



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:13 AM BST

PDB ID : 5ELC  
Title : Cholera toxin El Tor B-pentamer in complex with Lewis-y  
Authors : Heggelund, J.E.; Burschowsky, D.; Krengel, U.  
Deposited on : 2015-11-04  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

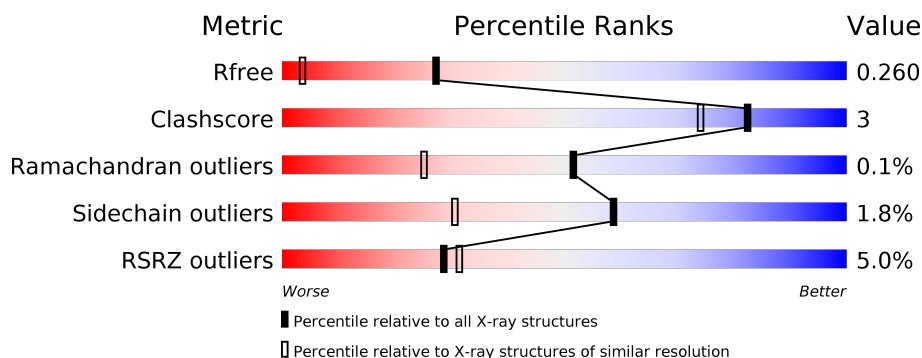
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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.



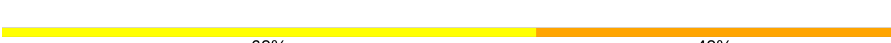
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>4%</div> <div>91%</div> <div>8%</div> </div>
1	B	103	<div> <div>3%</div> <div>93%</div> <div>7%</div> </div>
1	C	103	<div> <div>3%</div> <div>93%</div> <div>7%</div> </div>
1	D	103	<div> <div>5%</div> <div>95%</div> <div>5%</div> </div>
1	E	103	<div> <div>4%</div> <div>87%</div> <div>13%</div> </div>
1	F	103	<div> <div>10%</div> <div>93%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	103	
1	H	103	
1	I	103	
1	J	103	
2	K	4	
2	O	4	
2	Q	4	
2	S	4	
3	L	5	
3	M	5	
3	R	5	
4	N	4	
4	P	4	

## 2 Entry composition [i](#)

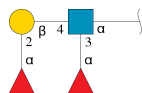
There are 8 unique types of molecules in this entry. The entry contains 9536 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			817	516	140	156	5			
1	B	103	Total	C	N	O	S	0	0	0
			817	516	140	156	5			
1	C	103	Total	C	N	O	S	0	1	0
			820	518	140	156	6			
1	D	103	Total	C	N	O	S	0	1	0
			823	521	141	156	5			
1	E	103	Total	C	N	O	S	0	1	0
			821	520	140	156	5			
1	F	103	Total	C	N	O	S	0	0	0
			817	516	140	156	5			
1	G	103	Total	C	N	O	S	0	0	0
			817	516	140	156	5			
1	H	103	Total	C	N	O	S	0	1	0
			823	520	141	157	5			
1	I	103	Total	C	N	O	S	0	2	0
			825	523	140	156	6			
1	J	103	Total	C	N	O	S	0	0	0
			817	516	140	156	5			

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



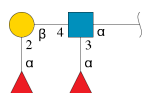
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	4	Total	C	N	O	0	0	0
			46	26	1	19			
2	O	4	Total	C	N	O	0	0	0
			46	26	1	19			

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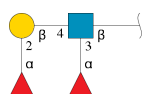
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	4	Total	C	N	O	0	0	0
			46	26	1	19			
2	S	4	Total	C	N	O	0	0	0
			46	26	1	19			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	L	4	Total	C	N	O	0	4	0
			92	52	2	38			
3	M	4	Total	C	N	O	0	4	0
			92	52	2	38			
3	R	4	Total	C	N	O	0	4	0
			92	52	2	38			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	N	4	Total	C	N	O	0	0	0
			46	26	1	19			
4	P	4	Total	C	N	O	0	0	0
			46	26	1	19			

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

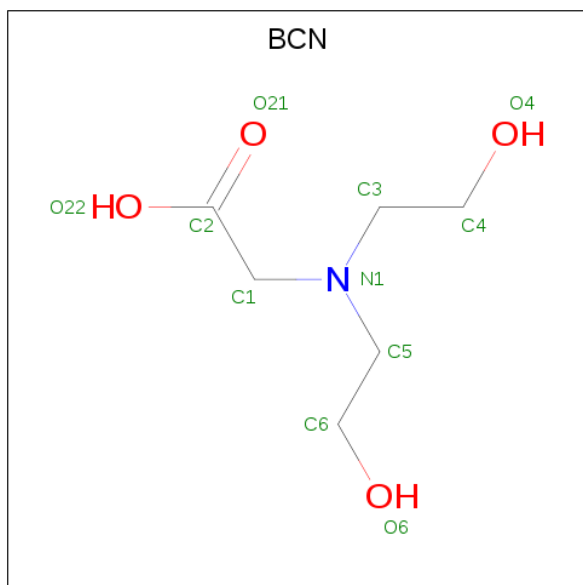
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	A	2	Total	Ca	0	0
			2	2		

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

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



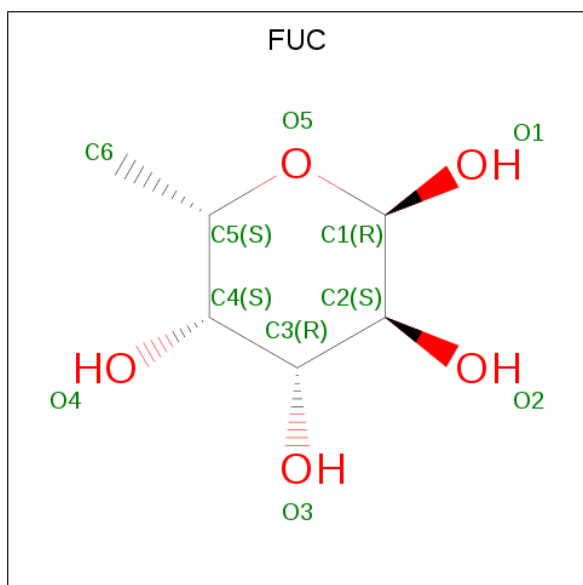
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			11	6	1	4		
6	A	1	Total	C	N	O	0	0
			11	6	1	4		
6	B	1	Total	C	N	O	0	0
			11	6	1	4		
6	B	1	Total	C	N	O	0	0
			11	6	1	4		
6	C	1	Total	C	N	O	0	0
			11	6	1	4		
6	C	1	Total	C	N	O	0	0
			11	6	1	4		
6	D	1	Total	C	N	O	0	0
			11	6	1	4		
6	D	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	62	Total	O	0	0
			62	62		
8	B	80	Total	O	0	0
			80	80		
8	C	77	Total	O	0	0
			77	77		
8	D	70	Total	O	0	0
			70	70		
8	E	64	Total	O	0	0
			64	64		
8	F	51	Total	O	0	1
			52	52		

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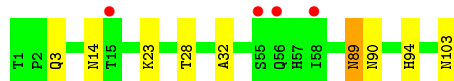
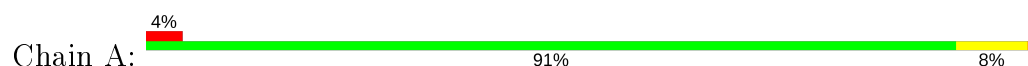
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	59	Total 59	O 59	0	0
8	H	60	Total 60	O 60	0	0
8	I	74	Total 75	O 75	0	1
8	J	57	Total 57	O 57	0	0



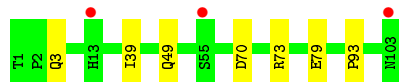
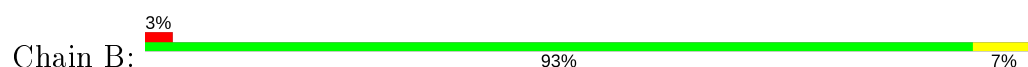
### 3 Residue-property plots [i](#)

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 subunit B



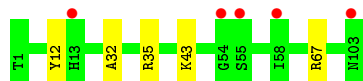
- Molecule 1: Cholera enterotoxin subunit B



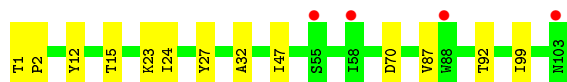
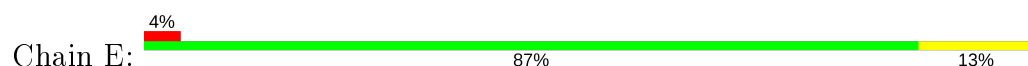
- Molecule 1: Cholera enterotoxin subunit B



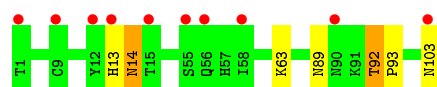
- Molecule 1: Cholera enterotoxin subunit B



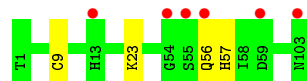
- Molecule 1: Cholera enterotoxin subunit B



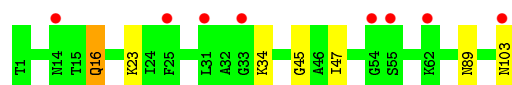
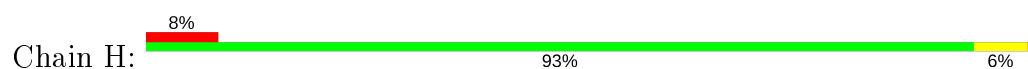
- Molecule 1: Cholera enterotoxin subunit B



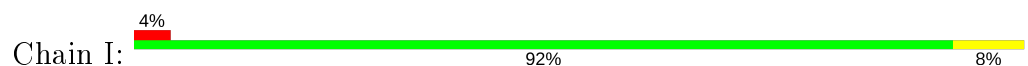
- Molecule 1: Cholera enterotoxin subunit B



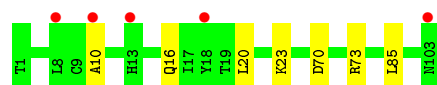
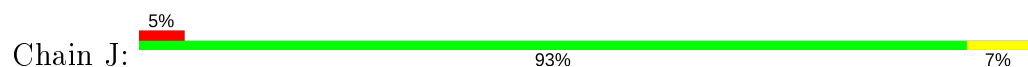
- Molecule 1: Cholera enterotoxin subunit B



- Molecule 1: Cholera enterotoxin subunit B



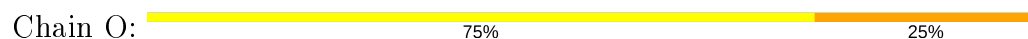
- Molecule 1: Cholera enterotoxin subunit B




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



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



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

Chain Q:  75% 25%

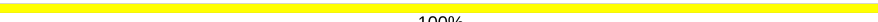
NDG1  
GAL2  
FUC3  
FUC4

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

Chain S:  100%

NDG1  
GAL2  
FUC3  
FUC4

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

Chain L:  100%

NDG1  
NAG1  
GAL2  
FUC3  
FUC4

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

Chain M:  60% 40%

NDG1  
NAG1  
GAL2  
FUC3  
FUC4

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

Chain R:  40% 60%

NDG1  
NAG1  
GAL2  
FUC3  
FUC4

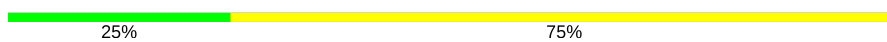
- Molecule 4: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  25% 75%

NAG1  
GAL2  
FUC3  
FUC4

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

Chain P:



HM1
GAL2
FUC3
FUC4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.67Å 80.92Å 95.77Å 90.00° 96.07° 90.00°	Depositor
Resolution (Å)	47.62 – 1.50 47.62 – 1.50	Depositor EDS
% Data completeness (in resolution range)	94.5 (47.62-1.50) 94.4 (47.62-1.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.221 , 0.260 0.224 , 0.260	Depositor DCC
$R_{free}$ test set	7329 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9536	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCN, NAG, CA, NDG, 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	0.70	0/831	0.90	0/1122
1	B	0.85	1/831 (0.1%)	0.95	4/1122 (0.4%)
1	C	0.84	0/837	0.96	3/1130 (0.3%)
1	D	0.69	0/840	0.89	1/1133 (0.1%)
1	E	0.69	0/838	0.88	0/1133
1	F	0.69	0/831	0.88	1/1122 (0.1%)
1	G	0.61	0/831	0.80	0/1122
1	H	0.73	0/840	0.84	0/1134
1	I	0.80	0/845	1.04	3/1141 (0.3%)
1	J	0.76	0/831	0.88	2/1122 (0.2%)
All	All	0.74	1/8355 (0.0%)	0.90	14/11281 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	GLU	CD-OE1	6.70	1.33	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	73	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	C	73	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	I	73	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	C	73	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	73	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	J	73	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	J	70	ASP	CB-CG-OD1	6.03	123.73	118.30
1	B	79	GLU	CG-CD-OE1	5.69	129.67	118.30
1	C	67	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	70	ASP	CB-CG-OD1	5.21	122.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	F	89	ASN	CB-CA-C	-5.12	100.16	110.40
1	D	35	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	I	70	ASP	CB-CG-OD1	5.03	122.83	118.30

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	817	0	823	8	0
1	B	817	0	823	5	0
1	C	820	0	828	3	0
1	D	823	0	836	3	0
1	E	821	0	832	11	0
1	F	817	0	823	2	0
1	G	817	0	823	1	0
1	H	823	0	831	8	0
1	I	825	0	839	3	0
1	J	817	0	823	2	0
2	K	46	0	39	2	0
2	O	46	0	39	1	0
2	Q	46	0	39	5	0
2	S	46	0	39	0	0
3	L	92	0	81	0	0
3	M	92	0	81	1	0
3	R	92	0	81	1	0
4	N	46	0	42	0	0
4	P	46	0	42	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	22	0	20	0	0
6	C	22	0	20	0	0
6	D	22	0	20	0	0
6	E	22	0	20	0	0
7	F	11	0	12	0	0
8	A	62	0	0	1	0
8	B	80	0	0	6	0
8	C	77	0	0	0	0
8	D	70	0	0	1	0
8	E	64	0	0	4	0
8	F	52	0	0	0	0
8	G	59	0	0	0	0
8	H	60	0	0	1	0
8	I	75	0	0	0	0
8	J	57	0	0	2	0
All	All	9536	0	8876	43	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:HG12	8:B:349:HOH:O	1.69	0.92
1:H:47:ILE:HD11	2:Q:1:NDG:H8C2	1.53	0.89
1:E:27:TYR:HB2	8:E:343:HOH:O	1.75	0.87
1:E:24:ILE:HG21	8:E:343:HOH:O	1.78	0.84
1:H:47:ILE:CD1	2:Q:1:NDG:H8C2	2.15	0.75
1:H:103:ASN:HA	8:H:350:HOH:O	1.93	0.68
1:E:92:THR:OG1	8:E:301:HOH:O	2.11	0.67
1:F:13:HIS:O	1:F:14:ASN:OD1	2.16	0.63
1:B:49:GLN:HB3	8:B:349:HOH:O	1.98	0.62
1:B:49:GLN:CB	8:B:349:HOH:O	2.51	0.59
1:C:74:ILE:HD13	8:D:361:HOH:O	2.06	0.55
1:J:23:LYS:NZ	8:J:301:HOH:O	2.40	0.54
1:A:3:GLN:CD	8:B:301:HOH:O	2.45	0.54
1:E:47:ILE:HD11	2:O:1:NDG:H8C2	1.90	0.54
1:H:47:ILE:CG1	2:Q:1:NDG:H8C2	2.38	0.54
1:C:103:ASN:HD21	1:H:23:LYS:HD3	1.74	0.52
1:A:3:GLN:NE2	8:B:301:HOH:O	2.42	0.52
3:R:1[A]:NDG:O4	3:R:4[A]:FUC:H5	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:2[A]:GAL:H61	3:M:4[A]:FUC:H3	1.95	0.49
1:I:83:GLU:HG2	1:I:84:LYS:HG3	1.94	0.49
1:I:88:TRP:CZ3	1:I:97:ALA:HB2	2.50	0.46
1:A:94:HIS:CE1	2:K:1:NDG:O1	2.68	0.46
1:G:56:GLN:OE1	1:G:57:HIS:ND1	2.49	0.46
1:D:67:ARG:NH1	1:E:70:ASP:OD1	2.44	0.46
1:D:12:TYR:CZ	1:E:32:ALA:HB1	2.51	0.46
1:H:16:GLN:NE2	1:H:89:ASN:HD22	2.15	0.45
1:A:103:ASN:ND2	8:A:303:HOH:O	2.50	0.45
1:A:32:ALA:HB1	1:E:12:TYR:CZ	2.51	0.45
1:F:92:THR:HA	1:F:93:PRO:C	2.37	0.44
1:E:15:THR:HA	1:E:87:VAL:O	2.18	0.43
1:J:20:LEU:HD11	1:J:85:LEU:HD12	2.00	0.43
1:B:93:PRO:HA	8:B:301:HOH:O	2.18	0.43
1:A:90:ASN:OD1	1:A:90:ASN:N	2.48	0.42
1:E:23:LYS:CE	8:E:302:HOH:O	2.68	0.41
1:H:45:GLY:O	2:Q:1:NDG:H8C1	2.19	0.41
1:C:12:TYR:CZ	1:D:32:ALA:HB1	2.54	0.41
1:E:1:THR:HG23	1:E:2:PRO:HD2	2.02	0.41
1:H:47:ILE:HG13	2:Q:1:NDG:H8C2	2.02	0.41
1:A:89:ASN:HB2	1:A:94:HIS:CE1	2.55	0.41
1:B:3:GLN:HB3	1:B:3:GLN:HE21	1.61	0.41
1:A:28:THR:HA	1:E:99:ILE:O	2.21	0.41
1:I:74[B]:ILE:CD1	8:J:354:HOH:O	2.69	0.40
2:K:1:NDG:H8C1	2:K:1:NDG:H2	1.73	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	101/103 (98%)	98 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	C	102/103 (99%)	100 (98%)	2 (2%)	0	100	100
1	D	102/103 (99%)	101 (99%)	1 (1%)	0	100	100
1	E	102/103 (99%)	100 (98%)	2 (2%)	0	100	100
1	F	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	G	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
1	H	102/103 (99%)	98 (96%)	4 (4%)	0	100	100
1	I	103/103 (100%)	100 (97%)	3 (3%)	0	100	100
1	J	101/103 (98%)	99 (98%)	1 (1%)	1 (1%)	15	3
All	All	1016/1030 (99%)	994 (98%)	21 (2%)	1 (0%)	51	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	10	ALA

### 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	89/89 (100%)	86 (97%)	3 (3%)	37	9
1	B	89/89 (100%)	89 (100%)	0	100	100
1	C	90/89 (101%)	87 (97%)	3 (3%)	38	10
1	D	90/89 (101%)	89 (99%)	1 (1%)	73	53
1	E	90/89 (101%)	90 (100%)	0	100	100
1	F	89/89 (100%)	85 (96%)	4 (4%)	27	5
1	G	89/89 (100%)	87 (98%)	2 (2%)	52	22
1	H	90/89 (101%)	88 (98%)	2 (2%)	52	22
1	I	91/89 (102%)	90 (99%)	1 (1%)	73	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	89/89 (100%)	88 (99%)	1 (1%)	73	53
All	All	896/890 (101%)	879 (98%)	17 (2%)	59	27

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	23	LYS
1	A	89	ASN
1	C	9[A]	CYS
1	C	9[B]	CYS
1	C	92	THR
1	D	43	LYS
1	F	14	ASN
1	F	63	LYS
1	F	92	THR
1	F	103	ASN
1	G	9	CYS
1	G	23	LYS
1	H	16	GLN
1	H	34	LYS
1	I	59	ASP
1	J	16	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	89	ASN
1	A	94	HIS
1	A	103	ASN
1	B	3	GLN
1	D	13	HIS
1	F	14	ASN
1	F	94	HIS
1	G	14	ASN
1	H	16	GLN
1	H	103	ASN
1	I	3	GLN

### 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 ⓘ

48 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	NDG	K	1	2	15,15,15	1.18	1 (6%)	21,21,21	1.39	3 (14%)
2	GAL	K	2	2	11,11,12	0.61	0	15,15,17	1.13	2 (13%)
2	FUC	K	3	2	10,10,11	1.67	2 (20%)	14,14,16	1.33	1 (7%)
2	FUC	K	4	2	10,10,11	0.63	0	14,14,16	0.74	0
3	NAG	L	1[B]	3	15,15,15	0.81	0	21,21,21	1.56	4 (19%)
3	NDG	L	1[A]	3	15,15,15	0.76	0	21,21,21	1.44	2 (9%)
3	GAL	L	2[A]	3	11,11,12	0.80	0	15,15,17	1.10	1 (6%)
3	GAL	L	2[B]	3	11,11,12	0.77	0	15,15,17	1.35	1 (6%)
3	FUC	L	3[A]	3	10,10,11	0.77	0	14,14,16	1.03	1 (7%)
3	FUC	L	3[B]	3	10,10,11	0.76	0	14,14,16	0.98	1 (7%)
3	FUC	L	4[A]	3	10,10,11	0.89	0	14,14,16	1.50	3 (21%)
3	FUC	L	4[B]	3	10,10,11	0.77	0	14,14,16	1.87	4 (28%)
3	NAG	M	1[B]	3	15,15,15	0.72	0	21,21,21	1.12	1 (4%)
3	NDG	M	1[A]	3	15,15,15	1.30	2 (13%)	21,21,21	1.74	4 (19%)
3	GAL	M	2[A]	3	11,11,12	0.81	0	15,15,17	1.32	1 (6%)
3	GAL	M	2[B]	3	11,11,12	0.79	0	15,15,17	2.12	2 (13%)
3	FUC	M	3[A]	3	10,10,11	1.07	1 (10%)	14,14,16	0.84	0
3	FUC	M	3[B]	3	10,10,11	0.95	0	14,14,16	0.89	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUC	M	4[A]	3	10,10,11	0.59	0	14,14,16	1.26	2 (14%)
3	FUC	M	4[B]	3	10,10,11	0.57	0	14,14,16	1.11	1 (7%)
4	NAG	N	1	4	15,15,15	1.11	1 (6%)	21,21,21	1.37	4 (19%)
4	GAL	N	2	4	11,11,12	1.56	1 (9%)	15,15,17	1.97	4 (26%)
4	FUC	N	3	4	10,10,11	1.39	1 (10%)	14,14,16	0.88	0
4	FUC	N	4	4	10,10,11	1.02	0	14,14,16	0.89	0
2	NDG	O	1	2	15,15,15	1.48	2 (13%)	21,21,21	1.89	3 (14%)
2	GAL	O	2	2	11,11,12	0.66	0	15,15,17	1.82	3 (20%)
2	FUC	O	3	2	10,10,11	0.91	0	14,14,16	0.90	1 (7%)
2	FUC	O	4	2	10,10,11	1.00	1 (10%)	14,14,16	0.99	1 (7%)
4	NAG	P	1	4	15,15,15	1.52	3 (20%)	21,21,21	2.13	7 (33%)
4	GAL	P	2	4	11,11,12	0.70	0	15,15,17	1.05	0
4	FUC	P	3	4	10,10,11	1.37	1 (10%)	14,14,16	1.29	3 (21%)
4	FUC	P	4	4	10,10,11	1.09	1 (10%)	14,14,16	0.98	0
2	NDG	Q	1	2	15,15,15	1.27	1 (6%)	21,21,21	2.59	7 (33%)
2	GAL	Q	2	2	11,11,12	1.63	3 (27%)	15,15,17	1.99	5 (33%)
2	FUC	Q	3	2	10,10,11	0.82	1 (10%)	14,14,16	1.27	1 (7%)
2	FUC	Q	4	2	10,10,11	1.34	2 (20%)	14,14,16	0.98	1 (7%)
3	NAG	R	1[B]	3	15,15,15	1.20	1 (6%)	21,21,21	1.72	5 (23%)
3	NDG	R	1[A]	3	15,15,15	0.81	0	21,21,21	1.06	1 (4%)
3	GAL	R	2[A]	3	11,11,12	0.56	0	15,15,17	1.52	3 (20%)
3	GAL	R	2[B]	3	11,11,12	0.94	0	15,15,17	1.27	1 (6%)
3	FUC	R	3[A]	3	10,10,11	0.88	0	14,14,16	1.18	2 (14%)
3	FUC	R	3[B]	3	10,10,11	0.89	0	14,14,16	0.88	0
3	FUC	R	4[A]	3	10,10,11	0.72	0	14,14,16	1.86	3 (21%)
3	FUC	R	4[B]	3	10,10,11	1.23	1 (10%)	14,14,16	1.23	1 (7%)
2	NDG	S	1	2	15,15,15	1.16	3 (20%)	21,21,21	2.01	5 (23%)
2	GAL	S	2	2	11,11,12	1.23	1 (9%)	15,15,17	1.63	3 (20%)
2	FUC	S	3	2	10,10,11	1.32	2 (20%)	14,14,16	0.68	0
2	FUC	S	4	2	10,10,11	0.84	1 (10%)	14,14,16	0.77	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	NDG	K	1	2	-	2/6/26/26	0/1/1/1
2	GAL	K	2	2	-	2/2/19/22	0/1/1/1
2	FUC	K	3	2	-	-	0/1/1/1
2	FUC	K	4	2	-	-	0/1/1/1
3	NAG	L	1[B]	3	-	0/6/26/26	0/1/1/1
3	NDG	L	1[A]	3	-	0/6/26/26	0/1/1/1
3	GAL	L	2[A]	3	-	0/2/19/22	0/1/1/1
3	GAL	L	2[B]	3	-	0/2/19/22	0/1/1/1
3	FUC	L	3[A]	3	-	-	0/1/1/1
3	FUC	L	3[B]	3	-	-	0/1/1/1
3	FUC	L	4[A]	3	-	-	0/1/1/1
3	FUC	L	4[B]	3	-	-	0/1/1/1
3	NAG	M	1[B]	3	-	0/6/26/26	0/1/1/1
3	NDG	M	1[A]	3	-	2/6/26/26	0/1/1/1
3	GAL	M	2[A]	3	-	0/2/19/22	0/1/1/1
3	GAL	M	2[B]	3	-	2/2/19/22	0/1/1/1
3	FUC	M	3[A]	3	-	-	0/1/1/1
3	FUC	M	3[B]	3	-	-	0/1/1/1
3	FUC	M	4[A]	3	-	-	0/1/1/1
3	FUC	M	4[B]	3	-	-	0/1/1/1
4	NAG	N	1	4	-	0/6/26/26	0/1/1/1
4	GAL	N	2	4	-	0/2/19/22	0/1/1/1
4	FUC	N	3	4	-	-	0/1/1/1
4	FUC	N	4	4	-	-	0/1/1/1
2	NDG	O	1	2	-	2/6/26/26	0/1/1/1
2	GAL	O	2	2	-	1/2/19/22	0/1/1/1
2	FUC	O	3	2	-	-	0/1/1/1
2	FUC	O	4	2	-	-	0/1/1/1
4	NAG	P	1	4	-	2/6/26/26	0/1/1/1
4	GAL	P	2	4	-	0/2/19/22	0/1/1/1
4	FUC	P	3	4	-	-	0/1/1/1
4	FUC	P	4	4	-	-	0/1/1/1
2	NDG	Q	1	2	-	1/6/26/26	0/1/1/1
2	GAL	Q	2	2	-	2/2/19/22	0/1/1/1
2	FUC	Q	3	2	-	-	0/1/1/1
2	FUC	Q	4	2	-	-	0/1/1/1
3	NAG	R	1[B]	3	-	0/6/26/26	0/1/1/1
3	NDG	R	1[A]	3	-	0/6/26/26	0/1/1/1
3	GAL	R	2[A]	3	-	0/2/19/22	0/1/1/1
3	GAL	R	2[B]	3	-	0/2/19/22	0/1/1/1
3	FUC	R	3[A]	3	-	-	0/1/1/1
3	FUC	R	3[B]	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	R	4[A]	3	-	-	0/1/1/1
3	FUC	R	4[B]	3	-	-	0/1/1/1
2	NDG	S	1	2	-	2/6/26/26	0/1/1/1
2	GAL	S	2	2	-	0/2/19/22	0/1/1/1
2	FUC	S	3	2	-	-	0/1/1/1
2	FUC	S	4	2	-	-	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	2	GAL	O5-C1	3.95	1.50	1.43
4	P	3	FUC	O5-C1	-3.90	1.37	1.43
2	Q	2	GAL	C2-C3	3.80	1.58	1.52
2	O	1	NDG	C1-C2	-3.54	1.48	1.52
4	P	1	NAG	C3-C2	3.39	1.59	1.53
2	K	3	FUC	C2-C3	3.04	1.57	1.52
4	P	4	FUC	O5-C1	2.98	1.48	1.43
3	M	1[A]	NDG	C3-C2	2.93	1.58	1.53
4	N	3	FUC	O5-C5	2.87	1.49	1.43
4	N	1	NAG	C1-C2	-2.83	1.49	1.52
2	S	2	GAL	O5-C5	2.82	1.49	1.43
2	Q	2	GAL	C4-C3	2.74	1.59	1.52
3	R	4[B]	FUC	O5-C1	2.73	1.48	1.43
2	Q	1	NDG	C3-C2	-2.64	1.48	1.53
2	K	3	FUC	O4-C4	2.48	1.48	1.43
2	O	1	NDG	C4-C3	2.46	1.58	1.52
2	Q	4	FUC	O4-C4	2.44	1.48	1.43
4	P	1	NAG	O5-C5	-2.32	1.38	1.44
2	S	1	NDG	C8-C7	2.31	1.55	1.50
2	Q	2	GAL	O2-C2	2.28	1.48	1.43
2	O	4	FUC	C4-C3	2.25	1.58	1.52
3	R	1[B]	NAG	O1-C1	2.15	1.46	1.39
3	M	1[A]	NDG	C4-C5	-2.12	1.48	1.53
2	S	3	FUC	O5-C5	2.12	1.48	1.43
2	S	3	FUC	O5-C1	-2.11	1.40	1.43
4	P	1	NAG	C4-C3	-2.10	1.47	1.52
3	M	3[A]	FUC	O4-C4	2.10	1.47	1.43
2	Q	4	FUC	C2-C3	2.05	1.55	1.52
2	K	1	NDG	C8-C7	2.05	1.54	1.50
2	S	4	FUC	O5-C1	2.03	1.47	1.43
2	S	1	NDG	C3-C2	2.03	1.57	1.53
2	S	1	NDG	O4-C4	2.02	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	3	FUC	O5-C1	2.02	1.46	1.43

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	1	NDG	C1-C2-N2	-8.99	100.31	110.73
2	O	1	NDG	C1-C2-N2	-6.19	103.56	110.73
3	M	2[B]	GAL	C1-O5-C5	-5.83	104.29	112.19
4	N	2	GAL	O5-C5-C6	5.57	115.94	107.20
2	S	1	NDG	O5-C1-C2	5.39	114.94	109.52
2	O	2	GAL	O5-C5-C6	5.31	115.53	107.20
3	M	1[A]	NDG	C1-C2-N2	-5.23	104.67	110.73
2	Q	2	GAL	C1-O5-C5	-4.89	105.57	112.19
3	R	1[B]	NAG	C1-C2-N2	-4.66	105.33	110.73
4	P	1	NAG	C1-C2-N2	-4.65	105.35	110.73
3	L	1[A]	NDG	C1-C2-N2	-4.59	105.41	110.73
2	S	1	NDG	C1-C2-C3	4.41	116.56	110.54
4	P	1	NAG	O5-C1-C2	4.32	113.85	109.52
2	S	2	GAL	O5-C5-C6	4.27	113.90	107.20
3	L	1[B]	NAG	C1-O5-C5	-4.14	105.86	113.66
3	L	4[B]	FUC	C6-C5-C4	-3.91	105.85	113.07
3	M	1[A]	NDG	C1-O5-C5	-3.90	106.31	113.66
3	R	4[A]	FUC	C1-O5-C5	-3.87	104.01	112.78
3	M	2[B]	GAL	O5-C5-C6	3.86	113.26	107.20
3	R	2[A]	GAL	C1-O5-C5	-3.74	107.12	112.19
2	Q	1	NDG	C8-C7-N2	-3.61	109.99	116.10
3	M	2[A]	GAL	C1-O5-C5	3.54	116.99	112.19
2	K	3	FUC	O5-C5-C4	3.50	115.79	109.52
3	R	4[A]	FUC	C1-C2-C3	-3.41	105.48	109.67
2	S	1	NDG	C1-C2-N2	-3.37	106.83	110.73
4	P	1	NAG	C3-C2-N2	-3.33	104.34	110.62
3	L	1[B]	NAG	C1-C2-N2	-3.32	106.88	110.73
2	Q	1	NDG	O4-C4-C3	-3.32	102.68	110.35
4	P	1	NAG	C1-C2-C3	3.27	115.01	110.54
4	N	1	NAG	C1-C2-N2	-3.23	106.98	110.73
3	L	4[B]	FUC	O5-C5-C6	3.22	114.25	107.33
2	O	1	NDG	C1-O5-C5	-3.16	107.71	113.66
2	K	1	NDG	O5-C1-C2	-3.10	106.40	109.52
2	O	1	NDG	O5-C1-C2	-3.10	106.40	109.52
2	S	1	NDG	C4-C3-C2	2.94	114.66	110.34
2	K	2	GAL	O5-C5-C6	-2.94	102.60	107.20
2	Q	1	NDG	O7-C7-N2	2.93	127.34	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	4[A]	FUC	O3-C3-C2	2.93	115.60	109.99
3	L	2[B]	GAL	O5-C5-C6	2.92	111.79	107.20
3	R	1[B]	NAG	O5-C1-C2	2.88	112.41	109.52
3	M	1[B]	NAG	O4-C4-C3	-2.83	103.80	110.35
4	N	1	NAG	C1-O5-C5	-2.83	108.32	113.66
4	P	1	NAG	O5-C5-C6	-2.75	99.59	106.44
3	R	2[B]	GAL	C1-C2-C3	2.67	112.94	109.67
3	M	1[A]	NDG	O5-C1-C2	2.66	112.18	109.52
3	R	4[B]	FUC	O5-C1-C2	-2.62	106.73	110.77
2	Q	2	GAL	O5-C5-C4	-2.59	104.53	110.83
3	L	1[B]	NAG	O5-C5-C4	-2.57	105.03	109.69
2	Q	2	GAL	C6-C5-C4	2.55	118.98	113.00
3	L	4[B]	FUC	O3-C3-C2	2.53	114.83	109.99
3	R	3[A]	FUC	C1-O5-C5	-2.52	107.06	112.78
3	L	4[A]	FUC	C6-C5-C4	-2.51	108.42	113.07
4	P	3	FUC	O2-C2-C3	-2.51	105.12	110.14
3	R	1[B]	NAG	O3-C3-C4	-2.45	104.68	110.35
2	Q	2	GAL	O5-C1-C2	2.44	114.54	110.77
3	R	1[B]	NAG	C1-O5-C5	-2.44	109.06	113.66
3	M	4[B]	FUC	C6-C5-C4	-2.42	108.59	113.07
3	M	4[A]	FUC	C2-C3-C4	-2.40	106.73	110.89
2	Q	1	NDG	O5-C5-C6	-2.40	100.46	106.44
2	S	2	GAL	C6-C5-C4	-2.40	107.39	113.00
4	N	1	NAG	O1-C1-O5	-2.38	103.24	110.38
4	P	1	NAG	C4-C3-C2	2.38	113.82	110.34
3	R	4[A]	FUC	O5-C1-C2	-2.36	107.14	110.77
2	Q	3	FUC	O5-C5-C4	2.33	113.70	109.52
4	N	2	GAL	O2-C2-C3	2.33	114.81	110.14
2	Q	1	NDG	C3-C4-C5	2.33	114.39	110.24
3	R	2[A]	GAL	C1-C2-C3	2.31	112.51	109.67
3	L	2[A]	GAL	O6-C6-C5	-2.31	103.35	111.29
3	R	1[A]	NDG	O5-C1-C2	2.27	111.80	109.52
3	R	1[B]	NAG	O4-C4-C3	-2.27	105.09	110.35
2	Q	4	FUC	O4-C4-C5	2.27	114.69	109.67
3	M	3[B]	FUC	C1-C2-C3	-2.25	106.90	109.67
2	K	2	GAL	C1-C2-C3	-2.24	106.91	109.67
4	N	2	GAL	O2-C2-C1	-2.23	104.59	109.15
2	S	2	GAL	C1-O5-C5	2.23	115.21	112.19
4	N	2	GAL	C6-C5-C4	-2.22	107.80	113.00
2	S	1	NDG	C3-C2-N2	-2.22	106.42	110.62
2	O	2	GAL	O6-C6-C5	-2.21	103.70	111.29
3	M	1[A]	NDG	O3-C3-C2	2.20	114.09	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NDG	O4-C4-C3	-2.19	105.29	110.35
3	R	2[A]	GAL	O6-C6-C5	-2.18	103.83	111.29
2	Q	2	GAL	C2-C3-C4	2.17	114.64	110.89
3	L	3[B]	FUC	O3-C3-C2	-2.16	105.85	109.99
2	K	1	NDG	O5-C5-C4	2.13	113.56	109.69
2	O	4	FUC	O2-C2-C1	-2.12	104.82	109.15
3	L	1[B]	NAG	O3-C3-C4	-2.12	105.46	110.35
4	P	3	FUC	O5-C5-C6	2.10	111.84	107.33
3	R	3[A]	FUC	C6-C5-C4	-2.07	109.25	113.07
4	N	1	NAG	O7-C7-N2	2.07	125.75	121.95
2	O	2	GAL	O5-C1-C2	2.05	113.94	110.77
3	L	4[A]	FUC	O5-C5-C4	2.05	113.20	109.52
2	O	3	FUC	C3-C4-C5	-2.05	106.58	109.77
3	M	4[A]	FUC	C6-C5-C4	-2.05	109.29	113.07
3	L	1[A]	NDG	O7-C7-N2	2.03	125.69	121.95
3	L	4[B]	FUC	C1-O5-C5	-2.03	108.18	112.78
4	P	1	NAG	O4-C4-C3	-2.02	105.67	110.35
2	Q	1	NDG	C1-O5-C5	-2.02	109.85	113.66
4	P	3	FUC	C1-O5-C5	2.01	117.34	112.78
3	L	3[A]	FUC	C6-C5-C4	-2.01	109.36	113.07

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	2	GAL	O5-C5-C6-O6
2	K	2	GAL	O5-C5-C6-O6
2	K	2	GAL	C4-C5-C6-O6
2	Q	2	GAL	C4-C5-C6-O6
2	K	1	NDG	C8-C7-N2-C2
2	K	1	NDG	O7-C7-N2-C2
4	P	1	NAG	C8-C7-N2-C2
4	P	1	NAG	O7-C7-N2-C2
2	S	1	NDG	C8-C7-N2-C2
2	S	1	NDG	O7-C7-N2-C2
3	M	1[A]	NDG	O5-C5-C6-O6
3	M	1[A]	NDG	C4-C5-C6-O6
2	Q	1	NDG	O5-C5-C6-O6
3	M	2[B]	GAL	C4-C5-C6-O6
2	O	1	NDG	O5-C5-C6-O6
2	O	1	NDG	C4-C5-C6-O6
2	O	2	GAL	C4-C5-C6-O6

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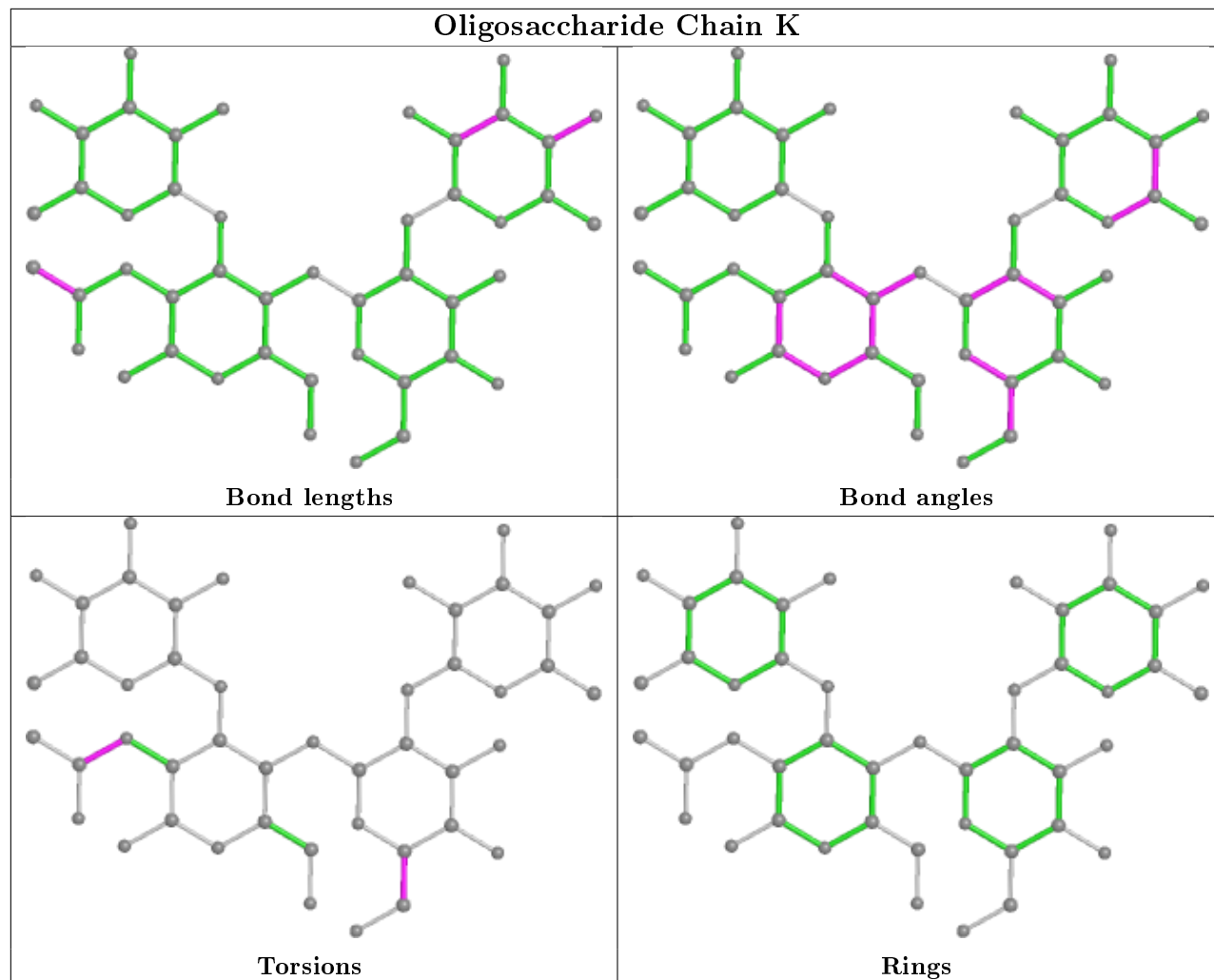
Mol	Chain	Res	Type	Atoms
3	M	2[B]	GAL	O5-C5-C6-O6

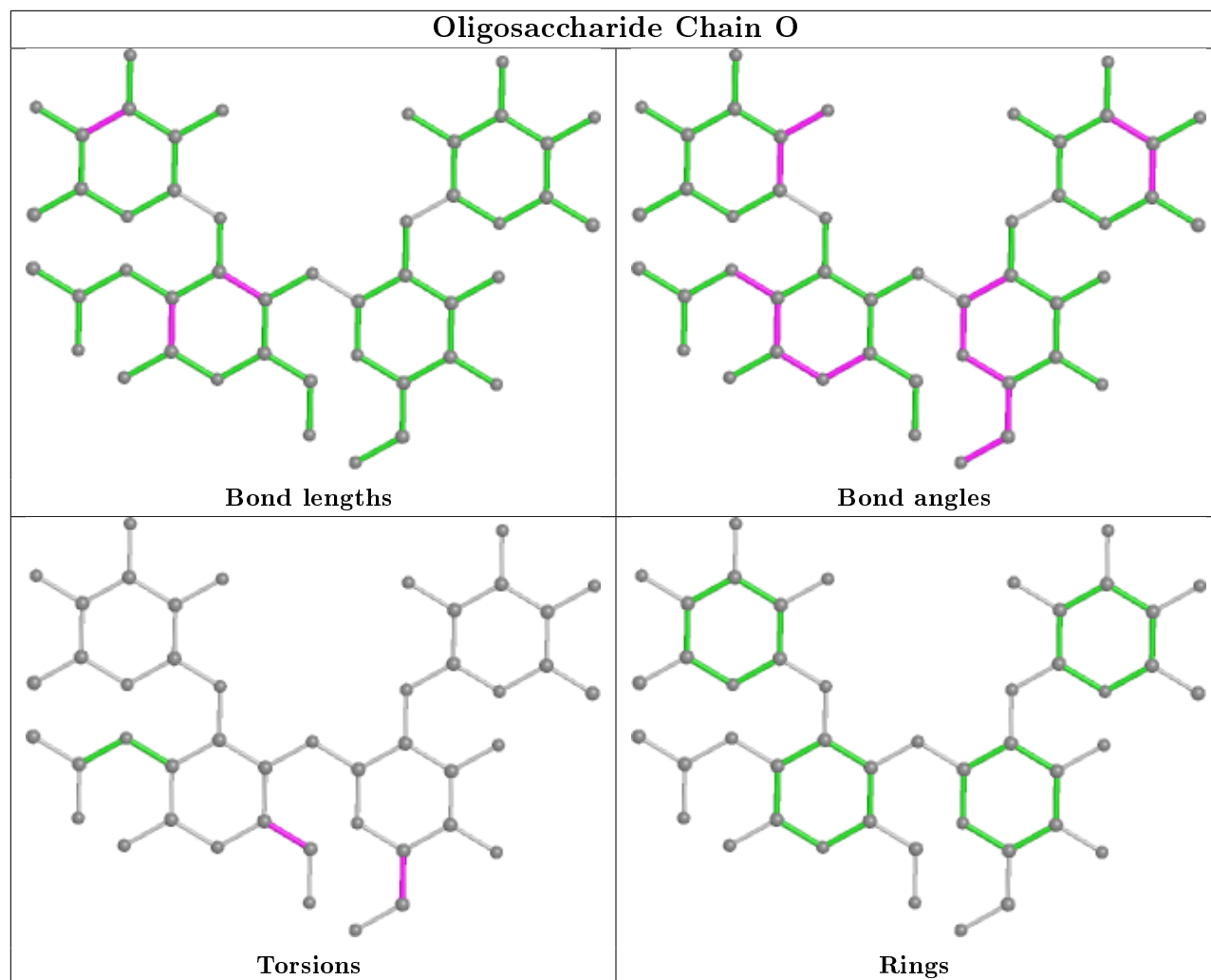
There are no ring outliers.

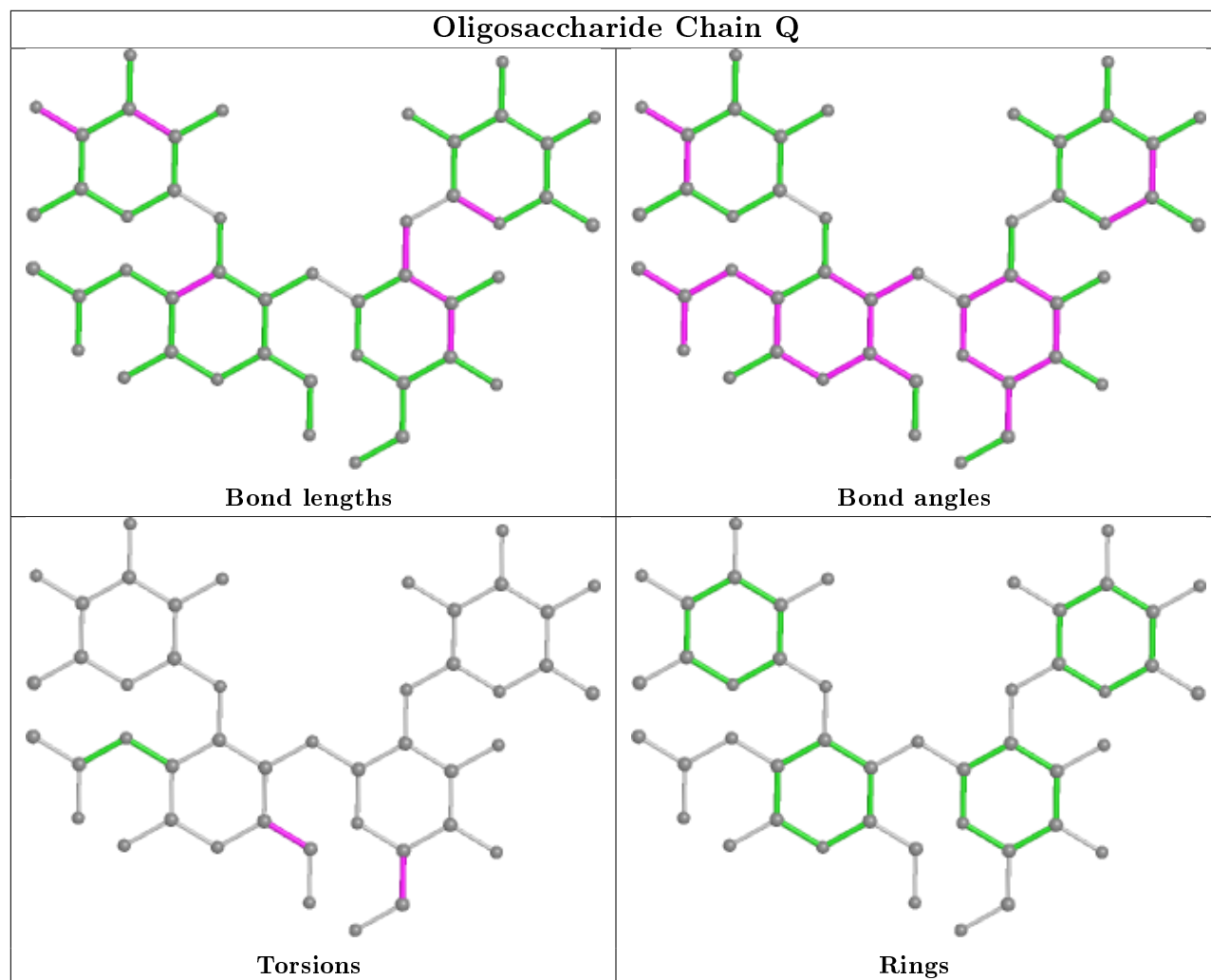
7 monomers are involved in 10 short contacts:

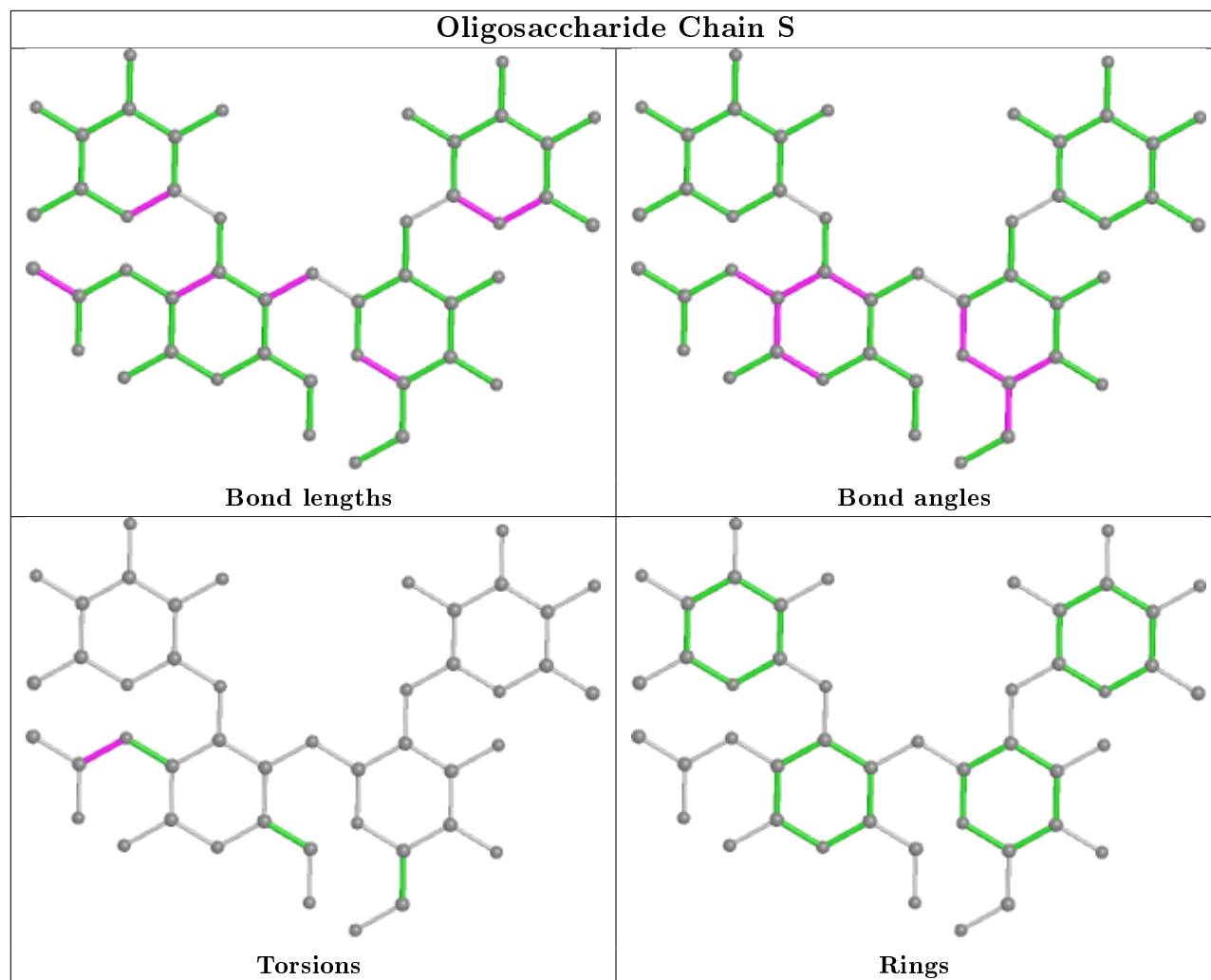
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	NDG	2	0
2	Q	1	NDG	5	0
2	O	1	NDG	1	0
3	R	4[A]	FUC	1	0
3	M	2[A]	GAL	1	0
3	M	4[A]	FUC	1	0
3	R	1[A]	NDG	1	0

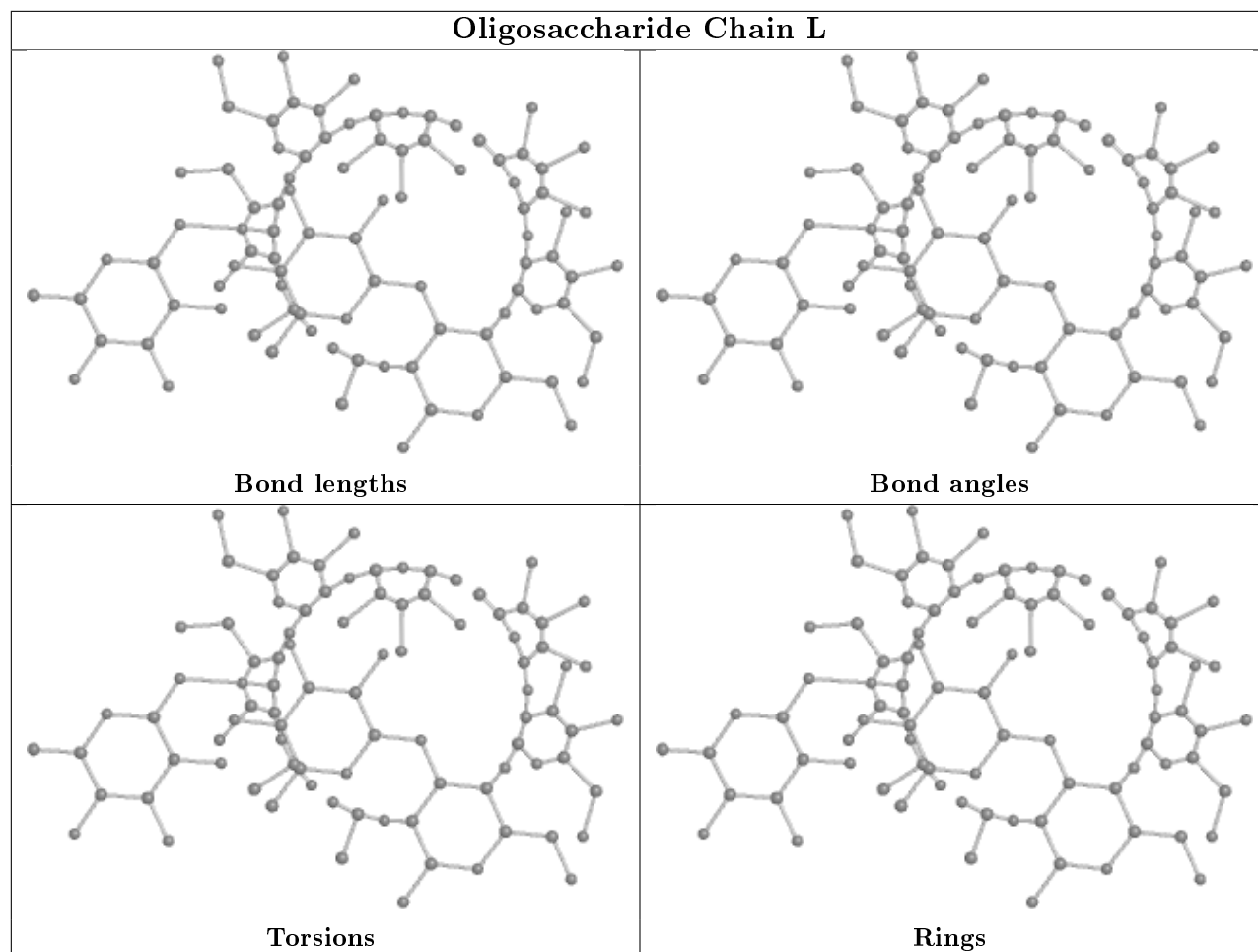
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

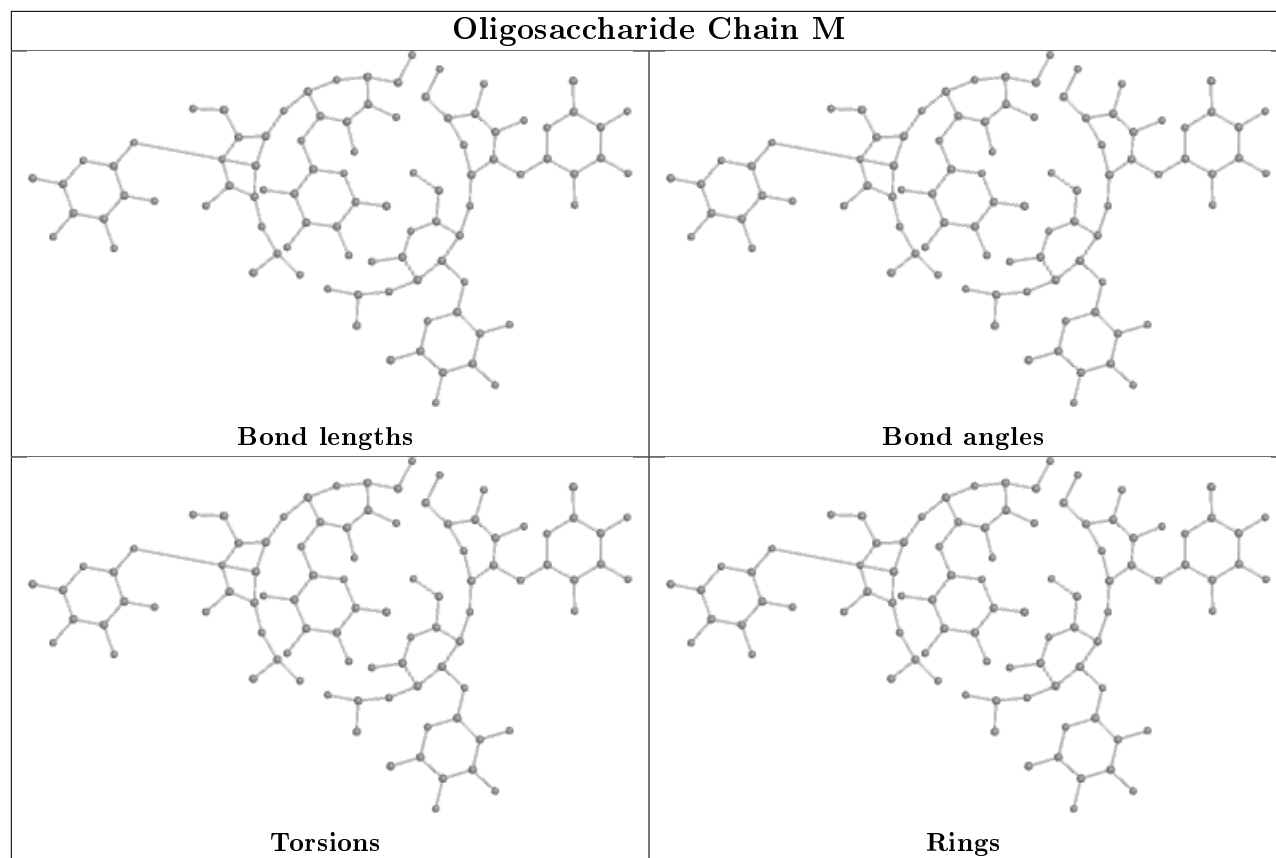






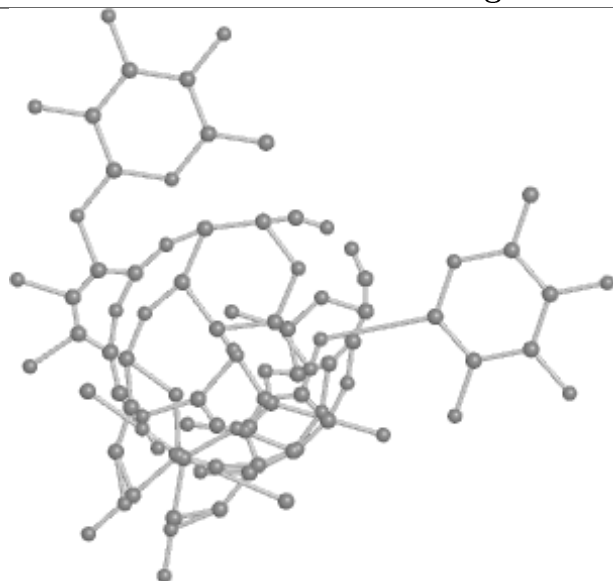




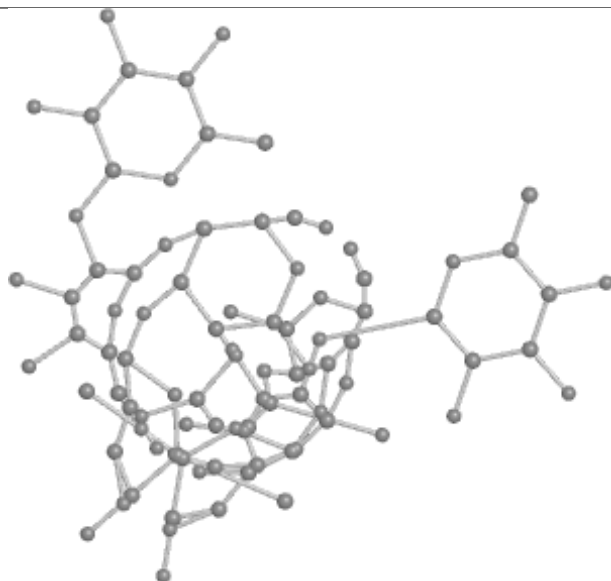




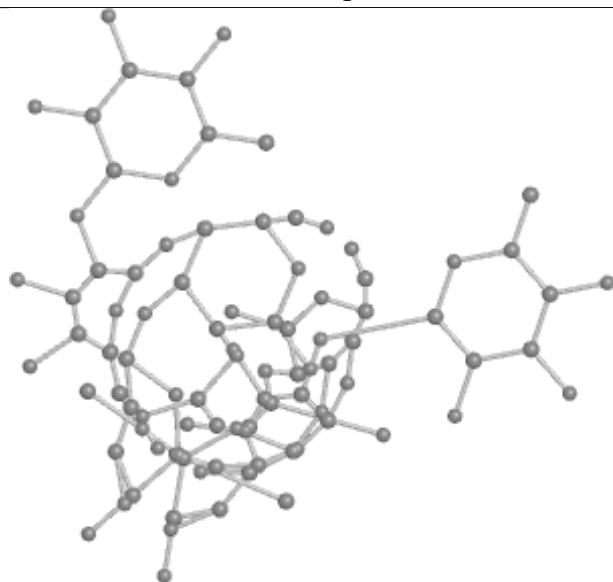
## Oligosaccharide Chain R



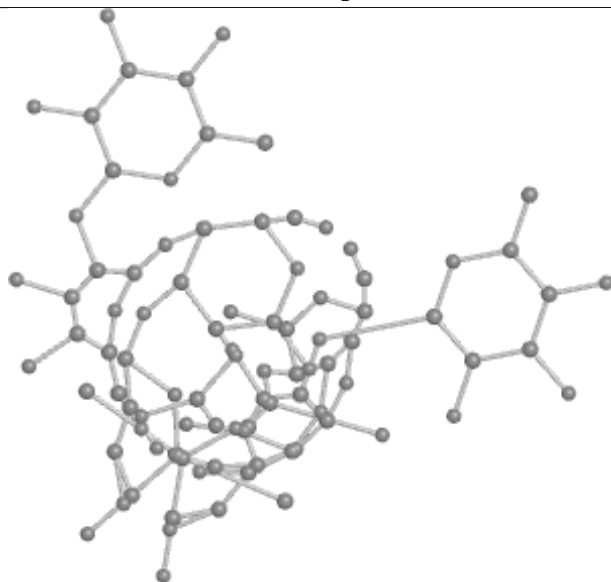
Bond lengths



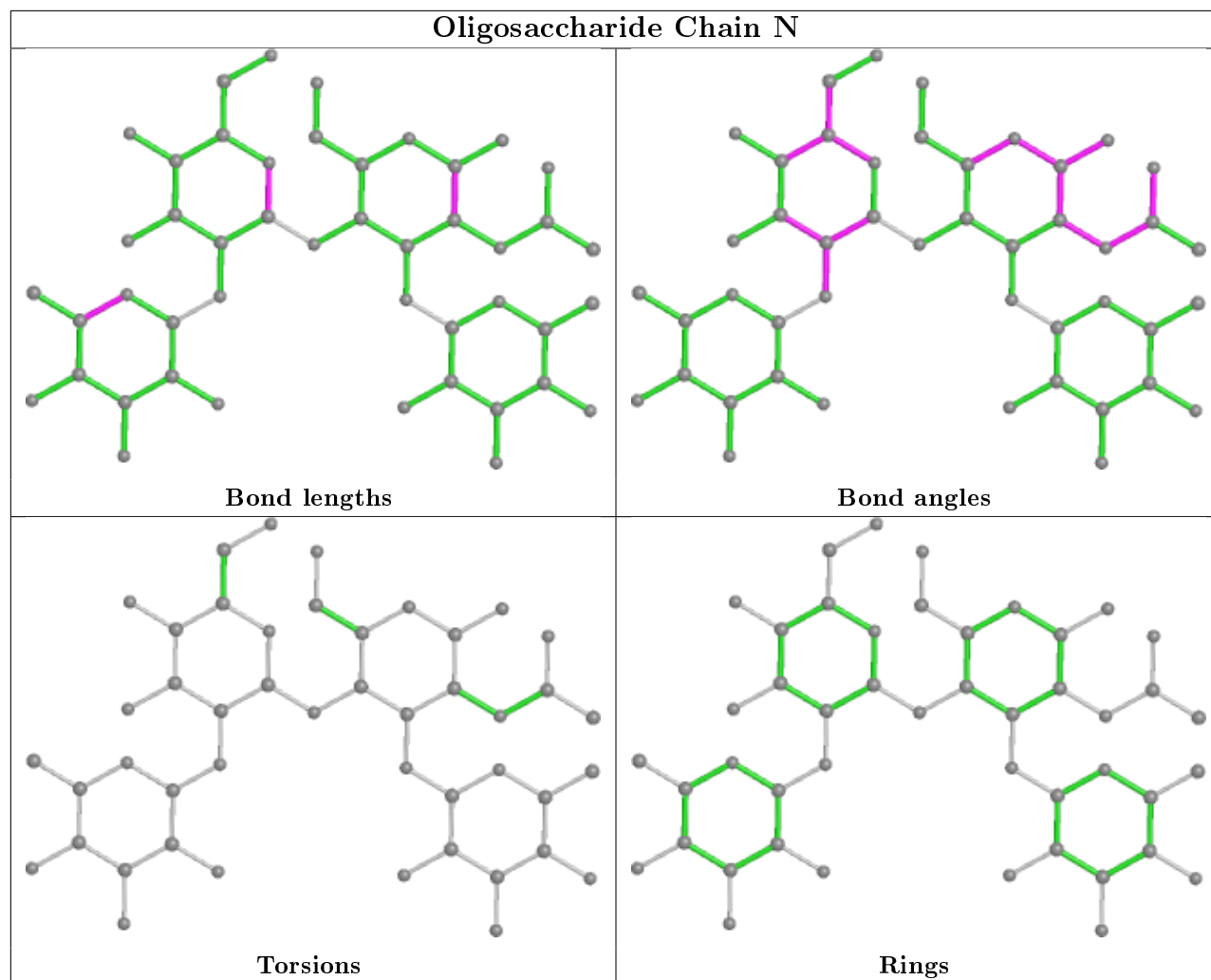
Bond angles

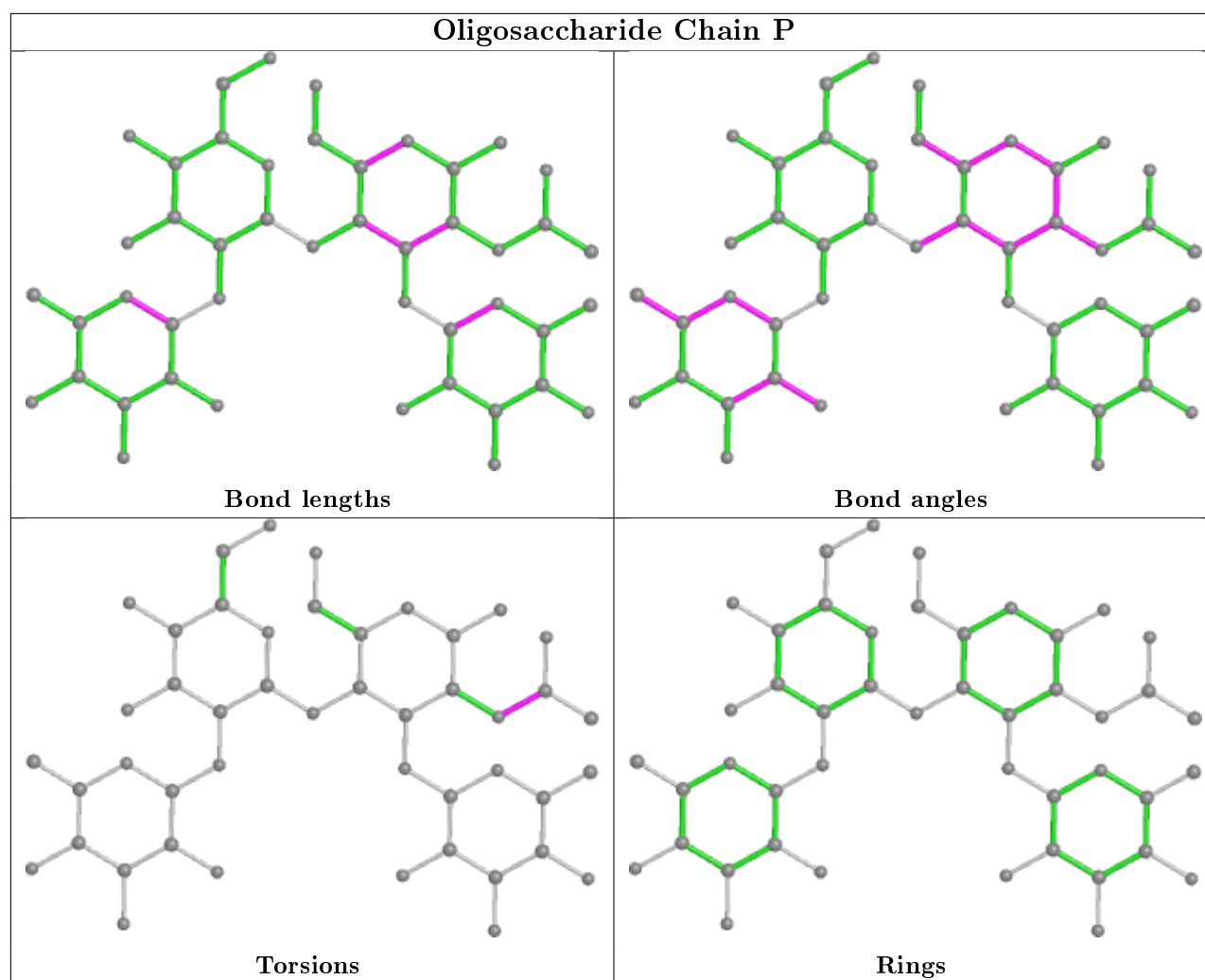


Torsions



Rings





## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 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	B	201	5	7,10,10	0.64	0	8,11,11	1.16	1 (12%)
6	BCN	E	204	5	7,10,10	0.67	0	8,11,11	2.92	2 (25%)
6	BCN	C	204	5	7,10,10	0.61	0	8,11,11	3.80	6 (75%)
6	BCN	B	203	5	7,10,10	0.42	0	8,11,11	4.01	3 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BCN	D	203	5	7,10,10	0.83	0	8,11,11	4.14	5 (62%)
6	BCN	C	202	5	7,10,10	0.54	0	8,11,11	3.94	6 (75%)
6	BCN	E	202	5	7,10,10	0.92	0	8,11,11	3.97	4 (50%)
6	BCN	D	201	5	7,10,10	0.58	0	8,11,11	1.26	1 (12%)
6	BCN	A	202	5	7,10,10	0.58	0	8,11,11	0.89	0
6	BCN	A	204	5	7,10,10	0.88	0	8,11,11	2.65	4 (50%)
7	FUC	F	201	-	11,11,11	0.66	0	15,16,16	1.14	1 (6%)

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	B	201	5	-	2/8/10/10	-
6	BCN	E	204	5	-	6/8/10/10	-
6	BCN	C	204	5	-	4/8/10/10	-
6	BCN	B	203	5	-	5/8/10/10	-
6	BCN	D	203	5	-	4/8/10/10	-
6	BCN	C	202	5	-	4/8/10/10	-
6	BCN	E	202	5	-	4/8/10/10	-
6	BCN	D	201	5	-	2/8/10/10	-
6	BCN	A	202	5	-	2/8/10/10	-
6	BCN	A	204	5	-	6/8/10/10	-
7	FUC	F	201	-	-	-	0/1/1/1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	203	BCN	C2-C1-N1	8.47	125.55	113.48
6	E	202	BCN	C1-N1-C3	8.23	128.67	111.29
6	B	203	BCN	C2-C1-N1	7.95	124.81	113.48
6	C	204	BCN	C2-C1-N1	7.42	124.05	113.48
6	C	202	BCN	C2-C1-N1	7.34	123.93	113.48
6	E	204	BCN	C1-N1-C5	7.31	126.72	111.29
6	C	202	BCN	C1-N1-C3	6.67	125.37	111.29
6	E	202	BCN	C2-C1-N1	6.60	122.88	113.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	203	BCN	C5-N1-C3	6.19	126.15	111.44
6	D	203	BCN	C1-N1-C3	5.88	123.71	111.29
6	A	204	BCN	C1-N1-C5	5.55	123.01	111.29
6	C	204	BCN	C1-N1-C3	5.34	122.57	111.29
6	B	203	BCN	C1-N1-C3	4.00	119.74	111.29
6	D	203	BCN	C5-N1-C3	3.93	120.79	111.44
6	C	204	BCN	C5-N1-C3	3.40	119.52	111.44
6	C	202	BCN	C1-N1-C5	3.22	118.08	111.29
6	C	204	BCN	C1-N1-C5	3.01	117.65	111.29
6	D	201	BCN	C2-C1-N1	-2.87	109.39	113.48
6	A	204	BCN	C2-C1-N1	2.81	117.48	113.48
6	A	204	BCN	C5-N1-C3	2.61	117.65	111.44
6	E	204	BCN	C2-C1-N1	2.56	117.13	113.48
6	D	203	BCN	C4-C3-N1	2.51	122.41	113.40
6	E	202	BCN	C4-C3-N1	2.42	122.08	113.40
6	D	203	BCN	C6-C5-N1	2.40	122.03	113.40
6	B	201	BCN	C2-C1-N1	-2.40	110.07	113.48
6	C	204	BCN	O6-C6-C5	-2.35	101.44	111.19
6	A	204	BCN	C4-C3-N1	2.30	121.64	113.40
6	C	204	BCN	C4-C3-N1	2.20	121.31	113.40
6	C	202	BCN	C4-C3-N1	2.20	121.30	113.40
6	C	202	BCN	C6-C5-N1	2.17	121.18	113.40
6	C	202	BCN	C5-N1-C3	2.14	116.52	111.44
7	F	201	FUC	O5-C5-C4	2.10	113.29	109.52
6	E	202	BCN	C1-N1-C5	-2.00	107.06	111.29

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	204	BCN	C6-C5-N1-C1
6	B	203	BCN	C6-C5-N1-C3
6	D	203	BCN	C4-C3-N1-C1
6	A	204	BCN	C6-C5-N1-C1
6	E	202	BCN	C2-C1-N1-C3
6	E	204	BCN	C2-C1-N1-C3
6	A	204	BCN	C4-C3-N1-C5
6	D	203	BCN	C6-C5-N1-C3
6	C	202	BCN	C6-C5-N1-C1
6	C	204	BCN	C4-C3-N1-C1
6	E	202	BCN	C4-C3-N1-C1
6	E	202	BCN	N1-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
6	E	204	BCN	C4-C3-N1-C5
6	B	203	BCN	C4-C3-N1-C1
6	E	204	BCN	C2-C1-N1-C5
6	D	203	BCN	C2-C1-N1-C5
6	A	204	BCN	N1-C5-C6-O6
6	C	202	BCN	C2-C1-N1-C3
6	B	203	BCN	N1-C5-C6-O6
6	A	204	BCN	C2-C1-N1-C5
6	E	202	BCN	N1-C5-C6-O6
6	A	202	BCN	C2-C1-N1-C5
6	D	201	BCN	C2-C1-N1-C5
6	E	204	BCN	N1-C5-C6-O6
6	A	204	BCN	C2-C1-N1-C3
6	B	201	BCN	C2-C1-N1-C5
6	C	204	BCN	C2-C1-N1-C5
6	C	204	BCN	N1-C3-C4-O4
6	D	203	BCN	N1-C3-C4-O4
6	B	201	BCN	C2-C1-N1-C3
6	D	201	BCN	C2-C1-N1-C3
6	C	202	BCN	C2-C1-N1-C5
6	A	202	BCN	C2-C1-N1-C3
6	C	202	BCN	C4-C3-N1-C1
6	C	204	BCN	C6-C5-N1-C3
6	B	203	BCN	C2-C1-N1-C5
6	E	204	BCN	C4-C3-N1-C1
6	A	204	BCN	C4-C3-N1-C1
6	B	203	BCN	C4-C3-N1-C5

There are no ring outliers.

No monomer is involved in short contacts.

## 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%)	0.59	4 (3%) 39 44	11, 17, 32, 49	0
1	B	103/103 (100%)	0.28	3 (2%) 51 56	9, 15, 25, 32	0
1	C	103/103 (100%)	0.18	3 (2%) 51 56	8, 15, 27, 35	0
1	D	103/103 (100%)	0.36	5 (4%) 29 32	10, 16, 34, 44	0
1	E	103/103 (100%)	0.45	4 (3%) 39 44	11, 17, 31, 41	0
1	F	103/103 (100%)	0.73	10 (9%) 7 8	13, 20, 31, 40	0
1	G	103/103 (100%)	0.59	6 (5%) 23 25	10, 18, 37, 48	0
1	H	103/103 (100%)	0.61	8 (7%) 13 13	11, 19, 32, 38	0
1	I	103/103 (100%)	0.22	4 (3%) 39 44	10, 16, 30, 35	0
1	J	103/103 (100%)	0.53	5 (4%) 29 32	11, 19, 28, 41	0
All	All	1030/1030 (100%)	0.46	52 (5%) 28 31	8, 17, 32, 49	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	ILE	4.7
1	G	13	HIS	4.5
1	G	55	SER	4.4
1	G	54	GLY	4.1
1	A	56	GLN	3.8
1	E	103	ASN	3.7
1	J	13	HIS	3.7
1	F	15	THR	3.3
1	D	103	ASN	3.3
1	F	58	ILE	3.3
1	F	103	ASN	3.3
1	A	55	SER	3.2
1	F	55	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	90	ASN	3.1
1	G	103	ASN	3.1
1	E	55	SER	3.0
1	D	13	HIS	2.9
1	F	56	GLN	2.9
1	F	12	TYR	2.8
1	B	103	ASN	2.8
1	J	103	ASN	2.8
1	H	25	PHE	2.8
1	D	54	GLY	2.7
1	H	103	ASN	2.7
1	H	54	GLY	2.7
1	D	55	SER	2.7
1	I	55	SER	2.7
1	B	13	HIS	2.6
1	C	103	ASN	2.6
1	D	58	ILE	2.6
1	A	15	THR	2.5
1	J	8	LEU	2.4
1	J	18	TYR	2.4
1	B	55	SER	2.4
1	F	9	CYS	2.4
1	I	58	ILE	2.4
1	H	31	LEU	2.4
1	G	59	ASP	2.4
1	F	13	HIS	2.3
1	C	1	THR	2.3
1	I	13	HIS	2.3
1	H	55	SER	2.2
1	I	1	THR	2.2
1	F	1	THR	2.2
1	H	33	GLY	2.2
1	H	14	ASN	2.2
1	G	56	GLN	2.1
1	J	10	ALA	2.1
1	E	58	ILE	2.1
1	H	62	LYS	2.1
1	C	55	SER	2.1
1	E	88	TRP	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	NDG	K	1	15/15	0.72	0.18	33,37,46,47	0
2	GAL	K	2	11/12	0.75	0.20	26,35,40,41	0
2	NDG	S	1	15/15	0.76	0.24	30,38,49,52	0
2	FUC	Q	3	10/11	0.77	0.18	29,30,32,33	0
2	NDG	Q	1	15/15	0.77	0.17	23,28,37,39	0
2	GAL	Q	2	11/12	0.78	0.18	30,36,42,43	0
4	NAG	P	1	15/15	0.78	0.17	23,28,37,37	0
2	FUC	K	3	10/11	0.79	0.18	21,23,24,27	0
2	NDG	O	1	15/15	0.80	0.14	24,26,28,31	0
4	NAG	N	1	15/15	0.82	0.14	21,24,29,30	0
2	FUC	S	4	10/11	0.83	0.12	32,34,39,40	0
2	FUC	O	3	10/11	0.83	0.13	28,28,29,31	0
4	GAL	N	2	11/12	0.85	0.13	19,21,27,32	0
2	FUC	K	4	10/11	0.86	0.11	30,32,33,35	0
4	FUC	N	4	10/11	0.87	0.11	21,22,25,27	0
2	FUC	Q	4	10/11	0.87	0.11	22,23,25,25	0
4	FUC	P	4	10/11	0.89	0.09	24,26,27,29	0
3	NAG	L	1[B]	15/15	0.90	0.12	15,16,18,18	15
4	FUC	N	3	10/11	0.90	0.11	17,19,20,20	0
2	GAL	O	2	11/12	0.91	0.10	27,29,31,33	0
4	GAL	P	2	11/12	0.91	0.10	20,21,23,26	0
2	GAL	S	2	11/12	0.91	0.12	24,28,33,35	0
3	NDG	L	1[A]	15/15	0.91	0.12	14,15,18,18	15
3	FUC	R	4[A]	10/11	0.91	0.11	15,17,18,18	10
3	FUC	R	4[B]	10/11	0.91	0.11	19,19,21,21	10
2	FUC	S	3	10/11	0.91	0.09	21,22,24,24	0
2	FUC	O	4	10/11	0.91	0.09	22,24,25,25	0
3	NAG	M	1[B]	15/15	0.92	0.09	16,17,18,19	15
3	NAG	R	1[B]	15/15	0.92	0.12	16,19,23,24	15
3	NDG	R	1[A]	15/15	0.92	0.14	18,21,26,26	15
3	GAL	R	2[A]	11/12	0.93	0.09	17,18,19,19	11
3	FUC	M	4[B]	10/11	0.93	0.10	20,22,24,24	10

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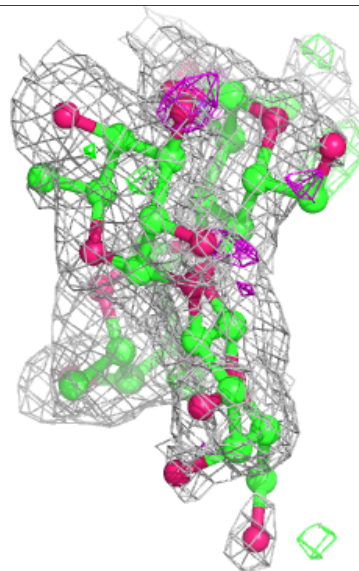
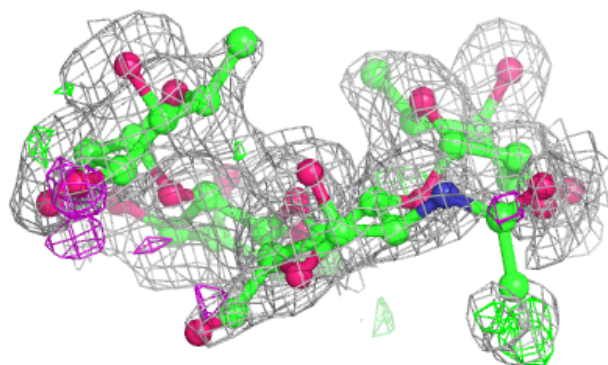
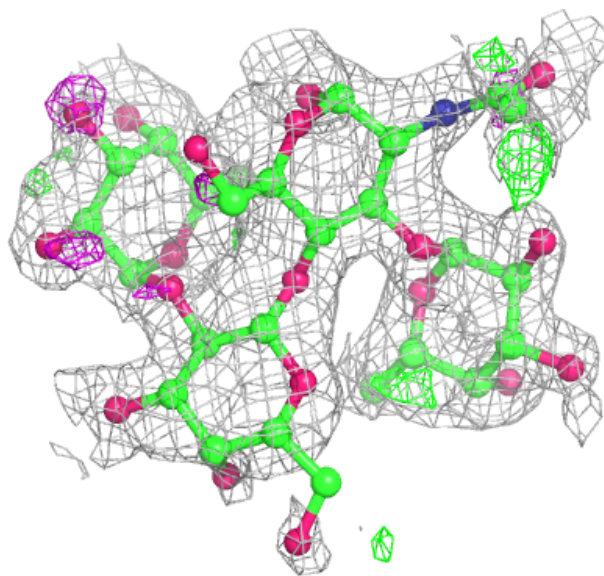
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FUC	M	3[A]	10/11	0.93	0.09	14,15,16,16	10
3	FUC	M	4[A]	10/11	0.93	0.10	17,19,20,21	10
3	GAL	R	2[B]	11/12	0.93	0.09	15,16,17,17	11
3	FUC	M	3[B]	10/11	0.93	0.09	15,16,17,18	10
3	NDG	M	1[A]	15/15	0.93	0.09	14,15,16,18	15
3	FUC	R	3[A]	10/11	0.94	0.11	17,18,18,18	10
3	GAL	L	2[A]	11/12	0.94	0.09	16,17,18,19	11
3	GAL	M	2[A]	11/12	0.94	0.10	14,15,18,20	11
3	FUC	L	3[B]	10/11	0.94	0.08	16,17,18,18	10
3	GAL	M	2[B]	11/12	0.94	0.10	16,17,20,20	11
3	FUC	L	3[A]	10/11	0.94	0.08	15,16,17,17	10
3	FUC	R	3[B]	10/11	0.94	0.11	15,16,18,18	10
4	FUC	P	3	10/11	0.94	0.08	19,21,21,21	0
3	GAL	L	2[B]	11/12	0.94	0.09	17,19,19,20	11
3	FUC	L	4[B]	10/11	0.95	0.09	14,15,17,18	10
3	FUC	L	4[A]	10/11	0.95	0.09	14,15,17,17	10

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.

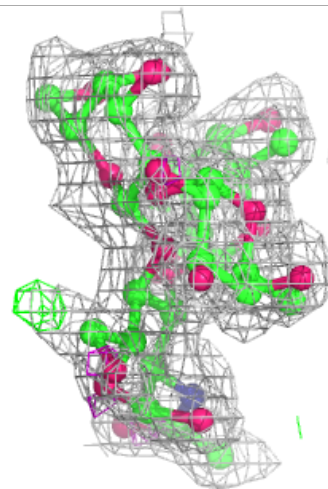
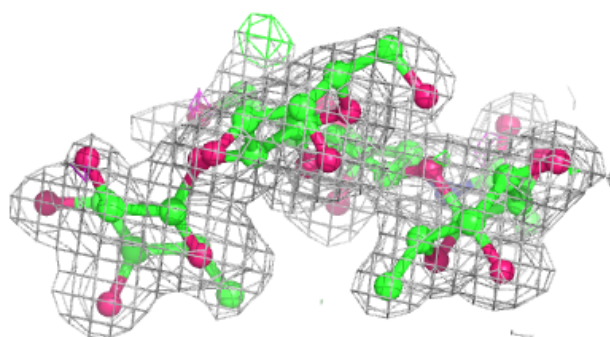
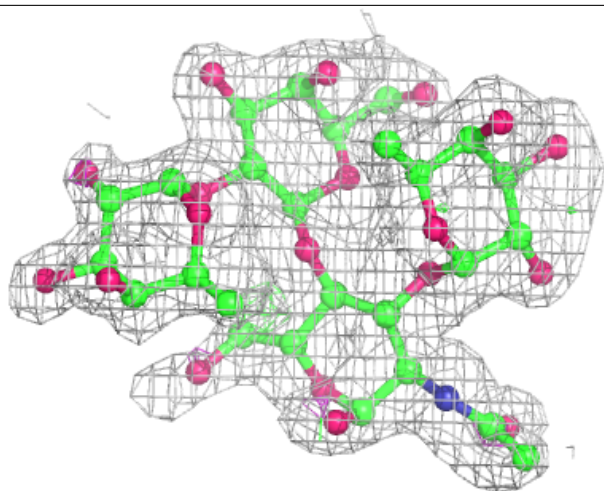
**Electron density around Chain K:**

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



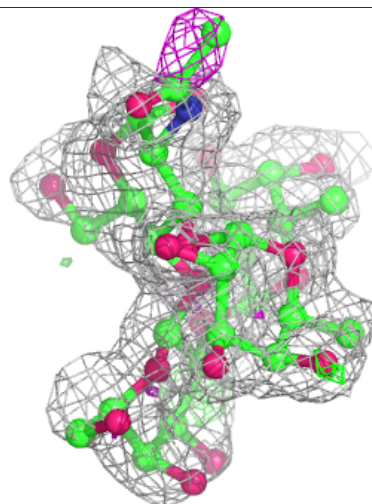
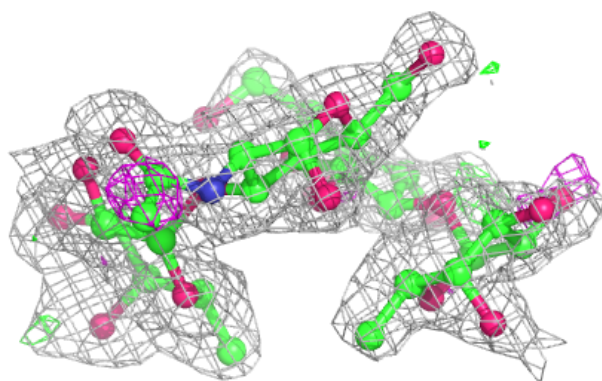
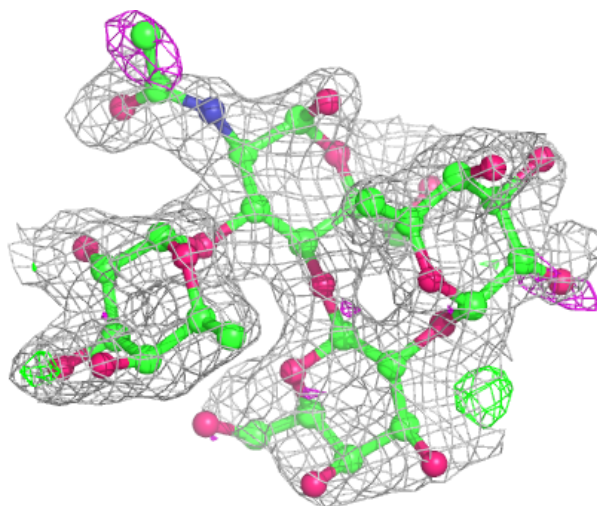
**Electron density around Chain O:**

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



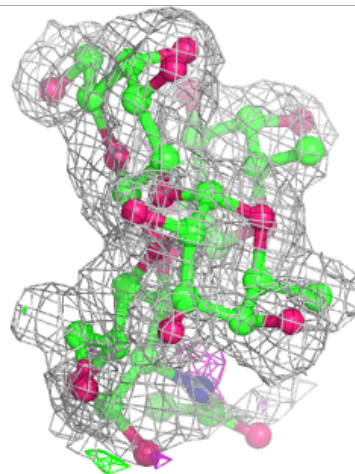
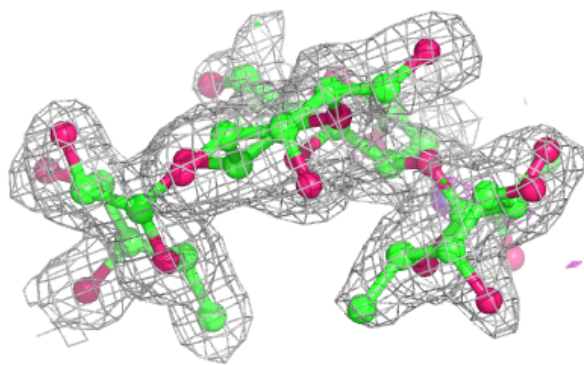
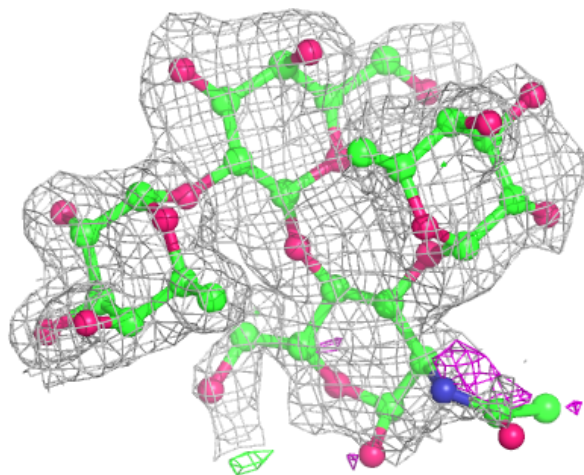
**Electron density around Chain Q:**

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



**Electron density around Chain S:**

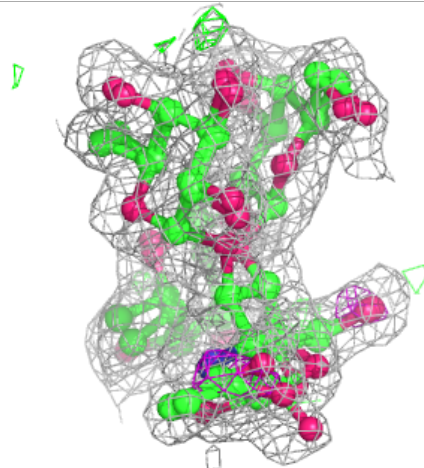
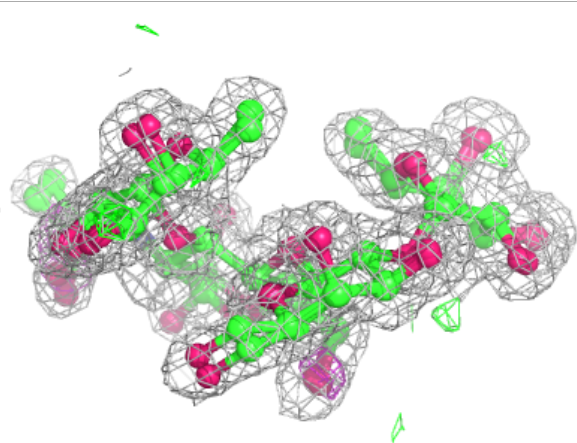
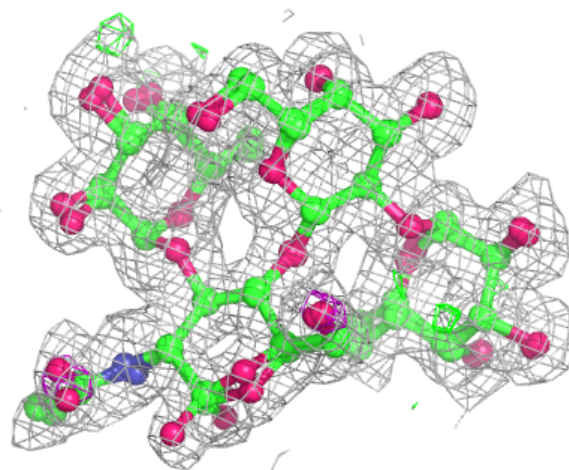
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





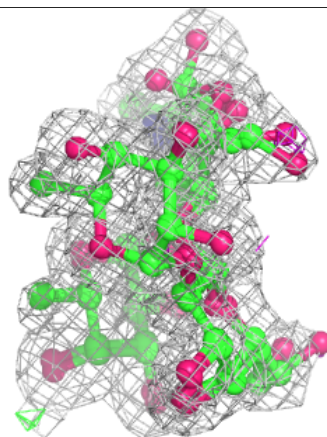
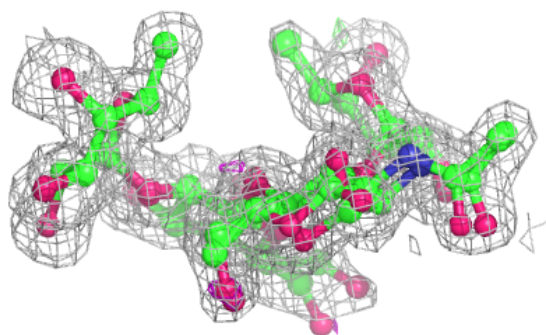
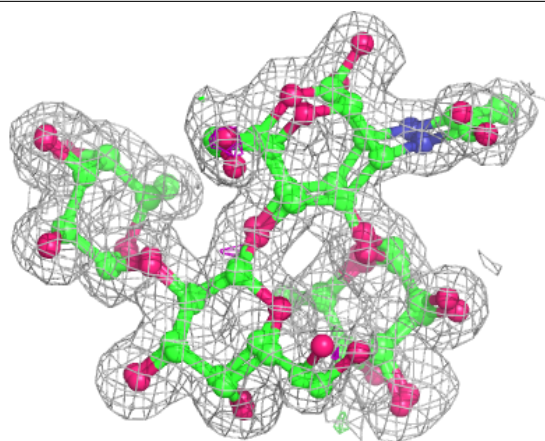
**Electron density around Chain L:**

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



**Electron density around Chain M:**

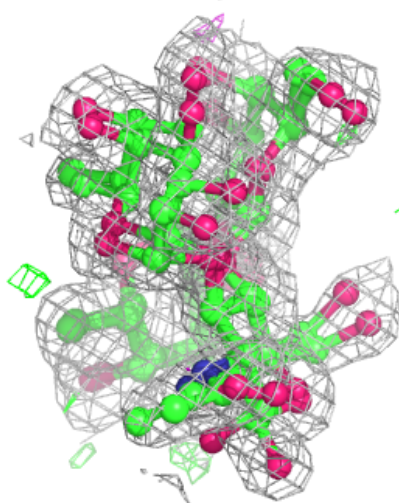
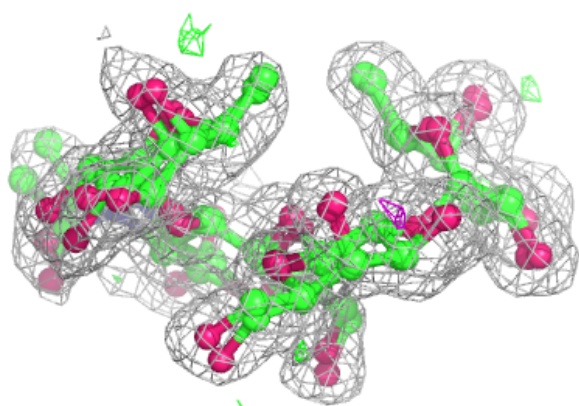
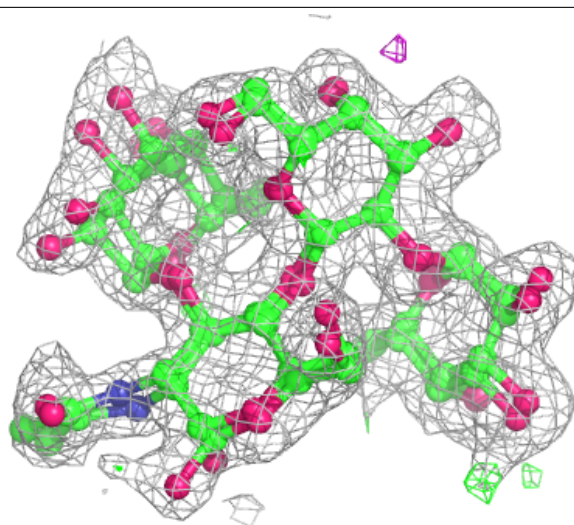
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





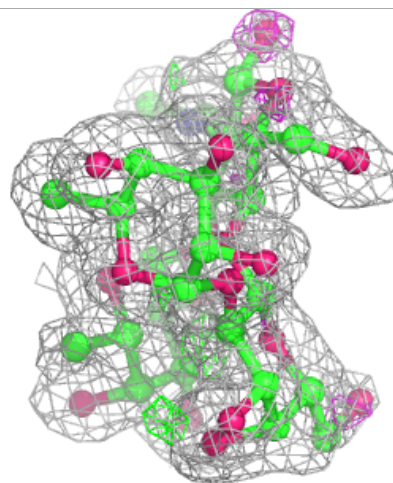
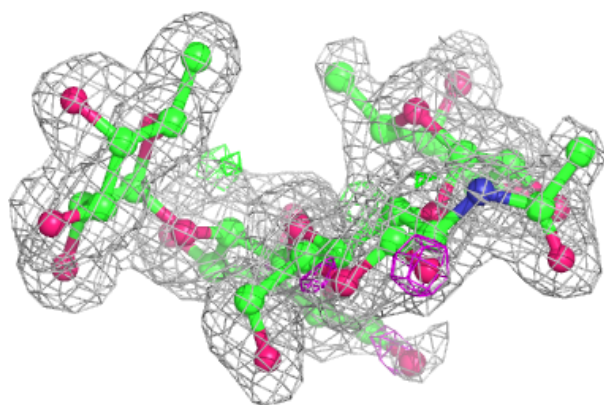
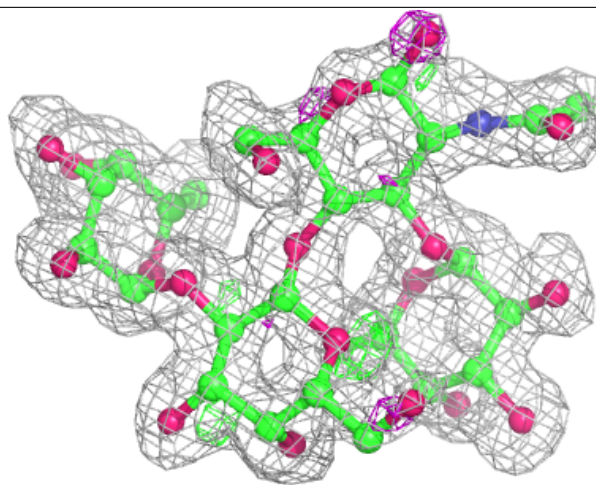
**Electron density around Chain R:**

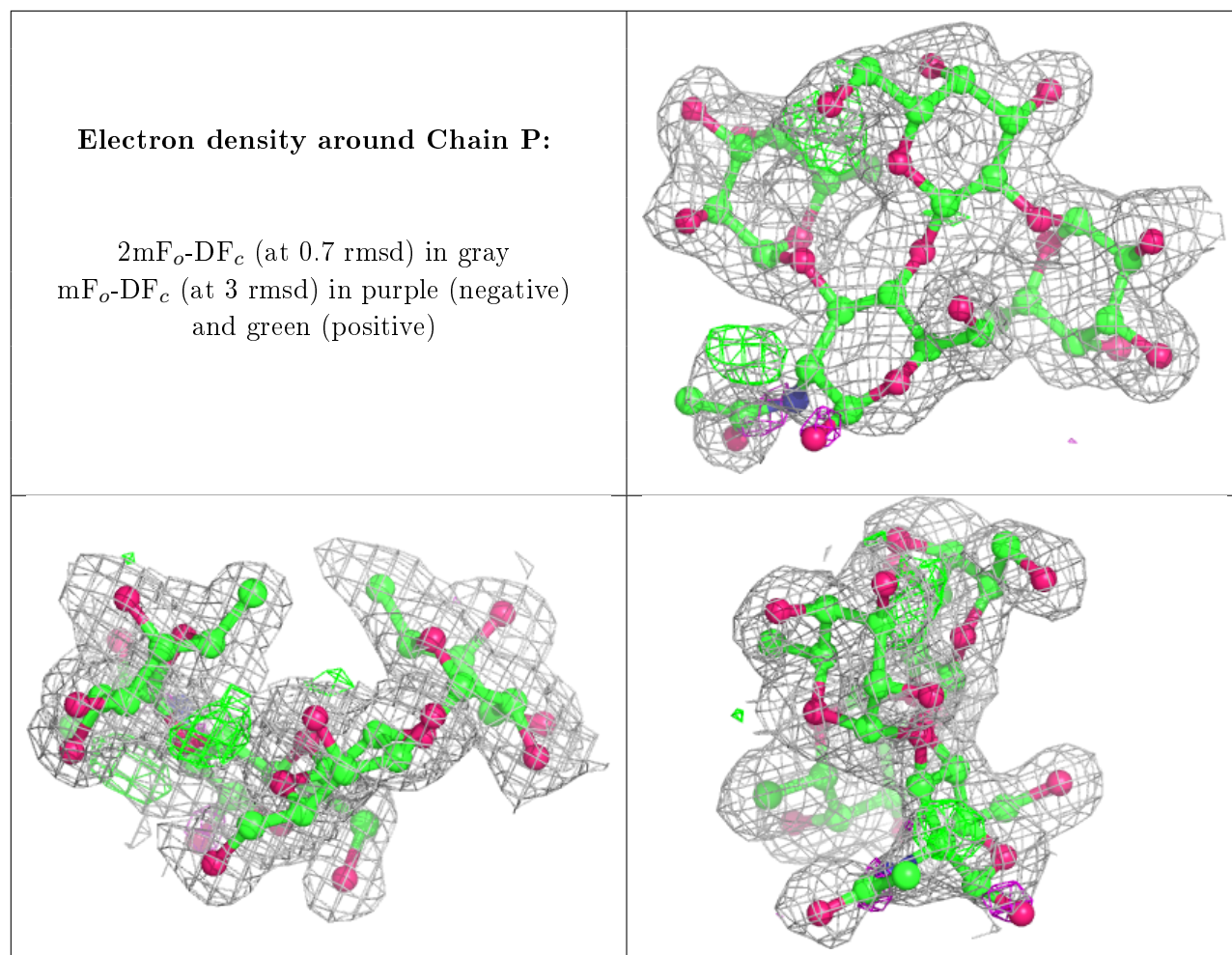
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain N:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.84	0.14	21,24,25,28	0
6	BCN	A	202	11/11	0.86	0.12	16,20,26,28	0
6	BCN	E	202	11/11	0.86	0.17	17,26,31,31	0
6	BCN	A	204	11/11	0.87	0.10	21,25,27,27	0
6	BCN	D	201	11/11	0.89	0.15	18,21,24,26	0
6	BCN	E	204	11/11	0.89	0.12	18,23,25,27	0
6	BCN	D	203	11/11	0.91	0.11	14,18,26,28	0
6	BCN	B	201	11/11	0.91	0.10	15,17,21,23	0
6	BCN	B	203	11/11	0.91	0.12	15,22,25,25	0
6	BCN	C	202	11/11	0.93	0.12	17,23,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	BCN	C	204	11/11	0.93	0.11	13,18,23,24	0
5	CA	B	204	1/1	0.98	0.06	14,14,14,14	0
5	CA	B	202	1/1	0.98	0.06	14,14,14,14	0
5	CA	D	202	1/1	0.99	0.08	14,14,14,14	0
5	CA	A	203	1/1	0.99	0.05	15,15,15,15	0
5	CA	C	201	1/1	0.99	0.06	14,14,14,14	0
5	CA	C	203	1/1	0.99	0.08	14,14,14,14	0
5	CA	D	204	1/1	0.99	0.05	13,13,13,13	0
5	CA	A	201	1/1	0.99	0.06	16,16,16,16	0
5	CA	E	203	1/1	0.99	0.08	15,15,15,15	0
5	CA	E	201	1/1	1.00	0.07	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.