



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 03:50 AM BST

PDB ID : 4POR  
Title : Structure of Human Polyomavirus 9 VP1 pentamer in complex with 3'-sialyllactose  
Authors : Khan, Z.M.; Stehle, T.  
Deposited on : 2014-02-26  
Resolution : 2.09 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

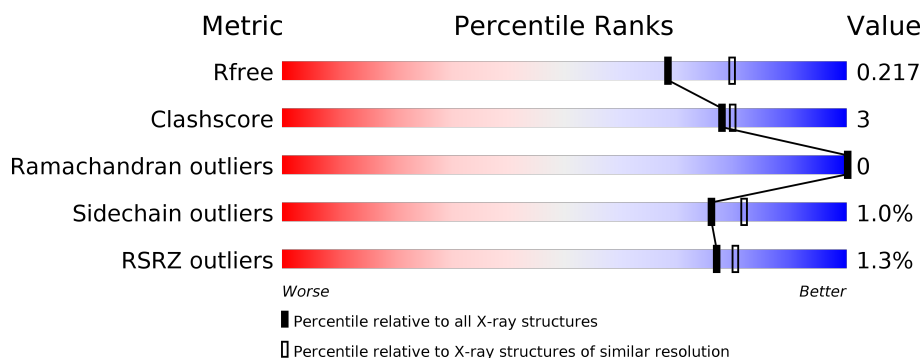
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	278	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </div> <div></div> </div>
1	B	278	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div></div> </div> <div></div> </div>
1	C	278	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div></div> </div> <div></div> </div>
1	D	278	<div> <div></div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> <div></div> </div>
1	E	278	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div> <div></div> </div>
1	F	278	<div> <div></div> <div> <div></div> <div>92%</div> <div>6%</div> <div></div> </div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
1	G	278	
1	H	278	
1	I	278	
1	J	278	
2	K	3	
2	L	3	
2	M	3	
2	N	3	
2	O	3	
2	P	3	
2	Q	3	
2	R	3	
2	S	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	C	403	-	-	X	-
4	EDO	H	404	-	-	X	-
4	EDO	I	403	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23567 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2059	1297	341	410	11			
1	B	270	Total	C	N	O	S	0	2	0
			2070	1304	341	414	11			
1	C	269	Total	C	N	O	S	0	0	0
			2050	1292	340	407	11			
1	D	270	Total	C	N	O	S	0	0	0
			2059	1297	341	410	11			
1	E	269	Total	C	N	O	S	0	2	0
			2066	1302	342	411	11			
1	F	272	Total	C	N	O	S	0	3	0
			2101	1324	346	420	11			
1	G	266	Total	C	N	O	S	0	1	0
			2035	1283	338	404	10			
1	H	270	Total	C	N	O	S	0	0	0
			2059	1297	341	410	11			
1	I	269	Total	C	N	O	S	0	0	0
			2052	1293	340	408	11			
1	J	273	Total	C	N	O	S	0	0	0
			2083	1313	344	415	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP E9NQ90
A	28	SER	-	expression tag	UNP E9NQ90
A	29	HIS	-	expression tag	UNP E9NQ90
A	30	MET	-	expression tag	UNP E9NQ90
B	27	GLY	-	expression tag	UNP E9NQ90
B	28	SER	-	expression tag	UNP E9NQ90
B	29	HIS	-	expression tag	UNP E9NQ90
B	30	MET	-	expression tag	UNP E9NQ90
C	27	GLY	-	expression tag	UNP E9NQ90

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Chain	Residue	Modelled	Actual	Comment	Reference
C	28	SER	-	expression tag	UNP E9NQ90
C	29	HIS	-	expression tag	UNP E9NQ90
C	30	MET	-	expression tag	UNP E9NQ90
D	27	GLY	-	expression tag	UNP E9NQ90
D	28	SER	-	expression tag	UNP E9NQ90
D	29	HIS	-	expression tag	UNP E9NQ90
D	30	MET	-	expression tag	UNP E9NQ90
E	27	GLY	-	expression tag	UNP E9NQ90
E	28	SER	-	expression tag	UNP E9NQ90
E	29	HIS	-	expression tag	UNP E9NQ90
E	30	MET	-	expression tag	UNP E9NQ90
F	27	GLY	-	expression tag	UNP E9NQ90
F	28	SER	-	expression tag	UNP E9NQ90
F	29	HIS	-	expression tag	UNP E9NQ90
F	30	MET	-	expression tag	UNP E9NQ90
G	27	GLY	-	expression tag	UNP E9NQ90
G	28	SER	-	expression tag	UNP E9NQ90
G	29	HIS	-	expression tag	UNP E9NQ90
G	30	MET	-	expression tag	UNP E9NQ90
H	27	GLY	-	expression tag	UNP E9NQ90
H	28	SER	-	expression tag	UNP E9NQ90
H	29	HIS	-	expression tag	UNP E9NQ90
H	30	MET	-	expression tag	UNP E9NQ90
I	27	GLY	-	expression tag	UNP E9NQ90
I	28	SER	-	expression tag	UNP E9NQ90
I	29	HIS	-	expression tag	UNP E9NQ90
I	30	MET	-	expression tag	UNP E9NQ90
J	27	GLY	-	expression tag	UNP E9NQ90
J	28	SER	-	expression tag	UNP E9NQ90
J	29	HIS	-	expression tag	UNP E9NQ90
J	30	MET	-	expression tag	UNP E9NQ90

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	3	Total	C	N	O	0	0	0
			43	23	1	19			

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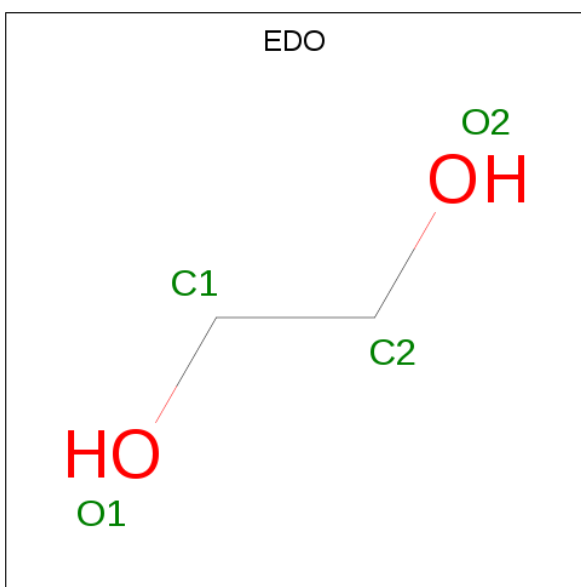
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	L	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	M	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	N	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	O	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	P	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	Q	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	R	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	S	3	Total	C	N	O	0	0	0
			43	23	1	19			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

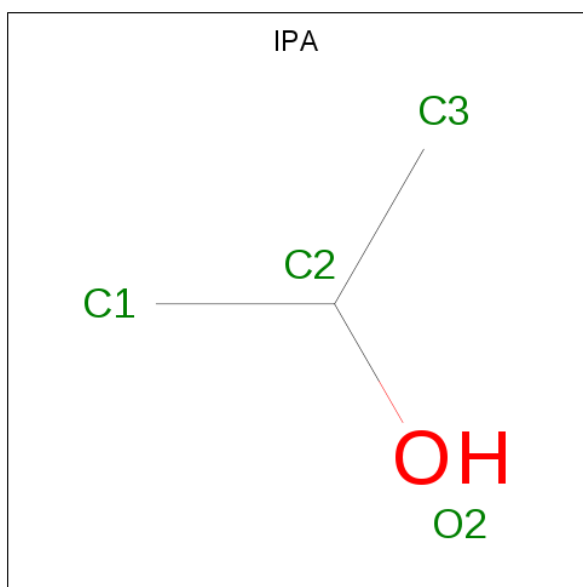
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	F	1	Total 4	C 2	O 2	0	0
4	F	1	Total 4	C 2	O 2	0	0
4	F	1	Total 4	C 2	O 2	0	0
4	G	1	Total 4	C 2	O 2	0	0
4	G	1	Total 4	C 2	O 2	0	0
4	G	1	Total 4	C 2	O 2	0	0
4	G	1	Total 4	C 2	O 2	0	0
4	H	1	Total 4	C 2	O 2	0	0
4	H	1	Total 4	C 2	O 2	0	0
4	H	1	Total 4	C 2	O 2	0	0
4	H	1	Total 4	C 2	O 2	0	0
4	I	1	Total 4	C 2	O 2	0	0
4	I	1	Total 4	C 2	O 2	0	0
4	I	1	Total 4	C 2	O 2	0	0
4	J	1	Total 4	C 2	O 2	0	0

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 3 1	0	0
5	B	1	Total C O 4 3 1	0	0
5	C	1	Total C O 4 3 1	0	0
5	D	1	Total C O 4 3 1	0	0
5	E	1	Total C O 4 3 1	0	0
5	F	1	Total C O 4 3 1	0	0
5	G	1	Total C O 4 3 1	0	0
5	H	1	Total C O 4 3 1	0	0
5	I	1	Total C O 4 3 1	0	0
5	J	1	Total C O 4 3 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	250	Total O 250 250	0	0
6	B	259	Total O 259 259	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	216	Total 216	O 216	0	0
6	D	207	Total 207	O 207	0	0
6	E	241	Total 241	O 241	0	0
6	F	230	Total 230	O 230	0	0
6	G	236	Total 236	O 236	0	0
6	H	250	Total 250	O 250	0	0
6	I	260	Total 260	O 260	0	0
6	J	215	Total 215	O 215	0	0




- Molecule 1: VP1

Chain F:  92% 6%

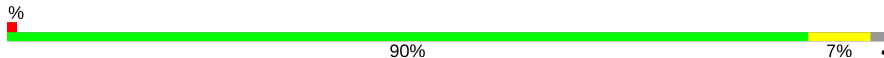


- Molecule 1: VP1

Chain G:  90% 6%



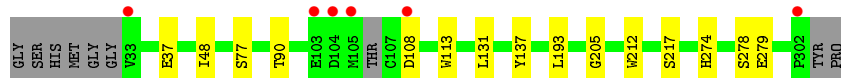
- Molecule 1: VP1

Chain H:  90% 7%



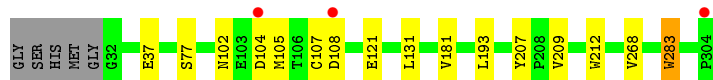
- Molecule 1: VP1

Chain I:  91% 5%

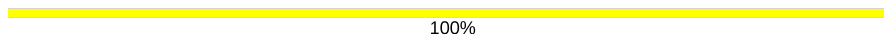


- Molecule 1: VP1

Chain J:  92% 5%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain K:  100%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain L:  67% 33%

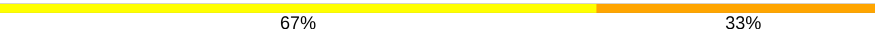


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain M:  33% 33% 33%

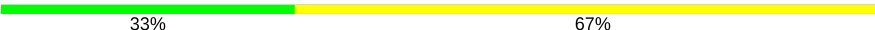


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain N:  67% 33%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain O:  33% 67%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain P:  33% 33% 33%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain Q:  33% 33% 33%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain R:  33% 33% 33%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain S:  33% 33% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.01Å 180.40Å 199.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	133.85 – 2.09 48.11 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.9 (133.85-2.09) 99.0 (48.11-2.09)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0025	Depositor
R, $R_{free}$	0.178 , 0.216 0.180 , 0.217	Depositor DCC
$R_{free}$ test set	10219 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: BGC, IPA, CA, EDO, SIA, GAL

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	0.58	1/2103 (0.0%)	0.65	0/2872
1	B	0.53	2/2120 (0.1%)	0.61	0/2895
1	C	0.50	0/2093	0.59	0/2857
1	D	0.51	0/2103	0.61	0/2872
1	E	0.52	2/2109 (0.1%)	0.61	0/2879
1	F	0.52	2/2147 (0.1%)	0.60	0/2932
1	G	0.50	1/2078 (0.0%)	0.60	0/2837
1	H	0.55	2/2103 (0.1%)	0.62	0/2872
1	I	0.52	2/2095 (0.1%)	0.61	0/2859
1	J	0.54	2/2129 (0.1%)	0.62	0/2907
All	All	0.53	14/21080 (0.1%)	0.61	0/28782

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	PRO	C-N	-8.00	1.15	1.34
1	F	113	TRP	CD2-CE2	5.65	1.48	1.41
1	F	283	TRP	CD2-CE2	5.56	1.48	1.41
1	J	212	TRP	CD2-CE2	5.48	1.48	1.41
1	E	113	TRP	CD2-CE2	5.44	1.47	1.41

There are no bond angle outliers.

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	2059	0	2036	14	0
1	B	2070	0	2047	14	0
1	C	2050	0	2031	19	0
1	D	2059	0	2038	11	0
1	E	2066	0	2044	15	0
1	F	2101	0	2071	14	0
1	G	2035	0	2012	11	0
1	H	2059	0	2037	16	0
1	I	2052	0	2029	11	0
1	J	2083	0	2057	11	0
2	K	43	0	37	2	0
2	L	43	0	37	1	0
2	M	43	0	37	3	0
2	N	43	0	37	2	0
2	O	43	0	37	2	0
2	P	43	0	37	2	0
2	Q	43	0	37	1	0
2	R	43	0	37	2	0
2	S	43	0	37	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	12	0	18	0	0
4	B	12	0	18	4	0
4	C	16	0	24	8	0
4	D	16	0	24	2	0
4	E	16	0	24	1	0
4	F	12	0	18	1	0
4	G	16	0	24	2	0
4	H	16	0	24	6	0
4	I	12	0	18	5	0
4	J	4	0	6	0	0
5	A	4	0	8	0	0
5	B	4	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	4	0	8	0	0
5	D	4	0	8	0	0
5	E	4	0	8	2	0
5	F	4	0	8	2	0
5	G	4	0	8	0	0
5	H	4	0	8	0	0
5	I	4	0	8	0	0
5	J	4	0	8	0	0
6	A	250	0	0	0	0
6	B	259	0	0	2	0
6	C	216	0	0	0	0
6	D	207	0	0	1	0
6	E	241	0	0	0	0
6	F	230	0	0	1	0
6	G	236	0	0	1	0
6	H	250	0	0	2	0
6	I	260	0	0	0	0
6	J	215	0	0	1	0
All	All	23567	0	21013	121	0

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

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:223:ARG:HD2	4:H:404:EDO:H22	1.19	1.12
1:H:223:ARG:CD	4:H:404:EDO:H22	2.03	0.86
1:B:104:ASP:OD1	1:B:106:THR:OG1	1.95	0.85
1:B:223:ARG:HD2	4:B:404:EDO:H21	1.60	0.83
1:F:51:TYR:CD2	4:G:403:EDO:H12	2.16	0.80

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	268/278 (96%)	257 (96%)	11 (4%)	0	100	100
1	B	270/278 (97%)	256 (95%)	14 (5%)	0	100	100
1	C	265/278 (95%)	254 (96%)	11 (4%)	0	100	100
1	D	268/278 (96%)	257 (96%)	11 (4%)	0	100	100
1	E	267/278 (96%)	258 (97%)	9 (3%)	0	100	100
1	F	273/278 (98%)	263 (96%)	10 (4%)	0	100	100
1	G	263/278 (95%)	254 (97%)	9 (3%)	0	100	100
1	H	268/278 (96%)	253 (94%)	15 (6%)	0	100	100
1	I	265/278 (95%)	252 (95%)	13 (5%)	0	100	100
1	J	271/278 (98%)	258 (95%)	13 (5%)	0	100	100
All	All	2678/2780 (96%)	2562 (96%)	116 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/240 (98%)	233 (99%)	2 (1%)	78	84
1	B	237/240 (99%)	235 (99%)	2 (1%)	81	86
1	C	234/240 (98%)	231 (99%)	3 (1%)	69	75
1	D	235/240 (98%)	232 (99%)	3 (1%)	69	75
1	E	236/240 (98%)	234 (99%)	2 (1%)	81	86
1	F	240/240 (100%)	238 (99%)	2 (1%)	81	86
1	G	232/240 (97%)	229 (99%)	3 (1%)	69	75
1	H	235/240 (98%)	233 (99%)	2 (1%)	78	84
1	I	234/240 (98%)	232 (99%)	2 (1%)	78	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	237/240 (99%)	235 (99%)	2 (1%)	81	86
All	All	2355/2400 (98%)	2332 (99%)	23 (1%)	76	82

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	121	GLU
1	F	121	GLU
1	J	121	GLU
1	E	193	LEU
1	F	193	LEU

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

Mol	Chain	Res	Type
1	D	274	HIS
1	H	239	GLN
1	F	274	HIS
1	D	47	GLN
1	F	47	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 ⓘ

27 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BGC	K	1	2	12,12,12	0.56	0	17,17,17	1.00	1 (5%)
2	GAL	K	2	2	11,11,12	0.59	0	15,15,17	0.92	1 (6%)
2	SIA	K	3	2	17,20,21	0.74	0	21,28,31	0.88	0
2	BGC	L	1	2	12,12,12	0.42	0	17,17,17	0.74	0
2	GAL	L	2	2	11,11,12	0.59	0	15,15,17	1.05	1 (6%)
2	SIA	L	3	2	17,20,21	0.78	0	21,28,31	0.75	0
2	BGC	M	1	2	12,12,12	0.49	0	17,17,17	0.64	0
2	GAL	M	2	2	11,11,12	0.54	0	15,15,17	1.60	2 (13%)
2	SIA	M	3	2	17,20,21	0.62	0	21,28,31	0.82	0
2	BGC	N	1	2	12,12,12	0.50	0	17,17,17	1.34	3 (17%)
2	GAL	N	2	2	11,11,12	0.59	0	15,15,17	1.20	1 (6%)
2	SIA	N	3	2	17,20,21	0.75	0	21,28,31	1.00	0
2	BGC	O	1	2	12,12,12	0.50	0	17,17,17	0.73	0
2	GAL	O	2	2	11,11,12	0.64	0	15,15,17	0.93	1 (6%)
2	SIA	O	3	2	17,20,21	0.53	0	21,28,31	0.72	0
2	BGC	P	1	2	12,12,12	0.45	0	17,17,17	0.60	0
2	GAL	P	2	2	11,11,12	0.56	0	15,15,17	1.36	2 (13%)
2	SIA	P	3	2	17,20,21	0.48	0	21,28,31	0.66	0
2	BGC	Q	1	2	12,12,12	0.44	0	17,17,17	0.99	1 (5%)
2	GAL	Q	2	2	11,11,12	0.67	0	15,15,17	1.26	2 (13%)
2	SIA	Q	3	2	17,20,21	0.65	0	21,28,31	0.72	0
2	BGC	R	1	2	12,12,12	0.45	0	17,17,17	0.90	0
2	GAL	R	2	2	11,11,12	0.63	0	15,15,17	0.87	1 (6%)
2	SIA	R	3	2	17,20,21	0.66	0	21,28,31	0.80	0
2	BGC	S	1	2	12,12,12	0.53	0	17,17,17	1.06	0
2	GAL	S	2	2	11,11,12	0.66	0	15,15,17	1.02	1 (6%)
2	SIA	S	3	2	17,20,21	0.63	0	21,28,31	0.99	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	K	1	2	-	0/2/22/22	0/1/1/1
2	GAL	K	2	2	-	1/2/19/22	0/1/1/1
2	SIA	K	3	2	-	0/14/34/38	0/1/1/1
2	BGC	L	1	2	-	0/2/22/22	0/1/1/1
2	GAL	L	2	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	L	3	2	-	0/14/34/38	0/1/1/1
2	BGC	M	1	2	-	0/2/22/22	0/1/1/1
2	GAL	M	2	2	-	1/2/19/22	0/1/1/1
2	SIA	M	3	2	-	4/14/34/38	0/1/1/1
2	BGC	N	1	2	-	0/2/22/22	0/1/1/1
2	GAL	N	2	2	-	2/2/19/22	0/1/1/1
2	SIA	N	3	2	-	0/14/34/38	0/1/1/1
2	BGC	O	1	2	-	0/2/22/22	0/1/1/1
2	GAL	O	2	2	-	1/2/19/22	0/1/1/1
2	SIA	O	3	2	-	1/14/34/38	0/1/1/1
2	BGC	P	1	2	-	0/2/22/22	0/1/1/1
2	GAL	P	2	2	-	1/2/19/22	0/1/1/1
2	SIA	P	3	2	-	0/14/34/38	0/1/1/1
2	BGC	Q	1	2	-	0/2/22/22	0/1/1/1
2	GAL	Q	2	2	-	1/2/19/22	0/1/1/1
2	SIA	Q	3	2	-	0/14/34/38	0/1/1/1
2	BGC	R	1	2	-	0/2/22/22	0/1/1/1
2	GAL	R	2	2	-	1/2/19/22	0/1/1/1
2	SIA	R	3	2	-	0/14/34/38	0/1/1/1
2	BGC	S	1	2	-	0/2/22/22	0/1/1/1
2	GAL	S	2	2	-	2/2/19/22	0/1/1/1
2	SIA	S	3	2	-	0/14/34/38	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	2	GAL	C1-O5-C5	4.69	118.55	112.19
2	P	2	GAL	C1-O5-C5	3.80	117.34	112.19
2	Q	2	GAL	C1-O5-C5	3.44	116.85	112.19
2	L	2	GAL	C1-O5-C5	2.91	116.14	112.19
2	N	1	BGC	C1-O5-C5	-2.80	108.39	113.66

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	2	GAL	O5-C5-C6-O6
2	N	2	GAL	O5-C5-C6-O6
2	S	2	GAL	O5-C5-C6-O6
2	L	2	GAL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	M	3	SIA	C6-C7-C8-O8

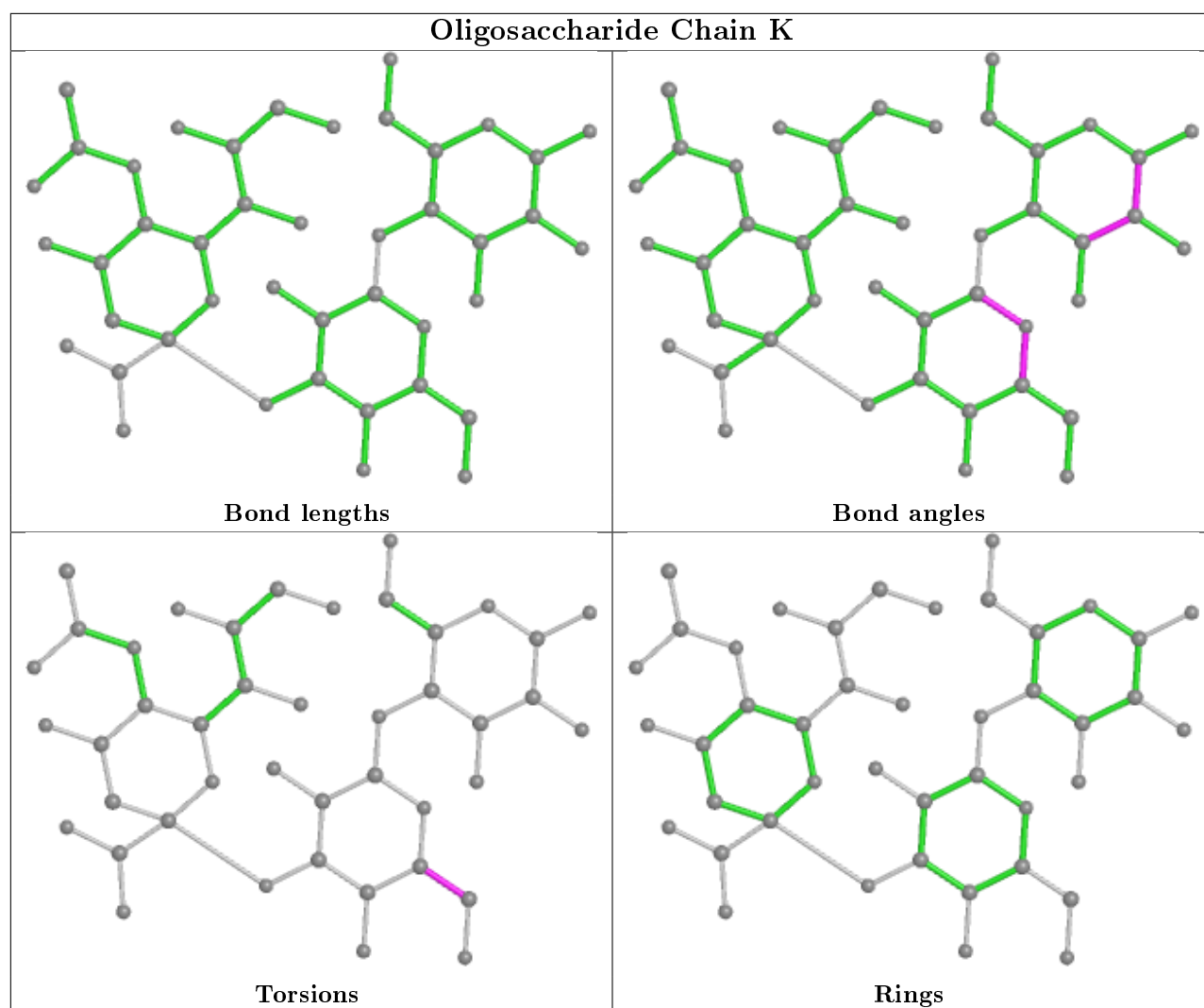
There are no ring outliers.

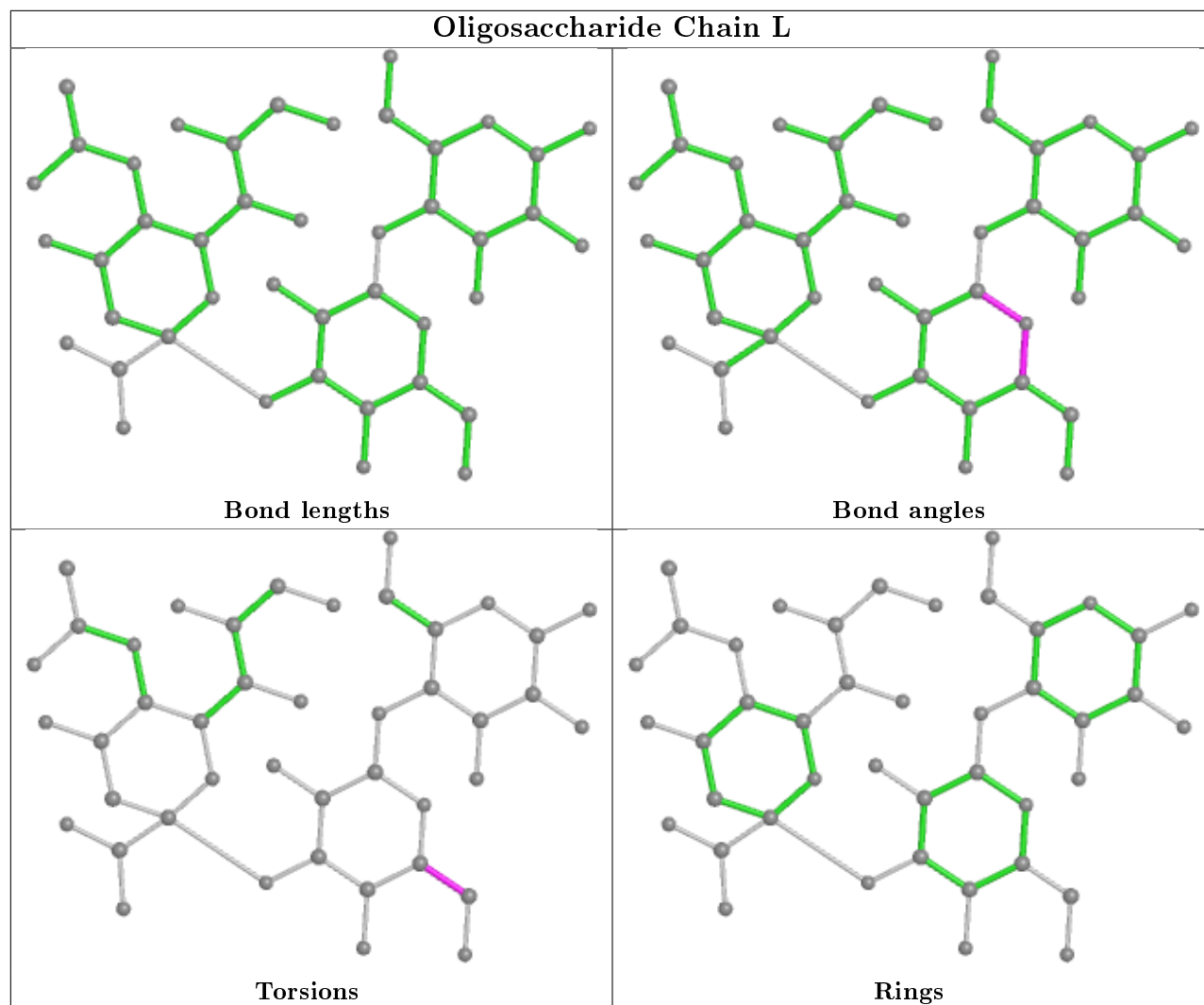
13 monomers are involved in 16 short contacts:

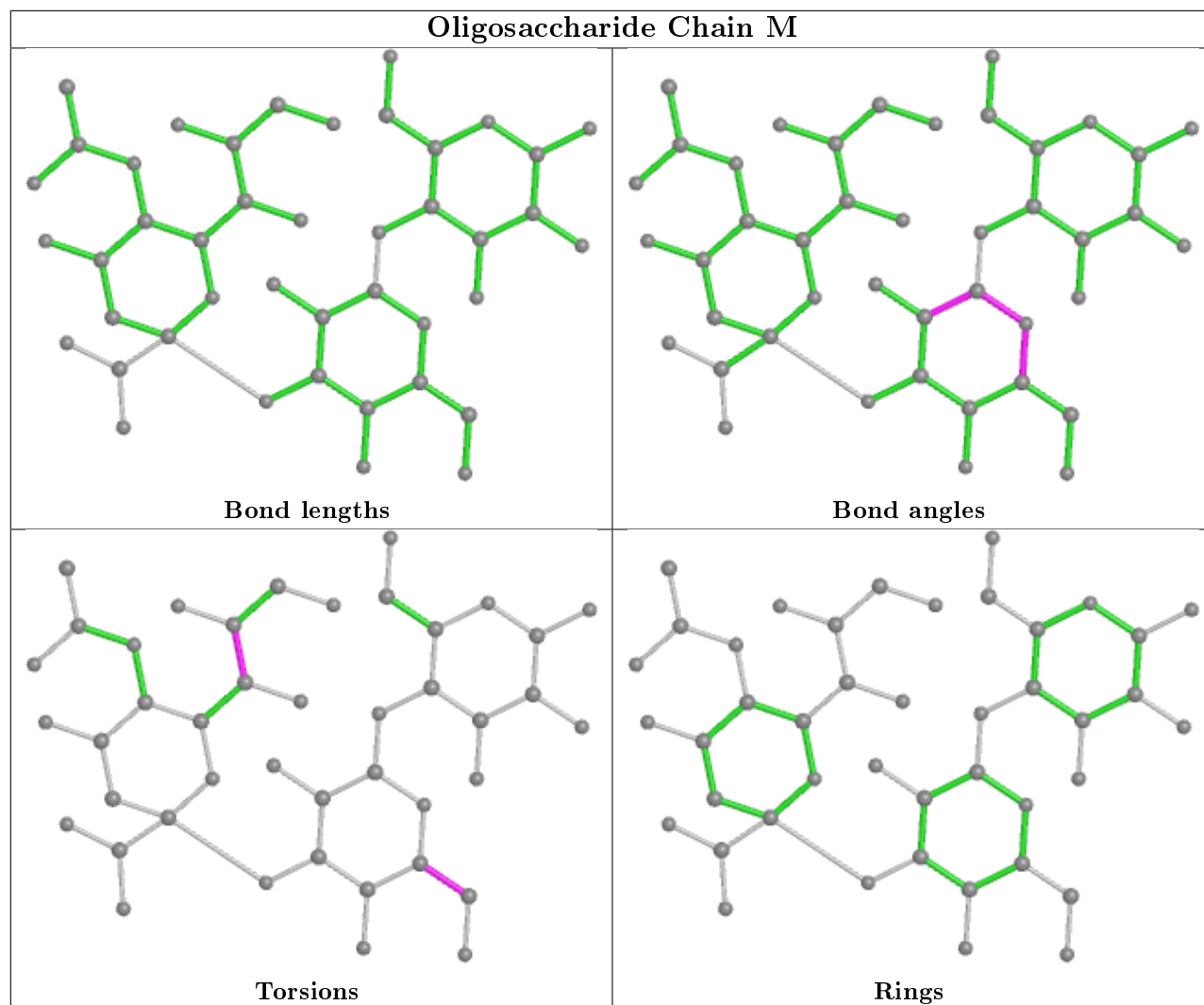
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	2	GAL	1	0
2	N	3	SIA	1	0
2	O	3	SIA	2	0
2	R	2	GAL	1	0
2	S	2	GAL	1	0
2	K	3	SIA	2	0
2	M	2	GAL	2	0
2	P	3	SIA	1	0
2	N	2	GAL	1	0
2	M	3	SIA	2	0
2	P	2	GAL	1	0
2	R	3	SIA	1	0
2	L	2	GAL	1	0

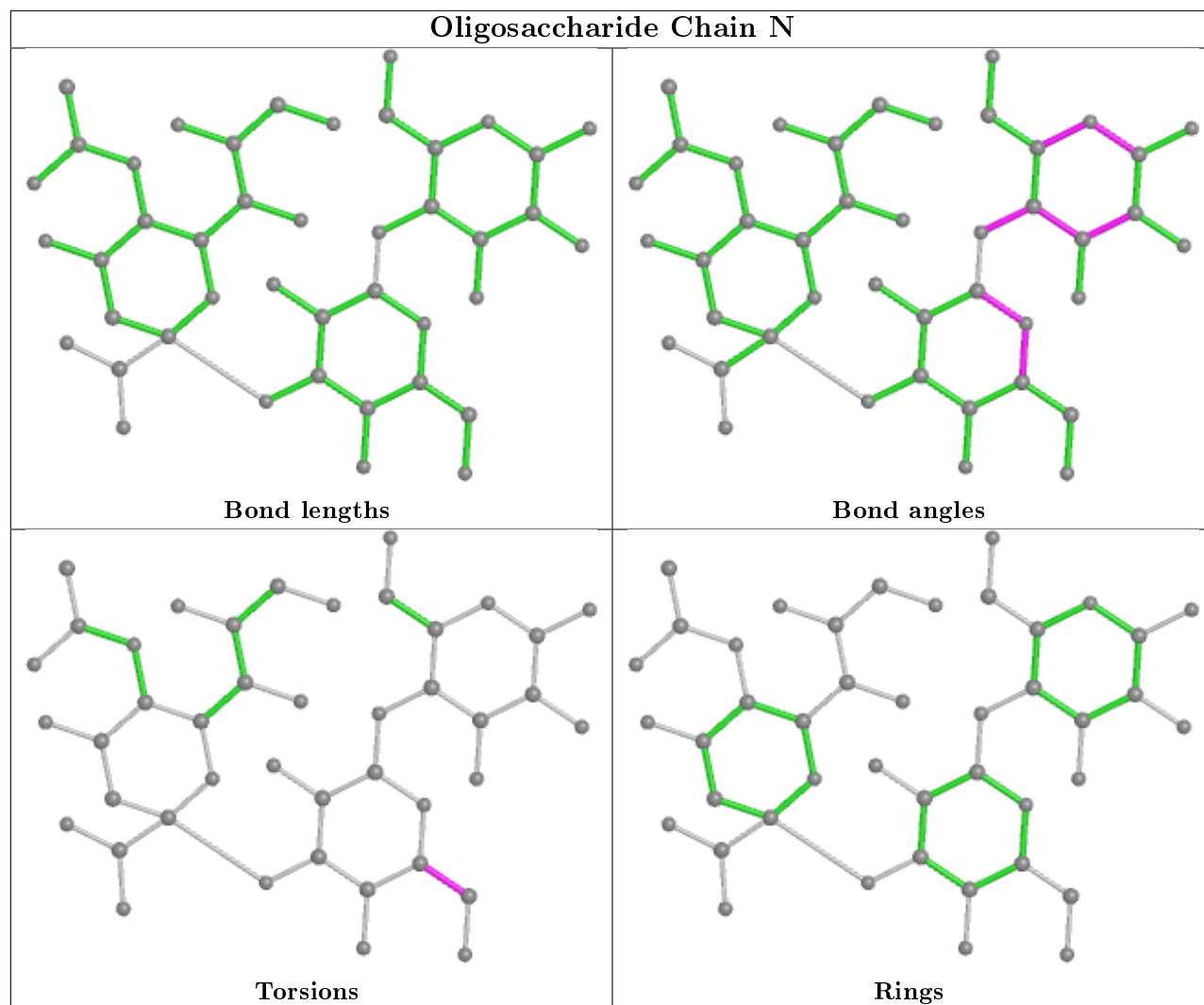
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

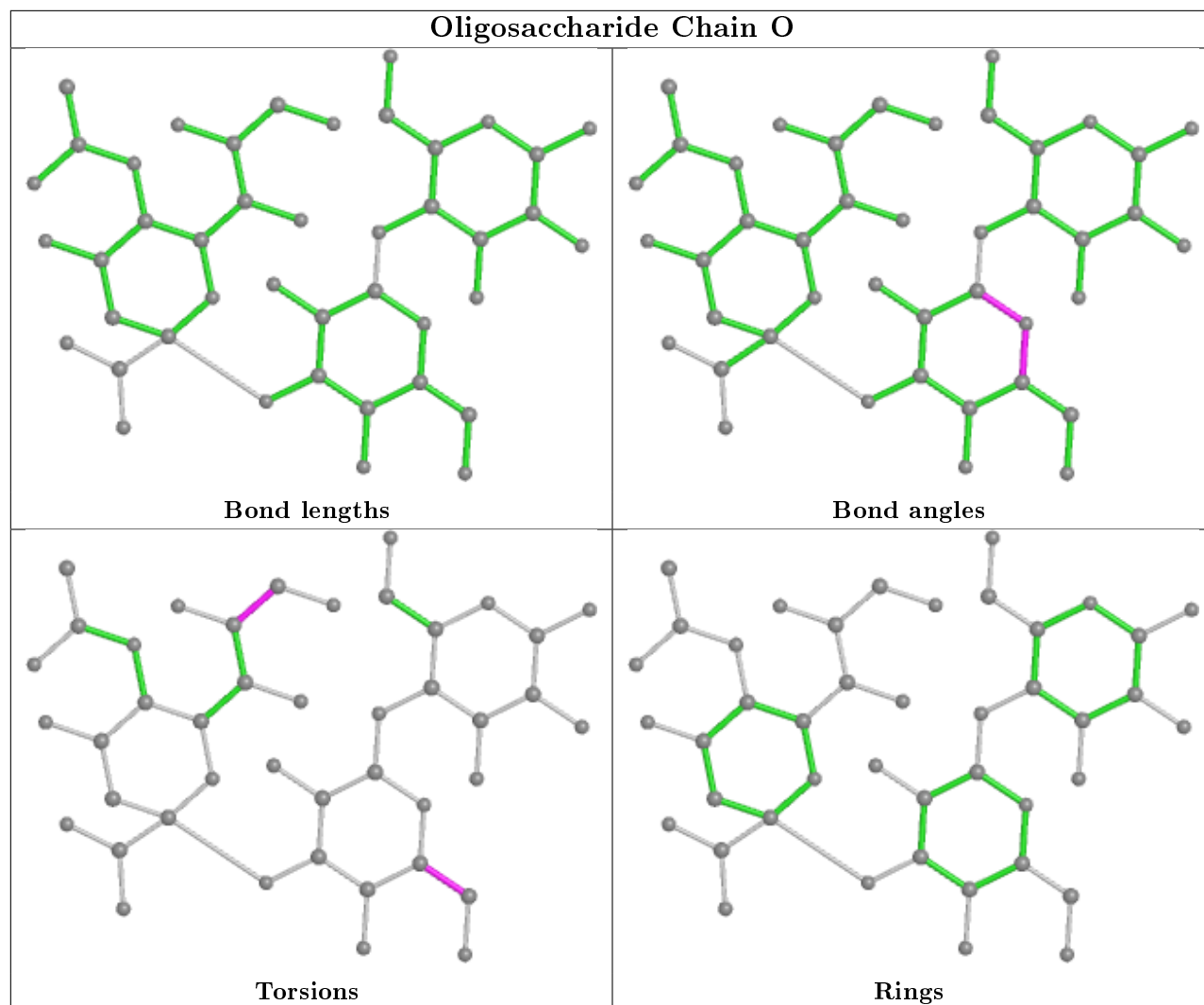


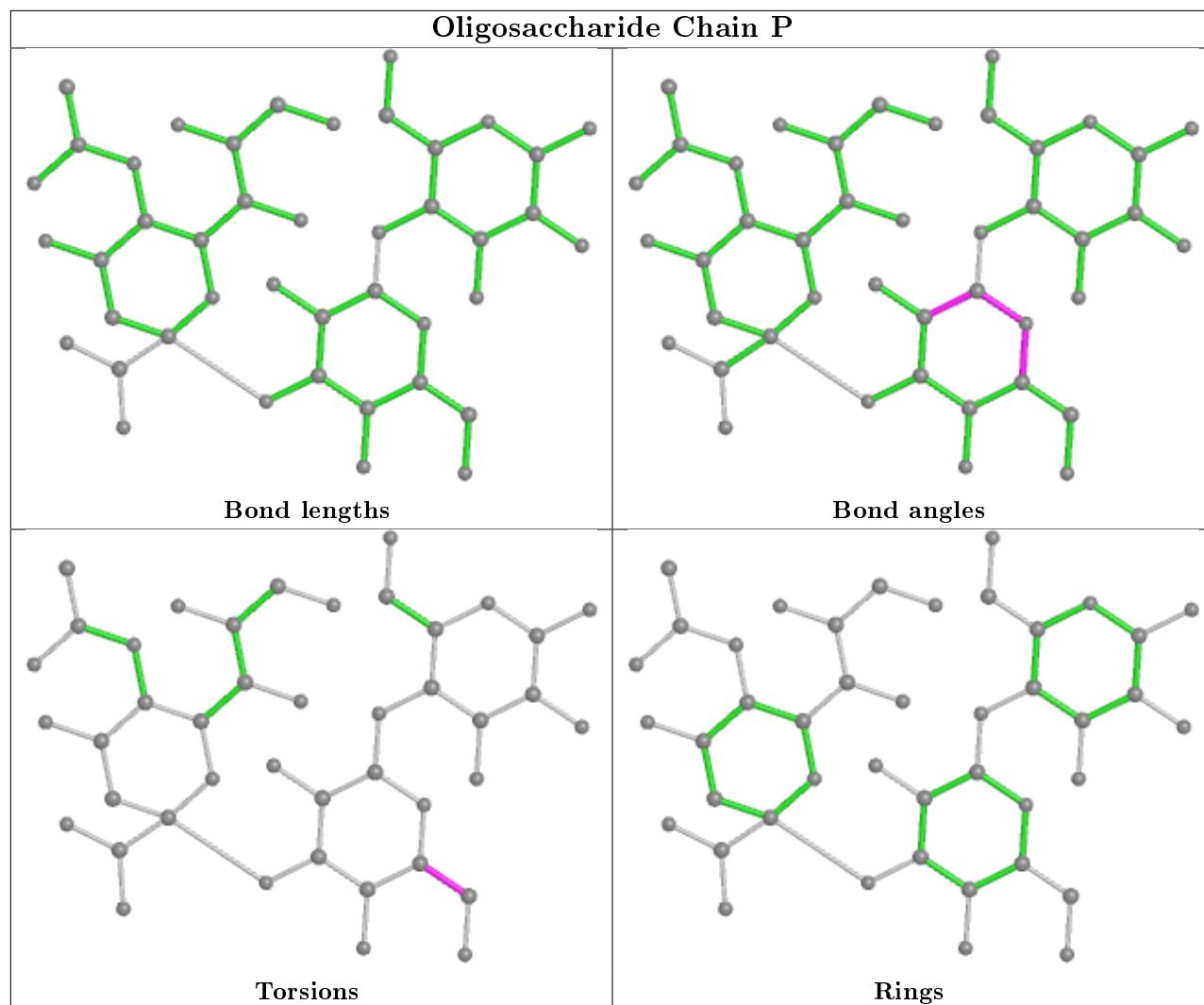


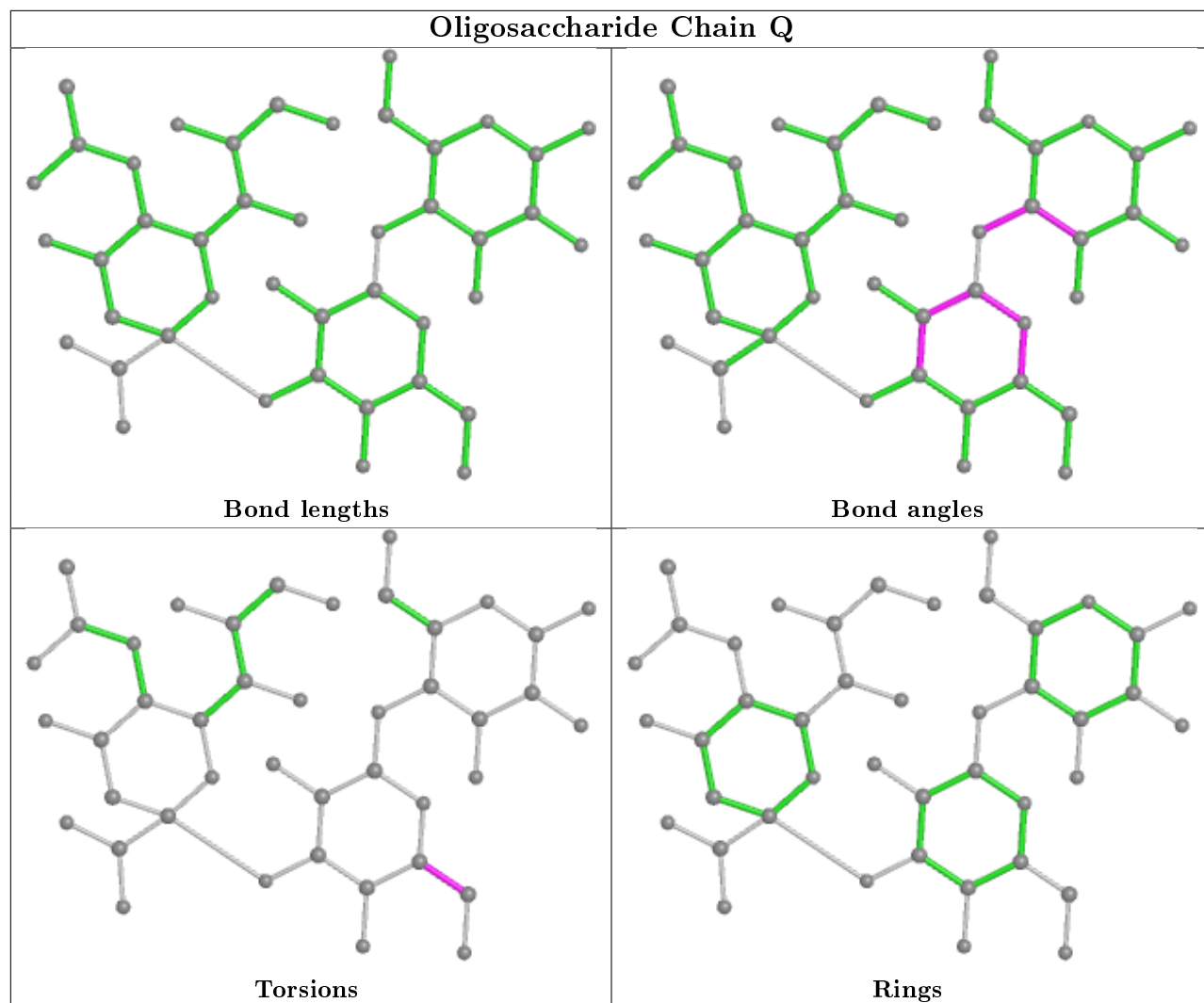


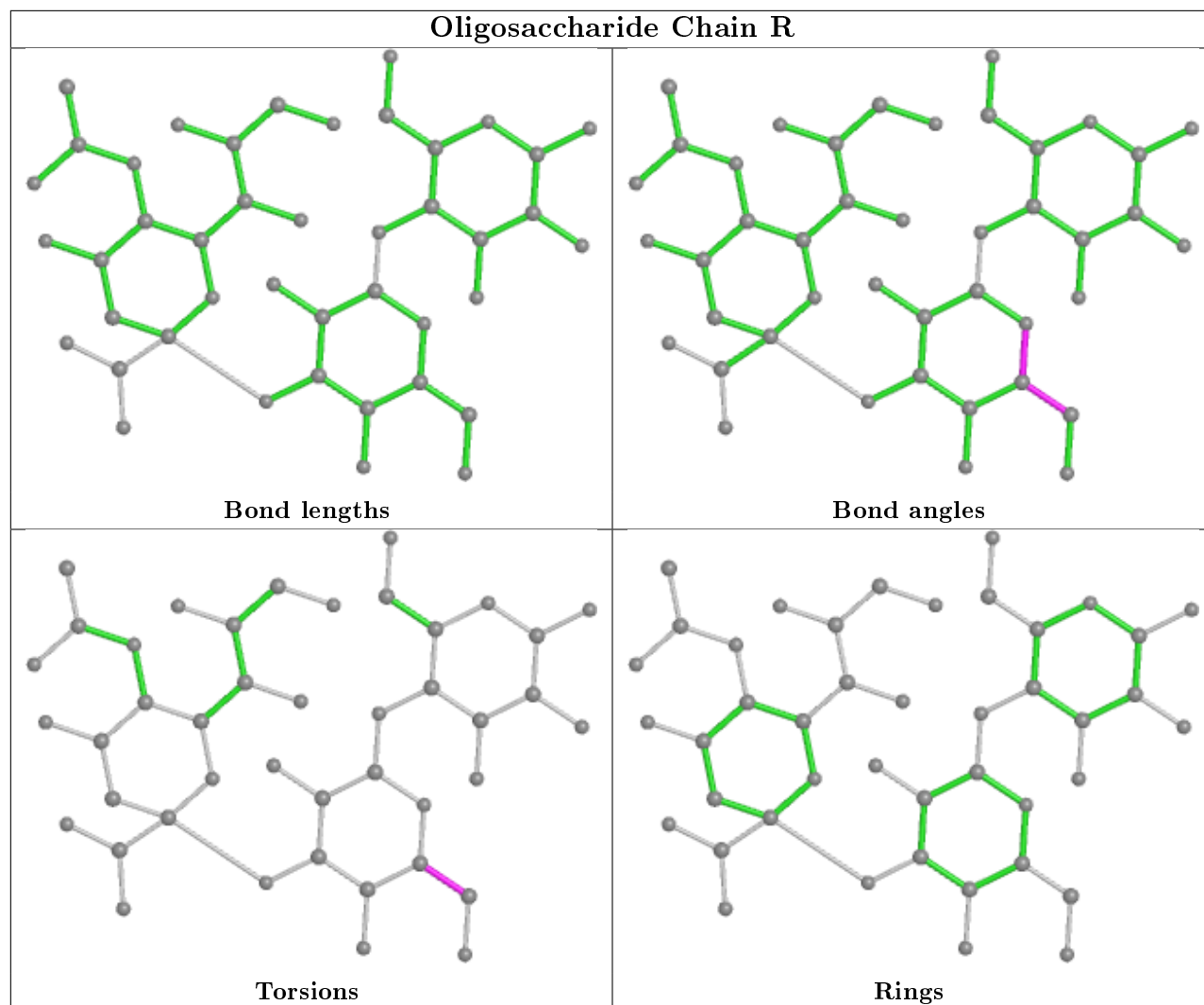




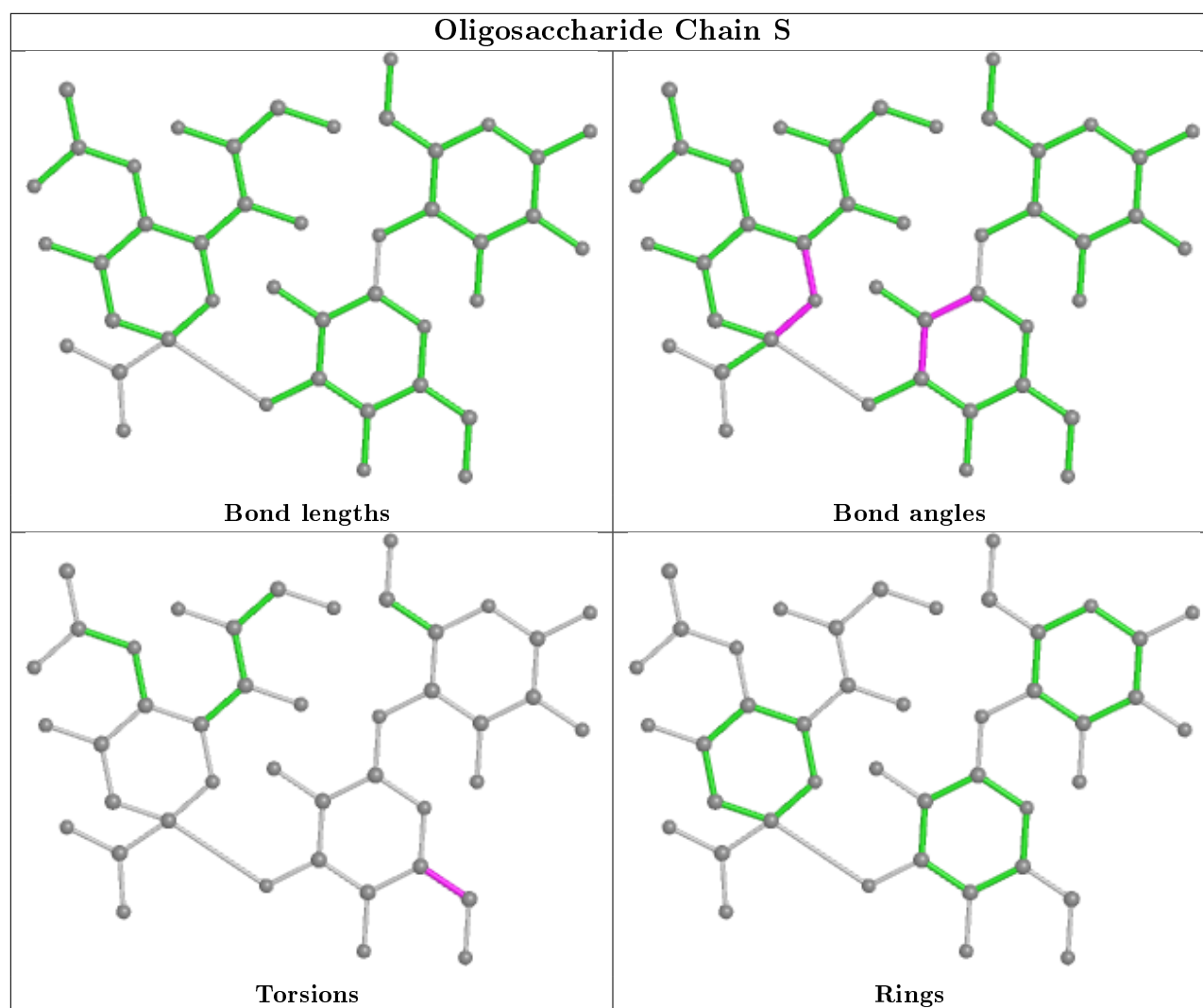












## 5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 10 are monoatomic - leaving 43 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	$\# Z  > 2$
4	EDO	C	402	-	3,3,3	0.49	0	2,2,2	0.18	0
4	EDO	I	402	-	3,3,3	0.41	0	2,2,2	0.45	0
4	EDO	H	402	-	3,3,3	0.52	0	2,2,2	0.29	0
4	EDO	H	403	-	3,3,3	0.48	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	B	404	-	3,3,3	0.37	0	2,2,2	0.50	0
5	IPA	B	405	-	3,3,3	0.44	0	3,3,3	0.49	0
5	IPA	D	406	-	3,3,3	0.46	0	3,3,3	0.58	0
4	EDO	A	402	-	3,3,3	0.47	0	2,2,2	0.32	0
4	EDO	I	403	-	3,3,3	0.42	0	2,2,2	0.27	0
5	IPA	G	406	-	3,3,3	0.52	0	3,3,3	0.53	0
4	EDO	F	404	-	3,3,3	0.45	0	2,2,2	0.44	0
5	IPA	E	406	-	3,3,3	0.49	0	3,3,3	0.44	0
4	EDO	C	403	-	3,3,3	0.54	0	2,2,2	0.23	0
4	EDO	E	403	-	3,3,3	0.50	0	2,2,2	0.30	0
4	EDO	F	402	-	3,3,3	0.60	0	2,2,2	0.23	0
4	EDO	D	402	-	3,3,3	0.34	0	2,2,2	0.75	0
4	EDO	G	402	-	3,3,3	0.42	0	2,2,2	0.52	0
4	EDO	D	403	-	3,3,3	0.53	0	2,2,2	0.36	0
5	IPA	I	405	-	3,3,3	0.47	0	3,3,3	0.34	0
4	EDO	C	405	-	3,3,3	0.48	0	2,2,2	0.27	0
4	EDO	F	403	-	3,3,3	0.51	0	2,2,2	0.31	0
5	IPA	H	406	-	3,3,3	0.47	0	3,3,3	0.53	0
4	EDO	C	404	-	3,3,3	0.57	0	2,2,2	0.18	0
5	IPA	F	405	-	3,3,3	0.45	0	3,3,3	0.52	0
4	EDO	A	403	-	3,3,3	0.53	0	2,2,2	0.33	0
4	EDO	D	405	-	3,3,3	0.47	0	2,2,2	0.36	0
4	EDO	G	403	-	3,3,3	0.52	0	2,2,2	0.24	0
4	EDO	H	405	-	3,3,3	0.47	0	2,2,2	0.39	0
4	EDO	E	405	-	3,3,3	0.69	0	2,2,2	0.24	0
5	IPA	C	406	-	3,3,3	0.42	0	3,3,3	0.61	0
4	EDO	G	405	-	3,3,3	0.44	0	2,2,2	0.61	0
4	EDO	B	403	-	3,3,3	0.52	0	2,2,2	0.33	0
4	EDO	G	404	-	3,3,3	0.51	0	2,2,2	0.43	0
4	EDO	D	404	-	3,3,3	0.52	0	2,2,2	0.24	0
5	IPA	A	405	-	3,3,3	0.53	0	3,3,3	0.41	0
4	EDO	E	404	-	3,3,3	0.53	0	2,2,2	0.30	0
4	EDO	A	404	-	3,3,3	0.36	0	2,2,2	0.68	0
4	EDO	J	402	-	3,3,3	0.37	0	2,2,2	0.67	0
4	EDO	H	404	-	3,3,3	0.53	0	2,2,2	0.25	0
5	IPA	J	403	-	3,3,3	0.48	0	3,3,3	0.44	0
4	EDO	I	404	-	3,3,3	0.53	0	2,2,2	0.37	0
4	EDO	B	402	-	3,3,3	0.50	0	2,2,2	0.56	0
4	EDO	E	402	-	3,3,3	0.53	0	2,2,2	0.20	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
4	EDO	C	402	-	-	0/1/1/1	-
4	EDO	I	402	-	-	0/1/1/1	-
4	EDO	H	402	-	-	0/1/1/1	-
4	EDO	H	403	-	-	1/1/1/1	-
4	EDO	B	404	-	-	1/1/1/1	-
4	EDO	A	402	-	-	0/1/1/1	-
4	EDO	I	403	-	-	1/1/1/1	-
4	EDO	F	404	-	-	0/1/1/1	-
4	EDO	C	403	-	-	1/1/1/1	-
4	EDO	E	403	-	-	1/1/1/1	-
4	EDO	F	402	-	-	0/1/1/1	-
4	EDO	D	402	-	-	1/1/1/1	-
4	EDO	G	402	-	-	0/1/1/1	-
4	EDO	D	403	-	-	1/1/1/1	-
4	EDO	C	405	-	-	0/1/1/1	-
4	EDO	F	403	-	-	1/1/1/1	-
4	EDO	C	404	-	-	1/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	D	405	-	-	0/1/1/1	-
4	EDO	G	403	-	-	0/1/1/1	-
4	EDO	H	405	-	-	1/1/1/1	-
4	EDO	E	405	-	-	1/1/1/1	-
4	EDO	G	405	-	-	1/1/1/1	-
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	G	404	-	-	1/1/1/1	-
4	EDO	D	404	-	-	0/1/1/1	-
4	EDO	E	404	-	-	1/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-
4	EDO	J	402	-	-	1/1/1/1	-
4	EDO	H	404	-	-	1/1/1/1	-
4	EDO	I	404	-	-	1/1/1/1	-
4	EDO	B	402	-	-	0/1/1/1	-
4	EDO	E	402	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	403	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	H	405	EDO	O1-C1-C2-O2
4	B	403	EDO	O1-C1-C2-O2
4	J	402	EDO	O1-C1-C2-O2
4	H	404	EDO	O1-C1-C2-O2

There are no ring outliers.

16 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	EDO	3	0
4	B	404	EDO	3	0
4	I	403	EDO	4	0
4	F	404	EDO	1	0
5	E	406	IPA	2	0
4	C	403	EDO	4	0
4	D	403	EDO	1	0
4	C	404	EDO	1	0
5	F	405	IPA	2	0
4	G	403	EDO	2	0
4	H	405	EDO	2	0
4	B	403	EDO	1	0
4	D	404	EDO	1	0
4	E	404	EDO	1	0
4	H	404	EDO	4	0
4	I	404	EDO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	54:PRO	C	55:ARG	N	1.15

## 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	270/278 (97%)	-0.42	6 (2%) 62 66	15, 21, 46, 82	2 (0%)
1	B	270/278 (97%)	-0.68	3 (1%) 80 84	16, 22, 43, 78	0
1	C	269/278 (96%)	-0.45	4 (1%) 73 77	19, 26, 49, 90	0
1	D	270/278 (97%)	-0.52	1 (0%) 92 93	18, 26, 46, 68	0
1	E	269/278 (96%)	-0.54	4 (1%) 73 77	15, 23, 45, 87	0
1	F	272/278 (97%)	-0.51	1 (0%) 92 93	21, 28, 41, 61	0
1	G	266/278 (95%)	-0.47	5 (1%) 66 71	18, 25, 44, 78	0
1	H	270/278 (97%)	-0.43	2 (0%) 87 89	14, 22, 43, 84	0
1	I	269/278 (96%)	-0.46	6 (2%) 62 66	18, 24, 46, 91	0
1	J	273/278 (98%)	-0.53	3 (1%) 80 84	20, 26, 48, 80	0
All	All	2698/2780 (97%)	-0.50	35 (1%) 77 80	14, 24, 46, 91	2 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	THR	4.9
1	I	105	MET	4.5
1	G	108	ASP	4.4
1	H	103	GLU	4.0
1	A	104	ASP	3.7

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

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

## 6.3 Carbohydrates ⓘ

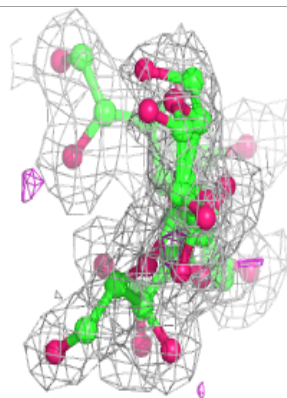
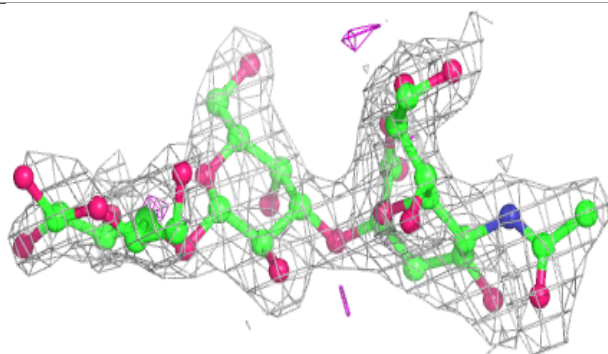
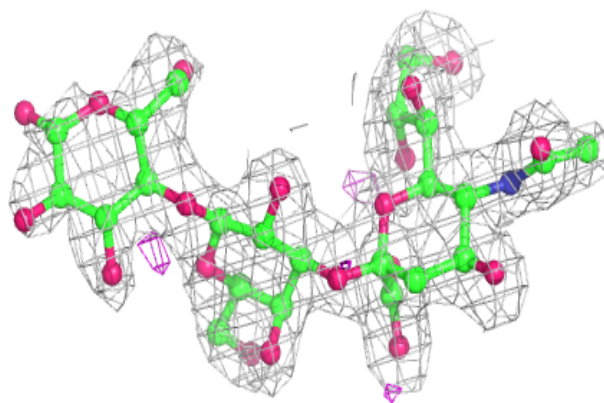
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	GAL	M	2	11/12	0.80	0.23	45,48,54,58	0
2	BGC	M	1	12/12	0.81	0.30	60,70,81,89	0
2	BGC	K	1	12/12	0.83	0.20	46,55,66,69	0
2	BGC	P	1	12/12	0.85	0.22	47,53,62,71	0
2	BGC	N	1	12/12	0.87	0.16	36,45,48,53	0
2	BGC	L	1	12/12	0.88	0.15	34,41,47,51	0
2	BGC	S	1	12/12	0.89	0.22	44,48,53,65	0
2	BGC	Q	1	12/12	0.90	0.14	29,36,45,50	0
2	SIA	M	3	20/21	0.90	0.15	27,38,40,40	0
2	BGC	O	1	12/12	0.90	0.17	39,48,52,57	0
2	GAL	P	2	11/12	0.92	0.14	31,35,39,41	0
2	GAL	S	2	11/12	0.92	0.16	30,34,38,43	0
2	BGC	R	1	12/12	0.93	0.19	37,45,57,59	0
2	GAL	K	2	11/12	0.93	0.13	31,38,42,43	0
2	SIA	P	3	20/21	0.93	0.10	22,28,31,32	0
2	SIA	K	3	20/21	0.94	0.09	28,31,33,33	0
2	SIA	O	3	20/21	0.94	0.09	25,28,31,32	0
2	GAL	L	2	11/12	0.94	0.14	24,27,36,41	0
2	GAL	O	2	11/12	0.94	0.10	31,34,37,42	0
2	SIA	S	3	20/21	0.95	0.14	23,27,29,30	0
2	SIA	N	3	20/21	0.95	0.08	16,23,25,27	0
2	GAL	N	2	11/12	0.96	0.09	24,27,32,33	0
2	SIA	R	3	20/21	0.96	0.09	19,24,29,30	0
2	GAL	R	2	11/12	0.96	0.11	27,32,35,41	0
2	GAL	Q	2	11/12	0.96	0.10	23,27,29,32	0
2	SIA	L	3	20/21	0.96	0.10	19,22,26,26	0
2	SIA	Q	3	20/21	0.97	0.07	15,20,23,23	0

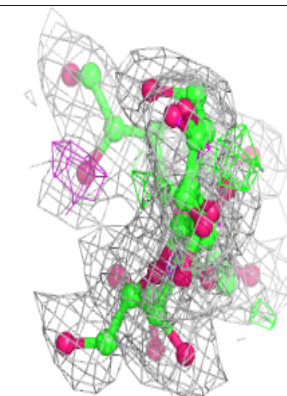
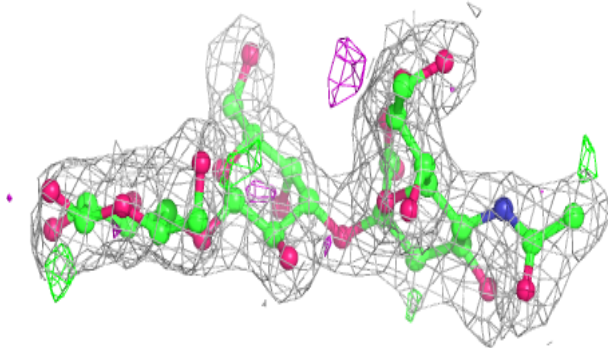
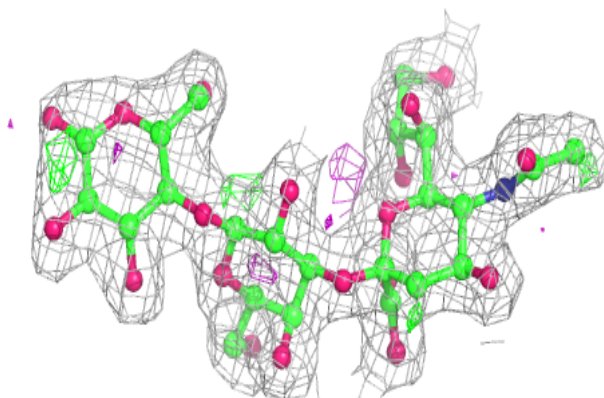
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain K:**

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

**Electron density around Chain L:**

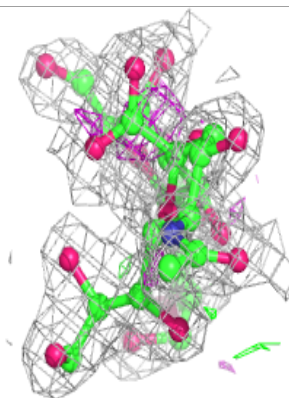
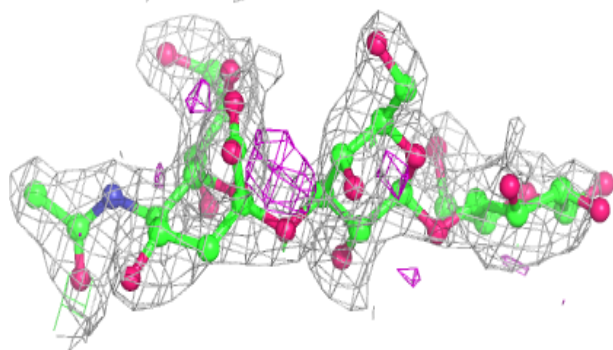
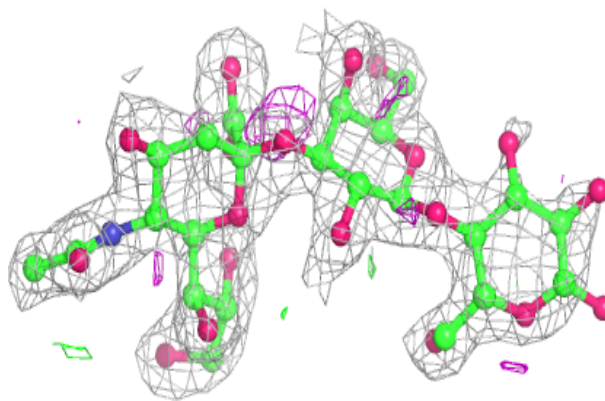
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



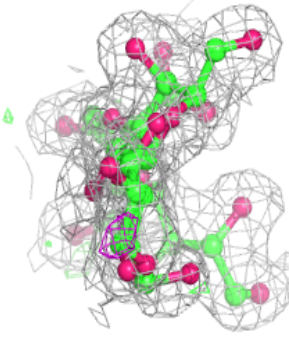
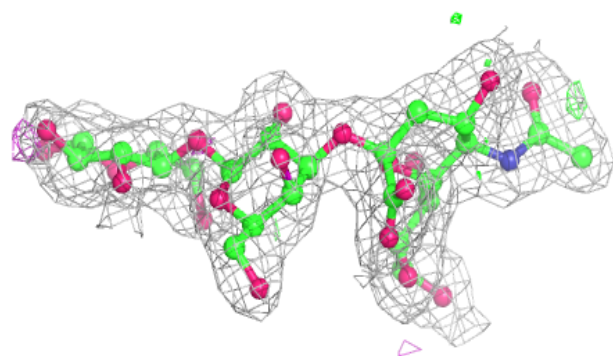
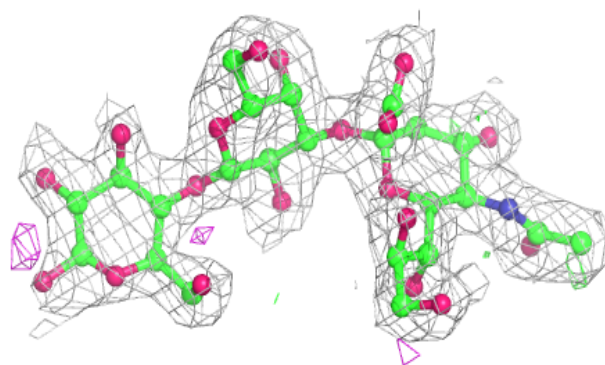


**Electron density around Chain M:**

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

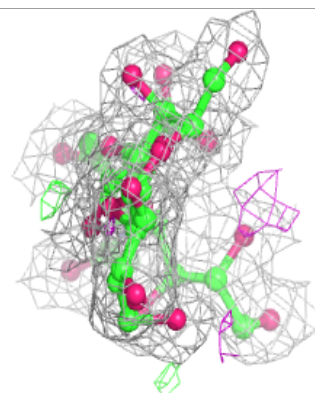
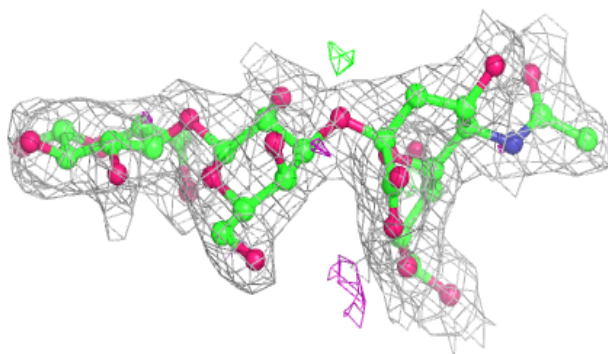
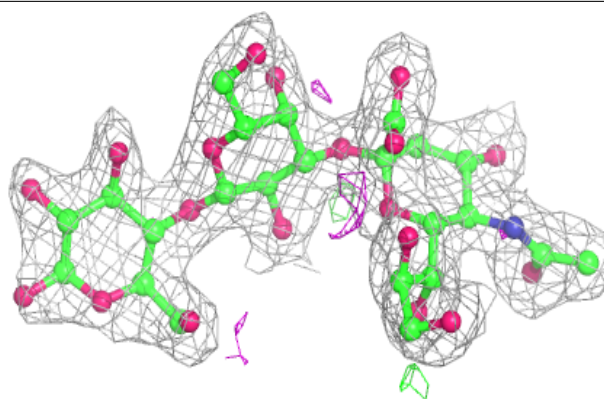
**Electron density around Chain N:**

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

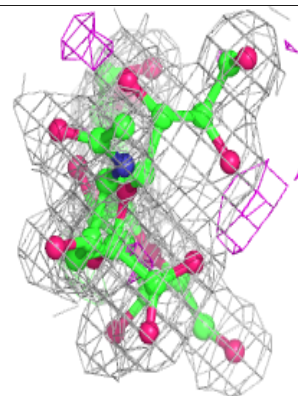
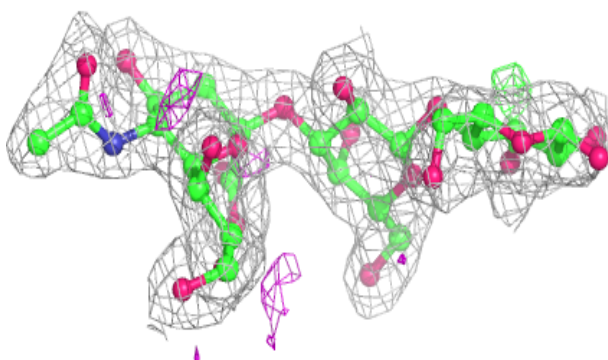
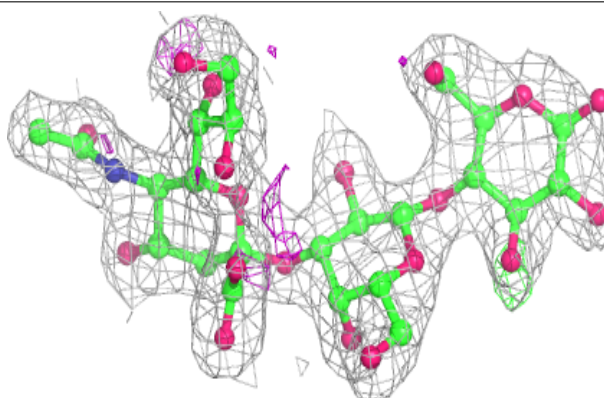


**Electron density around Chain O:**

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

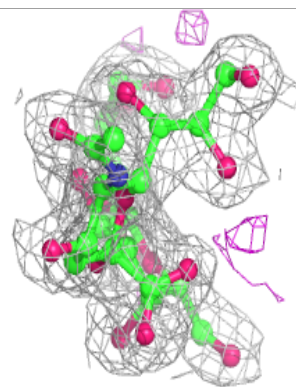
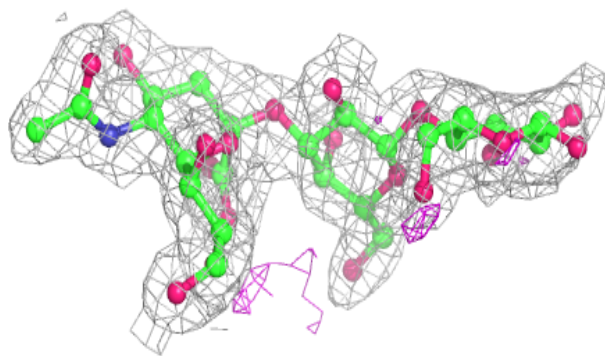
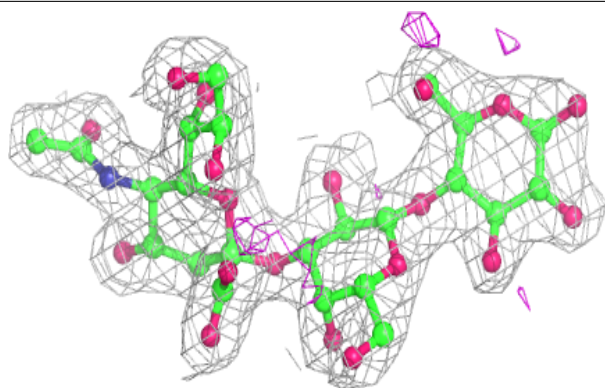
**Electron density around Chain P:**

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

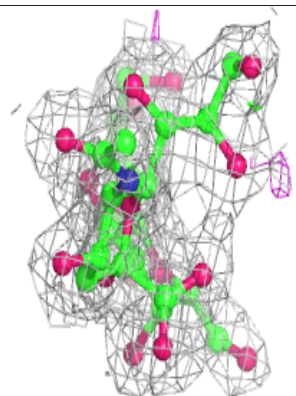
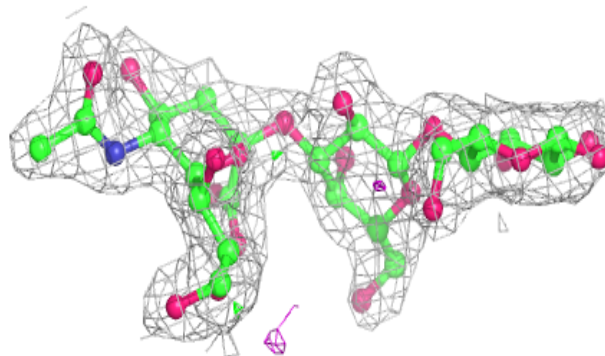
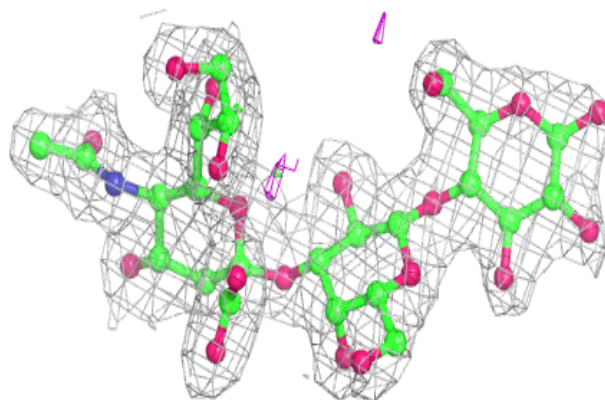


**Electron density around Chain Q:**

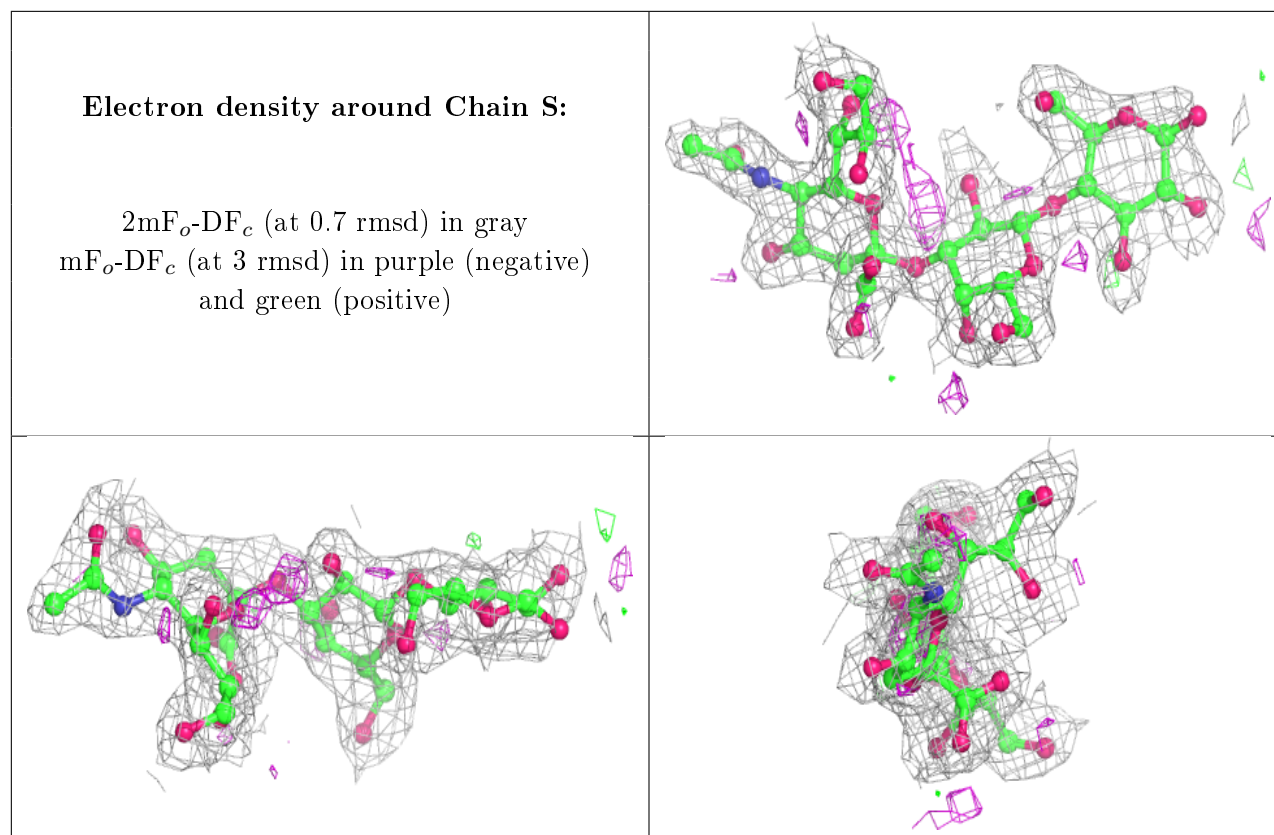
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain R:**

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







## 6.4 Ligands ⓘ

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
4	EDO	H	404	4/4	0.81	0.21	38,39,39,50	0
4	EDO	E	405	4/4	0.86	0.15	28,32,32,33	0
4	EDO	C	404	4/4	0.86	0.15	36,36,39,41	0
4	EDO	C	403	4/4	0.87	0.14	33,36,38,41	0
4	EDO	I	404	4/4	0.87	0.19	31,32,34,40	0
5	IPA	C	406	4/4	0.88	0.23	32,33,34,35	0
5	IPA	G	406	4/4	0.88	0.19	30,32,35,38	0
4	EDO	D	403	4/4	0.88	0.20	41,43,43,45	0
4	EDO	E	403	4/4	0.89	0.14	35,37,37,38	0
4	EDO	G	403	4/4	0.89	0.14	34,35,38,39	0
5	IPA	I	405	4/4	0.89	0.15	29,30,32,33	0
4	EDO	D	404	4/4	0.90	0.14	39,40,40,41	0
4	EDO	F	404	4/4	0.90	0.26	41,42,45,46	0
5	IPA	E	406	4/4	0.90	0.17	35,38,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	C	405	4/4	0.91	0.26	41,41,41,48	0
5	IPA	A	405	4/4	0.91	0.16	28,31,31,32	0
5	IPA	H	406	4/4	0.92	0.17	31,31,31,33	0
4	EDO	H	405	4/4	0.92	0.14	38,41,43,43	0
4	EDO	F	402	4/4	0.93	0.10	31,31,32,34	0
3	CA	F	401	1/1	0.93	0.04	42,42,42,42	0
5	IPA	F	405	4/4	0.93	0.19	32,34,35,36	0
4	EDO	A	403	4/4	0.93	0.14	26,27,33,36	0
4	EDO	F	403	4/4	0.94	0.11	41,42,43,45	0
5	IPA	B	405	4/4	0.94	0.13	26,27,28,29	0
4	EDO	E	404	4/4	0.94	0.12	35,40,41,45	0
4	EDO	A	404	4/4	0.94	0.15	30,32,33,45	0
4	EDO	B	404	4/4	0.94	0.18	31,31,32,34	0
5	IPA	J	403	4/4	0.94	0.13	34,34,35,35	0
4	EDO	B	403	4/4	0.94	0.14	28,30,30,37	0
4	EDO	G	404	4/4	0.95	0.07	29,31,32,35	0
4	EDO	J	402	4/4	0.95	0.08	32,34,35,35	0
4	EDO	D	405	4/4	0.95	0.17	29,34,39,46	0
5	IPA	D	406	4/4	0.95	0.15	29,30,31,33	0
4	EDO	A	402	4/4	0.95	0.11	29,31,31,34	0
4	EDO	B	402	4/4	0.95	0.07	26,27,29,29	0
4	EDO	E	402	4/4	0.95	0.10	27,28,29,29	0
4	EDO	H	403	4/4	0.96	0.09	31,32,34,40	0
4	EDO	I	403	4/4	0.96	0.11	26,28,31,36	0
3	CA	G	401	1/1	0.96	0.05	37,37,37,37	0
4	EDO	H	402	4/4	0.96	0.10	25,27,27,28	0
4	EDO	C	402	4/4	0.97	0.12	26,27,27,28	0
4	EDO	G	405	4/4	0.97	0.12	29,29,32,38	0
3	CA	E	401	1/1	0.97	0.04	36,36,36,36	0
3	CA	B	401	1/1	0.97	0.04	39,39,39,39	0
3	CA	C	401	1/1	0.97	0.03	41,41,41,41	0
4	EDO	D	402	4/4	0.97	0.10	23,26,26,29	0
4	EDO	G	402	4/4	0.97	0.12	28,29,30,30	0
4	EDO	I	402	4/4	0.98	0.09	24,25,29,33	0
3	CA	D	401	1/1	0.98	0.05	37,37,37,37	0
3	CA	J	401	1/1	0.98	0.06	43,43,43,43	0
3	CA	H	401	1/1	0.99	0.03	31,31,31,31	0
3	CA	I	401	1/1	0.99	0.04	37,37,37,37	0
3	CA	A	401	1/1	1.00	0.03	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.