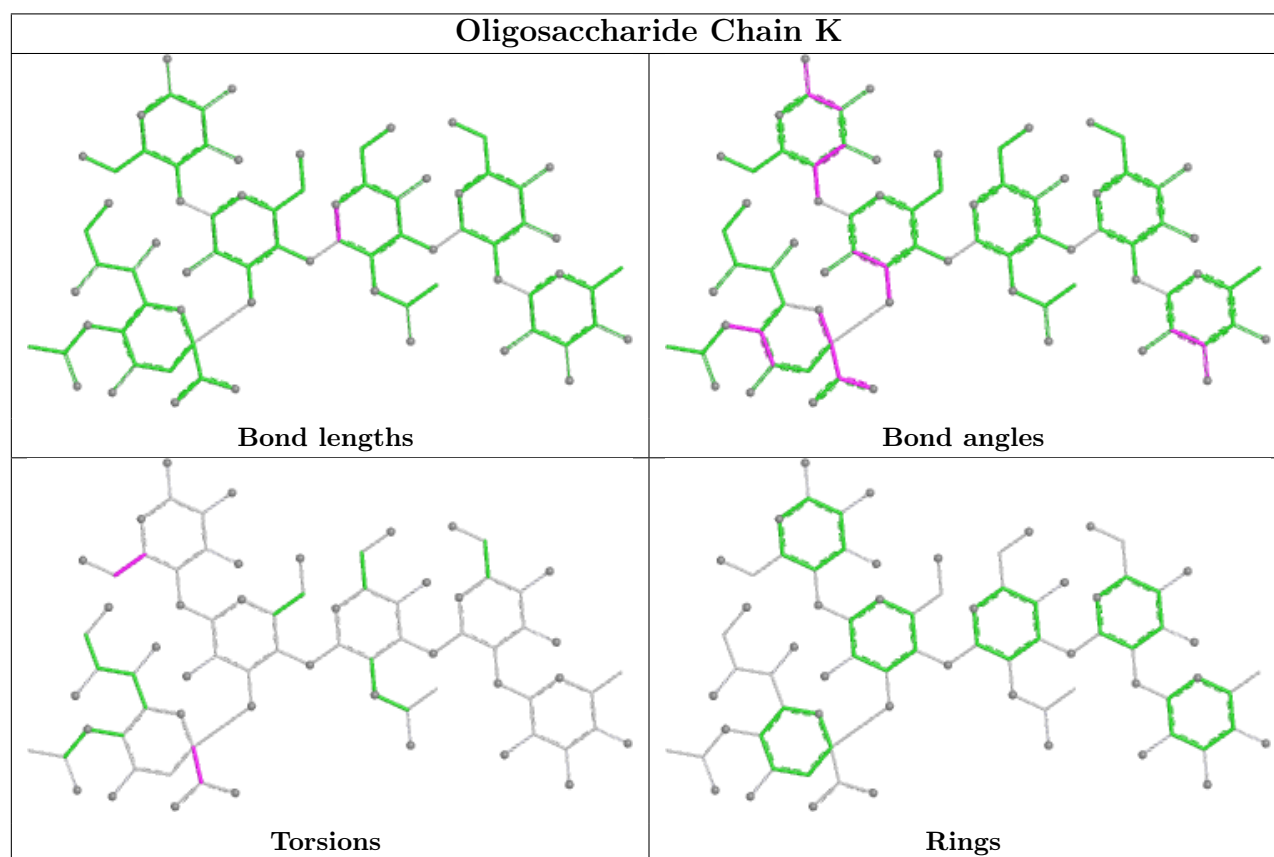
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	3[A]	NGA	3	0
3	L	5[A]	FUC	1	0
3	R	6[B]	SIA	1	0
4	Q	5[B]	FUC	1	0
2	O	3	NGA	1	0
2	T	6[B]	SIA	2	0
2	N	3[B]	NGA	4	0
4	Q	6[B]	SIA	1	0
4	M	3[A]	NGA	5	0
4	M	5[A]	FUC	4	0
3	R	5[B]	FUC	2	0
3	R	6[A]	SIA	1	0
2	N	5[B]	FUC	5	0
2	N	3[A]	NGA	1	0
3	L	3[B]	NGA	1	0
2	N	6[B]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

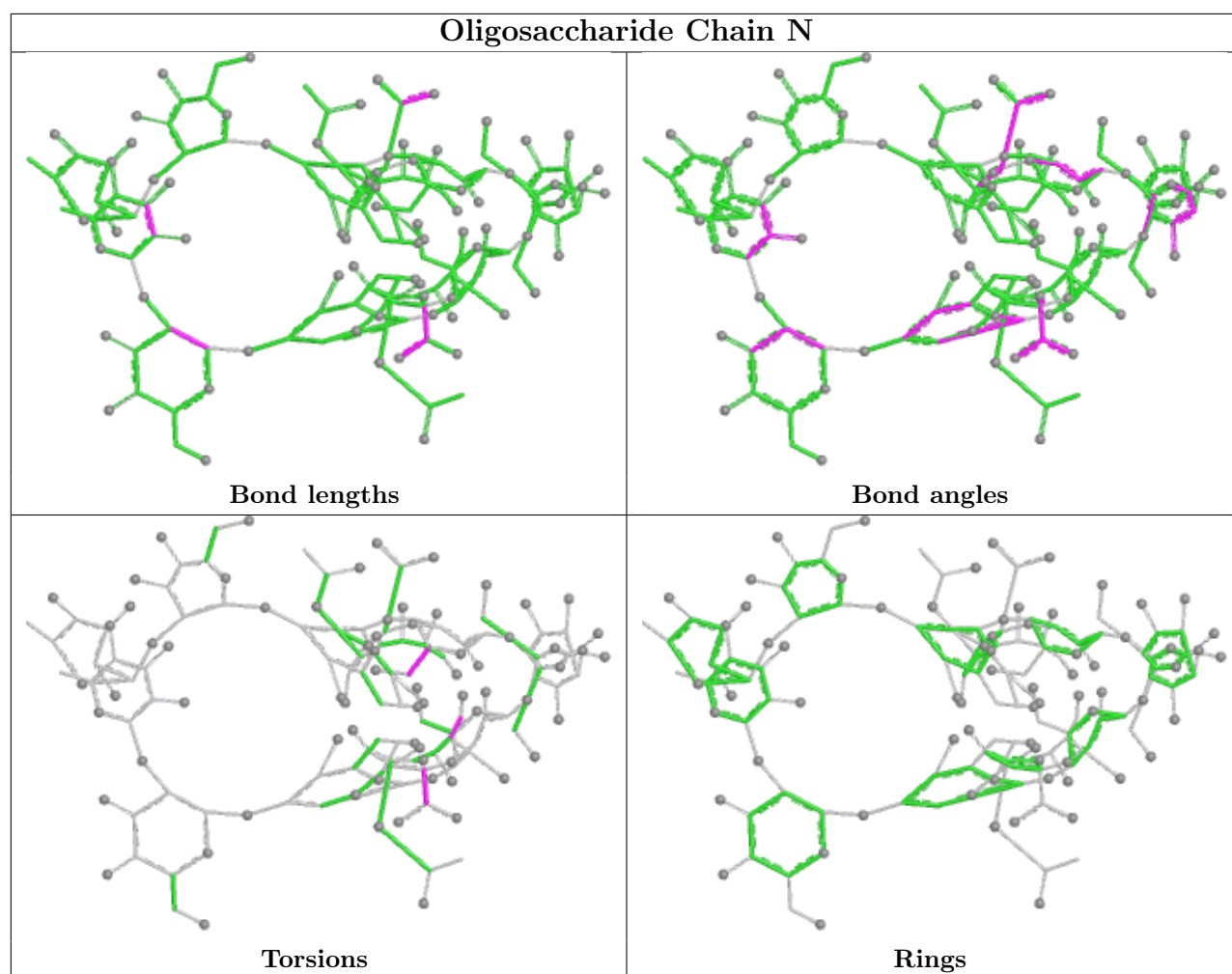
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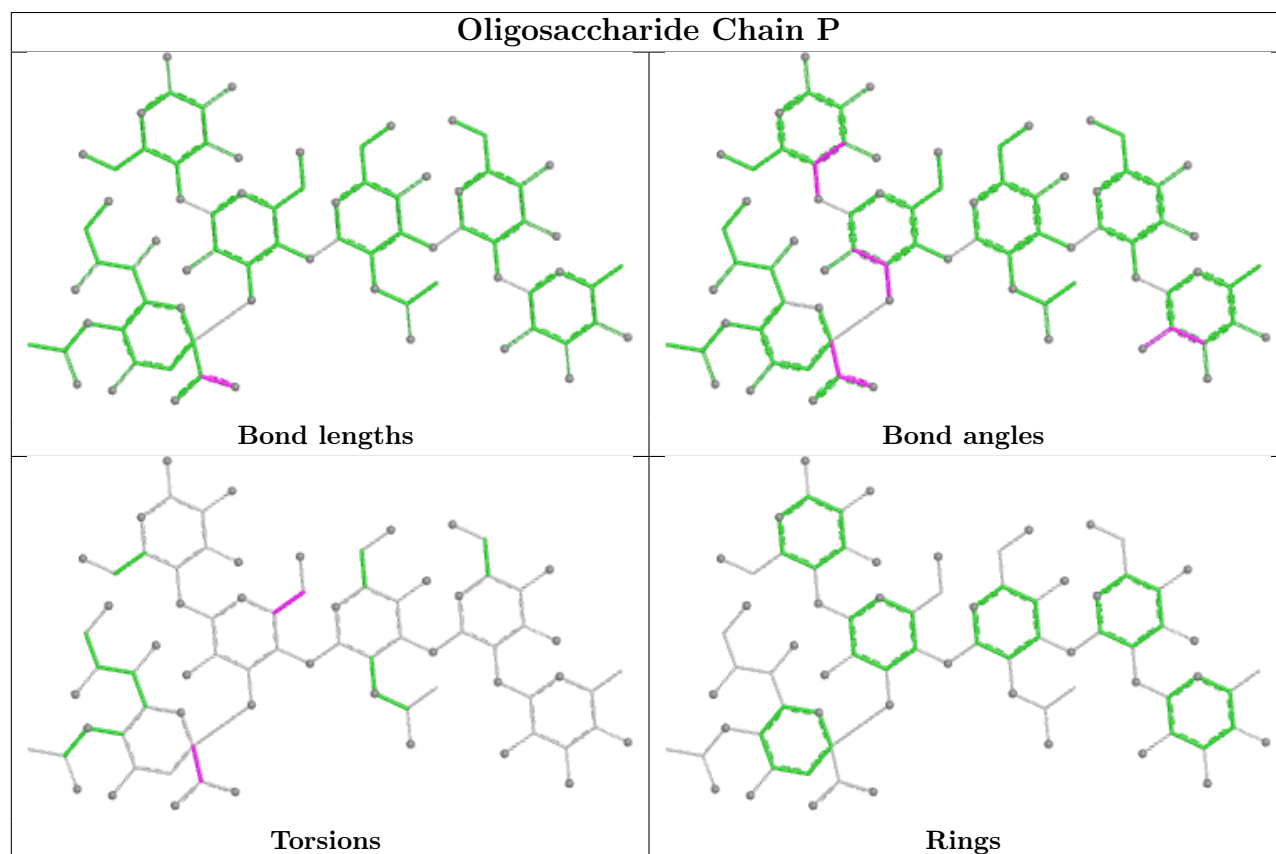
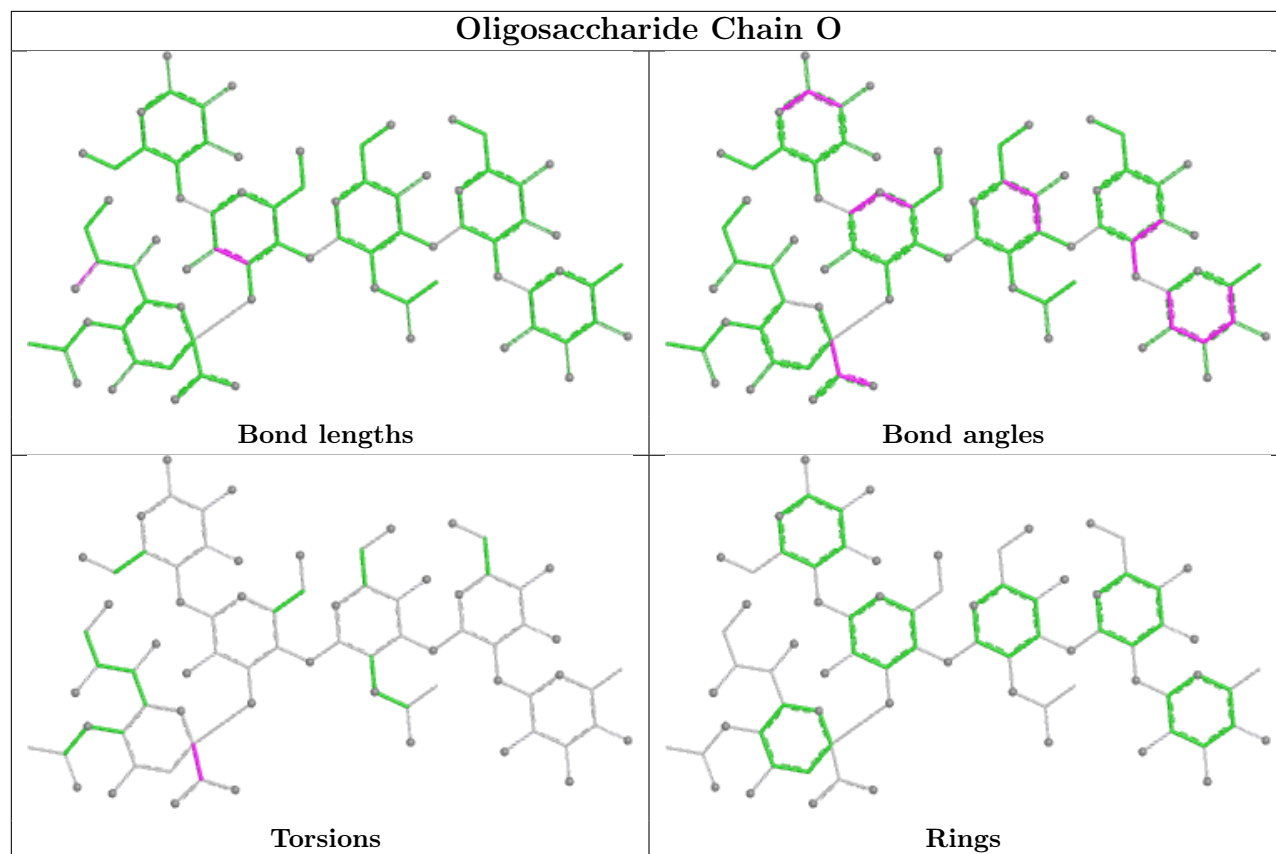
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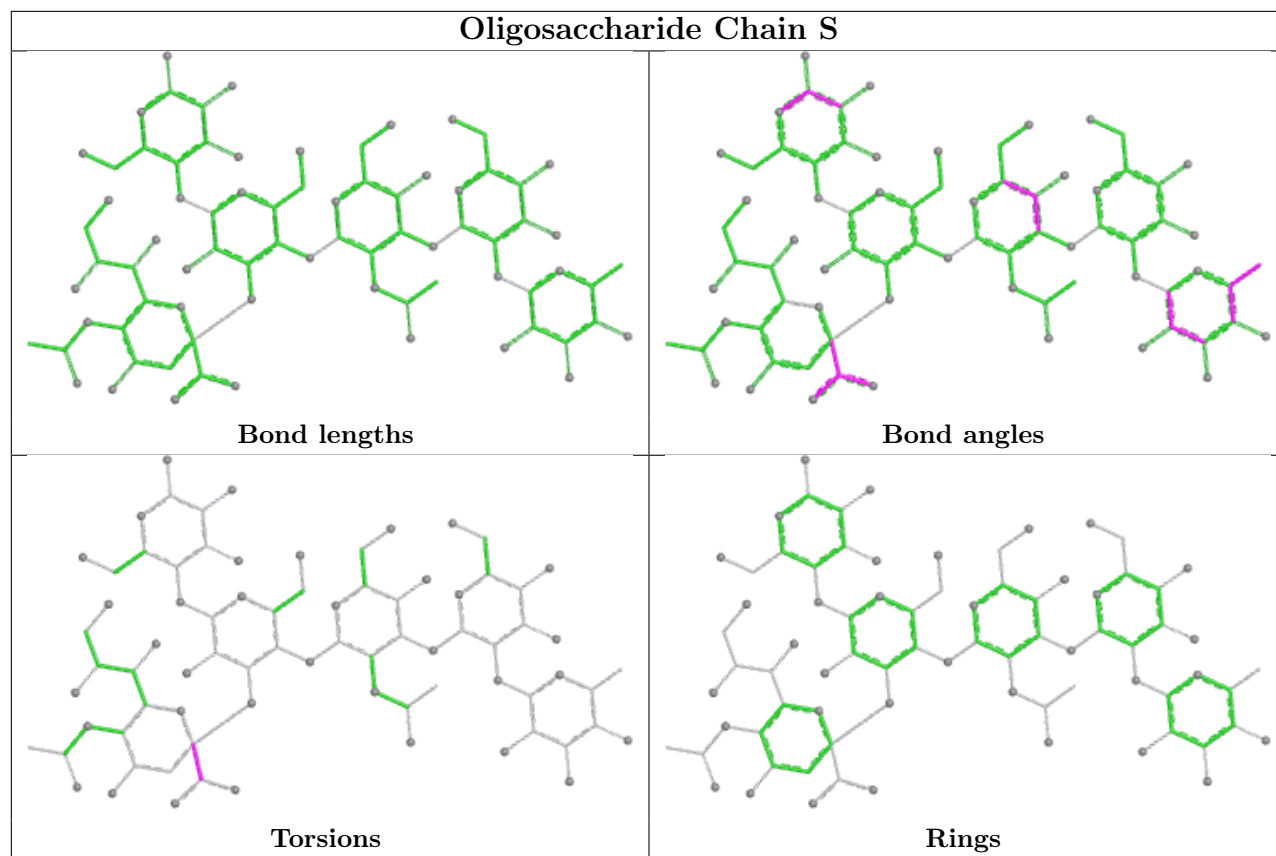
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	5	FUC	1	0
2	S	3	NGA	1	0
2	P	3	NGA	1	0
2	S	5	FUC	3	0
4	Q	3[B]	NGA	2	0
3	R	3[B]	NGA	2	0
2	T	3[B]	NGA	1	0
3	L	5[B]	FUC	2	0
2	T	4[A]	GAL	1	0
3	L	1[B]	GLC	0	1
2	T	5[A]	FUC	4	0
3	R	3[A]	NGA	1	0

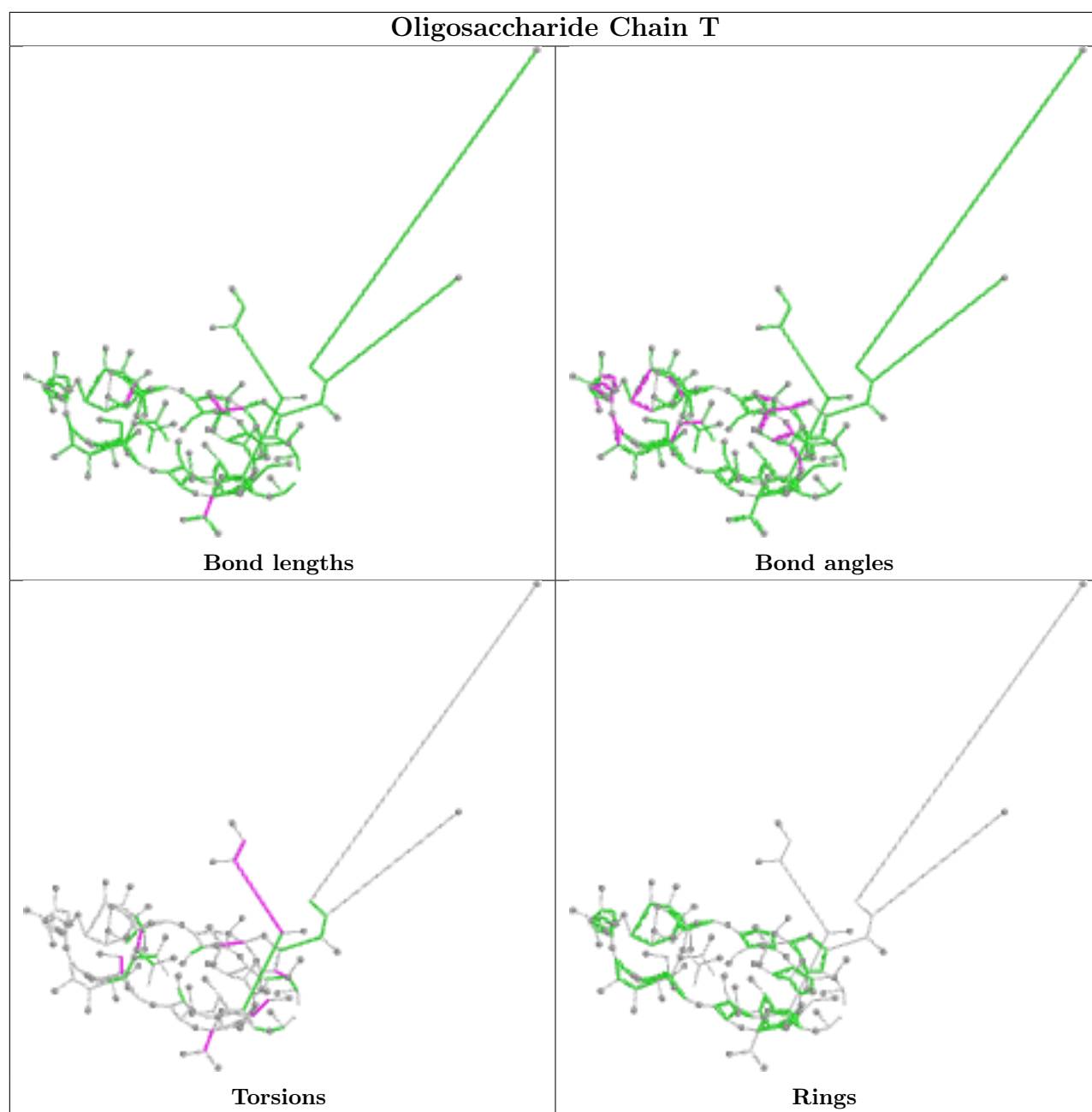
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

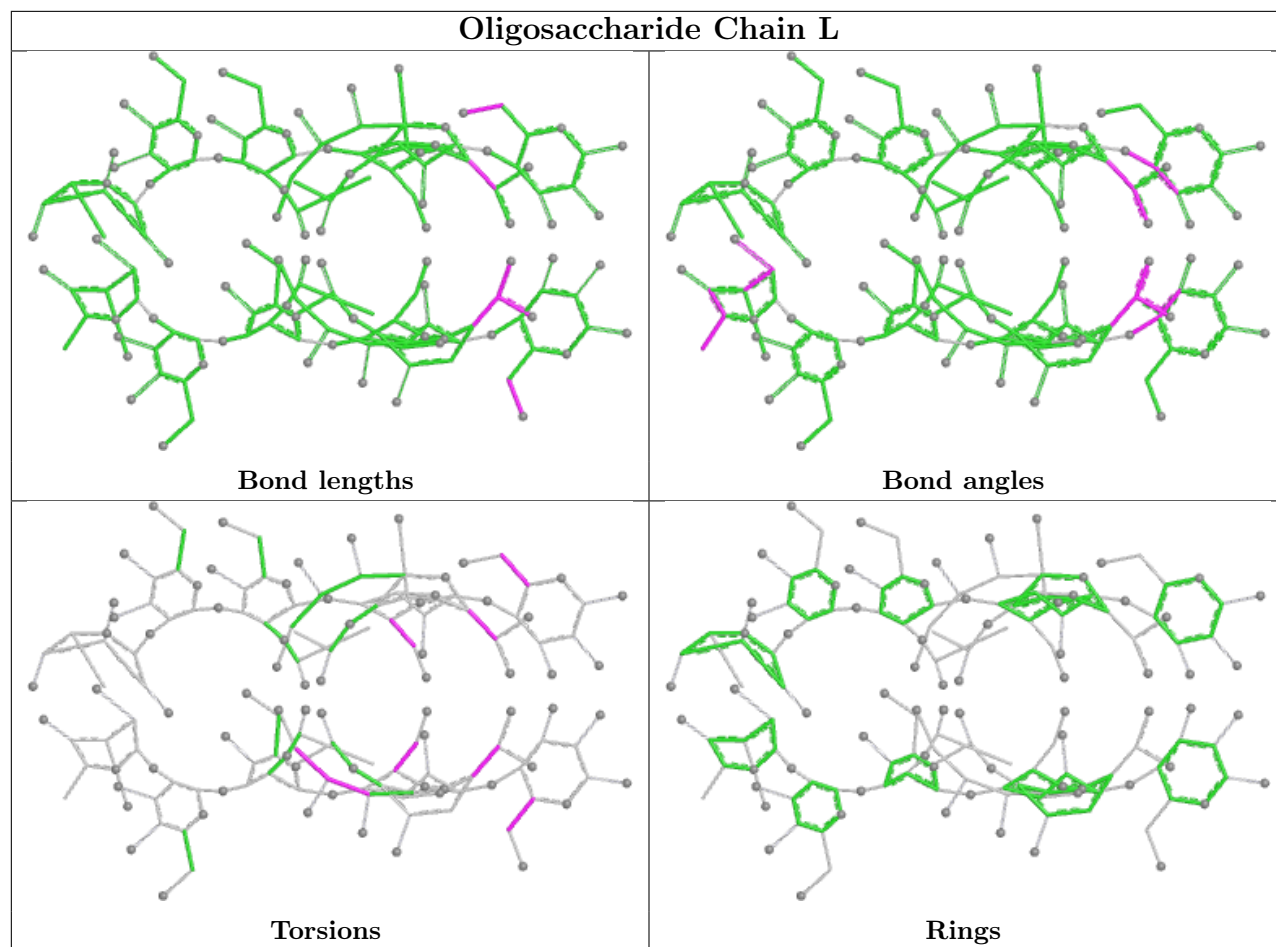




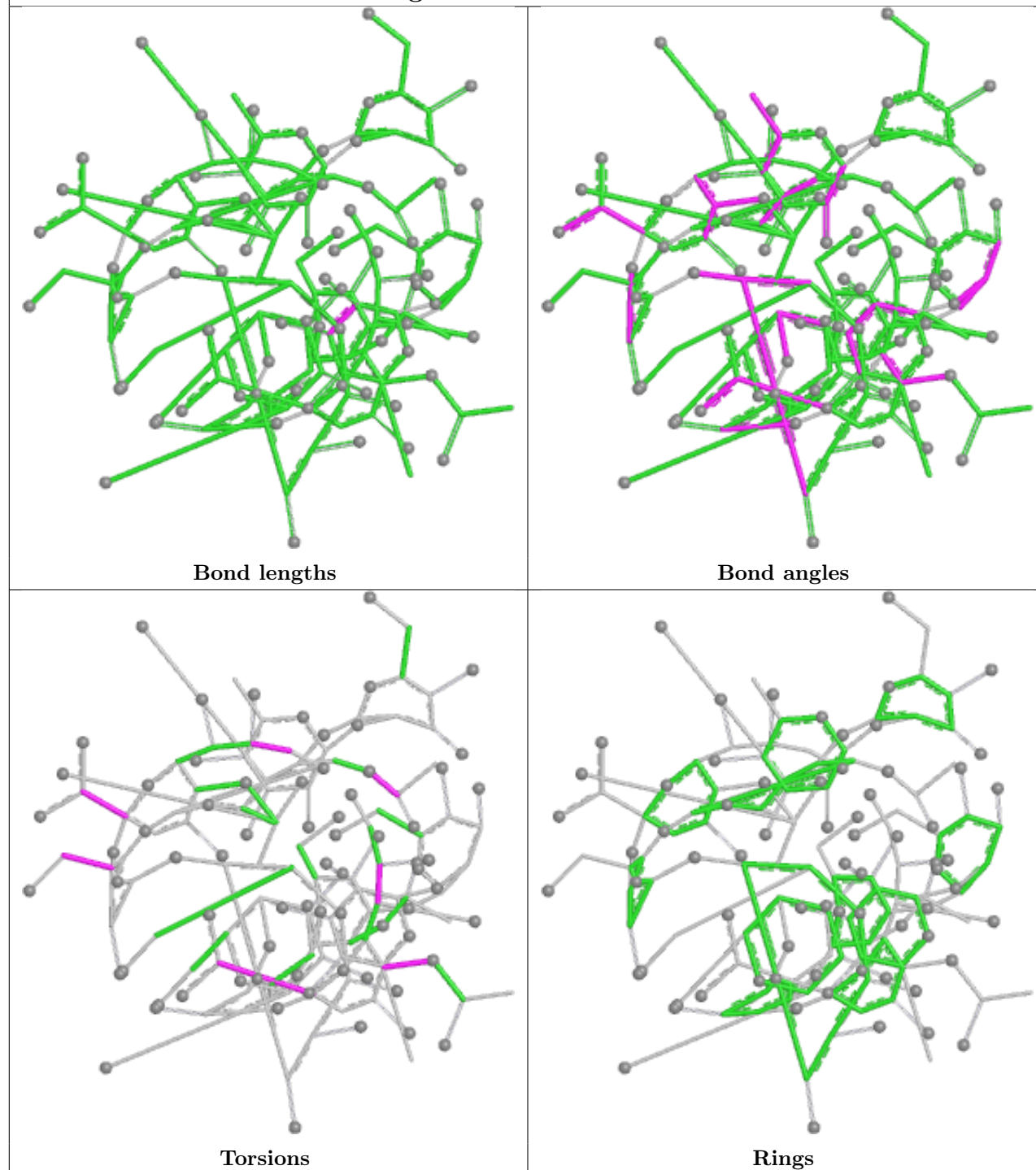


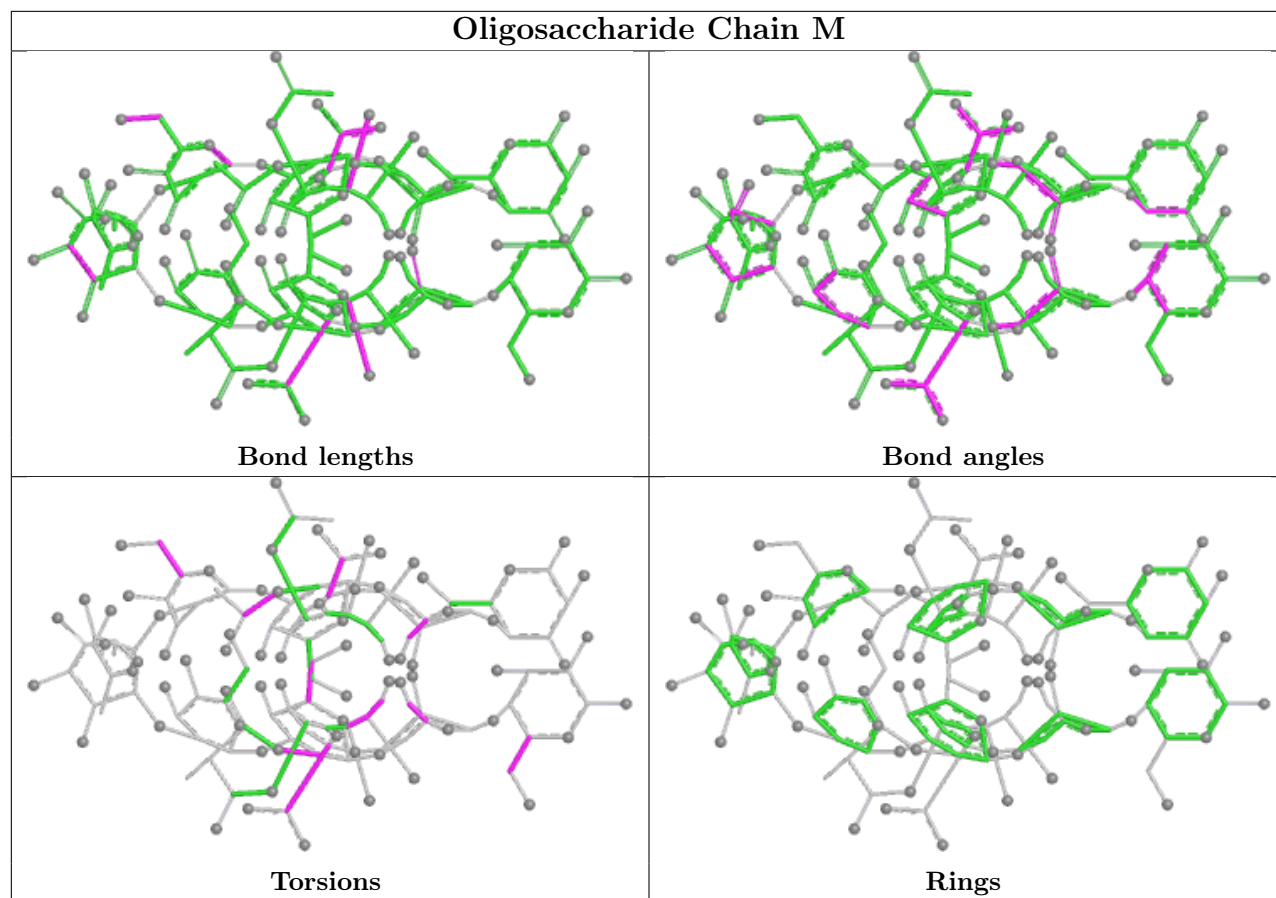


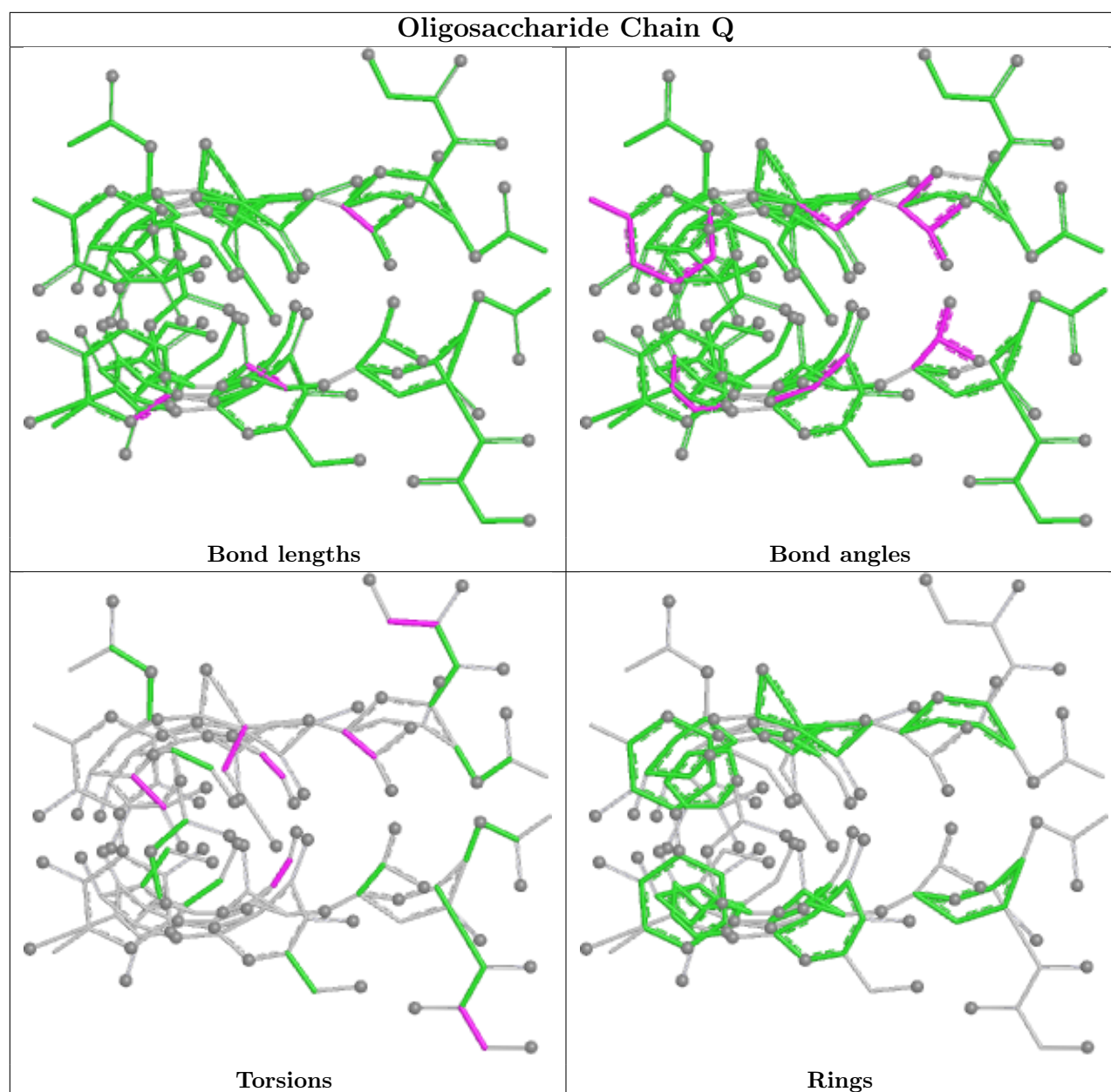




Oligosaccharide Chain R







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	I	203	5	10,10,10	0.65	0	11,11,11	0.93	0
6	BCN	J	201	5	10,10,10	0.87	0	11,11,11	0.87	0
6	BCN	F	201	5	10,10,10	0.60	0	11,11,11	0.94	1 (9%)
6	BCN	I	201	5	10,10,10	0.89	1 (10%)	11,11,11	0.80	0
7	FUC	J	203	-	11,11,11	0.71	0	16,16,16	1.23	0
6	BCN	D	202	5	10,10,10	1.04	1 (10%)	11,11,11	1.09	0
6	BCN	E	201	5	10,10,10	0.99	1 (10%)	11,11,11	1.06	0
6	BCN	A	202	5	10,10,10	1.20	1 (10%)	11,11,11	1.00	1 (9%)
6	BCN	C	202	5	10,10,10	0.81	0	11,11,11	0.98	0
7	FUC	F	203	-	11,11,11	1.01	0	16,16,16	2.30	6 (37%)
6	BCN	G	202	5	10,10,10	0.57	0	11,11,11	1.22	1 (9%)
6	BCN	B	202	5	10,10,10	0.59	0	11,11,11	0.80	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
6	BCN	I	203	5	-	2/10/10/10	-
6	BCN	J	201	5	-	2/10/10/10	-
6	BCN	F	201	5	-	1/10/10/10	-
6	BCN	I	201	5	-	0/10/10/10	-
7	FUC	J	203	-	-	-	0/1/1/1
6	BCN	D	202	5	-	0/10/10/10	-
6	BCN	E	201	5	-	2/10/10/10	-
6	BCN	A	202	5	-	2/10/10/10	-
6	BCN	C	202	5	-	3/10/10/10	-
7	FUC	F	203	-	-	-	0/1/1/1
6	BCN	G	202	5	-	1/10/10/10	-
6	BCN	B	202	5	-	1/10/10/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	201	BCN	O22-C2	-2.49	1.22	1.30
6	A	202	BCN	O21-C2	2.23	1.29	1.22
6	D	202	BCN	C1-N1	2.18	1.51	1.47
6	I	201	BCN	O22-C2	-2.07	1.24	1.30

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	203	FUC	O4-C4-C3	-4.76	99.15	110.38
7	F	203	FUC	O4-C4-C5	4.64	119.97	109.74
7	F	203	FUC	O3-C3-C4	-2.87	103.62	110.38
7	F	203	FUC	C4-C3-C2	-2.59	106.28	110.83
7	F	203	FUC	O5-C5-C4	2.38	113.83	109.55

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	203	BCN	C2-C1-N1-C3
6	I	203	BCN	C2-C1-N1-C5
6	A	202	BCN	C2-C1-N1-C3
6	J	201	BCN	C2-C1-N1-C3
6	C	202	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	C	202	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, 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	103/103 (100%)	-0.19	1 (0%) 79 83	5, 12, 20, 34	9 (8%)
1	B	103/103 (100%)	-0.23	1 (0%) 79 83	5, 12, 19, 24	11 (10%)
1	C	103/103 (100%)	-0.17	1 (0%) 79 83	5, 13, 20, 40	7 (6%)
1	D	103/103 (100%)	-0.31	0 100 100	5, 11, 16, 21	9 (8%)
1	E	103/103 (100%)	-0.25	1 (0%) 79 83	5, 12, 19, 33	7 (6%)
1	F	103/103 (100%)	-0.30	1 (0%) 79 83	5, 10, 16, 34	9 (8%)
1	G	103/103 (100%)	-0.33	0 100 100	5, 11, 17, 22	8 (7%)
1	H	103/103 (100%)	-0.11	1 (0%) 79 83	5, 13, 20, 27	10 (9%)
1	I	103/103 (100%)	-0.13	2 (1%) 66 70	4, 14, 22, 28	8 (7%)
1	J	103/103 (100%)	-0.19	2 (1%) 66 70	5, 12, 18, 31	9 (8%)
All	All	1030/1030 (100%)	-0.22	10 (0%) 79 83	4, 12, 20, 40	87 (8%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	103	ASN	4.4
1	C	103	ASN	3.6
1	E	103	ASN	3.4
1	J	103	ASN	3.1
1	H	103	ASN	2.7

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FUC	T	5[A]	10/11	0.58	0.38	18,20,20,21	10
2	FUC	T	5[B]	10/11	0.58	0.38	13,14,15,15	10
2	FUC	S	5	10/11	0.66	0.21	30,36,39,40	0
4	FUC	M	5[A]	10/11	0.69	0.20	23,25,27,27	10
4	FUC	M	5[B]	10/11	0.69	0.20	21,23,24,25	10
3	FUC	L	5[A]	10/11	0.70	0.17	20,21,23,23	10
3	FUC	L	5[B]	10/11	0.70	0.17	19,21,22,22	10
2	FUC	N	5[B]	10/11	0.74	0.20	18,20,22,22	10
2	FUC	N	5[A]	10/11	0.74	0.20	15,17,18,18	10
3	BGC	R	1[A]	12/12	0.78	0.15	23,26,28,30	12
4	GAL	M	2[A]	11/12	0.80	0.12	20,22,23,24	11
4	GAL	M	2[B]	11/12	0.80	0.12	21,23,25,25	11
2	FUC	O	5	10/11	0.80	0.18	27,32,34,35	0
2	BGC	S	1	12/12	0.80	0.13	30,37,41,43	0
4	FUC	Q	5[A]	10/11	0.80	0.19	16,18,19,20	10
4	FUC	Q	5[B]	10/11	0.80	0.19	16,18,20,21	10
3	FUC	R	5[A]	10/11	0.81	0.17	19,20,22,22	10
3	FUC	R	5[B]	10/11	0.81	0.17	18,19,21,21	10
4	GLC	M	1[A]	12/12	0.81	0.13	25,28,31,32	12
2	BGC	O	1	12/12	0.82	0.13	28,36,40,43	0
3	BGC	L	1[A]	12/12	0.82	0.13	21,23,25,26	12
4	GAL	M	4[A]	11/12	0.82	0.12	15,16,18,21	11
4	GAL	M	4[B]	11/12	0.82	0.12	15,16,18,19	11
2	FUC	K	5	10/11	0.83	0.13	25,29,31,31	0
2	FUC	P	5	10/11	0.84	0.14	19,22,25,28	0
2	BGC	K	1	12/12	0.85	0.13	29,35,37,41	0
2	BGC	N	1[A]	12/12	0.86	0.12	20,24,25,27	12
2	BGC	N	1[B]	12/12	0.86	0.12	20,23,25,26	12
4	SIA	M	6[A]	20/21	0.87	0.10	16,17,18,19	20
4	SIA	M	6[B]	20/21	0.87	0.10	16,18,20,20	20
2	BGC	T	1[B]	12/12	0.88	0.10	13,14,16,16	12
2	BGC	T	1[A]	12/12	0.88	0.10	16,18,20,20	12
2	SIA	T	6[B]	20/21	0.89	0.09	10,11,12,12	20
2	GAL	S	2	11/12	0.89	0.10	22,25,27,27	0
2	SIA	T	6[A]	20/21	0.89	0.09	12,13,14,15	20
2	GAL	K	2	11/12	0.91	0.10	21,24,26,27	0
2	GAL	O	2	11/12	0.91	0.09	20,23,25,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NGA	R	3[A]	14/15	0.92	0.08	16,17,18,18	14
3	NGA	R	3[B]	14/15	0.92	0.08	15,16,17,17	14
2	NGA	N	3[B]	14/15	0.92	0.08	14,15,15,15	14
2	NGA	N	3[A]	14/15	0.92	0.08	13,15,16,16	14
2	GAL	T	2[A]	11/12	0.92	0.08	14,15,15,16	11
2	GAL	T	2[B]	11/12	0.92	0.08	11,12,13,13	11
3	GAL	L	2[A]	11/12	0.92	0.08	17,19,20,21	11
3	GAL	L	2[B]	11/12	0.92	0.08	17,19,20,21	11
3	GAL	L	4[A]	11/12	0.92	0.08	14,15,16,18	11
3	GAL	L	4[B]	11/12	0.92	0.08	14,15,16,17	11
2	NGA	T	3[A]	14/15	0.92	0.08	13,13,14,14	14
2	NGA	T	3[B]	14/15	0.92	0.08	11,11,12,12	14
3	GLC	L	1[B]	12/12	-	-	22,24,26,26	12
2	SIA	S	6	20/21	0.92	0.09	18,20,22,22	0
4	NGA	Q	3[A]	14/15	0.92	0.08	11,11,12,12	14
4	NGA	Q	3[B]	14/15	0.92	0.08	11,11,12,12	14
3	GAL	R	2[A]	11/12	0.92	0.09	17,20,21,21	11
3	GAL	R	2[B]	11/12	0.92	0.09	17,19,21,21	11
4	GLC	Q	1[A]	12/12	0.93	0.07	14,16,17,17	12
3	NGA	L	3[A]	14/15	0.93	0.07	16,17,17,18	14
3	NGA	L	3[B]	14/15	0.93	0.07	16,17,18,18	14
3	SIA	L	6[A]	20/21	0.93	0.07	14,15,17,17	20
3	SIA	L	6[B]	20/21	0.93	0.07	14,15,17,17	20
2	NGA	S	3	14/15	0.94	0.07	19,21,23,23	0
3	GLC	R	1[B]	12/12	-	-	22,25,28,28	12
2	SIA	K	6	20/21	0.94	0.07	16,18,19,20	0
4	NGA	M	3[A]	14/15	0.94	0.07	18,19,20,21	14
4	NGA	M	3[B]	14/15	0.94	0.07	18,20,21,22	14
2	GAL	T	4[A]	11/12	0.94	0.07	11,12,14,16	11
2	GAL	T	4[B]	11/12	0.94	0.07	9,10,11,12	11
2	SIA	O	6	20/21	0.94	0.07	17,17,19,20	0
2	BGC	P	1	12/12	0.94	0.07	14,17,19,20	0
3	GAL	R	4[A]	11/12	0.94	0.07	13,14,15,17	11
3	GAL	R	4[B]	11/12	0.94	0.07	13,14,15,17	11
2	GAL	N	2[A]	11/12	0.94	0.07	16,18,19,19	11
4	GAL	Q	2[A]	11/12	0.94	0.07	12,12,13,14	11
4	BGC	M	1[B]	12/12	-	-	27,30,34,35	12
4	GAL	Q	2[B]	11/12	0.94	0.07	11,12,13,13	11
2	GAL	N	2[B]	11/12	0.94	0.07	15,17,18,18	11
3	SIA	R	6[A]	20/21	0.94	0.07	14,15,17,17	20
4	GAL	Q	4[A]	11/12	0.94	0.07	9,10,12,14	11
4	GAL	Q	4[B]	11/12	0.94	0.07	10,11,12,14	11

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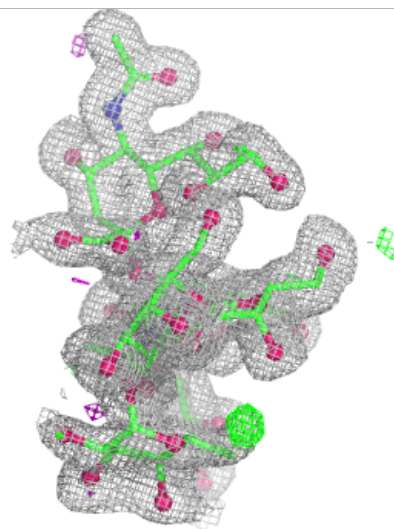
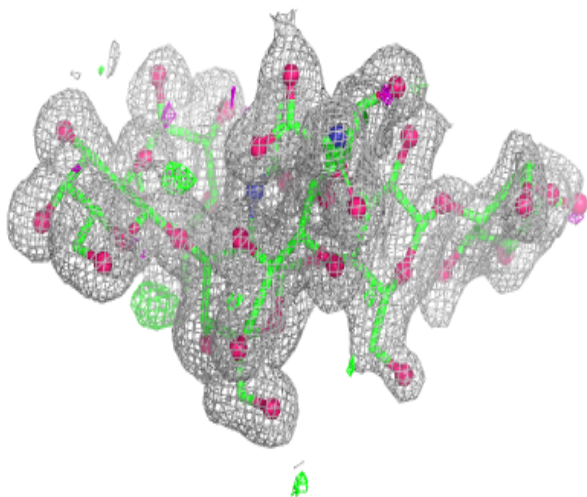
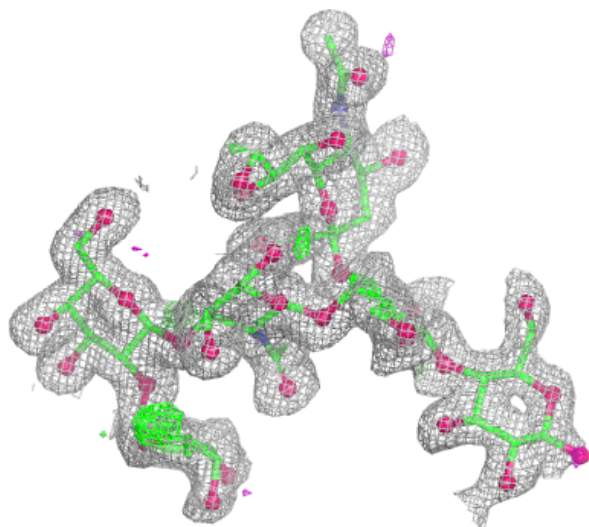
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SIA	R	6[B]	20/21	0.94	0.07	14,15,17,17	20
2	NGA	O	3	14/15	0.94	0.07	17,18,20,22	0
2	GAL	N	4[B]	11/12	0.95	0.07	11,12,14,16	11
2	GAL	N	4[A]	11/12	0.95	0.07	11,11,13,14	11
2	GAL	O	4	11/12	0.95	0.08	14,15,18,22	0
2	GAL	P	2	11/12	0.95	0.06	11,12,13,14	0
4	BGC	Q	1[B]	12/12	-	-	13,15,16,17	12
4	SIA	Q	6[A]	20/21	0.95	0.07	10,11,12,12	20
4	SIA	Q	6[B]	20/21	0.95	0.07	9,10,11,11	20
2	NGA	P	3	14/15	0.96	0.06	10,10,11,11	0
2	GAL	S	4	11/12	0.96	0.07	16,17,20,24	0
2	SIA	N	6[B]	20/21	0.96	0.06	12,13,15,15	20
2	SIA	P	6	20/21	0.96	0.06	10,11,12,12	0
2	NGA	K	3	14/15	0.96	0.06	19,20,22,23	0
2	SIA	N	6[A]	20/21	0.96	0.06	13,14,16,16	20
2	GAL	K	4	11/12	0.97	0.05	14,15,18,22	0
2	GAL	P	4	11/12	0.97	0.06	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.

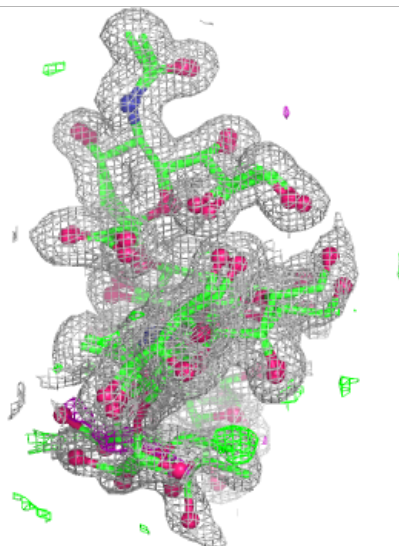
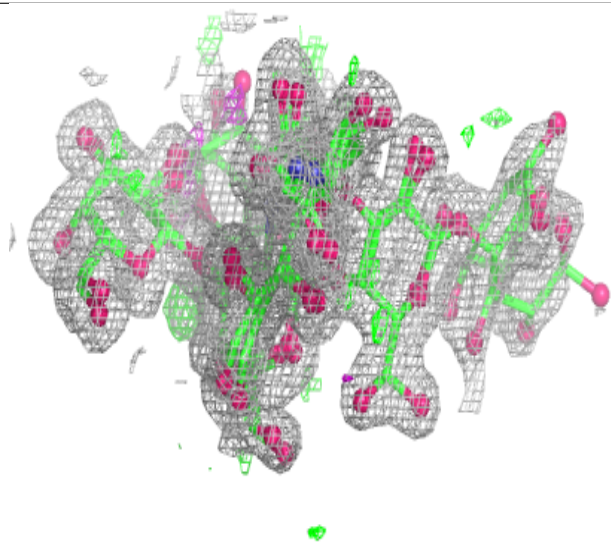
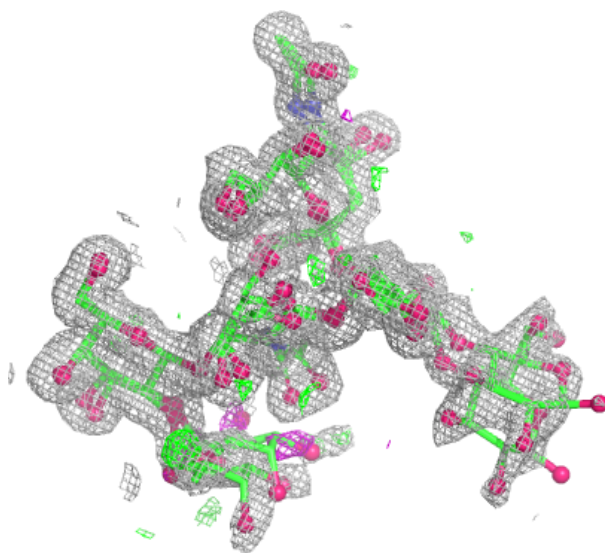
Electron density around Chain K:

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



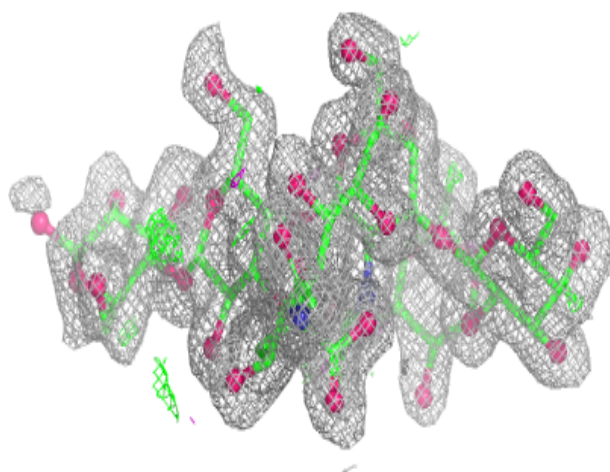
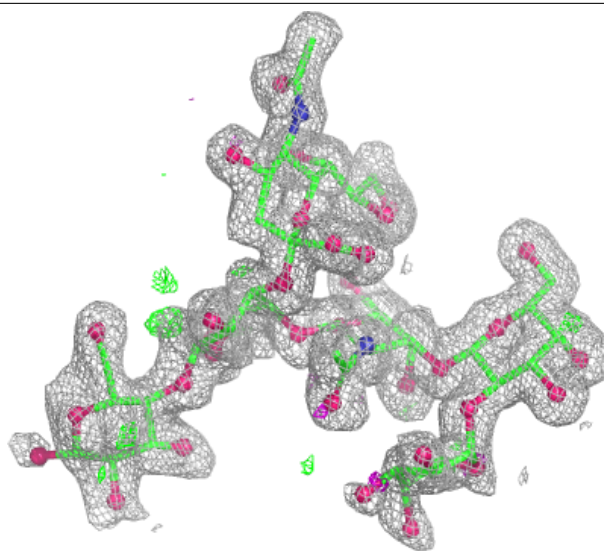
Electron density around Chain N:

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



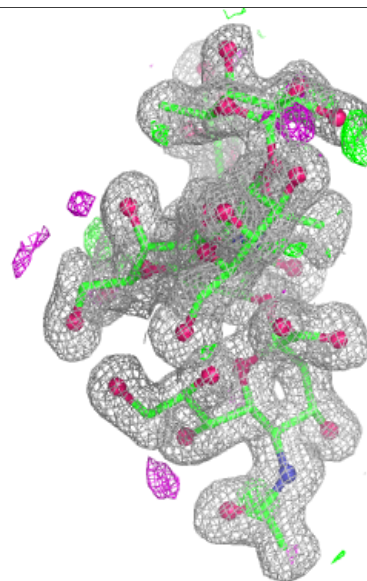
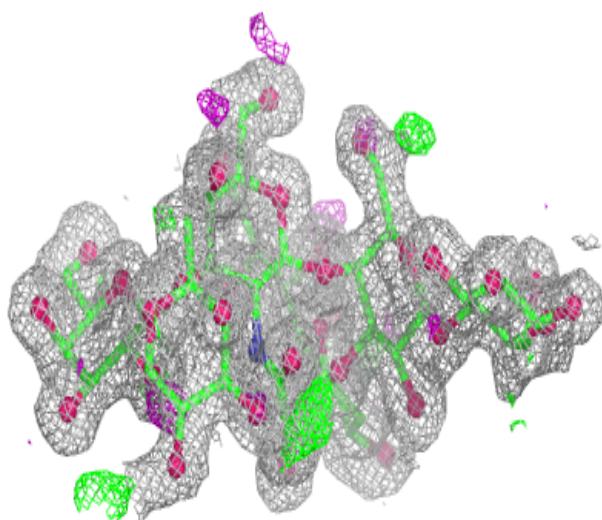
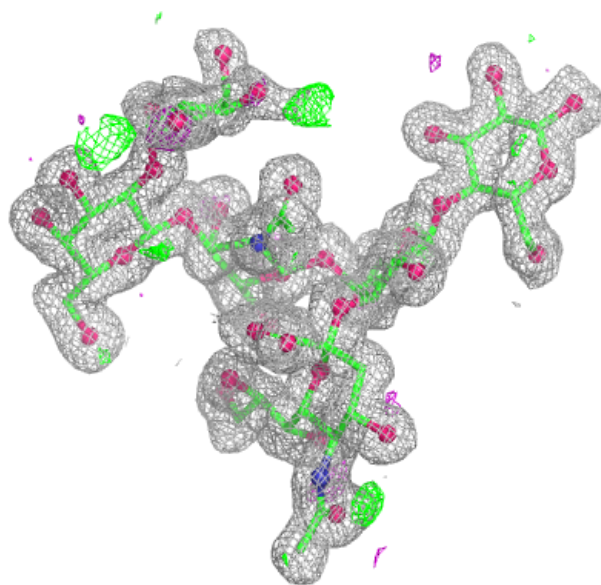
Electron density around Chain O:

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



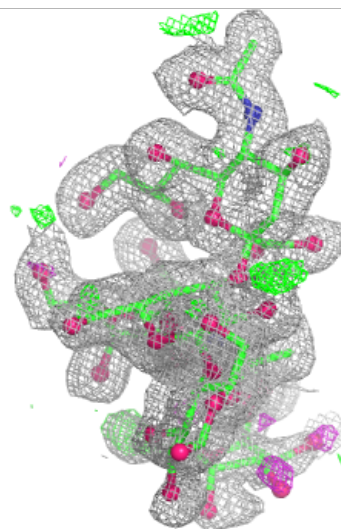
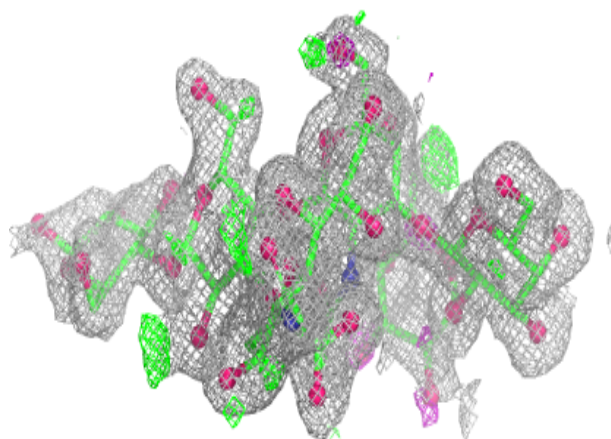
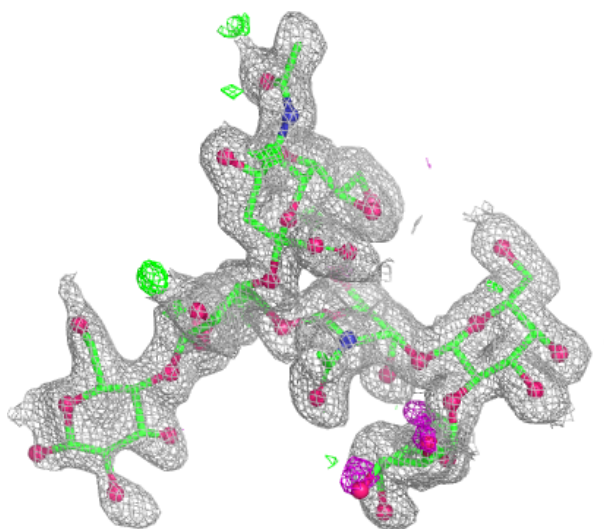
Electron density around Chain P:

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



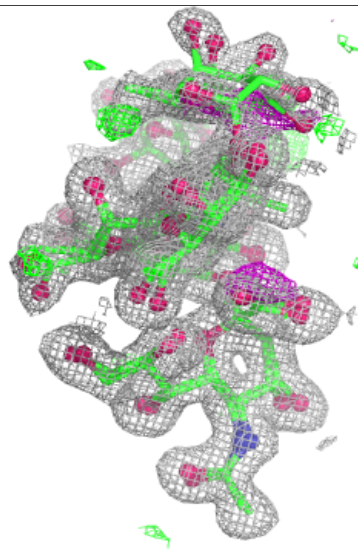
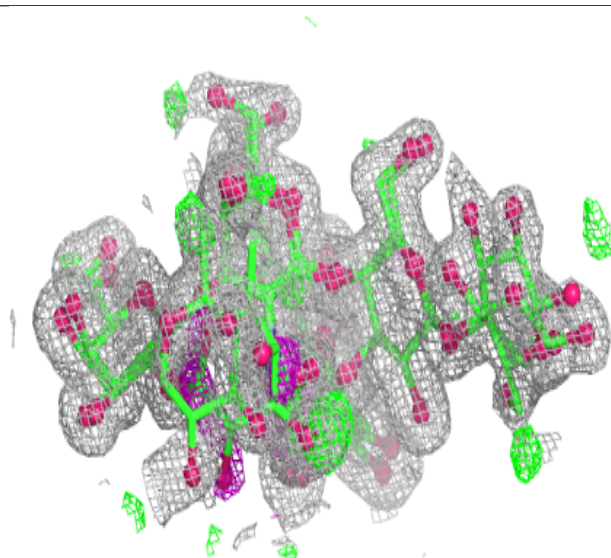
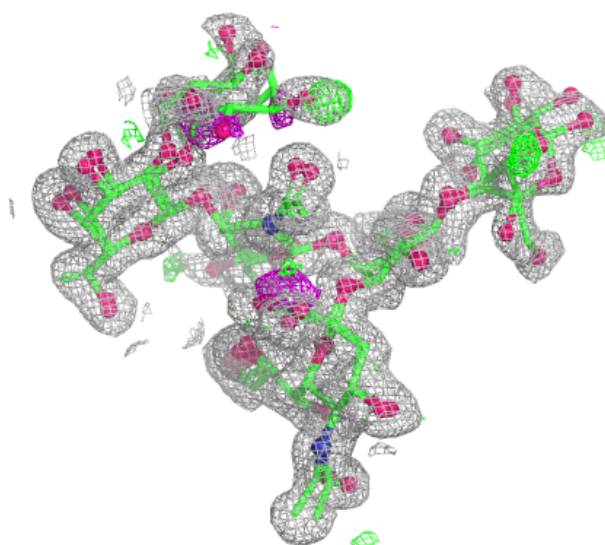
Electron density around Chain S:

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



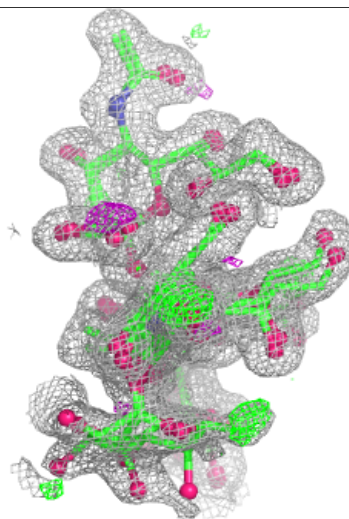
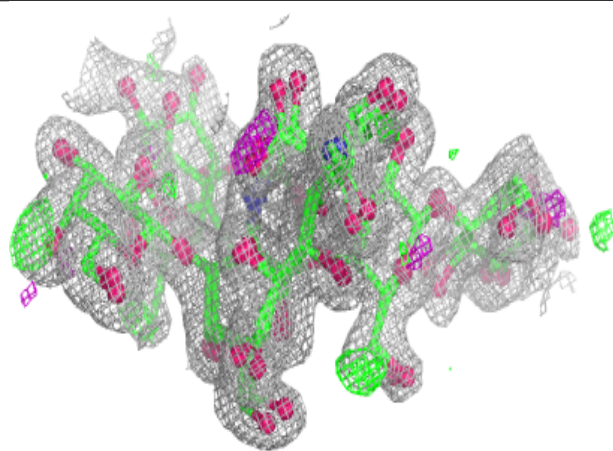
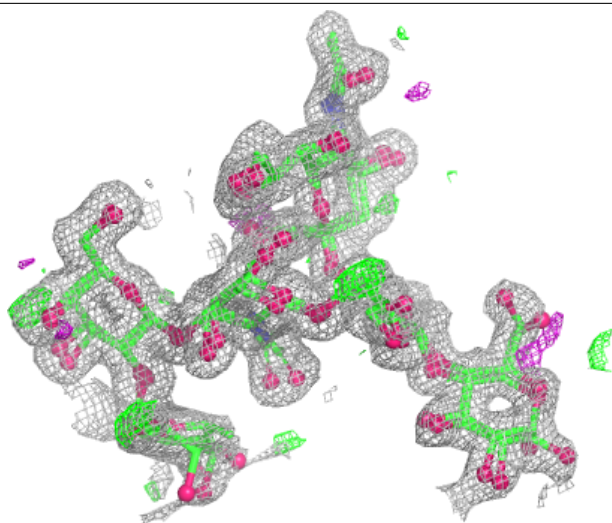
Electron density around Chain T:

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



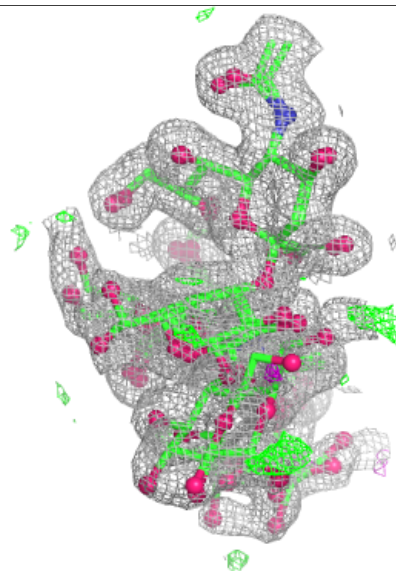
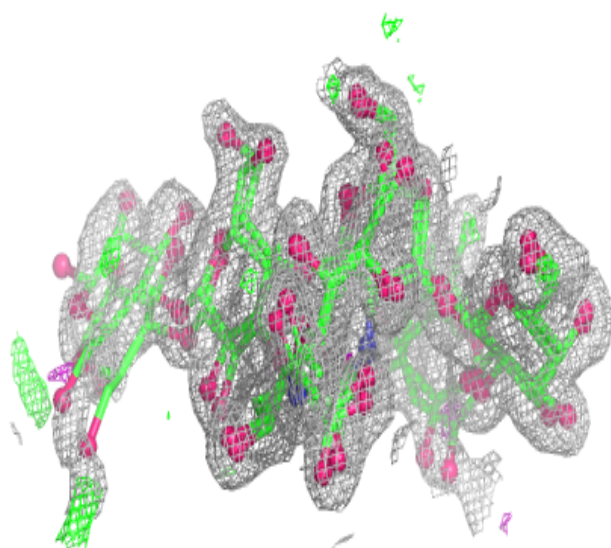
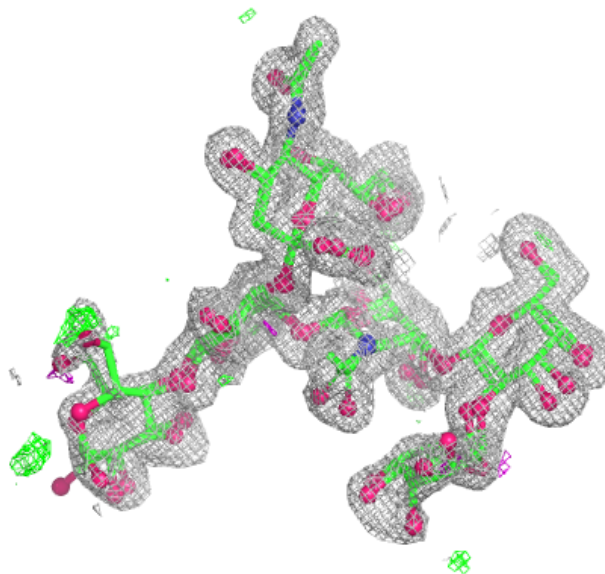
Electron density around Chain L:

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



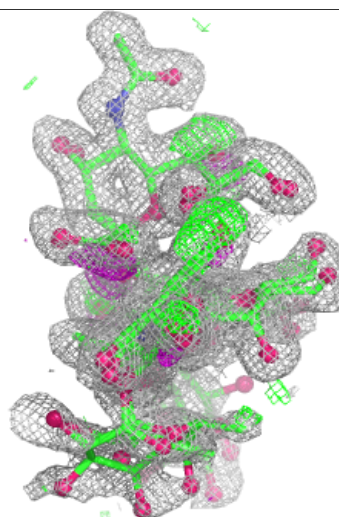
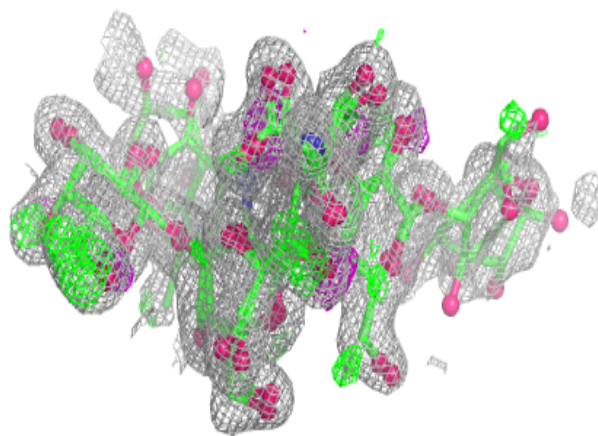
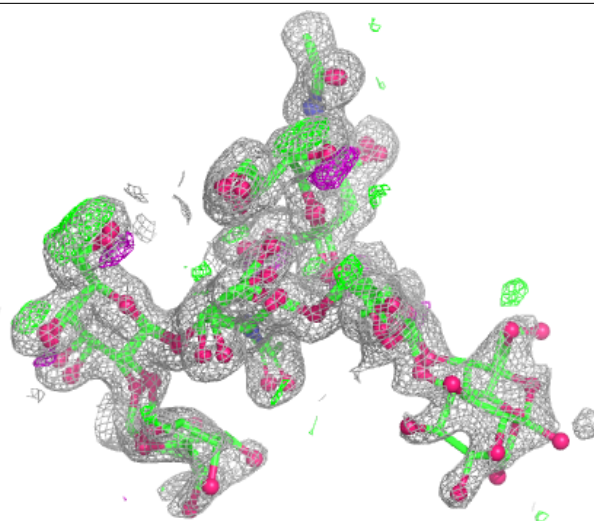
Electron density around Chain R:

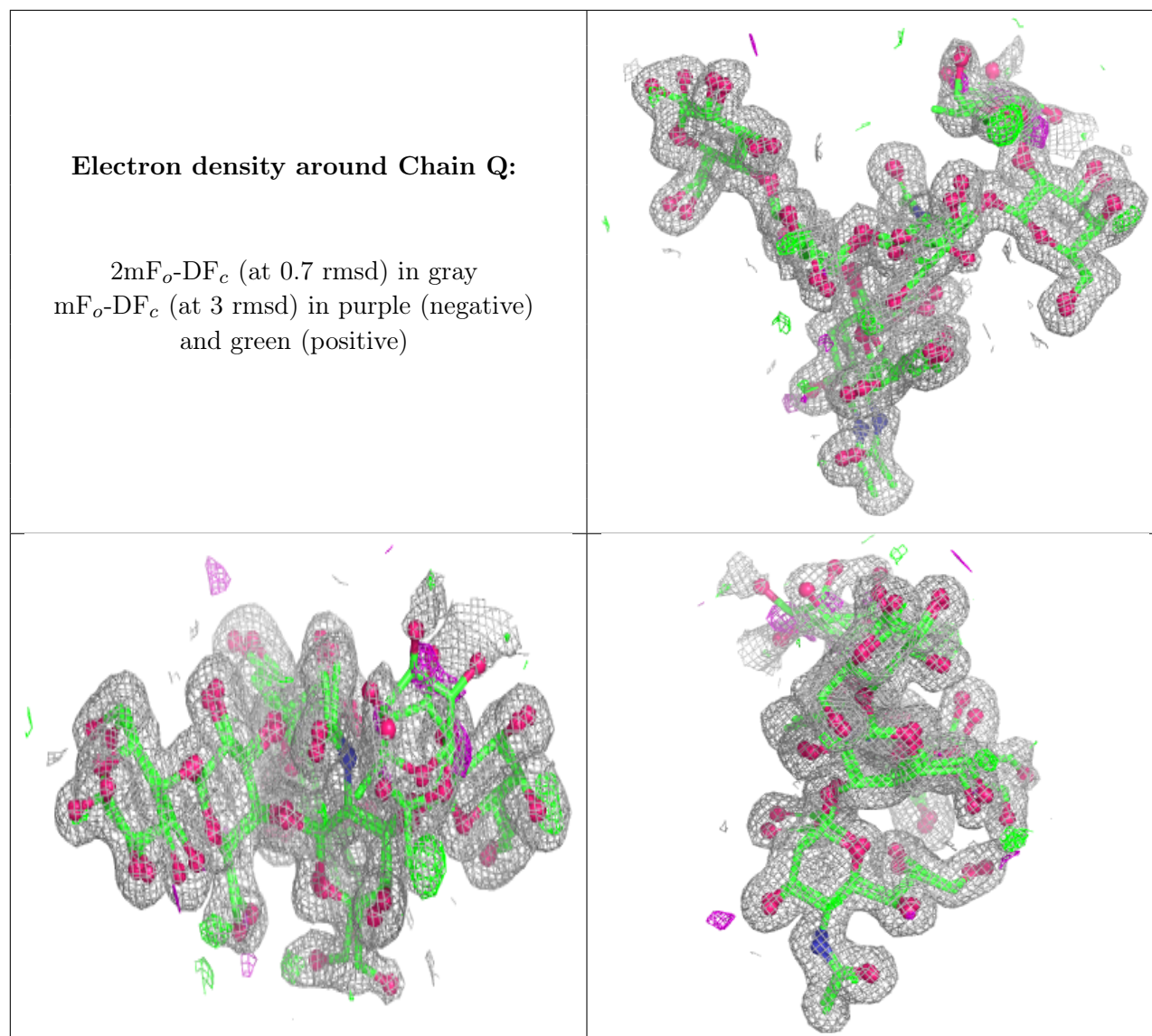
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	FUC	F	203	11/11	0.81	0.14	17,19,22,23	11
7	FUC	J	203	11/11	0.82	0.14	23,25,26,26	11
6	BCN	A	202	11/11	0.92	0.10	13,17,21,23	0
6	BCN	I	203	11/11	0.94	0.09	15,20,22,22	0
6	BCN	C	202	11/11	0.94	0.08	13,18,20,21	0
6	BCN	E	201	11/11	0.94	0.09	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	J	201	11/11	0.95	0.08	12,17,22,23	0
6	BCN	I	201	11/11	0.95	0.07	14,18,20,20	0
6	BCN	D	202	11/11	0.95	0.07	13,15,22,25	0
6	BCN	G	202	11/11	0.96	0.07	12,15,23,25	0
6	BCN	B	202	11/11	0.96	0.07	13,18,21,22	0
6	BCN	F	201	11/11	0.96	0.07	13,17,20,21	0
5	CA	F	202	1/1	0.98	0.04	10,10,10,10	0
5	CA	B	201	1/1	0.99	0.04	11,11,11,11	0
5	CA	H	201	1/1	0.99	0.03	11,11,11,11	0
5	CA	I	202	1/1	0.99	0.03	10,10,10,10	0
5	CA	D	201	1/1	0.99	0.03	11,11,11,11	0
5	CA	E	202	1/1	0.99	0.05	11,11,11,11	0
5	CA	G	201	1/1	1.00	0.02	10,10,10,10	0
5	CA	C	201	1/1	1.00	0.03	11,11,11,11	0
5	CA	A	201	1/1	1.00	0.03	10,10,10,10	0
5	CA	J	202	1/1	1.00	0.02	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.