



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 05:25 PM EDT

PDB ID : 4YEF
Title : beta1 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 : 1.72 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-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

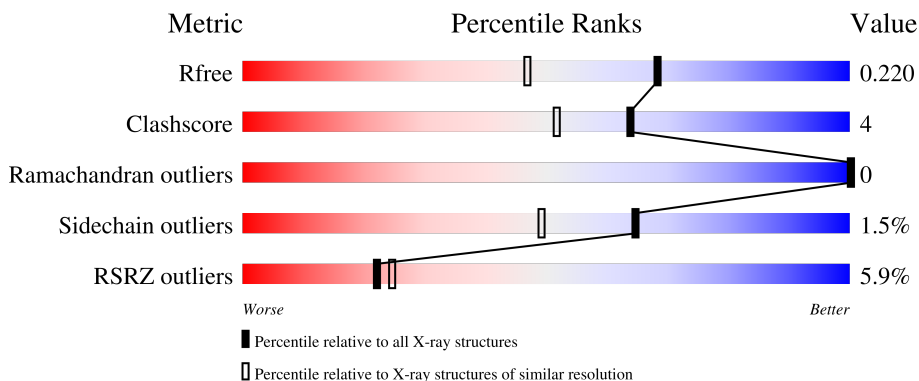
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	89	 2% 84% 6% 10%
1	B	89	 % 90% 7% .
1	C	89	 81% 8% 11%
1	D	89	 7% 81% 6% 13%
1	E	89	 2% 91% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	89	<p>7% 80% 7% 13%</p>
1	G	89	<p>18% 58% 20% 16%</p>
2	H	7	<p>14% 86%</p>
2	I	7	<p>43% 57%</p>
2	J	7	<p>86% 14%</p>
2	K	7	<p>29% 71%</p>
2	L	7	<p>14% 86%</p>
2	M	7	<p>14% 86%</p>
2	N	7	<p>29% 43% 29%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6310 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-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	80	648	416	111	121	0	1	0
1	B	86	682	434	118	130	0	0	0
1	C	79	637	410	107	120	0	1	0
1	D	77	597	386	101	110	0	0	0
1	E	85	686	437	118	131	0	1	0
1	F	77	596	386	102	108	0	0	0
1	G	75	1122	726	186	210	0	75	0

There are 56 discrepancies between the modelled and reference sequences:

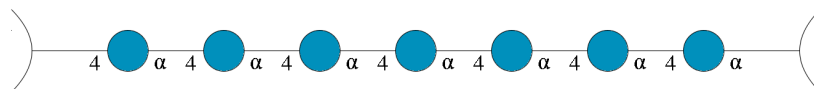
Chain	Residue	Modelled	Actual	Comment	Reference
A	68	GLY	-	expression tag	UNP P80386
A	69	PRO	-	expression tag	UNP P80386
A	70	LEU	-	expression tag	UNP P80386
A	71	GLY	-	expression tag	UNP P80386
A	72	SER	-	expression tag	UNP P80386
A	73	PRO	-	expression tag	UNP P80386
A	74	ASN	-	expression tag	UNP P80386
A	75	SER	-	expression tag	UNP P80386
B	68	GLY	-	expression tag	UNP P80386
B	69	PRO	-	expression tag	UNP P80386
B	70	LEU	-	expression tag	UNP P80386
B	71	GLY	-	expression tag	UNP P80386
B	72	SER	-	expression tag	UNP P80386
B	73	PRO	-	expression tag	UNP P80386
B	74	ASN	-	expression tag	UNP P80386

Continued on next page...

Continued from previous page...

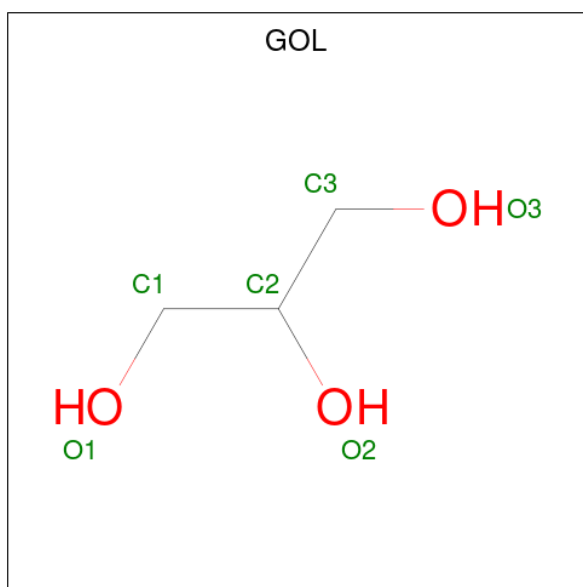
Chain	Residue	Modelled	Actual	Comment	Reference
B	75	SER	-	expression tag	UNP P80386
C	68	GLY	-	expression tag	UNP P80386
C	69	PRO	-	expression tag	UNP P80386
C	70	LEU	-	expression tag	UNP P80386
C	71	GLY	-	expression tag	UNP P80386
C	72	SER	-	expression tag	UNP P80386
C	73	PRO	-	expression tag	UNP P80386
C	74	ASN	-	expression tag	UNP P80386
C	75	SER	-	expression tag	UNP P80386
D	68	GLY	-	expression tag	UNP P80386
D	69	PRO	-	expression tag	UNP P80386
D	70	LEU	-	expression tag	UNP P80386
D	71	GLY	-	expression tag	UNP P80386
D	72	SER	-	expression tag	UNP P80386
D	73	PRO	-	expression tag	UNP P80386
D	74	ASN	-	expression tag	UNP P80386
D	75	SER	-	expression tag	UNP P80386
E	68	GLY	-	expression tag	UNP P80386
E	69	PRO	-	expression tag	UNP P80386
E	70	LEU	-	expression tag	UNP P80386
E	71	GLY	-	expression tag	UNP P80386
E	72	SER	-	expression tag	UNP P80386
E	73	PRO	-	expression tag	UNP P80386
E	74	ASN	-	expression tag	UNP P80386
E	75	SER	-	expression tag	UNP P80386
F	68	GLY	-	expression tag	UNP P80386
F	69	PRO	-	expression tag	UNP P80386
F	70	LEU	-	expression tag	UNP P80386
F	71	GLY	-	expression tag	UNP P80386
F	72	SER	-	expression tag	UNP P80386
F	73	PRO	-	expression tag	UNP P80386
F	74	ASN	-	expression tag	UNP P80386
F	75	SER	-	expression tag	UNP P80386
G	68	GLY	-	expression tag	UNP P80386
G	69	PRO	-	expression tag	UNP P80386
G	70	LEU	-	expression tag	UNP P80386
G	71	GLY	-	expression tag	UNP P80386
G	72	SER	-	expression tag	UNP P80386
G	73	PRO	-	expression tag	UNP P80386
G	74	ASN	-	expression tag	UNP P80386
G	75	SER	-	expression tag	UNP P80386

- Molecule 2 is an oligosaccharide called Cycloheptakis-(1-4)-(alpha-D-glucopyranose).



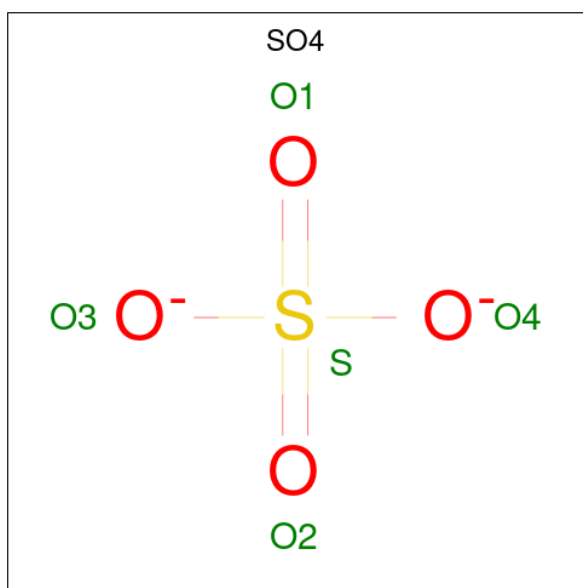
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	H	7	Total	C	O	0	0	0
			77	42	35			
2	I	7	Total	C	O	0	0	0
			77	42	35			
2	J	7	Total	C	O	0	0	0
			77	42	35			
2	K	7	Total	C	O	0	0	0
			77	42	35			
2	L	7	Total	C	O	0	0	0
			77	42	35			
2	M	7	Total	C	O	0	0	0
			77	42	35			
2	N	7	Total	C	O	0	7	0
			154	84	70			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	115	Total O 115 115	0	0
5	B	157	Total O 157 157	0	0
5	C	115	Total O 115 115	0	0
5	D	60	Total O 60 60	0	0
5	E	151	Total O 151 151	0	0

Continued on next page...

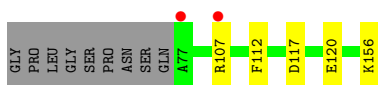
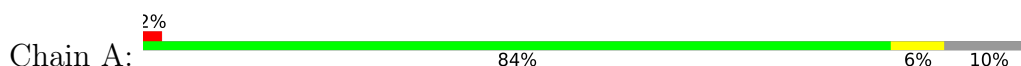
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	61	Total O 61 61	0	0
5	G	25	Total O 25 25	0	0

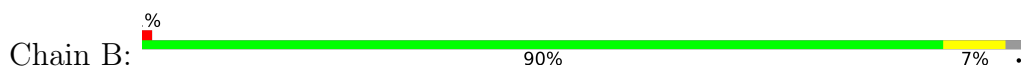
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

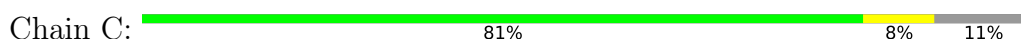
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-1



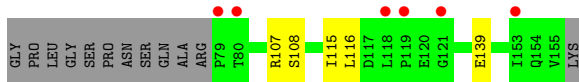
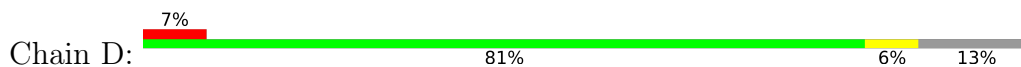
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-1



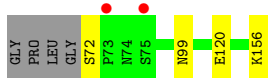
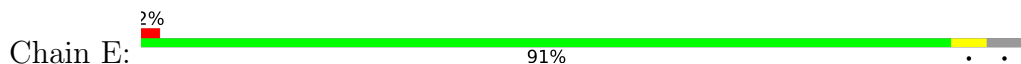
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-1



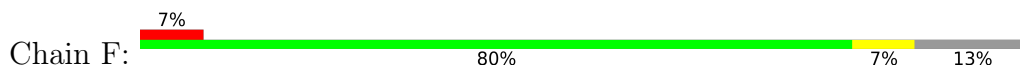
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-1



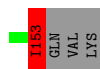
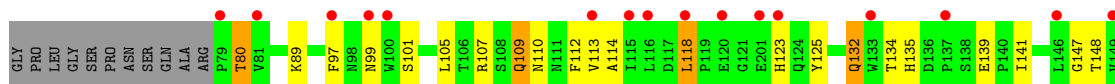
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-1



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



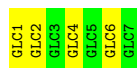
- Molecule 1: 5'-AMP-activated protein kinase subunit beta-1



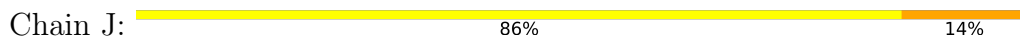
- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)



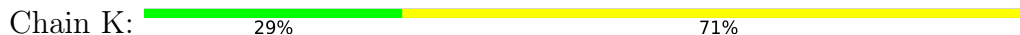
- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)



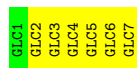
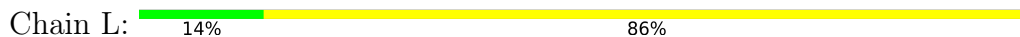
- Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)




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



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



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

Chain M:  14% 86%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7

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

Chain N:  29% 43% 29%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.72Å 68.39Å 92.21Å 111.72° 95.56° 90.06°	Depositor
Resolution (Å)	43.71 – 1.72 43.71 – 1.72	Depositor EDS
% Data completeness (in resolution range)	97.1 (43.71-1.72) 96.9 (43.71-1.72)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.72Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.178 , 0.213 0.186 , 0.220	Depositor DCC
R_{free} test set	4768 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtrriage
Anisotropy	0.487	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.479 for -h,k,-k-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6310	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, GLC

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	0.66	0/670	0.74	0/912
1	B	0.69	0/702	0.76	0/956
1	C	0.67	0/659	0.74	0/898
1	D	0.59	0/616	0.73	0/843
1	E	0.73	0/709	0.76	0/965
1	F	0.57	0/615	0.75	0/841
1	G	151.82	26/1180 (2.2%)	4.95	42/1610 (2.6%)
All	All	72.67	26/5151 (0.5%)	2.46	42/7025 (0.6%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	109[A]	GLN	CD-OE1	2102.00	47.48	1.24
1	G	109[B]	GLN	CD-OE1	2102.00	47.48	1.24
1	G	109[A]	GLN	CD-NE2	1872.02	48.12	1.32
1	G	109[B]	GLN	CD-NE2	1872.02	48.12	1.32
1	G	89[A]	LYS	C-O	1623.10	32.07	1.23
1	G	89[B]	LYS	C-O	1623.10	32.07	1.23
1	G	89[A]	LYS	CG-CD	905.23	32.30	1.52
1	G	89[B]	LYS	CG-CD	905.23	32.30	1.52
1	G	99[A]	ASN	CG-OD1	884.25	20.69	1.24
1	G	99[B]	ASN	CG-OD1	884.25	20.69	1.24
1	G	99[A]	ASN	CG-ND2	857.64	22.77	1.32
1	G	99[B]	ASN	CG-ND2	857.64	22.77	1.32
1	G	80[A]	THR	CB-OG1	511.09	11.65	1.43
1	G	80[B]	THR	CB-OG1	511.09	11.65	1.43
1	G	153[A]	ILE	CB-CG1	374.67	12.03	1.54
1	G	153[B]	ILE	CB-CG1	374.67	12.03	1.54
1	G	80[A]	THR	CB-CG2	328.13	12.35	1.52
1	G	80[B]	THR	CB-CG2	328.13	12.35	1.52
1	G	132[A]	GLN	CB-CG	295.10	9.49	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	132[B]	GLN	CB-CG	295.10	9.49	1.52
1	G	153[A]	ILE	CB-CG2	266.01	9.77	1.52
1	G	153[B]	ILE	CB-CG2	266.01	9.77	1.52
1	G	123[A]	HIS	CB-CG	143.70	4.08	1.50
1	G	123[B]	HIS	CB-CG	143.70	4.08	1.50
1	G	118[A]	LEU	CB-CG	128.63	5.25	1.52
1	G	118[B]	LEU	CB-CG	128.63	5.25	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	89[A]	LYS	O-C-N	-63.56	21.01	122.70
1	G	89[B]	LYS	O-C-N	-63.56	21.01	122.70
1	G	99[A]	ASN	OD1-CG-ND2	-51.99	2.32	121.90
1	G	99[B]	ASN	OD1-CG-ND2	-51.99	2.32	121.90
1	G	109[A]	GLN	OE1-CD-NE2	-51.88	2.57	121.90
1	G	109[B]	GLN	OE1-CD-NE2	-51.88	2.57	121.90
1	G	153[A]	ILE	CG1-CB-CG2	-48.02	5.77	111.40
1	G	153[B]	ILE	CG1-CB-CG2	-48.02	5.77	111.40
1	G	80[A]	THR	OG1-CB-CG2	-43.02	11.07	110.00
1	G	80[B]	THR	OG1-CB-CG2	-43.02	11.07	110.00
1	G	123[A]	HIS	CA-CB-CG	34.17	171.69	113.60
1	G	123[B]	HIS	CA-CB-CG	34.17	171.69	113.60
1	G	80[A]	THR	CA-CB-CG2	29.68	153.96	112.40
1	G	80[B]	THR	CA-CB-CG2	29.68	153.96	112.40
1	G	132[A]	GLN	CB-CG-CD	-29.65	34.52	111.60
1	G	132[B]	GLN	CB-CG-CD	-29.65	34.52	111.60
1	G	109[A]	GLN	CG-CD-OE1	-22.03	77.54	121.60
1	G	109[B]	GLN	CG-CD-OE1	-22.03	77.54	121.60
1	G	118[A]	LEU	CB-CG-CD1	-20.59	76.00	111.00
1	G	118[B]	LEU	CB-CG-CD1	-20.59	76.00	111.00
1	G	99[A]	ASN	CB-CG-OD1	-18.77	84.07	121.60
1	G	99[B]	ASN	CB-CG-OD1	-18.77	84.07	121.60
1	G	80[A]	THR	CA-CB-OG1	17.79	146.36	109.00
1	G	80[B]	THR	CA-CB-OG1	17.79	146.36	109.00
1	G	109[A]	GLN	CG-CD-NE2	-15.46	79.60	116.70
1	G	109[B]	GLN	CG-CD-NE2	-15.46	79.60	116.70
1	G	89[A]	LYS	CB-CG-CD	-14.98	72.65	111.60
1	G	89[B]	LYS	CB-CG-CD	-14.98	72.65	111.60
1	G	118[A]	LEU	CB-CG-CD2	-14.34	86.62	111.00
1	G	118[B]	LEU	CB-CG-CD2	-14.34	86.62	111.00
1	G	99[A]	ASN	CB-CG-ND2	-13.83	83.51	116.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	99[B]	ASN	CB-CG-ND2	-13.83	83.51	116.70
1	G	123[A]	HIS	CB-CG-ND1	-11.74	93.85	123.20
1	G	123[B]	HIS	CB-CG-ND1	-11.74	93.85	123.20
1	G	132[A]	GLN	CA-CB-CG	-10.72	89.82	113.40
1	G	132[B]	GLN	CA-CB-CG	-10.72	89.82	113.40
1	G	89[A]	LYS	CA-C-O	-8.72	101.78	120.10
1	G	89[B]	LYS	CA-C-O	-8.72	101.78	120.10
1	G	123[A]	HIS	CB-CG-CD2	-8.15	105.53	130.80
1	G	123[B]	HIS	CB-CG-CD2	-8.15	105.53	130.80
1	G	153[A]	ILE	CB-CG1-CD1	-6.79	94.89	113.90
1	G	153[B]	ILE	CB-CG1-CD1	-6.79	94.89	113.90

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	648	0	621	4	0
1	B	682	0	647	4	0
1	C	637	0	605	5	0
1	D	597	0	554	9	0
1	E	686	0	657	3	0
1	F	596	0	553	5	0
1	G	1122	0	991	22	0
2	H	77	0	63	0	0
2	I	77	0	63	0	0
2	J	77	0	63	1	0
2	K	77	0	63	0	0
2	L	77	0	63	0	0
2	M	77	0	63	0	0
2	N	154	0	83	4	0
3	A	6	0	8	0	0
3	C	6	0	8	1	0
4	B	10	0	0	0	0
4	D	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	10	0	0	0	0
4	F	5	0	0	0	0
5	A	115	0	0	1	1
5	B	157	0	0	1	1
5	C	115	0	0	1	2
5	D	60	0	0	2	0
5	E	151	0	0	1	2
5	F	61	0	0	2	1
5	G	25	0	0	7	1
All	All	6310	0	5105	45	4

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 4.

All (45) 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:D:115:ILE:O	1:G:141[A]:ILE:HG12	1.61	1.00
1:G:147[A]:GLY:O	5:G:301:HOH:O	1.87	0.93
1:G:153[B]:ILE:C	5:G:304:HOH:O	2.09	0.91
5:G:314:HOH:O	2:N:4[A]:GLC:O2	1.90	0.88
1:G:107[B]:ARG:HD3	1:G:112[B]:PHE:CZ	2.11	0.86
5:G:321:HOH:O	2:N:4[B]:GLC:H4	1.80	0.79
1:G:147[B]:GLY:O	5:G:302:HOH:O	2.02	0.77
1:G:110[A]:ASN:ND2	5:G:303:HOH:O	2.18	0.76
1:D:139:GLU:OE1	5:D:301:HOH:O	2.12	0.67
1:E:120:GLU:OE2	1:E:156:LYS:OXT	2.13	0.65
1:B:120:GLU:OE2	1:B:156:LYS:OXT	2.16	0.64
1:F:97:PHE:CE1	1:F:116:LEU:HD21	2.33	0.63
1:G:134[A]:THR:HG21	5:G:324:HOH:O	1.98	0.63
1:F:139:GLU:OE1	5:F:301:HOH:O	2.16	0.62
1:B:105:LEU:HD22	1:B:114:ALA:HB2	1.83	0.61
1:A:107:ARG:NH2	5:A:301:HOH:O	2.34	0.61
1:B:122:GLU:OE2	5:B:301:HOH:O	2.16	0.59
1:F:110:ASN:ND2	2:J:2:GLC:O6	2.34	0.58
1:D:115:ILE:CG2	1:G:139[A]:GLU:O	2.54	0.55
1:D:115:ILE:HG21	1:G:139[A]:GLU:O	2.08	0.54
1:D:115:ILE:O	1:G:101[B]:SER:HB2	2.08	0.54
1:C:145[B]:GLN:NE2	5:C:301:HOH:O	2.20	0.52
1:F:99:ASN:HB2	5:F:308:HOH:O	2.11	0.51
1:A:107:ARG:HD2	1:A:112:PHE:CZ	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:346:HOH:O	1:G:135[A]:HIS:HE1	1.93	0.50
1:G:148[A]:THR:HG21	2:N:7[A]:GLC:H3	1.93	0.50
1:C:109:GLN:O	1:C:110:ASN:HB2	2.13	0.49
1:C:120:GLU:OE1	1:C:156:LYS:OXT	2.31	0.49
1:G:105[A]:LEU:HD22	1:G:114[A]:ALA:HB2	1.96	0.48
1:D:116:LEU:HD23	1:G:141[A]:ILE:HG13	1.96	0.47
1:G:109[A]:GLN:O	1:G:110[A]:ASN:CB	2.63	0.47
1:G:113[B]:VAL:HG12	1:G:114[B]:ALA:N	2.31	0.45
1:A:120:GLU:OE1	1:A:156:LYS:OXT	2.35	0.44
1:G:109[A]:GLN:O	1:G:110[A]:ASN:HB3	2.18	0.44
1:D:115:ILE:O	1:G:141[A]:ILE:CG1	2.48	0.43
1:B:74:ASN:HB2	1:C:115:ILE:O	2.18	0.43
1:F:97:PHE:CE1	1:F:116:LEU:CD2	3.01	0.42
1:A:117:ASP:OD2	1:E:72:SER:N	2.53	0.42
1:G:97[B]:PHE:HE2	1:G:125[B]:TYR:HB3	1.85	0.42
1:G:148[B]:THR:HG21	2:N:7[B]:GLC:H3	2.01	0.42
1:D:115:ILE:HG23	1:G:139[A]:GLU:O	2.19	0.41
1:C:97:PHE:HA	3:C:201:GOL:H32	2.01	0.41
1:G:109[B]:GLN:O	1:G:110[B]:ASN:HB3	2.19	0.41
1:D:115:ILE:O	1:D:115:ILE:HG23	2.21	0.41
1:E:99:ASN:ND2	5:E:304:HOH:O	2.53	0.41

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:338:HOH:O	5:C:352:HOH:O[1_655]	1.86	0.34
5:A:326:HOH:O	5:E:330:HOH:O[1_655]	1.98	0.22
5:F:306:HOH:O	5:G:317:HOH:O[1_644]	1.99	0.21
5:C:413:HOH:O	5:E:446:HOH:O[1_545]	2.11	0.09

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	79/89 (89%)	78 (99%)	1 (1%)	0	100	100
1	B	84/89 (94%)	82 (98%)	2 (2%)	0	100	100
1	C	78/89 (88%)	77 (99%)	1 (1%)	0	100	100
1	D	75/89 (84%)	74 (99%)	1 (1%)	0	100	100
1	E	84/89 (94%)	82 (98%)	2 (2%)	0	100	100
1	F	75/89 (84%)	74 (99%)	1 (1%)	0	100	100
1	G	145/89 (163%)	143 (99%)	2 (1%)	0	100	100
All	All	620/623 (100%)	610 (98%)	10 (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	71/78 (91%)	71 (100%)	0	100	100
1	B	75/78 (96%)	75 (100%)	0	100	100
1	C	70/78 (90%)	70 (100%)	0	100	100
1	D	63/78 (81%)	61 (97%)	2 (3%)	39	18
1	E	77/78 (99%)	77 (100%)	0	100	100
1	F	62/78 (80%)	61 (98%)	1 (2%)	62	47
1	G	118/78 (151%)	110 (93%)	8 (7%)	16	3
All	All	536/546 (98%)	525 (98%)	11 (2%)	65	35

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	107	ARG
1	D	108	SER
1	F	108	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	80[A]	THR
1	G	80[B]	THR
1	G	118[A]	LEU
1	G	118[B]	LEU
1	G	132[A]	GLN
1	G	132[B]	GLN
1	G	153[A]	ILE
1	G	153[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	110	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](#)

56 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	H	1	2	11,11,12	0.54	0	15,15,17	1.13	1 (6%)
2	GLC	H	2	2	11,11,12	0.69	0	15,15,17	1.30	0
2	GLC	H	3	2	11,11,12	0.45	0	15,15,17	1.19	1 (6%)
2	GLC	H	4	2	11,11,12	0.33	0	15,15,17	1.00	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	H	5	2	11,11,12	0.39	0	15,15,17	1.28	2 (13%)
2	GLC	H	6	2	11,11,12	0.75	0	15,15,17	2.14	4 (26%)
2	GLC	H	7	2	11,11,12	1.00	0	15,15,17	1.32	1 (6%)
2	GLC	I	1	2	11,11,12	0.45	0	15,15,17	1.17	2 (13%)
2	GLC	I	2	2	11,11,12	0.53	0	15,15,17	1.24	2 (13%)
2	GLC	I	3	2	11,11,12	0.37	0	15,15,17	0.75	0
2	GLC	I	4	2	11,11,12	0.37	0	15,15,17	1.43	1 (6%)
2	GLC	I	5	2	11,11,12	0.51	0	15,15,17	1.09	0
2	GLC	I	6	2	11,11,12	0.85	0	15,15,17	2.07	2 (13%)
2	GLC	I	7	2	11,11,12	0.58	0	15,15,17	1.01	0
2	GLC	J	1	2	11,11,12	0.67	0	15,15,17	1.18	1 (6%)
2	GLC	J	2	2	11,11,12	0.58	0	15,15,17	1.28	2 (13%)
2	GLC	J	3	2	11,11,12	0.51	0	15,15,17	1.02	2 (13%)
2	GLC	J	4	2	11,11,12	0.28	0	15,15,17	1.00	1 (6%)
2	GLC	J	5	2	11,11,12	0.40	0	15,15,17	1.33	2 (13%)
2	GLC	J	6	2	11,11,12	0.62	0	15,15,17	2.06	4 (26%)
2	GLC	J	7	2	11,11,12	0.87	0	15,15,17	1.20	1 (6%)
2	GLC	K	1	2	11,11,12	0.47	0	15,15,17	1.11	1 (6%)
2	GLC	K	2	2	11,11,12	0.25	0	15,15,17	0.93	0
2	GLC	K	3	2	11,11,12	0.42	0	15,15,17	1.14	2 (13%)
2	GLC	K	4	2	11,11,12	0.37	0	15,15,17	1.23	2 (13%)
2	GLC	K	5	2	11,11,12	0.35	0	15,15,17	1.05	1 (6%)
2	GLC	K	6	2	11,11,12	0.47	0	15,15,17	1.79	4 (26%)
2	GLC	K	7	2	11,11,12	0.39	0	15,15,17	0.97	0
2	GLC	L	1	2	11,11,12	0.69	0	15,15,17	0.95	0
2	GLC	L	2	2	11,11,12	0.53	0	15,15,17	1.14	1 (6%)
2	GLC	L	3	2	11,11,12	0.31	0	15,15,17	0.96	1 (6%)
2	GLC	L	4	2	11,11,12	0.40	0	15,15,17	1.25	2 (13%)
2	GLC	L	5	2	11,11,12	0.35	0	15,15,17	1.20	1 (6%)
2	GLC	L	6	2	11,11,12	0.68	0	15,15,17	1.79	3 (20%)
2	GLC	L	7	2	11,11,12	0.62	0	15,15,17	1.18	2 (13%)
2	GLC	M	1	2	11,11,12	0.52	0	15,15,17	1.08	1 (6%)
2	GLC	M	2	2	11,11,12	0.35	0	15,15,17	0.79	0
2	GLC	M	3	2	11,11,12	0.31	0	15,15,17	1.27	2 (13%)
2	GLC	M	4	2	11,11,12	0.34	0	15,15,17	1.14	1 (6%)
2	GLC	M	5	2	11,11,12	0.42	0	15,15,17	1.32	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	M	6	2	11,11,12	0.48	0	15,15,17	1.52	3 (20%)
2	GLC	M	7	2	11,11,12	0.61	0	15,15,17	1.13	2 (13%)
2	GLC	N	1[A]	2	11,11,12	0.29	0	15,15,17	0.68	0
2	GLC	N	1[B]	2	11,11,12	0.36	0	15,15,17	0.89	0
2	GLC	N	2[A]	2	11,11,12	0.45	0	15,15,17	0.95	1 (6%)
2	GLC	N	2[B]	2	11,11,12	0.38	0	15,15,17	0.85	0
2	GLC	N	3[A]	2	11,11,12	0.24	0	15,15,17	1.02	0
2	GLC	N	3[B]	2	11,11,12	0.39	0	15,15,17	1.20	1 (6%)
2	GLC	N	4[A]	2	11,11,12	0.23	0	15,15,17	1.07	1 (6%)
2	GLC	N	4[B]	2	11,11,12	0.24	0	15,15,17	1.22	1 (6%)
2	GLC	N	5[A]	2	11,11,12	0.39	0	15,15,17	0.69	0
2	GLC	N	5[B]	2	11,11,12	0.35	0	15,15,17	0.77	0
2	GLC	N	6[A]	2	11,11,12	0.21	0	15,15,17	2.40	4 (26%)
2	GLC	N	6[B]	2	11,11,12	0.22	0	15,15,17	2.01	4 (26%)
2	GLC	N	7[A]	2	11,11,12	0.27	0	15,15,17	0.74	0
2	GLC	N	7[B]	2	11,11,12	0.38	0	15,15,17	0.95	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	H	1	2	-	0/2/19/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	3	2	-	0/2/19/22	0/1/1/1
2	GLC	H	4	2	-	0/2/19/22	0/1/1/1
2	GLC	H	5	2	-	0/2/19/22	0/1/1/1
2	GLC	H	6	2	-	2/2/19/22	0/1/1/1
2	GLC	H	7	2	-	0/2/19/22	0/1/1/1
2	GLC	I	1	2	-	0/2/19/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
2	GLC	I	3	2	-	0/2/19/22	0/1/1/1
2	GLC	I	4	2	-	2/2/19/22	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	J	1	2	-	0/2/19/22	0/1/1/1
2	GLC	J	2	2	-	0/2/19/22	0/1/1/1
2	GLC	J	3	2	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	J	4	2	-	2/2/19/22	0/1/1/1
2	GLC	J	5	2	-	0/2/19/22	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	K	1	2	-	0/2/19/22	0/1/1/1
2	GLC	K	2	2	-	0/2/19/22	0/1/1/1
2	GLC	K	3	2	-	0/2/19/22	0/1/1/1
2	GLC	K	4	2	-	0/2/19/22	0/1/1/1
2	GLC	K	5	2	-	0/2/19/22	0/1/1/1
2	GLC	K	6	2	-	2/2/19/22	0/1/1/1
2	GLC	K	7	2	-	0/2/19/22	0/1/1/1
2	GLC	L	1	2	-	0/2/19/22	0/1/1/1
2	GLC	L	2	2	-	0/2/19/22	0/1/1/1
2	GLC	L	3	2	-	1/2/19/22	0/1/1/1
2	GLC	L	4	2	-	2/2/19/22	0/1/1/1
2	GLC	L	5	2	-	1/2/19/22	0/1/1/1
2	GLC	L	6	2	-	2/2/19/22	0/1/1/1
2	GLC	L	7	2	-	0/2/19/22	0/1/1/1
2	GLC	M	1	2	-	0/2/19/22	0/1/1/1
2	GLC	M	2	2	-	0/2/19/22	0/1/1/1
2	GLC	M	3	2	-	0/2/19/22	0/1/1/1
2	GLC	M	4	2	-	0/2/19/22	0/1/1/1
2	GLC	M	5	2	-	0/2/19/22	0/1/1/1
2	GLC	M	6	2	-	2/2/19/22	0/1/1/1
2	GLC	M	7	2	-	0/2/19/22	0/1/1/1
2	GLC	N	1[A]	2	-	0/2/19/22	0/1/1/1
2	GLC	N	1[B]	2	-	0/2/19/22	0/1/1/1
2	GLC	N	2[A]	2	-	0/2/19/22	0/1/1/1
2	GLC	N	2[B]	2	-	0/2/19/22	0/1/1/1
2	GLC	N	3[A]	2	-	2/2/19/22	0/1/1/1
2	GLC	N	3[B]	2	-	2/2/19/22	0/1/1/1
2	GLC	N	4[A]	2	-	0/2/19/22	0/1/1/1
2	GLC	N	4[B]	2	-	0/2/19/22	0/1/1/1
2	GLC	N	5[A]	2	-	0/2/19/22	0/1/1/1
2	GLC	N	5[B]	2	-	2/2/19/22	0/1/1/1
2	GLC	N	6[A]	2	-	1/2/19/22	0/1/1/1
2	GLC	N	6[B]	2	-	2/2/19/22	0/1/1/1
2	GLC	N	7[A]	2	-	0/2/19/22	0/1/1/1
2	GLC	N	7[B]	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	6[A]	GLC	C1-O5-C5	7.40	122.22	112.19
2	I	6	GLC	C1-O5-C5	6.25	120.65	112.19
2	J	6	GLC	C1-O5-C5	5.85	120.12	112.19
2	H	6	GLC	C1-O5-C5	5.74	119.97	112.19
2	N	6[B]	GLC	C1-O5-C5	5.51	119.65	112.19
2	L	6	GLC	C1-O5-C5	4.82	118.72	112.19
2	I	4	GLC	O5-C5-C6	4.50	114.26	107.20
2	K	6	GLC	C1-O5-C5	4.35	118.08	112.19
2	H	7	GLC	C1-O5-C5	4.19	117.86	112.19
2	N	4[B]	GLC	C1-O5-C5	3.66	117.15	112.19
2	N	6[A]	GLC	O5-C5-C4	3.62	119.62	110.83
2	L	4	GLC	O5-C5-C6	3.46	112.62	107.20
2	N	4[A]	GLC	C1-O5-C5	3.39	116.78	112.19
2	M	6	GLC	C1-O5-C5	3.28	116.64	112.19
2	M	3	GLC	O5-C5-C6	3.28	112.35	107.20
2	M	1	GLC	C1-O5-C5	3.28	116.64	112.19
2	J	1	GLC	C1-O5-C5	3.22	116.55	112.19
2	K	1	GLC	C1-O5-C5	3.20	116.52	112.19
2	J	6	GLC	O5-C5-C4	3.17	118.54	110.83
2	M	5	GLC	C1-O5-C5	3.13	116.43	112.19
2	H	1	GLC	C1-O5-C5	3.11	116.40	112.19
2	J	5	GLC	C1-O5-C5	3.07	116.34	112.19
2	M	4	GLC	O4-C4-C3	-3.06	103.27	110.35
2	N	6[B]	GLC	O5-C5-C4	3.03	118.20	110.83
2	J	7	GLC	C1-O5-C5	3.01	116.27	112.19
2	N	6[B]	GLC	O5-C5-C6	2.96	111.85	107.20
2	L	6	GLC	O6-C6-C5	-2.95	101.18	111.29
2	J	6	GLC	O6-C6-C5	-2.94	101.21	111.29
2	H	6	GLC	C3-C4-C5	2.92	115.45	110.24
2	K	4	GLC	O4-C4-C3	-2.91	103.62	110.35
2	K	6	GLC	O3-C3-C4	-2.83	103.80	110.35
2	H	5	GLC	C1-O5-C5	2.82	116.01	112.19
2	I	6	GLC	O6-C6-C5	-2.77	101.78	111.29
2	I	1	GLC	C1-O5-C5	2.73	115.89	112.19
2	M	6	GLC	O5-C5-C6	2.70	111.44	107.20
2	H	6	GLC	O6-C6-C5	-2.63	102.26	111.29
2	H	3	GLC	C1-O5-C5	2.63	115.75	112.19
2	I	2	GLC	O4-C4-C3	-2.62	104.30	110.35
2	L	5	GLC	O2-C2-C1	-2.59	103.86	109.15
2	I	1	GLC	O5-C5-C6	2.59	111.26	107.20
2	N	6[A]	GLC	C3-C4-C5	2.58	114.84	110.24
2	N	7[B]	GLC	O5-C1-C2	-2.58	106.79	110.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	4	GLC	O5-C5-C6	2.50	111.12	107.20
2	L	2	GLC	O4-C4-C3	-2.49	104.58	110.35
2	K	3	GLC	O5-C5-C6	2.46	111.07	107.20
2	H	6	GLC	O5-C5-C4	2.45	116.78	110.83
2	M	3	GLC	O3-C3-C2	-2.39	105.42	109.99
2	K	6	GLC	O6-C6-C5	-2.37	103.16	111.29
2	N	3[B]	GLC	O5-C5-C6	-2.35	103.52	107.20
2	L	4	GLC	C1-O5-C5	2.33	115.35	112.19
2	N	6[B]	GLC	C3-C4-C5	2.33	114.39	110.24
2	J	2	GLC	O5-C5-C4	-2.33	105.16	110.83
2	N	2[A]	GLC	O2-C2-C1	-2.30	104.45	109.15
2	J	3	GLC	C1-O5-C5	2.29	115.29	112.19
2	K	5	GLC	C1-O5-C5	2.28	115.28	112.19
2	L	6	GLC	O5-C5-C4	2.24	116.28	110.83
2	M	7	GLC	O4-C4-C3	-2.23	105.20	110.35
2	I	2	GLC	C1-O5-C5	2.17	115.14	112.19
2	N	6[A]	GLC	O3-C3-C4	-2.15	105.38	110.35
2	M	5	GLC	O4-C4-C3	-2.14	105.39	110.35
2	J	4	GLC	O2-C2-C3	-2.14	105.84	110.14
2	L	7	GLC	C1-O5-C5	2.13	115.08	112.19
2	H	5	GLC	O5-C1-C2	-2.13	107.48	110.77
2	J	5	GLC	O6-C6-C5	-2.13	103.98	111.29
2	K	3	GLC	C1-O5-C5	2.11	115.05	112.19
2	J	6	GLC	C3-C4-C5	2.10	113.99	110.24
2	M	6	GLC	O6-C6-C5	-2.09	104.11	111.29
2	L	7	GLC	O5-C1-C2	-2.09	107.54	110.77
2	K	6	GLC	C3-C4-C5	2.08	113.94	110.24
2	L	3	GLC	C1-C2-C3	2.08	112.22	109.67
2	M	7	GLC	C1-O5-C5	2.07	114.99	112.19
2	J	3	GLC	O6-C6-C5	-2.05	104.26	111.29
2	H	4	GLC	O2-C2-C3	-2.04	106.05	110.14
2	J	2	GLC	O4-C4-C3	-2.02	105.67	110.35

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	4	GLC	O5-C5-C6-O6
2	L	4	GLC	O5-C5-C6-O6
2	J	6	GLC	C4-C5-C6-O6
2	N	6[B]	GLC	C4-C5-C6-O6
2	J	4	GLC	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

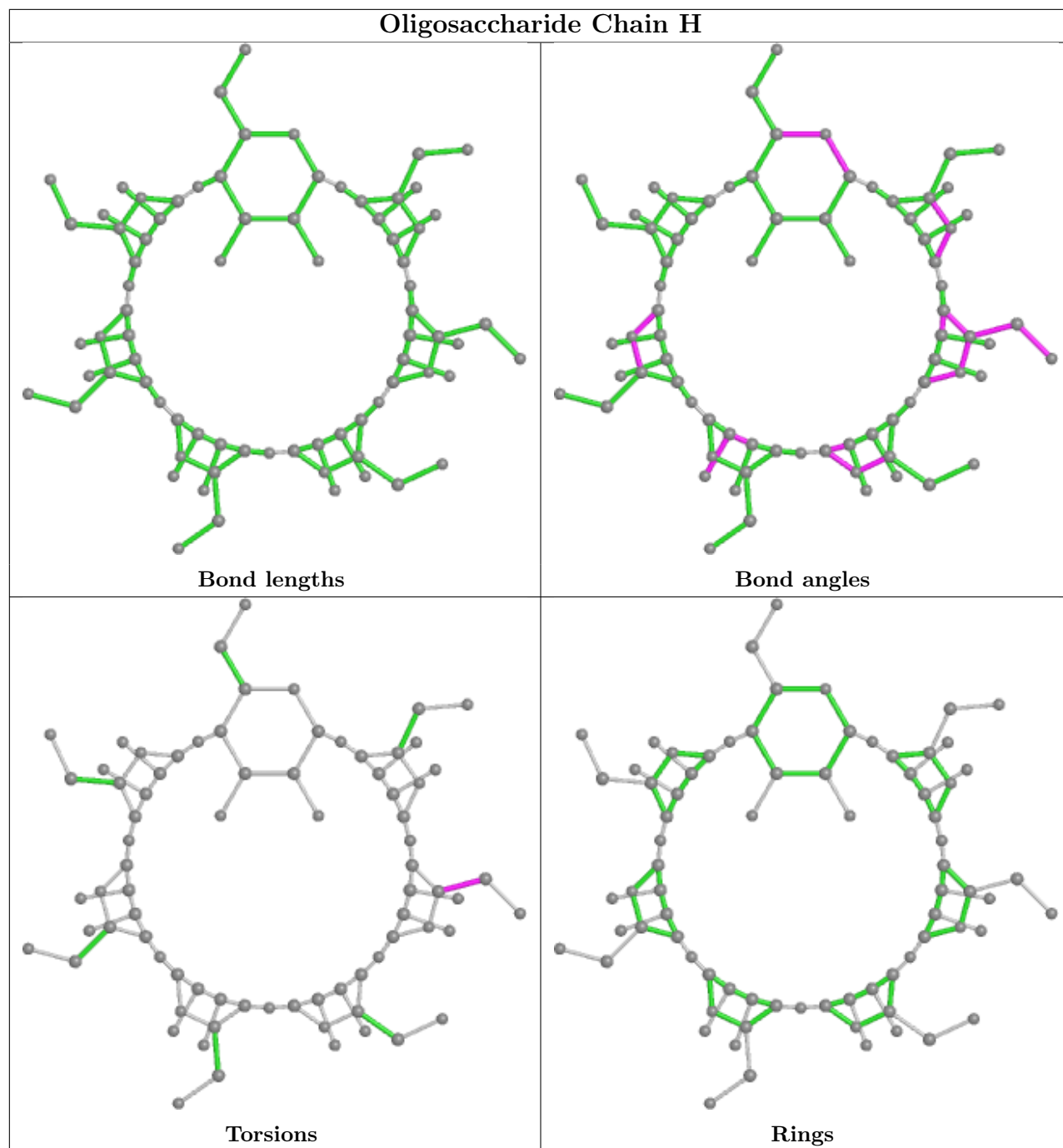
Mol	Chain	Res	Type	Atoms
2	N	3[A]	GLC	C4-C5-C6-O6
2	L	4	GLC	C4-C5-C6-O6
2	N	3[B]	GLC	O5-C5-C6-O6
2	N	3[A]	GLC	O5-C5-C6-O6
2	H	6	GLC	C4-C5-C6-O6
2	L	6	GLC	C4-C5-C6-O6
2	M	6	GLC	C4-C5-C6-O6
2	I	6	GLC	C4-C5-C6-O6
2	K	6	GLC	C4-C5-C6-O6
2	N	3[B]	GLC	C4-C5-C6-O6
2	N	6[B]	GLC	O5-C5-C6-O6
2	I	4	GLC	O5-C5-C6-O6
2	N	5[B]	GLC	C4-C5-C6-O6
2	J	6	GLC	O5-C5-C6-O6
2	L	3	GLC	O5-C5-C6-O6
2	N	5[B]	GLC	O5-C5-C6-O6
2	L	6	GLC	O5-C5-C6-O6
2	M	6	GLC	O5-C5-C6-O6
2	K	6	GLC	O5-C5-C6-O6
2	H	6	GLC	O5-C5-C6-O6
2	I	6	GLC	O5-C5-C6-O6
2	L	5	GLC	C4-C5-C6-O6
2	N	6[A]	GLC	C4-C5-C6-O6
2	I	4	GLC	C4-C5-C6-O6

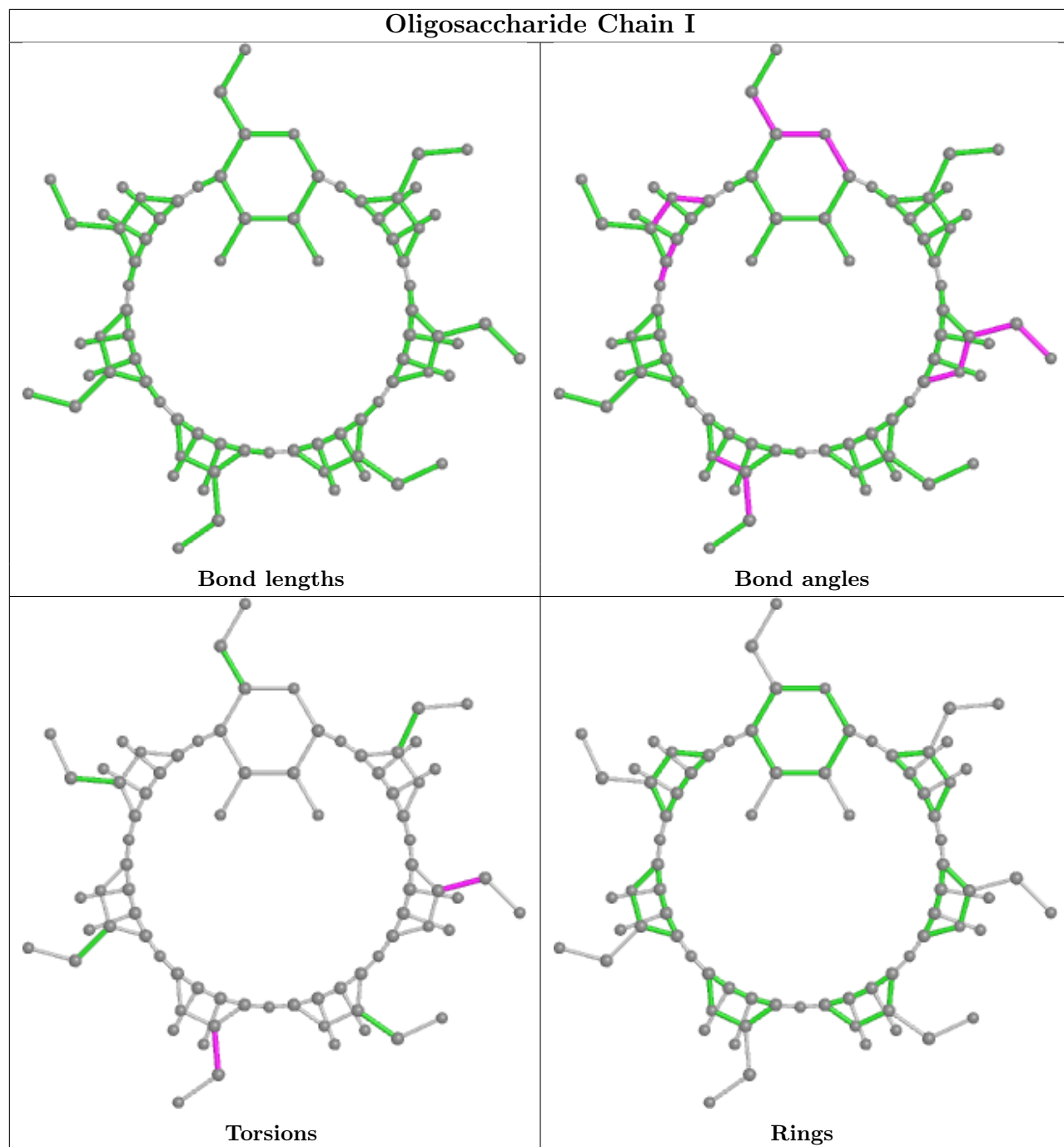
There are no ring outliers.

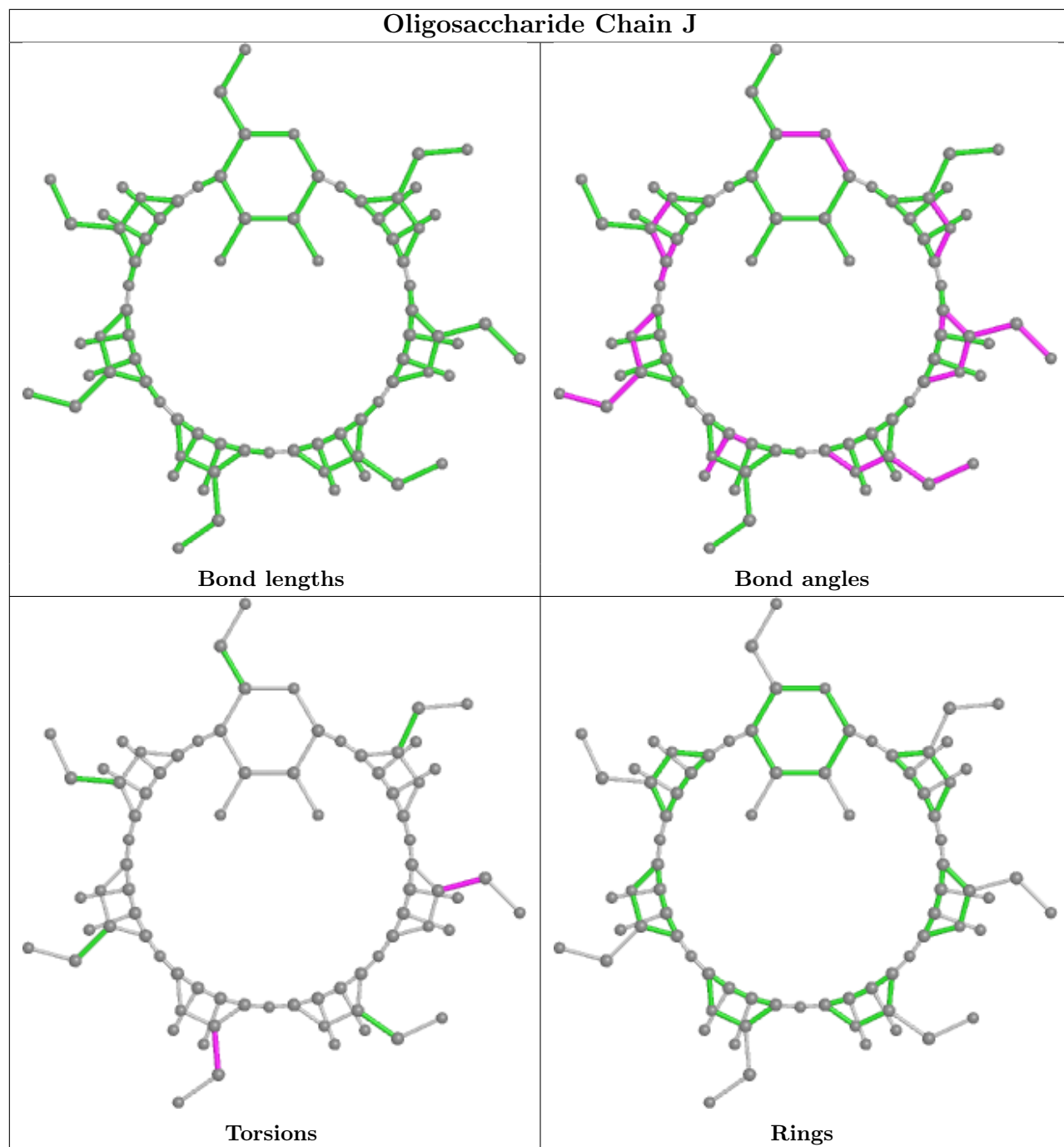
5 monomers are involved in 5 short contacts:

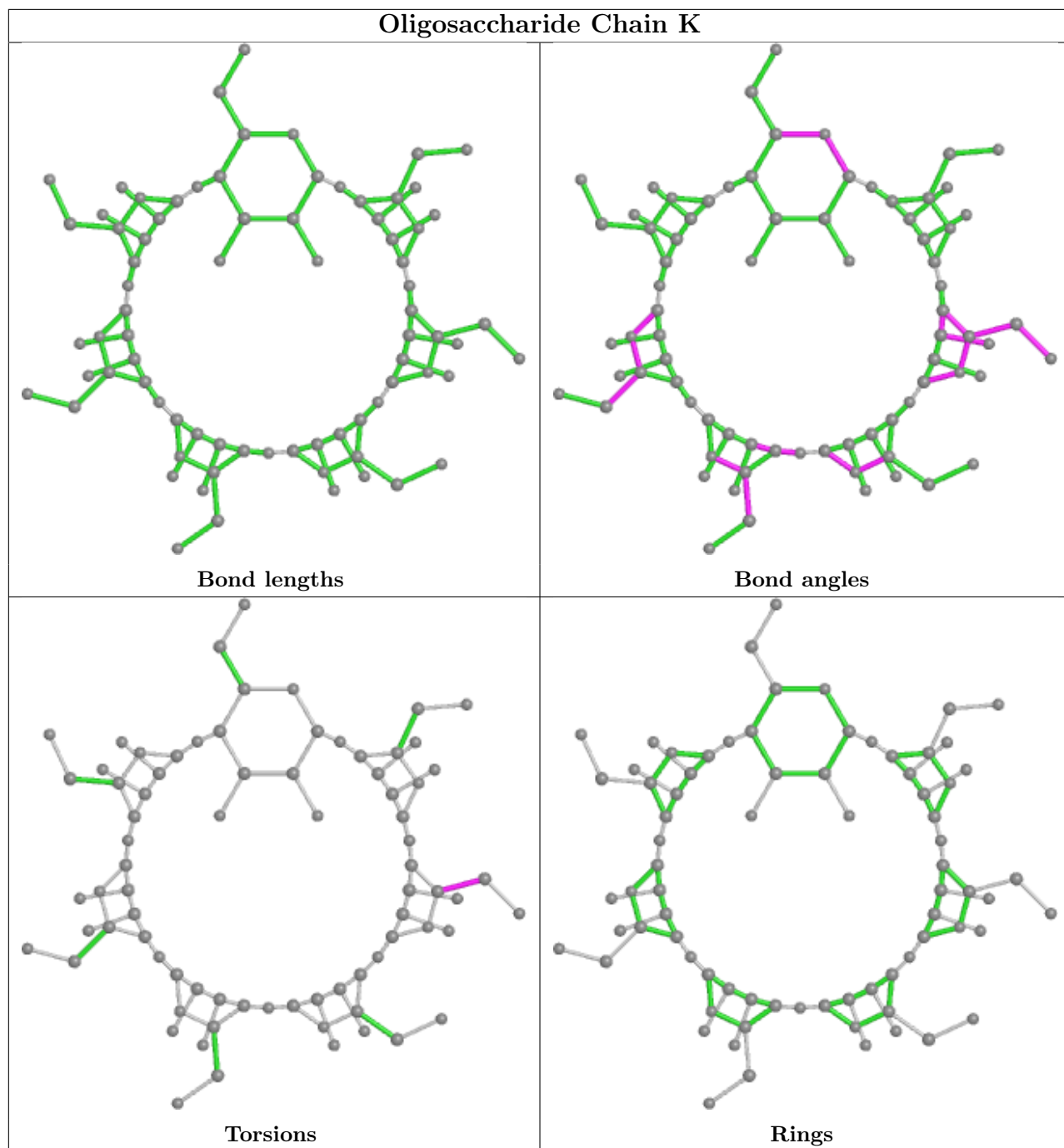
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	7[B]	GLC	1	0
2	N	7[A]	GLC	1	0
2	N	4[A]	GLC	1	0
2	J	2	GLC	1	0
2	N	4[B]	GLC	1	0

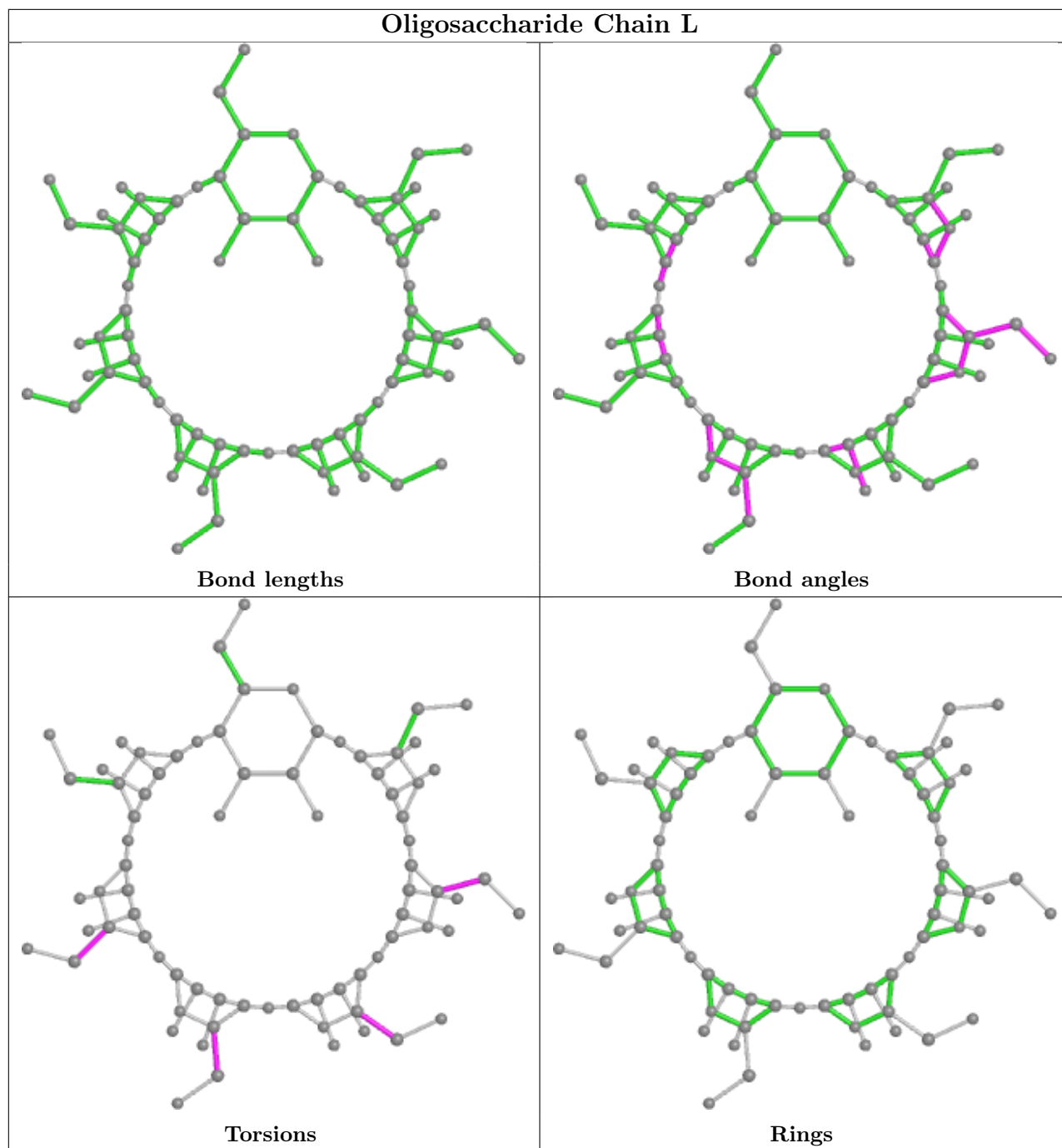
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

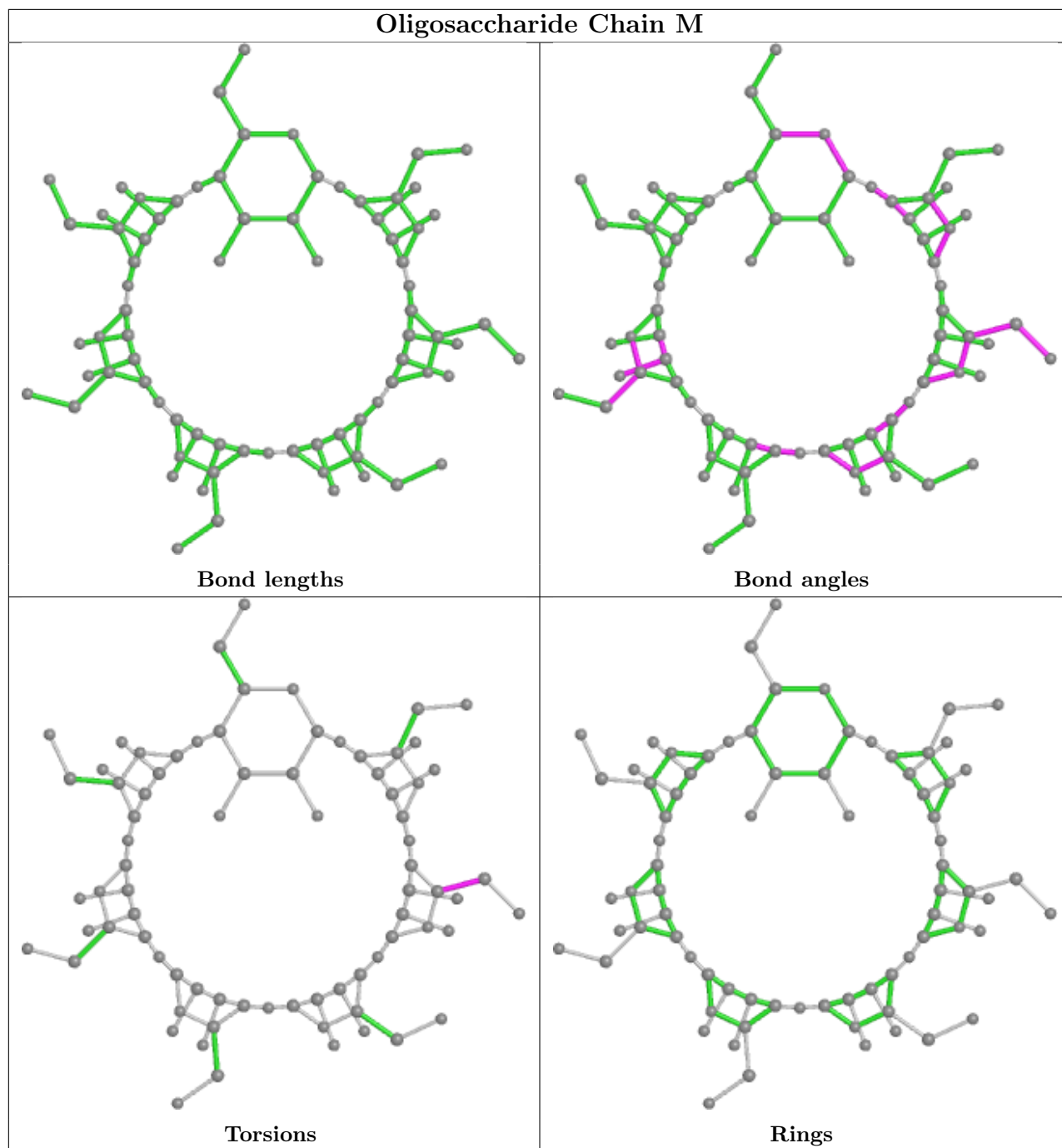


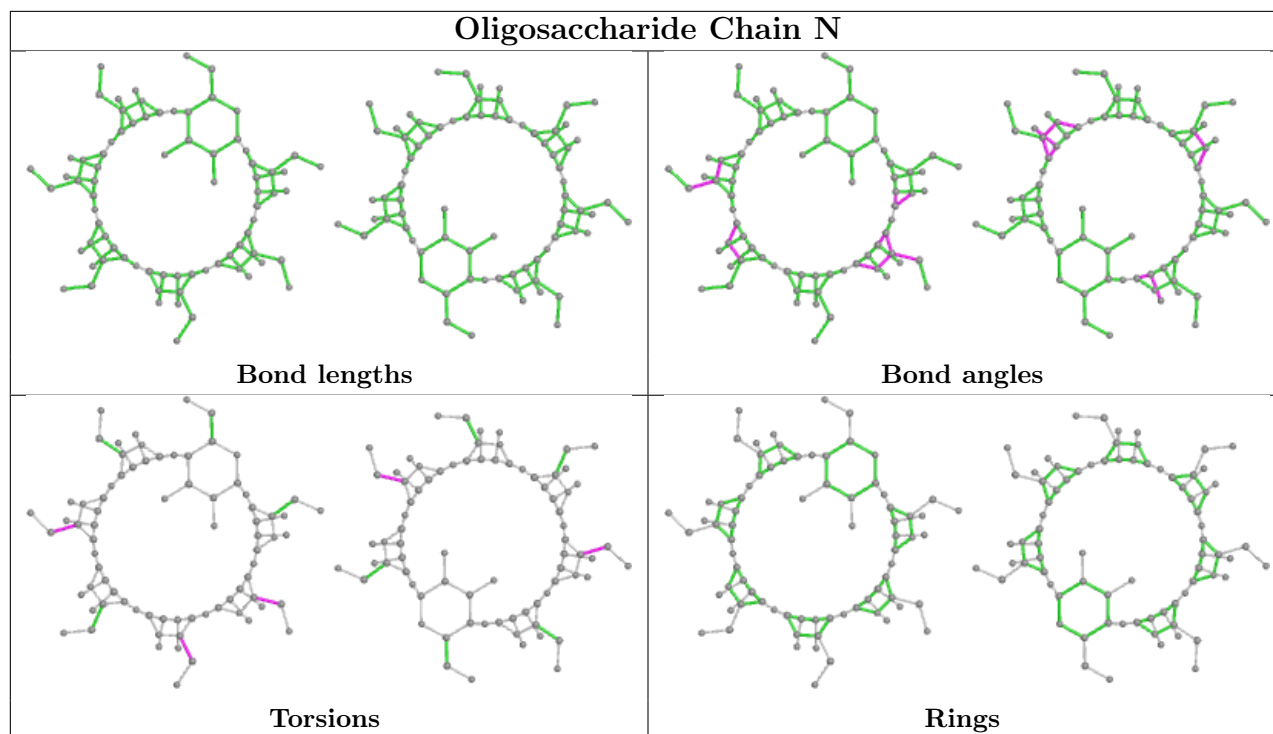












5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	B	202	-	4,4,4	0.21	0	6,6,6	0.57	0
4	SO4	D	201	-	4,4,4	0.58	0	6,6,6	0.32	0
3	GOL	C	201	-	5,5,5	0.54	0	5,5,5	0.69	0
3	GOL	A	201	-	5,5,5	0.60	0	5,5,5	1.46	1 (20%)
4	SO4	B	201	-	4,4,4	0.56	0	6,6,6	0.53	0
4	SO4	F	201	-	4,4,4	0.58	0	6,6,6	0.25	0
4	SO4	E	202	-	4,4,4	0.42	0	6,6,6	0.43	0
4	SO4	E	201	-	4,4,4	0.62	0	6,6,6	0.90	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
3	GOL	A	201	-	-	2/4/4/4	-
3	GOL	C	201	-	-	1/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	GOL	O2-C2-C3	2.03	118.08	109.12

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	GOL	C1-C2-C3-O3
3	A	201	GOL	O2-C2-C3-O3
3	C	201	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	201	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	80/89 (89%)	-0.11	2 (2%) 57 61	12, 19, 48, 60	0
1	B	86/89 (96%)	-0.12	1 (1%) 79 83	12, 18, 42, 70	0
1	C	79/89 (88%)	-0.18	0 100 100	12, 19, 40, 59	0
1	D	77/89 (86%)	0.28	6 (7%) 13 15	14, 31, 57, 72	0
1	E	85/89 (95%)	-0.05	2 (2%) 59 63	11, 18, 42, 54	0
1	F	77/89 (86%)	0.22	6 (7%) 13 15	14, 32, 57, 67	0
1	G	75/89 (84%)	1.18	16 (21%) 0 0	18, 26, 45, 54	9 (12%)
All	All	559/623 (89%)	0.16	33 (5%) 22 24	11, 21, 51, 72	9 (1%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	73	PRO	5.6
1	G	81[A]	VAL	4.7
1	B	73	PRO	4.2
1	G	79[A]	PRO	4.0
1	F	155	VAL	3.9
1	G	115[A]	ILE	3.4
1	D	118	LEU	3.4
1	G	100[A]	TRP	3.3
1	F	121	GLY	3.1
1	G	201[B]	GLU	3.0
1	G	146[A]	LEU	3.0
1	G	123[A]	HIS	2.9
1	D	121	GLY	2.9
1	F	115	ILE	2.9
1	A	77	ALA	2.9
1	G	120[A]	GLU	2.8
1	G	137[A]	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	113[A]	VAL	2.7
1	D	119	PRO	2.7
1	G	116[A]	LEU	2.7
1	G	118[A]	LEU	2.7
1	E	75	SER	2.5
1	A	107	ARG	2.4
1	F	79	PRO	2.3
1	G	149[A]	VAL	2.2
1	D	153	ILE	2.2
1	F	119	PRO	2.2
1	G	133[A]	TRP	2.2
1	D	79	PRO	2.2
1	F	80	THR	2.0
1	G	99[A]	ASN	2.0
1	G	97[A]	PHE	2.0
1	D	80	THR	2.0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	N	5[A]	11/12	0.73	0.23	37,38,39,40	11
2	GLC	N	5[B]	11/12	0.73	0.23	38,39,40,41	11
2	GLC	N	6[A]	11/12	0.78	0.19	33,36,38,40	11
2	GLC	N	6[B]	11/12	0.78	0.19	33,36,38,39	11
2	GLC	N	3[A]	11/12	0.83	0.16	37,38,40,41	11
2	GLC	N	3[B]	11/12	0.83	0.16	38,39,41,41	11
2	GLC	M	5	11/12	0.88	0.10	32,37,40,44	0
2	GLC	L	3	11/12	0.89	0.15	34,38,43,45	0
2	GLC	N	2[A]	11/12	0.89	0.21	32,34,35,36	11
2	GLC	N	2[B]	11/12	0.89	0.21	32,33,36,36	11
2	GLC	M	4	11/12	0.90	0.10	34,34,37,44	0
2	GLC	K	6	11/12	0.90	0.09	25,29,34,42	0

Continued on next page...

Continued from previous page...

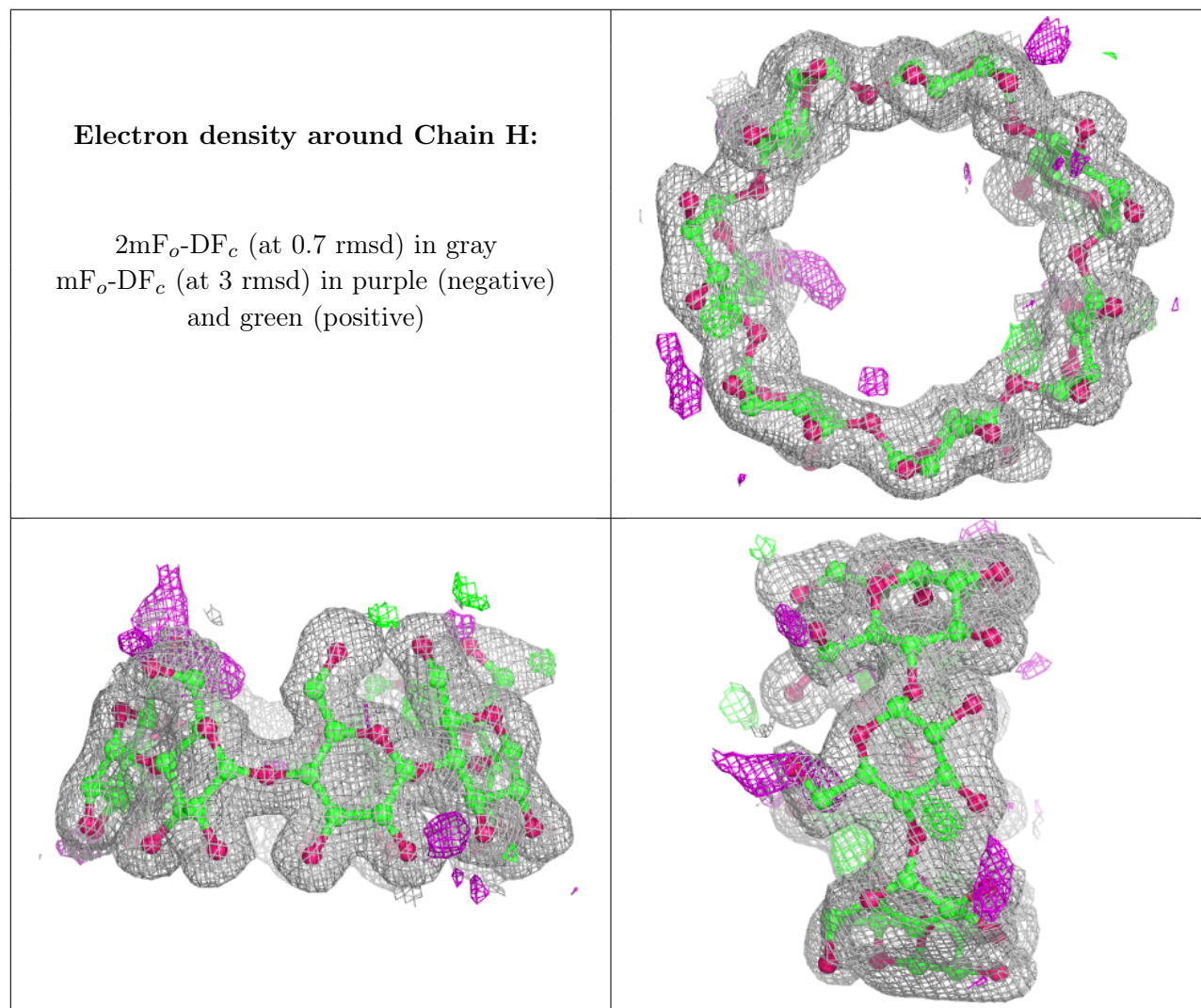
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	J	4	11/12	0.90	0.14	40,43,51,58	0
2	GLC	L	4	11/12	0.90	0.14	42,46,50,56	0
2	GLC	L	6	11/12	0.90	0.11	25,30,35,40	0
2	GLC	J	3	11/12	0.91	0.09	29,31,34,37	0
2	GLC	H	3	11/12	0.91	0.13	28,31,34,36	0
2	GLC	J	6	11/12	0.91	0.09	22,28,31,35	0
2	GLC	K	4	11/12	0.91	0.10	33,35,38,45	0
2	GLC	H	4	11/12	0.91	0.14	40,43,48,54	0
2	GLC	I	5	11/12	0.91	0.12	33,41,44,48	0
2	GLC	J	5	11/12	0.92	0.11	31,36,39,44	0
2	GLC	I	6	11/12	0.92	0.10	25,29,34,38	0
2	GLC	L	5	11/12	0.92	0.10	33,40,43,46	0
2	GLC	N	4[A]	11/12	0.92	0.13	37,38,39,39	11
2	GLC	N	4[B]	11/12	0.92	0.13	38,39,41,41	11
2	GLC	K	3	11/12	0.92	0.10	28,29,32,35	0
2	GLC	I	3	11/12	0.92	0.09	34,36,41,42	0
2	GLC	H	6	11/12	0.92	0.10	22,28,31,34	0
2	GLC	L	2	11/12	0.92	0.10	21,24,29,31	0
2	GLC	N	7[A]	11/12	0.92	0.12	27,29,31,32	11
2	GLC	N	7[B]	11/12	0.92	0.12	27,29,30,31	11
2	GLC	I	4	11/12	0.93	0.09	43,45,50,55	0
2	GLC	M	6	11/12	0.93	0.09	24,29,33,41	0
2	GLC	J	2	11/12	0.94	0.09	20,22,28,32	0
2	GLC	M	7	11/12	0.94	0.08	18,20,23,25	0
2	GLC	K	5	11/12	0.94	0.10	33,36,38,42	0
2	GLC	H	2	11/12	0.94	0.09	20,22,28,31	0
2	GLC	M	3	11/12	0.94	0.08	28,29,32,35	0
2	GLC	K	2	11/12	0.94	0.07	21,23,26,27	0
2	GLC	I	2	11/12	0.94	0.09	21,24,29,30	0
2	GLC	H	5	11/12	0.95	0.08	31,36,38,41	0
2	GLC	N	1[A]	11/12	0.95	0.10	26,28,30,30	11
2	GLC	N	1[B]	11/12	0.95	0.10	26,28,29,30	11
2	GLC	I	7	11/12	0.95	0.09	17,20,22,26	0
2	GLC	H	1	11/12	0.95	0.07	15,16,18,20	0
2	GLC	M	2	11/12	0.96	0.07	20,22,25,26	0
2	GLC	K	7	11/12	0.96	0.07	18,21,24,27	0
2	GLC	J	7	11/12	0.96	0.11	16,19,21,21	0
2	GLC	H	7	11/12	0.96	0.07	16,19,21,21	0
2	GLC	L	7	11/12	0.96	0.09	17,21,23,26	0
2	GLC	K	1	11/12	0.97	0.06	17,19,21,22	0
2	GLC	L	1	11/12	0.97	0.07	15,17,19,20	0
2	GLC	I	1	11/12	0.97	0.08	15,17,19,19	0

Continued on next page...

Continued from previous page...

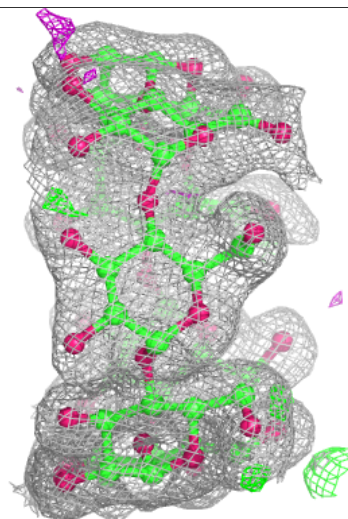
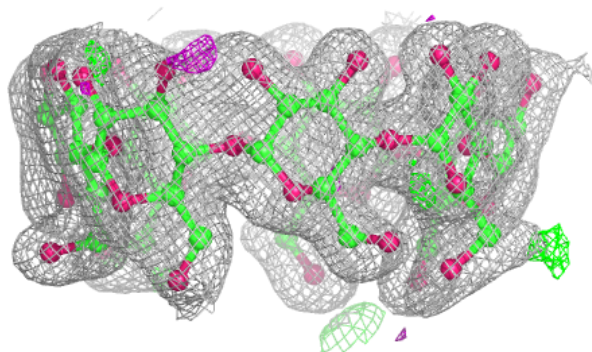
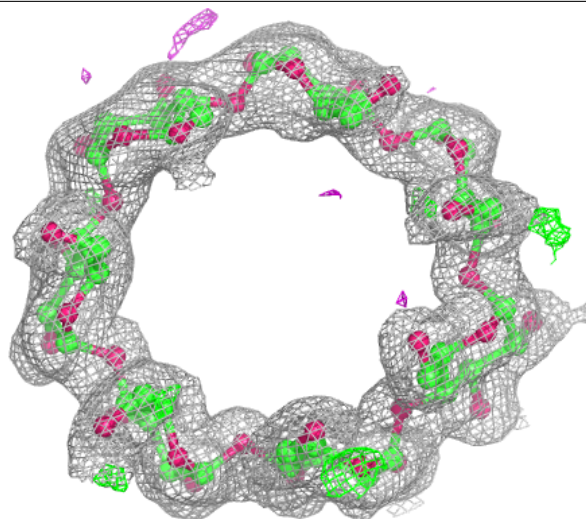
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	J	1	11/12	0.97	0.09	15,16,19,20	0
2	GLC	M	1	11/12	0.97	0.07	17,19,22,24	0

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.



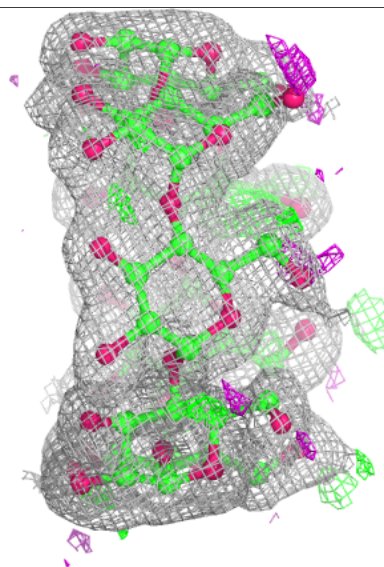
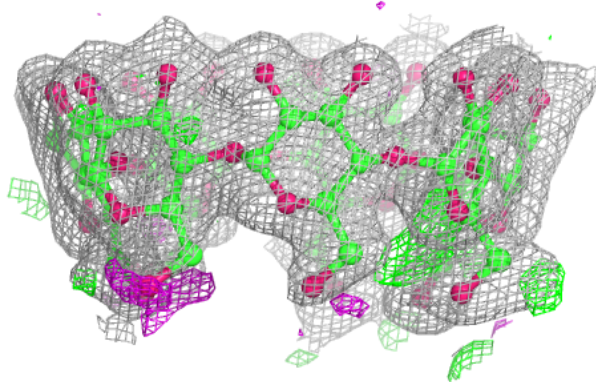
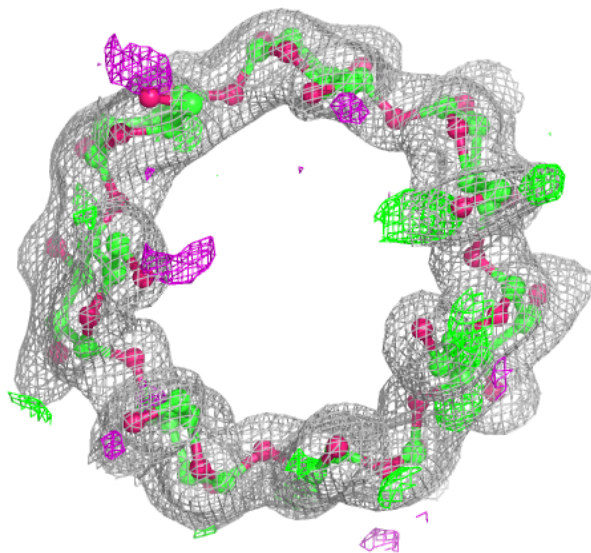
Electron density around Chain I:

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



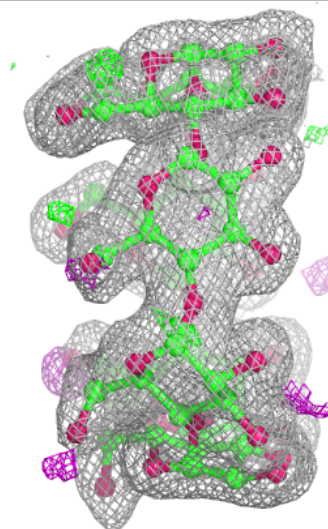
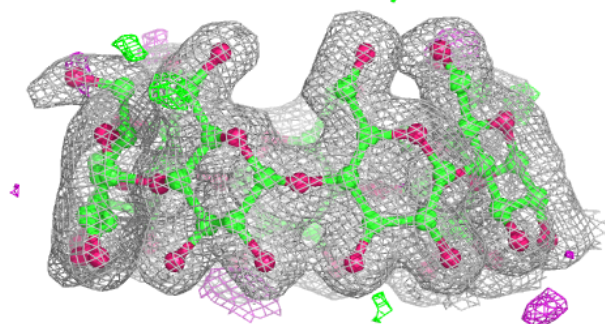
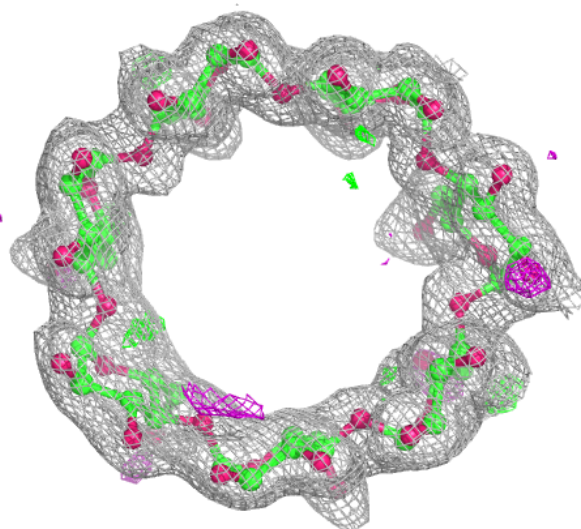
Electron density around Chain J:

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



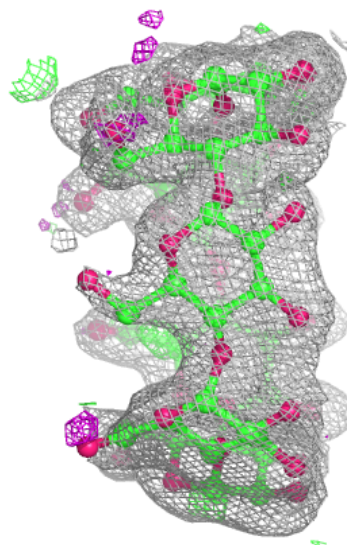
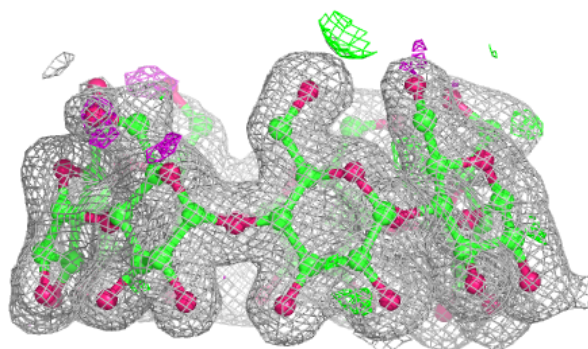
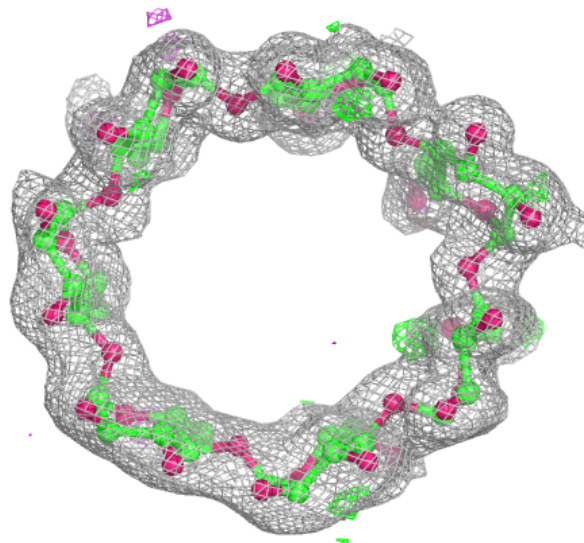
Electron density around Chain K:

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



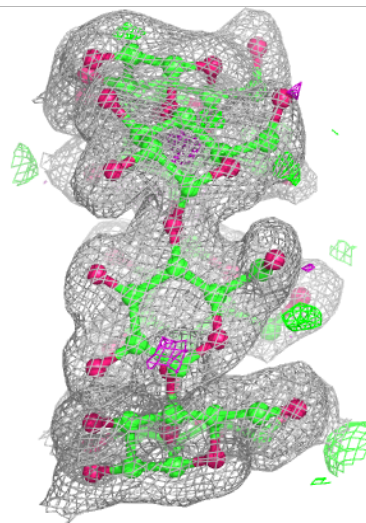
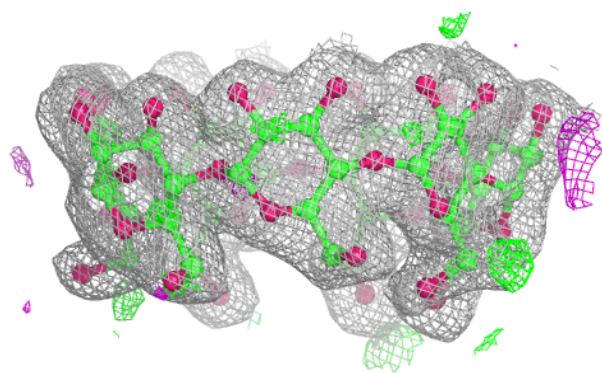
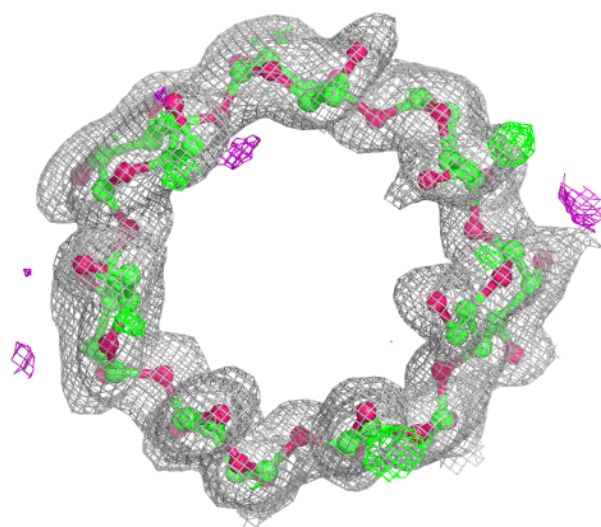
Electron density around Chain L:

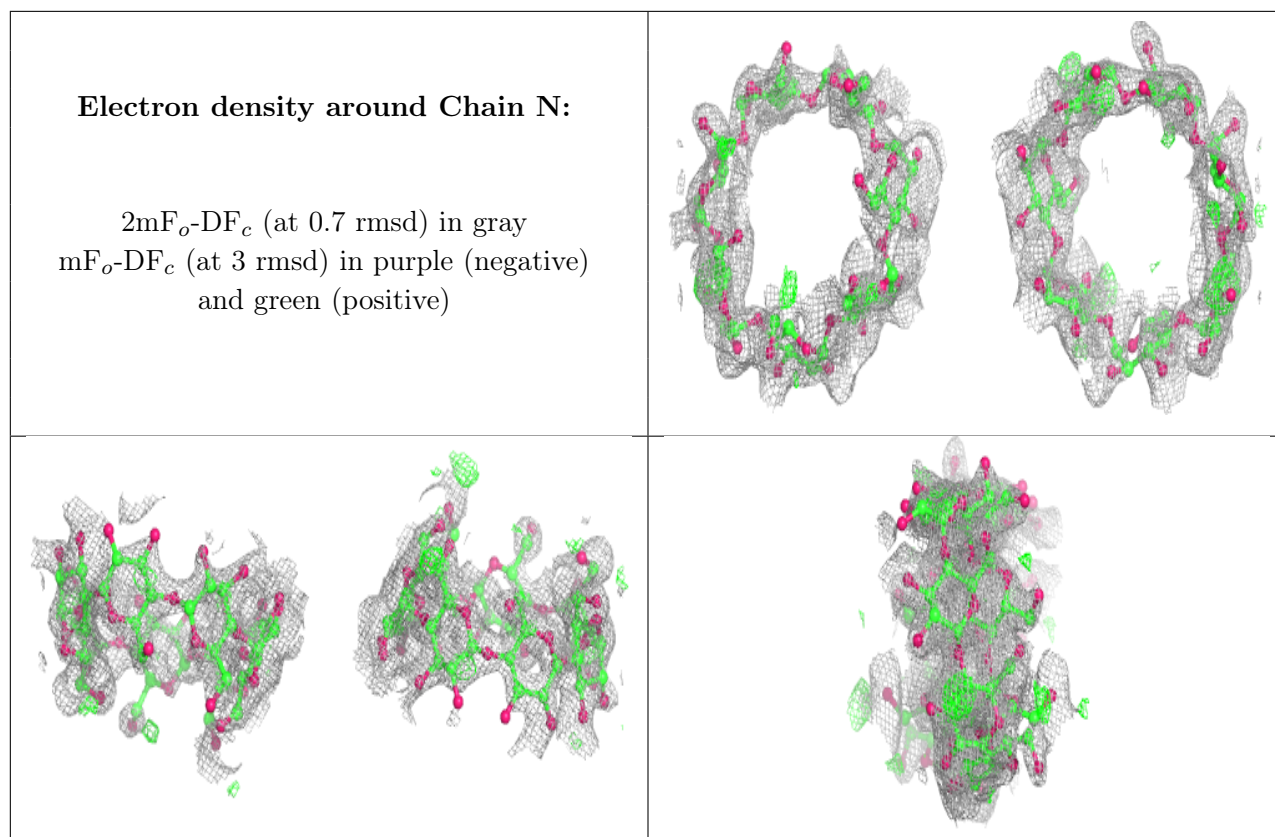
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	C	201	6/6	0.82	0.22	33,35,38,46	0
3	GOL	A	201	6/6	0.91	0.19	35,38,41,42	0
4	SO4	F	201	5/5	0.94	0.27	45,46,49,49	0
4	SO4	D	201	5/5	0.97	0.14	43,43,46,47	0
4	SO4	B	201	5/5	0.98	0.10	18,21,21,26	0
4	SO4	B	202	5/5	0.98	0.09	34,35,39,42	0
4	SO4	E	202	5/5	0.99	0.08	34,36,41,45	0
4	SO4	E	201	5/5	0.99	0.09	19,20,22,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.