



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:27 AM BST

PDB ID : 4DVK  
Title : Crystal structure of the glycoprotein Erns from the pestivirus BVDV-1 strain NCP-7  
Authors : Krey, T.; Bontems, F.; Vonrhein, C.; Vaney, M.-C.; Bricogne, G.; Ruemenapf, T.; Rey, F.A.  
Deposited on : 2012-02-23  
Resolution : 2.21 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

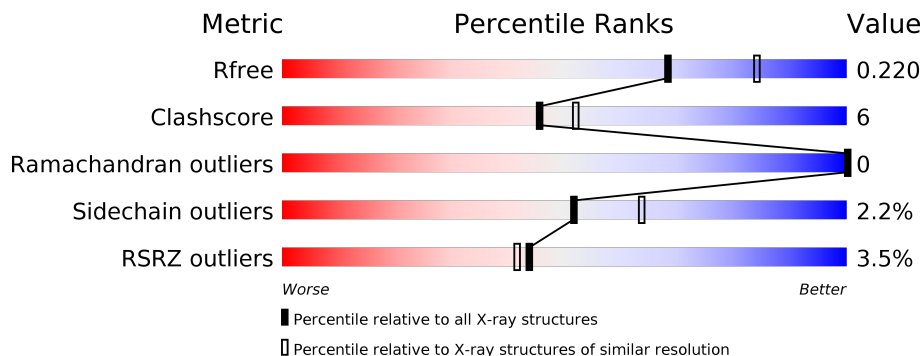
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	165	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4%      83%      11%      • 5%</p>
1	B	165	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      85%      8%      •• 5%</p>
2	C	6	<div style="width: 100%; height: 10px; background-color: yellow;"></div> <p style="text-align: center;">100%</p>
3	D	2	<div style="width: 100%; height: 10px; background-color: yellow;"></div> <p style="text-align: center;">100%</p>
3	F	2	<div style="width: 100%; height: 10px; background-color: yellow;"></div> <p style="text-align: center;">100%</p>
3	G	2	<div style="width: 100%; height: 10px; background-color: yellow;"></div> <p style="text-align: center;">100%</p>

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Mol	Chain	Length	Quality of chain
4	E	7	 100%

## 2 Entry composition [i](#)

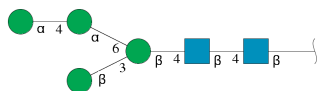
There are 7 unique types of molecules in this entry. The entry contains 3193 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 E(rns) glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	157	1301	806	234	241	20	0	10	0
1	B	157	1314	811	243	240	20	0	10	0

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



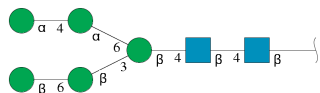
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	6	72	40	2	30	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



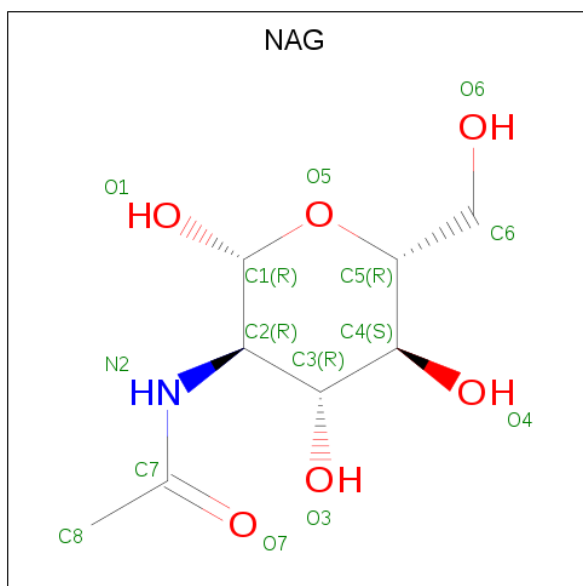
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	2	28	16	2	10	0	0	0
3	F	2	28	16	2	10	0	0	0
3	G	2	28	16	2	10	0	0	0

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



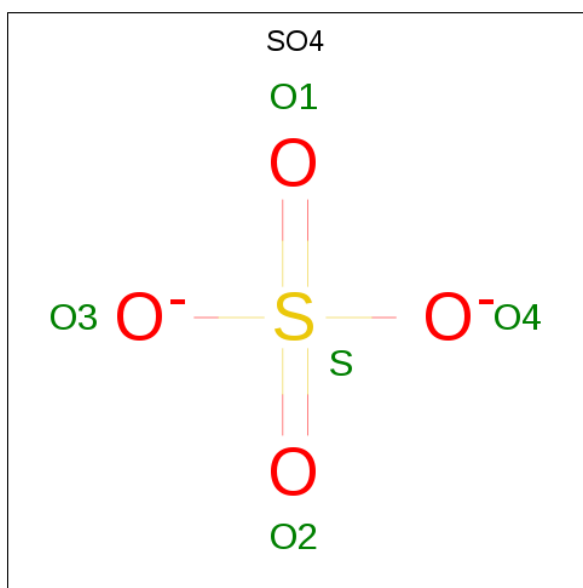
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	7	83	46	2	35	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	94	Total O 94 94	0	0

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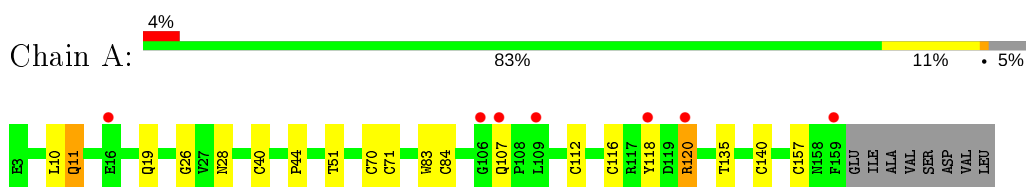
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	B	111	Total 111	O 111	0	0

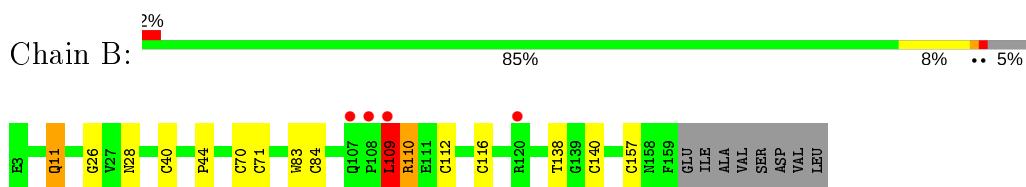
### 3 Residue-property plots [i](#)

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.

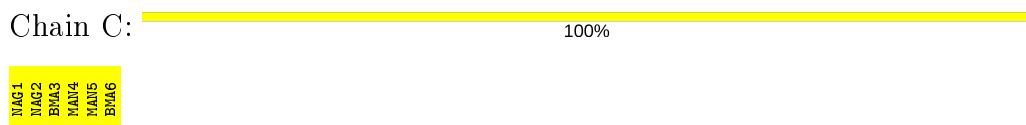
- Molecule 1: E(rns) glycoprotein



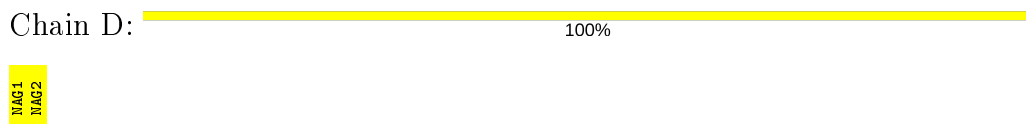
- Molecule 1: E(rns) glycoprotein



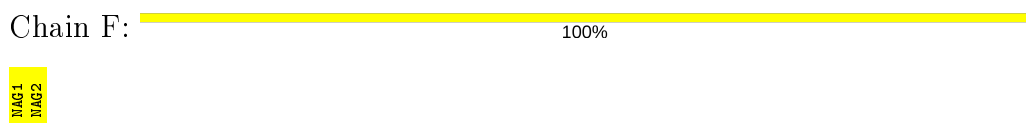
- Molecule 2: alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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




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





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

Chain G:  100%

MAG1  
MAG2

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

Chain E:  100%

MAG1  
MAG2  
EMAA3  
EMAA4  
EMAA5  
MANG  
MANT

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.04Å 106.04Å 211.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.92 – 2.21 45.92 – 2.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.92-2.21) 96.7 (45.92-2.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.20Å)	Xtrriage
Refinement program	BUSTER-TNT BUSTER 2.9.2, BUSTER 2.9.2	Depositor
R, $R_{free}$	0.209 , 0.225 0.210 , 0.220	Depositor DCC
$R_{free}$ test set	1785 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtrriage
Anisotropy	0.416	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 68.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3193	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, BMA, NAG, MAN

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	0.56	0/1349	0.71	0/1828
1	B	0.56	0/1353	0.71	1/1832 (0.1%)
All	All	0.56	0/2702	0.71	1/3660 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	LEU	N-CA-C	-6.12	94.47	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1301	0	1240	18	0
1	B	1314	0	1253	16	0
2	C	72	0	61	0	0
3	D	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
4	E	83	0	70	0	0
5	A	42	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	42	0	39	1	0
6	A	15	0	0	0	0
6	B	35	0	0	0	0
7	A	94	0	0	1	0
7	B	111	0	0	0	0
All	All	3193	0	2777	33	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116[B]:CYS:HB2	1:A:140[B]:CYS:SG	2.13	0.89
1:B:116[B]:CYS:HB2	1:B:140[B]:CYS:SG	2.16	0.86
1:A:40[B]:CYS:HG	1:A:84[B]:CYS:HG	0.95	0.85
1:B:40[B]:CYS:HG	1:B:84[B]:CYS:HG	0.81	0.81
1:B:70[B]:CYS:SG	1:B:71[B]:CYS:HB3	2.21	0.80
1:A:116[B]:CYS:HG	1:A:140[B]:CYS:HG	1.30	0.79
1:A:70[B]:CYS:SG	1:A:71[B]:CYS:HB3	2.25	0.77
1:A:118:TYR:HE2	1:A:120:ARG:HD3	1.52	0.73
1:A:116[B]:CYS:CB	1:A:140[B]:CYS:SG	2.83	0.66
1:B:116[B]:CYS:CB	1:B:140[B]:CYS:SG	2.85	0.65
1:A:116[B]:CYS:CB	1:A:140[B]:CYS:HG	2.12	0.62
1:A:70[B]:CYS:SG	1:A:71[B]:CYS:CB	2.89	0.60
1:B:70[B]:CYS:SG	1:B:71[B]:CYS:CB	2.88	0.60
1:A:118:TYR:CE2	1:A:120:ARG:HD3	2.35	0.59
1:A:112[B]:CYS:HG	1:A:157[B]:CYS:HG	1.52	0.54
1:B:116[B]:CYS:CB	1:B:140[B]:CYS:HG	2.22	0.51
1:A:26:GLY:O	5:A:1107:NAG:H82	2.10	0.51
1:A:11:GLN:HG2	1:A:28:ASN:HA	1.93	0.51
1:B:26:GLY:O	5:B:1108:NAG:H82	2.12	0.50
1:B:112[B]:CYS:HG	1:B:157[B]:CYS:HG	1.58	0.49
1:A:70[B]:CYS:SG	1:A:71[B]:CYS:SG	3.10	0.49
1:B:70[B]:CYS:HG	1:B:71[B]:CYS:HB3	1.76	0.49
1:B:70[B]:CYS:SG	1:B:71[B]:CYS:SG	3.11	0.49
1:B:11:GLN:HG2	1:B:28:ASN:HA	1.95	0.49
1:B:109:LEU:HD12	1:B:110:ARG:H	1.78	0.48
1:A:51:THR:HG22	7:A:1285:HOH:O	2.14	0.47
1:A:44:PRO:HA	1:A:83:TRP:CD2	2.51	0.46
1:B:70[B]:CYS:HG	1:B:71[B]:CYS:CB	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:PRO:HA	1:B:83:TRP:CD2	2.52	0.45
1:A:10:LEU:O	1:A:19:GLN:HG3	2.19	0.43
1:A:135:THR:OG1	1:B:138:THR:HG23	2.19	0.42
1:B:70[B]:CYS:HA	1:B:71[B]:CYS:HA	1.79	0.42
1:A:70[B]:CYS:HA	1:A:71[B]:CYS:HA	1.82	0.42

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	164/165 (99%)	157 (96%)	7 (4%)	0	100	100
1	B	165/165 (100%)	158 (96%)	7 (4%)	0	100	100
All	All	329/330 (100%)	315 (96%)	14 (4%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	147/144 (102%)	144 (98%)	3 (2%)	55	67
1	B	147/144 (102%)	144 (98%)	3 (2%)	55	67
All	All	294/288 (102%)	288 (98%)	6 (2%)	52	67

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	107	GLN
1	A	120	ARG
1	B	11	GLN
1	B	109	LEU
1	B	110	ARG

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

Mol	Chain	Res	Type
1	A	24	GLN
1	B	24	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

19 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	NAG	C	1	1,2	14,14,15	0.90	1 (7%)	17,19,21	2.10	6 (35%)
2	NAG	C	2	2	14,14,15	0.92	1 (7%)	17,19,21	1.81	3 (17%)
2	BMA	C	3	2	11,11,12	0.82	0	15,15,17	1.25	1 (6%)
2	MAN	C	4	2	11,11,12	0.76	0	15,15,17	2.62	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	C	5	2	11,11,12	0.86	0	15,15,17	2.59	5 (33%)
2	BMA	C	6	2	11,11,12	0.87	0	15,15,17	5.06	8 (53%)
3	NAG	D	1	1,3	14,14,15	0.94	1 (7%)	17,19,21	1.68	5 (29%)
3	NAG	D	2	3	14,14,15	0.98	1 (7%)	17,19,21	1.72	4 (23%)
4	NAG	E	1	1,4	14,14,15	0.89	1 (7%)	17,19,21	2.39	8 (47%)
4	NAG	E	2	4	14,14,15	0.80	0	17,19,21	1.77	2 (11%)
4	BMA	E	3	4	11,11,12	0.82	0	15,15,17	1.91	4 (26%)
4	BMA	E	4	4	11,11,12	0.79	0	15,15,17	3.62	9 (60%)
4	BMA	E	5	4	11,11,12	0.84	0	15,15,17	2.15	4 (26%)
4	MAN	E	6	4	11,11,12	0.75	0	15,15,17	2.07	5 (33%)
4	MAN	E	7	4	11,11,12	0.82	0	15,15,17	2.46	5 (33%)
3	NAG	F	1	1,3	14,14,15	1.03	1 (7%)	17,19,21	2.99	7 (41%)
3	NAG	F	2	3	14,14,15	1.06	1 (7%)	17,19,21	2.28	5 (29%)
3	NAG	G	1	1,3	14,14,15	0.93	1 (7%)	17,19,21	1.43	2 (11%)
3	NAG	G	2	3	14,14,15	0.94	1 (7%)	17,19,21	1.71	3 (17%)

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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	0/1/1/1
2	BMA	C	6	2	-	0/2/19/22	1/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	BMA	E	4	4	-	1/2/19/22	1/1/1/1
4	BMA	E	5	4	-	1/2/19/22	0/1/1/1
4	MAN	E	6	4	-	1/2/19/22	1/1/1/1
4	MAN	E	7	4	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	C1-C2	2.70	1.56	1.52
3	D	2	NAG	C1-C2	2.49	1.56	1.52
3	F	2	NAG	C1-C2	2.44	1.56	1.52
2	C	2	NAG	C1-C2	2.41	1.55	1.52
3	G	2	NAG	C1-C2	2.37	1.55	1.52
3	G	1	NAG	C1-C2	2.22	1.55	1.52
3	D	1	NAG	C1-C2	2.19	1.55	1.52
4	E	1	NAG	C1-C2	2.19	1.55	1.52
2	C	1	NAG	C1-C2	2.05	1.55	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	BMA	O5-C1-C2	-11.36	93.24	110.77
3	F	1	NAG	O4-C4-C5	8.74	131.01	109.30
2	C	6	BMA	C3-C4-C5	-8.33	95.38	110.24
2	C	6	BMA	C1-O5-C5	7.32	122.11	112.19
2	C	6	BMA	C1-C2-C3	7.29	118.63	109.67
4	E	4	BMA	C3-C4-C5	-6.64	98.39	110.24
2	C	5	MAN	C1-O5-C5	6.21	120.61	112.19
4	E	7	MAN	C1-O5-C5	6.11	120.47	112.19
4	E	4	BMA	O5-C1-C2	-5.68	102.01	110.77
2	C	6	BMA	O3-C3-C2	5.49	120.50	109.99
2	C	4	MAN	C1-O5-C5	5.40	119.50	112.19
4	E	4	BMA	C1-O5-C5	5.27	119.33	112.19
4	E	5	BMA	O5-C1-C2	5.07	118.60	110.77
4	E	1	NAG	C1-C2-N2	5.01	119.04	110.49
3	D	2	NAG	C4-C3-C2	4.86	118.14	111.02
4	E	4	BMA	O3-C3-C2	4.82	119.23	109.99
2	C	6	BMA	O2-C2-C1	4.77	118.91	109.15
3	F	2	NAG	O5-C1-C2	4.76	118.81	111.29
3	G	2	NAG	C4-C3-C2	4.68	117.88	111.02
4	E	1	NAG	C8-C7-N2	-4.63	108.27	116.10
2	C	4	MAN	O2-C2-C1	4.46	118.28	109.15
4	E	2	NAG	O4-C4-C5	-4.26	98.73	109.30
2	C	2	NAG	C6-C5-C4	-4.22	103.11	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-C2-N2	4.22	117.69	110.49
4	E	6	MAN	O5-C1-C2	4.20	117.26	110.77
2	C	1	NAG	C8-C7-N2	-4.05	109.24	116.10
2	C	5	MAN	O2-C2-C1	4.04	117.42	109.15
3	F	2	NAG	O3-C3-C2	3.98	117.70	109.47
2	C	2	NAG	O4-C4-C5	-3.97	99.43	109.30
4	E	5	BMA	C1-O5-C5	3.96	117.55	112.19
2	C	5	MAN	O5-C1-C2	3.95	116.86	110.77
4	E	2	NAG	C6-C5-C4	-3.89	103.89	113.00
4	E	4	BMA	O5-C5-C6	3.89	113.30	107.20
3	F	1	NAG	C2-N2-C7	-3.82	117.46	122.90
4	E	4	BMA	O2-C2-C1	3.78	116.89	109.15
3	F	2	NAG	C3-C4-C5	3.78	116.97	110.24
3	F	1	NAG	O5-C5-C4	-3.75	101.70	110.83
4	E	7	MAN	O5-C1-C2	3.73	116.53	110.77
2	C	4	MAN	O5-C1-C2	3.72	116.51	110.77
3	G	1	NAG	C1-C2-N2	3.70	116.82	110.49
4	E	4	BMA	C1-C2-C3	3.70	114.22	109.67
4	E	3	BMA	O2-C2-C1	3.54	116.39	109.15
2	C	5	MAN	O2-C2-C3	-3.53	103.07	110.14
4	E	6	MAN	O2-C2-C3	3.49	117.14	110.14
4	E	3	BMA	C1-C2-C3	-3.46	105.41	109.67
3	D	1	NAG	C1-O5-C5	3.45	116.86	112.19
4	E	3	BMA	O6-C6-C5	-3.44	99.48	111.29
3	F	1	NAG	C4-C3-C2	-3.37	106.08	111.02
4	E	7	MAN	O2-C2-C1	3.37	116.05	109.15
3	F	1	NAG	O5-C1-C2	3.34	116.56	111.29
4	E	4	BMA	C6-C5-C4	3.31	120.75	113.00
4	E	6	MAN	O6-C6-C5	-3.23	100.20	111.29
4	E	5	BMA	C2-C3-C4	3.23	116.48	110.89
4	E	1	NAG	O6-C6-C5	-3.20	100.32	111.29
4	E	4	BMA	O2-C2-C3	3.17	116.49	110.14
2	C	6	BMA	C6-C5-C4	3.15	120.39	113.00
2	C	4	MAN	O4-C4-C3	-3.07	103.26	110.35
3	D	1	NAG	C1-C2-N2	3.03	115.66	110.49
4	E	6	MAN	O2-C2-C1	2.95	115.18	109.15
3	F	2	NAG	C2-N2-C7	-2.94	118.72	122.90
4	E	7	MAN	O2-C2-C3	-2.93	104.27	110.14
3	F	1	NAG	C6-C5-C4	2.88	119.75	113.00
2	C	1	NAG	O6-C6-C5	-2.84	101.53	111.29
3	G	2	NAG	C3-C4-C5	2.84	115.31	110.24
2	C	1	NAG	O4-C4-C3	-2.71	104.09	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C5-C6	-2.67	103.02	107.20
2	C	6	BMA	O4-C4-C5	2.66	115.89	109.30
3	D	2	NAG	C3-C4-C5	2.64	114.95	110.24
3	G	2	NAG	O3-C3-C2	-2.64	104.00	109.47
4	E	1	NAG	C1-O5-C5	2.61	115.73	112.19
3	D	1	NAG	C8-C7-N2	-2.60	111.70	116.10
4	E	1	NAG	O4-C4-C3	-2.58	104.38	110.35
4	E	3	BMA	C1-O5-C5	-2.58	108.70	112.19
2	C	3	BMA	O6-C6-C5	-2.55	102.54	111.29
3	D	1	NAG	O3-C3-C2	-2.49	104.31	109.47
3	D	2	NAG	O3-C3-C2	-2.49	104.31	109.47
3	F	2	NAG	O4-C4-C3	-2.44	104.71	110.35
4	E	1	NAG	O5-C5-C6	-2.44	103.38	107.20
3	F	1	NAG	O3-C3-C2	-2.38	104.53	109.47
4	E	1	NAG	O7-C7-C8	2.38	126.48	122.06
2	C	1	NAG	O7-C7-C8	2.36	126.44	122.06
4	E	7	MAN	O5-C5-C6	2.26	110.75	107.20
2	C	4	MAN	O3-C3-C2	2.23	114.26	109.99
2	C	2	NAG	O6-C6-C5	-2.23	103.65	111.29
4	E	6	MAN	O4-C4-C3	-2.21	105.24	110.35
2	C	5	MAN	C1-C2-C3	-2.21	106.95	109.67
4	E	1	NAG	O3-C3-C4	-2.20	105.25	110.35
3	D	2	NAG	C8-C7-N2	-2.12	112.50	116.10
3	G	1	NAG	C1-O5-C5	2.10	115.03	112.19
3	D	1	NAG	O5-C5-C6	-2.05	103.98	107.20
4	E	5	BMA	O5-C5-C6	2.05	110.41	107.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

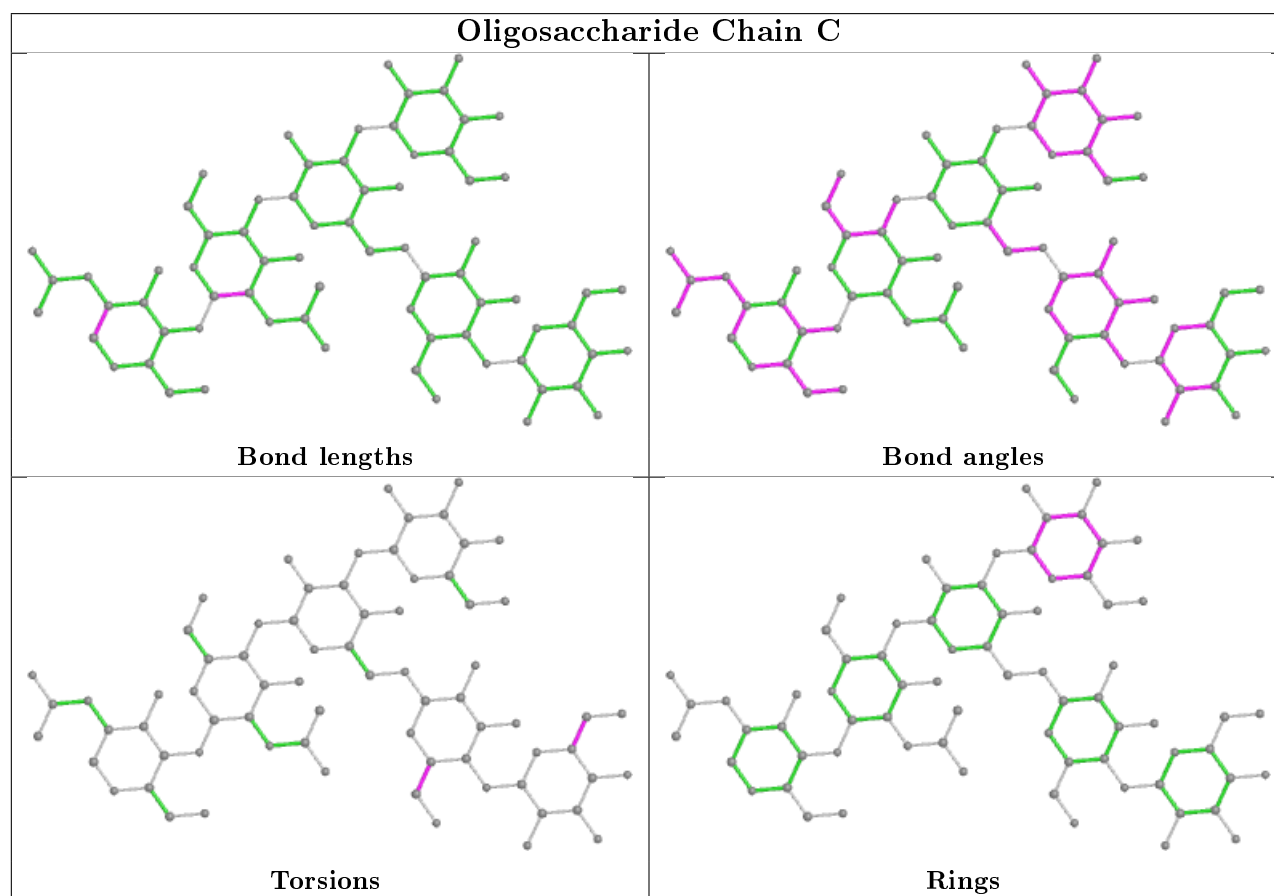
Mol	Chain	Res	Type	Atoms
2	C	4	MAN	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
4	E	4	BMA	O5-C5-C6-O6
4	E	7	MAN	C4-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
4	E	5	BMA	O5-C5-C6-O6
4	E	6	MAN	O5-C5-C6-O6
4	E	7	MAN	O5-C5-C6-O6

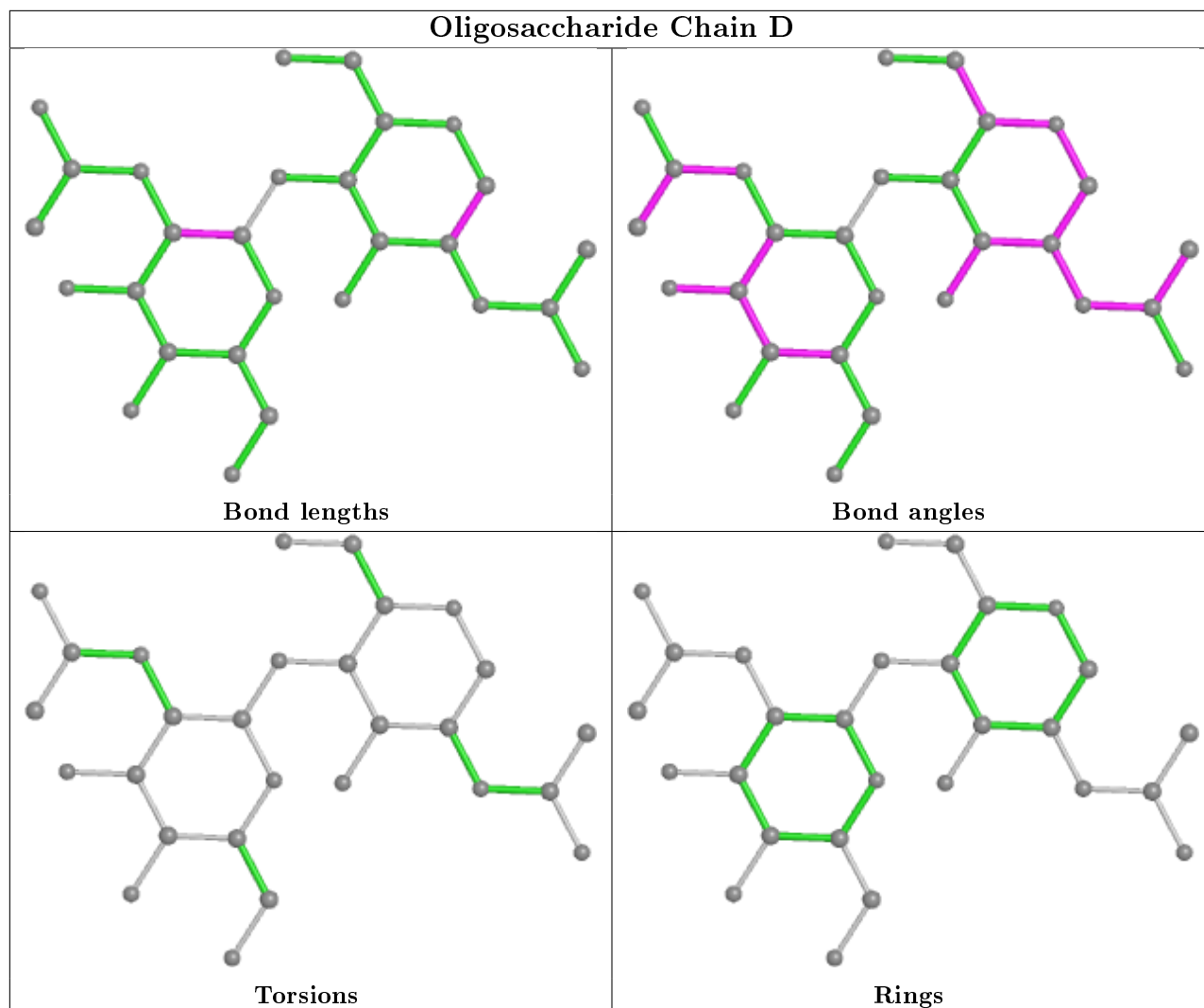
All (3) ring outliers are listed below:

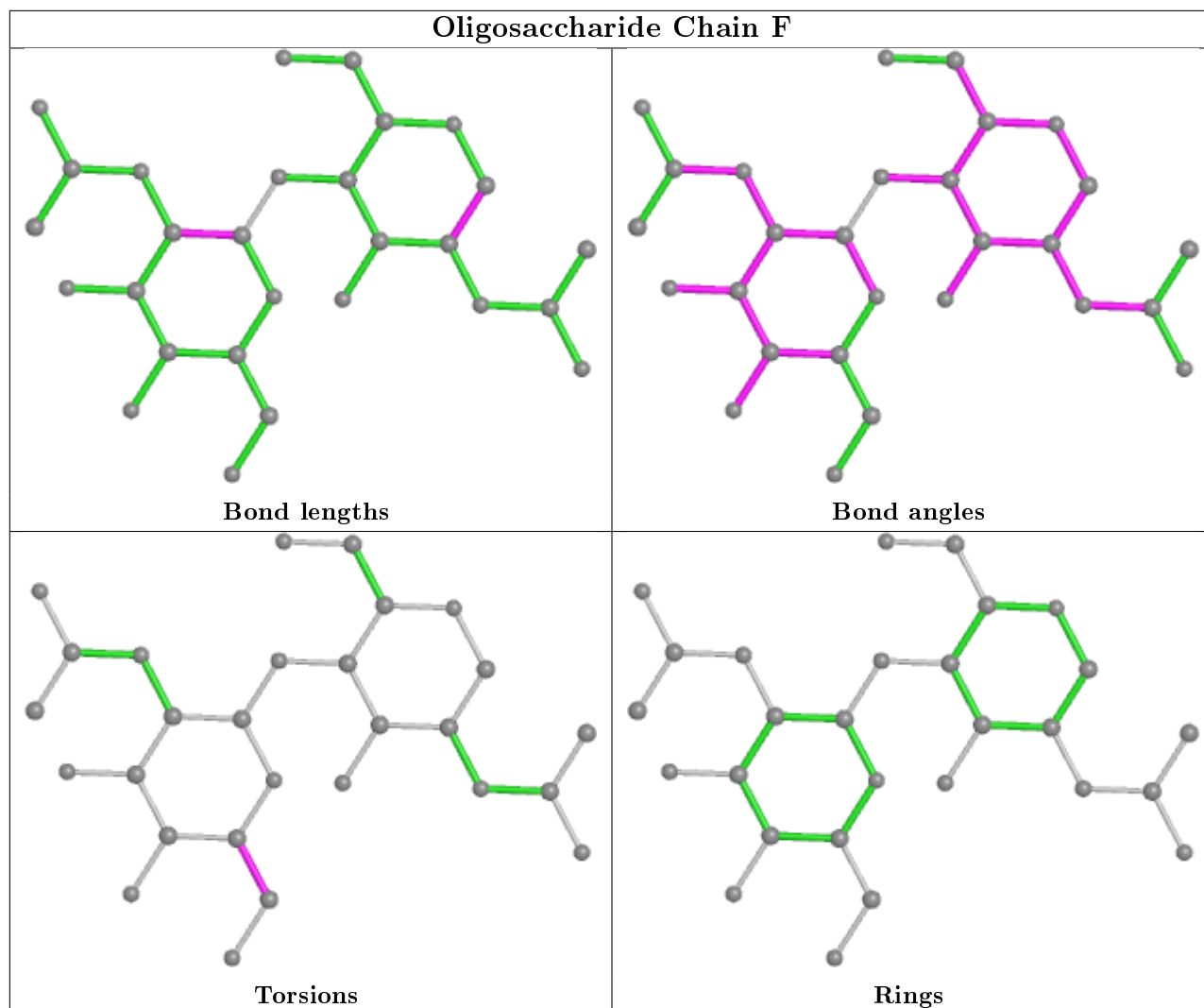
Mol	Chain	Res	Type	Atoms
4	E	6	MAN	C1-C2-C3-C4-C5-O5
4	E	4	BMA	C1-C2-C3-C4-C5-O5
2	C	6	BMA	C1-C2-C3-C4-C5-O5

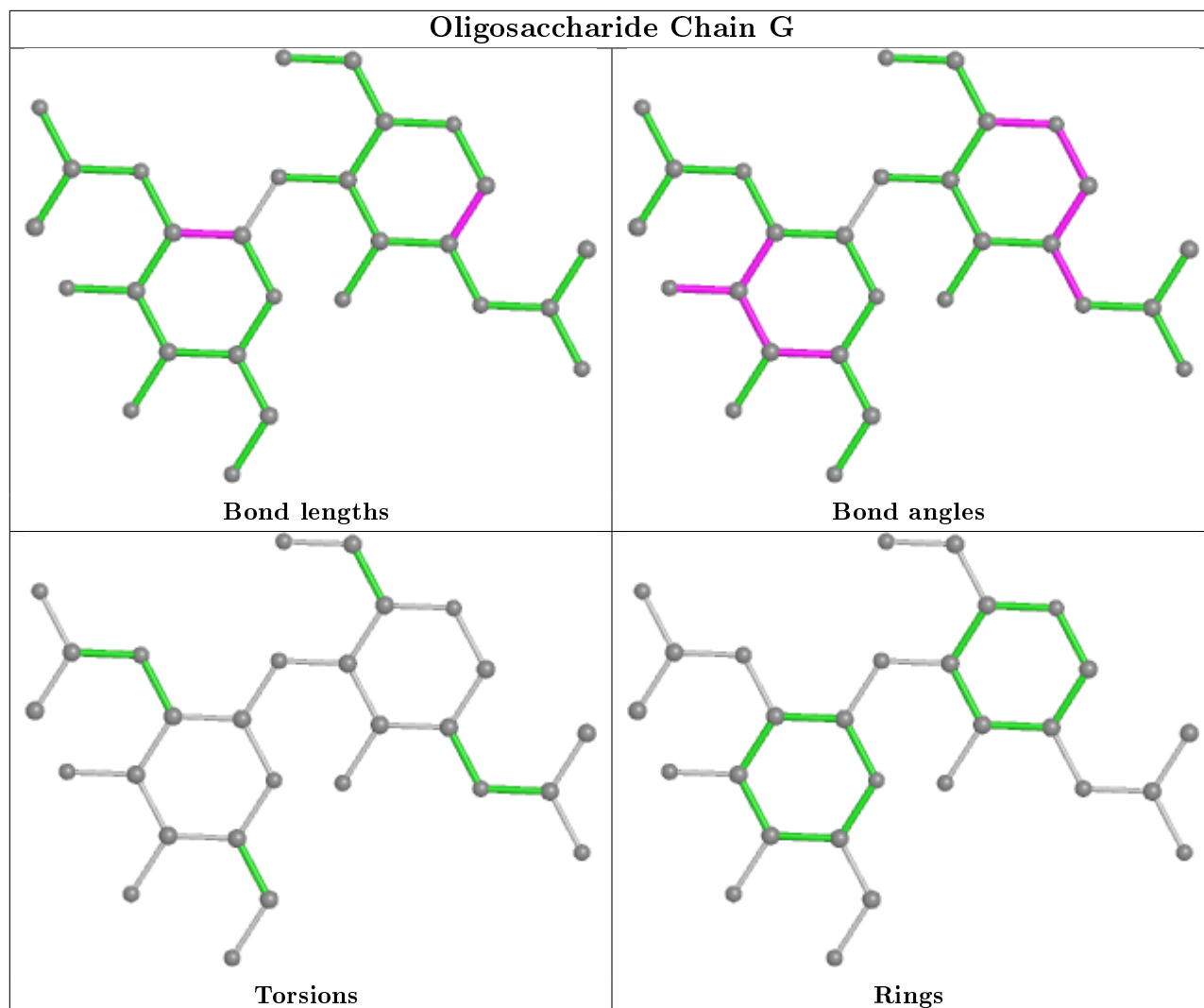
No monomer is involved in short contacts.

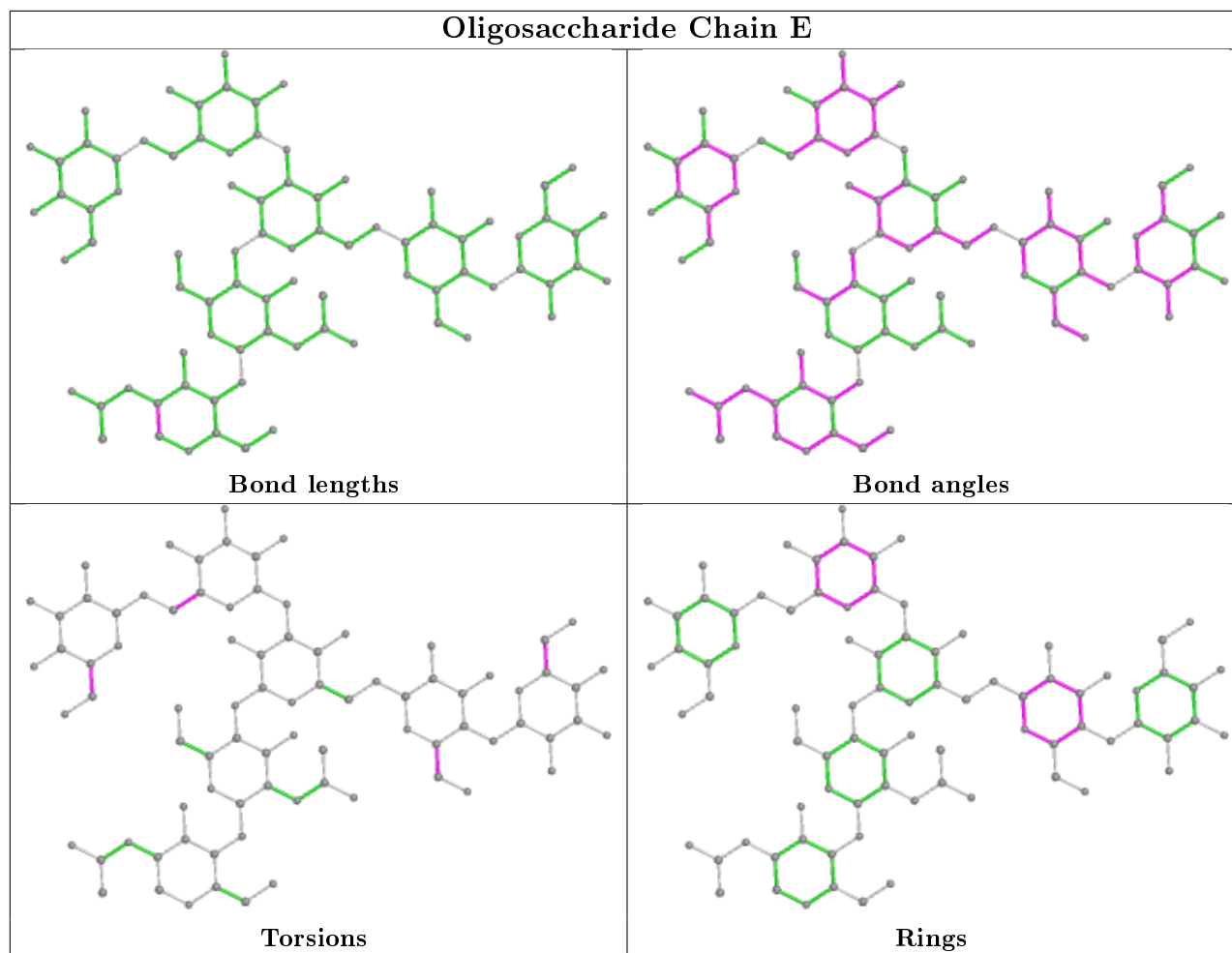
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	NAG	B	1114	1	14,14,15	0.93	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	B	1108	1	14,14,15	0.93	1 (7%)	17,19,21	1.02	1 (5%)
5	NAG	A	1109	1	14,14,15	1.11	1 (7%)	17,19,21	2.27	7 (41%)
6	SO4	A	1114	-	4,4,4	0.22	0	6,6,6	0.16	0
6	SO4	B	1117	-	4,4,4	0.15	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	A	1113	-	4,4,4	0.38	0	6,6,6	0.33	0
6	SO4	A	1112	-	4,4,4	0.54	0	6,6,6	0.40	0
5	NAG	A	1108	1	14,14,15	0.99	1 (7%)	17,19,21	1.94	5 (29%)
6	SO4	B	1121	-	4,4,4	0.38	0	6,6,6	0.41	0
5	NAG	A	1107	1	14,14,15	0.94	1 (7%)	17,19,21	1.08	2 (11%)
5	NAG	B	1109	1	14,14,15	0.98	1 (7%)	17,19,21	2.17	4 (23%)
6	SO4	B	1115	-	4,4,4	0.31	0	6,6,6	0.43	0
6	SO4	B	1120	-	4,4,4	0.42	0	6,6,6	0.40	0
6	SO4	B	1118	-	4,4,4	0.31	0	6,6,6	0.30	0
6	SO4	B	1116	-	4,4,4	0.94	0	6,6,6	0.71	0
6	SO4	B	1119	-	4,4,4	0.38	0	6,6,6	0.27	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
5	NAG	B	1114	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1108	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1109	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1108	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1107	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1109	1	-	3/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1109	NAG	C1-C2	2.75	1.56	1.52
5	A	1108	NAG	C1-C2	2.47	1.56	1.52
5	A	1107	NAG	C1-C2	2.37	1.55	1.52
5	B	1108	NAG	C1-C2	2.31	1.55	1.52
5	B	1114	NAG	C1-C2	2.28	1.55	1.52
5	B	1109	NAG	C1-C2	2.18	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1109	NAG	C1-C2-N2	6.63	121.81	110.49
5	A	1108	NAG	C1-C2-N2	5.59	120.04	110.49
5	A	1109	NAG	C2-N2-C7	-5.15	115.57	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1109	NAG	O4-C4-C3	-3.36	102.57	110.35
5	A	1109	NAG	O5-C1-C2	3.35	116.58	111.29
5	A	1109	NAG	O4-C4-C5	3.08	116.94	109.30
5	A	1109	NAG	C6-C5-C4	3.00	120.04	113.00
5	B	1109	NAG	C3-C4-C5	2.82	115.28	110.24
5	A	1109	NAG	C1-O5-C5	-2.76	108.45	112.19
5	A	1108	NAG	C3-C4-C5	2.66	114.98	110.24
5	A	1107	NAG	C1-O5-C5	2.60	115.71	112.19
5	B	1109	NAG	O4-C4-C3	-2.59	104.35	110.35
5	B	1108	NAG	C1-O5-C5	2.31	115.32	112.19
5	A	1107	NAG	O5-C1-C2	2.22	114.80	111.29
5	A	1108	NAG	O4-C4-C3	-2.21	105.25	110.35
5	B	1114	NAG	O5-C5-C6	2.17	110.61	107.20
5	B	1109	NAG	O6-C6-C5	2.12	118.57	111.29
5	A	1108	NAG	O5-C5-C6	2.06	110.43	107.20
5	A	1108	NAG	C1-O5-C5	2.03	114.95	112.19
5	A	1109	NAG	O7-C7-C8	2.00	125.77	122.06

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1108	NAG	C4-C5-C6-O6
5	B	1109	NAG	C4-C5-C6-O6
5	B	1109	NAG	O5-C5-C6-O6
5	A	1108	NAG	O5-C5-C6-O6
5	B	1114	NAG	C4-C5-C6-O6
5	B	1114	NAG	O5-C5-C6-O6
5	A	1108	NAG	C3-C2-N2-C7
5	B	1109	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1108	NAG	1	0
5	A	1107	NAG	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	157/165 (95%)	0.03	7 (4%) 33 31	25, 38, 66, 79	0
1	B	157/165 (95%)	-0.12	4 (2%) 57 55	23, 32, 65, 86	0
All	All	314/330 (95%)	-0.04	11 (3%) 44 41	23, 35, 66, 86	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	LEU	6.4
1	B	108	PRO	3.6
1	A	106	GLY	3.3
1	A	120	ARG	2.8
1	A	107	GLN	2.8
1	A	109	LEU	2.8
1	B	120[A]	ARG	2.4
1	A	16[A]	GLU	2.3
1	B	107	GLN	2.2
1	A	159	PHE	2.1
1	A	118	TYR	2.1

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

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

### 6.3 Carbohydrates [i](#)

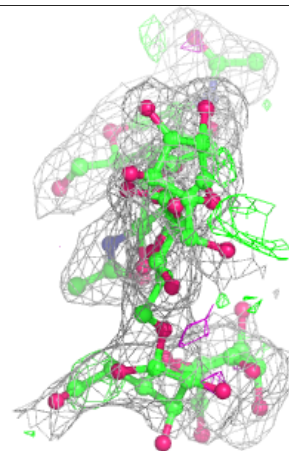
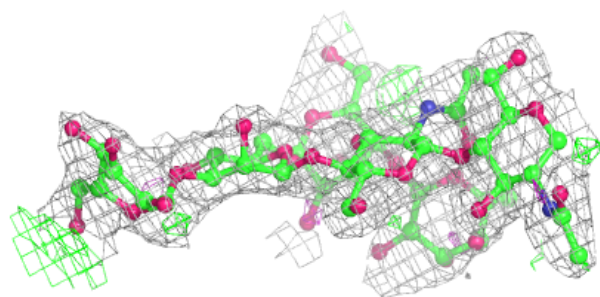
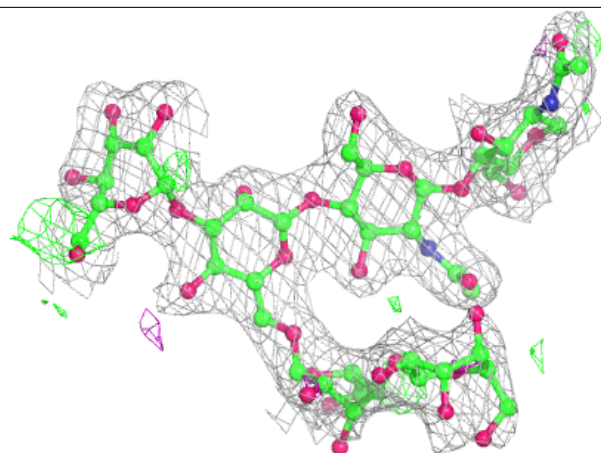
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	E	6	11/12	0.71	0.26	59,62,64,64	11
2	MAN	C	4	11/12	0.76	0.22	60,65,67,67	11
3	NAG	G	2	14/15	0.77	0.25	61,65,68,68	14
3	NAG	D	2	14/15	0.77	0.18	60,64,66,67	14
4	BMA	E	4	11/12	0.79	0.18	54,58,60,65	0
3	NAG	D	1	14/15	0.81	0.16	51,55,58,58	14
3	NAG	F	2	14/15	0.82	0.23	65,69,72,73	0
4	BMA	E	5	11/12	0.83	0.26	67,70,72,72	11
2	MAN	C	5	11/12	0.84	0.24	73,77,79,80	0
4	MAN	E	7	11/12	0.85	0.24	64,67,69,70	11
2	BMA	C	6	11/12	0.87	0.15	53,56,59,64	0
3	NAG	G	1	14/15	0.89	0.13	51,54,57,58	14
3	NAG	F	1	14/15	0.90	0.14	47,51,54,57	0
2	NAG	C	1	14/15	0.94	0.14	30,33,36,39	14
4	BMA	E	3	11/12	0.94	0.14	45,48,51,56	0
4	NAG	E	1	14/15	0.96	0.11	33,36,39,41	0
4	NAG	E	2	14/15	0.96	0.12	37,40,43,44	0
2	BMA	C	3	11/12	0.97	0.10	42,45,48,53	0
2	NAG	C	2	14/15	0.98	0.11	34,37,40,42	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.

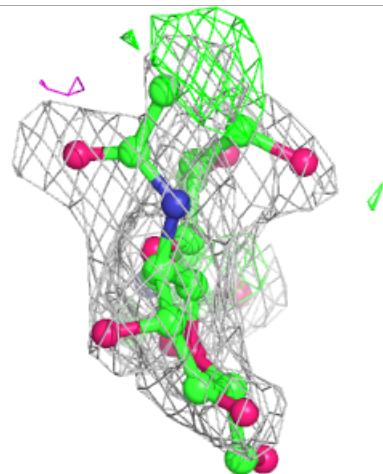
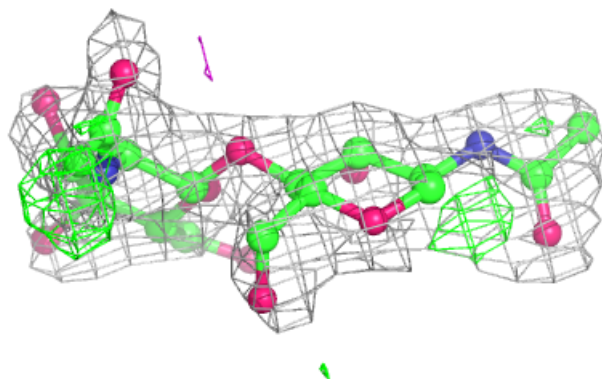
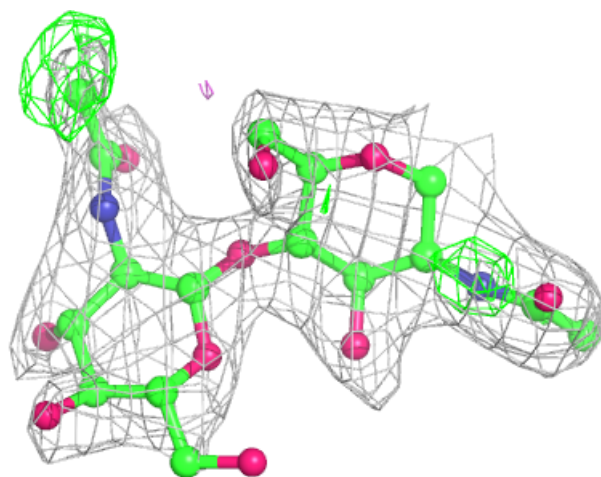
**Electron density around Chain C:**

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



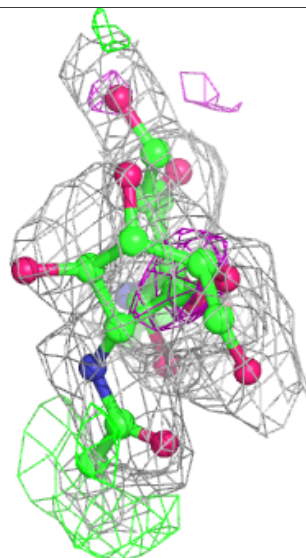
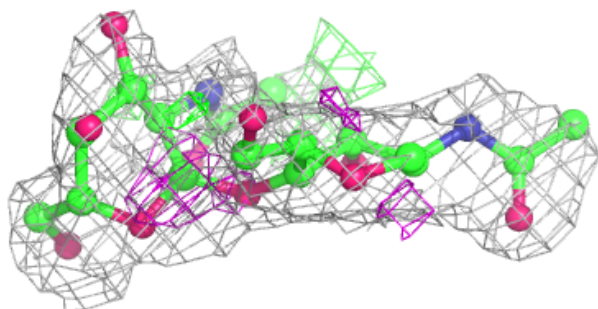
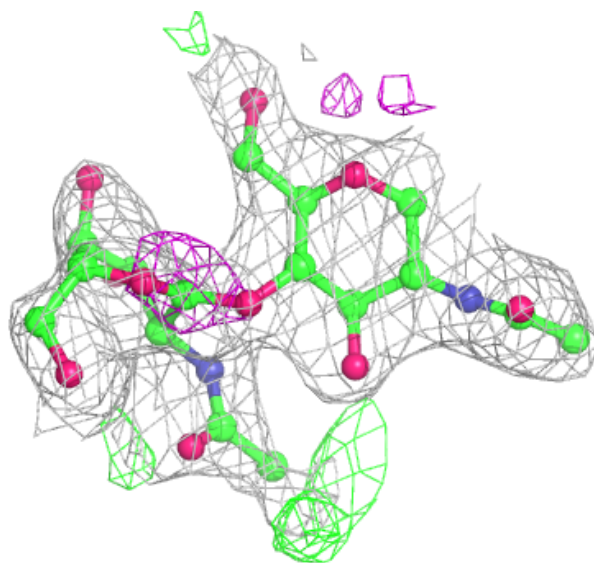
**Electron density around Chain D:**

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



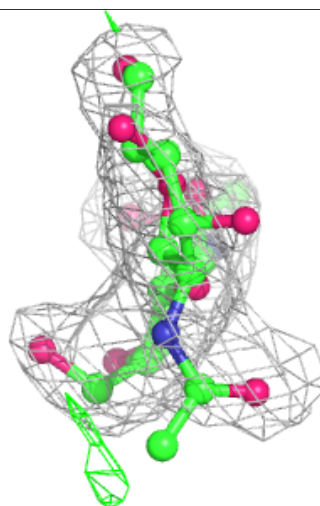
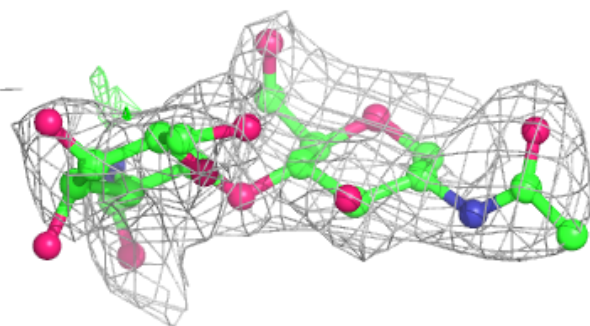
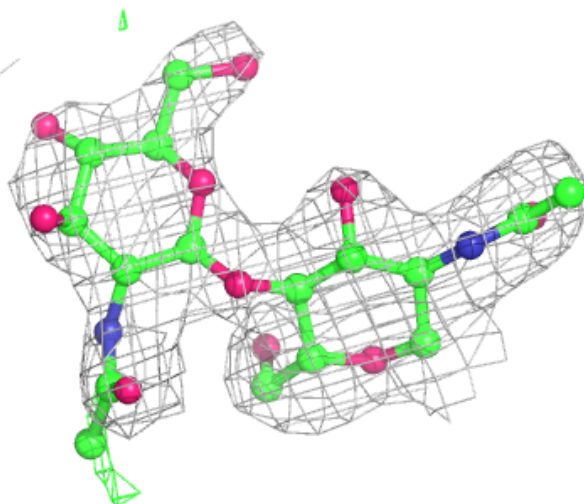
**Electron density around Chain F:**

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

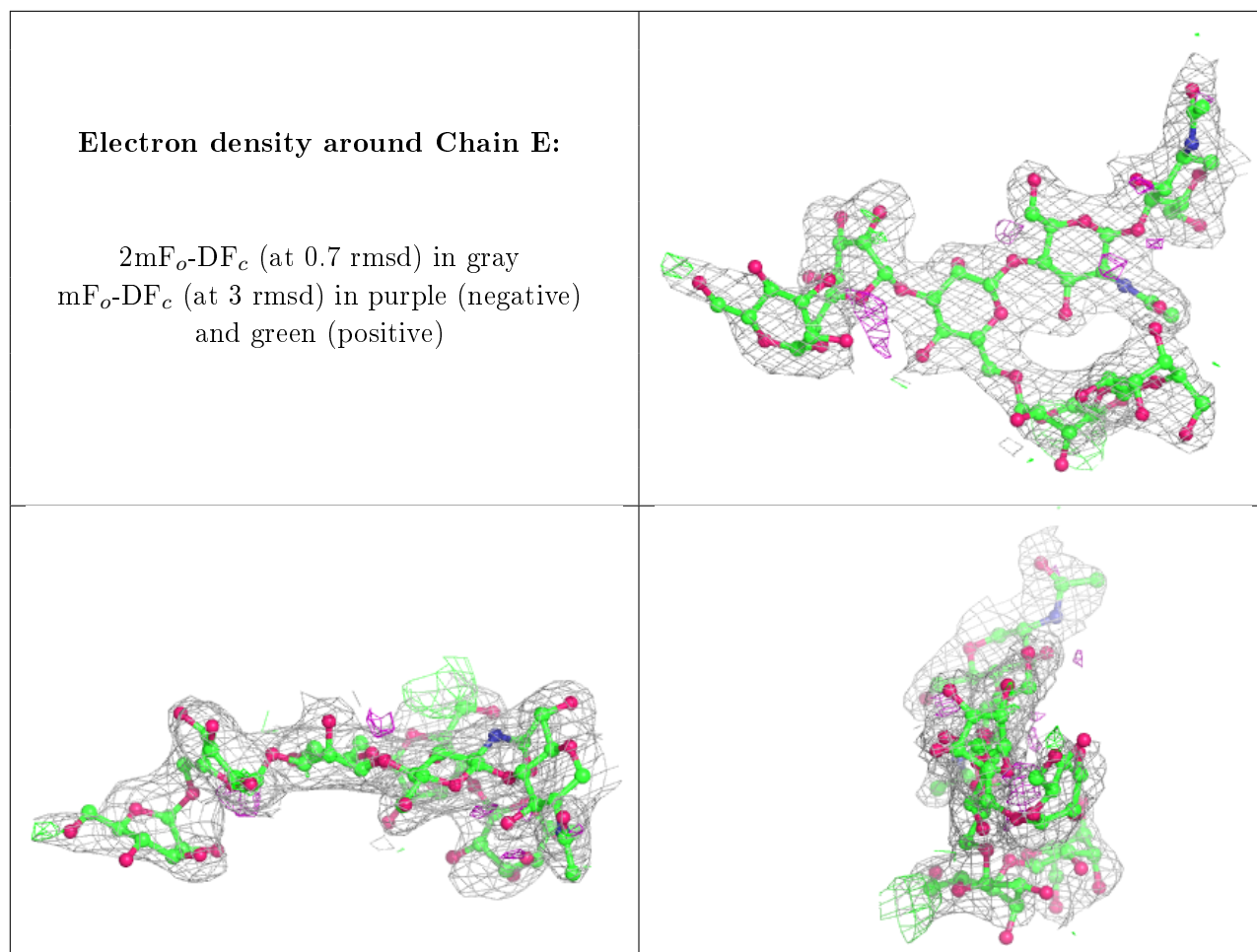


**Electron density around Chain G:**

$2mF_o-DF_c$  (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
5	NAG	A	1108	14/15	0.66	0.31	79,83,86,86	14
5	NAG	B	1109	14/15	0.66	0.21	49,53,56,57	14
5	NAG	B	1108	14/15	0.77	0.17	65,69,72,72	14
5	NAG	A	1109	14/15	0.80	0.17	47,50,53,54	0
6	SO4	B	1121	5/5	0.87	0.34	84,87,89,92	0
5	NAG	A	1107	14/15	0.88	0.14	68,72,75,75	14
5	NAG	B	1114	14/15	0.90	0.23	63,67,69,69	14
6	SO4	B	1117	5/5	0.91	0.21	74,79,79,80	5
6	SO4	A	1114	5/5	0.93	0.12	101,106,107,107	0
6	SO4	A	1113	5/5	0.95	0.20	50,53,56,56	5
6	SO4	B	1118	5/5	0.95	0.20	59,62,65,65	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	B	1119	5/5	0.96	0.23	57,59,62,63	5
6	SO4	A	1112	5/5	0.97	0.18	49,52,54,57	0
6	SO4	B	1120	5/5	0.98	0.24	24,26,30,31	5
6	SO4	B	1115	5/5	0.99	0.14	33,33,38,38	0
6	SO4	B	1116	5/5	1.00	0.15	27,30,31,33	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.