



# Full wwPDB X-ray Structure Validation Report i

Sep 17, 2023 – 06:04 PM EDT

PDB ID : 4YEE  
Title : beta2 carbohydrate binding module (CBM) of AMP-activated protein kinase (AMPK) in complex with glucosyl-beta-cyclodextrin  
Authors : Mobbs, J.; Gorman, M.A.; Parker, M.W.; Gooley, P.R.; Griffin, M.  
Deposited on : 2015-02-24  
Resolution : 2.00 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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) i) 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 : 2.35.1  
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) : 2.35.1

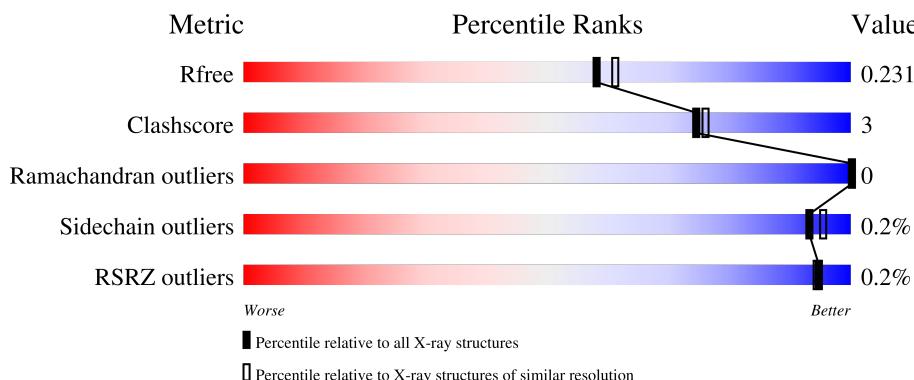
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



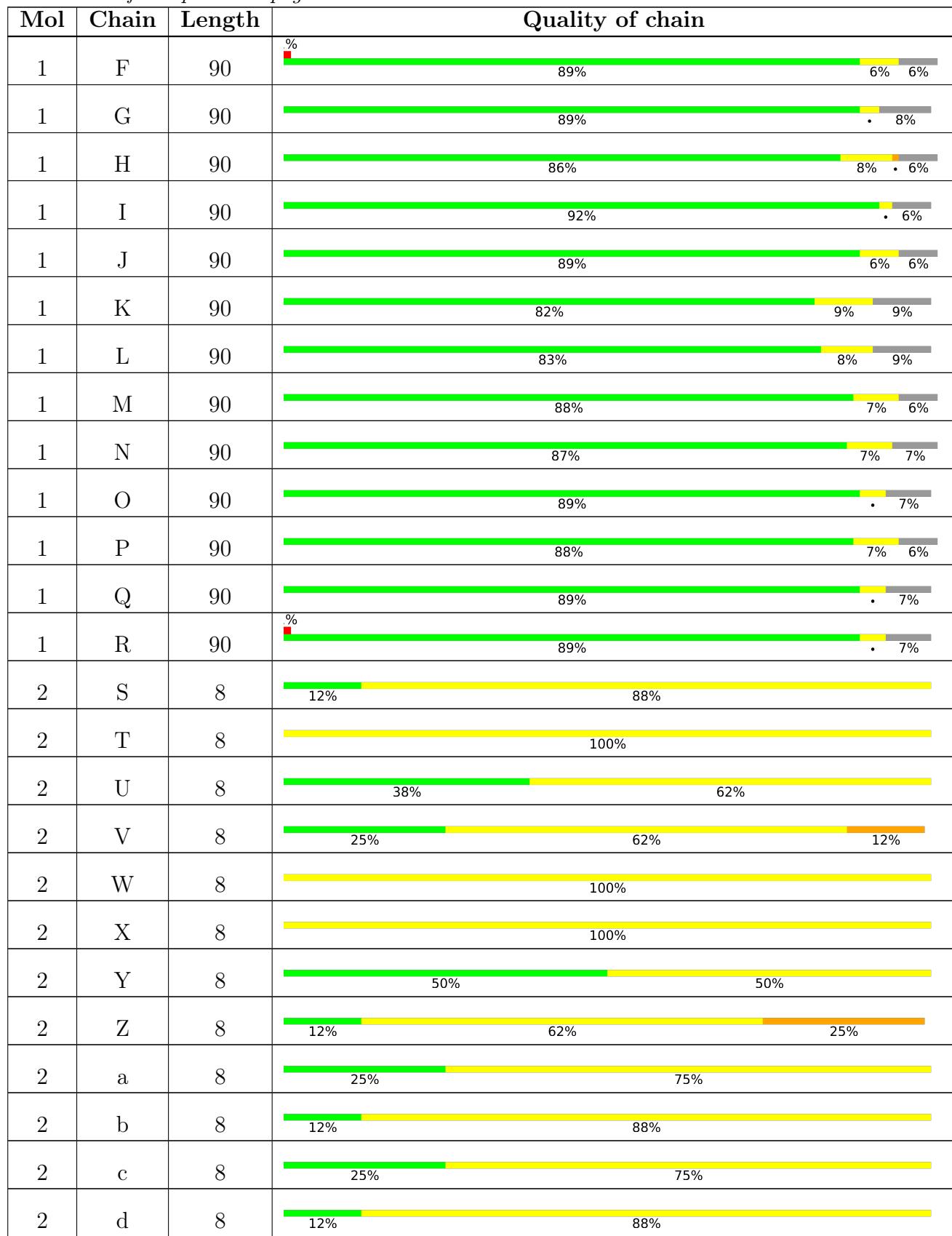
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.



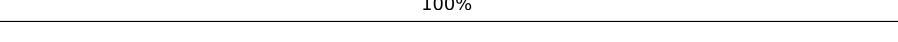
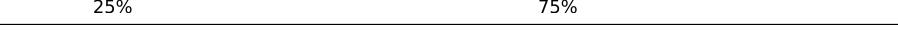
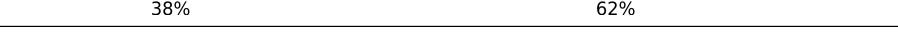
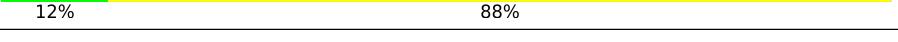
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Mol	Chain	Length	Quality of chain
2	e	8	<div style="width: 88%;">12%</div>
2	f	8	<div style="width: 100%;">100%</div>
2	g	8	<div style="width: 75%;">25%</div>
2	h	8	<div style="width: 62%;">38%</div>
2	i	8	<div style="width: 88%;">12%</div>
2	j	8	<div style="width: 75%;">25%</div>

## 2 Entry composition [\(i\)](#)

There are 4 unique types of molecules in this entry. The entry contains 15355 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 5'-AMP-activated protein kinase subunit beta-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	82	Total	C 652	N 421	O 110	121	0	0
1	B	83	Total	C 667	N 429	O 114	124	0	0
1	C	83	Total	C 662	N 428	O 111	123	0	1
1	D	79	Total	C 630	N 408	O 104	118	0	0
1	E	85	Total	C 685	N 440	O 118	127	0	1
1	F	85	Total	C 682	N 438	O 117	127	0	0
1	G	83	Total	C 666	N 429	O 113	124	0	1
1	H	85	Total	C 675	N 434	O 114	127	0	0
1	I	85	Total	C 666	N 429	O 113	124	0	0
1	J	85	Total	C 671	N 431	O 114	126	0	0
1	K	82	Total	C 639	N 414	O 103	122	0	0
1	L	82	Total	C 654	N 422	O 111	121	0	0
1	M	85	Total	C 679	N 437	O 116	126	0	0
1	N	84	Total	C 672	N 432	O 115	125	0	0
1	O	84	Total	C 675	N 433	O 116	126	0	0
1	P	85	Total	C 678	N 435	O 116	127	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Q	84	Total	C	N	O	0	0	0
			665	427	113	125			
1	R	84	Total	C	N	O	0	0	0
			662	425	111	126			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	GLY	-	expression tag	UNP Q9QZH4
A	68	PRO	-	expression tag	UNP Q9QZH4
A	69	LEU	-	expression tag	UNP Q9QZH4
A	70	GLY	-	expression tag	UNP Q9QZH4
A	71	SER	-	expression tag	UNP Q9QZH4
A	72	PRO	-	expression tag	UNP Q9QZH4
A	73	ASN	-	expression tag	UNP Q9QZH4
A	74	SER	-	expression tag	UNP Q9QZH4
B	67	GLY	-	expression tag	UNP Q9QZH4
B	68	PRO	-	expression tag	UNP Q9QZH4
B	69	LEU	-	expression tag	UNP Q9QZH4
B	70	GLY	-	expression tag	UNP Q9QZH4
B	71	SER	-	expression tag	UNP Q9QZH4
B	72	PRO	-	expression tag	UNP Q9QZH4
B	73	ASN	-	expression tag	UNP Q9QZH4
B	74	SER	-	expression tag	UNP Q9QZH4
C	67	GLY	-	expression tag	UNP Q9QZH4
C	68	PRO	-	expression tag	UNP Q9QZH4
C	69	LEU	-	expression tag	UNP Q9QZH4
C	70	GLY	-	expression tag	UNP Q9QZH4
C	71	SER	-	expression tag	UNP Q9QZH4
C	72	PRO	-	expression tag	UNP Q9QZH4
C	73	ASN	-	expression tag	UNP Q9QZH4
C	74	SER	-	expression tag	UNP Q9QZH4
D	67	GLY	-	expression tag	UNP Q9QZH4
D	68	PRO	-	expression tag	UNP Q9QZH4
D	69	LEU	-	expression tag	UNP Q9QZH4
D	70	GLY	-	expression tag	UNP Q9QZH4
D	71	SER	-	expression tag	UNP Q9QZH4
D	72	PRO	-	expression tag	UNP Q9QZH4
D	73	ASN	-	expression tag	UNP Q9QZH4
D	74	SER	-	expression tag	UNP Q9QZH4
E	67	GLY	-	expression tag	UNP Q9QZH4
E	68	PRO	-	expression tag	UNP Q9QZH4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	69	LEU	-	expression tag	UNP Q9QZH4
E	70	GLY	-	expression tag	UNP Q9QZH4
E	71	SER	-	expression tag	UNP Q9QZH4
E	72	PRO	-	expression tag	UNP Q9QZH4
E	73	ASN	-	expression tag	UNP Q9QZH4
E	74	SER	-	expression tag	UNP Q9QZH4
F	67	GLY	-	expression tag	UNP Q9QZH4
F	68	PRO	-	expression tag	UNP Q9QZH4
F	69	LEU	-	expression tag	UNP Q9QZH4
F	70	GLY	-	expression tag	UNP Q9QZH4
F	71	SER	-	expression tag	UNP Q9QZH4
F	72	PRO	-	expression tag	UNP Q9QZH4
F	73	ASN	-	expression tag	UNP Q9QZH4
F	74	SER	-	expression tag	UNP Q9QZH4
G	67	GLY	-	expression tag	UNP Q9QZH4
G	68	PRO	-	expression tag	UNP Q9QZH4
G	69	LEU	-	expression tag	UNP Q9QZH4
G	70	GLY	-	expression tag	UNP Q9QZH4
G	71	SER	-	expression tag	UNP Q9QZH4
G	72	PRO	-	expression tag	UNP Q9QZH4
G	73	ASN	-	expression tag	UNP Q9QZH4
G	74	SER	-	expression tag	UNP Q9QZH4
H	67	GLY	-	expression tag	UNP Q9QZH4
H	68	PRO	-	expression tag	UNP Q9QZH4
H	69	LEU	-	expression tag	UNP Q9QZH4
H	70	GLY	-	expression tag	UNP Q9QZH4
H	71	SER	-	expression tag	UNP Q9QZH4
H	72	PRO	-	expression tag	UNP Q9QZH4
H	73	ASN	-	expression tag	UNP Q9QZH4
H	74	SER	-	expression tag	UNP Q9QZH4
I	67	GLY	-	expression tag	UNP Q9QZH4
I	68	PRO	-	expression tag	UNP Q9QZH4
I	69	LEU	-	expression tag	UNP Q9QZH4
I	70	GLY	-	expression tag	UNP Q9QZH4
I	71	SER	-	expression tag	UNP Q9QZH4
I	72	PRO	-	expression tag	UNP Q9QZH4
I	73	ASN	-	expression tag	UNP Q9QZH4
I	74	SER	-	expression tag	UNP Q9QZH4
J	67	GLY	-	expression tag	UNP Q9QZH4
J	68	PRO	-	expression tag	UNP Q9QZH4
J	69	LEU	-	expression tag	UNP Q9QZH4
J	70	GLY	-	expression tag	UNP Q9QZH4

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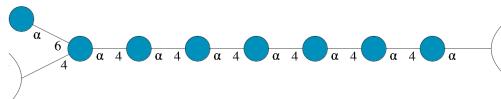
Chain	Residue	Modelled	Actual	Comment	Reference
J	71	SER	-	expression tag	UNP Q9QZH4
J	72	PRO	-	expression tag	UNP Q9QZH4
J	73	ASN	-	expression tag	UNP Q9QZH4
J	74	SER	-	expression tag	UNP Q9QZH4
K	67	GLY	-	expression tag	UNP Q9QZH4
K	68	PRO	-	expression tag	UNP Q9QZH4
K	69	LEU	-	expression tag	UNP Q9QZH4
K	70	GLY	-	expression tag	UNP Q9QZH4
K	71	SER	-	expression tag	UNP Q9QZH4
K	72	PRO	-	expression tag	UNP Q9QZH4
K	73	ASN	-	expression tag	UNP Q9QZH4
K	74	SER	-	expression tag	UNP Q9QZH4
L	67	GLY	-	expression tag	UNP Q9QZH4
L	68	PRO	-	expression tag	UNP Q9QZH4
L	69	LEU	-	expression tag	UNP Q9QZH4
L	70	GLY	-	expression tag	UNP Q9QZH4
L	71	SER	-	expression tag	UNP Q9QZH4
L	72	PRO	-	expression tag	UNP Q9QZH4
L	73	ASN	-	expression tag	UNP Q9QZH4
L	74	SER	-	expression tag	UNP Q9QZH4
M	67	GLY	-	expression tag	UNP Q9QZH4
M	68	PRO	-	expression tag	UNP Q9QZH4
M	69	LEU	-	expression tag	UNP Q9QZH4
M	70	GLY	-	expression tag	UNP Q9QZH4
M	71	SER	-	expression tag	UNP Q9QZH4
M	72	PRO	-	expression tag	UNP Q9QZH4
M	73	ASN	-	expression tag	UNP Q9QZH4
M	74	SER	-	expression tag	UNP Q9QZH4
N	67	GLY	-	expression tag	UNP Q9QZH4
N	68	PRO	-	expression tag	UNP Q9QZH4
N	69	LEU	-	expression tag	UNP Q9QZH4
N	70	GLY	-	expression tag	UNP Q9QZH4
N	71	SER	-	expression tag	UNP Q9QZH4
N	72	PRO	-	expression tag	UNP Q9QZH4
N	73	ASN	-	expression tag	UNP Q9QZH4
N	74	SER	-	expression tag	UNP Q9QZH4
O	67	GLY	-	expression tag	UNP Q9QZH4
O	68	PRO	-	expression tag	UNP Q9QZH4
O	69	LEU	-	expression tag	UNP Q9QZH4
O	70	GLY	-	expression tag	UNP Q9QZH4
O	71	SER	-	expression tag	UNP Q9QZH4
O	72	PRO	-	expression tag	UNP Q9QZH4

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Chain	Residue	Modelled	Actual	Comment	Reference
O	73	ASN	-	expression tag	UNP Q9QZH4
O	74	SER	-	expression tag	UNP Q9QZH4
P	67	GLY	-	expression tag	UNP Q9QZH4
P	68	PRO	-	expression tag	UNP Q9QZH4
P	69	LEU	-	expression tag	UNP Q9QZH4
P	70	GLY	-	expression tag	UNP Q9QZH4
P	71	SER	-	expression tag	UNP Q9QZH4
P	72	PRO	-	expression tag	UNP Q9QZH4
P	73	ASN	-	expression tag	UNP Q9QZH4
P	74	SER	-	expression tag	UNP Q9QZH4
Q	67	GLY	-	expression tag	UNP Q9QZH4
Q	68	PRO	-	expression tag	UNP Q9QZH4
Q	69	LEU	-	expression tag	UNP Q9QZH4
Q	70	GLY	-	expression tag	UNP Q9QZH4
Q	71	SER	-	expression tag	UNP Q9QZH4
Q	72	PRO	-	expression tag	UNP Q9QZH4
Q	73	ASN	-	expression tag	UNP Q9QZH4
Q	74	SER	-	expression tag	UNP Q9QZH4
R	67	GLY	-	expression tag	UNP Q9QZH4
R	68	PRO	-	expression tag	UNP Q9QZH4
R	69	LEU	-	expression tag	UNP Q9QZH4
R	70	GLY	-	expression tag	UNP Q9QZH4
R	71	SER	-	expression tag	UNP Q9QZH4
R	72	PRO	-	expression tag	UNP Q9QZH4
R	73	ASN	-	expression tag	UNP Q9QZH4
R	74	SER	-	expression tag	UNP Q9QZH4

- Molecule 2 is an oligosaccharide called Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose.



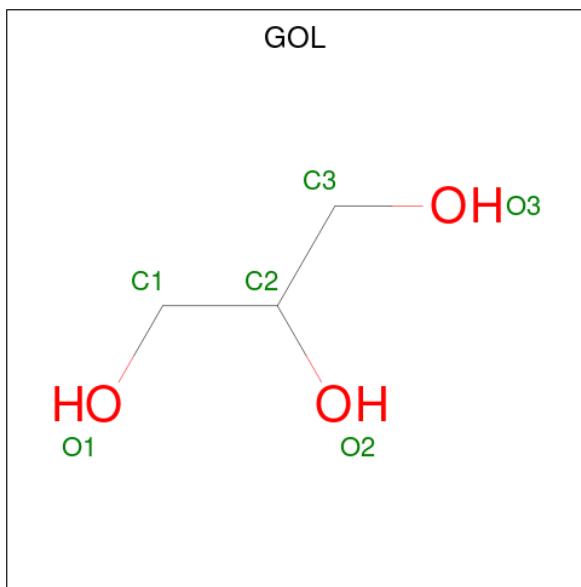
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	S	8	Total C O 88 48 40	0	0	0
2	T	8	Total C O 88 48 40	0	0	0
2	U	8	Total C O 88 48 40	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	V	8	Total C O 88 48 40	0	0	0
2	W	8	Total C O 88 48 40	0	0	0
2	X	8	Total C O 88 48 40	0	0	0
2	Y	8	Total C O 88 48 40	0	0	0
2	Z	8	Total C O 88 48 40	0	0	0
2	a	8	Total C O 88 48 40	0	0	0
2	b	8	Total C O 88 48 40	0	0	0
2	c	8	Total C O 88 48 40	0	0	0
2	d	8	Total C O 88 48 40	0	0	0
2	e	8	Total C O 88 48 40	0	0	0
2	f	8	Total C O 88 48 40	0	0	0
2	g	8	Total C O 88 48 40	0	0	0
2	h	8	Total C O 88 48 40	0	0	0
2	i	8	Total C O 88 48 40	0	0	0
2	j	8	Total C O 88 48 40	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	1	Total C O 6 3 3	0	0
3	M	1	Total C O 6 3 3	0	0
3	N	1	Total C O 6 3 3	0	0
3	N	1	Total C O 6 3 3	0	0
3	P	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	126	Total O 126 126	0	0
4	B	110	Total O 110 110	0	0
4	C	112	Total O 112 112	0	0
4	D	107	Total O 107 107	0	0
4	E	120	Total O 120 120	0	0
4	F	101	Total O 101 101	0	0
4	G	97	Total O 97 97	0	0
4	H	86	Total O 86 86	0	0
4	I	87	Total O 87 87	0	0
4	J	84	Total O 84 84	0	0
4	K	70	Total O 70 70	0	0
4	L	79	Total O 79 79	0	0
4	M	112	Total O 112 112	0	0
4	N	75	Total O 75 75	0	0

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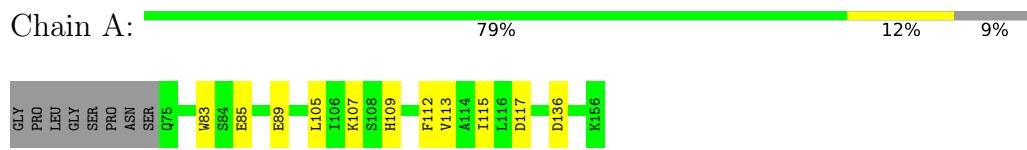
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	94	Total O 94 94	0	0
4	P	80	Total O 80 80	0	0
4	Q	76	Total O 76 76	0	0
4	R	61	Total O 61 61	0	0

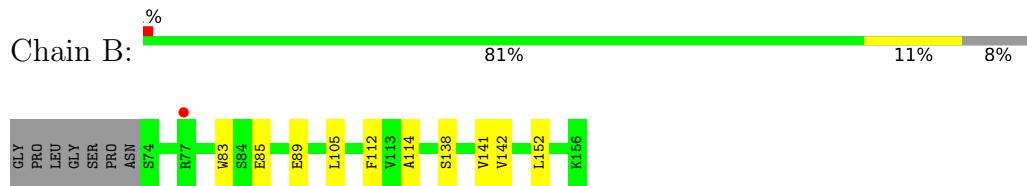
### 3 Residue-property plots

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.

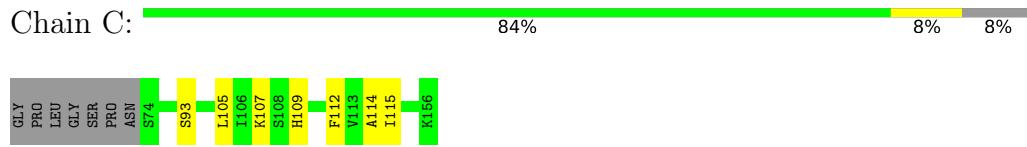
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2



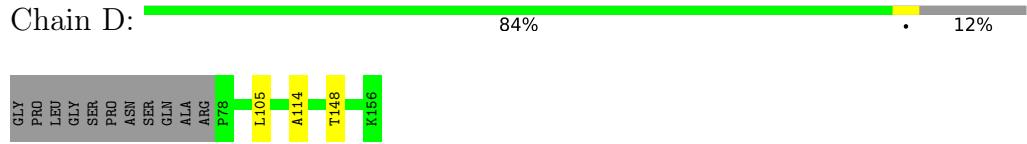
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2



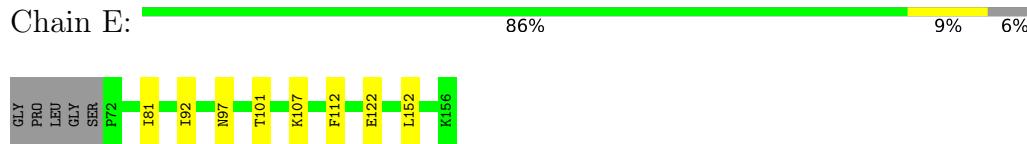
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2



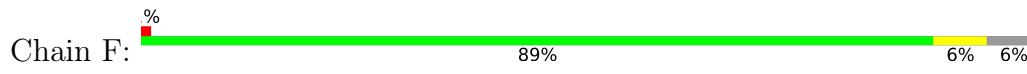
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2





- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain G: 89% • 8%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain H: 86% • 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain I: 92% • 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain J: 89% 6% 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain K: 82% 9% 9%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain L: 83% 8% 9%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain M: 88% 7% 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain N: 87% 7% 7%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain O: 89% • 7%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain P: 88% 7% 6%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain Q: 89% • 7%



- Molecule 1: 5'-AMP-activated protein kinase subunit beta-2

Chain R: 89% • 7%



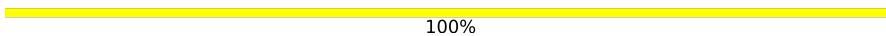
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain S: 12% 88%



- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-

## 4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain T:  100%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain U:  38% 62%

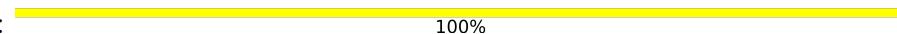
GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain V:  25% 62% 12%

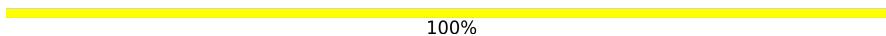
GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain W:  100%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain X:  100%

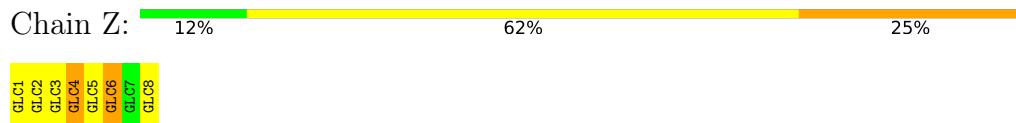
GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain Y:  50% 50%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose



- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose



- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose



- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

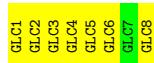


- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose



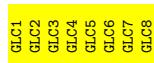
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose





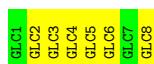
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain f: 100%



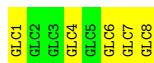
- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain g: 25% 75%



- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain h: 38% 62%



- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain i: 12% 88%



- Molecule 2: Cyclic alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose

Chain j: 25% 75%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.54Å    96.43Å    118.72Å 90.00°    125.46°    90.00°	Depositor
Resolution (Å)	43.38 – 2.00 48.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.38-2.00) 99.9 (48.38-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle^1$	2.44 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
$R$ , $R_{free}$	0.169 , 0.225 0.177 , 0.231	Depositor DCC
$R_{free}$ test set	6385 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15355	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% 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: GLC, GOL

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	0.69	0/672	0.79	2/916 (0.2%)
1	B	0.72	0/687	0.77	0/934
1	C	0.76	1/685 (0.1%)	0.73	0/934
1	D	0.71	0/650	0.71	0/886
1	E	0.64	0/710	0.74	0/967
1	F	0.61	0/703	0.71	0/956
1	G	0.60	0/689	0.69	0/938
1	H	0.59	0/695	0.70	1/946 (0.1%)
1	I	0.60	0/687	0.71	0/938
1	J	0.60	0/692	0.68	0/944
1	K	0.59	0/658	0.70	0/899
1	L	0.66	0/674	0.77	1/918 (0.1%)
1	M	0.63	0/700	0.72	0/952
1	N	0.65	0/692	0.74	1/941 (0.1%)
1	O	0.63	0/695	0.69	0/945
1	P	0.60	0/699	0.73	0/952
1	Q	0.57	0/685	0.70	0/934
1	R	0.48	0/682	0.64	0/931
All	All	0.63	1/12355 (0.0%)	0.72	5/16831 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	93	SER	CB-OG	5.32	1.49	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	N	111	ASP	CB-CG-OD1	5.70	123.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASP	CB-CG-OD1	5.67	123.41	118.30
1	L	111	ASP	CB-CG-OD1	5.45	123.21	118.30
1	H	146	LEU	CA-CB-CG	5.10	127.03	115.30

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 MolProbit. 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	652	0	618	7	0
1	B	667	0	645	9	0
1	C	662	0	632	6	0
1	D	630	0	597	2	0
1	E	685	0	655	6	0
1	F	682	0	659	4	0
1	G	666	0	638	2	0
1	H	675	0	647	8	0
1	I	666	0	624	1	0
1	J	671	0	633	3	0
1	K	639	0	597	4	1
1	L	654	0	625	4	0
1	M	679	0	655	5	0
1	N	672	0	647	4	0
1	O	675	0	651	2	0
1	P	678	0	648	5	0
1	Q	665	0	627	2	0
1	R	662	0	620	2	0
2	S	88	0	72	0	0
2	T	88	0	72	0	0
2	U	88	0	72	0	0
2	V	88	0	72	1	0
2	W	88	0	72	0	0
2	X	88	0	72	0	0
2	Y	88	0	72	0	0
2	Z	88	0	72	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	a	88	0	72	0	0
2	b	88	0	72	0	0
2	c	88	0	72	0	0
2	d	88	0	72	0	0
2	e	88	0	72	0	0
2	f	88	0	72	0	0
2	g	88	0	72	0	0
2	h	88	0	72	0	0
2	i	88	0	72	0	0
2	j	88	0	72	0	0
3	A	12	0	16	1	0
3	B	12	0	16	2	0
3	C	12	0	16	2	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	H	12	0	16	2	0
3	I	12	0	16	0	0
3	K	6	0	8	1	0
3	L	6	0	8	0	0
3	M	6	0	8	0	0
3	N	12	0	16	0	0
3	P	6	0	8	2	0
4	A	126	0	0	1	0
4	B	110	0	0	1	0
4	C	112	0	0	0	0
4	D	107	0	0	1	0
4	E	120	0	0	0	0
4	F	101	0	0	3	0
4	G	97	0	0	1	0
4	H	86	0	0	2	0
4	I	87	0	0	0	0
4	J	84	0	0	1	0
4	K	70	0	0	1	0
4	L	79	0	0	1	1
4	M	112	0	0	3	0
4	N	75	0	0	1	0
4	O	94	0	0	0	1
4	P	80	0	0	0	1
4	Q	76	0	0	1	0
4	R	61	0	0	0	0
All	All	15355	0	12866	77	3

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 (77) 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:J:139:GLU:OE1	4:J:370:HOH:O	1.95	0.82
2:Z:4:GLC:O3	2:Z:5:GLC:O2	2.02	0.73
1:B:142:VAL:HG11	1:B:152:LEU:HD22	1.71	0.71
1:H:148:THR:HG21	2:Z:6:GLC:H3	1.75	0.69
1:B:89:GLU:OE2	3:B:201:GOL:O2	2.14	0.66
1:F:145:GLN:NE2	4:F:301:HOH:O	2.28	0.65
1:I:122:GLU:OE2	1:I:154:HIS:NE2	2.32	0.61
1:C:107:LYS:HE2	1:C:109:HIS:O	2.02	0.59
1:E:122:GLU:CG	1:E:152:LEU:HD11	2.33	0.58
1:C:107:LYS:HD3	1:C:112:PHE:CZ	2.39	0.57
1:P:122:GLU:HG3	1:P:152:LEU:HD11	1.87	0.57
1:E:122:GLU:HG3	1:E:152:LEU:HD11	1.87	0.56
3:K:201:GOL:O1	4:K:343:HOH:O	2.18	0.56
1:P:122:GLU:CG	1:P:152:LEU:HD11	2.35	0.55
1:A:117:ASP:OD2	4:A:386:HOH:O	2.18	0.54
1:H:139:GLU:HG3	3:H:201:GOL:H12	1.89	0.53
2:Z:4:GLC:HO3	2:Z:5:GLC:HO2	1.26	0.52
1:M:120:GLU:HG2	4:M:366:HOH:O	2.09	0.52
1:E:97:ASN:ND2	1:E:101:THR:HG22	2.26	0.51
1:F:88:LYS:NZ	4:F:384:HOH:O	2.25	0.51
1:A:89:GLU:HG2	3:A:202:GOL:H11	1.91	0.51
1:H:122:GLU:HG2	1:H:154:HIS:CD2	2.47	0.50
1:B:105:LEU:HG	1:B:114:ALA:HB2	1.94	0.49
1:R:126:LYS:HE2	1:R:133:TRP:HB3	1.95	0.49
1:B:89:GLU:HB2	3:B:201:GOL:H12	1.93	0.49
1:H:139:GLU:HG3	3:H:201:GOL:C1	2.43	0.48
1:C:105:LEU:HB3	1:C:112:PHE:HB3	1.94	0.48
1:F:73:ASN:HB3	4:F:304:HOH:O	2.13	0.48
1:N:154:HIS:HB2	4:N:364:HOH:O	2.14	0.48
1:P:106:ILE:HD11	3:P:201:GOL:H12	1.94	0.48
1:R:105:LEU:HG	1:R:114:ALA:HB2	1.95	0.48
1:L:83:TRP:CZ2	1:L:85:GLU:HB2	2.49	0.47
1:G:78:PRO:HD2	4:G:339:HOH:O	2.15	0.47
1:P:106:ILE:HD11	3:P:201:GOL:C1	2.45	0.47
1:O:122:GLU:HG2	1:O:154:HIS:CD2	2.50	0.47
1:F:105:LEU:HB3	1:F:112:PHE:HB3	1.97	0.46
1:B:141:VAL:HG23	1:N:141:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:83:TRP:CZ2	1:K:85:GLU:HB2	2.51	0.46
1:H:134:VAL:CG2	4:H:308:HOH:O	2.63	0.46
1:E:107:LYS:HD3	1:E:112:PHE:CZ	2.50	0.46
1:J:105:LEU:HB3	1:J:112:PHE:HB3	1.97	0.45
1:D:105:LEU:HG	1:D:114:ALA:HB2	1.97	0.45
1:B:83:TRP:CZ2	1:B:85:GLU:HB2	2.52	0.45
1:G:83:TRP:CZ2	1:G:85:GLU:HB2	2.52	0.45
1:H:146:LEU:HD13	1:H:148:THR:HG23	1.97	0.45
1:J:122:GLU:HG3	1:J:152:LEU:HD11	1.99	0.45
1:C:114:ALA:HB1	3:C:202:GOL:H12	1.97	0.45
1:D:148:THR:HG21	2:V:6:GLC:H3	1.99	0.45
1:B:105:LEU:HB3	1:B:112:PHE:HB3	1.99	0.44
1:M:120:GLU:CG	4:M:366:HOH:O	2.65	0.44
1:E:81:ILE:HG21	1:E:92:ILE:HD12	1.97	0.44
1:L:105:LEU:HG	1:L:114:ALA:HB2	1.99	0.44
1:M:105:LEU:HB3	1:M:112:PHE:HB3	2.00	0.44
1:L:134:VAL:HG22	4:L:379:HOH:O	2.17	0.44
1:A:107:LYS:HD2	1:A:109:HIS:O	2.17	0.44
1:E:107:LYS:CD	1:E:112:PHE:CZ	3.01	0.43
1:H:83:TRP:CZ2	1:H:85:GLU:HB2	2.53	0.43
1:A:83:TRP:CZ2	1:A:85:GLU:HB2	2.53	0.43
1:A:115:ILE:HD12	3:C:202:GOL:O2	2.18	0.43
1:H:154:HIS:CD2	4:H:307:HOH:O	2.72	0.43
1:M:154:HIS:HB3	4:M:381:HOH:O	2.18	0.43
1:B:142:VAL:CG1	1:B:152:LEU:HD22	2.44	0.42
1:M:122:GLU:CG	1:M:152:LEU:HD11	2.49	0.42
1:O:105:LEU:HB3	1:O:112:PHE:HB3	2.02	0.42
1:Q:105:LEU:HB3	1:Q:112:PHE:HB3	2.02	0.42
1:K:94:GLY:HA2	1:K:99:TRP:CH2	2.55	0.42
1:Q:120:GLU:OE1	4:Q:301:HOH:O	2.22	0.42
1:L:105:LEU:HB3	1:L:112:PHE:HB3	2.01	0.42
1:B:138:SER:OG	4:B:375:HOH:O	2.22	0.41
1:C:105:LEU:HG	1:C:114:ALA:HB2	2.03	0.41
1:A:113:VAL:HG23	1:C:115:ILE:HD11	2.02	0.41
1:P:128:PHE:CZ	1:P:131:GLY:HA2	2.56	0.41
1:N:105:LEU:HB3	1:N:112:PHE:HB3	2.01	0.41
1:K:105:LEU:HB3	1:K:112:PHE:HB3	2.03	0.41
1:A:105:LEU:HB3	1:A:112:PHE:HB3	2.03	0.41
4:D:396:HOH:O	1:N:88:LYS:HE3	2.21	0.41
1:K:105:LEU:HG	1:K:114:ALA:HB2	2.02	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:110:ASN:OD1	1:K:110:ASN:OD1[2_656]	1.85	0.35
4:O:322:HOH:O	4:O:322:HOH:O[2_655]	2.08	0.12
4:L:302:HOH:O	4:P:311:HOH:O[2_655]	2.15	0.05

## 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	80/90 (89%)	79 (99%)	1 (1%)	0	100 100
1	B	81/90 (90%)	78 (96%)	3 (4%)	0	100 100
1	C	82/90 (91%)	80 (98%)	2 (2%)	0	100 100
1	D	77/90 (86%)	76 (99%)	1 (1%)	0	100 100
1	E	84/90 (93%)	83 (99%)	1 (1%)	0	100 100
1	F	83/90 (92%)	81 (98%)	2 (2%)	0	100 100
1	G	82/90 (91%)	81 (99%)	1 (1%)	0	100 100
1	H	83/90 (92%)	81 (98%)	2 (2%)	0	100 100
1	I	83/90 (92%)	81 (98%)	2 (2%)	0	100 100
1	J	83/90 (92%)	82 (99%)	1 (1%)	0	100 100
1	K	80/90 (89%)	79 (99%)	1 (1%)	0	100 100
1	L	80/90 (89%)	79 (99%)	1 (1%)	0	100 100
1	M	83/90 (92%)	82 (99%)	1 (1%)	0	100 100
1	N	82/90 (91%)	81 (99%)	1 (1%)	0	100 100
1	O	82/90 (91%)	81 (99%)	1 (1%)	0	100 100
1	P	83/90 (92%)	81 (98%)	2 (2%)	0	100 100
1	Q	82/90 (91%)	81 (99%)	1 (1%)	0	100 100
1	R	82/90 (91%)	81 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1472/1620 (91%)	1447 (98%)	25 (2%)	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	71/80 (89%)	71 (100%)	0	100 100
1	B	75/80 (94%)	75 (100%)	0	100 100
1	C	73/80 (91%)	73 (100%)	0	100 100
1	D	70/80 (88%)	70 (100%)	0	100 100
1	E	77/80 (96%)	77 (100%)	0	100 100
1	F	77/80 (96%)	77 (100%)	0	100 100
1	G	74/80 (92%)	74 (100%)	0	100 100
1	H	75/80 (94%)	75 (100%)	0	100 100
1	I	72/80 (90%)	72 (100%)	0	100 100
1	J	74/80 (92%)	74 (100%)	0	100 100
1	K	69/80 (86%)	69 (100%)	0	100 100
1	L	72/80 (90%)	72 (100%)	0	100 100
1	M	76/80 (95%)	76 (100%)	0	100 100
1	N	75/80 (94%)	75 (100%)	0	100 100
1	O	76/80 (95%)	76 (100%)	0	100 100
1	P	76/80 (95%)	75 (99%)	1 (1%)	69 74
1	Q	73/80 (91%)	72 (99%)	1 (1%)	67 72
1	R	73/80 (91%)	73 (100%)	0	100 100
All	All	1328/1440 (92%)	1326 (100%)	2 (0%)	93 95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	89	GLU
1	Q	122	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	110	ASN
1	C	110	ASN
1	F	145	GLN
1	N	75	GLN
1	Q	73	ASN

### 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 [\(i\)](#)

144 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	GLC	S	1	2	11,11,12	0.57	0	15,15,17	1.19	1 (6%)
2	GLC	S	2	2	11,11,12	0.72	0	15,15,17	1.74	6 (40%)
2	GLC	S	3	2	11,11,12	0.46	0	15,15,17	1.21	2 (13%)
2	GLC	S	4	2	11,11,12	0.57	0	15,15,17	1.43	3 (20%)
2	GLC	S	5	2	11,11,12	0.57	0	15,15,17	1.31	2 (13%)
2	GLC	S	6	2	11,11,12	0.62	0	15,15,17	1.70	4 (26%)







Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	g	3	2	11,11,12	0.54	0	15,15,17	1.03	1 (6%)
2	GLC	g	4	2	11,11,12	0.28	0	15,15,17	1.86	1 (6%)
2	GLC	g	5	2	11,11,12	0.58	0	15,15,17	1.28	2 (13%)
2	GLC	g	6	2	11,11,12	0.53	0	15,15,17	1.58	3 (20%)
2	GLC	g	7	2	11,11,12	0.43	0	15,15,17	1.06	0
2	GLC	g	8	2	11,11,12	0.68	0	15,15,17	1.06	1 (6%)
2	GLC	h	1	2	11,11,12	0.35	0	15,15,17	1.34	2 (13%)
2	GLC	h	2	2	11,11,12	0.23	0	15,15,17	0.74	0
2	GLC	h	3	2	11,11,12	0.24	0	15,15,17	0.79	0
2	GLC	h	4	2	11,11,12	0.26	0	15,15,17	1.73	3 (20%)
2	GLC	h	5	2	11,11,12	0.50	0	15,15,17	0.94	0
2	GLC	h	6	2	11,11,12	0.48	0	15,15,17	1.58	5 (33%)
2	GLC	h	7	2	11,11,12	0.54	0	15,15,17	1.22	1 (6%)
2	GLC	h	8	2	11,11,12	0.44	0	15,15,17	1.44	2 (13%)
2	GLC	i	1	2	11,11,12	0.57	0	15,15,17	1.31	1 (6%)
2	GLC	i	2	2	11,11,12	0.30	0	15,15,17	1.18	2 (13%)
2	GLC	i	3	2	11,11,12	0.43	0	15,15,17	1.44	3 (20%)
2	GLC	i	4	2	11,11,12	0.24	0	15,15,17	1.24	3 (20%)
2	GLC	i	5	2	11,11,12	0.46	0	15,15,17	0.89	0
2	GLC	i	6	2	11,11,12	0.64	0	15,15,17	1.49	4 (26%)
2	GLC	i	7	2	11,11,12	0.87	0	15,15,17	1.29	1 (6%)
2	GLC	i	8	2	11,11,12	0.46	0	15,15,17	1.20	1 (6%)
2	GLC	j	1	2	11,11,12	0.71	0	15,15,17	0.90	0
2	GLC	j	2	2	11,11,12	0.56	0	15,15,17	1.46	2 (13%)
2	GLC	j	3	2	11,11,12	0.37	0	15,15,17	1.60	4 (26%)
2	GLC	j	4	2	11,11,12	0.55	0	15,15,17	0.88	0
2	GLC	j	5	2	11,11,12	0.46	0	15,15,17	1.43	2 (13%)
2	GLC	j	6	2	11,11,12	0.41	0	15,15,17	2.22	6 (40%)
2	GLC	j	7	2	11,11,12	0.67	0	15,15,17	1.22	2 (13%)
2	GLC	j	8	2	11,11,12	0.41	0	15,15,17	1.74	3 (20%)

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	GLC	S	1	2	-	0/2/19/22	0/1/1/1
2	GLC	S	2	2	-	2/2/19/22	0/1/1/1
2	GLC	S	3	2	-	2/2/19/22	0/1/1/1
2	GLC	S	4	2	-	0/2/19/22	0/1/1/1
2	GLC	S	5	2	-	0/2/19/22	0/1/1/1
2	GLC	S	6	2	-	1/2/19/22	0/1/1/1
2	GLC	S	7	2	-	0/2/19/22	0/1/1/1
2	GLC	S	8	2	-	0/2/19/22	0/1/1/1
2	GLC	T	1	2	-	2/2/19/22	0/1/1/1
2	GLC	T	2	2	-	2/2/19/22	0/1/1/1
2	GLC	T	3	2	-	0/2/19/22	0/1/1/1
2	GLC	T	4	2	-	0/2/19/22	0/1/1/1
2	GLC	T	5	2	-	0/2/19/22	0/1/1/1
2	GLC	T	6	2	-	0/2/19/22	0/1/1/1
2	GLC	T	7	2	-	0/2/19/22	0/1/1/1
2	GLC	T	8	2	-	0/2/19/22	0/1/1/1
2	GLC	U	1	2	-	1/2/19/22	0/1/1/1
2	GLC	U	2	2	-	2/2/19/22	0/1/1/1
2	GLC	U	3	2	-	2/2/19/22	0/1/1/1
2	GLC	U	4	2	-	2/2/19/22	0/1/1/1
2	GLC	U	5	2	-	0/2/19/22	0/1/1/1
2	GLC	U	6	2	-	1/2/19/22	0/1/1/1
2	GLC	U	7	2	-	0/2/19/22	0/1/1/1
2	GLC	U	8	2	-	0/2/19/22	0/1/1/1
2	GLC	V	1	2	-	0/2/19/22	0/1/1/1
2	GLC	V	2	2	-	1/2/19/22	0/1/1/1
2	GLC	V	3	2	-	0/2/19/22	0/1/1/1
2	GLC	V	4	2	-	0/2/19/22	0/1/1/1
2	GLC	V	5	2	-	0/2/19/22	0/1/1/1
2	GLC	V	6	2	-	1/2/19/22	0/1/1/1
2	GLC	V	7	2	-	0/2/19/22	0/1/1/1
2	GLC	V	8	2	-	0/2/19/22	0/1/1/1
2	GLC	W	1	2	-	0/2/19/22	0/1/1/1
2	GLC	W	2	2	-	0/2/19/22	0/1/1/1
2	GLC	W	3	2	-	1/2/19/22	0/1/1/1
2	GLC	W	4	2	-	0/2/19/22	0/1/1/1
2	GLC	W	5	2	-	0/2/19/22	0/1/1/1
2	GLC	W	6	2	-	0/2/19/22	0/1/1/1
2	GLC	W	7	2	-	0/2/19/22	0/1/1/1
2	GLC	W	8	2	-	1/2/19/22	0/1/1/1
2	GLC	X	1	2	-	0/2/19/22	0/1/1/1
2	GLC	X	2	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	X	3	2	-	0/2/19/22	0/1/1/1
2	GLC	X	4	2	-	2/2/19/22	0/1/1/1
2	GLC	X	5	2	-	0/2/19/22	0/1/1/1
2	GLC	X	6	2	-	0/2/19/22	0/1/1/1
2	GLC	X	7	2	-	0/2/19/22	0/1/1/1
2	GLC	X	8	2	-	0/2/19/22	0/1/1/1
2	GLC	Y	1	2	-	0/2/19/22	0/1/1/1
2	GLC	Y	2	2	-	2/2/19/22	0/1/1/1
2	GLC	Y	3	2	-	0/2/19/22	0/1/1/1
2	GLC	Y	4	2	-	0/2/19/22	0/1/1/1
2	GLC	Y	5	2	-	0/2/19/22	0/1/1/1
2	GLC	Y	6	2	-	1/2/19/22	0/1/1/1
2	GLC	Y	7	2	-	0/2/19/22	0/1/1/1
2	GLC	Y	8	2	-	0/2/19/22	0/1/1/1
2	GLC	Z	1	2	-	2/2/19/22	0/1/1/1
2	GLC	Z	2	2	-	2/2/19/22	0/1/1/1
2	GLC	Z	3	2	-	2/2/19/22	0/1/1/1
2	GLC	Z	4	2	-	0/2/19/22	0/1/1/1
2	GLC	Z	5	2	-	0/2/19/22	0/1/1/1
2	GLC	Z	6	2	-	1/2/19/22	0/1/1/1
2	GLC	Z	7	2	-	0/2/19/22	0/1/1/1
2	GLC	Z	8	2	-	0/2/19/22	0/1/1/1
2	GLC	a	1	2	-	2/2/19/22	0/1/1/1
2	GLC	a	2	2	-	2/2/19/22	0/1/1/1
2	GLC	a	3	2	-	1/2/19/22	0/1/1/1
2	GLC	a	4	2	-	2/2/19/22	0/1/1/1
2	GLC	a	5	2	-	0/2/19/22	0/1/1/1
2	GLC	a	6	2	-	2/2/19/22	0/1/1/1
2	GLC	a	7	2	-	0/2/19/22	0/1/1/1
2	GLC	a	8	2	-	0/2/19/22	0/1/1/1
2	GLC	b	1	2	-	0/2/19/22	0/1/1/1
2	GLC	b	2	2	-	0/2/19/22	0/1/1/1
2	GLC	b	3	2	-	0/2/19/22	0/1/1/1
2	GLC	b	4	2	-	2/2/19/22	0/1/1/1
2	GLC	b	5	2	-	0/2/19/22	0/1/1/1
2	GLC	b	6	2	-	1/2/19/22	0/1/1/1
2	GLC	b	7	2	-	0/2/19/22	0/1/1/1
2	GLC	b	8	2	-	0/2/19/22	0/1/1/1
2	GLC	c	1	2	-	0/2/19/22	0/1/1/1
2	GLC	c	2	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	c	3	2	-	1/2/19/22	0/1/1/1
2	GLC	c	4	2	-	2/2/19/22	0/1/1/1
2	GLC	c	5	2	-	0/2/19/22	0/1/1/1
2	GLC	c	6	2	-	2/2/19/22	0/1/1/1
2	GLC	c	7	2	-	0/2/19/22	0/1/1/1
2	GLC	c	8	2	-	0/2/19/22	0/1/1/1
2	GLC	d	1	2	-	2/2/19/22	0/1/1/1
2	GLC	d	2	2	-	1/2/19/22	0/1/1/1
2	GLC	d	3	2	-	1/2/19/22	0/1/1/1
2	GLC	d	4	2	-	2/2/19/22	0/1/1/1
2	GLC	d	5	2	-	0/2/19/22	0/1/1/1
2	GLC	d	6	2	-	2/2/19/22	0/1/1/1
2	GLC	d	7	2	-	0/2/19/22	0/1/1/1
2	GLC	d	8	2	-	0/2/19/22	0/1/1/1
2	GLC	e	1	2	-	0/2/19/22	0/1/1/1
2	GLC	e	2	2	-	0/2/19/22	0/1/1/1
2	GLC	e	3	2	-	0/2/19/22	0/1/1/1
2	GLC	e	4	2	-	2/2/19/22	0/1/1/1
2	GLC	e	5	2	-	1/2/19/22	0/1/1/1
2	GLC	e	6	2	-	2/2/19/22	0/1/1/1
2	GLC	e	7	2	-	0/2/19/22	0/1/1/1
2	GLC	e	8	2	-	0/2/19/22	0/1/1/1
2	GLC	f	1	2	-	2/2/19/22	0/1/1/1
2	GLC	f	2	2	-	2/2/19/22	0/1/1/1
2	GLC	f	3	2	-	1/2/19/22	0/1/1/1
2	GLC	f	4	2	-	0/2/19/22	0/1/1/1
2	GLC	f	5	2	-	2/2/19/22	0/1/1/1
2	GLC	f	6	2	-	0/2/19/22	0/1/1/1
2	GLC	f	7	2	-	0/2/19/22	0/1/1/1
2	GLC	f	8	2	-	2/2/19/22	0/1/1/1
2	GLC	g	1	2	-	0/2/19/22	0/1/1/1
2	GLC	g	2	2	-	2/2/19/22	0/1/1/1
2	GLC	g	3	2	-	2/2/19/22	0/1/1/1
2	GLC	g	4	2	-	2/2/19/22	0/1/1/1
2	GLC	g	5	2	-	0/2/19/22	0/1/1/1
2	GLC	g	6	2	-	1/2/19/22	0/1/1/1
2	GLC	g	7	2	-	0/2/19/22	0/1/1/1
2	GLC	g	8	2	-	0/2/19/22	0/1/1/1
2	GLC	h	1	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	h	2	2	-	0/2/19/22	0/1/1/1
2	GLC	h	3	2	-	2/2/19/22	0/1/1/1
2	GLC	h	4	2	-	1/2/19/22	0/1/1/1
2	GLC	h	5	2	-	0/2/19/22	0/1/1/1
2	GLC	h	6	2	-	0/2/19/22	0/1/1/1
2	GLC	h	7	2	-	0/2/19/22	0/1/1/1
2	GLC	h	8	2	-	0/2/19/22	0/1/1/1
2	GLC	i	1	2	-	2/2/19/22	0/1/1/1
2	GLC	i	2	2	-	1/2/19/22	0/1/1/1
2	GLC	i	3	2	-	0/2/19/22	0/1/1/1
2	GLC	i	4	2	-	0/2/19/22	0/1/1/1
2	GLC	i	5	2	-	0/2/19/22	0/1/1/1
2	GLC	i	6	2	-	2/2/19/22	0/1/1/1
2	GLC	i	7	2	-	0/2/19/22	0/1/1/1
2	GLC	i	8	2	-	0/2/19/22	0/1/1/1
2	GLC	j	1	2	-	1/2/19/22	0/1/1/1
2	GLC	j	2	2	-	0/2/19/22	0/1/1/1
2	GLC	j	3	2	-	2/2/19/22	0/1/1/1
2	GLC	j	4	2	-	2/2/19/22	0/1/1/1
2	GLC	j	5	2	-	1/2/19/22	0/1/1/1
2	GLC	j	6	2	-	2/2/19/22	0/1/1/1
2	GLC	j	7	2	-	0/2/19/22	0/1/1/1
2	GLC	j	8	2	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	6	GLC	O5-C1	-2.65	1.39	1.43
2	f	1	GLC	C2-C3	2.29	1.55	1.52
2	f	4	GLC	C2-C3	2.28	1.55	1.52
2	U	5	GLC	O5-C1	-2.00	1.40	1.43

All (291) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	4	GLC	C1-C2-C3	6.88	118.12	109.67
2	U	4	GLC	C1-O5-C5	6.27	120.69	112.19
2	g	4	GLC	C1-O5-C5	6.08	120.43	112.19
2	f	1	GLC	C1-C2-C3	6.06	117.11	109.67
2	b	4	GLC	C1-O5-C5	5.84	120.11	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	8	GLC	C1-O5-C5	5.27	119.33	112.19
2	c	4	GLC	C1-O5-C5	5.21	119.25	112.19
2	X	6	GLC	C1-O5-C5	4.95	118.89	112.19
2	h	4	GLC	C1-O5-C5	4.77	118.66	112.19
2	j	6	GLC	O5-C1-C2	-4.74	103.46	110.77
2	d	4	GLC	C1-O5-C5	4.64	118.47	112.19
2	f	5	GLC	O5-C1-C2	-4.59	103.69	110.77
2	d	6	GLC	O4-C4-C3	-4.49	99.96	110.35
2	c	6	GLC	C1-O5-C5	4.48	118.27	112.19
2	f	2	GLC	O5-C1-C2	-4.40	103.97	110.77
2	V	6	GLC	O5-C5-C6	4.26	113.88	107.20
2	a	4	GLC	C1-O5-C5	4.20	117.88	112.19
2	W	8	GLC	O5-C5-C6	4.16	113.72	107.20
2	e	4	GLC	C1-O5-C5	4.14	117.80	112.19
2	U	6	GLC	O5-C5-C6	4.04	113.53	107.20
2	j	2	GLC	C1-C2-C3	4.00	114.58	109.67
2	X	4	GLC	C1-O5-C5	3.95	117.55	112.19
2	Y	6	GLC	O5-C5-C6	3.83	113.21	107.20
2	f	6	GLC	C6-C5-C4	3.80	121.91	113.00
2	Z	3	GLC	O3-C3-C2	3.75	117.17	109.99
2	h	8	GLC	C1-O5-C5	3.74	117.25	112.19
2	Z	2	GLC	O5-C1-C2	-3.57	105.26	110.77
2	e	5	GLC	C1-O5-C5	3.54	116.99	112.19
2	Z	6	GLC	O5-C5-C6	3.53	112.74	107.20
2	X	6	GLC	O5-C5-C6	3.52	112.72	107.20
2	f	6	GLC	O2-C2-C3	3.49	117.14	110.14
2	S	6	GLC	C3-C4-C5	3.49	116.46	110.24
2	T	6	GLC	O5-C5-C6	3.49	112.67	107.20
2	f	3	GLC	C1-C2-C3	3.45	113.91	109.67
2	e	2	GLC	C1-O5-C5	3.42	116.82	112.19
2	W	4	GLC	C1-O5-C5	3.39	116.79	112.19
2	X	5	GLC	O6-C6-C5	-3.39	99.65	111.29
2	V	2	GLC	C1-O5-C5	3.35	116.73	112.19
2	Z	4	GLC	C2-C3-C4	-3.33	105.14	110.89
2	Z	4	GLC	O5-C5-C6	3.31	112.39	107.20
2	T	8	GLC	C1-O5-C5	3.30	116.67	112.19
2	j	6	GLC	C1-O5-C5	3.29	116.66	112.19
2	f	6	GLC	O6-C6-C5	-3.28	100.03	111.29
2	g	6	GLC	C3-C4-C5	3.27	116.08	110.24
2	j	6	GLC	O5-C5-C6	3.25	112.30	107.20
2	S	6	GLC	C1-O5-C5	3.24	116.58	112.19
2	d	6	GLC	C3-C4-C5	3.23	116.00	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	5	GLC	C1-O5-C5	3.21	116.54	112.19
2	d	7	GLC	O2-C2-C3	3.20	116.55	110.14
2	S	4	GLC	C1-O5-C5	3.18	116.50	112.19
2	d	3	GLC	O5-C1-C2	-3.16	105.89	110.77
2	a	8	GLC	C1-O5-C5	3.16	116.48	112.19
2	T	4	GLC	C1-O5-C5	3.15	116.46	112.19
2	Z	2	GLC	C1-O5-C5	3.14	116.44	112.19
2	U	3	GLC	O5-C5-C6	3.13	112.11	107.20
2	f	3	GLC	C1-O5-C5	3.12	116.42	112.19
2	e	6	GLC	O5-C5-C6	3.11	112.09	107.20
2	h	4	GLC	O4-C4-C3	-3.11	103.15	110.35
2	T	1	GLC	C1-O5-C5	3.11	116.41	112.19
2	S	1	GLC	C1-O5-C5	3.10	116.40	112.19
2	W	8	GLC	C1-O5-C5	3.10	116.39	112.19
2	j	3	GLC	O5-C1-C2	-3.09	105.99	110.77
2	d	6	GLC	C6-C5-C4	3.09	120.24	113.00
2	f	4	GLC	C1-O5-C5	3.08	116.37	112.19
2	Z	6	GLC	C3-C4-C5	3.08	115.73	110.24
2	U	5	GLC	O2-C2-C3	-3.07	103.98	110.14
2	W	7	GLC	C3-C4-C5	3.07	115.72	110.24
2	e	3	GLC	O4-C4-C3	-3.07	103.25	110.35
2	U	3	GLC	C1-O5-C5	3.06	116.34	112.19
2	a	3	GLC	O4-C4-C3	-3.05	103.29	110.35
2	j	5	GLC	O3-C3-C4	-3.04	103.33	110.35
2	e	1	GLC	C1-O5-C5	3.03	116.30	112.19
2	e	6	GLC	O4-C4-C3	-3.03	103.35	110.35
2	U	1	GLC	O2-C2-C3	-3.01	104.10	110.14
2	W	4	GLC	O5-C1-C2	3.01	115.42	110.77
2	b	1	GLC	C1-O5-C5	2.99	116.25	112.19
2	h	6	GLC	C3-C4-C5	2.99	115.58	110.24
2	a	7	GLC	O3-C3-C2	2.99	115.72	109.99
2	i	2	GLC	O5-C1-C2	-2.99	106.15	110.77
2	T	3	GLC	C1-O5-C5	2.97	116.22	112.19
2	j	3	GLC	C1-C2-C3	2.96	113.30	109.67
2	g	2	GLC	O2-C2-C3	-2.94	104.24	110.14
2	i	1	GLC	C1-O5-C5	2.93	116.17	112.19
2	i	3	GLC	C1-O5-C5	2.92	116.15	112.19
2	g	2	GLC	O4-C4-C3	-2.91	103.62	110.35
2	T	2	GLC	O5-C5-C6	2.90	111.75	107.20
2	V	1	GLC	O6-C6-C5	-2.90	101.34	111.29
2	V	2	GLC	O4-C4-C3	-2.88	103.68	110.35
2	Z	3	GLC	O4-C4-C3	-2.88	103.68	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	6	GLC	C1-O5-C5	2.88	116.09	112.19
2	V	6	GLC	O3-C3-C2	2.84	115.44	109.99
2	g	6	GLC	C1-O5-C5	2.84	116.04	112.19
2	b	6	GLC	C3-C4-C5	2.82	115.27	110.24
2	e	6	GLC	C3-C4-C5	2.81	115.25	110.24
2	X	5	GLC	C2-C3-C4	2.81	115.76	110.89
2	f	4	GLC	O2-C2-C1	-2.81	103.41	109.15
2	b	6	GLC	C1-O5-C5	2.81	115.99	112.19
2	f	4	GLC	C2-C3-C4	2.80	115.74	110.89
2	e	3	GLC	C1-O5-C5	2.79	115.97	112.19
2	X	6	GLC	O3-C3-C4	-2.79	103.91	110.35
2	S	6	GLC	O5-C5-C6	2.78	111.56	107.20
2	i	7	GLC	O3-C3-C2	2.78	115.31	109.99
2	b	2	GLC	C1-O5-C5	2.76	115.93	112.19
2	i	8	GLC	O2-C2-C3	-2.76	104.62	110.14
2	f	2	GLC	C1-O5-C5	2.75	115.92	112.19
2	U	1	GLC	O6-C6-C5	-2.73	101.92	111.29
2	i	6	GLC	O4-C4-C3	-2.73	104.04	110.35
2	d	7	GLC	O3-C3-C4	-2.71	104.08	110.35
2	T	2	GLC	O2-C2-C3	-2.70	104.72	110.14
2	T	5	GLC	O6-C6-C5	-2.70	102.02	111.29
2	S	2	GLC	O5-C1-C2	-2.68	106.64	110.77
2	W	5	GLC	O5-C1-C2	-2.68	106.64	110.77
2	S	3	GLC	O5-C1-C2	-2.68	106.64	110.77
2	W	6	GLC	O5-C5-C6	2.67	111.38	107.20
2	d	4	GLC	C3-C4-C5	2.67	114.99	110.24
2	S	8	GLC	O5-C5-C6	2.66	111.38	107.20
2	f	1	GLC	C3-C4-C5	-2.66	105.49	110.24
2	W	6	GLC	C3-C4-C5	2.65	114.97	110.24
2	X	8	GLC	C1-O5-C5	2.65	115.79	112.19
2	j	5	GLC	C1-O5-C5	2.65	115.78	112.19
2	i	3	GLC	O2-C2-C3	-2.64	104.85	110.14
2	g	2	GLC	C1-O5-C5	2.64	115.77	112.19
2	S	8	GLC	C1-C2-C3	2.62	112.89	109.67
2	X	5	GLC	O4-C4-C3	-2.62	104.30	110.35
2	i	6	GLC	C6-C5-C4	2.62	119.14	113.00
2	i	4	GLC	C1-O5-C5	2.61	115.73	112.19
2	U	6	GLC	C3-C4-C5	2.60	114.88	110.24
2	Z	8	GLC	O3-C3-C2	-2.60	105.02	109.99
2	S	3	GLC	C1-O5-C5	2.60	115.71	112.19
2	U	3	GLC	O5-C1-C2	-2.60	106.76	110.77
2	Z	4	GLC	O5-C5-C4	-2.57	104.57	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	3	GLC	C6-C5-C4	-2.57	106.98	113.00
2	T	4	GLC	O4-C4-C3	-2.57	104.41	110.35
2	c	3	GLC	O4-C4-C3	-2.57	104.42	110.35
2	V	6	GLC	C3-C4-C5	2.56	114.81	110.24
2	X	6	GLC	O3-C3-C2	2.55	114.88	109.99
2	j	6	GLC	C1-C2-C3	-2.54	106.54	109.67
2	f	8	GLC	O4-C4-C3	-2.54	104.48	110.35
2	X	3	GLC	O2-C2-C1	-2.53	103.98	109.15
2	X	5	GLC	O5-C5-C4	-2.52	104.69	110.83
2	c	4	GLC	C1-C2-C3	2.51	112.76	109.67
2	T	2	GLC	O2-C2-C1	2.51	114.28	109.15
2	f	3	GLC	O3-C3-C2	2.50	114.79	109.99
2	b	1	GLC	O5-C1-C2	-2.50	106.92	110.77
2	S	2	GLC	O2-C2-C3	-2.49	105.14	110.14
2	j	3	GLC	O2-C2-C3	-2.49	105.15	110.14
2	a	3	GLC	O5-C1-C2	-2.49	106.92	110.77
2	T	4	GLC	O2-C2-C3	-2.48	105.18	110.14
2	X	7	GLC	C1-O5-C5	2.48	115.55	112.19
2	i	6	GLC	C1-O5-C5	2.47	115.54	112.19
2	c	5	GLC	C1-C2-C3	2.47	112.71	109.67
2	T	6	GLC	C3-C4-C5	2.47	114.65	110.24
2	e	5	GLC	O5-C1-C2	-2.47	106.97	110.77
2	f	7	GLC	O2-C2-C3	2.46	115.08	110.14
2	S	2	GLC	O4-C4-C3	-2.46	104.65	110.35
2	T	1	GLC	O5-C1-C2	-2.46	106.98	110.77
2	T	7	GLC	O2-C2-C3	2.44	115.03	110.14
2	g	6	GLC	C6-C5-C4	2.43	118.70	113.00
2	U	6	GLC	C1-O5-C5	2.42	115.47	112.19
2	d	7	GLC	O5-C5-C6	2.42	111.00	107.20
2	h	1	GLC	C1-O5-C5	2.41	115.46	112.19
2	V	2	GLC	O2-C2-C3	-2.41	105.31	110.14
2	V	1	GLC	O5-C5-C6	-2.41	103.43	107.20
2	f	4	GLC	O3-C3-C4	-2.40	104.79	110.35
2	S	2	GLC	O3-C3-C2	2.39	114.58	109.99
2	Y	1	GLC	C1-O5-C5	2.39	115.43	112.19
2	S	2	GLC	C3-C4-C5	-2.38	106.00	110.24
2	g	5	GLC	C1-O5-C5	2.38	115.41	112.19
2	b	6	GLC	C6-C5-C4	2.38	118.57	113.00
2	Y	6	GLC	O2-C2-C1	-2.37	104.29	109.15
2	d	6	GLC	O3-C3-C2	2.36	114.52	109.99
2	a	6	GLC	C6-C5-C4	2.36	118.53	113.00
2	i	4	GLC	O4-C4-C3	-2.36	104.90	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	1	GLC	O6-C6-C5	-2.36	103.21	111.29
2	S	5	GLC	O6-C6-C5	-2.35	103.23	111.29
2	X	3	GLC	O3-C3-C4	-2.35	104.92	110.35
2	X	1	GLC	O6-C6-C5	-2.35	103.24	111.29
2	Z	3	GLC	C1-O5-C5	2.34	115.37	112.19
2	a	3	GLC	O3-C3-C4	-2.34	104.94	110.35
2	c	6	GLC	C3-C4-C5	2.34	114.41	110.24
2	j	6	GLC	O2-C2-C1	2.34	113.93	109.15
2	Z	3	GLC	C1-C2-C3	2.33	112.53	109.67
2	f	7	GLC	C1-O5-C5	2.32	115.33	112.19
2	c	2	GLC	C1-O5-C5	2.31	115.33	112.19
2	c	7	GLC	O2-C2-C3	2.30	114.75	110.14
2	g	8	GLC	O4-C4-C3	-2.30	105.04	110.35
2	i	6	GLC	C3-C4-C5	2.29	114.33	110.24
2	V	6	GLC	O4-C4-C3	-2.29	105.06	110.35
2	W	6	GLC	C1-O5-C5	2.29	115.29	112.19
2	a	7	GLC	O2-C2-C3	2.28	114.71	110.14
2	f	8	GLC	O5-C5-C6	2.28	110.78	107.20
2	S	2	GLC	O5-C5-C6	2.28	110.78	107.20
2	j	7	GLC	O5-C5-C6	2.27	110.77	107.20
2	d	7	GLC	O3-C3-C2	2.27	114.34	109.99
2	Y	6	GLC	C6-C5-C4	2.26	118.31	113.00
2	h	6	GLC	C6-C5-C4	2.26	118.30	113.00
2	X	8	GLC	O3-C3-C2	-2.26	105.66	109.99
2	d	8	GLC	O2-C2-C1	2.26	113.78	109.15
2	e	4	GLC	O5-C5-C6	-2.26	103.67	107.20
2	b	7	GLC	C1-C2-C3	-2.26	106.89	109.67
2	X	3	GLC	O3-C3-C2	2.26	114.31	109.99
2	a	1	GLC	O3-C3-C4	-2.25	105.14	110.35
2	W	7	GLC	O3-C3-C2	2.25	114.30	109.99
2	Z	1	GLC	O3-C3-C4	-2.25	105.15	110.35
2	S	6	GLC	O5-C1-C2	2.25	114.24	110.77
2	Y	4	GLC	C1-C2-C3	2.25	112.43	109.67
2	W	1	GLC	C6-C5-C4	2.25	118.26	113.00
2	Y	6	GLC	O5-C1-C2	-2.24	107.31	110.77
2	j	7	GLC	O2-C2-C1	2.24	113.73	109.15
2	j	6	GLC	C6-C5-C4	2.24	118.25	113.00
2	U	1	GLC	C1-O5-C5	2.23	115.21	112.19
2	f	3	GLC	O5-C5-C4	2.23	116.24	110.83
2	Y	4	GLC	C1-O5-C5	2.23	115.21	112.19
2	c	5	GLC	O2-C2-C3	-2.22	105.68	110.14
2	Z	1	GLC	C1-C2-C3	2.22	112.40	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	6	GLC	C1-O5-C5	2.22	115.20	112.19
2	e	5	GLC	O3-C3-C4	-2.22	105.22	110.35
2	T	4	GLC	O4-C4-C5	2.22	114.80	109.30
2	W	2	GLC	C1-O5-C5	2.21	115.19	112.19
2	g	3	GLC	O5-C1-C2	-2.21	107.36	110.77
2	d	8	GLC	O3-C3-C2	-2.21	105.76	109.99
2	W	1	GLC	O2-C2-C1	-2.21	104.63	109.15
2	c	6	GLC	O5-C5-C6	2.21	110.67	107.20
2	c	5	GLC	C3-C4-C5	-2.21	106.30	110.24
2	Z	3	GLC	O5-C1-C2	-2.20	107.37	110.77
2	W	7	GLC	C2-C3-C4	-2.20	107.09	110.89
2	X	6	GLC	C6-C5-C4	2.20	118.16	113.00
2	c	4	GLC	O4-C4-C3	-2.20	105.27	110.35
2	j	3	GLC	O5-C5-C6	2.20	110.65	107.20
2	f	1	GLC	O2-C2-C1	-2.20	104.66	109.15
2	X	5	GLC	C3-C4-C5	-2.18	106.36	110.24
2	X	2	GLC	O4-C4-C3	-2.18	105.32	110.35
2	h	7	GLC	O5-C5-C6	2.17	110.61	107.20
2	W	3	GLC	O4-C4-C3	-2.17	105.33	110.35
2	T	2	GLC	O4-C4-C3	-2.16	105.35	110.35
2	a	1	GLC	C1-O5-C5	2.16	115.11	112.19
2	T	5	GLC	O4-C4-C3	-2.15	105.37	110.35
2	W	1	GLC	C3-C4-C5	-2.15	106.40	110.24
2	g	5	GLC	O4-C4-C3	-2.15	105.38	110.35
2	d	7	GLC	O5-C1-C2	2.15	114.09	110.77
2	j	8	GLC	C2-C3-C4	-2.15	107.18	110.89
2	Y	4	GLC	O4-C4-C3	-2.14	105.39	110.35
2	S	4	GLC	O4-C4-C3	-2.14	105.39	110.35
2	V	3	GLC	O5-C5-C6	2.13	110.55	107.20
2	f	1	GLC	O5-C5-C6	2.13	110.55	107.20
2	h	6	GLC	O6-C6-C5	-2.13	103.98	111.29
2	V	2	GLC	O5-C5-C6	-2.13	103.87	107.20
2	j	8	GLC	C6-C5-C4	-2.13	108.02	113.00
2	h	4	GLC	C1-C2-C3	2.13	112.28	109.67
2	f	7	GLC	O4-C4-C3	-2.12	105.44	110.35
2	h	6	GLC	C1-O5-C5	2.12	115.07	112.19
2	a	7	GLC	O5-C5-C4	-2.12	105.66	110.83
2	Y	8	GLC	O5-C5-C6	2.12	110.53	107.20
2	Z	1	GLC	C2-C3-C4	2.12	114.56	110.89
2	a	7	GLC	O2-C2-C1	-2.12	104.82	109.15
2	X	4	GLC	O2-C2-C3	-2.10	105.92	110.14
2	e	3	GLC	O2-C2-C3	-2.10	105.93	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	4	GLC	O4-C4-C3	-2.10	105.50	110.35
2	e	8	GLC	O5-C5-C6	2.10	110.49	107.20
2	X	7	GLC	O2-C2-C1	-2.10	104.86	109.15
2	j	2	GLC	C2-C3-C4	2.09	114.52	110.89
2	h	1	GLC	O6-C6-C5	-2.08	104.15	111.29
2	V	6	GLC	O5-C1-C2	-2.08	107.56	110.77
2	a	7	GLC	O5-C1-C2	-2.08	107.56	110.77
2	f	1	GLC	O5-C5-C4	-2.08	105.78	110.83
2	V	8	GLC	C1-O5-C5	2.07	115.00	112.19
2	V	8	GLC	O3-C3-C2	-2.07	106.03	109.99
2	V	5	GLC	C3-C4-C5	-2.07	106.55	110.24
2	Z	6	GLC	C1-O5-C5	2.06	114.98	112.19
2	i	4	GLC	O2-C2-C3	-2.06	106.01	110.14
2	b	2	GLC	O5-C1-C2	-2.06	107.59	110.77
2	d	4	GLC	O3-C3-C4	-2.06	105.59	110.35
2	h	8	GLC	C1-C2-C3	2.05	112.19	109.67
2	i	2	GLC	C1-O5-C5	2.05	114.97	112.19
2	i	3	GLC	O5-C1-C2	-2.05	107.61	110.77
2	d	2	GLC	O4-C4-C5	2.05	114.38	109.30
2	b	5	GLC	O4-C4-C5	2.04	114.36	109.30
2	h	6	GLC	O5-C5-C6	2.04	110.40	107.20
2	c	5	GLC	O5-C5-C6	2.03	110.39	107.20
2	W	6	GLC	O3-C3-C2	2.03	113.88	109.99
2	X	3	GLC	O5-C1-C2	-2.03	107.64	110.77
2	T	3	GLC	O5-C5-C6	2.02	110.38	107.20
2	b	6	GLC	O6-C6-C5	-2.02	104.35	111.29
2	S	4	GLC	O5-C5-C6	-2.02	104.05	107.20
2	d	6	GLC	O5-C5-C6	2.01	110.36	107.20
2	S	8	GLC	C2-C3-C4	-2.01	107.41	110.89
2	W	5	GLC	C3-C4-C5	-2.01	106.65	110.24
2	b	3	GLC	O2-C2-C1	-2.01	105.04	109.15
2	f	2	GLC	O5-C5-C4	2.01	115.71	110.83
2	a	6	GLC	O6-C6-C5	-2.00	104.42	111.29
2	d	1	GLC	C1-C2-C3	2.00	112.12	109.67

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	U	2	GLC	O5-C5-C6-O6
2	Z	2	GLC	O5-C5-C6-O6
2	a	2	GLC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	c	4	GLC	O5-C5-C6-O6
2	f	5	GLC	O5-C5-C6-O6
2	U	2	GLC	C4-C5-C6-O6
2	Z	2	GLC	C4-C5-C6-O6
2	U	3	GLC	O5-C5-C6-O6
2	Y	2	GLC	O5-C5-C6-O6
2	j	3	GLC	O5-C5-C6-O6
2	X	4	GLC	O5-C5-C6-O6
2	e	4	GLC	O5-C5-C6-O6
2	j	6	GLC	O5-C5-C6-O6
2	f	5	GLC	C4-C5-C6-O6
2	j	6	GLC	C4-C5-C6-O6
2	d	4	GLC	O5-C5-C6-O6
2	a	2	GLC	C4-C5-C6-O6
2	c	4	GLC	C4-C5-C6-O6
2	d	6	GLC	C4-C5-C6-O6
2	a	4	GLC	O5-C5-C6-O6
2	g	2	GLC	O5-C5-C6-O6
2	g	4	GLC	O5-C5-C6-O6
2	j	4	GLC	O5-C5-C6-O6
2	a	6	GLC	C4-C5-C6-O6
2	b	4	GLC	C4-C5-C6-O6
2	c	6	GLC	C4-C5-C6-O6
2	g	2	GLC	C4-C5-C6-O6
2	i	6	GLC	C4-C5-C6-O6
2	g	4	GLC	C4-C5-C6-O6
2	j	3	GLC	C4-C5-C6-O6
2	j	8	GLC	C4-C5-C6-O6
2	f	1	GLC	O5-C5-C6-O6
2	a	1	GLC	C4-C5-C6-O6
2	j	4	GLC	C4-C5-C6-O6
2	T	2	GLC	O5-C5-C6-O6
2	e	6	GLC	C4-C5-C6-O6
2	Z	3	GLC	O5-C5-C6-O6
2	b	4	GLC	O5-C5-C6-O6
2	f	1	GLC	C4-C5-C6-O6
2	S	3	GLC	O5-C5-C6-O6
2	f	2	GLC	O5-C5-C6-O6
2	Y	6	GLC	C4-C5-C6-O6
2	a	4	GLC	C4-C5-C6-O6
2	d	4	GLC	C4-C5-C6-O6
2	g	3	GLC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	S	2	GLC	O5-C5-C6-O6
2	U	4	GLC	O5-C5-C6-O6
2	T	1	GLC	C4-C5-C6-O6
2	h	3	GLC	O5-C5-C6-O6
2	U	3	GLC	C4-C5-C6-O6
2	V	6	GLC	C4-C5-C6-O6
2	S	3	GLC	C4-C5-C6-O6
2	S	2	GLC	C4-C5-C6-O6
2	f	8	GLC	C4-C5-C6-O6
2	Z	6	GLC	C4-C5-C6-O6
2	i	1	GLC	C4-C5-C6-O6
2	a	1	GLC	O5-C5-C6-O6
2	f	8	GLC	O5-C5-C6-O6
2	d	2	GLC	O5-C5-C6-O6
2	j	8	GLC	O5-C5-C6-O6
2	a	6	GLC	O5-C5-C6-O6
2	T	1	GLC	O5-C5-C6-O6
2	g	6	GLC	C4-C5-C6-O6
2	d	6	GLC	O5-C5-C6-O6
2	Z	1	GLC	C4-C5-C6-O6
2	h	1	GLC	C4-C5-C6-O6
2	a	3	GLC	O5-C5-C6-O6
2	T	2	GLC	C4-C5-C6-O6
2	V	2	GLC	O5-C5-C6-O6
2	d	3	GLC	O5-C5-C6-O6
2	S	6	GLC	C4-C5-C6-O6
2	Z	3	GLC	C4-C5-C6-O6
2	i	2	GLC	O5-C5-C6-O6
2	f	3	GLC	O5-C5-C6-O6
2	c	3	GLC	O5-C5-C6-O6
2	Y	2	GLC	C4-C5-C6-O6
2	X	4	GLC	C4-C5-C6-O6
2	d	1	GLC	C4-C5-C6-O6
2	c	6	GLC	O5-C5-C6-O6
2	i	1	GLC	O5-C5-C6-O6
2	i	6	GLC	O5-C5-C6-O6
2	U	1	GLC	C4-C5-C6-O6
2	h	4	GLC	C4-C5-C6-O6
2	b	6	GLC	O5-C5-C6-O6
2	U	6	GLC	C4-C5-C6-O6
2	e	5	GLC	C4-C5-C6-O6
2	W	8	GLC	C4-C5-C6-O6

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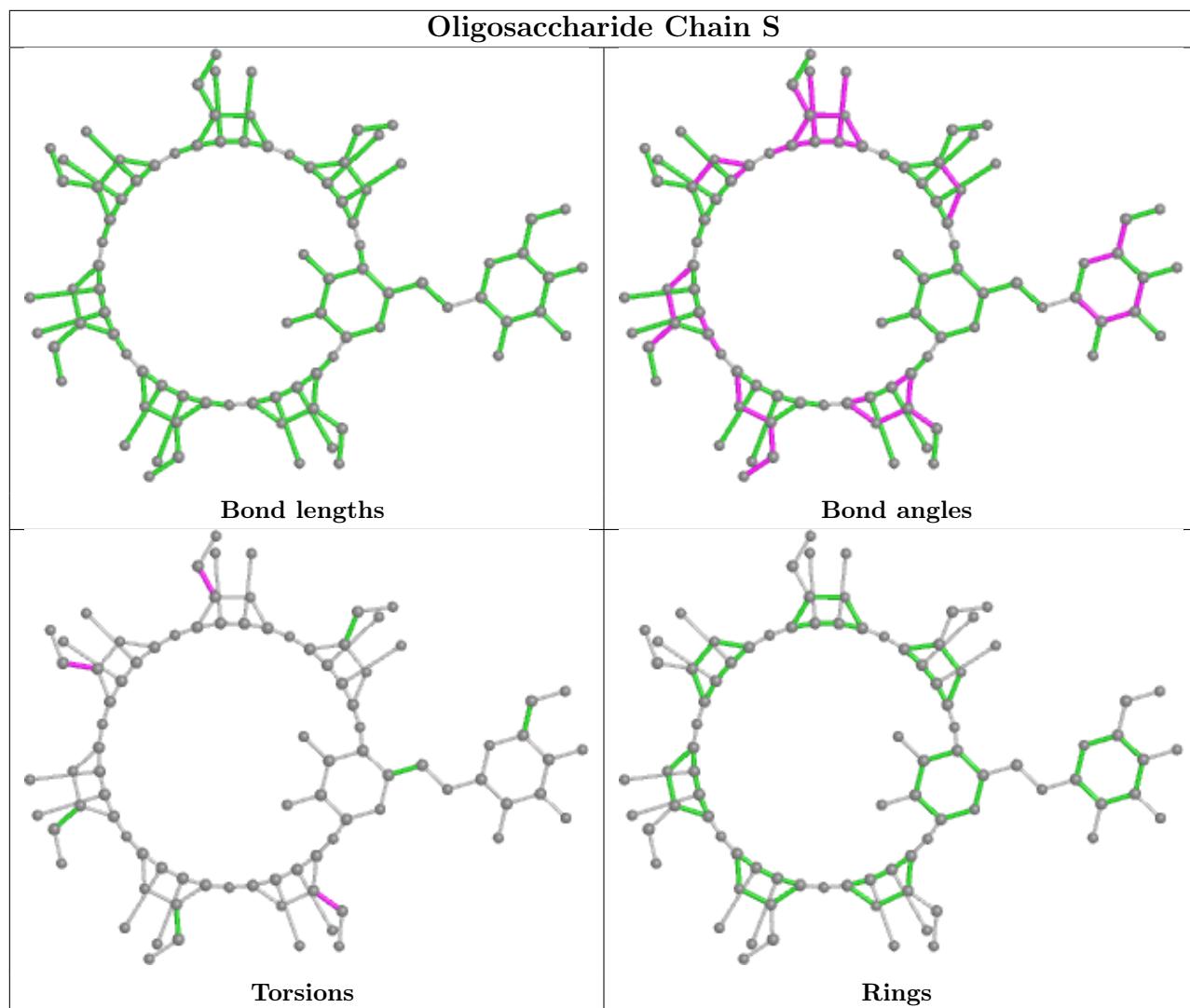
Mol	Chain	Res	Type	Atoms
2	U	4	GLC	C4-C5-C6-O6
2	f	2	GLC	C4-C5-C6-O6
2	j	1	GLC	C4-C5-C6-O6
2	g	3	GLC	C4-C5-C6-O6
2	h	3	GLC	C4-C5-C6-O6
2	h	1	GLC	O5-C5-C6-O6
2	d	1	GLC	O5-C5-C6-O6
2	e	4	GLC	C4-C5-C6-O6
2	W	3	GLC	O5-C5-C6-O6
2	j	5	GLC	C4-C5-C6-O6
2	Z	1	GLC	O5-C5-C6-O6
2	e	6	GLC	O5-C5-C6-O6

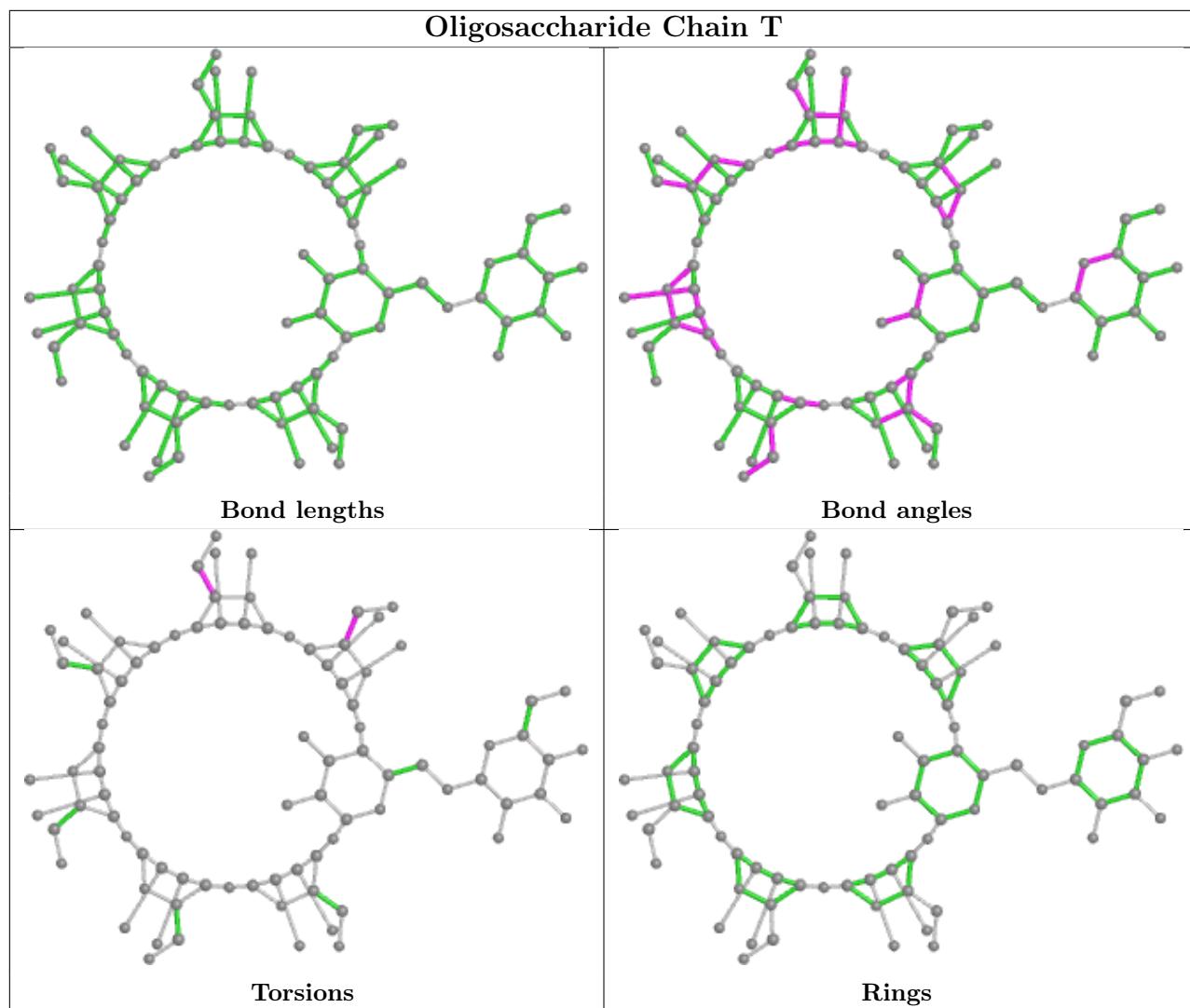
There are no ring outliers.

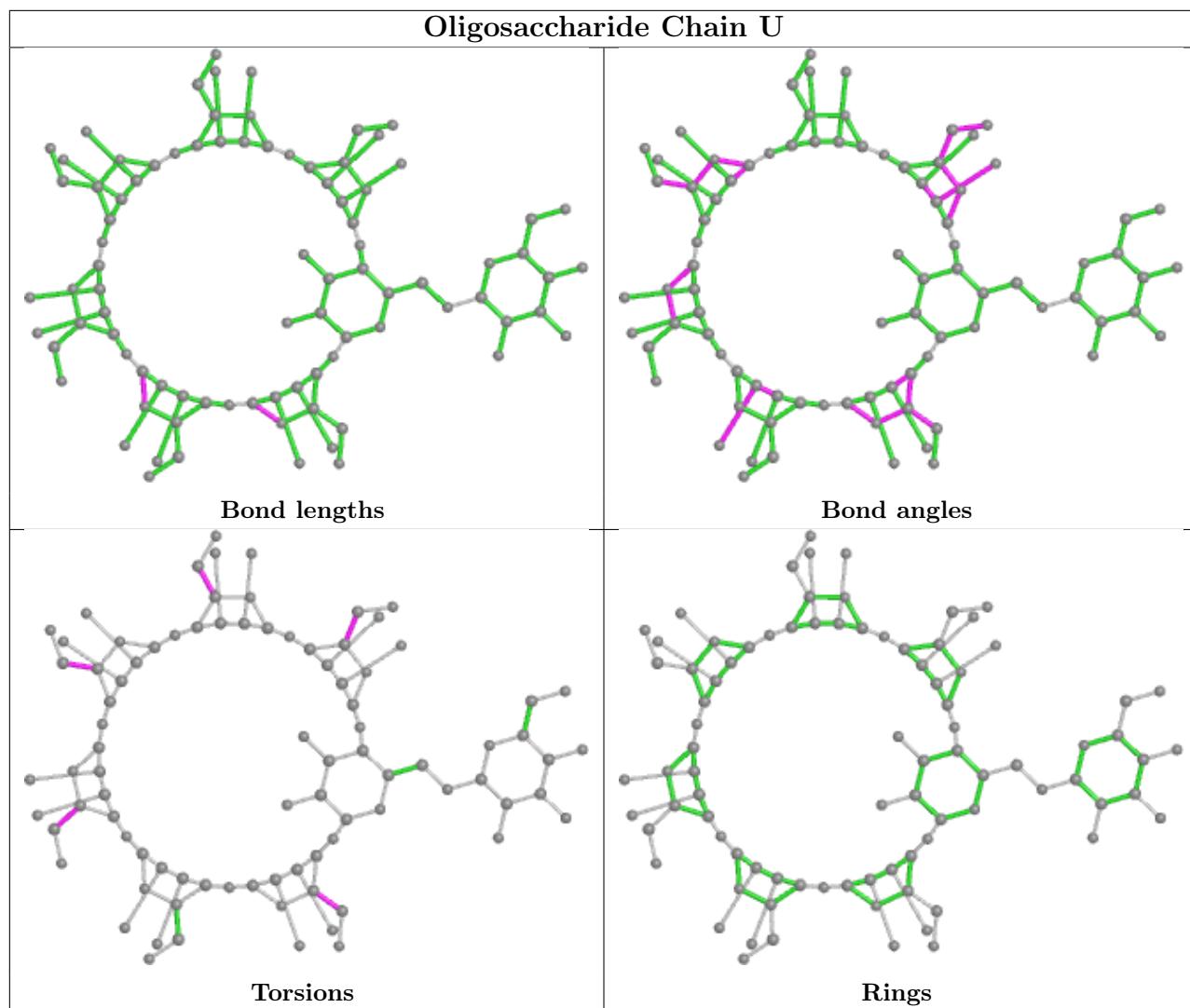
4 monomers are involved in 4 short contacts:

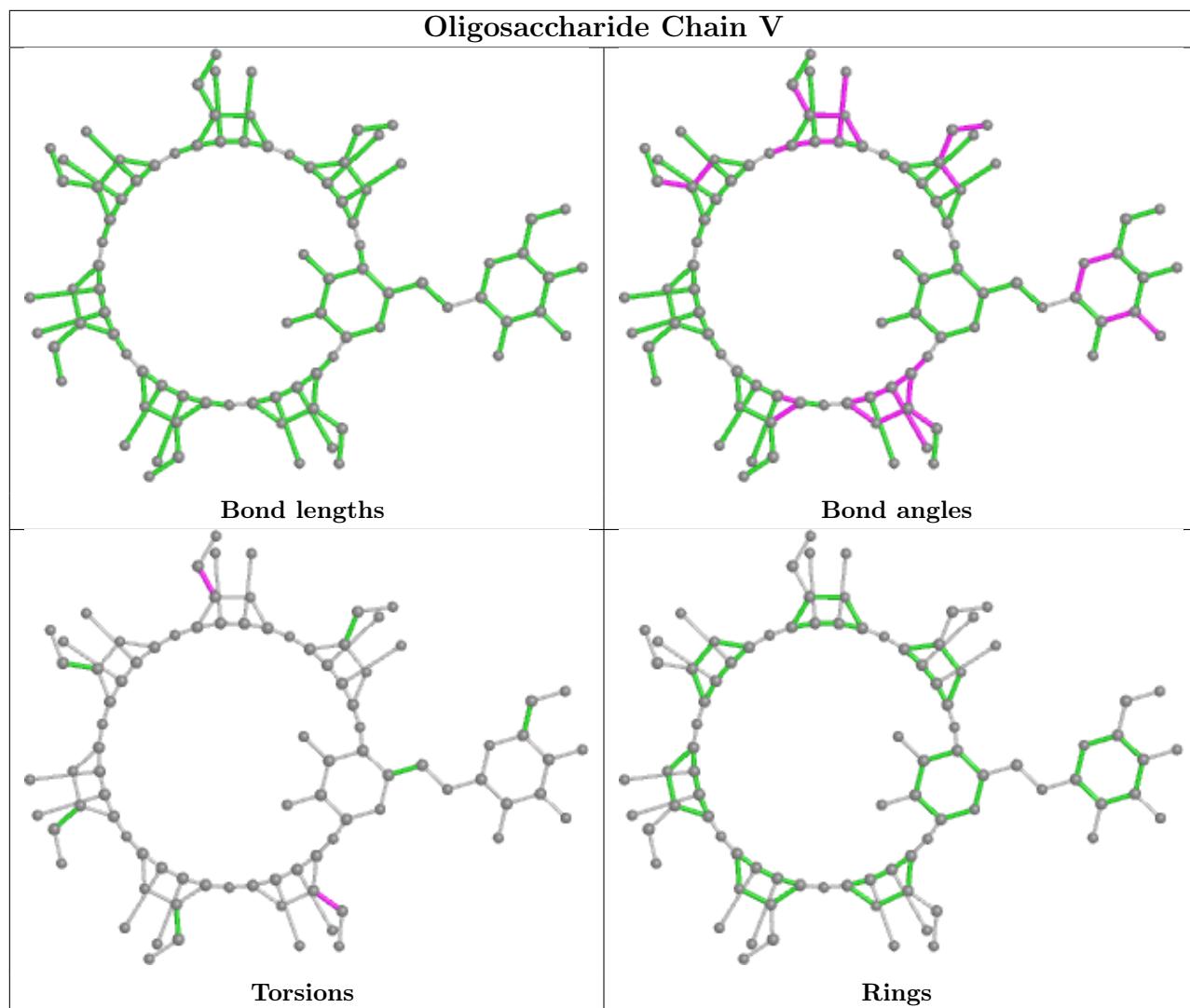
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	6	GLC	1	0
2	Z	4	GLC	2	0
2	V	6	GLC	1	0
2	Z	5	GLC	2	0

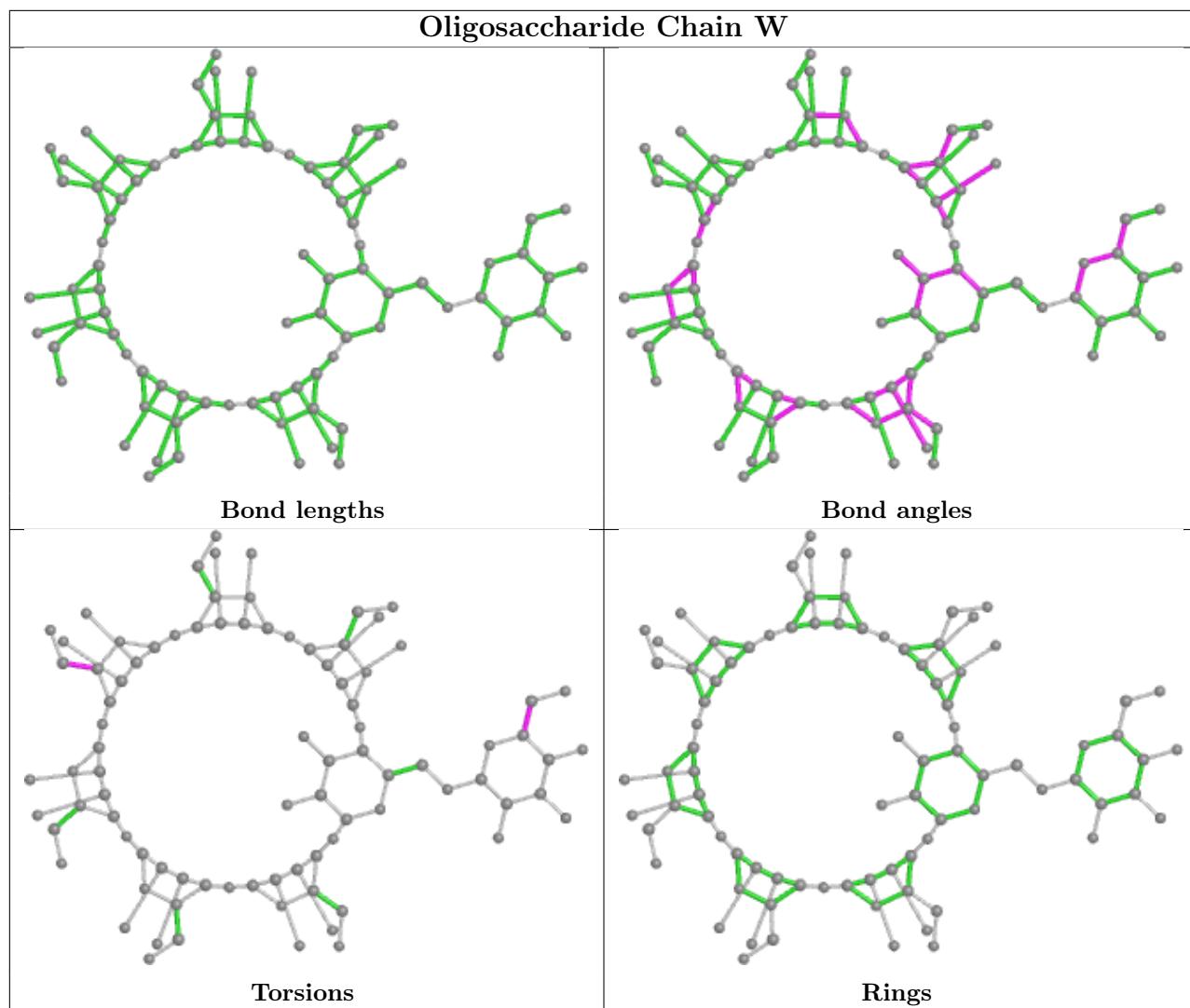
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

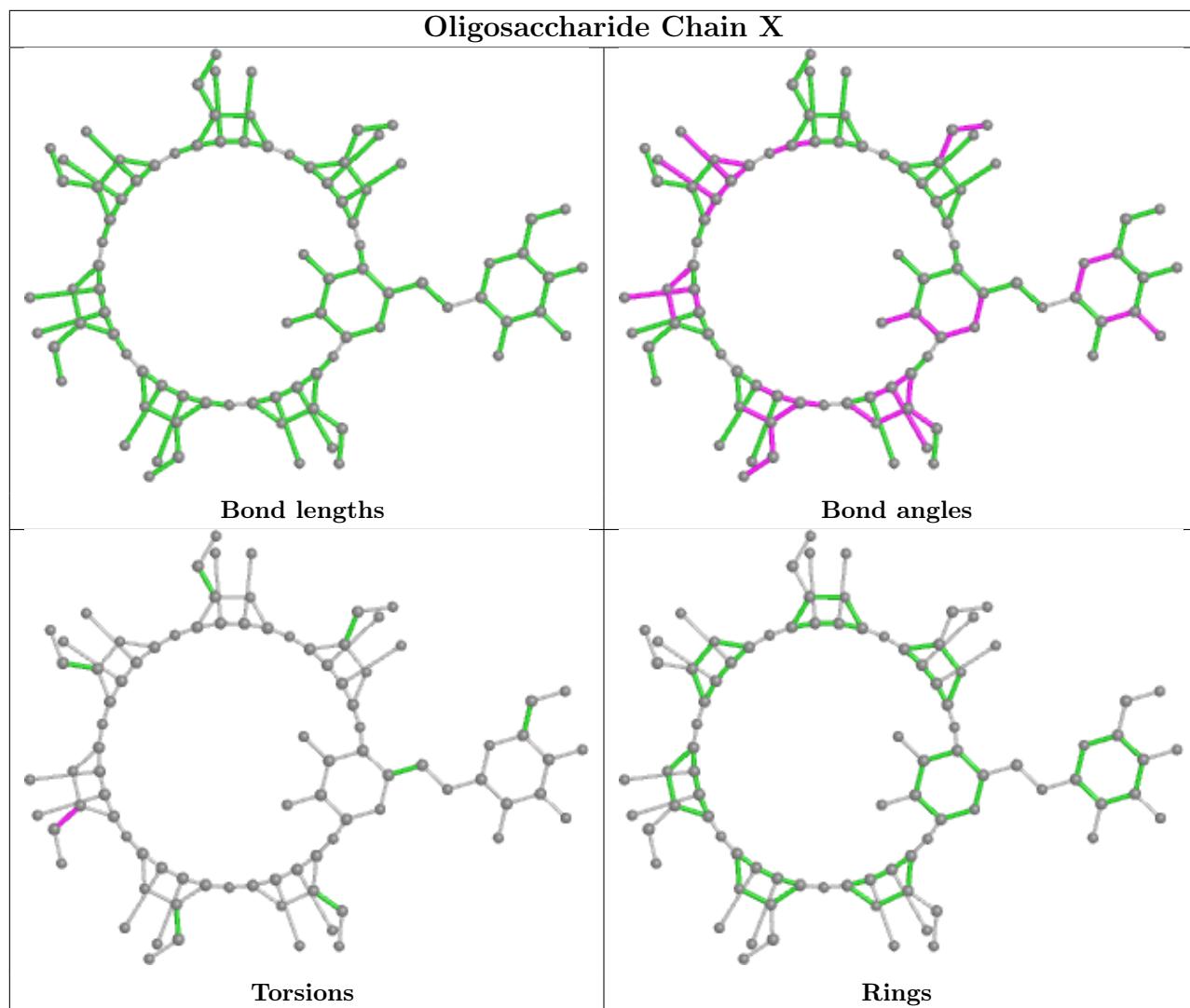


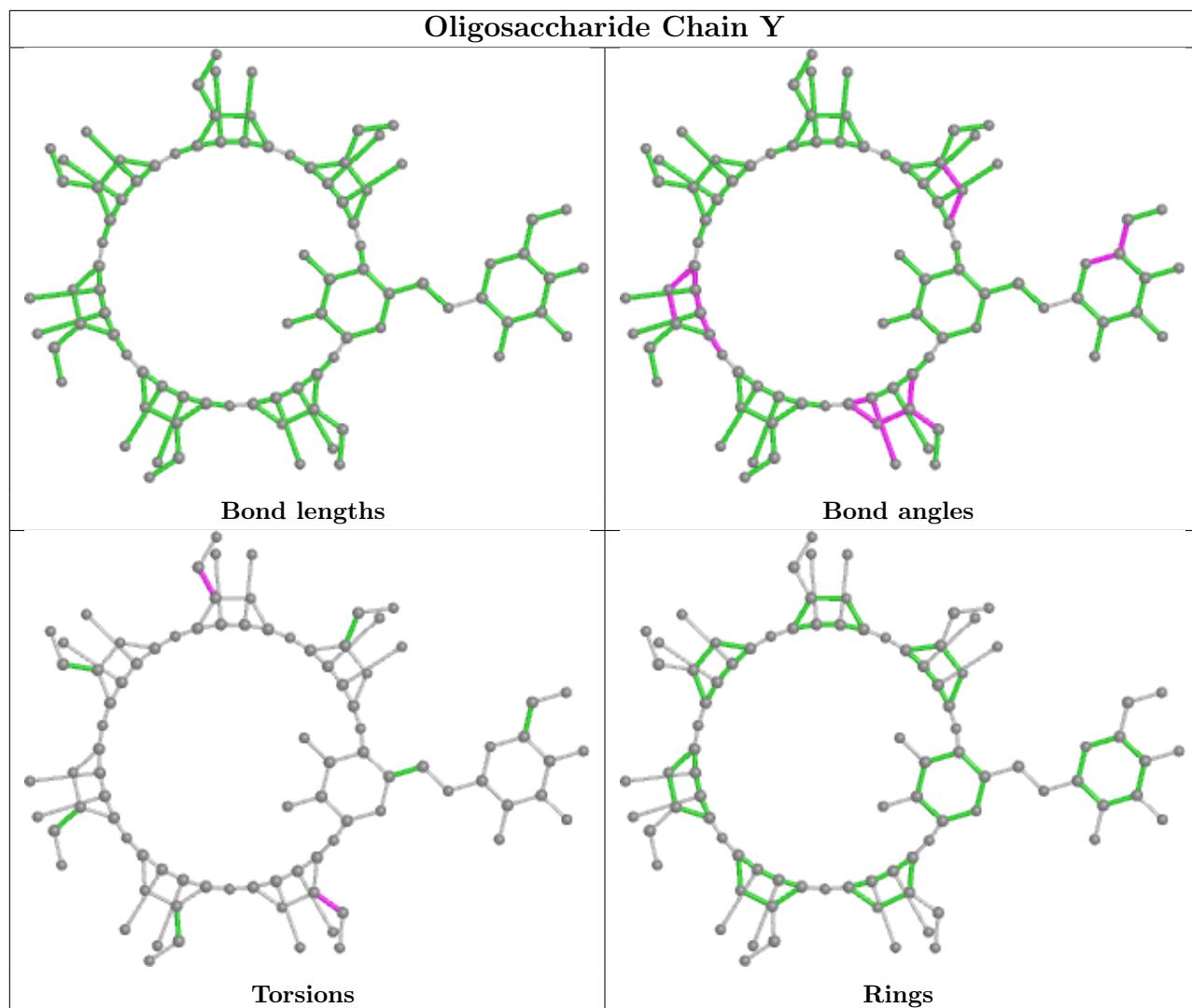


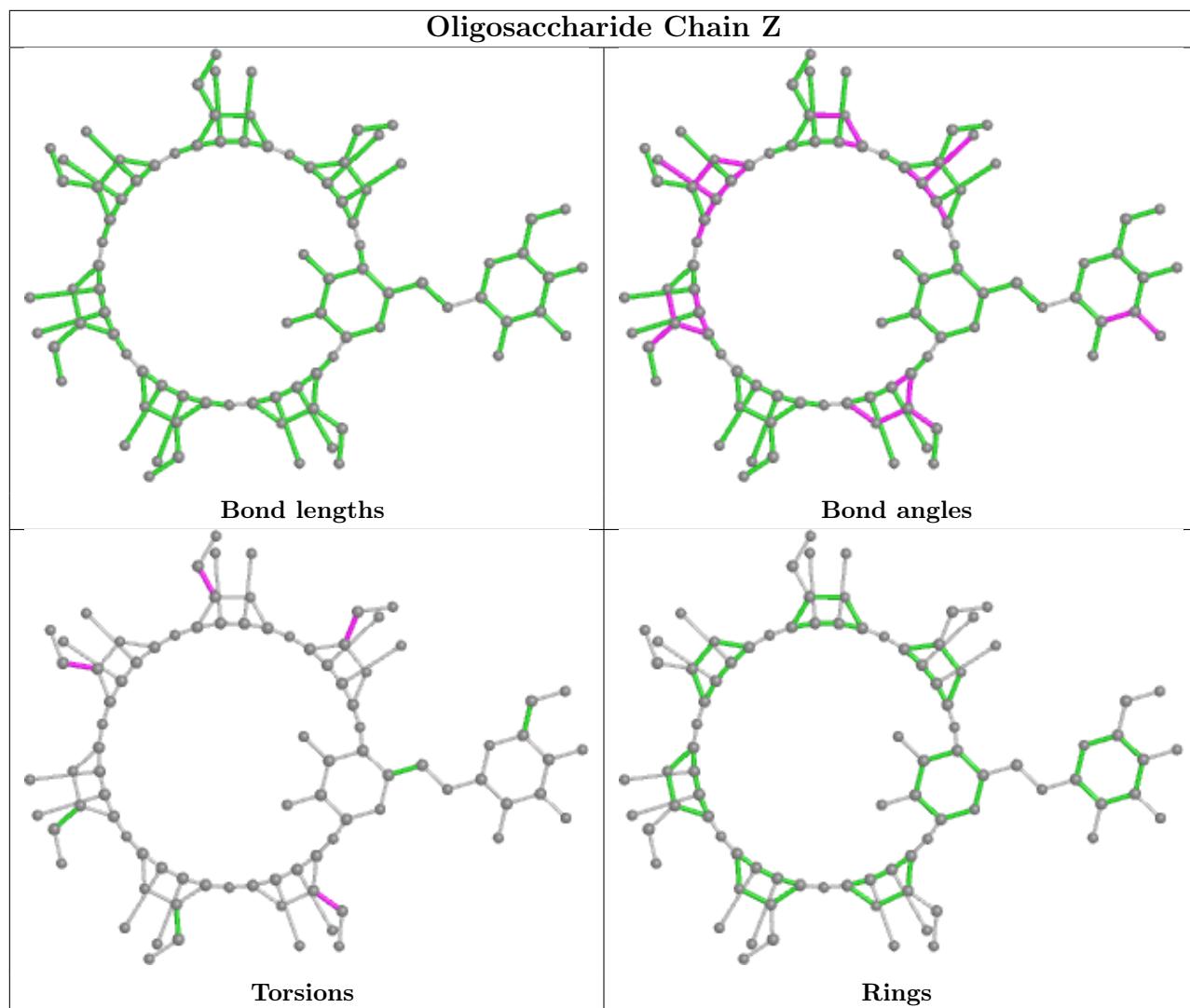


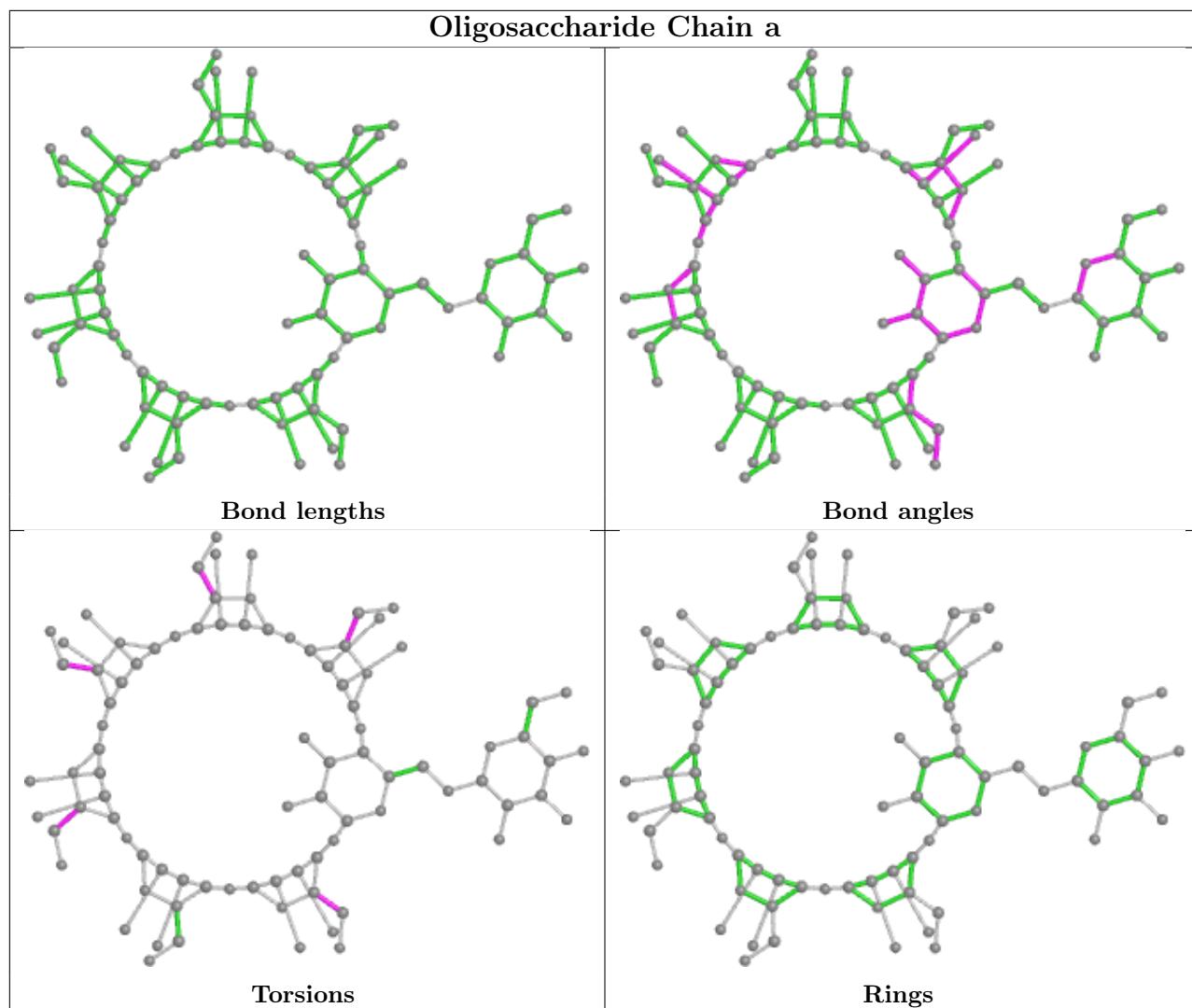


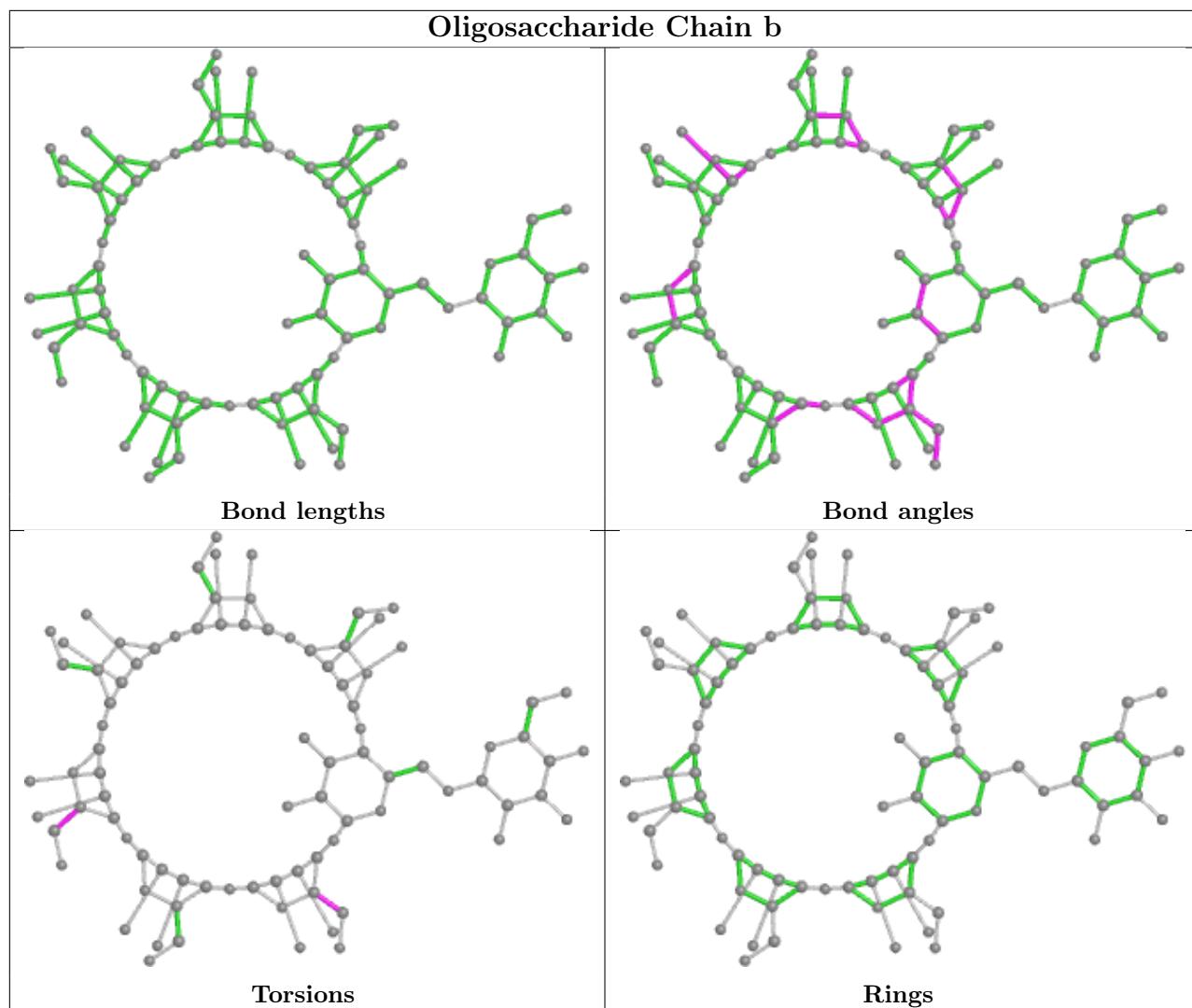


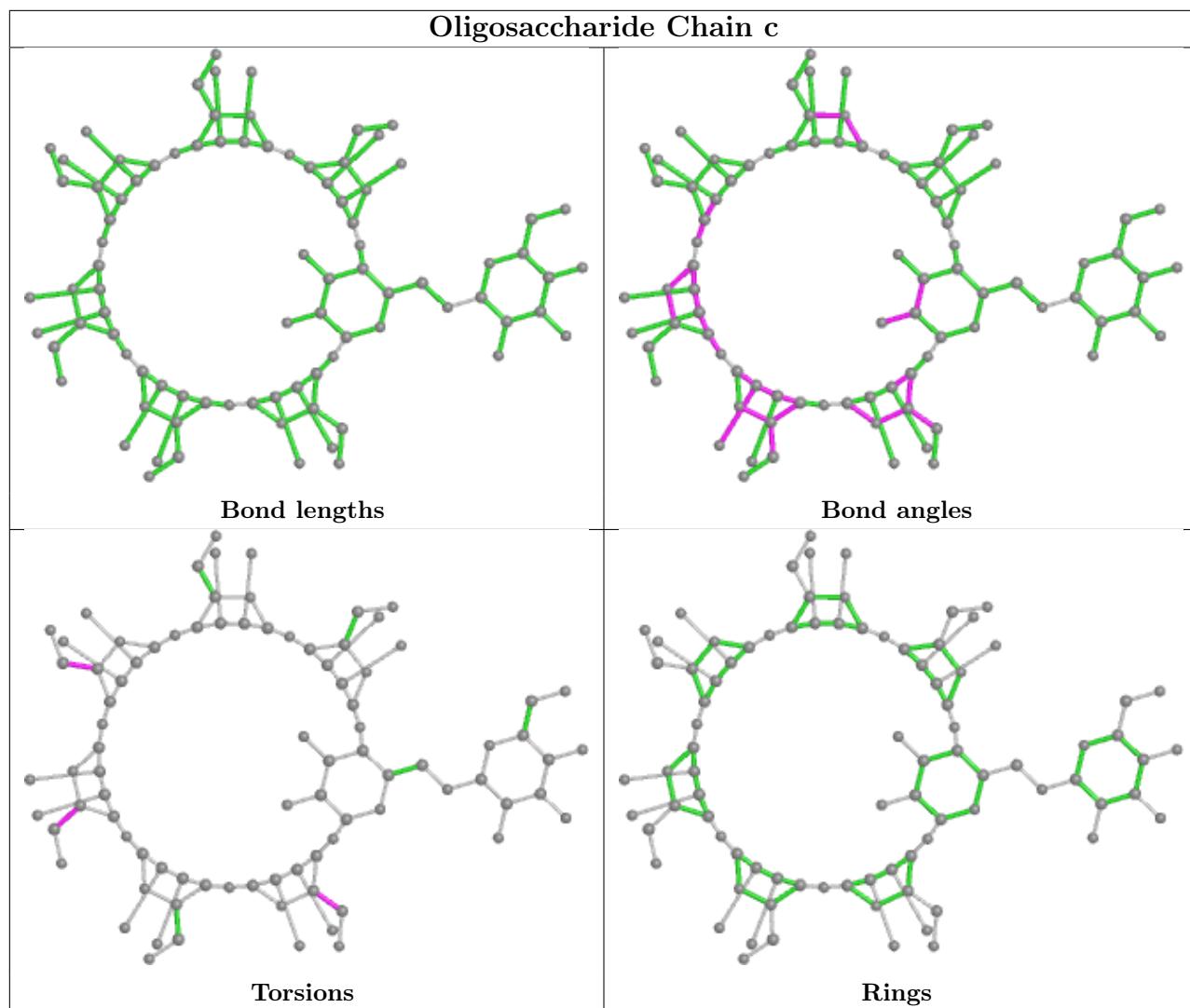


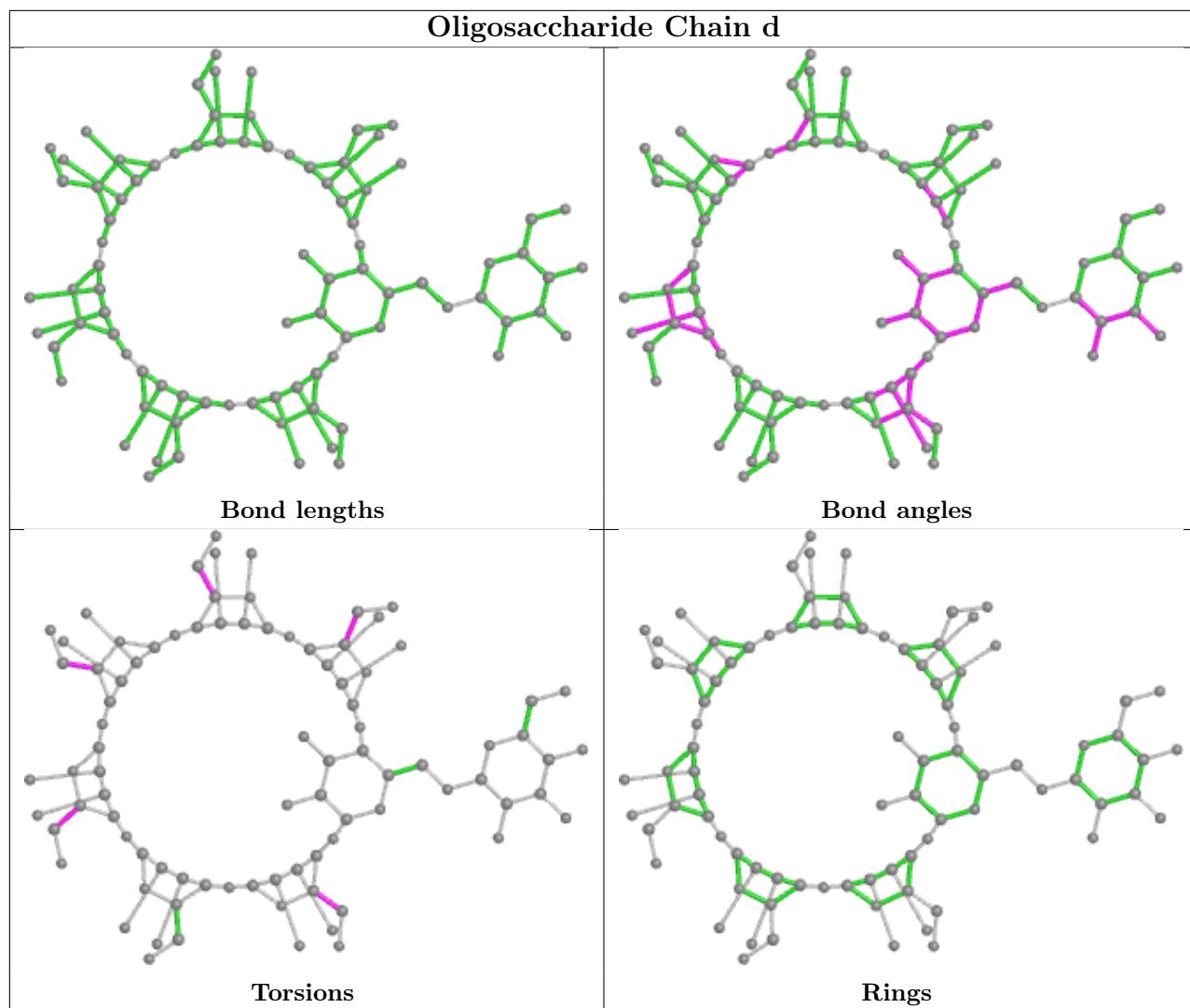


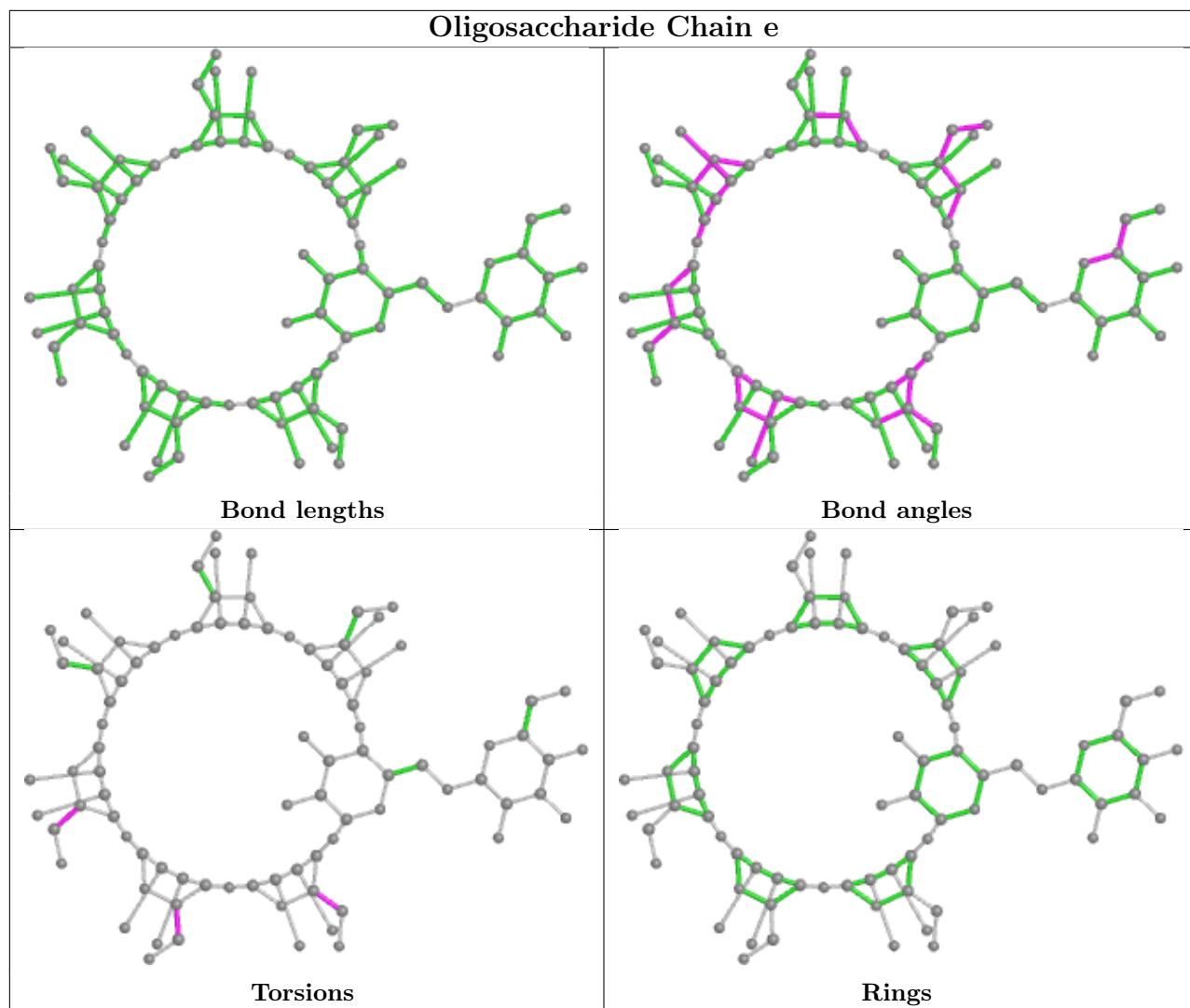


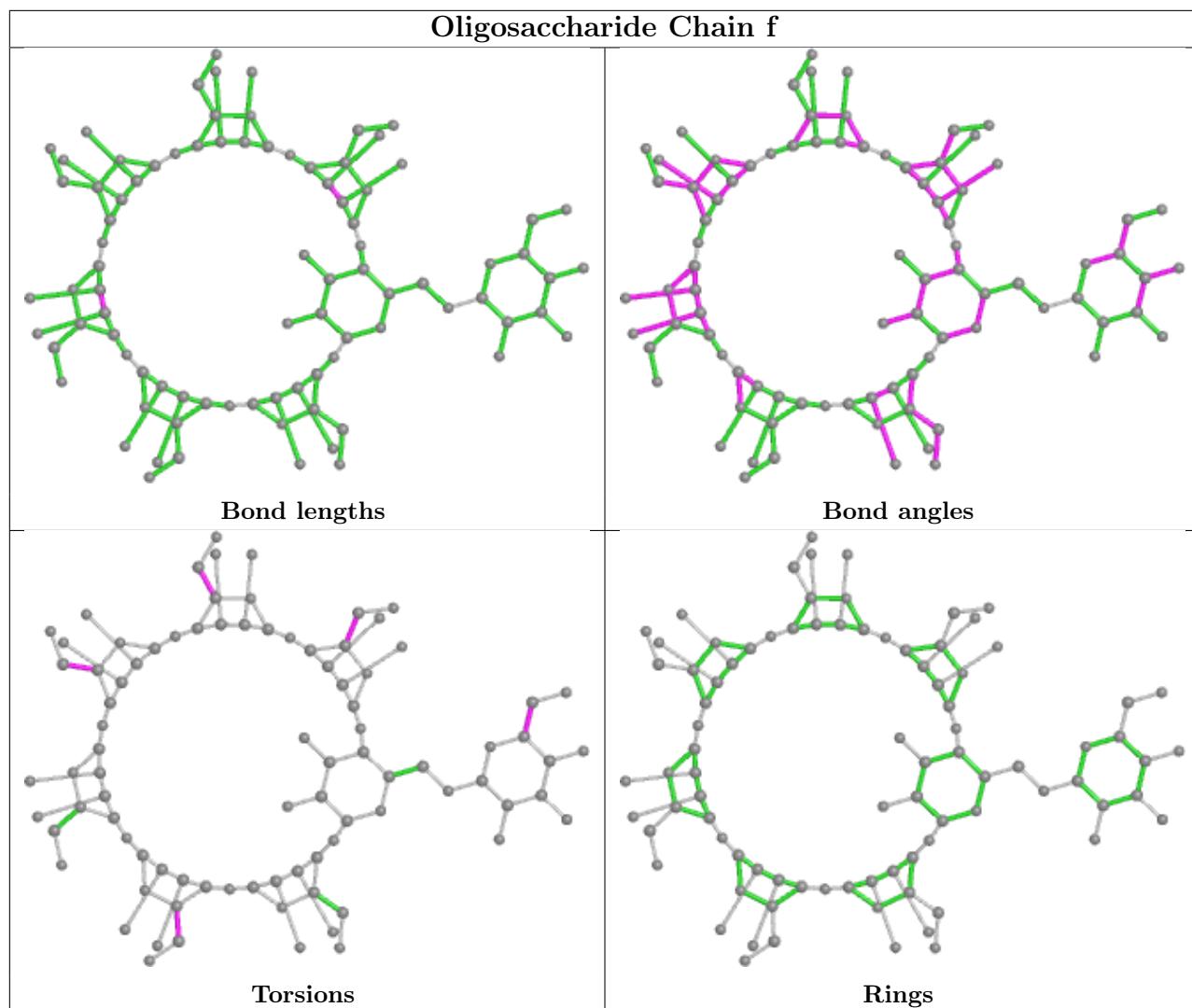


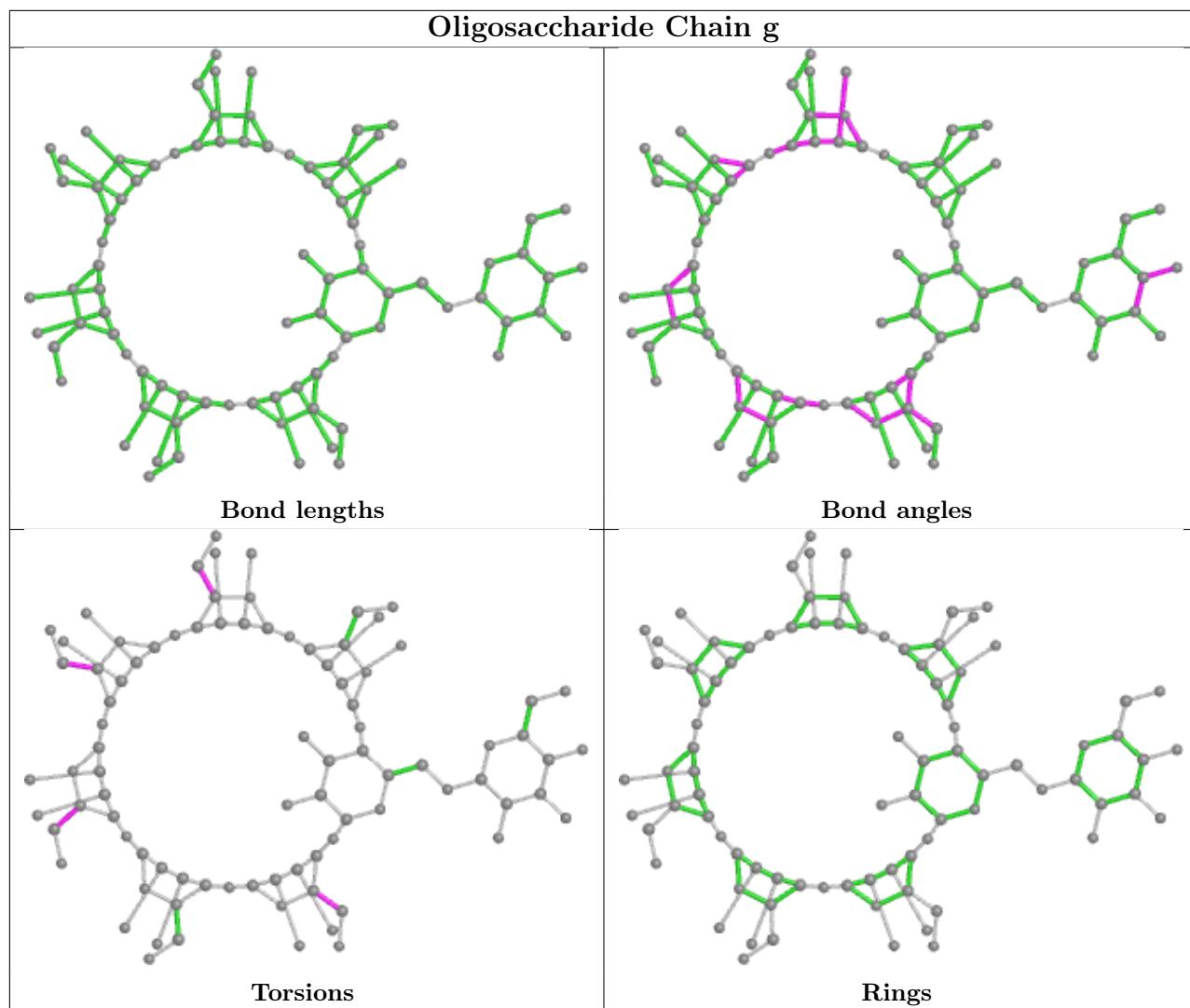


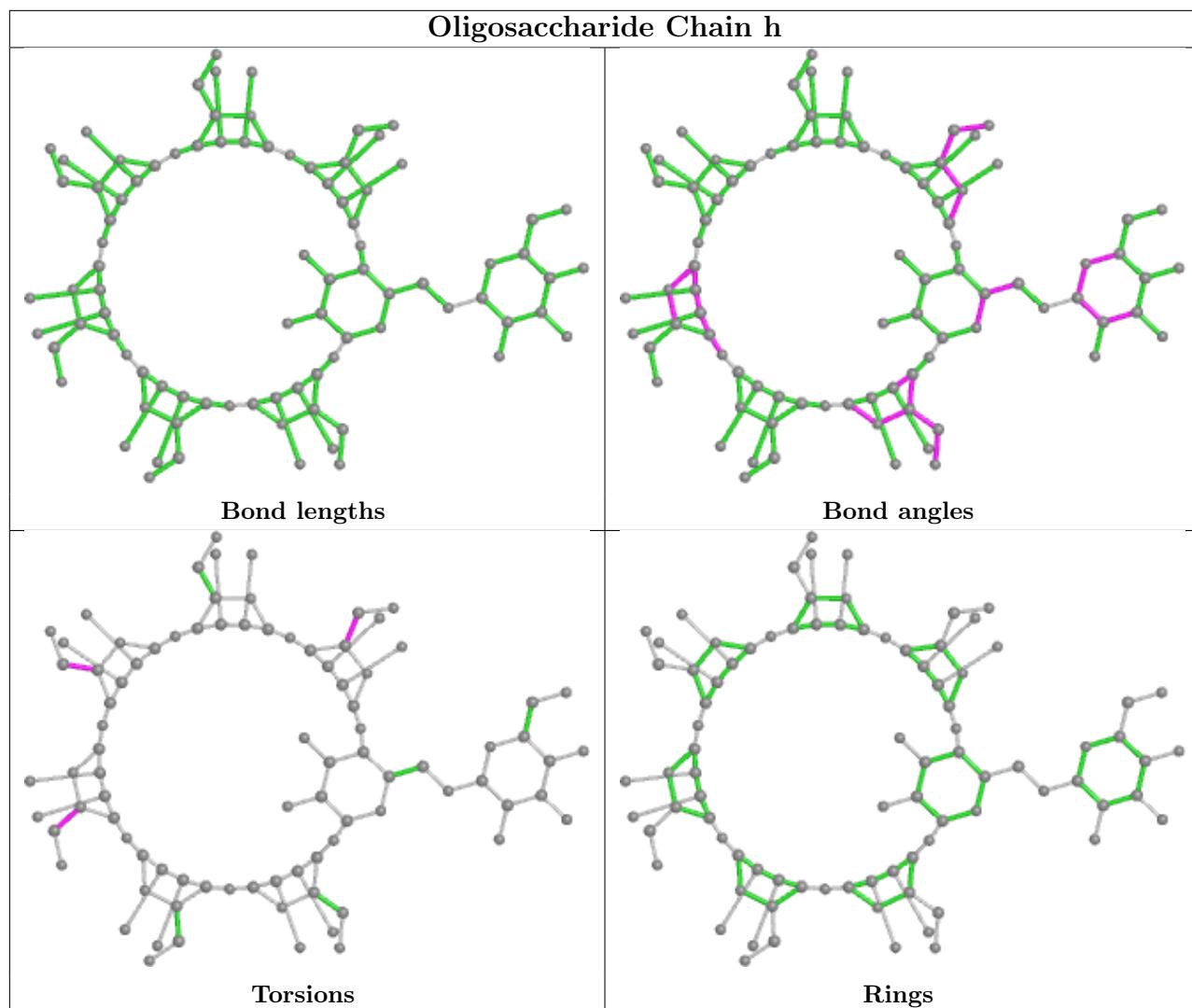


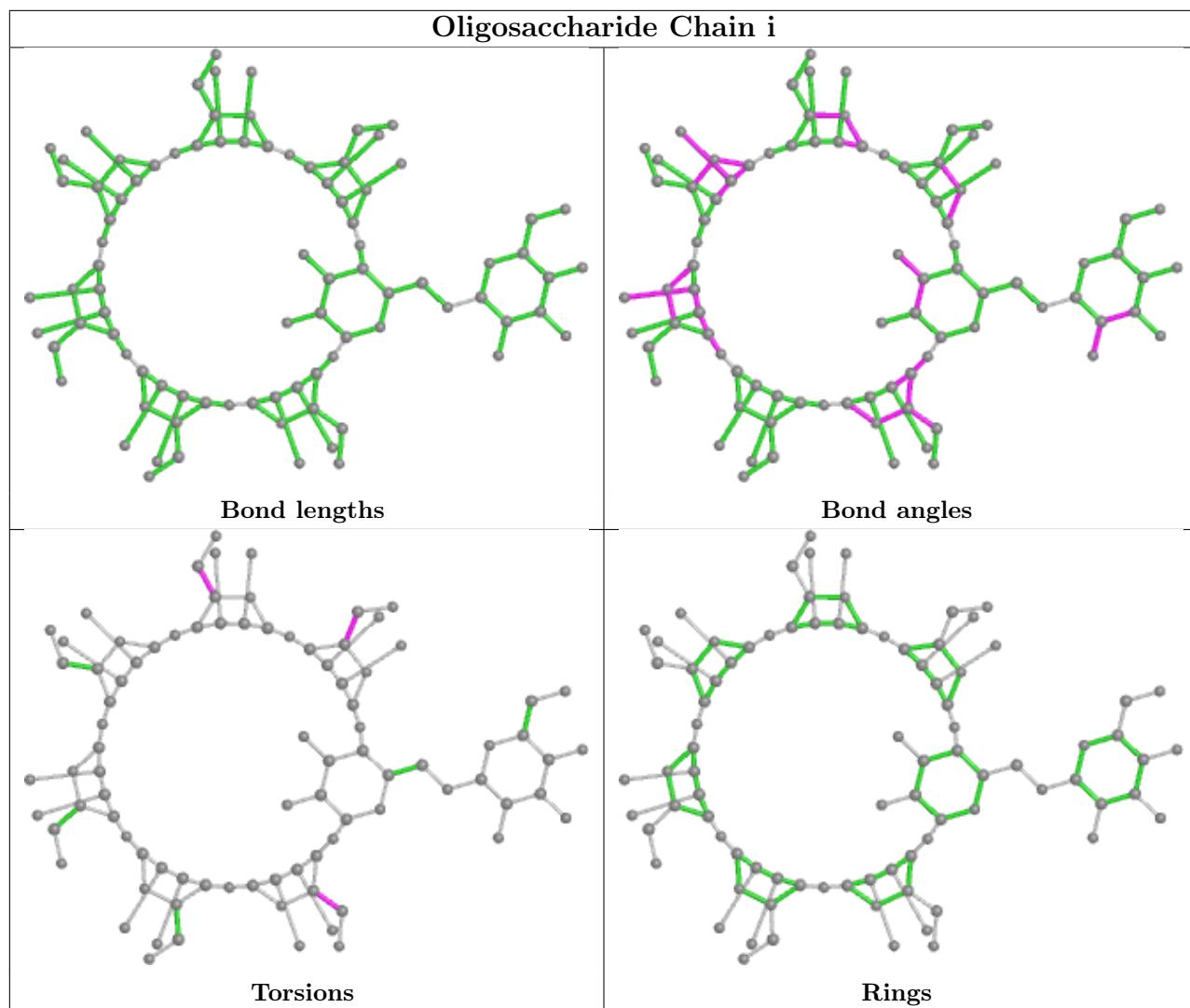


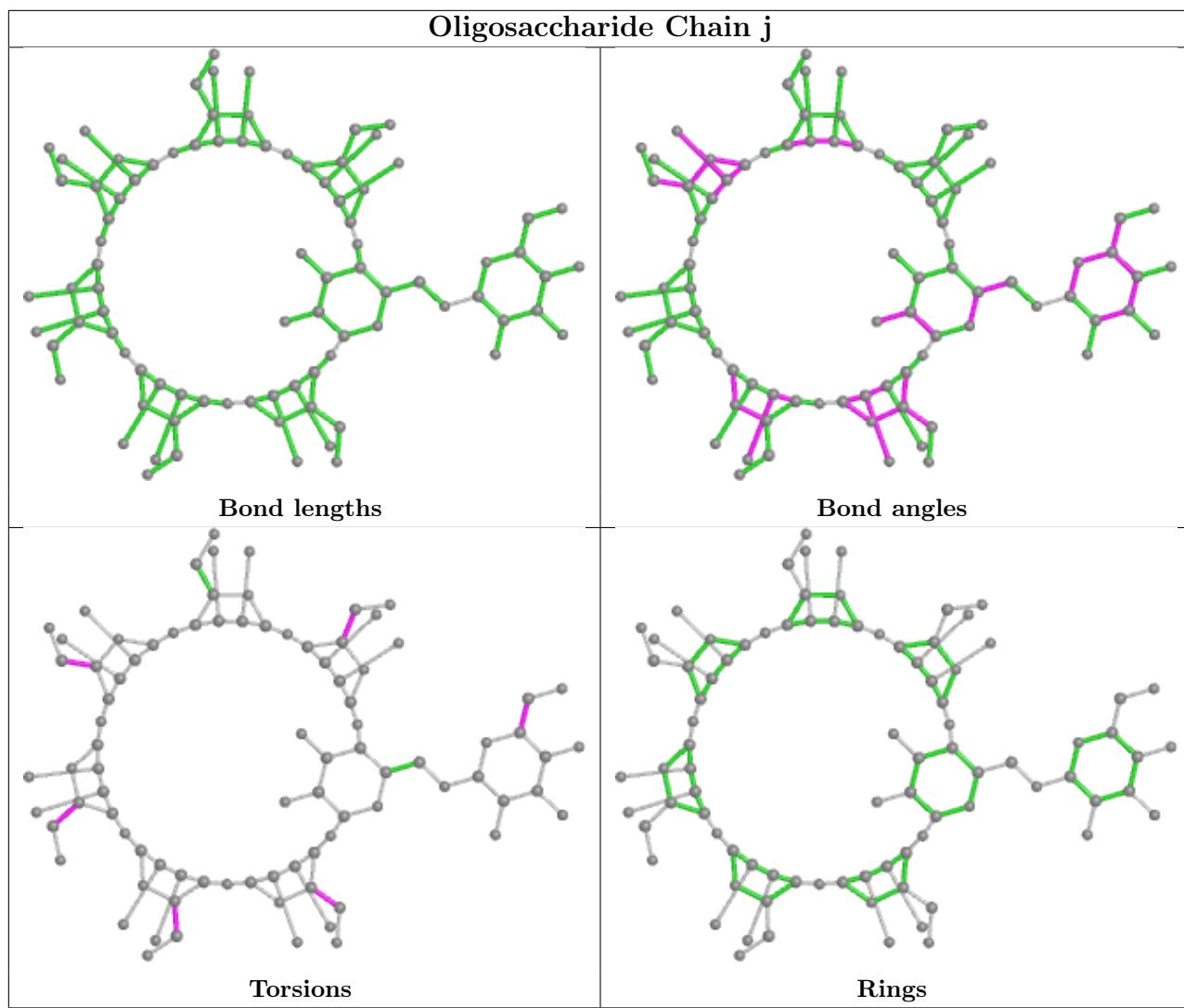












## 5.6 Ligand geometry [\(i\)](#)

19 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).

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Link</b>	<b>Bond lengths</b>			<b>Bond angles</b>		
					<b>Counts</b>	<b>RMSZ</b>	<b># Z  &gt; 2</b>	<b>Counts</b>	<b>RMSZ</b>	<b># Z  &gt; 2</b>
3	GOL	F	201	-	5,5,5	0.39	0	5,5,5	0.75	0
3	GOL	N	201	-	5,5,5	0.59	0	5,5,5	0.88	0
3	GOL	I	201	-	5,5,5	0.32	0	5,5,5	0.47	0





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Mol	Chain	Res	Type	Atoms
3	K	201	GOL	O2-C2-C3-O3
3	B	201	GOL	O2-C2-C3-O3
3	F	201	GOL	O2-C2-C3-O3
3	N	201	GOL	O2-C2-C3-O3
3	H	201	GOL	O2-C2-C3-O3
3	H	201	GOL	C1-C2-C3-O3
3	L	201	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	202	GOL	2	0
3	A	202	GOL	1	0
3	H	201	GOL	2	0
3	K	201	GOL	1	0
3	B	201	GOL	2	0
3	P	201	GOL	2	0

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

### 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	82/90 (91%)	-0.67	0 [100] [100]	15, 21, 39, 51	0
1	B	83/90 (92%)	-0.43	1 (1%) [79] [78]	15, 24, 49, 59	0
1	C	83/90 (92%)	-0.47	0 [100] [100]	14, 20, 45, 60	0
1	D	79/90 (87%)	-0.68	0 [100] [100]	16, 24, 40, 52	0
1	E	85/90 (94%)	-0.45	0 [100] [100]	16, 25, 38, 57	0
1	F	85/90 (94%)	-0.43	1 (1%) [79] [78]	17, 29, 49, 79	0
1	G	83/90 (92%)	-0.61	0 [100] [100]	21, 30, 48, 67	0
1	H	85/90 (94%)	-0.53	0 [100] [100]	24, 34, 52, 61	0
1	I	85/90 (94%)	-0.50	0 [100] [100]	23, 33, 48, 55	0
1	J	85/90 (94%)	-0.53	0 [100] [100]	22, 31, 50, 59	0
1	K	82/90 (91%)	-0.46	0 [100] [100]	24, 32, 52, 68	0
1	L	82/90 (91%)	-0.55	0 [100] [100]	20, 31, 50, 70	0
1	M	85/90 (94%)	-0.57	0 [100] [100]	20, 26, 47, 63	0
1	N	84/90 (93%)	-0.41	0 [100] [100]	20, 32, 52, 67	0
1	O	84/90 (93%)	-0.67	0 [100] [100]	20, 27, 41, 48	0
1	P	85/90 (94%)	-0.52	0 [100] [100]	24, 33, 49, 58	0
1	Q	84/90 (93%)	-0.50	0 [100] [100]	23, 36, 60, 73	0
1	R	84/90 (93%)	-0.24	1 (1%) [79] [78]	38, 49, 62, 79	0
All	All	1505/1620 (92%)	-0.51	3 (0%) [95] [94]	14, 30, 54, 79	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	154	HIS	2.3
1	F	74	SER	2.3
1	B	77	ARG	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(Å <sup>2</sup> )	Q<0.9
2	GLC	f	2	11/12	0.54	0.23	67,75,79,79	0
2	GLC	f	4	11/12	0.68	0.20	50,62,65,66	0
2	GLC	f	1	11/12	0.76	0.23	49,56,62,75	0
2	GLC	d	5	11/12	0.79	0.19	40,45,51,53	0
2	GLC	f	5	11/12	0.80	0.27	44,51,53,53	0
2	GLC	Z	3	11/12	0.83	0.12	48,56,61,62	0
2	GLC	i	4	11/12	0.83	0.15	53,62,64,65	0
2	GLC	Y	3	11/12	0.84	0.13	54,55,60,63	0
2	GLC	Z	4	11/12	0.84	0.17	59,60,63,65	0
2	GLC	Z	5	11/12	0.84	0.24	50,65,69,71	0
2	GLC	f	3	11/12	0.85	0.16	47,54,58,59	0
2	GLC	a	5	11/12	0.86	0.22	44,51,55,62	0
2	GLC	g	3	11/12	0.86	0.12	46,48,54,54	0
2	GLC	g	4	11/12	0.86	0.11	44,51,55,58	0
2	GLC	Z	8	11/12	0.86	0.13	38,47,52,56	0
2	GLC	Z	1	11/12	0.87	0.13	43,48,53,57	0
2	GLC	j	5	11/12	0.87	0.14	46,51,60,61	0
2	GLC	h	5	11/12	0.88	0.14	44,52,57,58	0
2	GLC	T	3	11/12	0.88	0.11	39,41,47,53	0
2	GLC	j	2	11/12	0.88	0.15	50,54,61,64	0
2	GLC	d	2	11/12	0.88	0.18	43,47,51,52	0
2	GLC	f	8	11/12	0.89	0.16	35,44,51,53	0
2	GLC	h	3	11/12	0.89	0.09	52,60,62,63	0
2	GLC	j	4	11/12	0.89	0.14	49,53,58,61	0
2	GLC	Y	2	11/12	0.89	0.15	42,48,55,58	0
2	GLC	b	3	11/12	0.90	0.12	45,46,49,53	0
2	GLC	h	4	11/12	0.90	0.17	58,61,67,70	0
2	GLC	j	3	11/12	0.90	0.13	38,47,51,54	0
2	GLC	e	3	11/12	0.90	0.11	45,48,53,53	0
2	GLC	i	1	11/12	0.90	0.12	31,36,42,43	0
2	GLC	j	6	11/12	0.90	0.10	41,46,47,50	0
2	GLC	j	8	11/12	0.90	0.14	40,45,51,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLC	c	8	11/12	0.91	0.09	28,32,36,36	0
2	GLC	d	1	11/12	0.91	0.10	33,36,39,43	0
2	GLC	g	5	11/12	0.91	0.13	36,39,44,50	0
2	GLC	X	8	11/12	0.91	0.09	28,30,35,36	0
2	GLC	d	4	11/12	0.91	0.17	48,53,55,55	0
2	GLC	Z	2	11/12	0.91	0.16	61,67,74,74	0
2	GLC	c	3	11/12	0.91	0.09	41,45,51,53	0
2	GLC	i	2	11/12	0.92	0.12	45,48,57,64	0
2	GLC	i	3	11/12	0.92	0.10	53,54,61,61	0
2	GLC	a	3	11/12	0.92	0.13	46,50,53,57	0
2	GLC	j	1	11/12	0.92	0.11	38,45,51,57	0
2	GLC	d	3	11/12	0.92	0.12	42,45,51,59	0
2	GLC	g	8	11/12	0.92	0.11	30,37,39,41	0
2	GLC	f	6	11/12	0.92	0.14	40,42,47,51	0
2	GLC	Z	6	11/12	0.92	0.15	47,49,53,53	0
2	GLC	g	2	11/12	0.92	0.13	40,46,50,53	0
2	GLC	Y	1	11/12	0.92	0.14	36,41,46,51	0
2	GLC	c	4	11/12	0.93	0.11	47,51,53,54	0
2	GLC	W	4	11/12	0.93	0.12	26,35,40,51	0
2	GLC	e	4	11/12	0.93	0.10	39,44,52,54	0
2	GLC	Y	8	11/12	0.93	0.10	34,41,46,47	0
2	GLC	h	8	11/12	0.93	0.10	35,39,42,42	0
2	GLC	S	2	11/12	0.93	0.11	30,33,38,43	0
2	GLC	b	4	11/12	0.93	0.09	44,50,56,57	0
2	GLC	a	2	11/12	0.93	0.16	42,45,47,48	0
2	GLC	b	8	11/12	0.94	0.14	29,36,38,42	0
2	GLC	g	1	11/12	0.94	0.11	29,37,44,47	0
2	GLC	c	2	11/12	0.94	0.08	41,44,47,49	0
2	GLC	X	5	11/12	0.94	0.09	21,24,27,34	0
2	GLC	S	3	11/12	0.94	0.12	34,37,42,49	0
2	GLC	U	3	11/12	0.94	0.09	34,36,38,47	0
2	GLC	d	7	11/12	0.94	0.09	26,30,32,32	0
2	GLC	h	1	11/12	0.94	0.08	33,36,45,46	0
2	GLC	U	4	11/12	0.94	0.12	33,39,45,52	0
2	GLC	V	4	11/12	0.94	0.11	38,40,43,47	0
2	GLC	Y	4	11/12	0.94	0.11	48,58,60,63	0
2	GLC	a	1	11/12	0.94	0.12	35,38,42,47	0
2	GLC	i	7	11/12	0.94	0.08	25,28,31,32	0
2	GLC	Y	5	11/12	0.94	0.13	36,43,48,48	0
2	GLC	d	6	11/12	0.94	0.09	30,32,35,37	0
2	GLC	e	2	11/12	0.94	0.09	36,40,48,49	0
2	GLC	Y	6	11/12	0.94	0.09	31,33,36,37	0

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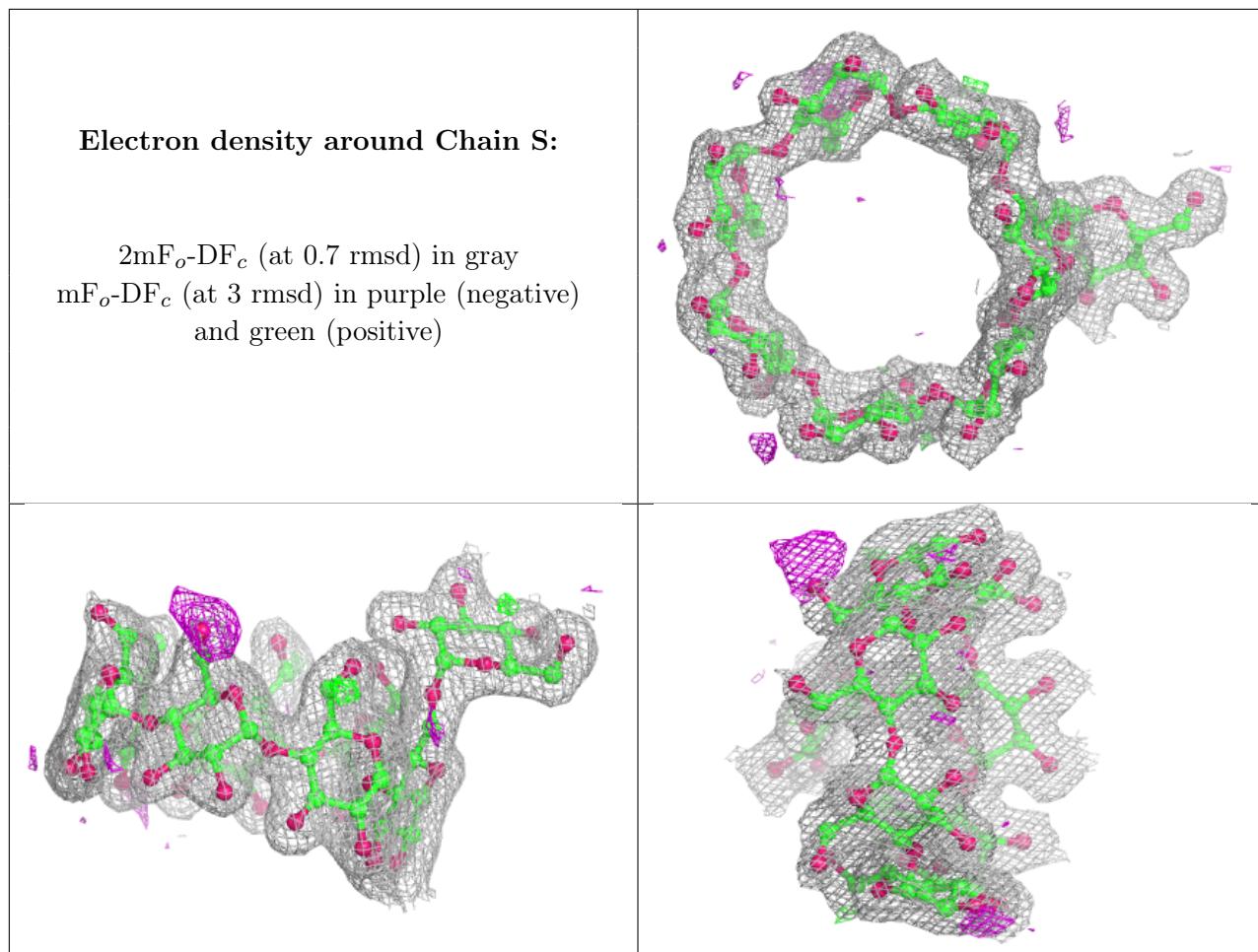
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLC	j	7	11/12	0.94	0.10	35,38,45,47	0
2	GLC	a	4	11/12	0.94	0.13	50,55,62,63	0
2	GLC	S	4	11/12	0.94	0.09	30,34,39,40	0
2	GLC	a	8	11/12	0.94	0.13	31,38,43,44	0
2	GLC	b	2	11/12	0.94	0.14	38,40,43,45	0
2	GLC	Z	7	11/12	0.94	0.09	39,40,43,44	0
2	GLC	W	5	11/12	0.94	0.10	23,27,30,35	0
2	GLC	b	5	11/12	0.94	0.09	38,40,43,47	0
2	GLC	W	1	11/12	0.95	0.09	22,25,29,32	0
2	GLC	T	5	11/12	0.95	0.10	24,28,30,36	0
2	GLC	T	6	11/12	0.95	0.07	18,20,21,21	0
2	GLC	W	8	11/12	0.95	0.08	23,27,31,33	0
2	GLC	a	6	11/12	0.95	0.09	32,39,43,43	0
2	GLC	g	6	11/12	0.95	0.07	28,32,35,36	0
2	GLC	X	1	11/12	0.95	0.09	19,21,23,29	0
2	GLC	h	7	11/12	0.95	0.09	27,31,34,36	0
2	GLC	b	1	11/12	0.95	0.09	29,31,35,36	0
2	GLC	X	4	11/12	0.95	0.09	23,26,31,39	0
2	GLC	d	8	11/12	0.95	0.12	23,27,32,38	0
2	GLC	e	1	11/12	0.95	0.08	24,30,36,45	0
2	GLC	T	2	11/12	0.95	0.09	28,37,40,46	0
2	GLC	S	5	11/12	0.95	0.08	24,25,29,33	0
2	GLC	V	3	11/12	0.95	0.08	35,39,45,51	0
2	GLC	e	5	11/12	0.95	0.09	34,38,44,47	0
2	GLC	e	6	11/12	0.95	0.09	28,29,33,37	0
2	GLC	f	7	11/12	0.95	0.10	35,39,41,42	0
2	GLC	i	5	11/12	0.95	0.11	35,50,52,57	0
2	GLC	i	6	11/12	0.95	0.09	28,34,39,39	0
2	GLC	b	6	11/12	0.95	0.09	26,30,35,36	0
2	GLC	T	4	11/12	0.95	0.11	32,39,45,48	0
2	GLC	c	7	11/12	0.95	0.09	28,31,33,33	0
2	GLC	V	5	11/12	0.95	0.10	31,34,37,41	0
2	GLC	a	7	11/12	0.95	0.09	26,31,33,34	0
2	GLC	V	6	11/12	0.95	0.08	25,26,29,31	0
2	GLC	c	5	11/12	0.95	0.11	32,41,45,48	0
2	GLC	g	7	11/12	0.95	0.08	27,31,34,34	0
2	GLC	Y	7	11/12	0.96	0.07	30,32,36,42	0
2	GLC	U	2	11/12	0.96	0.10	25,29,35,43	0
2	GLC	U	5	11/12	0.96	0.09	20,23,27,29	0
2	GLC	h	2	11/12	0.96	0.11	44,50,61,69	0
2	GLC	i	8	11/12	0.96	0.11	33,36,42,43	0
2	GLC	V	7	11/12	0.96	0.09	22,23,25,25	0

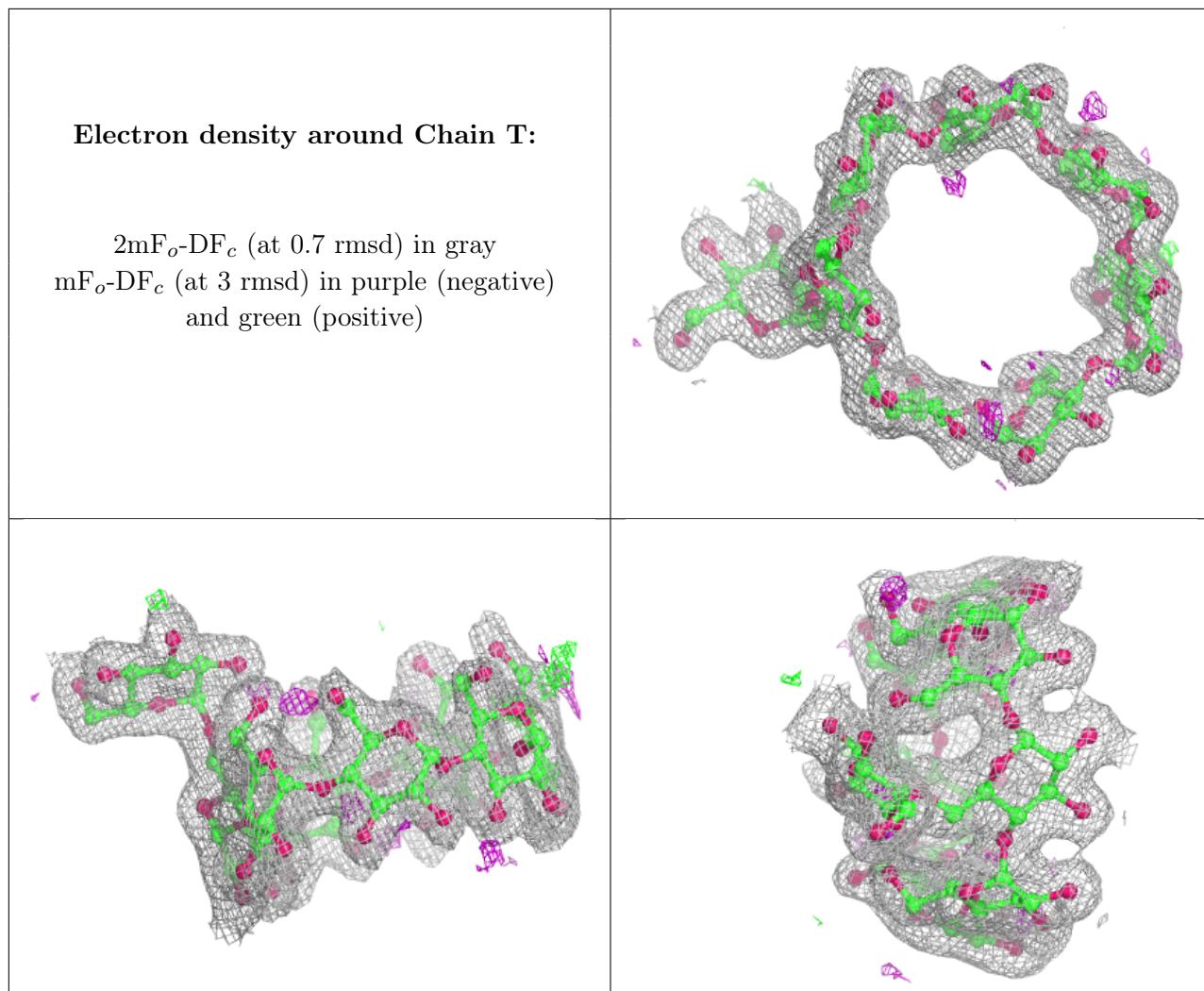
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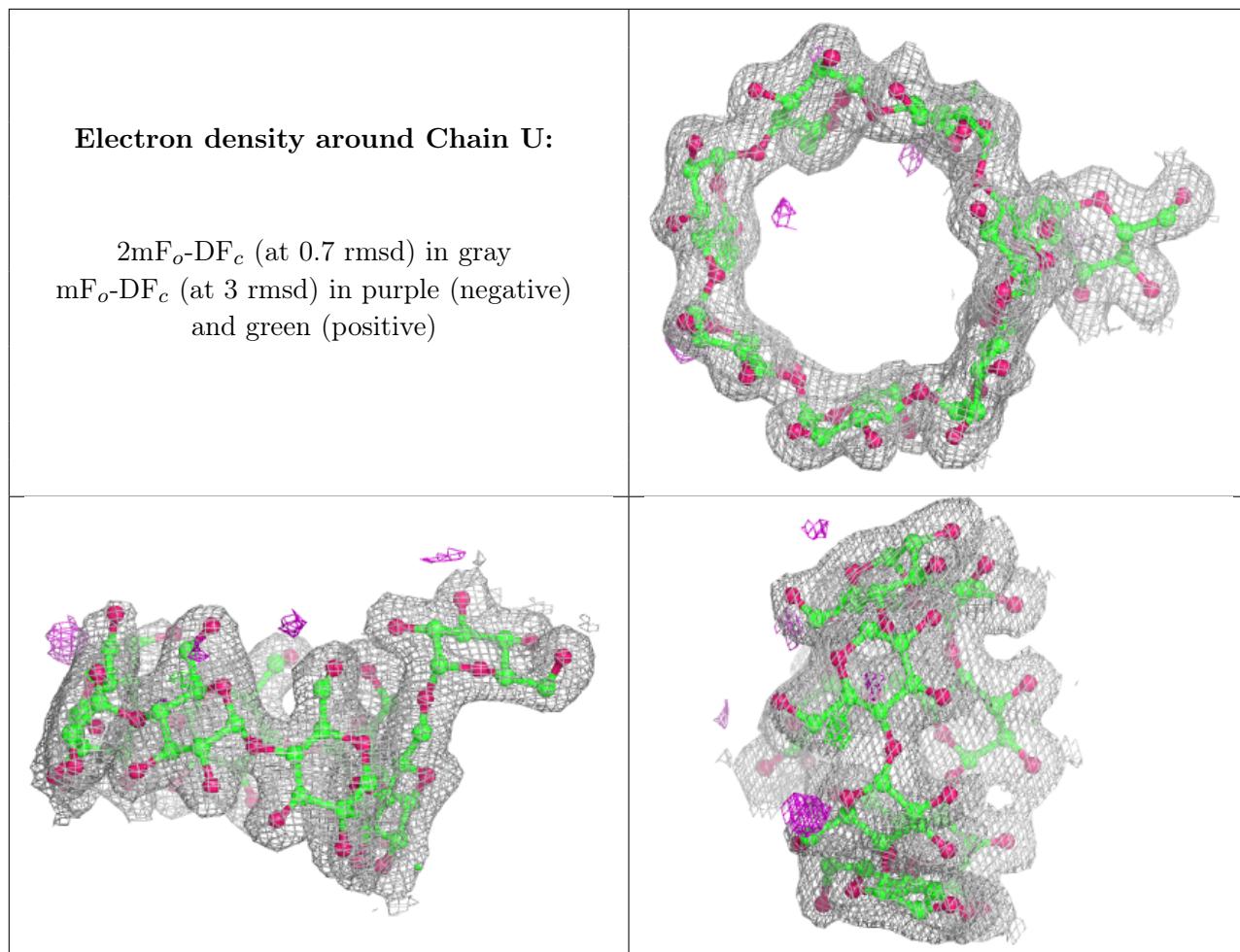
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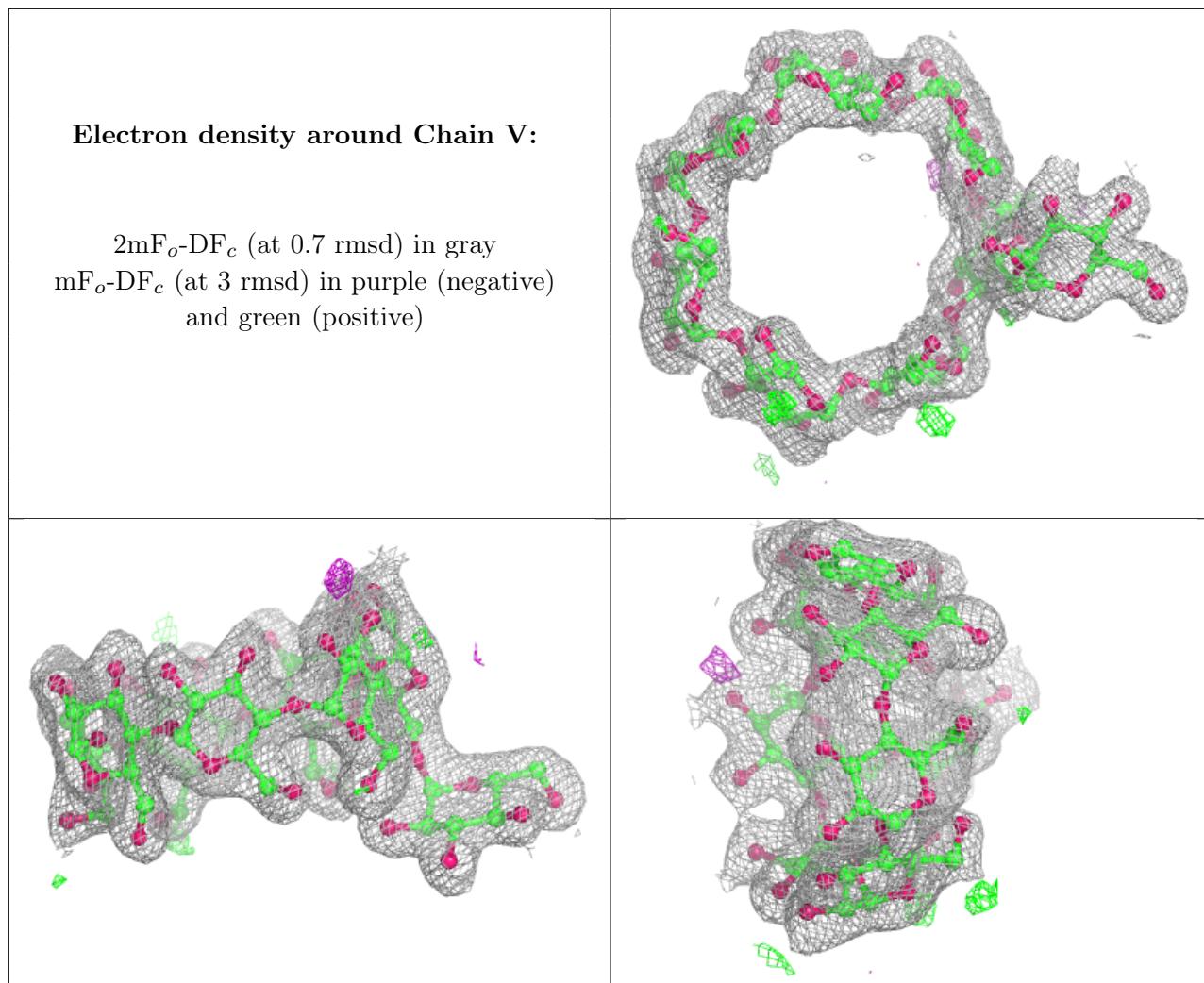
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLC	V	1	11/12	0.96	0.07	23,27,33,34	0
2	GLC	X	3	11/12	0.96	0.08	21,22,28,29	0
2	GLC	h	6	11/12	0.96	0.10	32,38,42,43	0
2	GLC	V	2	11/12	0.96	0.10	32,34,44,50	0
2	GLC	W	2	11/12	0.96	0.08	27,28,33,35	0
2	GLC	W	3	11/12	0.96	0.08	27,30,36,38	0
2	GLC	c	6	11/12	0.96	0.08	31,33,35,35	0
2	GLC	X	6	11/12	0.97	0.08	19,22,24,25	0
2	GLC	S	1	11/12	0.97	0.09	19,23,29,34	0
2	GLC	c	1	11/12	0.97	0.08	33,38,41,43	0
2	GLC	e	8	11/12	0.97	0.08	31,34,35,37	0
2	GLC	b	7	11/12	0.97	0.06	23,26,28,32	0
2	GLC	X	7	11/12	0.97	0.08	18,19,21,22	0
2	GLC	S	8	11/12	0.97	0.08	17,18,21,25	0
2	GLC	X	2	11/12	0.97	0.08	21,24,26,27	0
2	GLC	T	8	11/12	0.97	0.08	15,18,21,21	0
2	GLC	U	1	11/12	0.97	0.07	20,22,25,30	0
2	GLC	T	1	11/12	0.97	0.09	21,25,31,37	0
2	GLC	V	8	11/12	0.98	0.07	21,23,24,28	0
2	GLC	W	7	11/12	0.98	0.08	20,20,22,23	0
2	GLC	e	7	11/12	0.98	0.08	22,25,27,30	0
2	GLC	S	6	11/12	0.98	0.07	19,20,22,23	0
2	GLC	U	7	11/12	0.98	0.09	14,17,18,20	0
2	GLC	S	7	11/12	0.98	0.08	17,18,19,20	0
2	GLC	U	6	11/12	0.98	0.09	17,18,20,20	0
2	GLC	U	8	11/12	0.98	0.08	16,18,20,22	0
2	GLC	W	6	11/12	0.98	0.09	20,23,25,25	0
2	GLC	T	7	11/12	0.98	0.10	18,19,21,22	0

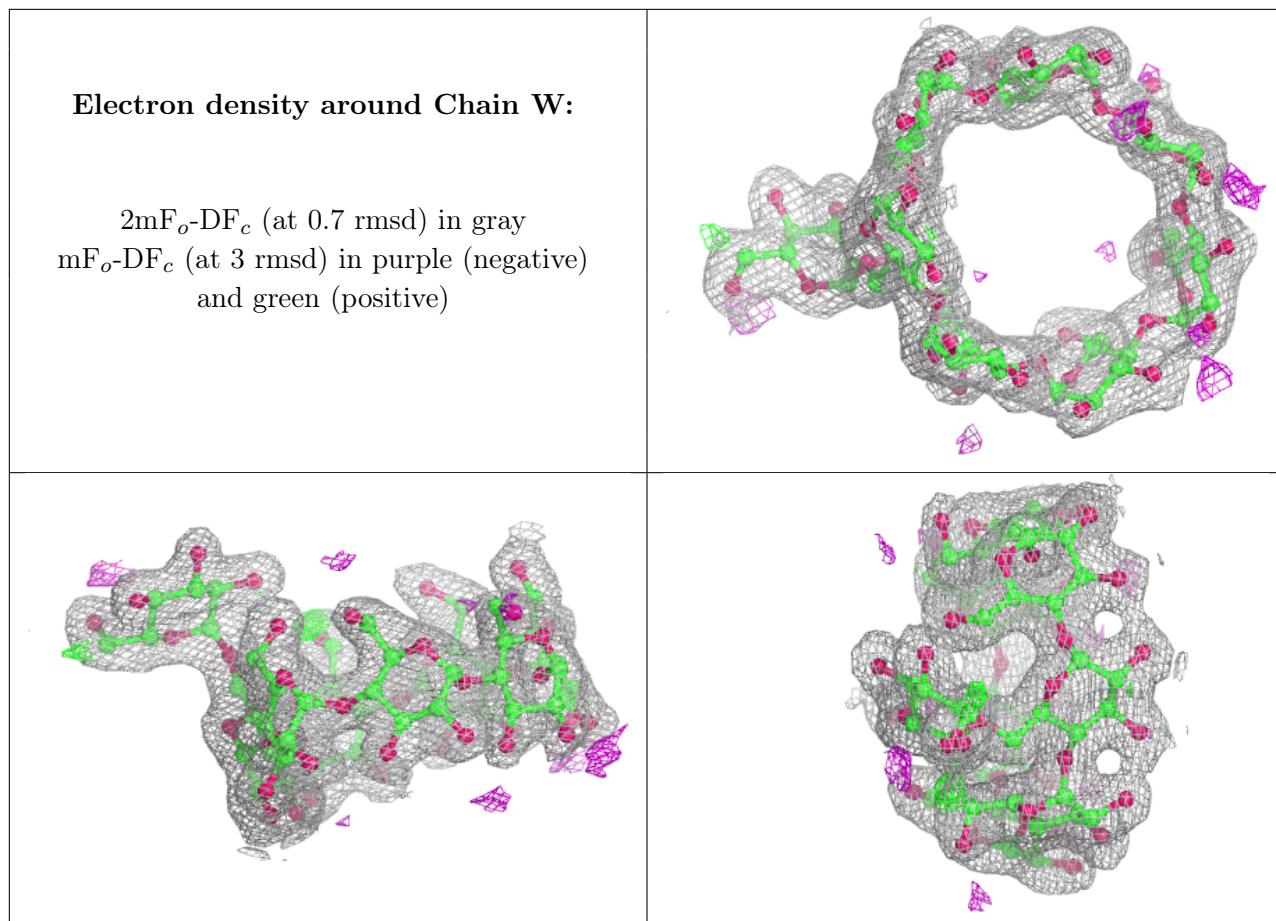
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

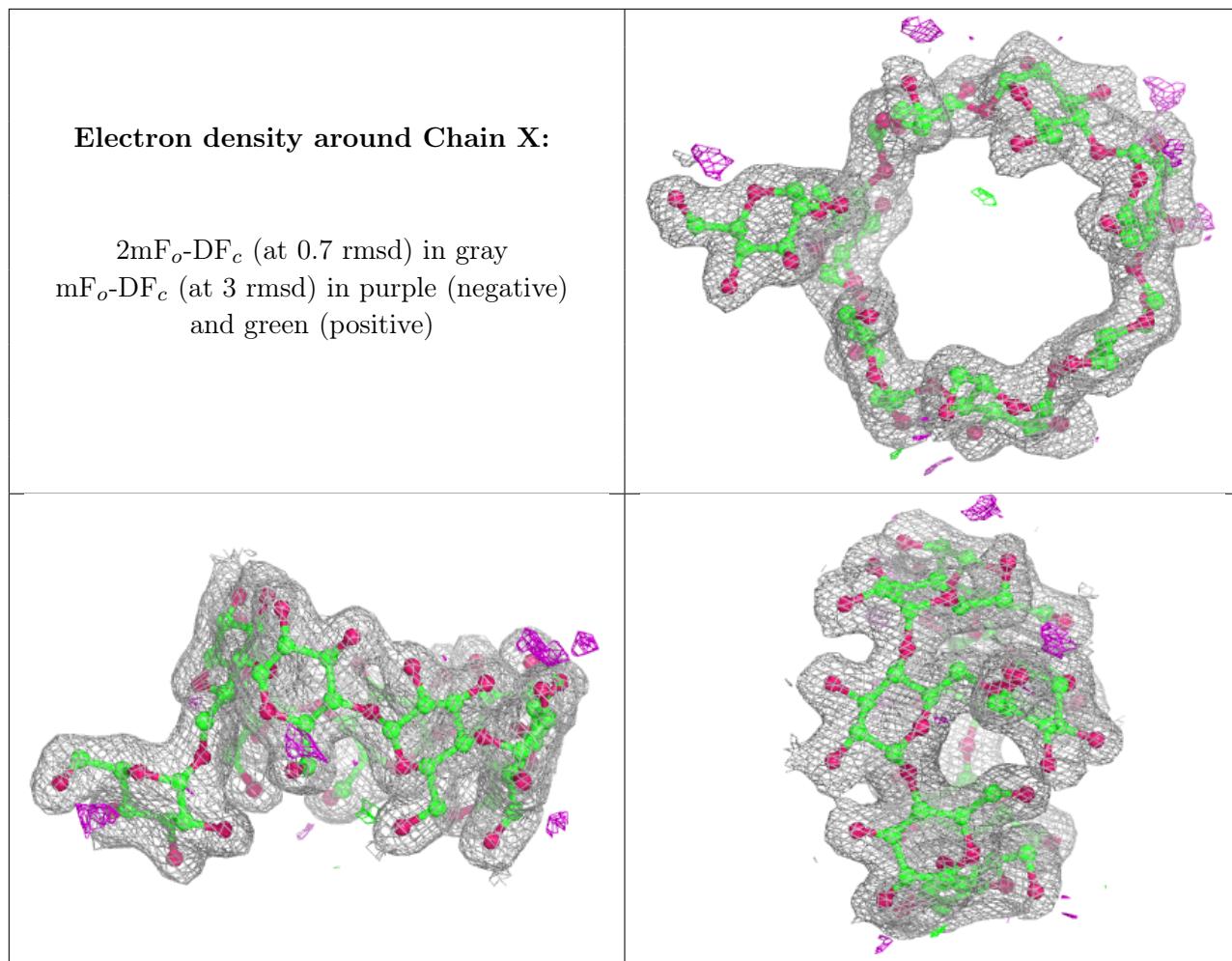


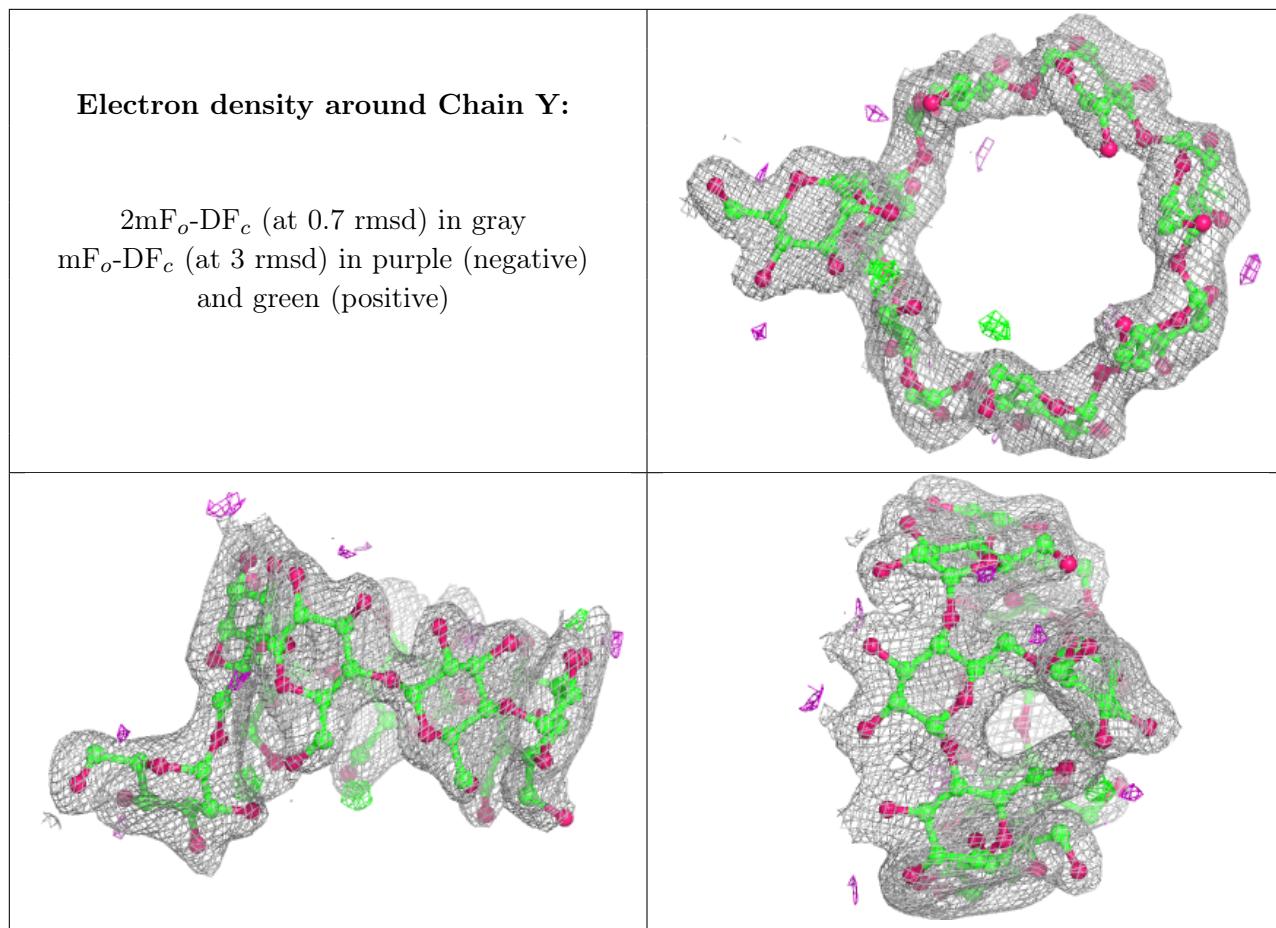


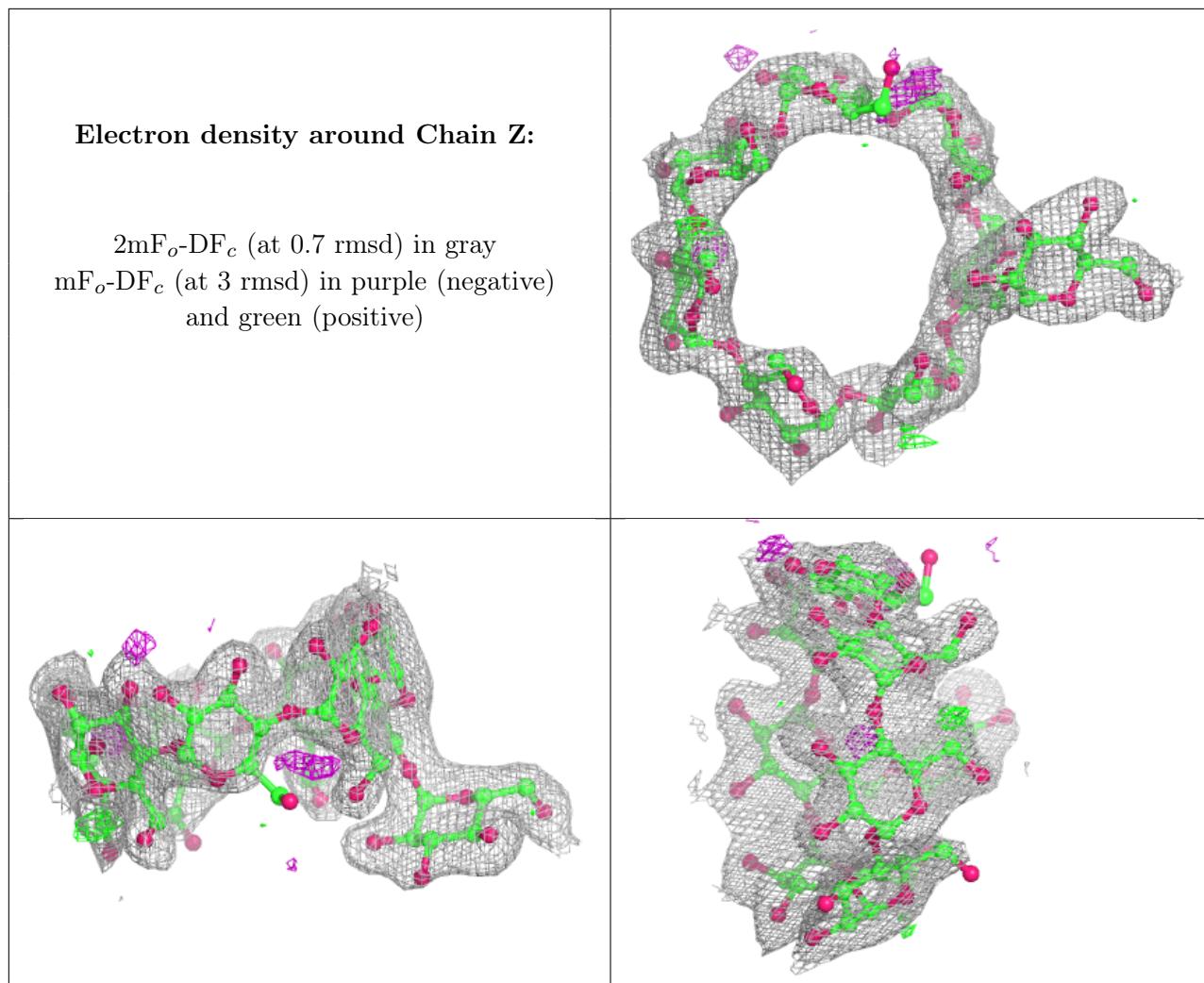


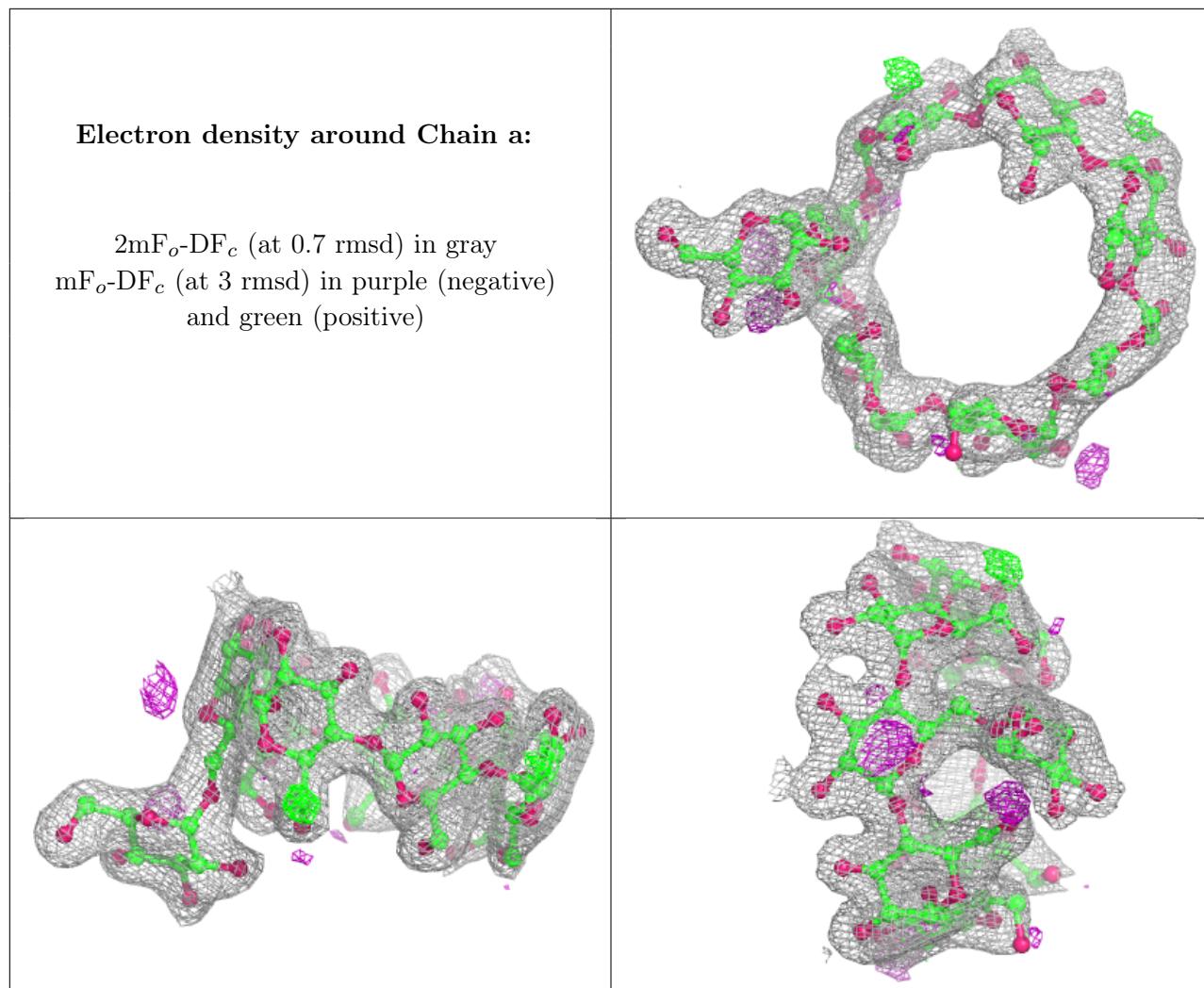


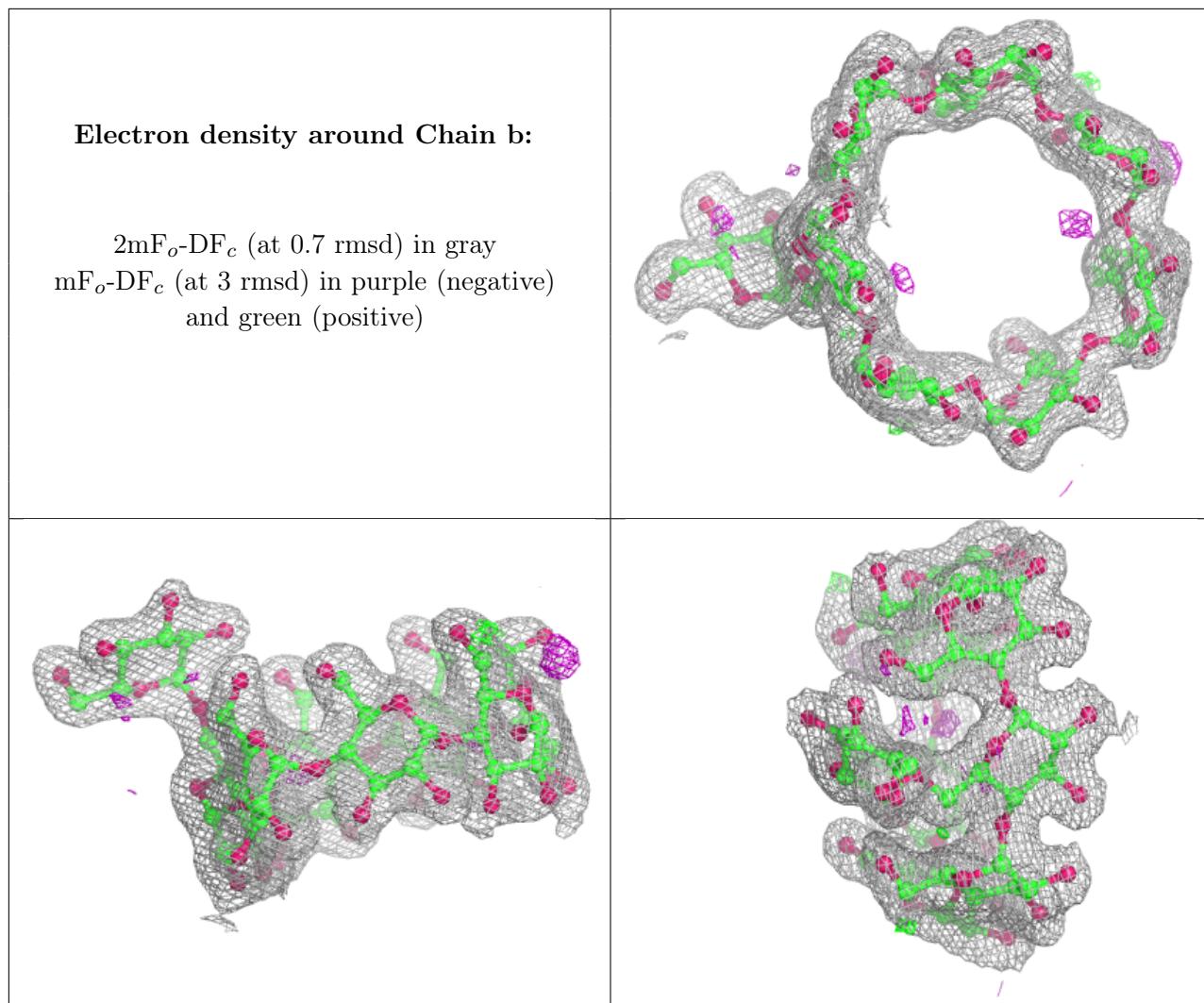


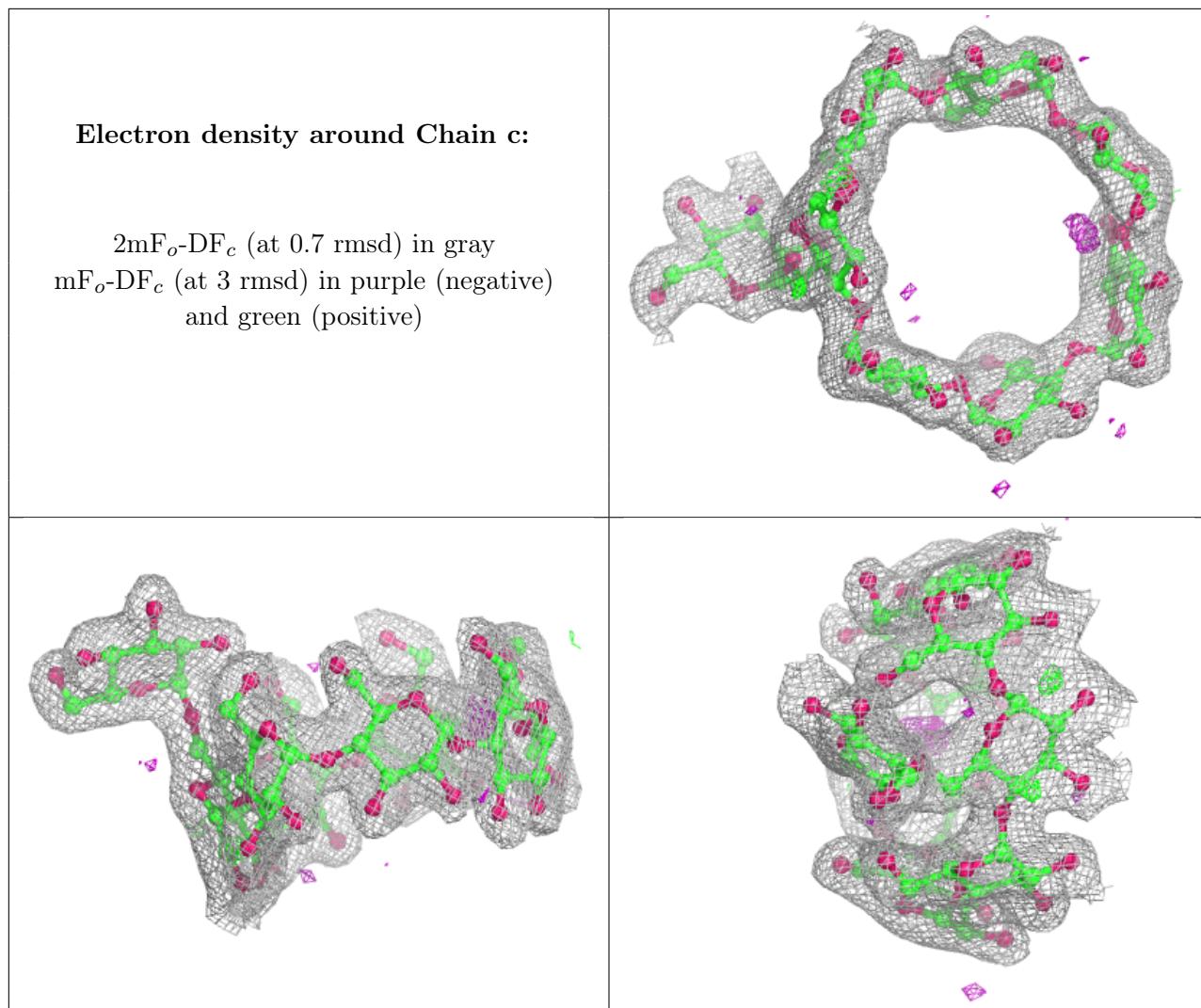


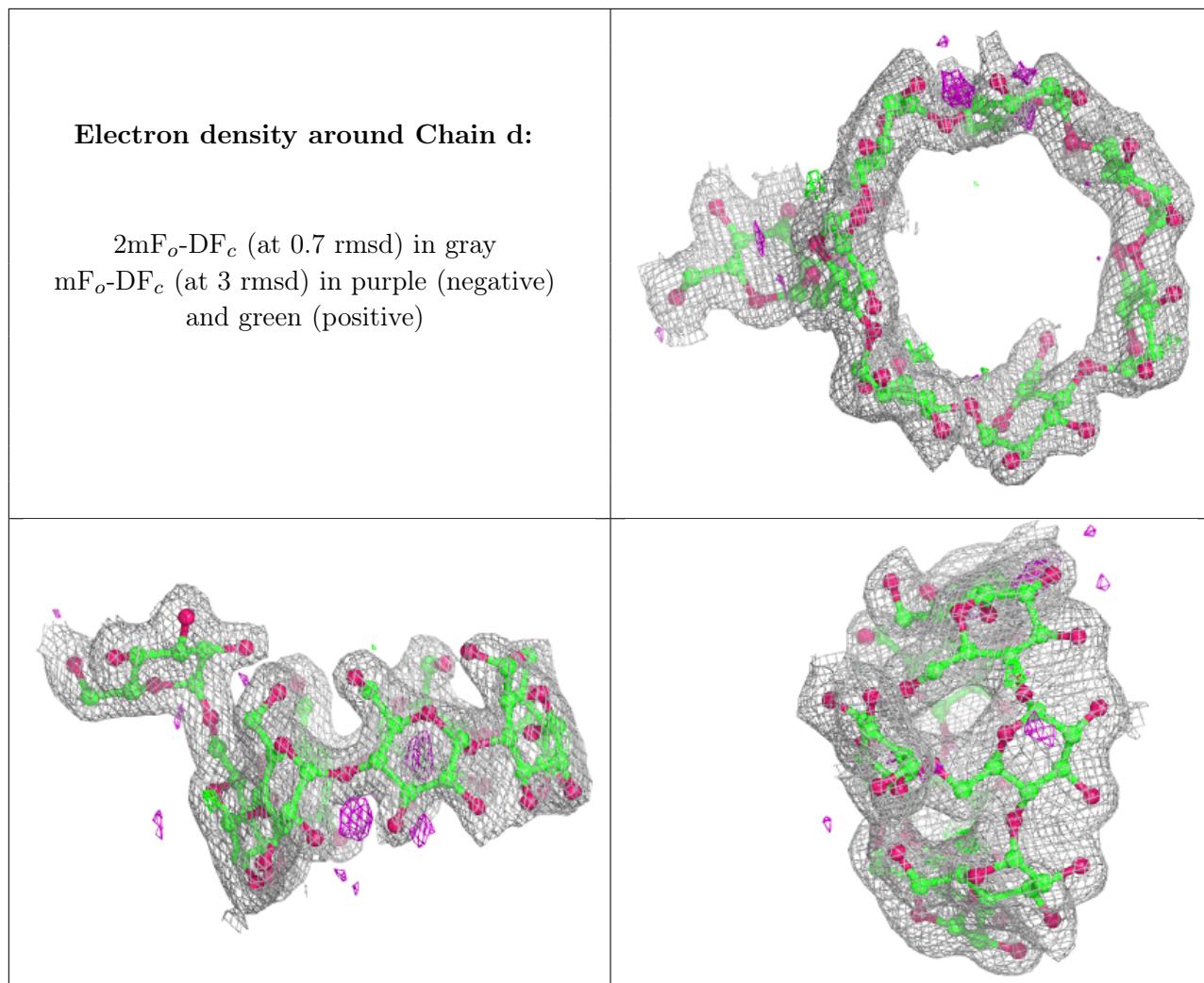


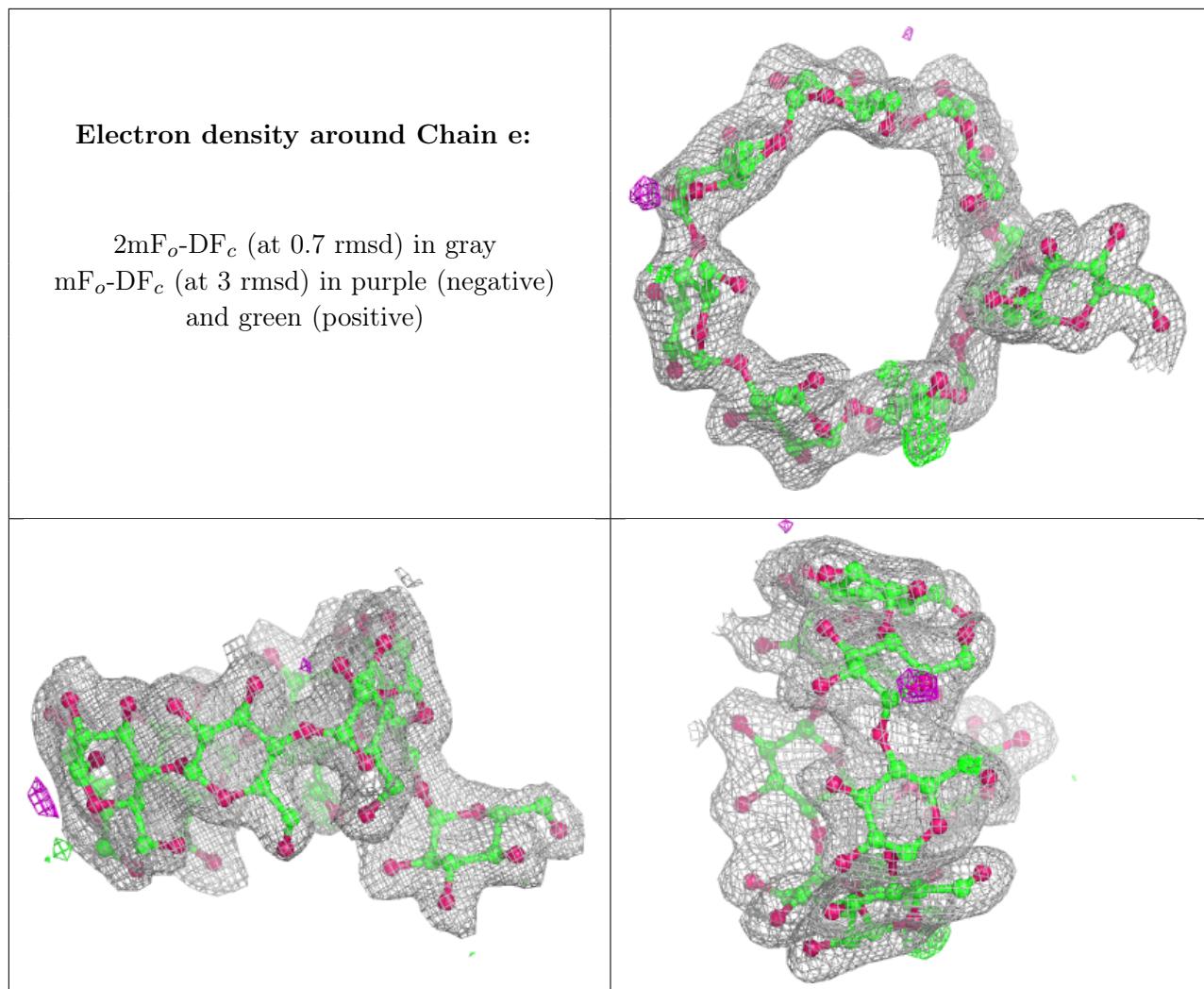


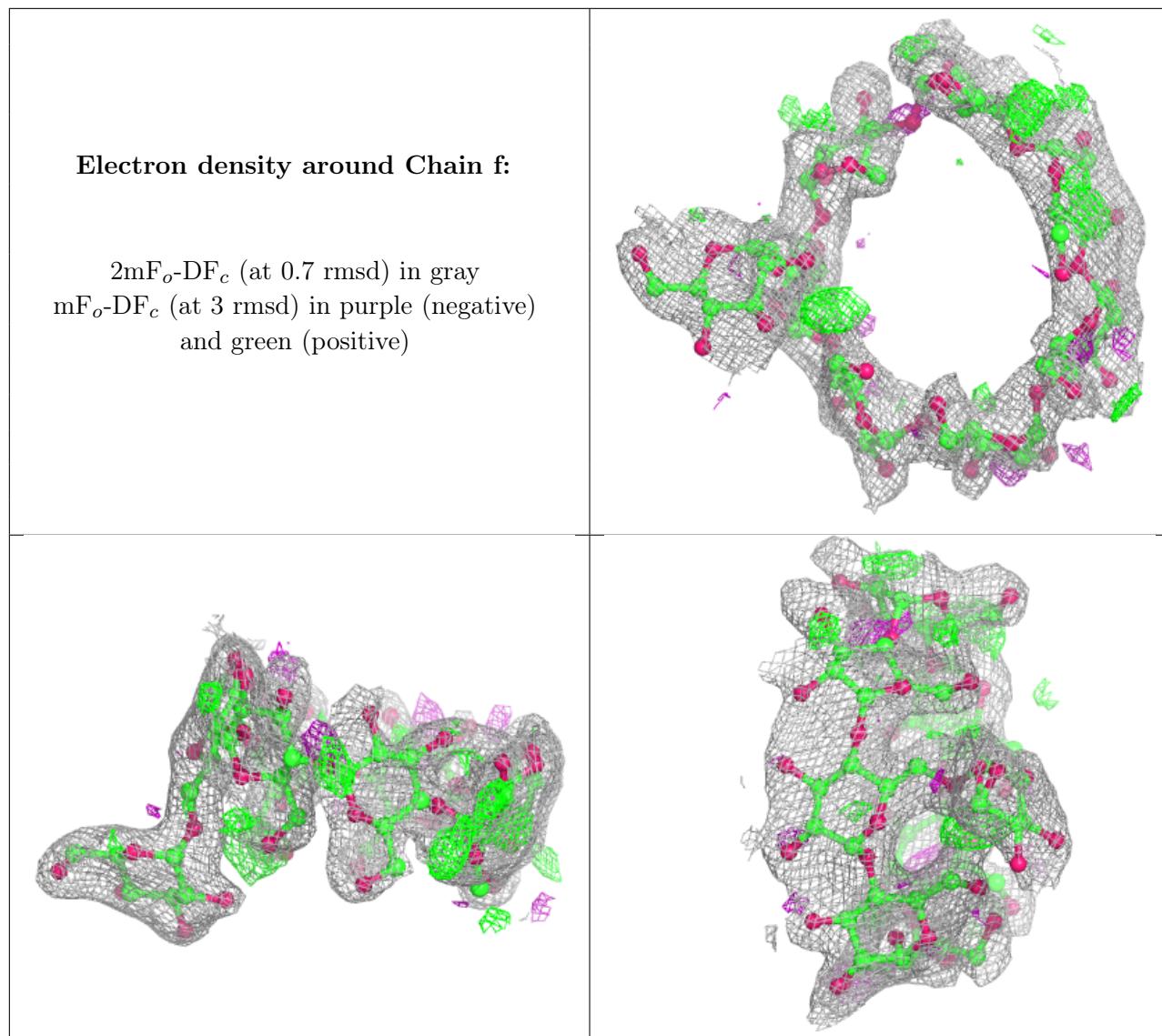


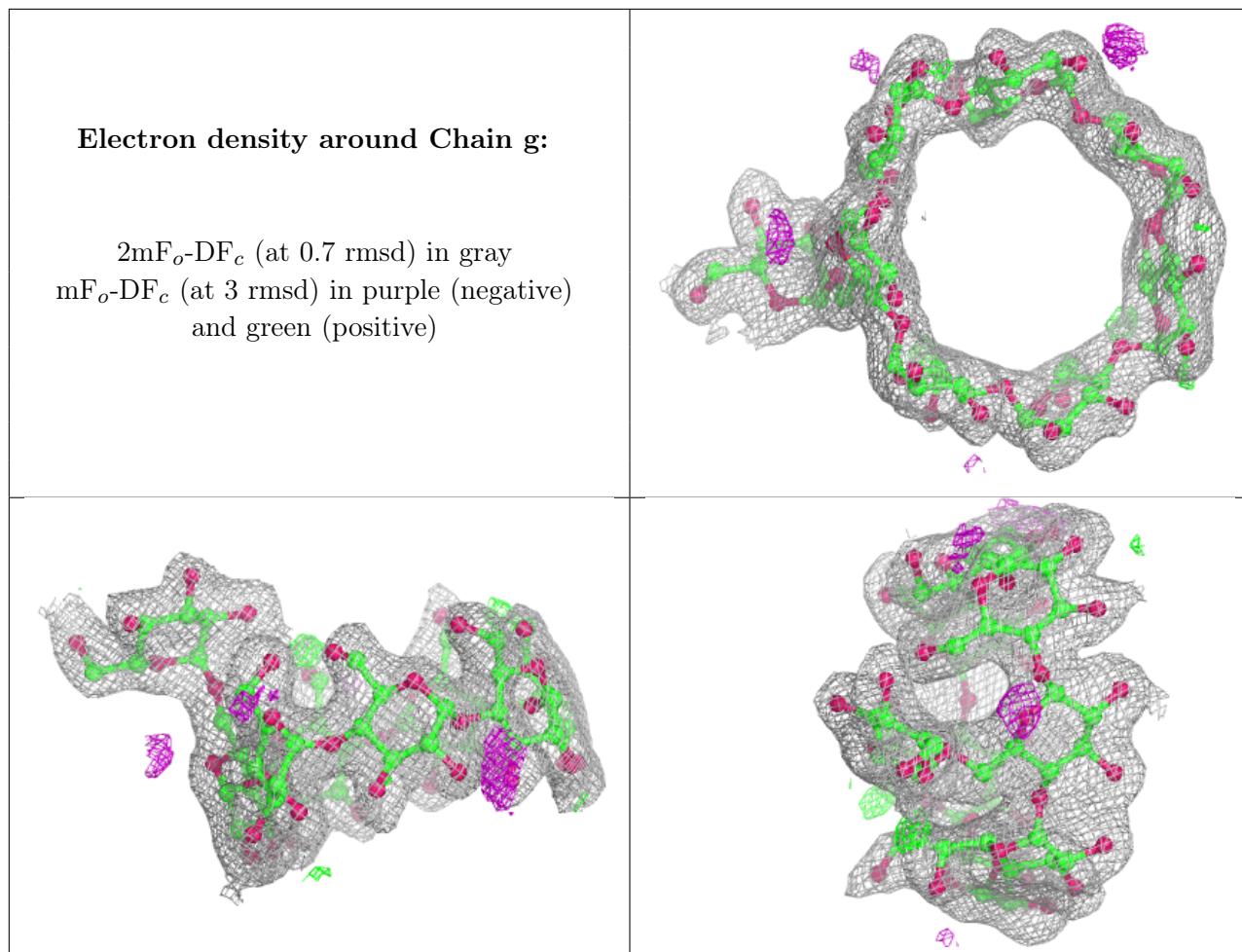


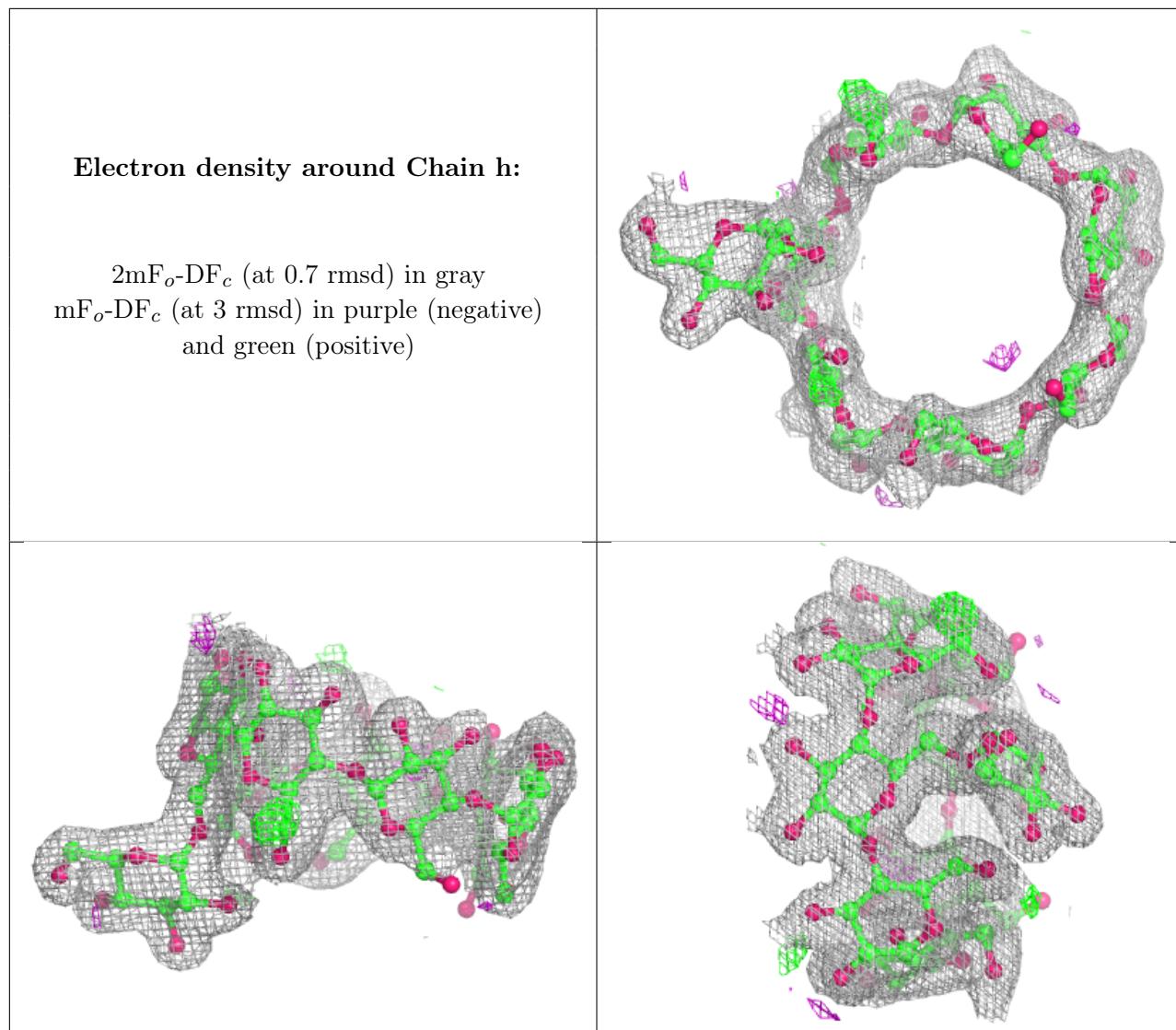


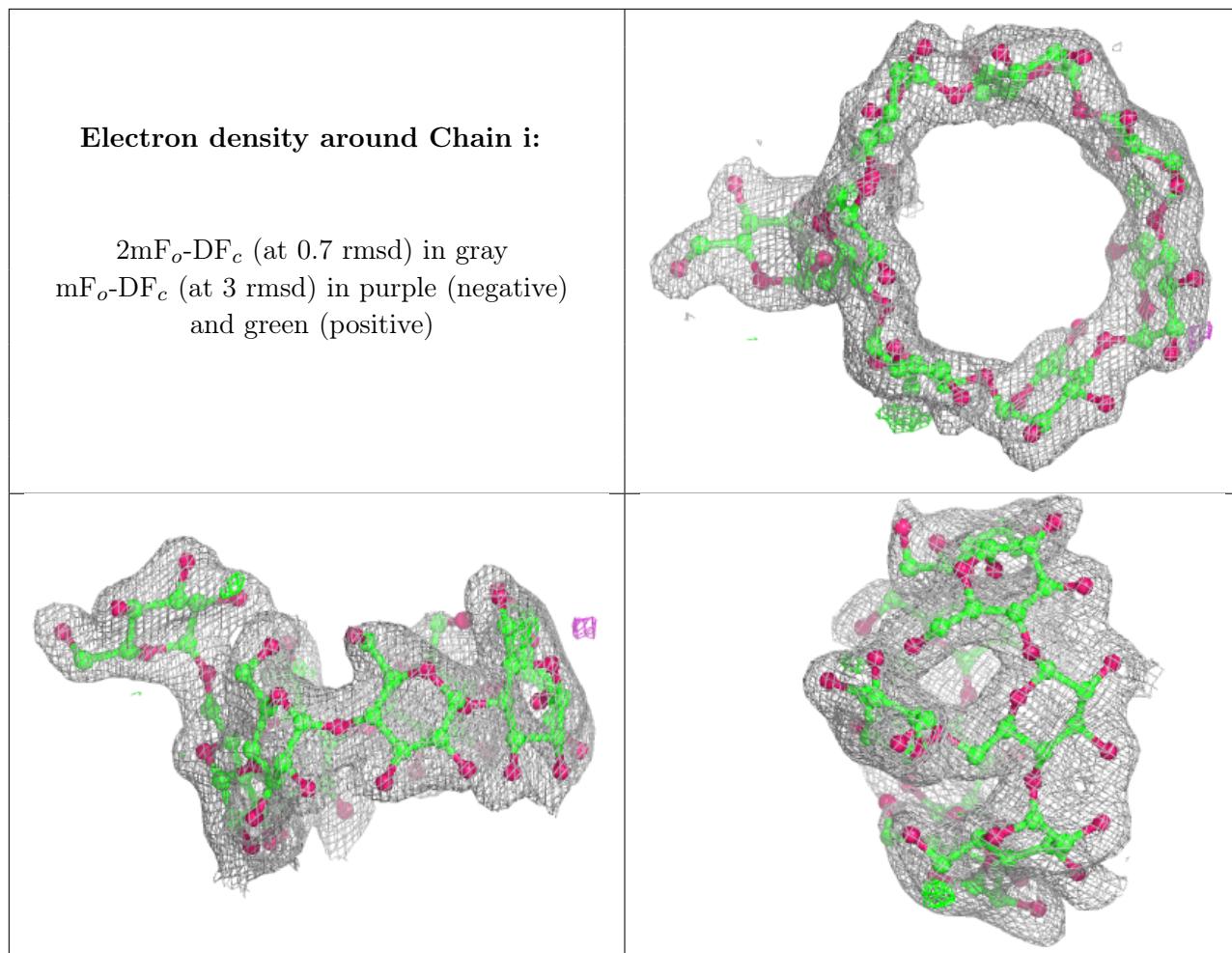


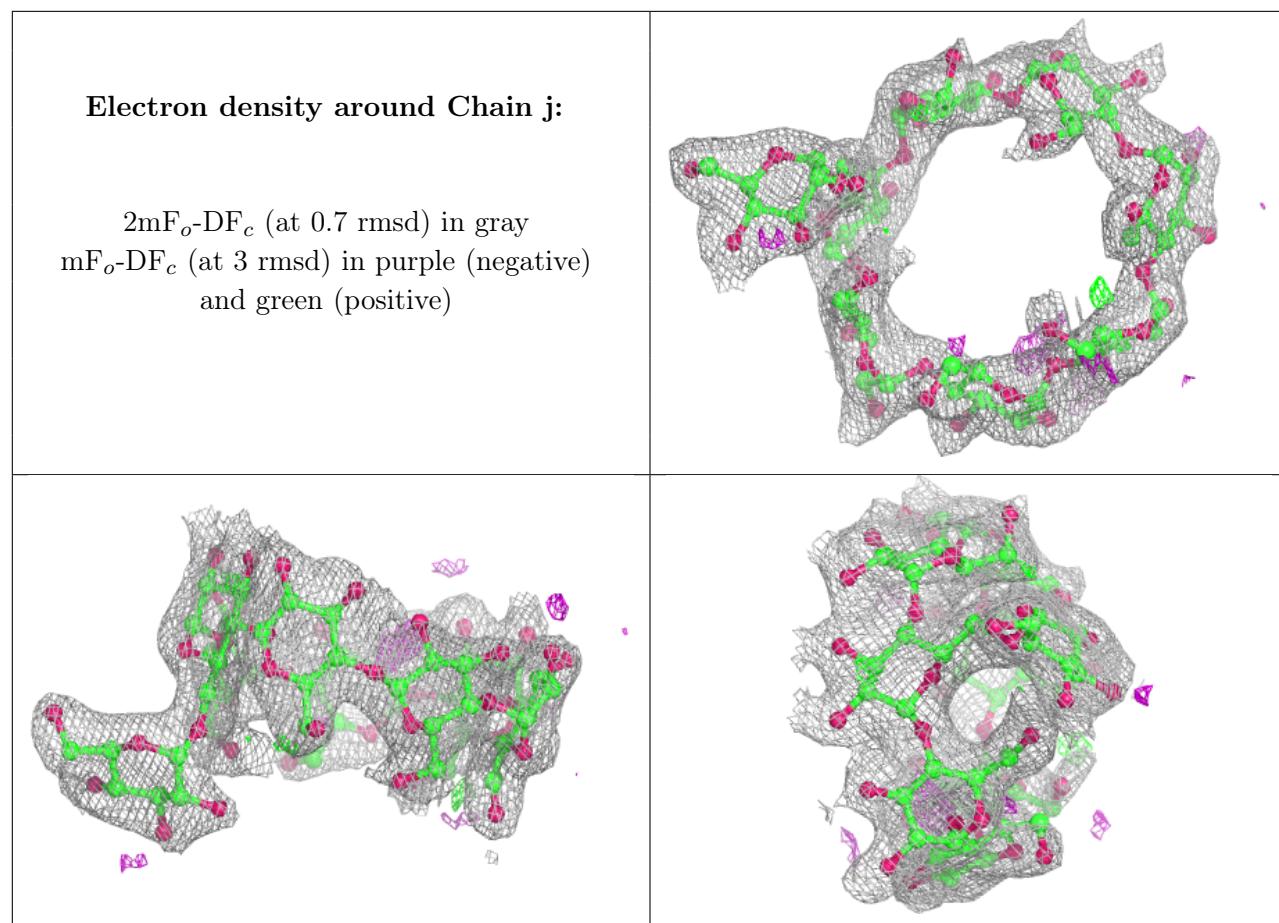












## 6.4 Ligands (i)

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
3	GOL	H	201	6/6	0.86	0.22	28,41,47,47	0
3	GOL	I	202	6/6	0.88	0.18	32,40,44,44	0
3	GOL	C	201	6/6	0.89	0.20	34,53,60,66	0
3	GOL	K	201	6/6	0.89	0.21	30,45,48,58	0
3	GOL	M	201	6/6	0.89	0.13	33,37,41,41	0
3	GOL	N	202	6/6	0.89	0.12	34,44,48,48	0
3	GOL	B	201	6/6	0.90	0.17	27,30,31,40	0
3	GOL	H	202	6/6	0.90	0.36	46,48,52,54	0
3	GOL	F	201	6/6	0.90	0.13	41,42,47,52	0
3	GOL	E	201	6/6	0.91	0.14	30,34,38,45	0
3	GOL	I	201	6/6	0.91	0.11	40,47,47,55	0
3	GOL	A	202	6/6	0.94	0.15	21,31,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	P	201	6/6	0.94	0.18	38,48,51,55	0
3	GOL	A	201	6/6	0.95	0.13	32,34,36,37	0
3	GOL	C	202	6/6	0.95	0.10	28,30,31,33	0
3	GOL	N	201	6/6	0.96	0.09	27,31,32,35	0
3	GOL	B	202	6/6	0.97	0.10	20,26,27,32	0
3	GOL	L	201	6/6	0.97	0.11	22,26,29,31	0
3	GOL	D	201	6/6	0.97	0.12	25,28,31,31	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.